



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 12:16 am GMT

PDB ID : 5MEI  
Title : Crystal structure of Agelastatin A bound to the 80S ribosome  
Authors : McClary, B.; Zinshteyn, B.; Meyer, M.; Jouanneau, M.; Pellegrino, S.; Yusupova, G.; Schuller, A.; Reyes, J.C.P.; Lu, J.; Luo, C.; Dang, Y.; Romo, D.; Yusupov, M.; Green, R.; Liu, J.O.  
Deposited on : 2016-11-15  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

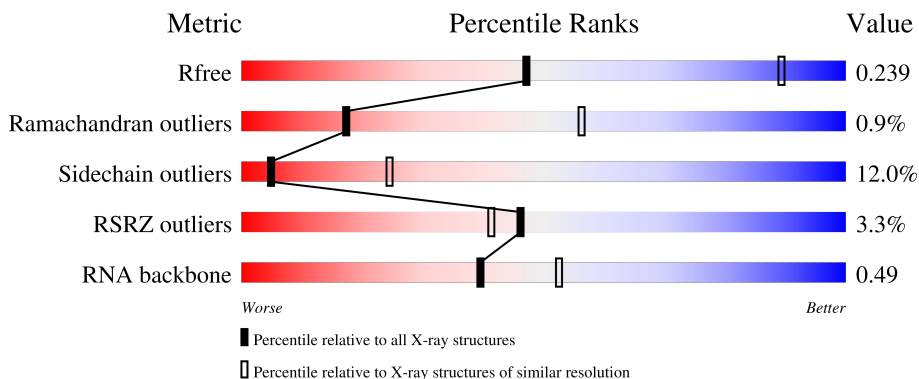
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






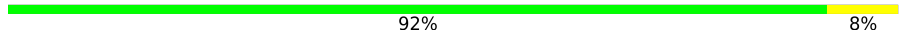





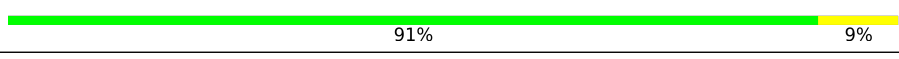


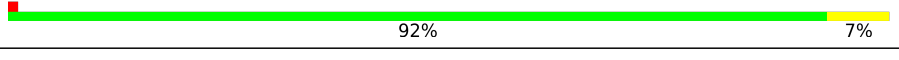
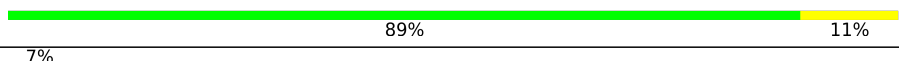
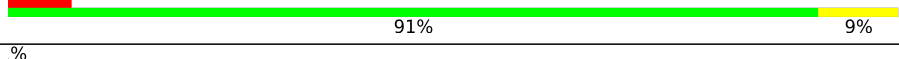
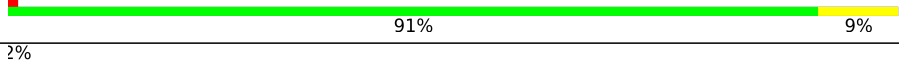





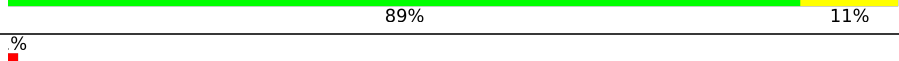
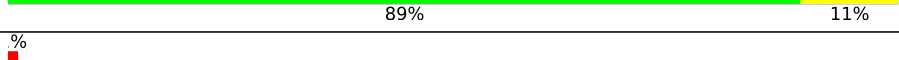
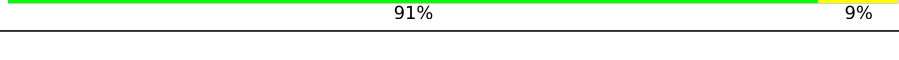

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1659 (3.60-3.40)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	3396	
1	AR	3396	
2	3	121	
2	AS	121	

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Mol	Chain	Length	Quality of chain
3	4	158	 % 77% 23%
3	AT	158	 % 79% 20%
4	CD	252	 % 89% 11%
4	j	252	 % 92% 8%
5	CE	386	 % 88% 12%
5	k	386	 % 86% 14%
6	CF	361	 % 90% 9%
6	l	361	 % 90% 10%
7	CG	296	 % 88% 12%
7	m	296	 % 91% 9%
8	CH	175	 % 79% 10% 11%
8	n	175	 % 81% 7% 11%
9	CI	222	 % 92% 7%
9	o	222	 % 89% 11%
10	CJ	233	 7% 91% 9%
10	p	233	 % 91% 9%
11	CK	191	 2% 83% 17%
11	q	191	 % 88% 12%
12	CL	220	 2% 84% 12%
12	r	220	 % 85% 11%
13	CM	169	 % 85% 15%
13	s	169	 % 89% 11%
14	CN	193	 % 89% 11%
14	t	193	 % 91% 9%
15	CO	136	 % 85% 15%

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Mol	Chain	Length	Quality of chain
15	u	136	90% 10%
16	CP	203	90% 10%
16	v	203	90% 10%
17	CQ	197	88% 12% .
17	w	197	87% 12% .
18	CR	183	14% 86% 14%
18	x	183	4% 87% 13%
19	CS	185	95% 5%
19	y	185	91% 9%
20	CT	188	2% 87% 13%
20	z	188	2% 93% 6% .
21	0	172	% 89% 10% .
21	CU	172	87% 13%
22	2	159	84% 16%
22	CV	159	87% 13%
23	5	100	7% 89% 11%
23	CW	100	7% 87% 13%
24	CX	136	93% 7%
24	l2	136	90% 10%
25	6	1800	4% 75% 22% ..
25	A	1800	5% 74% 24% ..
26	7	98	34% 93% 7%
26	CY	98	12% 92% 8%
27	8	121	86% 14%
27	CZ	121	2% 88% 11% .

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Mol	Chain	Length	Quality of chain	
28	9	126	%	91% 8%
28	DA	126	%	90% 10%
29	AA	135	3%	92% 8%
29	DB	135	3%	90% 10%
30	AB	148		90% 10%
30	DC	148		91% 9%
31	AC	58		88% 10%
31	DD	58		86% 14%
32	AD	97	4%	89% 11%
32	DE	97	%	94% 6%
33	AE	109	2%	89% 11%
33	DF	109		83% 17%
34	AF	127	2%	89% 11%
34	DG	127	%	87% 13%
35	AG	106		92% 8%
35	DH	106		92% 8%
36	AH	112		89% 11%
36	DI	112		88% 12%
37	AI	119	%	88% 12%
37	DJ	119	2%	86% 14%
38	AJ	99	2%	87% 13%
38	DK	99	2%	85% 15%
39	AK	87		92% 8%
39	DL	87	2%	90% 10%
40	AL	77	%	87% 13%

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Mol	Chain	Length	Quality of chain
40	DM	77	13% 88% 12%
41	AM	50	90% 10%
41	DN	50	94% 6%
42	AN	52	90% 10%
42	DO	52	90% 10%
43	AO	25	72% 28%
43	DP	25	84% 16%
44	AP	105	2% 86% 13%
44	DQ	105	88% 12%
45	AQ	91	90% 10%
45	DR	91	87% 13%
46	i	168	11% 86% 8% 5%
47	p0	220	11% 57% 8% 35%
48	sM	104	4% 92% 7%
49	B	206	5% 90% 10%
49	s0	206	88% 12%
50	C	216	15% 87% 12%
50	s1	216	88% 11%
51	D	217	2% 88% 12%
51	s2	217	85% 14%
52	E	223	3% 89% 11%
52	s3	223	4% 92% 8%
53	F	260	2% 88% 12%
53	s4	260	90% 10%
54	G	206	11% 91% 9%

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Mol	Chain	Length	Quality of chain
54	s5	206	6% 92% 8%
55	H	226	3% 91% 9%
55	s6	226	3% 85% 12% .
56	I	186	5% 85% 13% ..
56	s7	186	4% 92% 7% .
57	J	199	5% 85% 9% . 6%
57	s8	199	3% 86% 8% . 6%
58	K	185	9% 85% 14% .
58	s9	185	2% 89% 11%
59	L	105	2% 84% 7% . 9%
59	c0	105	26% 79% 10% . 9%
60	M	155	10% 92% 7% .
60	c1	155	5% 82% 12% 6%
61	N	124	19% 84% 15% .
61	c2	124	37% 81% 18% .
62	O	150	2% 91% 9%
62	c3	150	91% 9% .
63	P	128	12% 88% 12% .
63	c4	128	8% 91% 9%
64	Q	141	4% 80% 8% 12%
64	c5	141	8% 87% 8% . .
65	R	142	12% 86% 13% ..
65	c6	142	% 87% 13%
66	S	125	2% 85% 10% . . .
67	T	145	7% 88% 11% .

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Mol	Chain	Length	Quality of chain
67	c8	145	90% 9%
68	U	143	87% 13% 5%
68	c9	143	93% 7%
69	V	110	87% 10% 7%
69	d0	110	90% 10% 21%
70	W	87	87% 13% 5%
70	d1	87	91% 9%
71	X	129	88% 10%
71	d2	129	91% 9%
72	Y	144	87% 13%
72	d3	144	92% 8%
73	Z	134	94% 6% 4%
73	d4	134	90% 10% 2%
74	a	70	80% 20% 14%
74	d5	70	93% 6% 4%
75	b	97	82% 18% 8%
75	d6	97	90% 10%
76	c	81	94% 6% 11%
76	d7	81	90% 10% 6%
77	d	63	90% 10% 21%
77	d8	63	89% 11% 13%
78	d9	53	87% 11% 2%
78	e	53	91% 9% 2%
79	e0	62	76% 24% 3%
79	f	62	85% 11% 10%

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Mol	Chain	Length	Quality of chain
80	g	71	
81	h	318	
81	sR	318	
82	c7	121	
83	e1	51	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
84	OHX	1	3675	-	-	-	X
84	OHX	1	3722	-	-	-	X
85	MG	1	3758	-	-	-	X
85	MG	1	3789	-	-	-	X
85	MG	1	3801	-	-	-	X
85	MG	1	3830	-	-	-	X
85	MG	1	3949	-	-	-	X
85	MG	1	4008	-	-	-	X
85	MG	1	4010	-	-	-	X
85	MG	1	4063	-	-	-	X
85	MG	1	4140	-	-	-	X
85	MG	1	4175	-	-	-	X
85	MG	1	4183	-	-	-	X
85	MG	1	4192	-	-	-	X
85	MG	1	4206	-	-	-	X
85	MG	4	217	-	-	-	X
85	MG	6	2065	-	-	-	X
85	MG	6	2170	-	-	-	X
85	MG	6	2181	-	-	-	X
85	MG	6	2185	-	-	-	X
85	MG	6	2190	-	-	-	X
85	MG	6	2193	-	-	-	X
85	MG	A	2073	-	-	-	X
85	MG	A	2089	-	-	-	X
85	MG	A	2098	-	-	-	X
85	MG	A	2103	-	-	-	X
85	MG	A	2112	-	-	-	X
85	MG	A	2118	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	MG	A	2124	-	-	-	X
85	MG	A	2129	-	-	-	X
85	MG	A	2135	-	-	-	X
85	MG	AR	3804	-	-	-	X
85	MG	AR	3812	-	-	-	X
85	MG	AR	3820	-	-	-	X
85	MG	AR	3826	-	-	-	X
85	MG	AR	3880	-	-	-	X
85	MG	AR	3893	-	-	-	X
85	MG	AR	3958	-	-	-	X
85	MG	AR	4024	-	-	-	X
85	MG	AR	4101	-	-	-	X
85	MG	AR	4122	-	-	-	X
85	MG	AR	4167	-	-	-	X
85	MG	AR	4173	-	-	-	X
85	MG	AR	4193	-	-	-	X
85	MG	AR	4202	-	-	-	X
85	MG	AR	4214	-	-	-	X
85	MG	AR	4233	-	-	-	X
85	MG	AR	4241	-	-	-	X
85	MG	AT	223	-	-	-	X
85	MG	CK	202	-	-	-	X
85	MG	CO	202	-	-	-	X
85	MG	l	402	-	-	-	X

## 2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 409590 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3149	Total 67355	C 30086	N 12142	O 21978	P 3149	0	0	0
1	AR	3149	Total 67355	C 30086	N 12142	O 21978	P 3149	0	0	0

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	Total 2579	C 1152	N 461	O 845	P 121	0	0	0
2	AS	121	Total 2579	C 1152	N 461	O 845	P 121	0	0	0

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	158	Total 3353	C 1500	N 586	O 1109	P 158	0	0	0
3	AT	158	Total 3353	C 1500	N 586	O 1109	P 158	0	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	252	Total 1914	C 1191	N 388	O 334	S 1	0	0	0
4	CD	252	Total 1914	C 1191	N 388	O 334	S 1	0	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			
5	CE	386	Total	C	N	O	S	0	0	0
			3075	1950	584	533	8			

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			
6	CF	361	Total	C	N	O	S	0	0	0
			2748	1729	522	494	3			

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			
7	CG	296	Total	C	N	O	S	0	0	0
			2375	1501	414	458	2			

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	n	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			
8	CH	156	Total	C	N	O	S	0	0	0
			1239	800	222	216	1			

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			
9	CI	222	Total	C	N	O	S	0	0	0
			1784	1151	324	308	1			

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	233	Total	C	N	O	S	0	0	0
			1804	1151	323	327	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CJ	233	1804	1151	323	327	3	0	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	q	191	1518	963	274	277	4	0	0	0
11	CK	191	1518	963	274	277	4	0	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	r	211	1705	1083	322	294	6	0	0	0
12	CL	211	1705	1083	322	294	6	0	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	s	169	1353	847	253	249	4	0	0	0
13	CM	169	1353	847	253	249	4	0	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	t	193	1543	962	315	266	0	0	0
14	CN	193	1543	962	315	266	0	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	u	136	1053	675	199	177	2	0	0	0
15	CO	136	1053	675	199	177	2	0	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	v	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			
16	CP	203	Total	C	N	O	S	0	0	0
			1720	1077	361	281	1			

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	w	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			
17	CQ	197	Total	C	N	O	S	0	0	0
			1555	1003	289	262	1			

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	x	183	Total	C	N	O	0	0	0
			1420	882	281	257			
18	CR	183	Total	C	N	O	0	0	0
			1420	882	281	257			

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	y	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			
19	CS	185	Total	C	N	O	S	0	0	0
			1441	908	290	241	2			

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
20	z	188	Total	C	N	O	0	0	0
			1521	935	326	260			
20	CT	188	Total	C	N	O	0	0	0
			1521	935	326	260			

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	0	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			
21	CU	172	Total	C	N	O	S	0	0	0
			1445	930	267	244	4			

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	2	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			
22	CV	159	Total	C	N	O	S	0	0	0
			1276	805	246	221	4			

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O	0	0	0
			796	516	131	149			
23	CW	100	Total	C	N	O	0	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	12	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			
24	CX	136	Total	C	N	O	S	0	0	0
			1003	628	189	179	7			

- Molecule 25 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	6	1783	Total	C	N	O	P	0	0	0
			37990	16984	6723	12500	1783			
25	A	1781	Total	C	N	O	P	0	0	0
			37948	16965	6715	12487	1781			

- Molecule 26 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	7	98	Total	C	N	O	S	0	0	0
			699	443	137	118	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	CY	98	699	443	137	118	1	0	0	0

- Molecule 27 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	8	121	964	620	169	173	2	0	0	0
27	CZ	121	964	620	169	173	2	0	0	0

- Molecule 28 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
28	9	126	993	625	192	176	0	0	0
28	DA	126	993	625	192	176	0	0	0

- Molecule 29 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
29	AA	135	1092	710	202	180	0	0	0
29	DB	135	1092	710	202	180	0	0	0

- Molecule 30 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	AB	148	1173	749	231	190	3	0	0	0
30	DC	148	1173	749	231	190	3	0	0	0

- Molecule 31 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
31	AC	58	462	289	100	73	0	0	0
31	DD	58	462	289	100	73	0	0	0



- Molecule 32 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AD	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			
32	DE	97	Total	C	N	O	S	0	0	0
			743	479	124	139	1			

- Molecule 33 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AE	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			
33	DF	109	Total	C	N	O	S	0	0	0
			876	556	167	152	1			

- Molecule 34 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	AF	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			
34	DG	127	Total	C	N	O	S	0	0	0
			1020	647	205	167	1			

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	AG	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			
35	DH	106	Total	C	N	O	S	0	0	0
			850	540	165	144	1			

- Molecule 36 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	AH	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			
36	DI	112	Total	C	N	O	S	0	0	0
			880	545	179	152	4			

- Molecule 37 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AI	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			
37	DJ	119	Total	C	N	O	S	0	0	0
			969	615	186	167	1			

- Molecule 38 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AJ	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			
38	DK	99	Total	C	N	O	S	0	0	0
			771	481	156	132	2			

- Molecule 39 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	AK	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			
39	DL	87	Total	C	N	O	S	0	0	0
			681	414	148	114	5			

- Molecule 40 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AL	77	Total	C	N	O	0	0	0
			612	391	115	106			
40	DM	77	Total	C	N	O	0	0	0
			612	391	115	106			

- Molecule 41 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AM	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			
41	DN	50	Total	C	N	O	S	0	0	0
			436	272	97	65	2			

- Molecule 42 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AN	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DO	52	Total	C	N	O	S	0	0	0
			417	259	86	67	5			

- Molecule 43 is a protein called 60S ribosomal protein L41-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	AO	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			
43	DP	25	Total	C	N	O	S	0	0	0
			233	142	63	27	1			

- Molecule 44 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	AP	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			
44	DQ	105	Total	C	N	O	S	0	0	0
			847	534	170	138	5			

- Molecule 45 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	AQ	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			
45	DR	91	Total	C	N	O	S	0	0	0
			694	429	138	121	6			

- Molecule 46 is a protein called Suppressor protein STM1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	i	159	Total	C	N	O	0	0	0
			1104	652	221	231			

- Molecule 47 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	p0	143	Total	C	N	O	S	0	0	0
			1077	687	192	195	3			

- Molecule 48 is a protein called Suppressor protein STM1,Suppressor protein STM1,Suppressor protein Stm1 - Mol B.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
48	sM	104	680	403	140	137	0	0	0

- Molecule 49 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	B	206	1577	1014	278	283	2	0	0	0
49	s0	206	1583	1017	281	283	2	0	0	0

- Molecule 50 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	C	214	1709	1084	310	311	4	0	0	0
50	s1	216	1722	1091	312	315	4	0	0	0

- Molecule 51 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	D	217	1635	1047	289	297	2	0	0	0
51	s2	217	1635	1047	289	297	2	0	0	0

- Molecule 52 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	E	223	1734	1101	313	314	6	0	0	0
52	s3	223	1734	1101	313	314	6	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	F	260	2068	1316	389	360	3	0	0	0
53	s4	260	2068	1316	389	360	3	0	0	0

- Molecule 54 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	G	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			
54	s5	206	Total	C	N	O	S	0	0	0
			1609	1007	300	299	3			

- Molecule 55 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	H	226	Total	C	N	O	S	0	0	0
			1799	1129	346	321	3			
55	s6	218	Total	C	N	O	S	0	0	0
			1755	1102	337	313	3			

- Molecule 56 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	I	184	Total	C	N	O	0	0	0
			1481	951	265	265			
56	s7	186	Total	C	N	O	0	0	0
			1491	957	267	267			

- Molecule 57 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	J	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			
57	s8	188	Total	C	N	O	S	0	0	0
			1489	925	298	264	2			

- Molecule 58 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	K	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			
58	s9	185	Total	C	N	O	S	0	0	0
			1494	943	289	261	1			

- Molecule 59 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	L	96	Total	C	N	O	S	0	0	0
			772	499	126	145	2			
59	c0	96	Total	C	N	O	S	0	0	0
			761	490	125	144	2			

- Molecule 60 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	M	155	Total	C	N	O	S	0	0	0
			1213	774	230	206	3			
60	c1	146	Total	C	N	O	S	0	0	0
			1168	747	221	197	3			

- Molecule 61 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	N	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			
61	c2	124	Total	C	N	O	S	0	0	0
			890	560	156	172	2			

- Molecule 62 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	O	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			
62	c3	150	Total	C	N	O	S	0	0	0
			1192	759	224	207	2			

- Molecule 63 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	P	127	Total	C	N	O	S	0	0	0
			891	545	182	163	1			
63	c4	128	Total	C	N	O	S	0	0	0
			949	582	188	176	3			

- Molecule 64 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
64	Q	124	Total	C	N	O	S	0	0	0
			977	622	182	166	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	c5	135	1039	658	196	178	7	0	0	0

- Molecule 65 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
65	R	141	1105	708	203	194		0	0	0
65	c6	142	1111	711	204	196		0	0	0

- Molecule 66 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	S	120	926	577	177	170	2	0	0	0

- Molecule 67 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	T	145	1192	743	237	210	2	0	0	0
67	c8	145	1192	743	237	210	2	0	0	0

- Molecule 68 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	U	143	1112	694	208	208	2	0	0	0
68	c9	143	1112	694	208	208	2	0	0	0

- Molecule 69 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
69	V	107	855	539	156	159	1	0	0	0
69	d0	110	882	554	161	166	1	0	0	0

- Molecule 70 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	W	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			
70	d1	87	Total	C	N	O	S	0	0	0
			684	420	125	137	2			

- Molecule 71 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
71	X	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			
71	d2	129	Total	C	N	O	S	0	0	0
			1021	650	188	180	3			

- Molecule 72 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	Y	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			
72	d3	144	Total	C	N	O	S	0	0	0
			1121	708	220	191	2			

- Molecule 73 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
73	Z	134	Total	C	N	O	0	0	0
			1073	676	208	189			
73	d4	134	Total	C	N	O	0	0	0
			1073	676	208	189			

- Molecule 74 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
74	a	70	Total	C	N	O	0	0	0
			563	360	104	99			
74	d5	69	Total	C	N	O	0	0	0
			558	357	103	98			

- Molecule 75 is a protein called 40S ribosomal protein S26-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	b	97	Total	C	N	O	S	0	0	0
			769	475	160	129	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
75	d6	97	769	475	160	129	5	0	0	0

- Molecule 76 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	c	81	610	382	110	113	5	0	0	0
76	d7	81	610	382	110	113	5	0	0	0

- Molecule 77 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	d	63	497	306	99	91	1	0	0	0
77	d8	63	497	306	99	91	1	0	0	0

- Molecule 78 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	e	53	442	274	92	72	4	0	0	0
78	d9	53	442	274	92	72	4	0	0	0

- Molecule 79 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	f	60	475	299	98	77	1	0	0	0
79	e0	62	491	309	101	80	1	0	0	0

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	g	71	566	362	106	94	4	0	0	0

- Molecule 81 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	h	318	Total	C	N	O	S	0	0	0
			2437	1541	418	470	8			
81	sR	318	Total	C	N	O	S	0	0	0
			2442	1544	418	472	8			

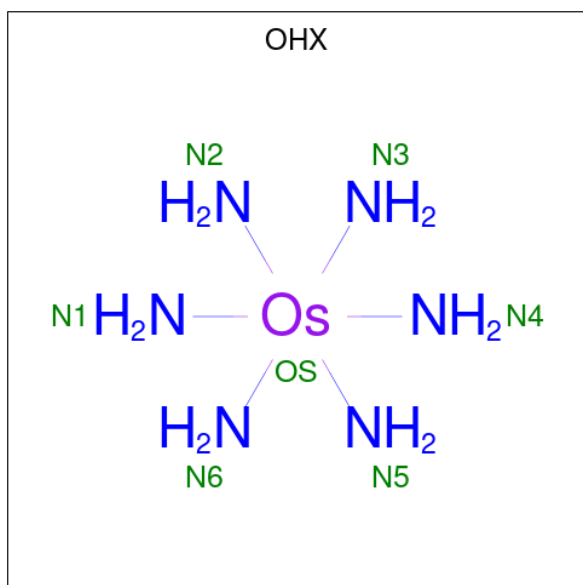
- Molecule 82 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	c7	117	Total	C	N	O	S	0	0	0
			906	563	174	167	2			

- Molecule 83 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
83	e1	51	Total	C	N	O	S	0	0	0
			397	249	73	71	4			

- Molecule 84 is osmium (III) hexammine (three-letter code: OHX) (formula: H<sub>12</sub>N<sub>6</sub>Os).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0
84	1	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		
84	1	1	Total	N	Os	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	1	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0
84	3	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	4	1	7	6	1	0	0
84	k	1	7	6	1	0	0
84	k	1	7	6	1	0	0
84	l	1	7	6	1	0	0
84	r	1	7	6	1	0	0
84	v	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	x	1	7	6	1	0	0
84	y	1	7	6	1	0	0
84	z	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	2	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
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84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
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84	6	1	Total 7	N 6	Os 1	0	0
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84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0
84	6	1	Total 7	N 6	Os 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0
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84	6	1	7	6	1	0	0
84	6	1	7	6	1	0	0
84	AC	1	7	6	1	0	0
84	AE	1	7	6	1	0	0
84	AG	1	7	6	1	0	0
84	AK	1	7	6	1	0	0
84	AK	1	7	6	1	0	0
84	AP	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
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84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AR	1	7	6	1	0	0
84	AS	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AS	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	AT	1	7	6	1	0	0
84	CE	1	7	6	1	0	0
84	CE	1	7	6	1	0	0
84	CF	1	7	6	1	0	0
84	CF	1	7	6	1	0	0
84	CG	1	7	6	1	0	0
84	CG	1	7	6	1	0	0
84	CG	1	7	6	1	0	0
84	CK	1	7	6	1	0	0
84	CL	1	7	6	1	0	0
84	CL	1	7	6	1	0	0
84	CM	1	7	6	1	0	0
84	CO	1	7	6	1	0	0
84	CP	1	7	6	1	0	0
84	CV	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	CX	1	7	6	1	0	0
84	CZ	1	7	6	1	0	0
84	DD	1	7	6	1	0	0
84	DG	1	7	6	1	0	0
84	DH	1	7	6	1	0	0
84	DI	1	7	6	1	0	0
84	DL	1	7	6	1	0	0
84	DL	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	Os		
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	A	1	7	6	1	0	0
84	H	1	7	6	1	0	0
84	J	1	7	6	1	0	0
84	M	1	7	6	1	0	0
84	O	1	7	6	1	0	0
84	Q	1	7	6	1	0	0
84	T	1	7	6	1	0	0
84	e	1	7	6	1	0	0
84	h	1	7	6	1	0	0
84	s8	1	7	6	1	0	0
84	c3	1	7	6	1	0	0
84	c5	1	7	6	1	0	0
84	c8	1	7	6	1	0	0
84	d9	1	7	6	1	0	0
84	sR	1	7	6	1	0	0

- Molecule 85 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	490	Total 490	Mg 490	0	0
85	3	12	Total 12	Mg 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	4	21	Total 21	Mg 21	0	0
85	j	2	Total 2	Mg 2	0	0
85	k	2	Total 2	Mg 2	0	0
85	l	2	Total 2	Mg 2	0	0
85	o	3	Total 3	Mg 3	0	0
85	r	1	Total 1	Mg 1	0	0
85	s	1	Total 1	Mg 1	0	0
85	t	2	Total 2	Mg 2	0	0
85	v	1	Total 1	Mg 1	0	0
85	w	1	Total 1	Mg 1	0	0
85	x	5	Total 5	Mg 5	0	0
85	z	2	Total 2	Mg 2	0	0
85	l2	2	Total 2	Mg 2	0	0
85	6	141	Total 141	Mg 141	0	0
85	9	1	Total 1	Mg 1	0	0
85	AB	4	Total 4	Mg 4	0	0
85	AF	2	Total 2	Mg 2	0	0
85	AH	1	Total 1	Mg 1	0	0
85	AK	1	Total 1	Mg 1	0	0
85	AP	1	Total 1	Mg 1	0	0
85	i	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AR	504	Total 504	Mg 504	0	0
85	AS	20	Total 20	Mg 20	0	0
85	AT	12	Total 12	Mg 12	0	0
85	CD	2	Total 2	Mg 2	0	0
85	CE	4	Total 4	Mg 4	0	0
85	CF	1	Total 1	Mg 1	0	0
85	CI	1	Total 1	Mg 1	0	0
85	CK	1	Total 1	Mg 1	0	0
85	CO	2	Total 2	Mg 2	0	0
85	CP	2	Total 2	Mg 2	0	0
85	CQ	4	Total 4	Mg 4	0	0
85	CR	6	Total 6	Mg 6	0	0
85	CU	2	Total 2	Mg 2	0	0
85	CX	2	Total 2	Mg 2	0	0
85	DA	1	Total 1	Mg 1	0	0
85	DC	4	Total 4	Mg 4	0	0
85	DD	1	Total 1	Mg 1	0	0
85	DE	1	Total 1	Mg 1	0	0
85	DF	1	Total 1	Mg 1	0	0
85	DG	1	Total 1	Mg 1	0	0
85	DH	2	Total 2	Mg 2	0	0

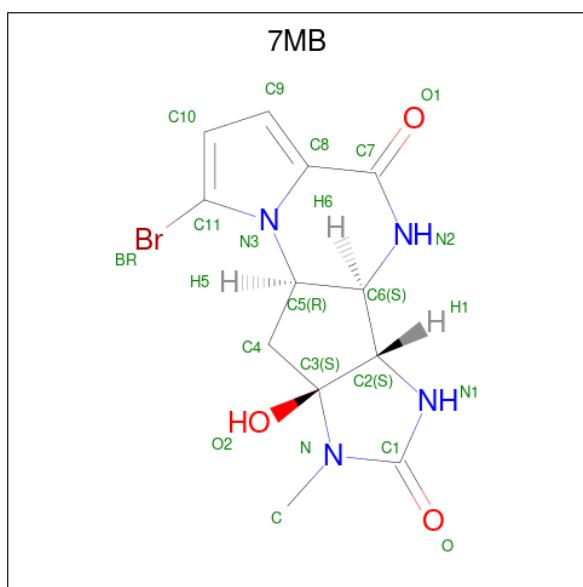
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	DI	1	Total Mg 1 1	0	0
85	DO	1	Total Mg 1 1	0	0
85	DP	1	Total Mg 1 1	0	0
85	DR	2	Total Mg 2 2	0	0
85	sM	1	Total Mg 1 1	0	0
85	A	111	Total Mg 111 111	0	0
85	D	1	Total Mg 1 1	0	0
85	F	1	Total Mg 1 1	0	0
85	Y	1	Total Mg 1 1	0	0
85	b	1	Total Mg 1 1	0	0
85	s1	1	Total Mg 1 1	0	0
85	s2	1	Total Mg 1 1	0	0
85	s6	1	Total Mg 1 1	0	0
85	s8	1	Total Mg 1 1	0	0
85	c6	1	Total Mg 1 1	0	0
85	c9	1	Total Mg 1 1	0	0
85	d3	3	Total Mg 3 3	0	0
85	d5	1	Total Mg 1 1	0	0
85	d6	1	Total Mg 1 1	0	0
85	d9	1	Total Mg 1 1	0	0

- Molecule 86 is Agelastatin A (three-letter code: 7MB) (formula:  $C_{12}H_{13}BrN_4O_3$ ).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
86	1	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		
86	AR	1	Total	Br	C	N	O	0	0
			20	1	12	4	3		

- Molecule 87 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
87	AK	1	Total	Zn	0	0
			1	1		
87	AN	1	Total	Zn	0	0
			1	1		
87	AP	1	Total	Zn	0	0
			1	1		
87	AQ	1	Total	Zn	0	0
			1	1		
87	DL	1	Total	Zn	0	0
			1	1		
87	DO	1	Total	Zn	0	0
			1	1		
87	DQ	1	Total	Zn	0	0
			1	1		
87	DR	1	Total	Zn	0	0
			1	1		
87	b	1	Total	Zn	0	0
			1	1		
87	c	1	Total	Zn	0	0
			1	1		

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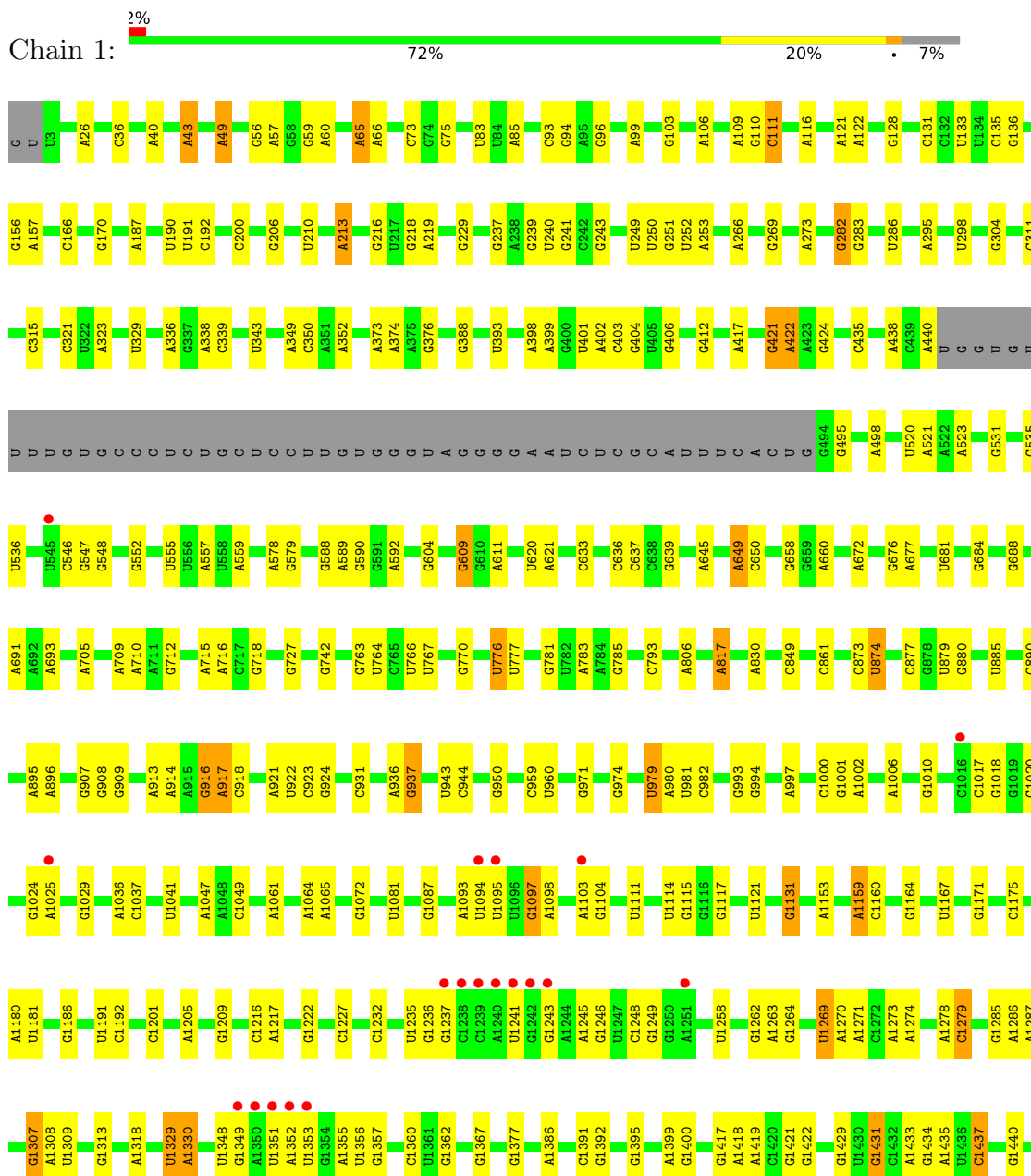
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
87	e	1	Total 1	Zn 1	0	0
87	g	1	Total 1	Zn 1	0	0
87	d6	1	Total 1	Zn 1	0	0
87	d7	1	Total 1	Zn 1	0	0
87	d9	1	Total 1	Zn 1	0	0
87	e1	1	Total 1	Zn 1	0	0

### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

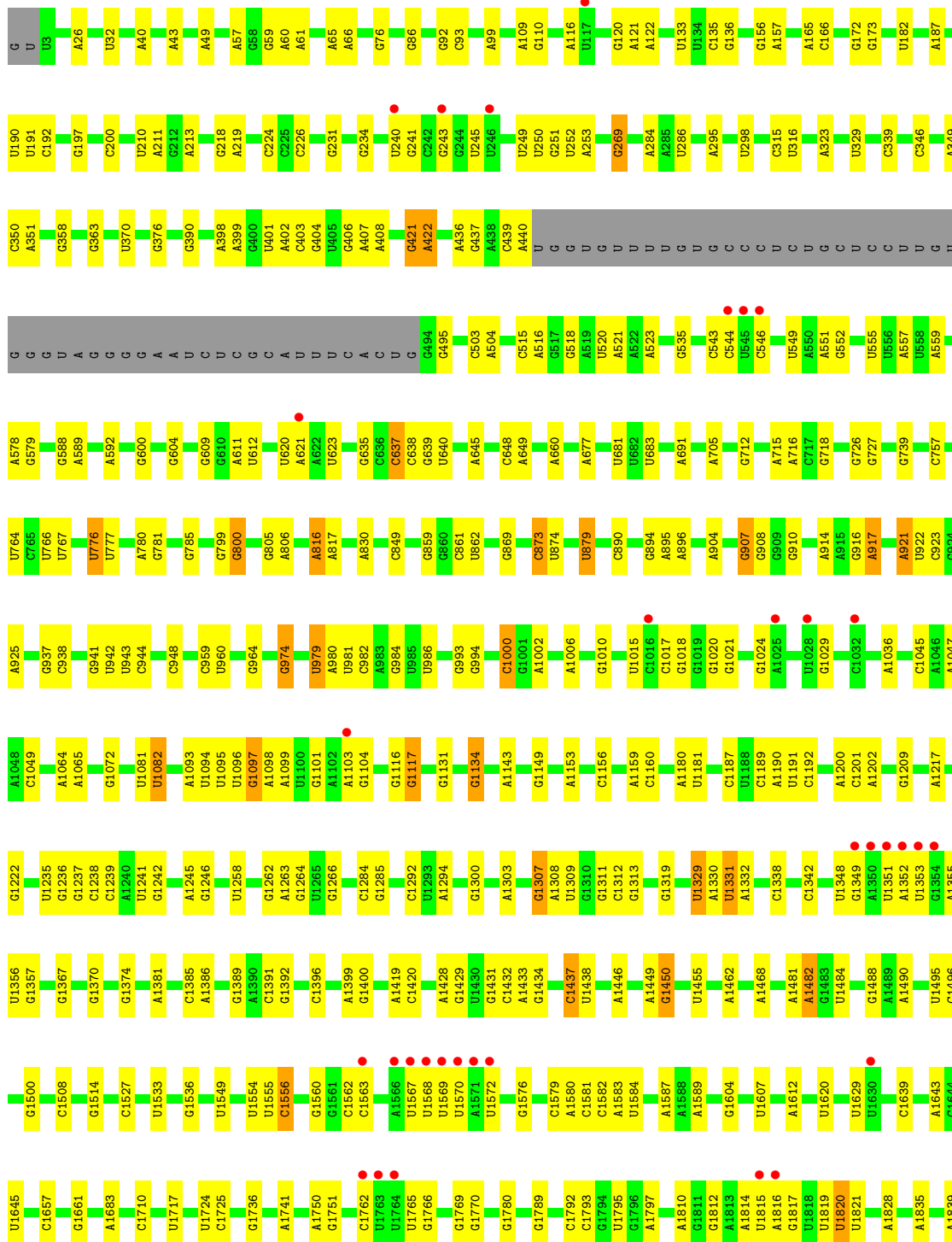
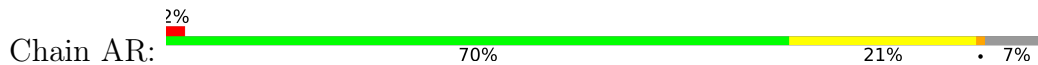
- Molecule 1: 25S ribosomal RNA

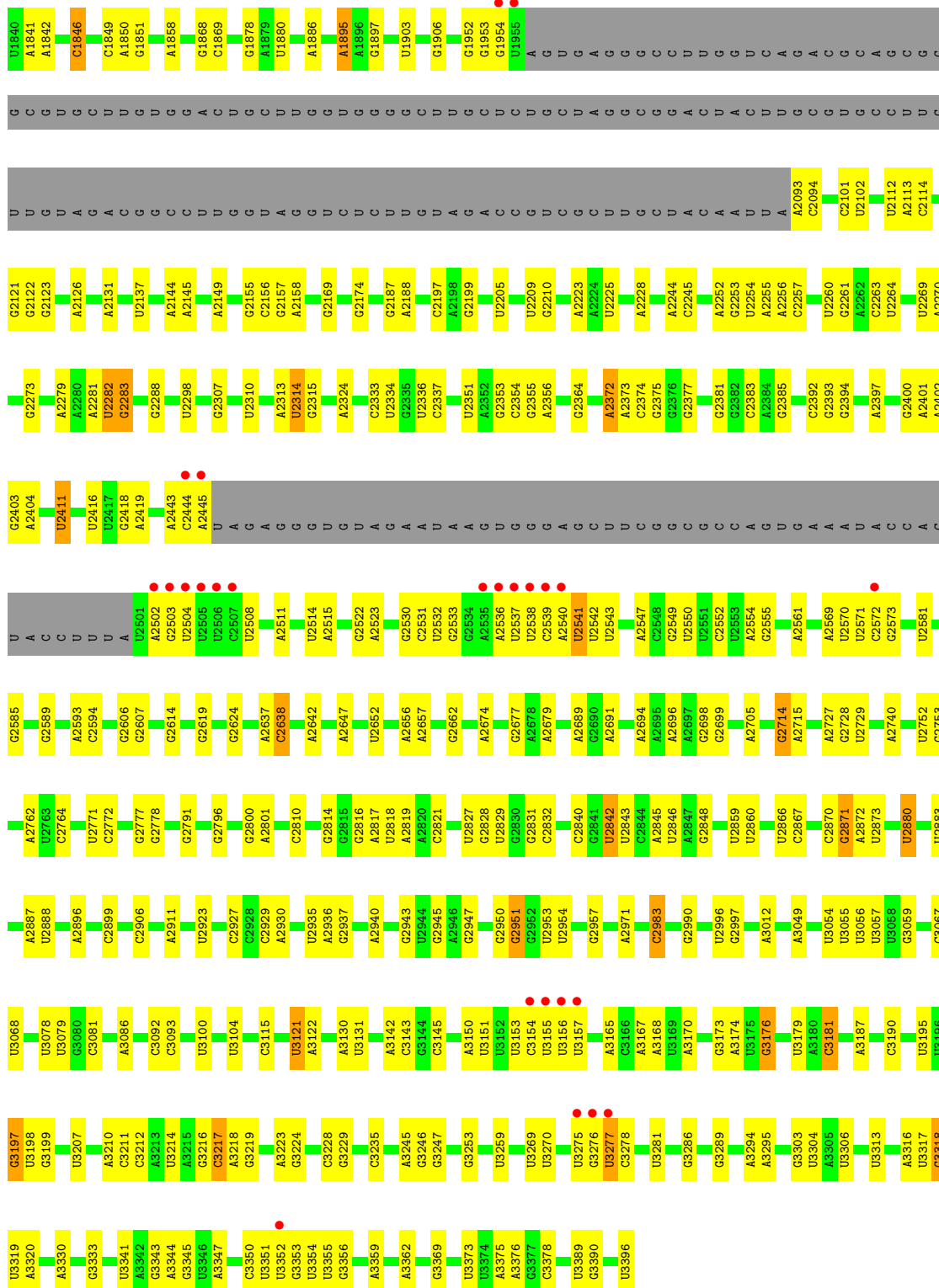


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A1482	U1716	G1852	A2131	C2306	A2445	U2506	G2615	A2802	C2942	A3142	G3271	G3348
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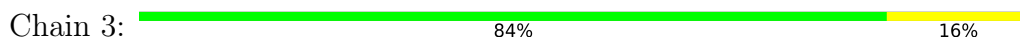
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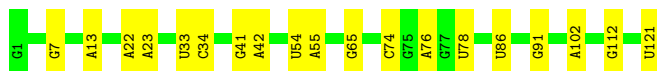
● Molecule 1: 25S ribosomal RNA



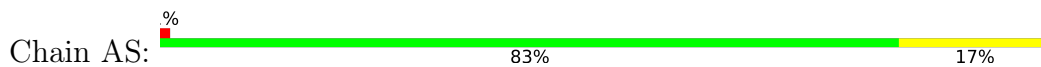


• Molecule 2: 5S ribosomal RNA

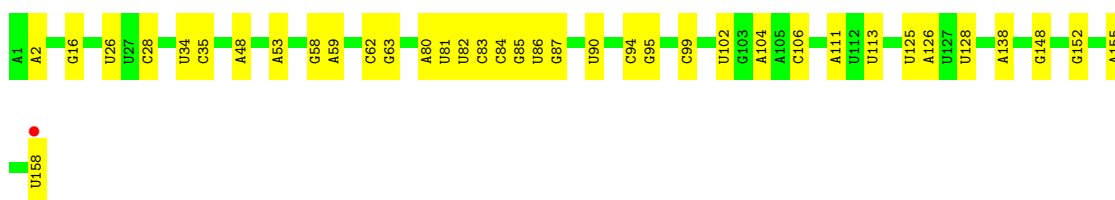
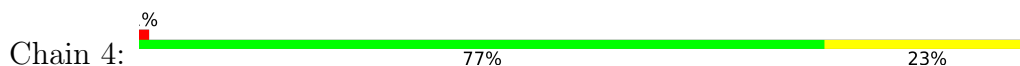




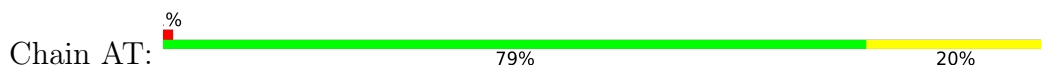
- Molecule 2: 5S ribosomal RNA



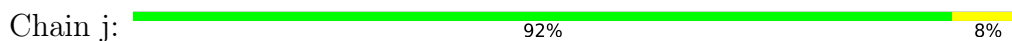
- Molecule 3: 5.8S ribosomal RNA



- Molecule 3: 5.8S ribosomal RNA



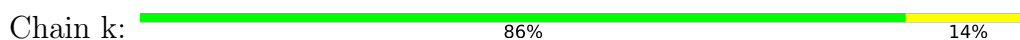
- Molecule 4: 60S ribosomal protein L2-A



- Molecule 4: 60S ribosomal protein L2-A

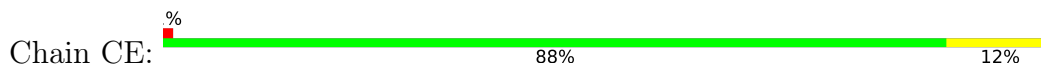


- Molecule 5: 60S ribosomal protein L3

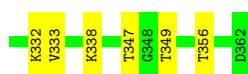
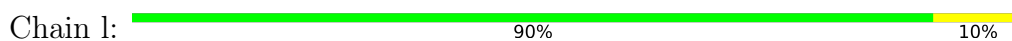




- Molecule 5: 60S ribosomal protein L3



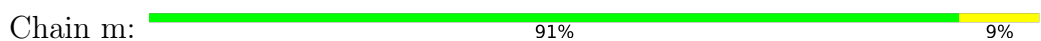
- Molecule 6: 60S ribosomal protein L4-A



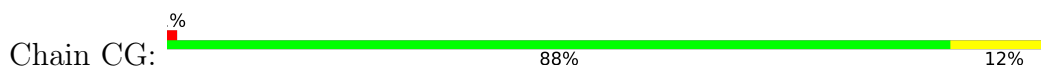
- Molecule 6: 60S ribosomal protein L4-A



- Molecule 7: 60S ribosomal protein L5



- Molecule 7: 60S ribosomal protein L5

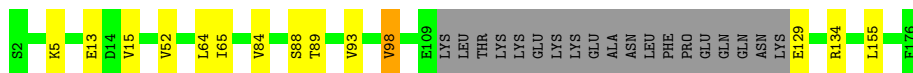






- Molecule 8: 60S ribosomal protein L6-A

Chain n: 81% 7% 11%



- Molecule 8: 60S ribosomal protein L6-A

Chain CH: 79% 10% 11%



- Molecule 9: 60S ribosomal protein L7-A

Chain o: 89% 11%



- Molecule 9: 60S ribosomal protein L7-A

Chain CI: 92% 7% 1%



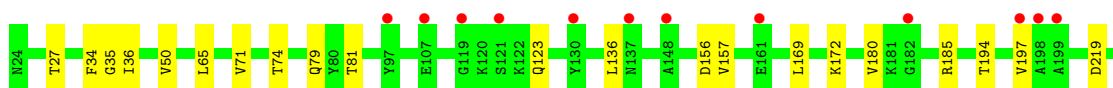
- Molecule 10: 60S ribosomal protein L8-A

Chain p: 91% 9% 1%

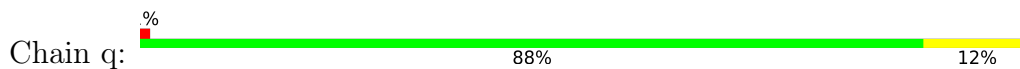


- Molecule 10: 60S ribosomal protein L8-A

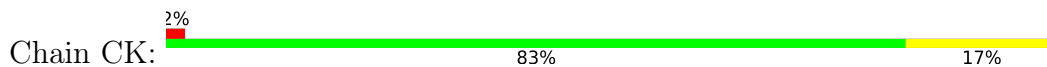
Chain CJ: 7% 91% 9%



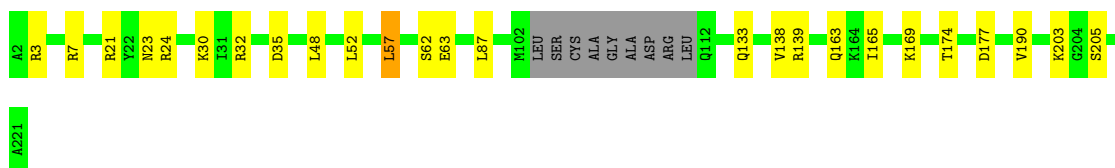
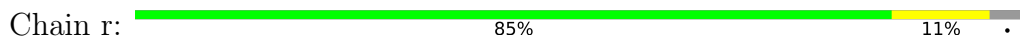
- Molecule 11: 60S ribosomal protein L9-A



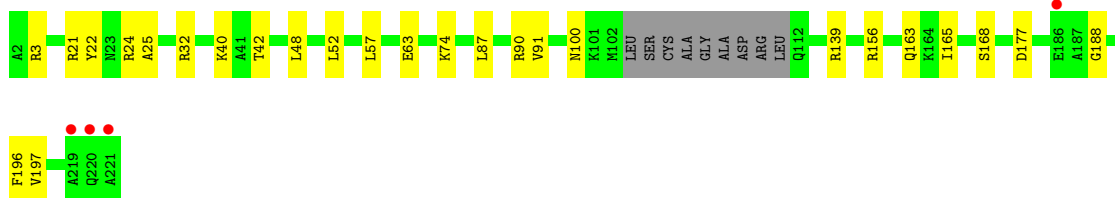
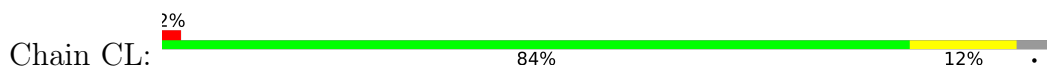
- Molecule 11: 60S ribosomal protein L9-A



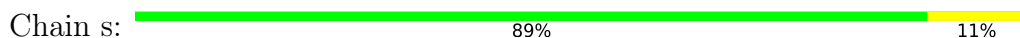
- Molecule 12: 60S ribosomal protein L10



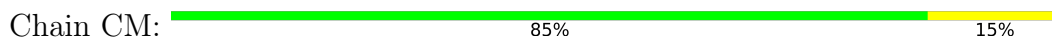
- Molecule 12: 60S ribosomal protein L10



- Molecule 13: 60S ribosomal protein L11-B

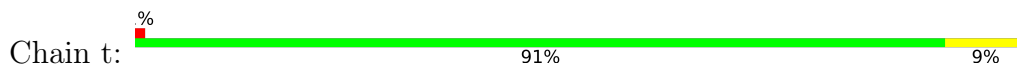


- Molecule 13: 60S ribosomal protein L11-B

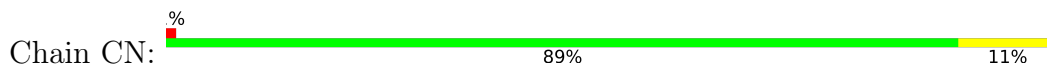




- Molecule 14: 60S ribosomal protein L13-A



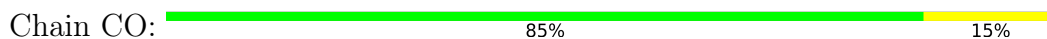
- Molecule 14: 60S ribosomal protein L13-A



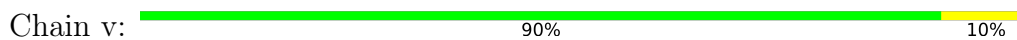
- Molecule 15: 60S ribosomal protein L14-A



- Molecule 15: 60S ribosomal protein L14-A



- Molecule 16: 60S ribosomal protein L15-A



- Molecule 16: 60S ribosomal protein L15-A

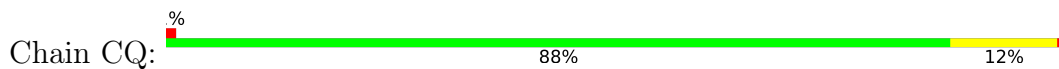


- Molecule 17: 60S ribosomal protein L16-A

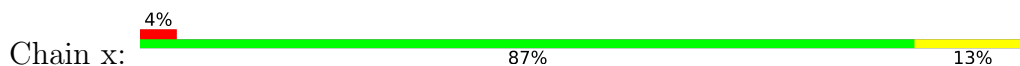




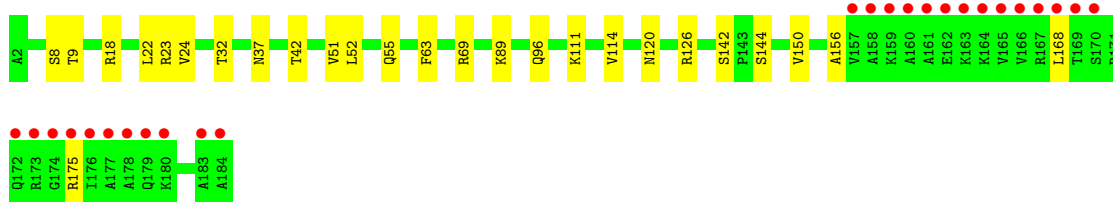
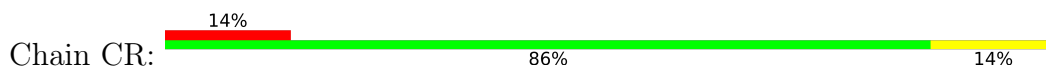
- Molecule 17: 60S ribosomal protein L16-A



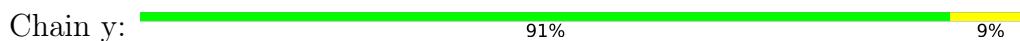
- Molecule 18: 60S ribosomal protein L17-A



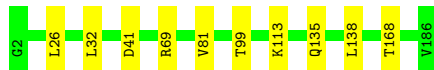
- Molecule 18: 60S ribosomal protein L17-A



- Molecule 19: 60S ribosomal protein L18-A



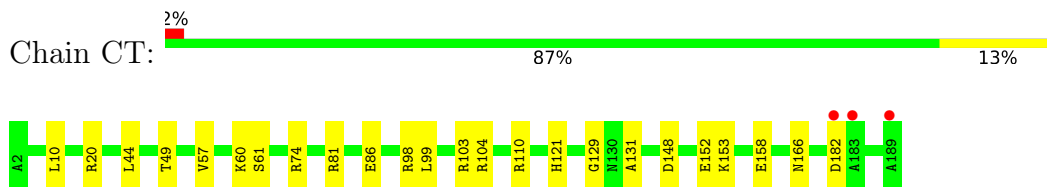
- Molecule 19: 60S ribosomal protein L18-A



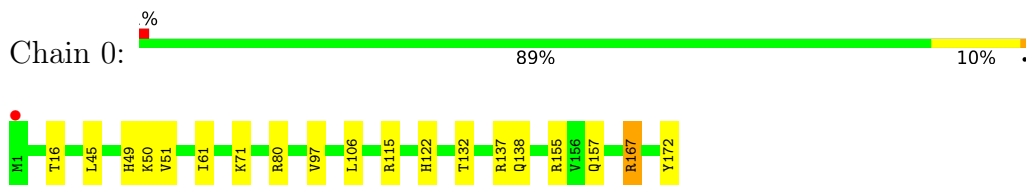
- Molecule 20: 60S ribosomal protein L19-A



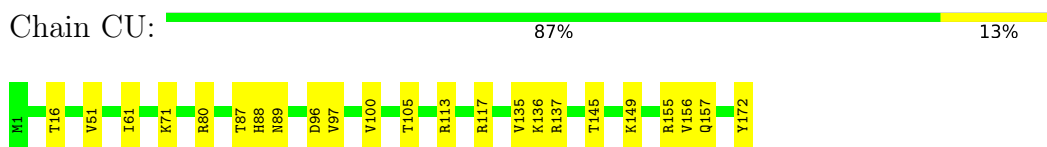
- Molecule 20: 60S ribosomal protein L19-A



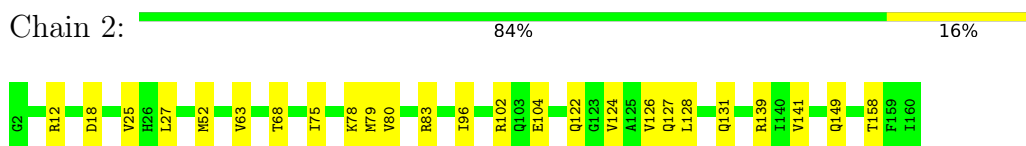
- Molecule 21: 60S ribosomal protein L20-A



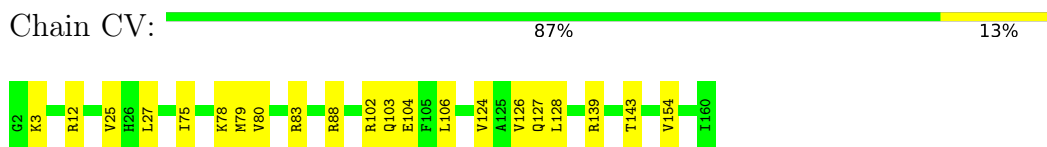
- Molecule 21: 60S ribosomal protein L20-A



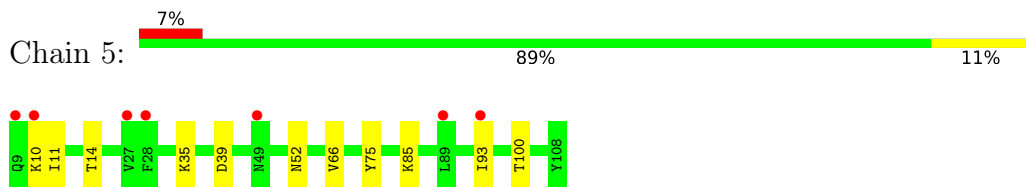
- Molecule 22: 60S ribosomal protein L21-A



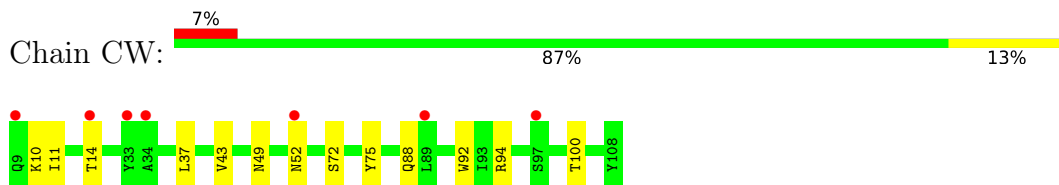
- Molecule 22: 60S ribosomal protein L21-A



- Molecule 23: 60S ribosomal protein L22-A



- Molecule 23: 60S ribosomal protein L22-A



- Molecule 24: 60S ribosomal protein L23-A

Chain l2: 90% 10%



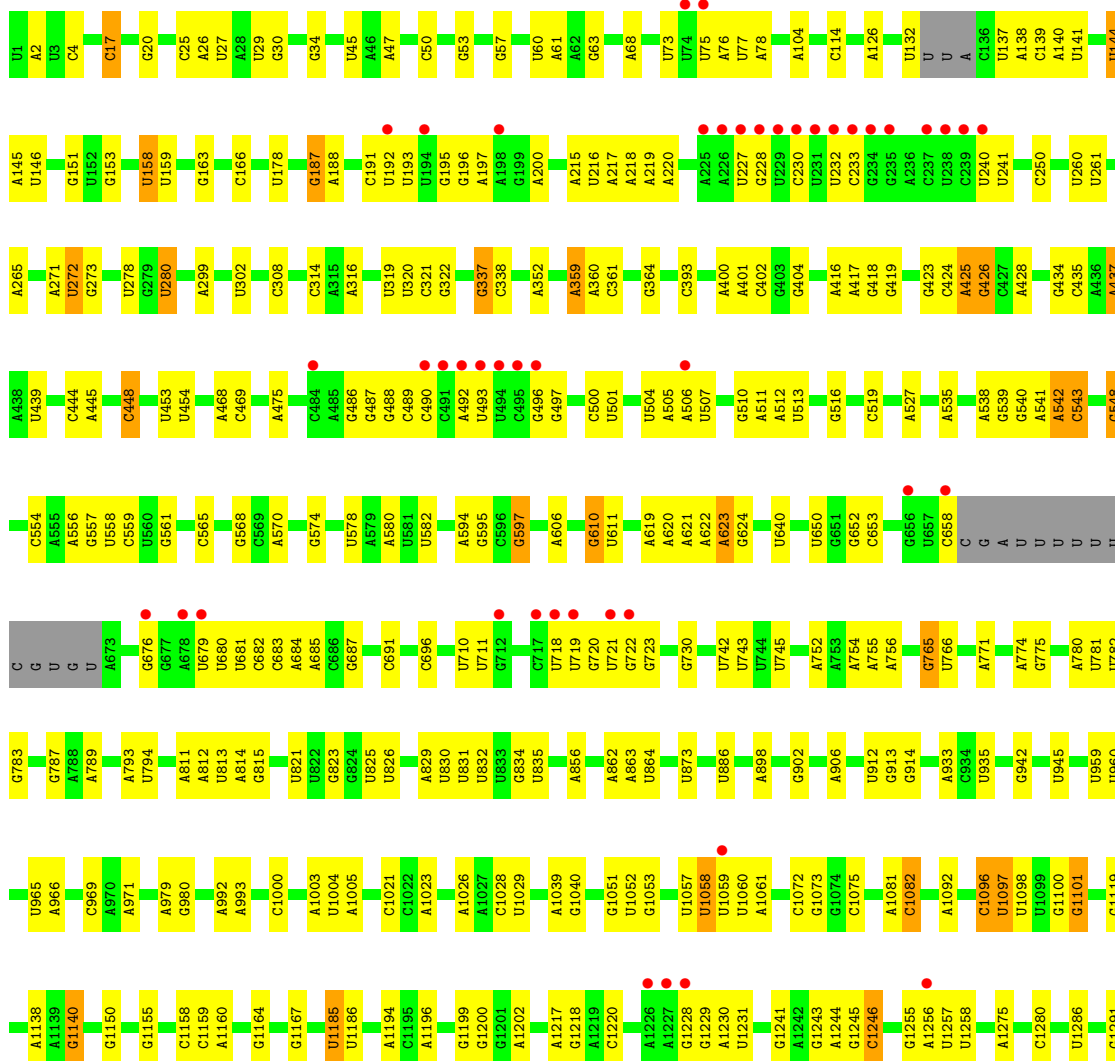
- Molecule 24: 60S ribosomal protein L23-A

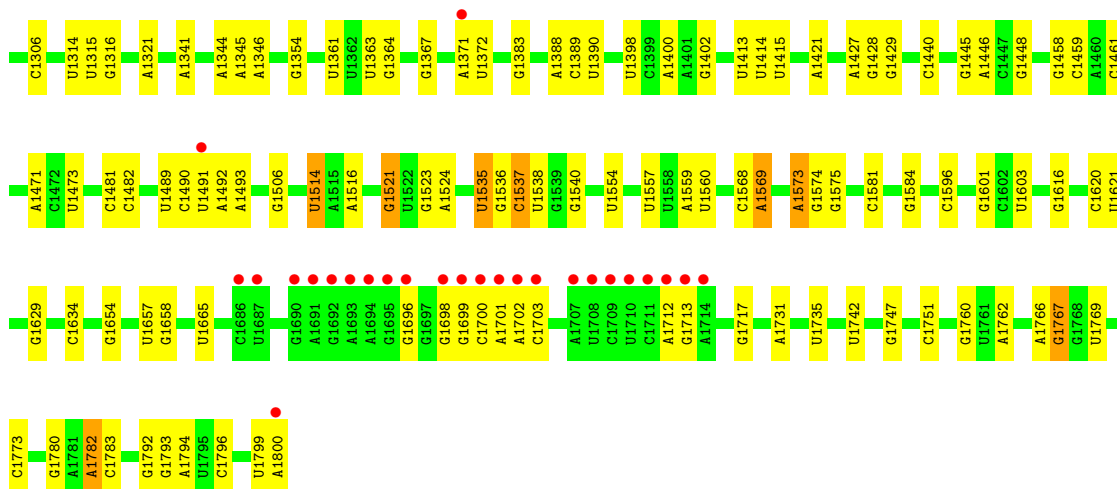
Chain CX: 93% 7%



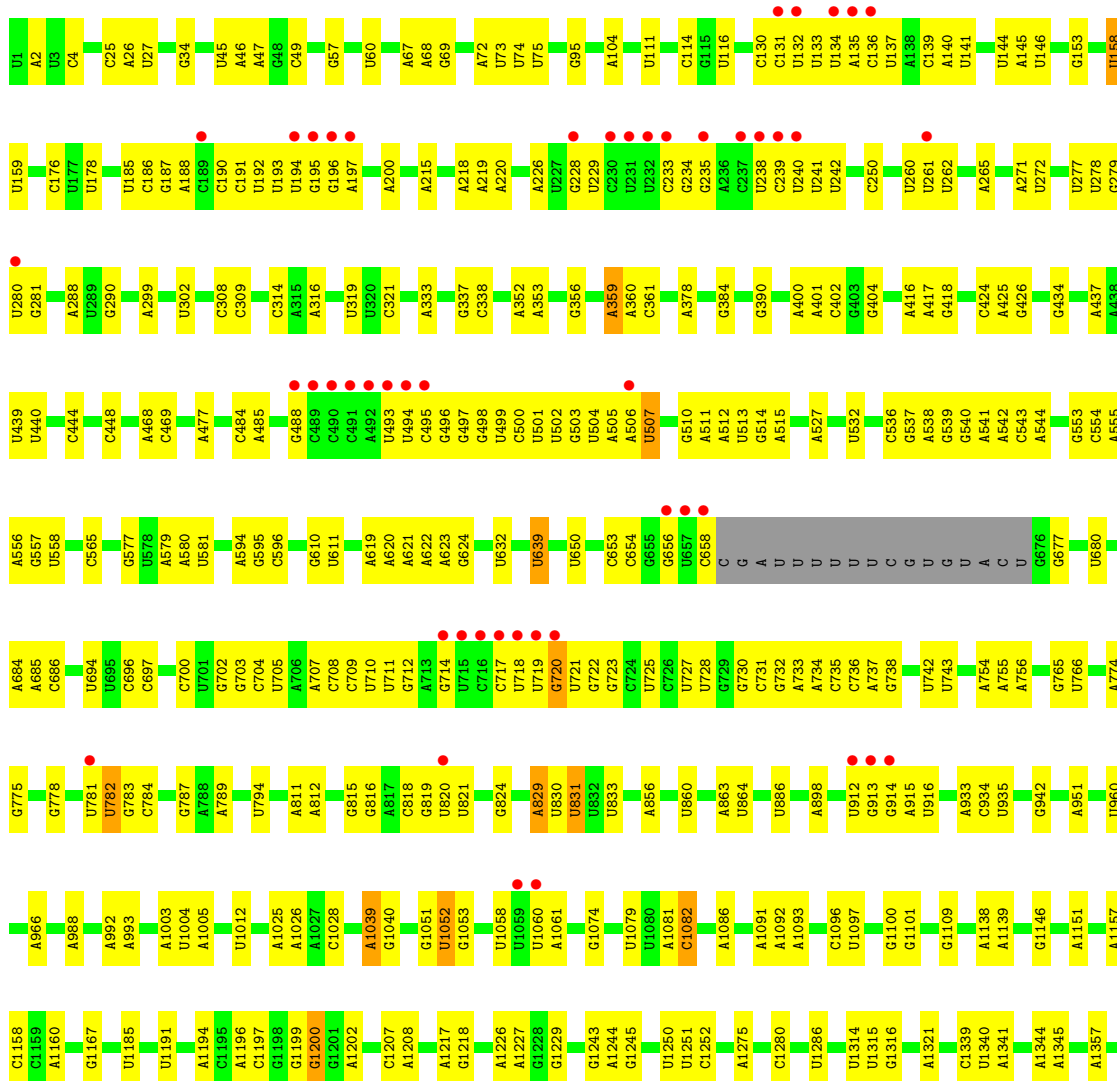
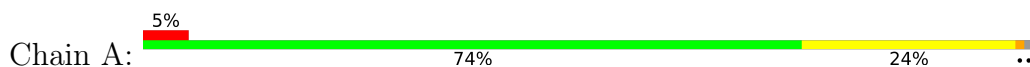
- Molecule 25: 18S ribosomal RNA

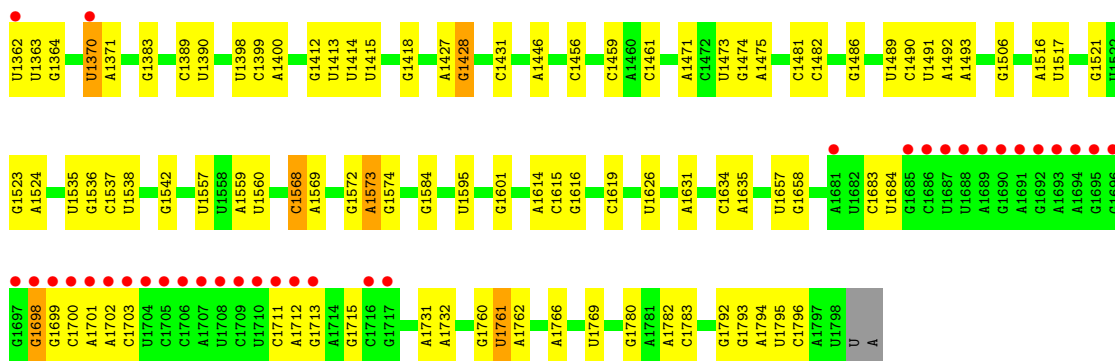
Chain 6: 4% 75% 22%



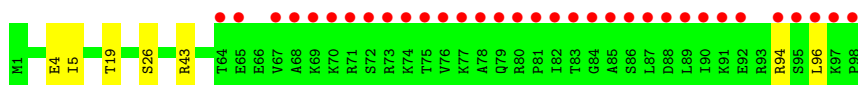


● Molecule 25: 18S ribosomal RNA

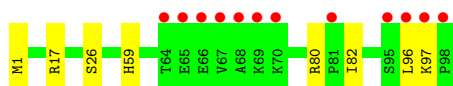




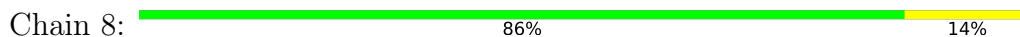
- Molecule 26: 60S ribosomal protein L24-A



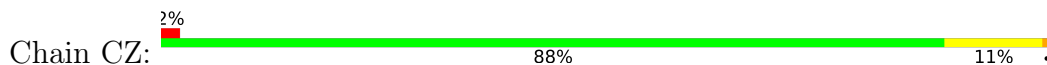
- Molecule 26: 60S ribosomal protein L24-A



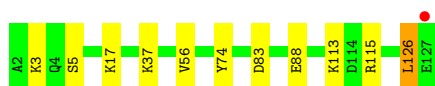
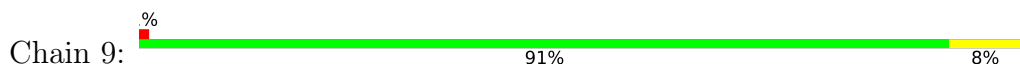
- Molecule 27: 60S ribosomal protein L25



- Molecule 27: 60S ribosomal protein L25

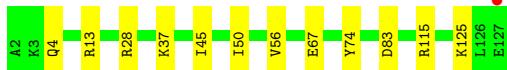


- Molecule 28: 60S ribosomal protein L26-A

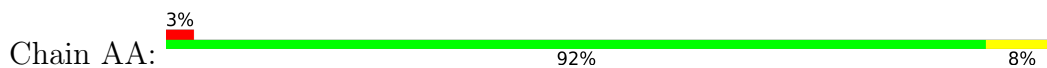


- Molecule 28: 60S ribosomal protein L26-A





- Molecule 29: 60S ribosomal protein L27-A



- Molecule 29: 60S ribosomal protein L27-A



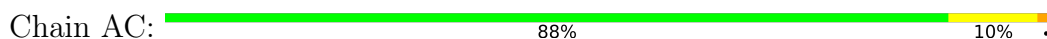
- Molecule 30: 60S ribosomal protein L28



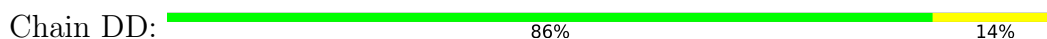
- Molecule 30: 60S ribosomal protein L28



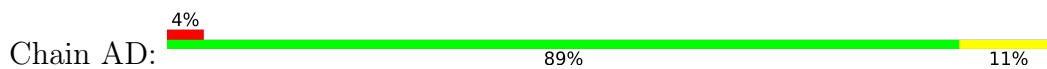
- Molecule 31: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L29



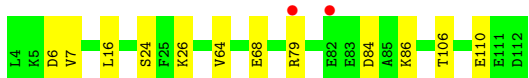
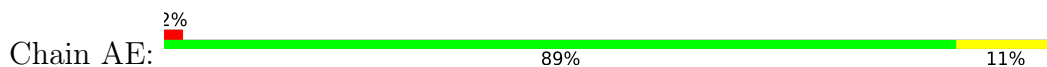
- Molecule 32: 60S ribosomal protein L30



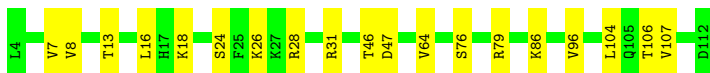
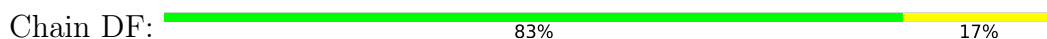
- Molecule 32: 60S ribosomal protein L30



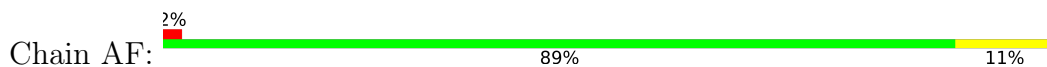
- Molecule 33: 60S ribosomal protein L31-A



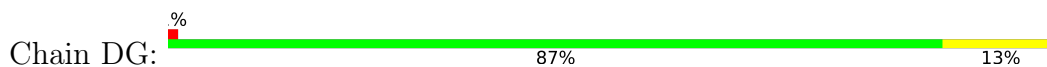
- Molecule 33: 60S ribosomal protein L31-A



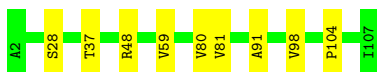
- Molecule 34: 60S ribosomal protein L32



- Molecule 34: 60S ribosomal protein L32



- Molecule 35: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L33-A

Chain DH:  92% 8%




- Molecule 36: 60S ribosomal protein L34-A

Chain AH:  89% 11%




- Molecule 36: 60S ribosomal protein L34-A

Chain DI:  88% 12%




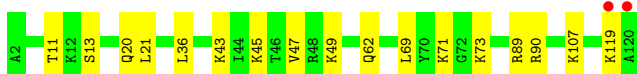
- Molecule 37: 60S ribosomal protein L35-A

Chain AI:  88% 12% 2%




- Molecule 37: 60S ribosomal protein L35-A

Chain DJ:  86% 14% 2%




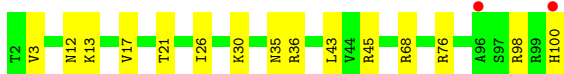
- Molecule 38: 60S ribosomal protein L36-A

Chain AJ:  87% 13% 2%



- Molecule 38: 60S ribosomal protein L36-A

Chain DK:  85% 15% 2%

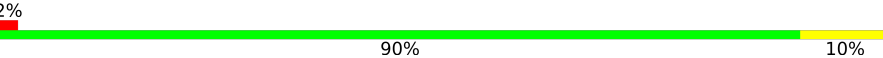


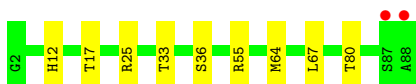
- Molecule 39: 60S ribosomal protein L37-A

Chain AK:  92% 8%




- Molecule 39: 60S ribosomal protein L37-A

Chain DL:  2% 90% 10%

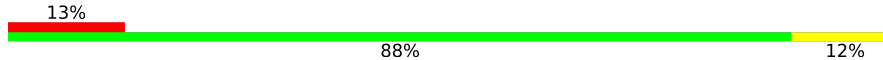


- Molecule 40: 60S ribosomal protein L38

Chain AL:  0% 87% 13%



- Molecule 40: 60S ribosomal protein L38

Chain DM:  13% 88% 12%



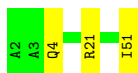
- Molecule 41: 60S ribosomal protein L39

Chain AM:  90% 10%



- Molecule 41: 60S ribosomal protein L39

Chain DN:  94% 6%



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain AN:  90% 10%



- Molecule 42: Ubiquitin-60S ribosomal protein L40

Chain DO:  90% 10%




- Molecule 43: 60S ribosomal protein L41-B

Chain AO:  72% 28%




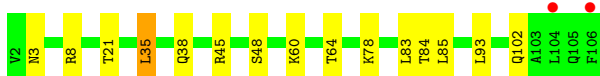
- Molecule 43: 60S ribosomal protein L41-B

Chain DP:  84% 16%




- Molecule 44: 60S ribosomal protein L42-A

Chain AP:  2% 86% 13%



- Molecule 44: 60S ribosomal protein L42-A

Chain DQ:  88% 12%




- Molecule 45: 60S ribosomal protein L43-A

Chain AQ:  90% 10%

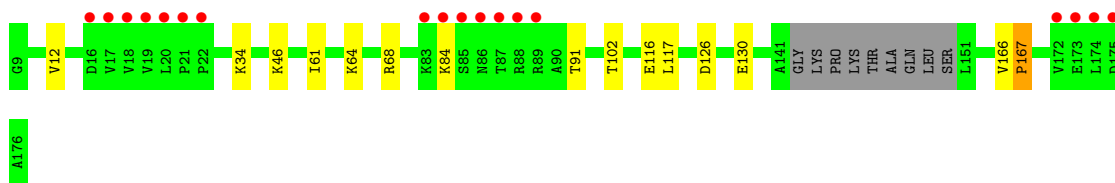
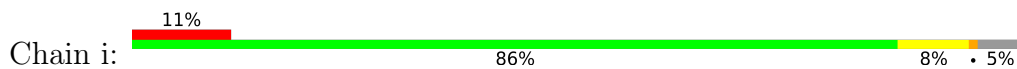


- Molecule 45: 60S ribosomal protein L43-A

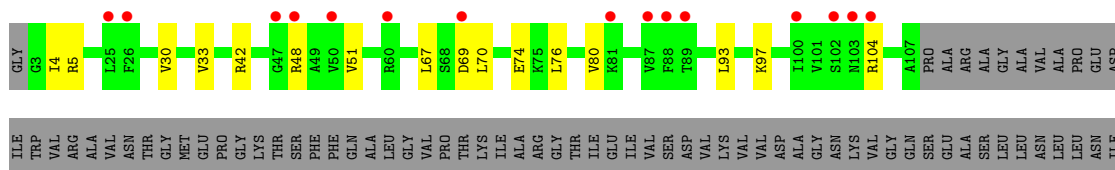
Chain DR:  87% 13%



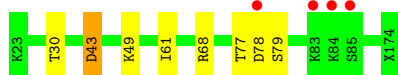
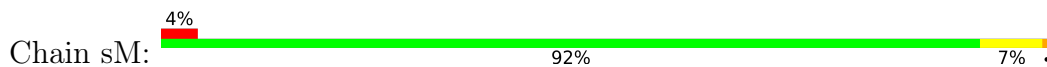
- Molecule 46: Suppressor protein STM1



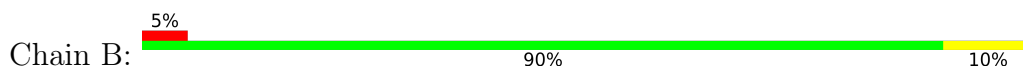
- Molecule 47: 60S acidic ribosomal protein P0



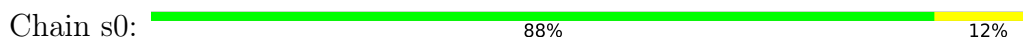
- Molecule 48: Suppressor protein STM1, Suppressor protein STM1, Suppressor protein Stm1 - Mol B



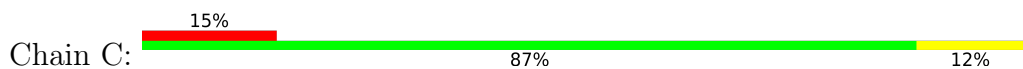
- Molecule 49: 40S ribosomal protein S0-A

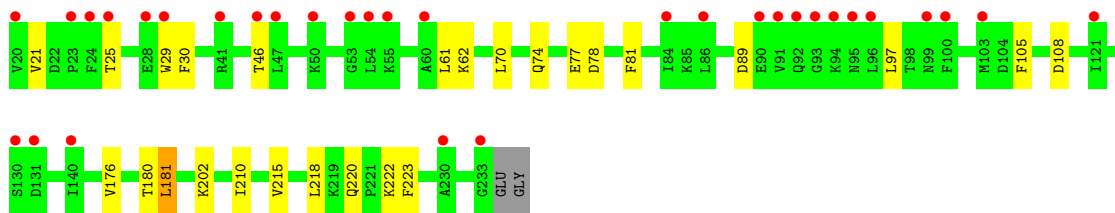


- Molecule 49: 40S ribosomal protein S0-A

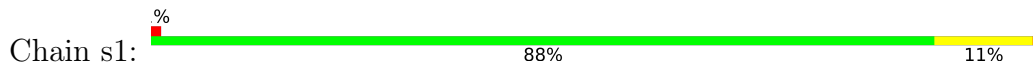


- Molecule 50: 40S ribosomal protein S1-A

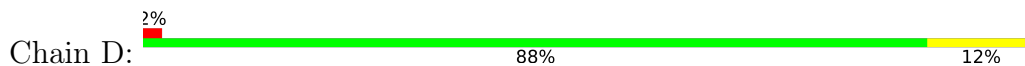




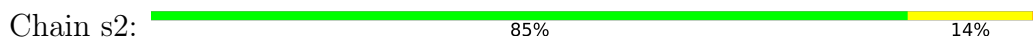
- Molecule 50: 40S ribosomal protein S1-A



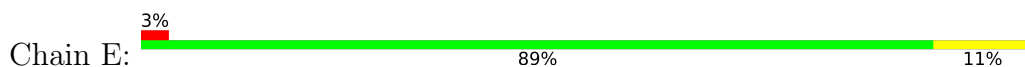
- Molecule 51: 40S ribosomal protein S2



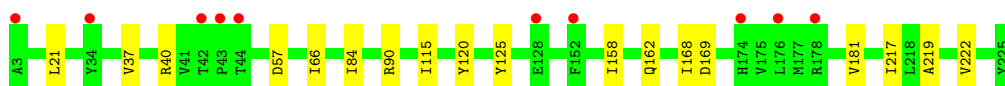
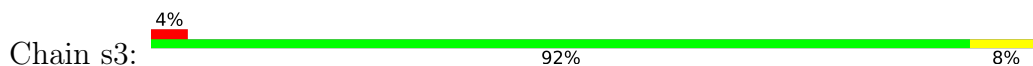
- Molecule 51: 40S ribosomal protein S2



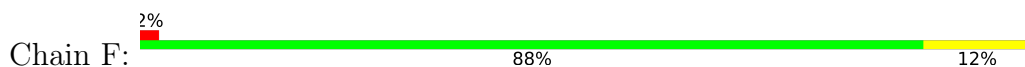
- Molecule 52: 40S ribosomal protein S3

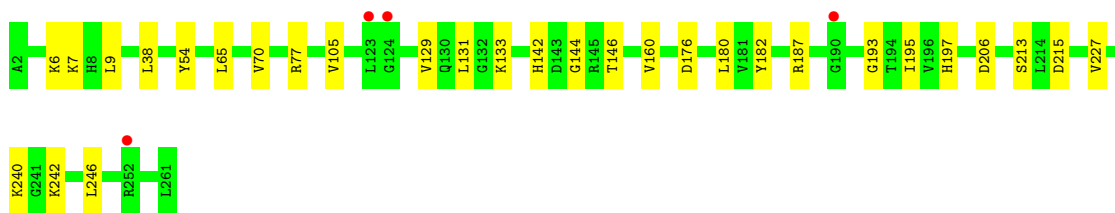


- Molecule 52: 40S ribosomal protein S3



- Molecule 53: 40S ribosomal protein S4-A





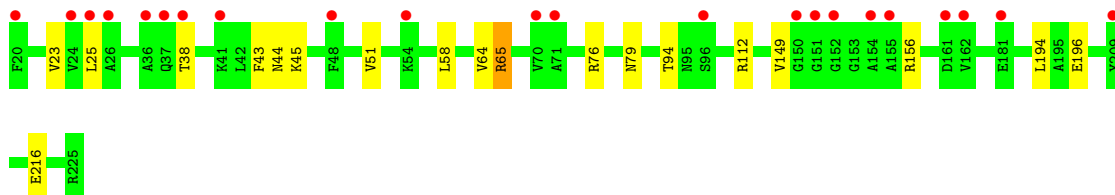
- Molecule 53: 40S ribosomal protein S4-A

Chain s4:  90% 10%



- Molecule 54: 40S ribosomal protein S5

Chain G:  11% 91% 9%



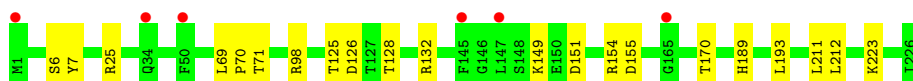
- Molecule 54: 40S ribosomal protein S5

Chain s5:  6% 92% 8%



- Molecule 55: 40S ribosomal protein S6-A

Chain H:  3% 91% 9%



- Molecule 55: 40S ribosomal protein S6-A

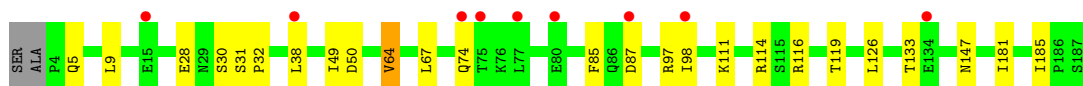
Chain s6:  3% 85% 12%



- Molecule 56: 40S ribosomal protein S7-A

Chain I:  5% 85% 13%

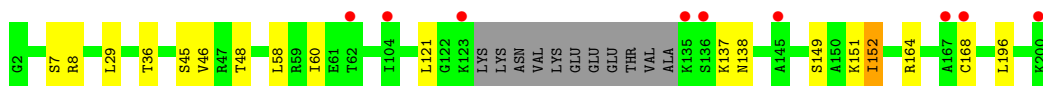
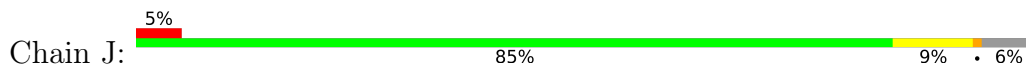




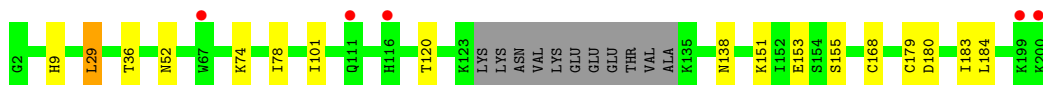
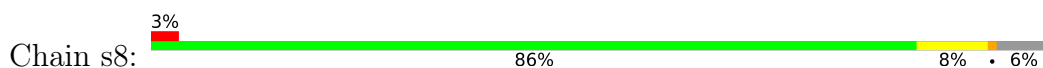
- Molecule 56: 40S ribosomal protein S7-A



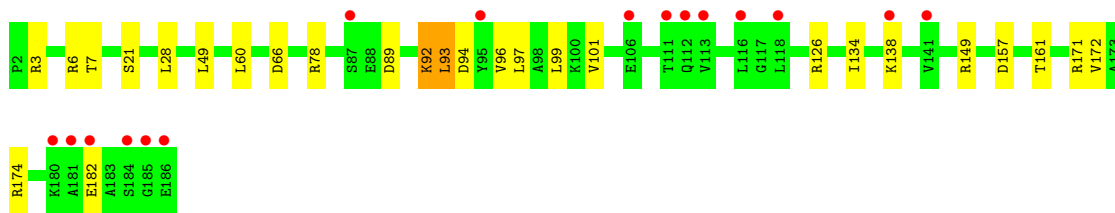
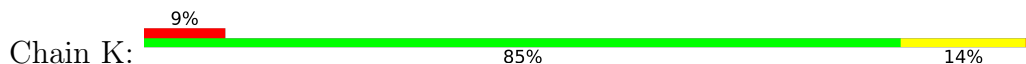
- Molecule 57: 40S ribosomal protein S8-A



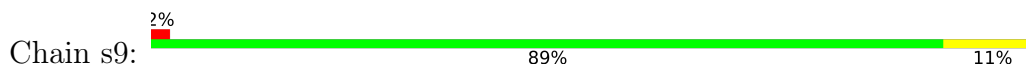
- Molecule 57: 40S ribosomal protein S8-A



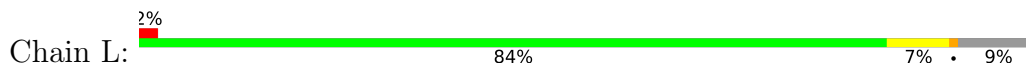
- Molecule 58: 40S ribosomal protein S9-A



- Molecule 58: 40S ribosomal protein S9-A

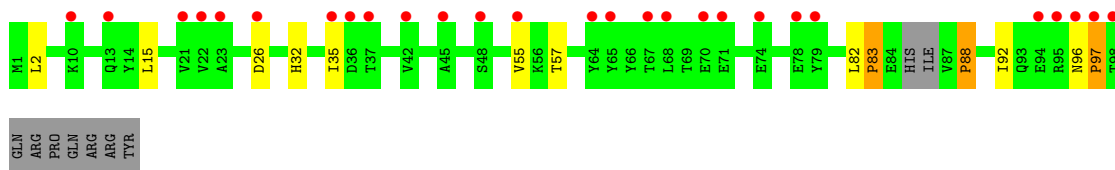
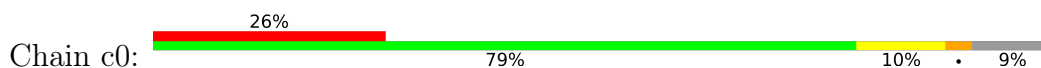


- Molecule 59: 40S ribosomal protein S10-A

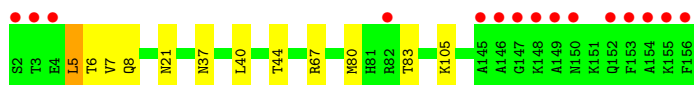




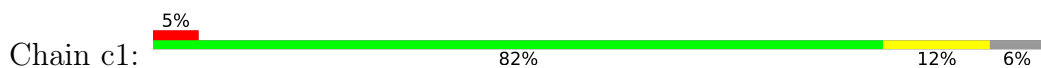
- Molecule 59: 40S ribosomal protein S10-A



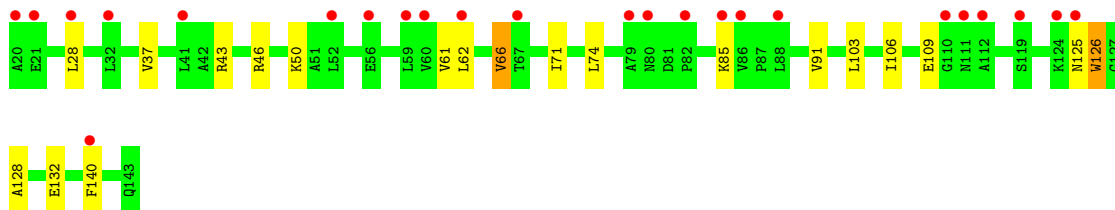
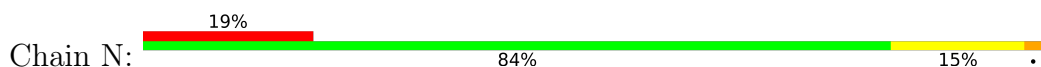
- Molecule 60: 40S ribosomal protein S11-A



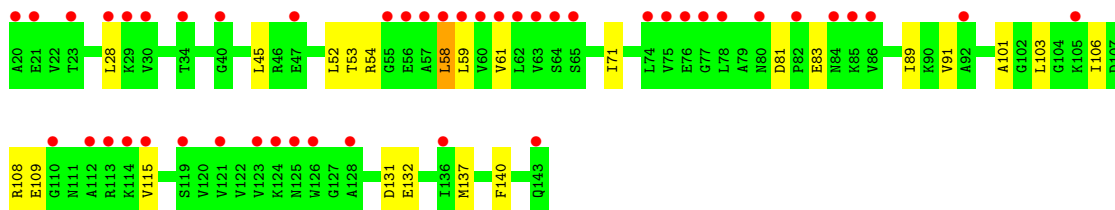
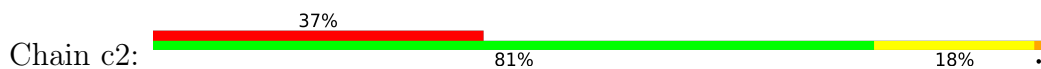
- Molecule 60: 40S ribosomal protein S11-A



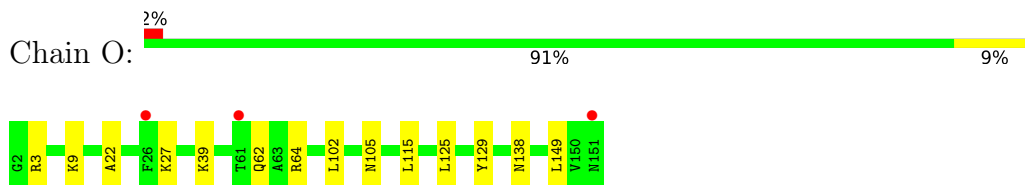
- Molecule 61: 40S ribosomal protein S12



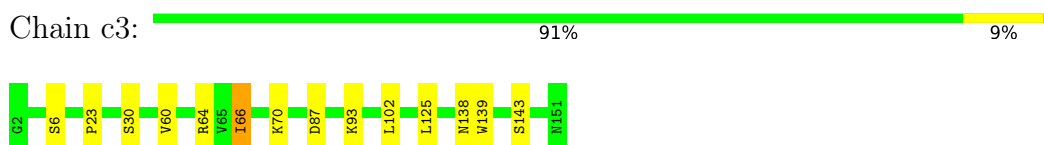
- Molecule 61: 40S ribosomal protein S12



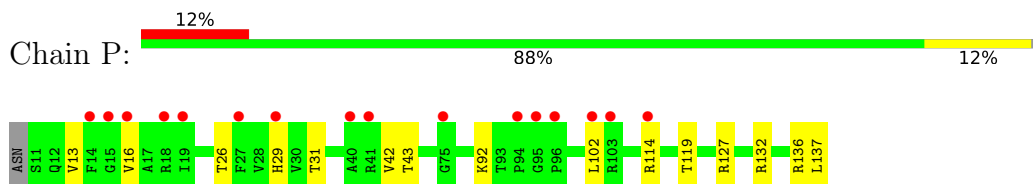
- Molecule 62: 40S ribosomal protein S13



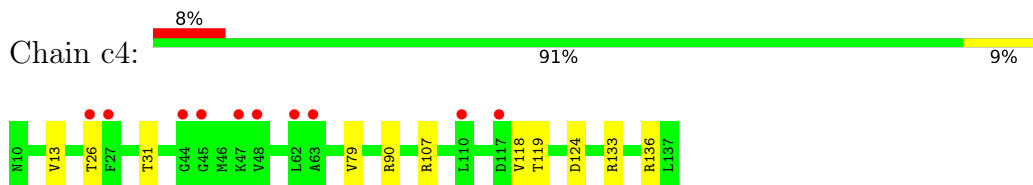
- Molecule 62: 40S ribosomal protein S13



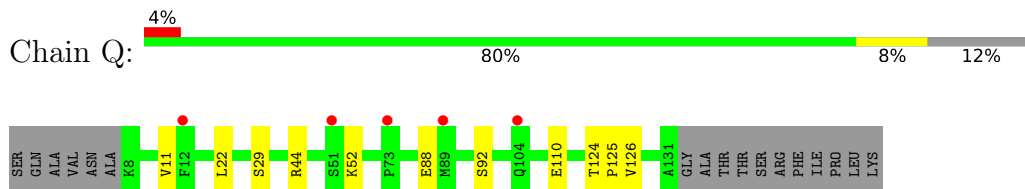
- Molecule 63: 40S ribosomal protein S14-B



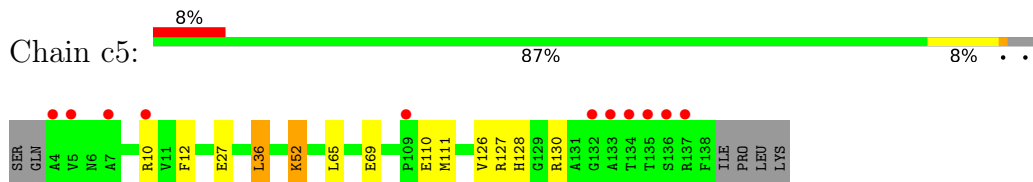
- Molecule 63: 40S ribosomal protein S14-B



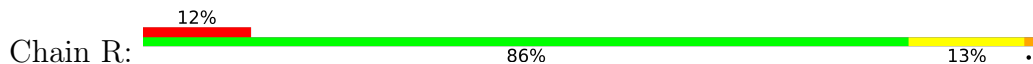
- Molecule 64: 40S ribosomal protein S15

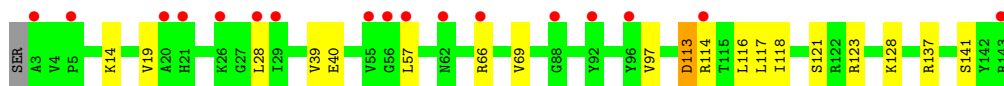


- Molecule 64: 40S ribosomal protein S15

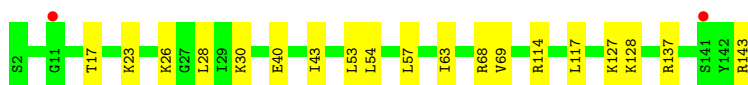
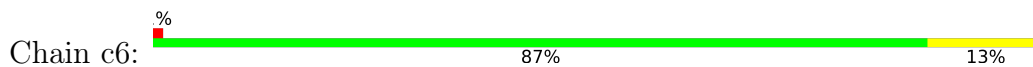


- Molecule 65: 40S ribosomal protein S16-A

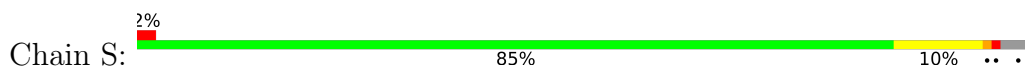




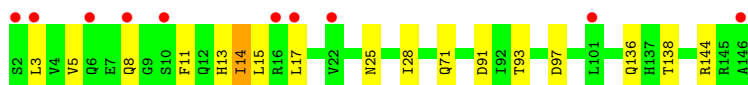
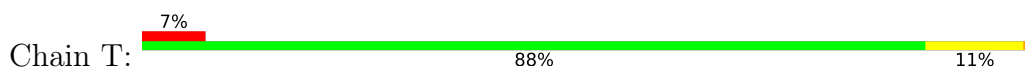
- Molecule 65: 40S ribosomal protein S16-A



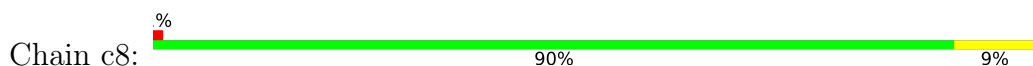
- Molecule 66: 40S ribosomal protein S17-B



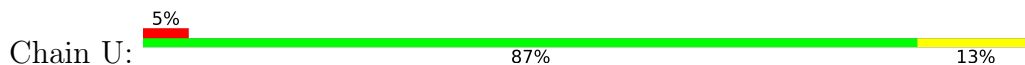
- Molecule 67: 40S ribosomal protein S18-A



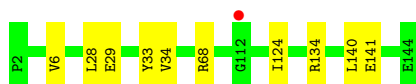
- Molecule 67: 40S ribosomal protein S18-A



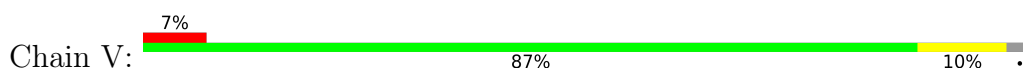
- Molecule 68: 40S ribosomal protein S19-A



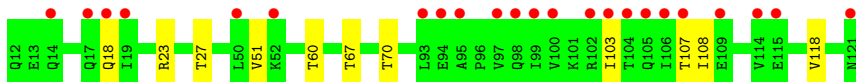
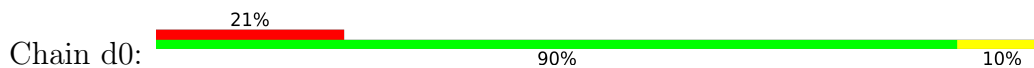
- Molecule 68: 40S ribosomal protein S19-A



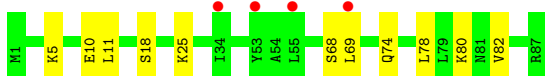
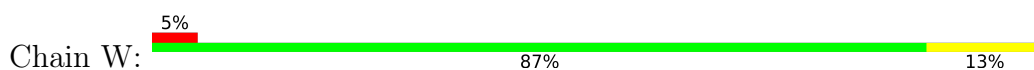
- Molecule 69: 40S ribosomal protein S20



- Molecule 69: 40S ribosomal protein S20



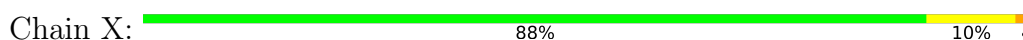
- Molecule 70: 40S ribosomal protein S21-A



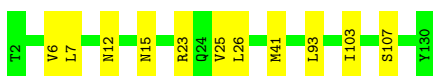
- Molecule 70: 40S ribosomal protein S21-A



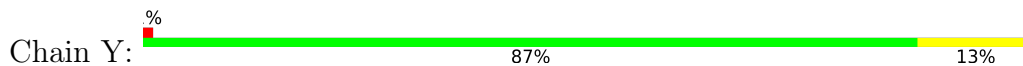
- Molecule 71: 40S ribosomal protein S22-A



- Molecule 71: 40S ribosomal protein S22-A



- Molecule 72: 40S ribosomal protein S23-A



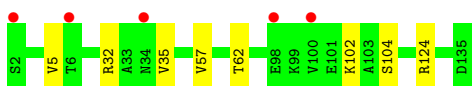
- Molecule 72: 40S ribosomal protein S23-A

Chain d3:  92% 8%

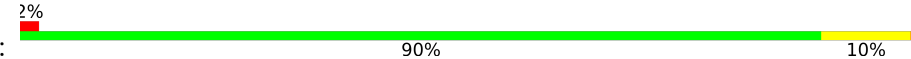


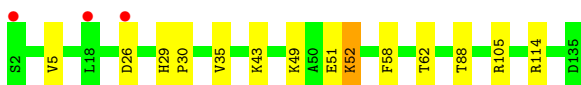
• Molecule 73: 40S ribosomal protein S24-A

Chain Z:  4% 94% 6%




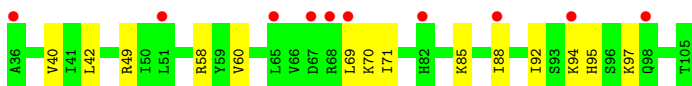
• Molecule 73: 40S ribosomal protein S24-A

Chain d4:  2% 90% 10%



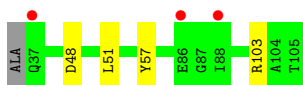
• Molecule 74: 40S ribosomal protein S25-A

Chain a:  14% 80% 20%




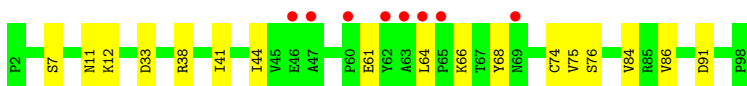
• Molecule 74: 40S ribosomal protein S25-A

Chain d5:  4% 93% 6%



• Molecule 75: 40S ribosomal protein S26-B

Chain b:  8% 82% 18%

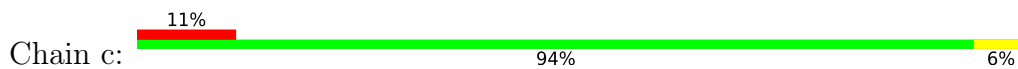


• Molecule 75: 40S ribosomal protein S26-B

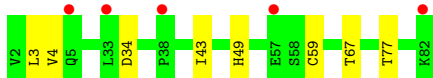
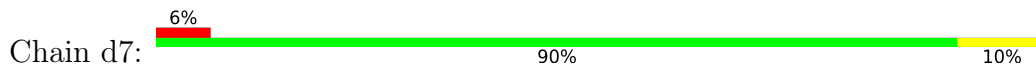
Chain d6:  90% 10%



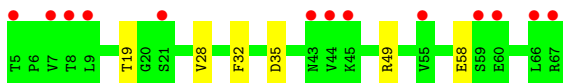
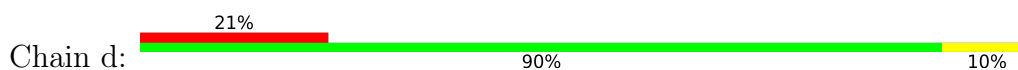
• Molecule 76: 40S ribosomal protein S27-A



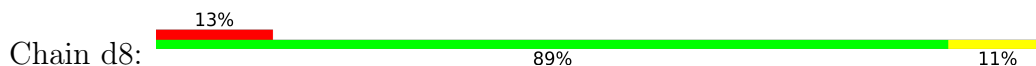
- Molecule 76: 40S ribosomal protein S27-A



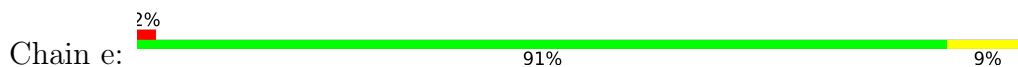
- Molecule 77: 40S ribosomal protein S28-A



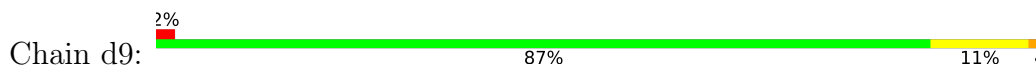
- Molecule 77: 40S ribosomal protein S28-A



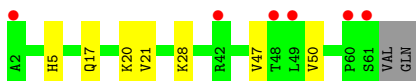
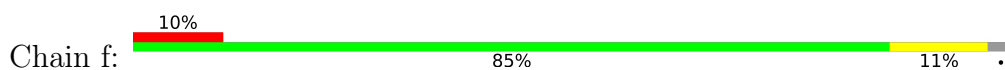
- Molecule 78: 40S ribosomal protein S29-A



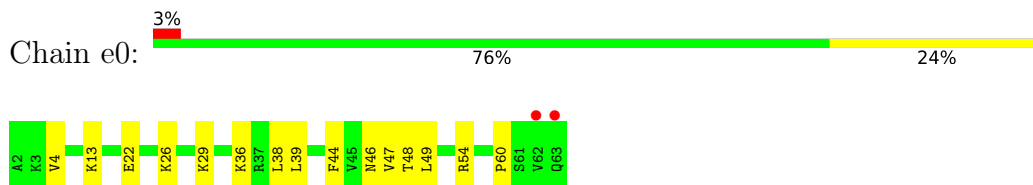
- Molecule 78: 40S ribosomal protein S29-A



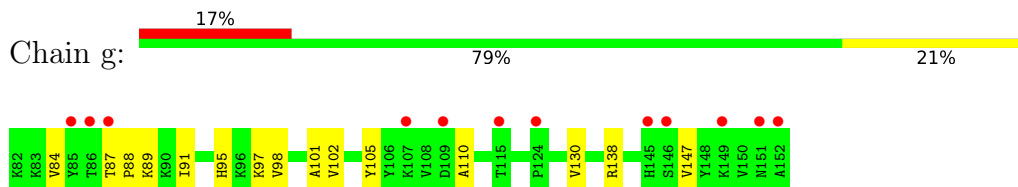
- Molecule 79: 40S ribosomal protein S30-A



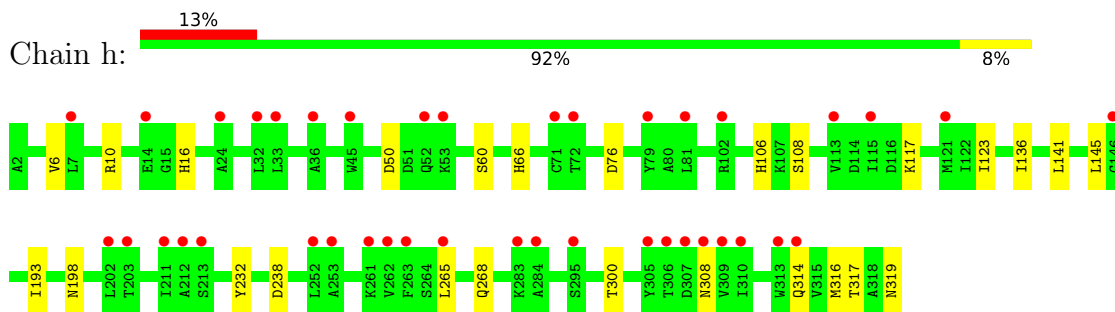
- Molecule 79: 40S ribosomal protein S30-A



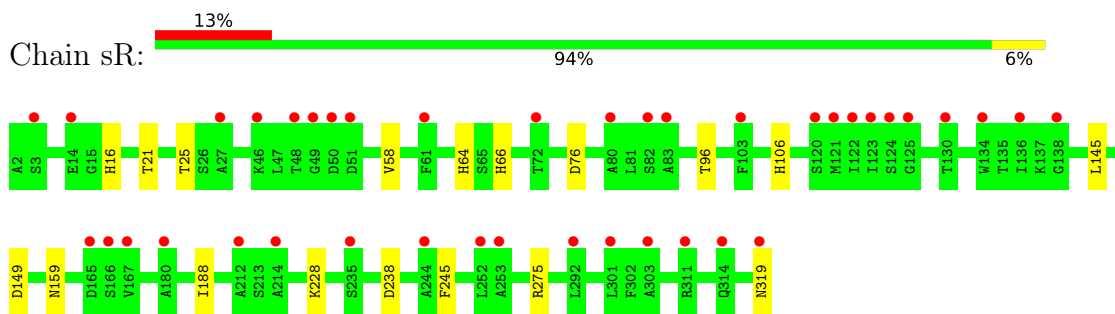
- Molecule 80: Ubiquitin-40S ribosomal protein S31



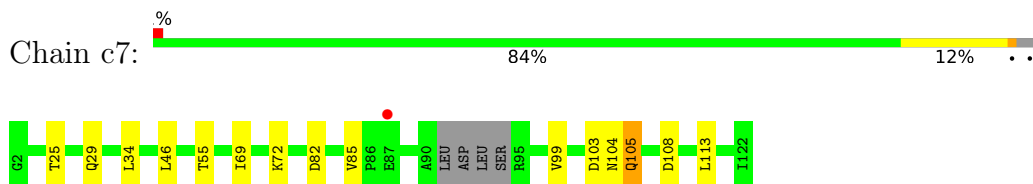
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



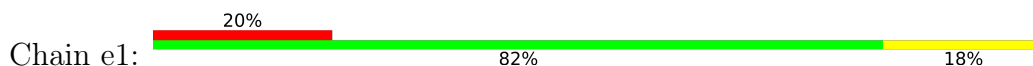
- Molecule 81: Guanine nucleotide-binding protein subunit beta-like protein



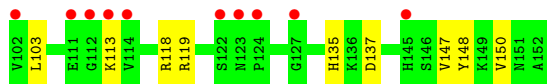
- Molecule 82: 40S ribosomal protein S17-A



- Molecule 83: Ubiquitin-40S ribosomal protein S31







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	304.08Å 286.55Å 436.55Å 90.00° 99.05° 90.00°	Depositor
Resolution (Å)	98.38 – 3.50 98.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.38-3.50) 100.0 (98.38-3.50)	Depositor EDS
$R_{merge}$	0.57	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.49Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.195 , 0.239 0.197 , 0.239	Depositor DCC
$R_{free}$ test set	18298 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.3	Xtrriage
Anisotropy	0.145	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 84.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	409590	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 7MB, OHX, MG, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.68	3/75394 (0.0%)	1.16	271/117545 (0.2%)
1	AR	0.72	2/75394 (0.0%)	1.19	322/117545 (0.3%)
2	3	0.63	0/2883	1.06	5/4491 (0.1%)
2	AS	0.68	0/2883	1.09	3/4491 (0.1%)
3	4	0.62	0/3746	1.11	7/5832 (0.1%)
3	AT	0.61	0/3746	1.07	7/5832 (0.1%)
4	CD	0.46	0/1948	0.67	0/2617
4	j	0.47	0/1948	0.66	1/2617 (0.0%)
5	CE	0.56	0/3146	0.69	0/4228
5	k	0.51	0/3146	0.65	0/4228
6	CF	0.49	0/2800	0.71	3/3790 (0.1%)
6	l	0.50	0/2800	0.70	1/3790 (0.0%)
7	CG	0.50	0/2425	0.62	0/3271
7	m	0.41	0/2425	0.58	0/3271
8	CH	0.51	0/1260	0.64	0/1694
8	n	0.50	0/1260	0.64	0/1694
9	CI	0.53	0/1821	0.67	0/2451
9	o	0.52	0/1821	0.66	1/2451 (0.0%)
10	CJ	0.38	0/1836	0.57	1/2481 (0.0%)
10	p	0.38	0/1836	0.56	0/2481
11	CK	0.52	0/1539	0.65	0/2073
11	q	0.46	0/1539	0.59	0/2073
12	CL	0.50	0/1741	0.64	0/2335
12	r	0.49	0/1741	0.62	1/2335 (0.0%)
13	CM	0.48	0/1374	0.64	0/1842
13	s	0.40	0/1374	0.60	0/1842
14	CN	0.47	0/1568	0.64	0/2106
14	t	0.49	0/1568	0.67	0/2106
15	CO	0.53	0/1068	0.64	0/1438
15	u	0.48	0/1068	0.64	0/1438
16	CP	0.47	0/1757	0.61	0/2354
16	v	0.52	0/1757	0.66	0/2354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	CQ	0.64	0/1585	0.70	1/2128 (0.0%)
17	w	0.56	0/1585	0.67	0/2128
18	CR	0.54	0/1443	0.67	0/1944
18	x	0.52	0/1443	0.66	0/1944
19	CS	0.47	0/1465	0.67	0/1965
19	y	0.51	0/1465	0.68	0/1965
20	CT	0.45	0/1538	0.64	0/2050
20	z	0.37	0/1538	0.55	0/2050
21	0	0.51	0/1481	0.68	0/1990
21	CU	0.55	0/1481	0.69	0/1990
22	2	0.52	0/1300	0.64	0/1743
22	CV	0.52	0/1300	0.64	0/1743
23	5	0.36	0/812	0.55	0/1099
23	CW	0.39	0/812	0.59	0/1099
24	CX	0.58	0/1018	0.69	0/1369
24	l2	0.47	0/1018	0.63	0/1369
25	6	0.57	0/42490	1.06	96/66207 (0.1%)
25	A	0.47	0/42443	0.97	50/66134 (0.1%)
26	7	0.39	0/712	0.55	0/958
26	CY	0.48	0/712	0.66	0/958
27	8	0.43	0/979	0.63	0/1321
27	CZ	0.45	0/979	0.63	1/1321 (0.1%)
28	9	0.45	0/1004	0.69	1/1341 (0.1%)
28	DA	0.44	0/1004	0.67	0/1341
29	AA	0.36	0/1118	0.53	0/1497
29	DB	0.36	0/1118	0.56	0/1497
30	AB	0.48	0/1204	0.70	0/1612
30	DC	0.49	0/1204	0.74	0/1612
31	AC	0.43	0/473	0.65	1/629 (0.2%)
31	DD	0.48	0/473	0.64	0/629
32	AD	0.33	0/751	0.51	0/1008
32	DE	0.38	0/751	0.55	0/1008
33	AE	0.42	0/890	0.58	0/1196
33	DF	0.49	0/890	0.65	0/1196
34	AF	0.55	0/1041	0.66	0/1394
34	DG	0.55	0/1041	0.64	0/1394
35	AG	0.55	0/868	0.70	0/1168
35	DH	0.55	0/868	0.67	0/1168
36	AH	0.40	0/890	0.57	0/1189
36	DI	0.39	0/890	0.60	0/1189
37	AI	0.44	0/978	0.58	0/1301
37	DJ	0.42	0/978	0.53	0/1301
38	AJ	0.44	0/778	0.61	0/1034

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	DK	0.41	0/778	0.58	0/1034
39	AK	0.49	0/696	0.72	0/923
39	DL	0.44	0/696	0.63	0/923
40	AL	0.36	0/618	0.52	0/826
40	DM	0.38	0/618	0.55	0/826
41	AM	0.46	0/443	0.67	0/588
41	DN	0.44	0/443	0.63	0/588
42	AN	0.50	0/423	0.67	0/562
42	DO	0.56	0/423	0.73	1/562 (0.2%)
43	AO	0.42	0/234	0.64	0/300
43	DP	0.49	0/234	0.58	0/300
44	AP	0.48	0/860	0.72	1/1136 (0.1%)
44	DQ	0.48	0/860	0.68	0/1136
45	AQ	0.44	0/701	0.61	0/934
45	DR	0.48	0/701	0.71	1/934 (0.1%)
46	i	0.37	0/1113	0.57	1/1502 (0.1%)
47	p0	0.36	0/1092	0.53	0/1474
48	sM	0.41	0/480	0.64	0/642
49	B	0.37	0/1617	0.59	0/2215
49	s0	0.39	0/1623	0.59	0/2222
50	C	0.32	0/1735	0.57	1/2335 (0.0%)
50	s1	0.36	0/1748	0.60	1/2352 (0.0%)
51	D	0.36	0/1665	0.57	0/2263
51	s2	0.43	0/1665	0.62	0/2263
52	E	0.35	0/1759	0.56	0/2368
52	s3	0.33	0/1759	0.53	0/2368
53	F	0.36	0/2109	0.61	1/2839 (0.0%)
53	s4	0.41	0/2109	0.63	0/2839
54	G	0.32	0/1629	0.52	0/2202
54	s5	0.36	0/1629	0.56	0/2202
55	H	0.34	0/1823	0.53	0/2439
55	s6	0.40	0/1779	0.54	0/2379
56	I	0.33	0/1506	0.59	0/2028
56	s7	0.35	0/1516	0.57	0/2043
57	J	0.40	0/1514	0.60	0/2021
57	s8	0.44	0/1514	0.65	1/2021 (0.0%)
58	K	0.32	0/1519	0.58	0/2035
58	s9	0.40	0/1519	0.58	0/2035
59	L	0.35	0/789	0.66	1/1067 (0.1%)
59	c0	0.33	0/776	0.64	3/1047 (0.3%)
60	M	0.43	0/1239	0.62	1/1673 (0.1%)
60	c1	0.47	0/1194	0.62	0/1610
61	N	0.34	0/898	0.63	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
61	c2	0.29	0/898	0.59	1/1220 (0.1%)
62	O	0.35	0/1215	0.55	0/1638
62	c3	0.41	0/1215	0.59	0/1638
63	P	0.34	0/901	0.61	0/1217
63	c4	0.40	0/960	0.66	0/1290
64	Q	0.34	0/998	0.59	0/1341
64	c5	0.38	0/1060	0.62	1/1426 (0.1%)
65	R	0.35	0/1125	0.58	0/1510
65	c6	0.39	0/1131	0.57	0/1518
66	S	0.37	0/935	0.65	2/1254 (0.2%)
67	T	0.35	0/1211	0.55	0/1628
67	c8	0.39	0/1211	0.59	0/1628
68	U	0.33	0/1130	0.53	0/1517
68	c9	0.36	0/1130	0.53	0/1517
69	V	0.37	0/865	0.60	0/1169
69	d0	0.37	0/892	0.58	0/1205
70	W	0.35	0/693	0.53	0/935
70	d1	0.38	0/693	0.60	0/935
71	X	0.36	0/1038	0.67	2/1395 (0.1%)
71	d2	0.45	0/1038	0.62	0/1395
72	Y	0.44	0/1139	0.64	0/1518
72	d3	0.51	0/1139	0.67	0/1518
73	Z	0.34	0/1087	0.50	0/1449
73	d4	0.40	0/1087	0.61	0/1449
74	a	0.33	0/571	0.60	0/768
74	d5	0.34	0/566	0.56	0/761
75	b	0.37	0/782	0.59	0/1047
75	d6	0.42	0/782	0.60	0/1047
76	c	0.33	0/620	0.56	0/838
76	d7	0.36	0/620	0.58	0/838
77	d	0.29	0/499	0.52	0/670
77	d8	0.32	0/499	0.54	0/670
78	d9	0.40	0/452	0.57	0/600
78	e	0.42	0/452	0.61	0/600
79	e0	0.41	0/499	0.70	0/665
79	f	0.36	0/483	0.60	0/643
80	g	0.41	0/577	0.73	0/770
81	h	0.31	0/2490	0.51	0/3389
81	sR	0.32	0/2495	0.51	0/3395
82	c7	0.37	0/914	0.58	0/1224
83	e1	0.33	0/404	0.67	0/542
All	All	0.56	5/429965 (0.0%)	0.96	792/631328 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	CG	0	1
10	CJ	0	1
12	CL	0	1
15	u	0	1
17	CQ	0	1
17	w	0	1
20	CT	0	1
22	2	0	1
26	7	0	1
26	CY	0	2
28	9	0	1
28	DA	0	1
29	DB	0	1
30	AB	0	1
31	AC	0	1
48	sM	0	1
49	B	0	1
50	s1	0	1
51	D	0	1
51	s2	0	1
52	E	0	1
52	s3	0	1
53	F	0	1
54	G	0	2
54	s5	0	1
56	I	0	2
56	s7	0	4
58	K	0	1
61	c2	0	4
64	Q	0	1
64	c5	0	1
65	R	0	2
65	c6	0	1
66	S	0	2
73	d4	0	2
74	a	0	1
80	g	0	2
82	c7	0	1
All	All	0	51

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AR	895	A	C5-C6	-5.81	1.35	1.41
1	1	936	A	N9-C4	-5.30	1.34	1.37
1	AR	2911	A	N9-C4	-5.05	1.34	1.37
1	1	1865	A	N9-C4	-5.05	1.34	1.37
1	1	3180	A	N9-C4	-5.03	1.34	1.37

All (792) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2821	C	C6-N1-C2	-9.74	116.40	120.30
1	1	637	C	C6-N1-C2	9.70	124.18	120.30
3	4	94	C	C6-N1-C2	9.68	124.17	120.30
1	1	2727	A	N1-C6-N6	-9.61	112.84	118.60
25	6	163	G	N3-C4-N9	-9.23	120.46	126.00
1	AR	2392	C	C6-N1-C2	9.20	123.98	120.30
1	AR	2937	G	N1-C6-O6	9.13	125.38	119.90
25	6	1537	C	C6-N1-C2	-9.11	116.66	120.30
1	AR	2714	G	N3-C4-C5	9.09	133.15	128.60
1	1	435	C	C6-N1-C2	9.04	123.91	120.30
1	AR	2866	U	N3-C2-O2	-8.90	115.97	122.20
1	AR	1897	G	N1-C6-O6	8.71	125.12	119.90
1	1	3217	C	C2-N1-C1'	8.57	128.23	118.80
1	AR	2353	G	N1-C6-O6	8.52	125.01	119.90
1	AR	921	A	N1-C6-N6	-8.42	113.55	118.60
1	AR	3217	C	N1-C2-O2	8.33	123.90	118.90
1	AR	2871	G	C5-C6-O6	-8.19	123.69	128.60
1	1	783	A	N1-C6-N6	8.14	123.48	118.60
1	AR	3093	C	C6-N1-C2	8.13	123.55	120.30
66	S	85	VAL	C-N-CD	-8.05	102.89	120.60
1	1	2866	U	N3-C2-O2	-8.05	116.56	122.20
1	1	676	G	C8-N9-C4	-7.89	103.25	106.40
1	AR	2257	C	C6-N1-C2	-7.83	117.17	120.30
25	A	728	U	C2-N1-C1'	7.82	127.08	117.70
1	AR	1307	G	P-O3'-C3'	7.80	129.06	119.70
1	AR	2263	C	C4-C5-C6	-7.71	113.54	117.40
25	6	163	G	N3-C2-N2	-7.69	114.52	119.90
1	AR	2906	C	C6-N1-C2	7.68	123.37	120.30
1	1	3217	C	C6-N1-C2	-7.65	117.24	120.30
1	AR	2137	U	O5'-P-OP1	-7.63	98.83	105.70
1	1	1367	G	N1-C6-O6	7.60	124.46	119.90
1	AR	2714	G	N3-C4-N9	-7.58	121.45	126.00
1	AR	3217	C	N3-C2-O2	-7.58	116.59	121.90

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1852	G	N1-C6-O6	7.58	124.45	119.90
1	AR	3214	U	N3-C2-O2	-7.57	116.90	122.20
1	1	676	G	C4-N9-C1'	7.53	136.29	126.50
1	1	3216	G	N1-C6-O6	7.52	124.41	119.90
25	A	553	G	N1-C6-O6	7.52	124.41	119.90
1	AR	1437	C	C6-N1-C2	-7.49	117.30	120.30
1	AR	1858	A	C8-N9-C4	-7.47	102.81	105.80
1	AR	1612	A	N1-C6-N6	7.46	123.08	118.60
1	1	3216	G	C5-C6-O6	-7.46	124.12	128.60
25	A	507	U	N1-C2-O2	7.46	128.02	122.80
25	A	728	U	N1-C2-O2	7.43	128.00	122.80
1	AR	2372	A	N1-C6-N6	7.41	123.05	118.60
1	AR	1116	G	O5'-P-OP1	-7.40	99.04	105.70
1	AR	3145	C	C6-N1-C2	7.40	123.26	120.30
1	AR	895	A	N1-C6-N6	7.39	123.03	118.60
1	1	937	G	N3-C4-C5	7.38	132.29	128.60
1	AR	1897	G	C4-C5-N7	7.33	113.73	110.80
12	r	57	LEU	CA-CB-CG	7.32	132.14	115.30
25	A	507	U	N3-C2-O2	-7.32	117.07	122.20
1	1	1115	G	C6-C5-N7	-7.30	126.02	130.40
1	AR	1858	A	N3-C4-C5	-7.28	121.70	126.80
1	AR	2197	C	C6-N1-C2	7.27	123.21	120.30
25	A	507	U	C2-N1-C1'	7.27	126.42	117.70
1	1	676	G	N3-C4-C5	-7.25	124.98	128.60
1	AR	1858	A	C2-N3-C4	7.21	114.21	110.60
3	AT	99	C	C6-N1-C2	7.20	123.18	120.30
25	6	1473	U	C2-N1-C1'	7.17	126.31	117.70
1	1	1167	U	N3-C2-O2	-7.16	117.19	122.20
1	AR	1149	G	N1-C6-O6	7.16	124.19	119.90
1	1	2946	A	N1-C6-N6	7.16	122.89	118.60
1	AR	1897	G	C5-C6-O6	-7.15	124.31	128.60
1	1	2930	A	C8-N9-C4	7.13	108.65	105.80
1	1	2987	A	N1-C6-N6	7.12	122.87	118.60
25	6	1773	C	N3-C4-C5	-7.12	119.05	121.90
1	AR	921	A	N9-C4-C5	7.03	108.61	105.80
1	AR	2699	G	N1-C6-O6	7.03	124.12	119.90
1	1	639	G	C5-C6-O6	-7.03	124.38	128.60
1	AR	2937	G	C5-C6-O6	-7.03	124.39	128.60
1	1	421	G	N3-C4-N9	7.01	130.21	126.00
1	1	2714	G	N3-C4-N9	-7.01	121.80	126.00
1	1	343	U	O5'-P-OP2	-7.00	99.40	105.70
1	AR	1303	A	C8-N9-C4	7.00	108.60	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	1367	G	C5-C6-N1	-6.99	108.00	111.50
25	6	965	U	N1-C2-O2	6.98	127.68	122.80
1	1	645	A	N1-C6-N6	-6.94	114.43	118.60
1	AR	2950	G	C8-N9-C4	-6.93	103.63	106.40
25	6	1000	C	C6-N1-C2	-6.93	117.53	120.30
1	1	1422	G	N1-C6-O6	6.93	124.06	119.90
1	AR	2354	C	N1-C2-O2	-6.93	114.74	118.90
2	AS	101	G	N1-C6-O6	6.92	124.05	119.90
25	A	1428	G	O5'-P-OP1	-6.92	99.47	105.70
1	1	1114	U	O5'-P-OP2	-6.91	99.48	105.70
1	AR	1342	C	C6-N1-C2	6.91	123.06	120.30
1	1	3092	C	C6-N1-C2	6.91	123.06	120.30
25	A	1280	C	C6-N1-C2	-6.90	117.54	120.30
1	AR	648	C	O5'-P-OP1	-6.89	99.50	105.70
1	AR	2353	G	C5-C6-O6	-6.89	124.47	128.60
1	AR	2416	U	O5'-P-OP2	-6.85	99.54	105.70
1	AR	2870	C	N1-C2-O2	-6.84	114.80	118.90
1	AR	2871	G	N1-C6-O6	6.84	124.00	119.90
1	1	639	G	N1-C6-O6	6.84	124.00	119.90
1	1	2871	G	C4-C5-N7	6.82	113.53	110.80
1	1	2831	G	N1-C6-O6	6.81	123.99	119.90
1	AR	895	A	C6-C5-N7	-6.80	127.54	132.30
1	AR	974	G	C8-N9-C4	-6.80	103.68	106.40
25	6	1473	U	N3-C2-O2	-6.79	117.45	122.20
1	1	2821	C	C6-N1-C2	-6.79	117.59	120.30
25	6	144	U	N3-C2-O2	-6.77	117.46	122.20
53	F	193	GLY	N-CA-C	6.74	129.95	113.10
25	A	728	U	N3-C2-O2	-6.73	117.49	122.20
61	c2	58	LEU	CA-CB-CG	6.72	130.77	115.30
1	1	645	A	N1-C2-N3	6.71	132.66	129.30
1	AR	2827	U	C5-C6-N1	-6.71	119.34	122.70
1	AR	637	C	P-O3'-C3'	6.70	127.74	119.70
25	6	980	G	N1-C6-O6	-6.70	115.88	119.90
6	l	182	LEU	CA-CB-CG	6.66	130.62	115.30
1	AR	1433	A	C8-N9-C4	-6.66	103.14	105.80
1	1	1279	C	C6-N1-C2	-6.65	117.64	120.30
1	1	1897	G	N1-C6-O6	6.64	123.89	119.90
1	1	793	C	C6-N1-C2	-6.63	117.65	120.30
46	i	167	PRO	N-CA-CB	6.63	111.25	103.30
1	1	2643	A	C8-N9-C4	6.62	108.45	105.80
1	AR	3306	U	C5-C4-O4	6.62	129.87	125.90
25	A	1389	C	N1-C2-O2	6.61	122.86	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	3344	A	C5-N7-C8	-6.61	100.60	103.90
1	1	917	A	O5'-P-OP2	-6.59	99.77	105.70
1	1	304	G	N3-C2-N2	-6.58	115.30	119.90
1	AR	2156	C	C6-N1-C2	6.58	122.93	120.30
1	AR	2353	G	C6-C5-N7	-6.58	126.45	130.40
1	AR	32	U	N3-C2-O2	-6.56	117.61	122.20
1	1	2287	C	C6-N1-C2	-6.54	117.68	120.30
1	AR	3344	A	N7-C8-N9	6.54	117.07	113.80
1	1	3217	C	N3-C2-O2	-6.53	117.33	121.90
1	AR	2870	C	N3-C2-O2	6.53	126.47	121.90
1	AR	1495	U	C5-C6-N1	-6.52	119.44	122.70
1	AR	2937	G	C4-C5-N7	6.52	113.41	110.80
1	AR	637	C	C2-N1-C1'	6.51	125.97	118.80
50	s1	231	LEU	CA-CB-CG	6.51	130.28	115.30
1	1	1131	G	C5-C6-O6	-6.51	124.69	128.60
1	AR	2714	G	C2-N3-C4	-6.51	108.64	111.90
25	6	1000	C	C2-N1-C1'	6.51	125.96	118.80
60	M	5	LEU	CA-CB-CG	6.51	130.27	115.30
1	1	2197	C	C6-N1-C2	6.50	122.90	120.30
1	1	1307	G	P-O3'-C3'	6.50	127.50	119.70
25	6	1082	C	C5-C6-N1	6.49	124.25	121.00
25	6	435	C	N1-C2-O2	6.48	122.79	118.90
1	1	2307	G	N1-C6-O6	-6.47	116.02	119.90
1	AR	504	A	N1-C6-N6	6.47	122.48	118.60
25	6	1096	C	C6-N1-C2	6.47	122.89	120.30
1	1	676	G	N7-C8-N9	6.47	116.34	113.10
1	AR	1661	G	C8-N9-C4	6.46	108.98	106.40
1	AR	800	G	N9-C4-C5	-6.45	102.82	105.40
1	1	1269	U	C2-N1-C1'	6.42	125.40	117.70
1	1	2943	G	N1-C6-O6	6.42	123.75	119.90
3	4	99	C	C6-N1-C2	6.42	122.87	120.30
1	AR	800	G	C8-N9-C4	6.41	108.96	106.40
45	DR	50	GLY	N-CA-C	-6.40	97.09	113.10
1	1	2764	C	C6-N1-C2	-6.40	117.74	120.30
1	1	111	C	C6-N1-C2	6.39	122.86	120.30
1	AR	1484	U	C6-N1-C2	6.39	124.84	121.00
25	A	1370	U	P-O3'-C3'	6.39	127.37	119.70
1	AR	3212	C	C6-N1-C2	6.39	122.86	120.30
1	AR	3343	G	N3-C4-N9	6.38	129.83	126.00
1	AR	1117	G	C5-C6-O6	-6.38	124.78	128.60
1	AR	1789	G	C4-N9-C1'	-6.37	118.22	126.50
1	1	2610	G	N1-C6-O6	6.37	123.72	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2866	U	N1-C2-O2	6.37	127.26	122.80
1	AR	346	C	N1-C2-O2	6.35	122.71	118.90
1	1	2874	G	C5-C6-O6	6.34	132.41	128.60
25	A	581	U	C2-N1-C1'	6.34	125.30	117.70
1	AR	2353	G	C4-C5-N7	6.32	113.33	110.80
25	6	337	G	C4-N9-C1'	6.32	134.72	126.50
1	1	2727	A	N9-C4-C5	6.32	108.33	105.80
1	1	1330	A	C2-N3-C4	-6.32	107.44	110.60
1	AR	2821	C	C5-C6-N1	6.32	124.16	121.00
1	1	1891	A	C8-N9-C4	6.31	108.33	105.80
1	AR	1500	G	C5-C6-O6	-6.31	124.81	128.60
25	A	1389	C	C2-N1-C1'	6.29	125.72	118.80
1	1	2827	U	C5-C6-N1	-6.29	119.56	122.70
25	A	1200	G	N1-C6-O6	6.29	123.67	119.90
1	AR	86	G	N3-C4-N9	6.29	129.77	126.00
1	1	336	A	N1-C6-N6	6.28	122.37	118.60
59	L	88	PRO	N-CA-CB	6.28	110.84	103.30
1	1	676	G	C6-C5-N7	-6.28	126.63	130.40
1	AR	1331	U	C5-C6-N1	-6.28	119.56	122.70
1	1	997	A	N1-C6-N6	-6.27	114.84	118.60
1	1	1360	C	C6-N1-C2	6.27	122.81	120.30
1	1	649	A	C8-N9-C4	6.27	108.31	105.80
1	AR	1604	G	C4-N9-C1'	6.27	134.65	126.50
1	AR	3344	A	C6-C5-N7	-6.27	127.91	132.30
1	AR	1897	G	C5-N7-C8	-6.27	101.17	104.30
1	AR	2355	G	C6-C5-N7	-6.26	126.64	130.40
1	1	2142	A	N1-C6-N6	-6.25	114.85	118.60
25	6	1596	C	C6-N1-C2	-6.24	117.81	120.30
1	AR	1495	U	C5-C4-O4	6.23	129.64	125.90
1	1	321	C	C6-N1-C2	-6.23	117.81	120.30
1	AR	3217	C	C2-N1-C1'	6.23	125.65	118.80
25	6	280	U	C2-N1-C1'	6.22	125.17	117.70
1	AR	2866	U	N1-C2-O2	6.22	127.16	122.80
25	A	554	C	N1-C2-O2	6.22	122.63	118.90
1	1	2927	C	N1-C2-O2	-6.22	115.17	118.90
1	AR	1189	C	C6-N1-C2	6.21	122.78	120.30
1	1	770	G	O4'-C1'-N9	6.21	113.17	108.20
1	1	3278	C	N1-C2-O2	6.21	122.62	118.90
1	AR	3211	C	C6-N1-C2	6.20	122.78	120.30
25	6	163	G	N3-C4-C5	6.20	131.70	128.60
1	AR	917	A	O5'-P-OP2	-6.20	100.12	105.70
1	AR	1367	G	N1-C6-O6	6.20	123.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	907	G	C5-C6-O6	-6.19	124.88	128.60
1	1	65	A	P-O3'-C3'	6.19	127.13	119.70
1	AR	3306	U	N3-C2-O2	-6.17	117.88	122.20
1	1	1429	G	N3-C4-N9	6.16	129.70	126.00
1	1	1847	A	N1-C6-N6	-6.15	114.91	118.60
1	1	2714	G	N3-C4-C5	6.15	131.67	128.60
1	AR	2871	G	C4-C5-N7	6.15	113.26	110.80
1	1	1724	U	O4'-C1'-N1	6.15	113.12	108.20
1	AR	422	A	C8-N9-C4	-6.14	103.34	105.80
1	1	3216	G	C4-C5-N7	6.14	113.26	110.80
1	AR	2197	C	N3-C2-O2	6.14	126.20	121.90
1	AR	1495	U	C4-C5-C6	6.14	123.38	119.70
1	1	1495	U	N1-C2-O2	-6.13	118.50	122.80
25	6	1246	C	N1-C2-O2	6.13	122.58	118.90
25	6	448	C	C6-N1-C2	-6.12	117.85	120.30
1	AR	2846	U	N3-C2-O2	-6.12	117.91	122.20
1	1	2871	G	C5-N7-C8	-6.12	101.24	104.30
1	1	1437	C	N3-C2-O2	-6.11	117.62	121.90
1	1	2871	G	N3-C4-C5	6.11	131.66	128.60
1	1	131	C	C6-N1-C2	-6.09	117.86	120.30
1	AR	2314	U	C2-N1-C1'	6.09	125.01	117.70
25	6	425	A	OP2-P-O3'	6.08	118.58	105.20
1	AR	718	G	C4-C5-N7	6.08	113.23	110.80
25	6	163	G	N9-C4-C5	6.08	107.83	105.40
1	AR	2764	C	N3-C2-O2	6.08	126.16	121.90
1	AR	3197	G	N3-C4-N9	-6.08	122.35	126.00
25	A	577	G	N1-C6-O6	6.08	123.55	119.90
1	AR	226	C	N1-C2-O2	6.07	122.54	118.90
1	AR	637	C	C5-C6-N1	6.06	124.03	121.00
1	1	2585	G	N3-C4-C5	-6.06	125.57	128.60
1	AR	895	A	C4-C5-N7	6.05	113.72	110.70
25	6	1747	G	C8-N9-C4	6.04	108.82	106.40
1	AR	2624	G	N1-C6-O6	6.04	123.53	119.90
25	6	1164	G	C5-C6-O6	-6.04	124.97	128.60
1	1	2381	G	C5-C6-O6	-6.03	124.98	128.60
2	3	86	U	C5-C4-O4	6.03	129.52	125.90
71	X	93	LEU	CA-CB-CG	6.03	129.18	115.30
2	AS	87	G	N1-C6-O6	6.03	123.52	119.90
2	3	34	C	C5-C6-N1	6.03	124.01	121.00
25	6	151	G	N9-C4-C5	6.03	107.81	105.40
25	A	353	A	C4-C5-N7	6.03	113.71	110.70
1	AR	1789	G	C6-C5-N7	6.02	134.01	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	86	G	N9-C4-C5	-6.02	102.99	105.40
1	AR	816	A	C8-N9-C4	-6.02	103.39	105.80
1	AR	2764	C	N1-C2-O2	-6.02	115.29	118.90
1	1	2727	A	C5-C6-N6	6.02	128.51	123.70
1	AR	1134	G	C4-C5-N7	-6.02	108.39	110.80
25	6	20	G	N1-C6-O6	6.02	123.51	119.90
1	AR	2381	G	N1-C6-O6	6.01	123.51	119.90
1	1	2828	G	N1-C6-O6	-6.01	116.30	119.90
1	AR	1495	U	N1-C2-N3	6.00	118.50	114.90
1	AR	2392	C	C2-N1-C1'	-6.00	112.19	118.80
1	1	2946	A	C4-C5-C6	5.99	119.99	117.00
1	AR	1450	G	N1-C6-O6	5.98	123.49	119.90
1	1	1269	U	N1-C2-O2	5.98	126.99	122.80
1	1	1851	G	C5-C6-O6	-5.98	125.01	128.60
1	1	2337	C	C6-N1-C2	-5.98	117.91	120.30
1	AR	645	A	N1-C6-N6	-5.98	115.01	118.60
1	1	971	G	N3-C4-N9	5.97	129.58	126.00
25	6	597	G	N1-C6-O6	5.96	123.47	119.90
25	6	1164	G	C4-C5-N7	5.96	113.18	110.80
1	1	36	C	N1-C2-O2	5.95	122.47	118.90
1	1	3129	A	C8-N9-C4	5.95	108.18	105.80
1	AR	1338	C	C6-N1-C2	-5.95	117.92	120.30
1	1	2169	G	N1-C6-O6	-5.95	116.33	119.90
1	1	916	G	N3-C4-N9	5.95	129.57	126.00
1	1	2643	A	N1-C6-N6	5.95	122.17	118.60
1	AR	406	G	O4'-C1'-N9	5.95	112.96	108.20
1	AR	2699	G	C5-C6-O6	-5.95	125.03	128.60
1	1	979	U	P-O3'-C3'	5.95	126.84	119.70
1	AR	873	C	C6-N1-C2	-5.95	117.92	120.30
1	1	1164	G	N1-C6-O6	-5.94	116.33	119.90
1	AR	2377	G	C8-N9-C4	5.94	108.78	106.40
1	1	2618	G	N1-C6-O6	-5.94	116.34	119.90
1	1	1061	A	C8-N9-C4	5.94	108.17	105.80
25	6	17	C	N3-C2-O2	-5.93	117.75	121.90
1	1	1437	C	C6-N1-C2	-5.93	117.93	120.30
25	6	965	U	N3-C2-O2	-5.93	118.05	122.20
25	6	1150	G	C8-N9-C4	5.93	108.77	106.40
1	AR	2870	C	C2-N1-C1'	-5.93	112.28	118.80
1	1	1115	G	N7-C8-N9	5.92	116.06	113.10
25	A	1039	A	O4'-C1'-N9	5.92	112.93	108.20
1	AR	3306	U	N3-C4-O4	-5.90	115.27	119.40
3	AT	3	A	C5-C6-N6	-5.90	118.98	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	c0	88	PRO	N-CA-CB	5.89	110.37	103.30
1	1	2928	C	N1-C2-O2	5.89	122.43	118.90
1	1	352	A	C8-N9-C4	5.89	108.16	105.80
1	AR	269	G	C8-N9-C4	5.88	108.75	106.40
1	AR	986	U	N1-C2-O2	5.88	126.91	122.80
1	AR	61	A	C8-N9-C4	-5.87	103.45	105.80
1	1	2827	U	C2-N3-C4	-5.87	123.48	127.00
1	AR	2337	C	N1-C2-O2	5.86	122.42	118.90
1	1	2372	A	N1-C6-N6	5.86	122.12	118.60
1	AR	1319	G	N1-C6-O6	5.86	123.42	119.90
1	AR	984	G	N3-C4-N9	5.86	129.51	126.00
1	AR	2400	G	N1-C6-O6	5.85	123.41	119.90
1	1	2366	C	C6-N1-C2	5.85	122.64	120.30
1	AR	346	C	N3-C2-O2	-5.85	117.80	121.90
1	1	2643	A	C5-C6-N6	-5.85	119.02	123.70
1	AR	2828	G	N1-C6-O6	-5.84	116.39	119.90
1	1	229	G	N1-C6-O6	5.84	123.41	119.90
1	1	2689	A	C8-N9-C4	-5.83	103.47	105.80
1	1	1431	G	C8-N9-C4	5.83	108.73	106.40
1	1	3278	C	C2-N1-C1'	5.83	125.21	118.80
25	6	1535	U	N3-C2-O2	-5.83	118.12	122.20
1	AR	437	G	N7-C8-N9	5.82	116.01	113.10
1	AR	504	A	C4-C5-N7	5.82	113.61	110.70
1	1	3201	C	C6-N1-C2	-5.82	117.97	120.30
1	AR	1396	C	C6-N1-C2	5.82	122.63	120.30
1	AR	2662	G	N1-C6-O6	-5.81	116.41	119.90
1	AR	2943	G	C5-C6-O6	-5.81	125.11	128.60
1	1	2221	G	N1-C6-O6	5.81	123.39	119.90
25	6	561	G	N1-C6-O6	5.81	123.38	119.90
1	AR	2642	A	N1-C6-N6	-5.80	115.12	118.60
25	A	1082	C	C6-N1-C2	-5.80	117.98	120.30
1	AR	518	G	C4-C5-N7	5.80	113.12	110.80
1	1	421	G	N9-C4-C5	-5.80	103.08	105.40
1	AR	943	U	N1-C2-O2	-5.80	118.74	122.80
25	A	934	C	C2-N1-C1'	5.80	125.17	118.80
1	1	2423	U	C5-C6-N1	5.79	125.60	122.70
1	AR	3344	A	N1-C6-N6	5.79	122.08	118.60
1	1	2663	G	N1-C6-O6	-5.79	116.42	119.90
1	AR	408	A	N1-C6-N6	-5.79	115.12	118.60
25	A	1280	C	N3-C4-C5	-5.79	119.58	121.90
1	1	742	G	N1-C6-O6	-5.79	116.43	119.90
1	1	273	A	C8-N9-C4	5.78	108.11	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	1665	U	C5-C6-N1	-5.78	119.81	122.70
1	AR	921	A	C5-C6-N6	5.78	128.32	123.70
1	AR	3054	U	C5-C4-O4	5.78	129.37	125.90
1	1	1851	G	N1-C6-O6	5.78	123.36	119.90
1	AR	2263	C	N3-C2-O2	5.78	125.94	121.90
1	1	783	A	C5-C6-N6	-5.77	119.08	123.70
1	AR	879	U	C5-C4-O4	-5.77	122.44	125.90
1	AR	2372	A	C6-C5-N7	-5.77	128.26	132.30
1	1	1115	G	C4-N9-C1'	5.77	134.00	126.50
1	1	2325	G	C4-C5-N7	5.76	113.11	110.80
1	AR	2383	C	C6-N1-C2	-5.76	118.00	120.30
1	1	1362	G	C8-N9-C4	5.76	108.70	106.40
1	AR	2943	G	N1-C6-O6	5.76	123.35	119.90
1	1	2914	G	C8-N9-C4	5.75	108.70	106.40
1	AR	3373	U	C5-C6-N1	-5.75	119.82	122.70
1	1	3216	G	C6-C5-N7	-5.75	126.95	130.40
25	6	1082	C	C6-N1-C2	-5.75	118.00	120.30
1	AR	921	A	C8-N9-C4	-5.74	103.50	105.80
25	A	720	G	OP1-P-O3'	5.74	117.84	105.20
1	AR	2983	C	C4-C5-C6	5.74	120.27	117.40
1	AR	1117	G	N1-C6-O6	5.73	123.34	119.90
1	1	2726	C	N3-C2-O2	-5.73	117.89	121.90
25	6	426	G	C8-N9-C4	-5.73	104.11	106.40
25	6	1000	C	N3-C2-O2	-5.73	117.89	121.90
44	AP	35	LEU	CA-CB-CG	5.72	128.46	115.30
1	AR	2832	C	C6-N1-C2	5.72	122.59	120.30
1	1	1097	G	P-O3'-C3'	5.71	126.56	119.70
1	AR	2337	C	N3-C2-O2	-5.71	117.90	121.90
1	AR	1462	A	C2-N3-C4	-5.71	107.74	110.60
1	AR	1495	U	C2-N1-C1'	-5.71	110.85	117.70
1	1	1269	U	N3-C2-O2	-5.70	118.21	122.20
25	6	1473	U	N1-C2-O2	5.70	126.79	122.80
3	4	26	U	N3-C2-O2	-5.70	118.21	122.20
1	AR	2364	G	N9-C4-C5	5.70	107.68	105.40
25	6	687	G	N3-C4-N9	-5.70	122.58	126.00
1	AR	925	A	O5'-P-OP1	-5.69	100.58	105.70
1	AR	3362	A	C5-N7-C8	-5.69	101.05	103.90
1	1	1440	G	N3-C4-C5	-5.69	125.75	128.60
2	3	34	C	C6-N1-C2	-5.69	118.03	120.30
31	AC	20	GLY	N-CA-C	5.69	127.32	113.10
25	A	639	U	N3-C2-O2	-5.69	118.22	122.20
1	AR	1000	C	C6-N1-C2	5.68	122.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1820	U	P-O3'-C3'	5.68	126.52	119.70
64	c5	36	LEU	CA-CB-CG	5.68	128.37	115.30
1	1	718	G	C4-C5-N7	5.68	113.07	110.80
1	AR	2245	C	N3-C4-C5	-5.68	119.63	121.90
25	A	639	U	N1-C2-O2	5.68	126.78	122.80
1	1	2383	C	C5-C4-N4	-5.68	116.23	120.20
1	AR	363	G	C5-C6-O6	-5.67	125.19	128.60
1	1	885	U	C5-C6-N1	-5.67	119.87	122.70
25	A	1052	U	C2-N1-C1'	5.67	124.50	117.70
1	AR	2282	U	O5'-P-OP2	-5.67	100.60	105.70
25	6	337	G	N7-C8-N9	5.66	115.93	113.10
25	A	359	A	C8-N9-C4	5.66	108.07	105.80
1	1	2550	U	N3-C2-O2	-5.66	118.24	122.20
25	6	1521	G	N3-C4-N9	5.66	129.40	126.00
1	1	128	G	N1-C6-O6	5.66	123.29	119.90
1	1	2392	C	C6-N1-C2	5.66	122.56	120.30
1	AR	2245	C	N1-C2-O2	-5.66	115.51	118.90
1	AR	2953	U	N3-C4-O4	5.65	123.36	119.40
25	6	453	U	C5-C6-N1	5.65	125.53	122.70
25	6	623	A	C8-N9-C4	5.65	108.06	105.80
1	AR	2647	A	N1-C6-N6	-5.65	115.21	118.60
25	6	1751	C	C6-N1-C2	5.64	122.56	120.30
1	AR	2714	G	C5-N7-C8	-5.64	101.48	104.30
25	6	1058	U	OP1-P-O3'	5.64	117.61	105.20
1	1	1796	G	C8-N9-C4	-5.63	104.15	106.40
1	1	96	G	N1-C6-O6	5.63	123.28	119.90
25	A	1698	G	P-O3'-C3'	5.63	126.46	119.70
4	j	191	LEU	CA-CB-CG	-5.63	102.35	115.30
25	6	543	C	N3-C4-N4	-5.62	114.06	118.00
1	AR	1820	U	OP2-P-O3'	5.62	117.57	105.20
1	AR	2698	G	C8-N9-C4	5.62	108.65	106.40
66	S	85	VAL	C-N-CA	5.62	145.60	122.00
1	1	2643	A	N9-C4-C5	-5.62	103.55	105.80
1	AR	1200	A	N1-C6-N6	5.62	121.97	118.60
28	9	126	LEU	CA-CB-CG	5.61	128.21	115.30
1	1	2372	A	C5-C6-N6	-5.61	119.21	123.70
1	1	676	G	N3-C4-N9	5.61	129.37	126.00
1	1	1121	U	N3-C2-O2	-5.61	118.28	122.20
2	3	86	U	N3-C4-O4	-5.61	115.47	119.40
1	AR	1604	G	N3-C4-C5	-5.60	125.80	128.60
1	AR	3176	G	N3-C2-N2	-5.60	115.98	119.90
1	1	895	A	C5-N7-C8	-5.60	101.10	103.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	1164	G	N1-C6-O6	5.60	123.26	119.90
1	AR	2831	G	C5-C6-O6	-5.59	125.24	128.60
1	1	609	G	C5-C6-O6	-5.59	125.25	128.60
1	1	3275	U	OP1-P-O3'	5.59	117.49	105.20
25	6	144	U	C6-N1-C2	-5.58	117.65	121.00
1	AR	640	U	N3-C2-O2	5.58	126.11	122.20
1	AR	986	U	N3-C2-O2	-5.58	118.29	122.20
1	AR	2930	A	C8-N9-C4	5.58	108.03	105.80
1	AR	2883	U	N1-C2-O2	-5.58	118.89	122.80
1	AR	2392	C	N1-C2-O2	-5.58	115.55	118.90
1	1	817	A	O5'-P-OP1	-5.57	100.69	105.70
1	AR	3121	U	OP1-P-O3'	5.57	117.45	105.20
1	1	658	G	N1-C6-O6	5.57	123.24	119.90
25	A	610	G	C4-N9-C1'	5.56	133.73	126.50
25	A	1560	U	N3-C2-O2	-5.56	118.31	122.20
25	A	1573	A	P-O3'-C3'	5.56	126.38	119.70
25	A	1568	C	P-O3'-C3'	5.56	126.37	119.70
1	1	1716	U	P-O3'-C3'	5.56	126.37	119.70
1	AR	2831	G	N1-C6-O6	5.56	123.23	119.90
1	AR	718	G	C5-N7-C8	-5.55	101.52	104.30
1	1	2946	A	C6-C5-N7	-5.55	128.41	132.30
1	AR	2940	A	N1-C2-N3	5.55	132.07	129.30
1	AR	421	G	N3-C4-C5	-5.54	125.83	128.60
1	AR	2333	C	C5-C6-N1	-5.54	118.23	121.00
1	1	931	C	N1-C2-O2	-5.54	115.58	118.90
25	6	548	G	N1-C6-O6	5.54	123.22	119.90
1	1	1440	G	C2-N3-C4	5.54	114.67	111.90
1	1	2899	C	C6-N1-C2	-5.54	118.08	120.30
1	1	688	G	N3-C4-C5	-5.54	125.83	128.60
1	AR	1556	C	C6-N1-C2	-5.53	118.09	120.30
25	6	1097	U	P-O3'-C3'	5.53	126.33	119.70
1	AR	3068	U	N3-C2-O2	-5.53	118.33	122.20
1	AR	873	C	P-O3'-C3'	5.52	126.33	119.70
1	1	718	G	C6-C5-N7	-5.51	127.09	130.40
1	1	2383	C	C5-C6-N1	5.51	123.76	121.00
1	AR	3343	G	N3-C4-C5	-5.51	125.84	128.60
1	1	922	U	C2-N1-C1'	5.51	124.31	117.70
1	AR	1604	G	C8-N9-C1'	-5.51	119.84	127.00
1	AR	917	A	N9-C4-C5	5.50	108.00	105.80
1	AR	1895	A	C5-N7-C8	-5.50	101.15	103.90
1	AR	2951	G	C5-C6-O6	-5.50	125.30	128.60
42	DO	103	LEU	CA-CB-CG	-5.50	102.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	907	G	C4-C5-N7	5.50	113.00	110.80
1	1	2937	G	C8-N9-C4	5.50	108.60	106.40
1	1	304	G	N1-C2-N2	5.49	121.14	116.20
25	6	1119	G	N1-C6-O6	-5.49	116.61	119.90
1	AR	1869	C	C6-N1-C2	5.49	122.50	120.30
1	1	2601	A	C8-N9-C4	5.49	108.00	105.80
25	A	1012	U	C5-C6-N1	5.49	125.44	122.70
1	1	2201	G	N1-C6-O6	5.48	123.19	119.90
1	1	2874	G	C5-C6-N1	-5.48	108.76	111.50
1	1	1159	A	N1-C6-N6	-5.48	115.31	118.60
1	1	406	G	O4'-C1'-N9	5.48	112.58	108.20
1	AR	284	A	C8-N9-C4	5.48	107.99	105.80
1	1	2112	U	P-O3'-C3'	5.47	126.27	119.70
59	c0	97	PRO	N-CA-CB	5.47	109.87	103.30
1	AR	948	C	C6-N1-C2	5.47	122.49	120.30
1	1	950	G	N1-C6-O6	5.47	123.18	119.90
1	1	417	A	C2-N3-C4	-5.46	107.87	110.60
1	1	1171	G	C4-C5-N7	-5.46	108.61	110.80
1	AR	2093	A	C2-N3-C4	5.46	113.33	110.60
1	AR	3190	C	N3-C4-C5	-5.46	119.72	121.90
3	AT	15	G	C8-N9-C4	5.46	108.58	106.40
1	1	676	G	C4-C5-C6	5.46	122.08	118.80
3	4	28	C	C6-N1-C2	-5.46	118.12	120.30
1	1	2836	C	N3-C2-O2	-5.45	118.08	121.90
1	AR	922	U	C2-N1-C1'	5.45	124.25	117.70
25	6	17	C	N1-C2-O2	5.45	122.17	118.90
1	AR	1846	C	C6-N1-C2	5.45	122.48	120.30
25	A	632	U	C5-C6-N1	5.45	125.42	122.70
1	AR	3057	U	N3-C2-O2	-5.44	118.39	122.20
1	1	56	G	C5-C6-O6	-5.44	125.33	128.60
25	6	979	A	N1-C6-N6	-5.44	115.33	118.60
1	1	2366	C	N3-C4-C5	5.44	124.08	121.90
25	6	1389	C	C2-N1-C1'	5.44	124.78	118.80
1	AR	1374	G	C4-C5-N7	5.44	112.98	110.80
25	A	158	U	P-O3'-C3'	5.44	126.23	119.70
1	1	645	A	C6-N1-C2	-5.43	115.34	118.60
1	1	2988	C	N3-C2-O2	-5.43	118.10	121.90
1	AR	639	G	C2-N3-C4	-5.43	109.18	111.90
1	AR	1149	G	C6-C5-N7	-5.43	127.14	130.40
1	AR	3150	A	N1-C6-N6	5.43	121.86	118.60
1	1	2308	C	N1-C2-O2	-5.43	115.64	118.90
1	AR	1370	G	C6-N1-C2	-5.43	121.84	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2123	G	N1-C6-O6	-5.43	116.64	119.90
1	AR	1082	U	C2-N1-C1'	5.43	124.21	117.70
1	1	2760	C	N1-C2-O2	-5.42	115.65	118.90
1	AR	2638	C	C6-N1-C2	-5.42	118.13	120.30
1	AR	1045	C	N1-C2-O2	-5.41	115.65	118.90
1	1	1175	C	C6-N1-C2	5.41	122.47	120.30
1	AR	1300	G	C5-C6-O6	-5.41	125.35	128.60
1	AR	2145	A	N1-C2-N3	5.41	132.01	129.30
1	AR	2950	G	N7-C8-N9	5.41	115.80	113.10
1	AR	942	U	N3-C4-C5	-5.41	111.36	114.60
1	AR	805	G	N1-C6-O6	5.40	123.14	119.90
1	AR	1868	G	N9-C4-C5	-5.40	103.24	105.40
1	1	2101	C	OP1-P-O3'	5.40	117.07	105.20
1	1	2101	C	P-O3'-C3'	5.39	126.17	119.70
1	1	2982	A	C6-N1-C2	-5.39	115.36	118.60
1	1	2935	U	N3-C4-C5	-5.39	111.37	114.60
1	1	2314	U	C5-C6-N1	5.38	125.39	122.70
1	1	3216	G	N9-C4-C5	-5.38	103.25	105.40
1	AR	86	G	C5-C6-O6	-5.38	125.37	128.60
59	c0	83	PRO	N-CA-CB	5.38	109.76	103.30
1	AR	2199	G	C4-C5-N7	5.38	112.95	110.80
1	AR	2840	C	C6-N1-C2	5.38	122.45	120.30
25	6	359	A	C4-C5-C6	-5.38	114.31	117.00
1	AR	2263	C	C5-C4-N4	-5.38	116.44	120.20
25	6	426	G	O5'-P-OP2	-5.37	100.86	105.70
1	AR	3067	C	C6-N1-C2	5.37	122.45	120.30
1	AR	3093	C	C5-C6-N1	-5.37	118.31	121.00
1	1	2257	C	O4'-C1'-N1	5.37	112.50	108.20
25	6	1569	A	N7-C8-N9	5.37	116.48	113.80
3	AT	96	A	C8-N9-C4	5.37	107.95	105.80
1	1	776	U	C5-C6-N1	-5.36	120.02	122.70
1	1	3217	C	N1-C2-O2	5.36	122.12	118.90
1	1	2762	A	N1-C6-N6	-5.36	115.39	118.60
1	AR	1134	G	N1-C6-O6	-5.36	116.69	119.90
25	A	1389	C	N3-C2-O2	-5.36	118.15	121.90
1	AR	2764	C	C5-C4-N4	-5.35	116.45	120.20
25	6	53	G	N1-C6-O6	5.35	123.11	119.90
1	1	49	A	N1-C6-N6	5.35	121.81	118.60
1	1	2287	C	N3-C2-O2	-5.35	118.16	121.90
1	1	2777	G	N9-C4-C5	5.35	107.54	105.40
1	AR	1143	A	N1-C6-N6	5.35	121.81	118.60
57	s8	29	LEU	CA-CB-CG	5.35	127.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2407	C	N1-C2-O2	-5.35	115.69	118.90
1	1	282	G	P-O3'-C3'	5.35	126.11	119.70
25	6	1140	G	N1-C6-O6	5.34	123.11	119.90
1	AR	1134	G	C5-C6-O6	5.34	131.81	128.60
1	AR	3190	C	C6-N1-C2	-5.34	118.16	120.30
1	AR	2871	G	C6-C5-N7	-5.34	127.20	130.40
1	AR	948	C	C5-C6-N1	-5.34	118.33	121.00
1	1	3344	A	N7-C8-N9	5.33	116.47	113.80
1	AR	3362	A	C4-C5-N7	5.33	113.37	110.70
25	6	568	G	N1-C6-O6	-5.33	116.70	119.90
1	1	2982	A	N1-C2-N3	5.33	131.97	129.30
1	AR	925	A	O5'-P-OP2	5.33	117.09	110.70
1	AR	2263	C	N3-C4-C5	5.33	124.03	121.90
1	1	2287	C	N1-C2-N3	5.33	122.93	119.20
1	1	2355	G	C6-C5-N7	-5.33	127.20	130.40
1	1	3278	C	N3-C2-O2	-5.33	118.17	121.90
1	1	2522	G	C4-N9-C1'	5.32	133.42	126.50
1	AR	3344	A	C2-N3-C4	-5.32	107.94	110.60
1	1	1367	G	C5-C6-N1	-5.32	108.84	111.50
1	AR	504	A	C5-C6-N6	-5.32	119.44	123.70
1	AR	1449	A	N1-C6-N6	5.32	121.79	118.60
25	6	1280	C	N3-C4-C5	-5.32	119.77	121.90
3	4	58	G	N1-C6-O6	5.31	123.09	119.90
1	1	1395	G	C8-N9-C4	5.31	108.52	106.40
1	AR	1187	C	C6-N1-C2	5.30	122.42	120.30
25	6	1654	G	N9-C4-C5	-5.30	103.28	105.40
1	1	421	G	C5-C6-N1	5.30	114.15	111.50
1	1	3217	C	C6-N1-C1'	-5.30	114.44	120.80
1	AR	3303	G	N1-C6-O6	-5.29	116.72	119.90
1	AR	197	G	C4-C5-N7	5.29	112.92	110.80
1	AR	3181	C	N1-C2-O2	5.29	122.08	118.90
1	1	1115	G	C5-N7-C8	-5.29	101.66	104.30
1	1	2337	C	N3-C2-O2	-5.29	118.20	121.90
25	A	1456	C	C2-N1-C1'	5.28	124.61	118.80
1	1	2870	C	C2-N1-C1'	-5.28	112.99	118.80
1	1	3000	A	C8-N9-C4	5.28	107.91	105.80
1	AR	2263	C	C6-N1-C1'	-5.28	114.46	120.80
1	AR	2937	G	C6-C5-N7	-5.28	127.23	130.40
25	A	720	G	P-O3'-C3'	5.28	126.03	119.70
6	CF	156	LEU	CA-CB-CG	5.27	127.42	115.30
25	A	782	U	OP2-P-O3'	5.27	116.80	105.20
1	AR	862	U	C6-N1-C2	5.27	124.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	874	U	C5-C4-O4	5.27	129.06	125.90
1	AR	504	A	C5-N7-C8	-5.27	101.27	103.90
1	1	922	U	N1-C2-O2	5.27	126.49	122.80
25	6	453	U	C2-N1-C1'	5.26	124.01	117.70
25	6	1573	A	P-O3'-C3'	5.26	126.01	119.70
25	6	1185	U	N1-C2-O2	5.26	126.48	122.80
25	6	1782	A	C8-N9-C4	-5.26	103.70	105.80
1	1	216	G	C5-C6-O6	-5.26	125.44	128.60
25	6	158	U	P-O3'-C3'	5.26	126.01	119.70
1	AR	3115	C	C6-N1-C2	-5.26	118.20	120.30
1	AR	1495	U	C6-N1-C1'	5.25	128.55	121.20
1	AR	3362	A	O4'-C1'-N9	5.25	112.40	108.20
1	AR	407	A	N1-C6-N6	5.25	121.75	118.60
71	X	65	LEU	CA-CB-CG	5.25	127.37	115.30
1	1	43	A	C5-C6-N6	5.24	127.89	123.70
2	3	33	U	N3-C2-O2	-5.24	118.53	122.20
1	AR	2377	G	N7-C8-N9	-5.24	110.48	113.10
1	1	710	A	N1-C6-N6	5.24	121.74	118.60
25	6	1440	C	C6-N1-C2	-5.24	118.20	120.30
1	AR	757	C	N1-C2-O2	-5.24	115.76	118.90
1	AR	1437	C	N3-C4-C5	-5.24	119.81	121.90
1	AR	1828	A	N1-C6-N6	5.24	121.74	118.60
1	1	979	U	N1-C2-N3	5.24	118.04	114.90
25	6	543	C	C5-C4-N4	5.24	123.86	120.20
25	6	1569	A	C8-N9-C4	-5.24	103.71	105.80
1	1	3344	A	O4'-C1'-N9	5.23	112.39	108.20
1	AR	2257	C	C2-N1-C1'	5.23	124.56	118.80
25	A	356	G	C6-C5-N7	-5.23	127.26	130.40
25	6	813	U	C2-N1-C1'	5.23	123.98	117.70
1	AR	2199	G	C5-C6-O6	-5.23	125.46	128.60
1	AR	3216	G	N3-C4-N9	5.23	129.14	126.00
25	A	1761	U	P-O3'-C3'	5.23	125.97	119.70
1	1	336	A	C5-C6-N6	-5.23	119.52	123.70
1	AR	2356	A	C4-C5-N7	5.22	113.31	110.70
1	AR	2541	U	P-O3'-C3'	5.22	125.97	119.70
1	1	936	A	C2-N3-C4	-5.22	107.99	110.60
1	AR	2324	A	N1-C6-N6	5.22	121.73	118.60
1	1	2593	A	P-O3'-C3'	5.22	125.96	119.70
1	AR	421	G	N3-C4-N9	5.22	129.13	126.00
1	1	1450	G	C4-C5-N7	5.21	112.89	110.80
1	AR	800	G	C5-C6-O6	-5.21	125.47	128.60
1	1	424	G	C6-C5-N7	-5.21	127.27	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	422	A	C8-N9-C4	-5.21	103.72	105.80
1	AR	895	A	C5-N7-C8	-5.21	101.30	103.90
25	6	1150	G	N9-C4-C5	-5.20	103.32	105.40
25	6	1767	G	C8-N9-C4	5.20	108.48	106.40
1	AR	2356	A	N9-C4-C5	-5.20	103.72	105.80
1	AR	2411	U	C5-C6-N1	-5.20	120.10	122.70
1	1	2305	G	N3-C4-C5	-5.20	126.00	128.60
1	AR	859	G	C5-C6-O6	-5.20	125.48	128.60
25	6	163	G	N1-C2-N2	5.20	120.88	116.20
1	1	645	A	N9-C4-C5	5.20	107.88	105.80
1	1	3298	C	C6-N1-C2	5.20	122.38	120.30
25	6	187	G	P-O3'-C3'	5.20	125.94	119.70
1	AR	2364	G	C4-C5-N7	-5.20	108.72	110.80
1	1	3277	U	N3-C2-O2	-5.19	118.56	122.20
25	A	782	U	P-O3'-C3'	5.19	125.93	119.70
1	1	2298	U	O4'-C1'-N1	5.19	112.35	108.20
25	6	1560	U	N3-C2-O2	-5.19	118.57	122.20
25	A	1560	U	C2-N1-C1'	5.19	123.92	117.70
1	1	971	G	N3-C4-C5	-5.18	126.01	128.60
1	AR	1389	G	C8-N9-C4	5.18	108.47	106.40
1	AR	358	G	N3-C4-C5	5.18	131.19	128.60
2	AS	89	G	N1-C6-O6	5.18	123.01	119.90
1	1	1792	C	O4'-C1'-N1	5.18	112.34	108.20
1	AR	1099	A	N1-C6-N6	5.18	121.71	118.60
1	AR	1851	G	C4-C5-N7	5.18	112.87	110.80
1	AR	2679	A	O4'-C1'-N9	5.18	112.34	108.20
3	AT	15	G	N7-C8-N9	-5.18	110.51	113.10
25	A	829	A	P-O3'-C3'	5.18	125.91	119.70
25	6	280	U	N1-C2-O2	5.17	126.42	122.80
1	AR	2943	G	C4-C5-N7	5.17	112.87	110.80
25	6	1581	C	C6-N1-C2	5.17	122.37	120.30
1	AR	3217	C	C6-N1-C2	-5.17	118.23	120.30
6	CF	324	LEU	CA-CB-CG	5.17	127.19	115.30
1	1	880	G	C4-N9-C1'	-5.17	119.78	126.50
1	1	1604	G	N3-C4-C5	-5.17	126.02	128.60
25	6	1735	U	N3-C2-O2	-5.17	118.58	122.20
1	AR	3057	U	N3-C4-O4	-5.17	115.78	119.40
1	1	1495	U	C5-C6-N1	-5.17	120.12	122.70
1	AR	2679	A	N1-C6-N6	5.16	121.70	118.60
1	1	1000	C	C5-C4-N4	-5.16	116.59	120.20
1	AR	942	U	N3-C4-O4	5.16	123.01	119.40
1	AR	2283	G	N3-C4-C5	5.16	131.18	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	918	C	C6-N1-C2	5.16	122.36	120.30
1	AR	3275	U	C5-C6-N1	5.15	125.28	122.70
1	1	880	G	N1-C6-O6	-5.15	116.81	119.90
1	1	2777	G	N3-C4-N9	-5.15	122.91	126.00
1	AR	1311	G	O5'-P-OP2	-5.15	101.07	105.70
1	1	1377	G	C5-C6-O6	-5.14	125.51	128.60
1	1	2550	U	N1-C2-O2	5.14	126.40	122.80
1	1	388	G	N3-C2-N2	-5.14	116.30	119.90
1	1	693	A	N1-C6-N6	5.14	121.69	118.60
25	6	158	U	OP1-P-O3'	5.14	116.51	105.20
25	6	902	G	N1-C6-O6	5.14	122.98	119.90
1	AR	1156	C	N1-C2-O2	-5.14	115.81	118.90
27	CZ	38	LEU	CA-CB-CG	5.14	127.13	115.30
1	1	1429	G	C8-N9-C1'	-5.14	120.32	127.00
1	AR	1789	G	C8-N9-C1'	5.14	133.68	127.00
1	AR	2351	U	N3-C2-O2	-5.14	118.60	122.20
1	1	2381	G	N1-C6-O6	5.13	122.98	119.90
1	1	877	C	N3-C4-C5	-5.13	119.85	121.90
6	CF	182	LEU	CA-CB-CG	5.13	127.10	115.30
1	1	2727	A	C4-C5-N7	-5.13	108.14	110.70
1	1	2943	G	C6-C5-N7	-5.13	127.32	130.40
1	1	3181	C	C6-N1-C2	-5.13	118.25	120.30
1	AR	805	G	C5-C6-O6	-5.13	125.52	128.60
1	AR	904	A	N1-C6-N6	5.13	121.68	118.60
1	AR	1134	G	N9-C4-C5	5.13	107.45	105.40
1	1	2121	G	N1-C6-O6	-5.13	116.82	119.90
1	1	2541	U	P-O3'-C3'	5.13	125.85	119.70
3	4	94	C	N3-C4-C5	5.13	123.95	121.90
1	AR	2842	U	C2-N1-C1'	5.13	123.85	117.70
25	A	831	U	C5-C6-N1	5.13	125.26	122.70
1	AR	938	C	C6-N1-C2	5.12	122.35	120.30
1	AR	1312	C	N3-C4-C5	-5.12	119.85	121.90
1	AR	3197	G	N3-C4-C5	5.12	131.16	128.60
1	AR	2848	G	N3-C4-C5	-5.12	126.04	128.60
1	1	94	G	O5'-P-OP1	-5.12	101.09	105.70
1	1	676	G	C8-N9-C1'	-5.12	120.35	127.00
1	1	1329	U	OP1-P-O3'	5.12	116.46	105.20
1	AR	2888	U	O5'-P-OP2	-5.12	101.10	105.70
3	AT	19	C	N1-C2-O2	-5.12	115.83	118.90
3	AT	36	G	N1-C6-O6	-5.12	116.83	119.90
1	1	688	G	N3-C4-N9	5.11	129.07	126.00
1	AR	515	C	C6-N1-C2	5.11	122.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2199	G	N1-C6-O6	5.11	122.97	119.90
25	6	30	G	N1-C6-O6	5.11	122.96	119.90
25	6	1023	A	C8-N9-C4	5.11	107.84	105.80
1	1	874	U	N3-C4-O4	-5.10	115.83	119.40
1	AR	1329	U	OP1-P-O3'	5.10	116.43	105.20
25	A	384	G	C4-N9-C1'	-5.10	119.87	126.50
25	6	364	G	C8-N9-C1'	-5.10	120.37	127.00
1	1	1111	U	C5-C6-N1	-5.10	120.15	122.70
25	6	1514	U	N3-C4-O4	-5.10	115.83	119.40
1	AR	776	U	C5-C6-N1	-5.09	120.15	122.70
3	4	58	G	C5-C6-O6	-5.09	125.54	128.60
25	6	20	G	C5-C6-O6	-5.09	125.55	128.60
1	AR	32	U	N1-C2-N3	5.09	117.95	114.90
1	AR	2263	C	C5-C6-N1	5.09	123.54	121.00
1	1	1435	A	C6-N1-C2	-5.09	115.55	118.60
25	6	1629	G	N3-C4-C5	-5.08	126.06	128.60
1	1	3212	C	C2-N1-C1'	-5.08	113.21	118.80
1	AR	1381	A	C2-N3-C4	-5.08	108.06	110.60
1	AR	2157	G	C8-N9-C4	5.08	108.43	106.40
1	1	672	A	N1-C6-N6	5.08	121.65	118.60
1	1	106	A	C8-N9-C4	5.08	107.83	105.80
1	1	650	C	N3-C2-O2	5.08	125.45	121.90
1	AR	1482	A	OP2-P-O3'	5.08	116.37	105.20
1	AR	2819	A	O5'-P-OP2	-5.07	101.14	105.70
1	1	633	C	C5-C6-N1	-5.07	118.46	121.00
1	1	650	C	N1-C2-O2	-5.07	115.86	118.90
25	6	272	U	P-O3'-C3'	5.07	125.78	119.70
1	1	2846	U	C2-N1-C1'	5.07	123.78	117.70
25	6	29	U	C4-C5-C6	5.07	122.74	119.70
1	AR	2880	U	C6-N1-C2	-5.07	117.96	121.00
1	1	2355	G	N1-C6-O6	5.07	122.94	119.90
1	AR	1858	A	C6-N1-C2	-5.06	115.56	118.60
1	AR	3277	U	N3-C2-O2	-5.06	118.66	122.20
25	A	1595	U	N1-C2-O2	-5.06	119.26	122.80
1	1	2281	A	O4'-C1'-N9	5.06	112.25	108.20
9	o	177	GLY	N-CA-C	-5.06	100.45	113.10
25	A	728	U	C6-N1-C1'	-5.06	114.12	121.20
1	AR	979	U	P-O3'-C3'	5.06	125.77	119.70
1	AR	2927	C	N1-C2-O2	-5.05	115.87	118.90
1	1	1115	G	N1-C6-O6	5.05	122.93	119.90
1	1	2283	G	N1-C6-O6	5.05	122.93	119.90
1	1	1897	G	C6-C5-N7	-5.05	127.37	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	3212	C	C5-C6-N1	-5.05	118.47	121.00
1	1	1916	U	C6-N1-C2	5.04	124.03	121.00
1	1	2659	G	C8-N9-C4	5.04	108.42	106.40
1	AR	3278	C	C6-N1-C2	-5.04	118.28	120.30
25	6	752	A	C8-N9-C4	5.04	107.82	105.80
1	AR	1319	G	C5-C6-N1	-5.04	108.98	111.50
1	AR	1370	G	N3-C4-C5	-5.04	126.08	128.60
1	AR	1429	G	C6-C5-N7	-5.04	127.38	130.40
1	1	913	A	C8-N9-C4	-5.04	103.78	105.80
1	AR	1101	G	C8-N9-C4	5.04	108.42	106.40
1	AR	1710	C	C6-N1-C2	5.04	122.31	120.30
1	AR	437	G	C8-N9-C4	-5.03	104.39	106.40
25	6	542	A	P-O3'-C3'	5.03	125.73	119.70
1	1	776	U	C4-C5-C6	5.02	122.71	119.70
1	AR	3344	A	C4-C5-N7	5.02	113.21	110.70
25	A	49	C	C6-N1-C2	-5.02	118.29	120.30
1	1	895	A	N7-C8-N9	5.02	116.31	113.80
1	1	75	G	N1-C6-O6	5.02	122.91	119.90
1	AR	941	G	O5'-P-OP2	-5.02	101.18	105.70
1	AR	1420	C	N1-C2-O2	-5.02	115.89	118.90
17	CQ	41	LEU	CA-CB-CG	5.02	126.84	115.30
25	6	1101	G	N1-C6-O6	5.02	122.91	119.90
1	AR	2550	U	N3-C2-O2	-5.02	118.69	122.20
1	AR	1903	U	C5-C4-O4	5.02	128.91	125.90
1	AR	2715	A	OP2-P-O3'	5.02	116.24	105.20
1	1	639	G	C4-C5-N7	5.01	112.81	110.80
25	6	610	G	C8-N9-C1'	-5.01	120.48	127.00
1	1	2417	U	C6-N1-C2	-5.01	117.99	121.00
1	AR	635	G	C5-C6-O6	-5.01	125.59	128.60
1	1	1604	G	C4-N9-C1'	5.01	133.01	126.50
10	CJ	35	GLY	N-CA-C	5.01	125.62	113.10
25	A	553	G	C5-C6-O6	-5.01	125.59	128.60
25	6	437	A	C8-N9-C4	5.01	107.80	105.80
25	6	765	G	N3-C4-C5	5.01	131.10	128.60
1	AR	739	G	N1-C6-O6	-5.01	116.90	119.90
1	AR	2637	A	O5'-P-OP1	-5.01	101.19	105.70
50	C	181	LEU	CA-CB-CG	5.01	126.82	115.30
1	1	213	A	N1-C6-N6	5.00	121.60	118.60
1	1	2726	C	C6-N1-C2	-5.00	118.30	120.30
25	6	1421	A	N1-C6-N6	5.00	121.60	118.60
1	AR	800	G	O4'-C1'-N9	-5.00	104.20	108.20
1	AR	1097	G	P-O3'-C3'	5.00	125.70	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AR	2283	G	C4-C5-N7	5.00	112.80	110.80
1	AR	3318	G	C6-C5-N7	-5.00	127.40	130.40
25	A	610	G	C8-N9-C1'	-5.00	120.50	127.00

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
22	2	122	GLN	Peptide
26	7	94	ARG	Peptide
28	9	83	ASP	Peptide
30	AB	46	ASP	Peptide
31	AC	20	GLY	Peptide
49	B	65	ALA	Peptide
7	CG	259	LYS	Peptide
10	CJ	34	PHE	Peptide
12	CL	188	GLY	Peptide
17	CQ	110	PRO	Peptide
20	CT	129	GLY	Peptide
26	CY	80	ARG	Peptide
26	CY	97	LYS	Peptide
51	D	106	ASP	Peptide
28	DA	83	ASP	Peptide
29	DB	3	LYS	Peptide
52	E	219	ALA	Peptide
53	F	213	SER	Peptide
54	G	44	ASN	Peptide
54	G	65	ARG	Peptide
56	I	31	SER	Peptide
56	I	64	VAL	Peptide
58	K	92	LYS	Peptide
64	Q	124	THR	Peptide
65	R	113	ASP	Peptide
65	R	40	GLU	Peptide
66	S	85	VAL	Peptide
66	S	86	PRO	Peptide
74	a	94	LYS	Peptide
61	c2	101	ALA	Peptide
61	c2	108	ARG	Peptide
61	c2	109	GLU	Peptide
61	c2	53	THR	Peptide
64	c5	52	LYS	Peptide

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Mol	Chain	Res	Type	Group
65	c6	40	GLU	Peptide
82	c7	103	ASP	Peptide
73	d4	29	HIS	Peptide
73	d4	51	GLU	Peptide
80	g	105	TYR	Peptide
80	g	110	ALA	Peptide
50	s1	152	ARG	Peptide
51	s2	106	ASP	Peptide
52	s3	219	ALA	Peptide
54	s5	44	ASN	Peptide
56	s7	130	VAL	Peptide
56	s7	62	VAL	Peptide
56	s7	63	PRO	Peptide
56	s7	64	VAL	Peptide
48	sM	79	SER	Peptide
15	u	28	SER	Peptide
17	w	110	PRO	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CD	250/252 (99%)	238 (95%)	12 (5%)	0	100	100
4	j	250/252 (99%)	232 (93%)	18 (7%)	0	100	100
5	CE	384/386 (100%)	355 (92%)	27 (7%)	2 (0%)	29	68
5	k	384/386 (100%)	351 (91%)	31 (8%)	2 (0%)	29	68
6	CF	359/361 (99%)	331 (92%)	28 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l	359/361 (99%)	326 (91%)	32 (9%)	1 (0%)	41	75
7	CG	294/296 (99%)	272 (92%)	22 (8%)	0	100	100
7	m	294/296 (99%)	271 (92%)	23 (8%)	0	100	100
8	CH	152/175 (87%)	144 (95%)	6 (4%)	2 (1%)	12	48
8	n	152/175 (87%)	145 (95%)	6 (4%)	1 (1%)	22	61
9	CI	220/222 (99%)	202 (92%)	15 (7%)	3 (1%)	11	46
9	o	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	11	46
10	CJ	231/233 (99%)	207 (90%)	21 (9%)	3 (1%)	12	48
10	p	231/233 (99%)	209 (90%)	18 (8%)	4 (2%)	9	42
11	CK	189/191 (99%)	178 (94%)	11 (6%)	0	100	100
11	q	189/191 (99%)	176 (93%)	12 (6%)	1 (0%)	29	68
12	CL	207/220 (94%)	195 (94%)	10 (5%)	2 (1%)	15	54
12	r	207/220 (94%)	199 (96%)	8 (4%)	0	100	100
13	CM	167/169 (99%)	146 (87%)	18 (11%)	3 (2%)	8	41
13	s	167/169 (99%)	149 (89%)	15 (9%)	3 (2%)	8	41
14	CN	191/193 (99%)	172 (90%)	18 (9%)	1 (0%)	29	68
14	t	191/193 (99%)	173 (91%)	15 (8%)	3 (2%)	9	43
15	CO	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	10	45
15	u	134/136 (98%)	122 (91%)	10 (8%)	2 (2%)	10	45
16	CP	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
16	v	201/203 (99%)	189 (94%)	12 (6%)	0	100	100
17	CQ	195/197 (99%)	189 (97%)	4 (2%)	2 (1%)	15	54
17	w	195/197 (99%)	188 (96%)	4 (2%)	3 (2%)	10	45
18	CR	181/183 (99%)	166 (92%)	14 (8%)	1 (1%)	25	64
18	x	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	25	64
19	CS	183/185 (99%)	171 (93%)	11 (6%)	1 (0%)	29	68
19	y	183/185 (99%)	173 (94%)	9 (5%)	1 (0%)	29	68
20	CT	186/188 (99%)	172 (92%)	13 (7%)	1 (0%)	29	68
20	z	186/188 (99%)	178 (96%)	7 (4%)	1 (0%)	29	68
21	0	170/172 (99%)	154 (91%)	15 (9%)	1 (1%)	25	64
21	CU	170/172 (99%)	158 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	2	157/159 (99%)	144 (92%)	12 (8%)	1 (1%)	25	64
22	CV	157/159 (99%)	147 (94%)	9 (6%)	1 (1%)	25	64
23	5	98/100 (98%)	88 (90%)	9 (9%)	1 (1%)	15	54
23	CW	98/100 (98%)	89 (91%)	8 (8%)	1 (1%)	15	54
24	CX	134/136 (98%)	132 (98%)	2 (2%)	0	100	100
24	l2	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
26	7	96/98 (98%)	85 (88%)	10 (10%)	1 (1%)	15	54
26	CY	96/98 (98%)	83 (86%)	11 (12%)	2 (2%)	7	38
27	8	119/121 (98%)	111 (93%)	8 (7%)	0	100	100
27	CZ	119/121 (98%)	111 (93%)	6 (5%)	2 (2%)	9	42
28	9	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
28	DA	124/126 (98%)	120 (97%)	4 (3%)	0	100	100
29	AA	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
29	DB	133/135 (98%)	121 (91%)	10 (8%)	2 (2%)	10	45
30	AB	146/148 (99%)	127 (87%)	17 (12%)	2 (1%)	11	46
30	DC	146/148 (99%)	130 (89%)	14 (10%)	2 (1%)	11	46
31	AC	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	41
31	DD	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	41
32	AD	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
32	DE	95/97 (98%)	93 (98%)	2 (2%)	0	100	100
33	AE	107/109 (98%)	101 (94%)	5 (5%)	1 (1%)	17	56
33	DF	107/109 (98%)	103 (96%)	3 (3%)	1 (1%)	17	56
34	AF	125/127 (98%)	122 (98%)	3 (2%)	0	100	100
34	DG	125/127 (98%)	119 (95%)	6 (5%)	0	100	100
35	AG	104/106 (98%)	98 (94%)	4 (4%)	2 (2%)	8	40
35	DH	104/106 (98%)	97 (93%)	6 (6%)	1 (1%)	15	54
36	AH	110/112 (98%)	104 (94%)	4 (4%)	2 (2%)	8	41
36	DI	110/112 (98%)	104 (94%)	6 (6%)	0	100	100
37	AI	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	DJ	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
38	AJ	97/99 (98%)	83 (86%)	13 (13%)	1 (1%)	15	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DK	97/99 (98%)	86 (89%)	10 (10%)	1 (1%)	15	54
39	AK	85/87 (98%)	77 (91%)	8 (9%)	0	100	100
39	DL	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
40	AL	75/77 (97%)	74 (99%)	1 (1%)	0	100	100
40	DM	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	12	48
41	AM	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
41	DN	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
42	AN	50/52 (96%)	45 (90%)	5 (10%)	0	100	100
42	DO	50/52 (96%)	46 (92%)	4 (8%)	0	100	100
43	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
43	DP	23/25 (92%)	23 (100%)	0	0	100	100
44	AP	103/105 (98%)	91 (88%)	12 (12%)	0	100	100
44	DQ	103/105 (98%)	90 (87%)	12 (12%)	1 (1%)	15	54
45	AQ	89/91 (98%)	77 (86%)	12 (14%)	0	100	100
45	DR	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
46	i	155/168 (92%)	129 (83%)	23 (15%)	3 (2%)	8	40
47	p0	139/220 (63%)	130 (94%)	8 (6%)	1 (1%)	22	61
48	sM	61/104 (59%)	47 (77%)	13 (21%)	1 (2%)	9	43
49	B	204/206 (99%)	175 (86%)	26 (13%)	3 (2%)	10	45
49	s0	204/206 (99%)	184 (90%)	17 (8%)	3 (2%)	10	45
50	C	212/216 (98%)	175 (82%)	35 (16%)	2 (1%)	17	56
50	s1	214/216 (99%)	196 (92%)	18 (8%)	0	100	100
51	D	215/217 (99%)	196 (91%)	18 (8%)	1 (0%)	29	68
51	s2	215/217 (99%)	199 (93%)	13 (6%)	3 (1%)	11	46
52	E	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	17	56
52	s3	221/223 (99%)	198 (90%)	21 (10%)	2 (1%)	17	56
53	F	258/260 (99%)	236 (92%)	20 (8%)	2 (1%)	19	58
53	s4	258/260 (99%)	233 (90%)	24 (9%)	1 (0%)	34	72
54	G	204/206 (99%)	179 (88%)	22 (11%)	3 (2%)	10	45
54	s5	204/206 (99%)	183 (90%)	21 (10%)	0	100	100
55	H	224/226 (99%)	207 (92%)	13 (6%)	4 (2%)	8	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	s6	216/226 (96%)	200 (93%)	14 (6%)	2 (1%)	17	56
56	I	182/186 (98%)	160 (88%)	17 (9%)	5 (3%)	5	33
56	s7	184/186 (99%)	162 (88%)	19 (10%)	3 (2%)	9	43
57	J	184/199 (92%)	160 (87%)	23 (12%)	1 (0%)	29	68
57	s8	184/199 (92%)	167 (91%)	15 (8%)	2 (1%)	14	52
58	K	183/185 (99%)	162 (88%)	19 (10%)	2 (1%)	14	52
58	s9	183/185 (99%)	172 (94%)	11 (6%)	0	100	100
59	L	94/105 (90%)	78 (83%)	14 (15%)	2 (2%)	7	38
59	c0	92/105 (88%)	63 (68%)	20 (22%)	9 (10%)	0	7
60	M	153/155 (99%)	138 (90%)	12 (8%)	3 (2%)	7	39
60	c1	144/155 (93%)	133 (92%)	10 (7%)	1 (1%)	22	61
61	N	122/124 (98%)	86 (70%)	30 (25%)	6 (5%)	2	19
61	c2	122/124 (98%)	91 (75%)	28 (23%)	3 (2%)	5	34
62	O	148/150 (99%)	134 (90%)	13 (9%)	1 (1%)	22	61
62	c3	148/150 (99%)	132 (89%)	15 (10%)	1 (1%)	22	61
63	P	125/128 (98%)	111 (89%)	13 (10%)	1 (1%)	19	58
63	c4	126/128 (98%)	114 (90%)	12 (10%)	0	100	100
64	Q	122/141 (86%)	107 (88%)	13 (11%)	2 (2%)	9	43
64	c5	133/141 (94%)	107 (80%)	24 (18%)	2 (2%)	10	45
65	R	139/142 (98%)	122 (88%)	14 (10%)	3 (2%)	6	37
65	c6	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
66	S	116/125 (93%)	99 (85%)	13 (11%)	4 (3%)	3	28
67	T	143/145 (99%)	127 (89%)	13 (9%)	3 (2%)	7	38
67	c8	143/145 (99%)	121 (85%)	18 (13%)	4 (3%)	5	32
68	U	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
68	c9	141/143 (99%)	129 (92%)	11 (8%)	1 (1%)	22	61
69	V	105/110 (96%)	93 (89%)	12 (11%)	0	100	100
69	d0	108/110 (98%)	92 (85%)	14 (13%)	2 (2%)	8	40
70	W	85/87 (98%)	76 (89%)	8 (9%)	1 (1%)	13	50
70	d1	85/87 (98%)	78 (92%)	7 (8%)	0	100	100
71	X	127/129 (98%)	120 (94%)	6 (5%)	1 (1%)	19	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
71	d2	127/129 (98%)	117 (92%)	9 (7%)	1 (1%)	19	58
72	Y	142/144 (99%)	119 (84%)	21 (15%)	2 (1%)	11	46
72	d3	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
73	Z	132/134 (98%)	121 (92%)	9 (7%)	2 (2%)	10	45
73	d4	132/134 (98%)	119 (90%)	10 (8%)	3 (2%)	6	36
74	a	68/70 (97%)	56 (82%)	10 (15%)	2 (3%)	4	31
74	d5	67/70 (96%)	59 (88%)	8 (12%)	0	100	100
75	b	95/97 (98%)	68 (72%)	24 (25%)	3 (3%)	4	29
75	d6	95/97 (98%)	76 (80%)	19 (20%)	0	100	100
76	c	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	12	48
76	d7	79/81 (98%)	75 (95%)	3 (4%)	1 (1%)	12	48
77	d	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
77	d8	61/63 (97%)	50 (82%)	11 (18%)	0	100	100
78	d9	51/53 (96%)	46 (90%)	4 (8%)	1 (2%)	7	39
78	e	51/53 (96%)	45 (88%)	6 (12%)	0	100	100
79	e0	60/62 (97%)	50 (83%)	8 (13%)	2 (3%)	4	28
79	f	58/62 (94%)	50 (86%)	7 (12%)	1 (2%)	9	42
80	g	69/71 (97%)	44 (64%)	19 (28%)	6 (9%)	1	9
81	h	316/318 (99%)	292 (92%)	23 (7%)	1 (0%)	41	75
81	sR	316/318 (99%)	292 (92%)	24 (8%)	0	100	100
82	c7	113/121 (93%)	102 (90%)	8 (7%)	3 (3%)	5	33
83	e1	49/51 (96%)	40 (82%)	9 (18%)	0	100	100
All	All	22260/22868 (97%)	20206 (91%)	1851 (8%)	203 (1%)	17	56

All (203) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	n	98	VAL
10	p	36	ILE
11	q	50	ASN
30	AB	48	TYR
46	i	167	PRO
8	CH	98	VAL
15	CO	8	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	CQ	111	PRO
58	K	134	ILE
59	L	88	PRO
61	N	126	TRP
66	S	85	VAL
66	S	86	PRO
71	X	83	ILE
73	Z	5	VAL
74	a	88	ILE
79	f	47	VAL
51	s2	164	SER
56	s7	67	LEU
59	c0	88	PRO
59	c0	97	PRO
62	c3	66	ILE
68	c9	34	VAL
71	d2	6	VAL
76	d7	59	CYS
17	w	111	PRO
18	x	156	ALA
19	y	99	THR
20	z	130	ASN
12	CL	25	ALA
22	CV	124	VAL
26	CY	82	ILE
29	DB	4	PHE
29	DB	18	TYR
40	DM	19	ASP
44	DQ	78	LYS
50	C	62	LYS
56	I	111	LYS
60	M	7	VAL
60	M	8	GLN
66	S	88	VAL
66	S	124	VAL
75	b	75	VAL
76	c	62	ILE
80	g	98	VAL
49	s0	189	VAL
52	s3	222	VAL
56	s7	63	PRO
59	c0	82	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
61	c2	91	VAL
82	c7	105	GLN
73	d4	52	LYS
9	o	25	GLN
10	p	37	GLY
15	u	8	LYS
17	w	110	PRO
22	2	124	VAL
13	CM	173	ASP
17	CQ	110	PRO
18	CR	156	ALA
26	CY	96	LEU
49	B	4	PRO
52	E	222	VAL
54	G	58	LEU
54	G	64	VAL
55	H	149	LYS
55	H	151	ASP
56	I	74	GLN
58	K	93	LEU
60	M	6	THR
65	R	39	VAL
65	R	113	ASP
73	Z	35	VAL
80	g	101	ALA
55	s6	70	PRO
82	c7	99	VAL
5	k	174	LYS
9	o	164	SER
10	p	123	GLN
13	s	8	PRO
14	t	47	ALA
26	7	96	LEU
35	AG	91	ALA
35	AG	104	PRO
36	AH	46	ASP
9	CI	24	GLU
9	CI	163	LEU
30	DC	48	TYR
35	DH	91	ALA
49	B	203	PHE
51	D	147	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
52	E	217	ILE
57	J	152	ILE
61	N	106	ILE
64	Q	126	VAL
67	T	91	ASP
70	W	82	VAL
80	g	102	VAL
52	s3	217	ILE
60	c1	7	VAL
61	c2	106	ILE
64	c5	128	HIS
82	c7	104	ASN
6	l	90	PHE
13	s	114	ILE
14	t	18	TRP
14	t	166	ALA
30	AB	47	LYS
5	CE	187	SER
8	CH	97	ASN
13	CM	8	PRO
14	CN	47	ALA
20	CT	131	ALA
30	DC	78	LEU
55	H	70	PRO
59	L	60	SER
61	N	109	GLU
64	Q	125	PRO
67	T	144	ARG
56	s7	64	VAL
59	c0	2	LEU
67	c8	8	GLN
67	c8	9	GLY
13	s	165	GLN
9	CI	25	GLN
10	CJ	36	ILE
10	CJ	123	GLN
10	CJ	157	VAL
12	CL	24	ARG
19	CS	99	THR
27	CZ	48	SER
53	F	144	GLY
53	F	195	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
56	I	5	GLN
61	N	128	ALA
72	Y	3	LYS
72	Y	30	LYS
80	g	88	PRO
59	c0	32	HIS
59	c0	83	PRO
69	d0	118	VAL
73	d4	30	PRO
73	d4	35	VAL
79	e0	47	VAL
9	o	26	VAL
10	p	157	VAL
38	AJ	3	VAL
13	CM	114	ILE
80	g	84	VAL
59	c0	35	ILE
59	c0	96	ASN
69	d0	51	VAL
78	d9	6	VAL
36	AH	12	PRO
46	i	166	VAL
15	CO	6	ILE
47	p0	33	VAL
49	B	158	VAL
55	H	69	LEU
56	I	32	PRO
61	N	91	VAL
63	P	42	VAL
80	g	87	THR
49	s0	158	VAL
57	s8	78	ILE
57	s8	101	ILE
79	e0	60	PRO
15	u	6	ILE
33	AE	7	VAL
23	CW	11	ILE
27	CZ	62	VAL
33	DF	7	VAL
50	C	210	ILE
54	G	51	VAL
56	I	98	ILE

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Mol	Chain	Res	Type
61	N	66	VAL
62	O	22	ALA
75	b	84	VAL
51	s2	163	GLY
59	c0	92	ILE
61	c2	115	VAL
5	k	317	ILE
17	w	16	VAL
21	0	167	ARG
23	5	11	ILE
46	i	12	VAL
5	CE	317	ILE
31	DD	21	ILE
65	R	97	VAL
67	T	14	ILE
74	a	71	ILE
75	b	86	VAL
81	h	6	VAL
49	s0	10	THR
53	s4	90	ILE
55	s6	69	LEU
64	c5	126	VAL
67	c8	14	ILE
31	AC	21	ILE
38	DK	3	VAL
48	sM	43	ASP
51	s2	121	VAL
67	c8	5	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	CD	193/194 (100%)	165 (86%)	28 (14%)	3	18
4	j	193/194 (100%)	174 (90%)	19 (10%)	8	33
5	CE	319/322 (99%)	273 (86%)	46 (14%)	3	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	k	319/322 (99%)	268 (84%)	51 (16%)	2	14
6	CF	288/288 (100%)	255 (88%)	33 (12%)	5	26
6	l	288/288 (100%)	254 (88%)	34 (12%)	5	25
7	CG	244/244 (100%)	209 (86%)	35 (14%)	3	19
7	m	244/244 (100%)	216 (88%)	28 (12%)	5	26
8	CH	134/152 (88%)	119 (89%)	15 (11%)	6	27
8	n	134/152 (88%)	120 (90%)	14 (10%)	7	31
9	CI	186/186 (100%)	171 (92%)	15 (8%)	11	41
9	o	186/186 (100%)	164 (88%)	22 (12%)	5	25
10	CJ	187/191 (98%)	170 (91%)	17 (9%)	9	36
10	p	187/191 (98%)	170 (91%)	17 (9%)	9	36
11	CK	171/171 (100%)	139 (81%)	32 (19%)	1	8
11	q	171/171 (100%)	150 (88%)	21 (12%)	4	23
12	CL	177/186 (95%)	154 (87%)	23 (13%)	4	21
12	r	177/186 (95%)	152 (86%)	25 (14%)	3	19
13	CM	147/147 (100%)	124 (84%)	23 (16%)	2	16
13	s	147/147 (100%)	131 (89%)	16 (11%)	6	29
14	CN	154/154 (100%)	134 (87%)	20 (13%)	4	21
14	t	154/154 (100%)	140 (91%)	14 (9%)	9	36
15	CO	107/107 (100%)	88 (82%)	19 (18%)	2	10
15	u	107/107 (100%)	96 (90%)	11 (10%)	7	32
16	CP	175/175 (100%)	155 (89%)	20 (11%)	5	26
16	v	175/175 (100%)	154 (88%)	21 (12%)	5	24
17	CQ	160/160 (100%)	138 (86%)	22 (14%)	3	20
17	w	160/160 (100%)	137 (86%)	23 (14%)	3	18
18	CR	140/145 (97%)	115 (82%)	25 (18%)	2	9
18	x	140/145 (97%)	117 (84%)	23 (16%)	2	13
19	CS	150/150 (100%)	141 (94%)	9 (6%)	19	52
19	y	150/150 (100%)	134 (89%)	16 (11%)	6	30
20	CT	153/153 (100%)	131 (86%)	22 (14%)	3	18
20	z	153/153 (100%)	140 (92%)	13 (8%)	10	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	0	156/156 (100%)	137 (88%)	19 (12%)	5	23
21	CU	156/156 (100%)	133 (85%)	23 (15%)	3	18
22	2	136/136 (100%)	113 (83%)	23 (17%)	2	12
22	CV	136/136 (100%)	116 (85%)	20 (15%)	3	18
23	5	87/87 (100%)	77 (88%)	10 (12%)	5	26
23	CW	87/87 (100%)	75 (86%)	12 (14%)	3	20
24	CX	104/104 (100%)	94 (90%)	10 (10%)	8	34
24	12	104/104 (100%)	91 (88%)	13 (12%)	4	23
26	7	57/86 (66%)	52 (91%)	5 (9%)	10	38
26	CY	57/86 (66%)	53 (93%)	4 (7%)	15	46
27	8	104/105 (99%)	87 (84%)	17 (16%)	2	13
27	CZ	104/105 (99%)	92 (88%)	12 (12%)	5	26
28	9	109/109 (100%)	99 (91%)	10 (9%)	9	36
28	DA	109/109 (100%)	98 (90%)	11 (10%)	7	32
29	AA	115/115 (100%)	104 (90%)	11 (10%)	8	34
29	DB	115/115 (100%)	105 (91%)	10 (9%)	10	38
30	AB	118/118 (100%)	106 (90%)	12 (10%)	7	32
30	DC	118/118 (100%)	107 (91%)	11 (9%)	9	35
31	AC	46/46 (100%)	41 (89%)	5 (11%)	6	29
31	DD	46/46 (100%)	39 (85%)	7 (15%)	3	17
32	AD	81/81 (100%)	70 (86%)	11 (14%)	3	20
32	DE	81/81 (100%)	75 (93%)	6 (7%)	13	44
33	AE	92/96 (96%)	81 (88%)	11 (12%)	5	24
33	DF	92/96 (96%)	74 (80%)	18 (20%)	1	7
34	AF	109/109 (100%)	95 (87%)	14 (13%)	4	22
34	DG	109/109 (100%)	93 (85%)	16 (15%)	3	18
35	AG	90/90 (100%)	83 (92%)	7 (8%)	12	42
35	DH	90/90 (100%)	83 (92%)	7 (8%)	12	42
36	AH	95/95 (100%)	85 (90%)	10 (10%)	7	31
36	DI	95/95 (100%)	82 (86%)	13 (14%)	3	20
37	AI	104/104 (100%)	90 (86%)	14 (14%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DJ	104/104 (100%)	87 (84%)	17 (16%)	2	13
38	AJ	81/81 (100%)	69 (85%)	12 (15%)	3	17
38	DK	81/81 (100%)	67 (83%)	14 (17%)	2	11
39	AK	70/70 (100%)	63 (90%)	7 (10%)	7	32
39	DL	70/70 (100%)	61 (87%)	9 (13%)	4	22
40	AL	68/68 (100%)	58 (85%)	10 (15%)	3	18
40	DM	68/68 (100%)	60 (88%)	8 (12%)	5	25
41	AM	45/45 (100%)	40 (89%)	5 (11%)	6	28
41	DN	45/45 (100%)	42 (93%)	3 (7%)	16	48
42	AN	47/47 (100%)	42 (89%)	5 (11%)	6	30
42	DO	47/47 (100%)	43 (92%)	4 (8%)	10	39
43	AO	23/23 (100%)	16 (70%)	7 (30%)	0	2
43	DP	23/23 (100%)	19 (83%)	4 (17%)	2	11
44	AP	90/90 (100%)	75 (83%)	15 (17%)	2	12
44	DQ	90/90 (100%)	78 (87%)	12 (13%)	4	21
45	AQ	71/71 (100%)	62 (87%)	9 (13%)	4	22
45	DR	71/71 (100%)	60 (84%)	11 (16%)	2	16
46	i	97/137 (71%)	85 (88%)	12 (12%)	4	23
47	p0	105/186 (56%)	89 (85%)	16 (15%)	3	17
48	sM	54/54 (100%)	47 (87%)	7 (13%)	4	21
49	B	164/173 (95%)	148 (90%)	16 (10%)	8	33
49	s0	165/173 (95%)	144 (87%)	21 (13%)	4	22
50	C	191/192 (100%)	167 (87%)	24 (13%)	4	22
50	s1	192/192 (100%)	166 (86%)	26 (14%)	4	21
51	D	176/176 (100%)	151 (86%)	25 (14%)	3	19
51	s2	176/176 (100%)	146 (83%)	30 (17%)	2	12
52	E	182/182 (100%)	160 (88%)	22 (12%)	5	24
52	s3	182/182 (100%)	167 (92%)	15 (8%)	11	40
53	F	221/221 (100%)	195 (88%)	26 (12%)	5	25
53	s4	221/221 (100%)	196 (89%)	25 (11%)	6	27
54	G	173/173 (100%)	158 (91%)	15 (9%)	10	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	s5	173/173 (100%)	158 (91%)	15 (9%)	10	38
55	H	188/193 (97%)	171 (91%)	17 (9%)	9	37
55	s6	187/193 (97%)	163 (87%)	24 (13%)	4	22
56	I	165/166 (99%)	146 (88%)	19 (12%)	5	26
56	s7	165/166 (99%)	155 (94%)	10 (6%)	18	51
57	J	150/160 (94%)	132 (88%)	18 (12%)	5	24
57	s8	150/160 (94%)	135 (90%)	15 (10%)	7	32
58	K	158/158 (100%)	132 (84%)	26 (16%)	2	13
58	s9	158/158 (100%)	138 (87%)	20 (13%)	4	22
59	L	77/98 (79%)	71 (92%)	6 (8%)	12	42
59	c0	73/98 (74%)	69 (94%)	4 (6%)	21	54
60	M	129/136 (95%)	120 (93%)	9 (7%)	15	46
60	c1	129/136 (95%)	111 (86%)	18 (14%)	3	19
61	N	88/100 (88%)	72 (82%)	16 (18%)	1	9
61	c2	88/100 (88%)	72 (82%)	16 (18%)	1	9
62	O	127/127 (100%)	114 (90%)	13 (10%)	7	32
62	c3	127/127 (100%)	113 (89%)	14 (11%)	6	29
63	P	81/97 (84%)	67 (83%)	14 (17%)	2	11
63	c4	97/97 (100%)	86 (89%)	11 (11%)	6	27
64	Q	101/117 (86%)	93 (92%)	8 (8%)	12	41
64	c5	103/117 (88%)	92 (89%)	11 (11%)	6	30
65	R	117/118 (99%)	102 (87%)	15 (13%)	4	22
65	c6	118/118 (100%)	100 (85%)	18 (15%)	2	17
66	S	94/113 (83%)	84 (89%)	10 (11%)	6	30
67	T	128/128 (100%)	113 (88%)	15 (12%)	5	26
67	c8	128/128 (100%)	117 (91%)	11 (9%)	10	38
68	U	115/115 (100%)	96 (84%)	19 (16%)	2	13
68	c9	115/115 (100%)	106 (92%)	9 (8%)	12	42
69	V	100/103 (97%)	89 (89%)	11 (11%)	6	29
69	d0	103/103 (100%)	94 (91%)	9 (9%)	10	38
70	W	74/74 (100%)	64 (86%)	10 (14%)	4	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	d1	74/74 (100%)	66 (89%)	8 (11%)	6	30
71	X	110/110 (100%)	96 (87%)	14 (13%)	4	22
71	d2	110/110 (100%)	100 (91%)	10 (9%)	9	36
72	Y	119/119 (100%)	102 (86%)	17 (14%)	3	19
72	d3	119/119 (100%)	107 (90%)	12 (10%)	7	32
73	Z	112/112 (100%)	106 (95%)	6 (5%)	22	55
73	d4	112/112 (100%)	102 (91%)	10 (9%)	9	37
74	a	61/61 (100%)	50 (82%)	11 (18%)	1	9
74	d5	61/61 (100%)	57 (93%)	4 (7%)	16	49
75	b	83/83 (100%)	69 (83%)	14 (17%)	2	12
75	d6	83/83 (100%)	73 (88%)	10 (12%)	5	24
76	c	70/70 (100%)	66 (94%)	4 (6%)	20	53
76	d7	70/70 (100%)	63 (90%)	7 (10%)	7	32
77	d	56/56 (100%)	50 (89%)	6 (11%)	6	30
77	d8	56/56 (100%)	49 (88%)	7 (12%)	4	23
78	d9	47/47 (100%)	40 (85%)	7 (15%)	3	17
78	e	47/47 (100%)	42 (89%)	5 (11%)	6	30
79	e0	53/53 (100%)	40 (76%)	13 (24%)	0	4
79	f	51/53 (96%)	45 (88%)	6 (12%)	5	25
80	g	62/62 (100%)	55 (89%)	7 (11%)	6	27
81	h	259/261 (99%)	234 (90%)	25 (10%)	8	33
81	sR	260/261 (100%)	242 (93%)	18 (7%)	15	47
82	c7	92/110 (84%)	80 (87%)	12 (13%)	4	21
83	e1	43/43 (100%)	34 (79%)	9 (21%)	1	6
All	All	18681/19177 (97%)	16432 (88%)	2249 (12%)	5	24

All (2249) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	j	32	LEU
4	j	44	ILE
4	j	45	VAL
4	j	72	ARG
4	j	74	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	j	88	ILE
4	j	96	LEU
4	j	101	VAL
4	j	116	VAL
4	j	134	VAL
4	j	157	VAL
4	j	165	VAL
4	j	179	LEU
4	j	190	ARG
4	j	204	MET
4	j	207	VAL
4	j	225	ILE
4	j	227	ARG
4	j	230	VAL
5	k	3	HIS
5	k	7	GLU
5	k	19	ARG
5	k	25	ILE
5	k	37	ARG
5	k	38	SER
5	k	55	THR
5	k	67	PHE
5	k	72	VAL
5	k	79	VAL
5	k	84	VAL
5	k	85	VAL
5	k	87	VAL
5	k	93	VAL
5	k	95	THR
5	k	100	ARG
5	k	103	THR
5	k	104	THR
5	k	112	ASP
5	k	114	VAL
5	k	123	TYR
5	k	139	GLN
5	k	140	ASP
5	k	156	SER
5	k	157	VAL
5	k	166	ILE
5	k	169	THR
5	k	183	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	k	188	ILE
5	k	192	VAL
5	k	196	ARG
5	k	201	LYS
5	k	208	VAL
5	k	211	GLN
5	k	212	ASN
5	k	226	PHE
5	k	229	VAL
5	k	236	LYS
5	k	238	LEU
5	k	241	LYS
5	k	274	SER
5	k	284	ARG
5	k	291	GLU
5	k	296	THR
5	k	305	ILE
5	k	306	THR
5	k	320	ASP
5	k	328	ILE
5	k	332	ARG
5	k	338	LEU
5	k	385	LYS
6	l	40	THR
6	l	47	ARG
6	l	60	THR
6	l	74	ILE
6	l	92	ASN
6	l	93	MET
6	l	105	THR
6	l	120	TYR
6	l	133	SER
6	l	136	LEU
6	l	138	ARG
6	l	141	ARG
6	l	150	LEU
6	l	153	SER
6	l	156	LEU
6	l	176	SER
6	l	179	LEU
6	l	193	LYS
6	l	220	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	l	222	VAL
6	l	230	VAL
6	l	246	ARG
6	l	258	LEU
6	l	270	SER
6	l	278	SER
6	l	310	THR
6	l	313	LEU
6	l	327	LEU
6	l	332	LYS
6	l	333	VAL
6	l	338	LYS
6	l	347	THR
6	l	349	THR
6	l	356	THR
7	m	5	LYS
7	m	23	ARG
7	m	32	GLN
7	m	41	LYS
7	m	58	LYS
7	m	80	SER
7	m	101	THR
7	m	105	ILE
7	m	110	LEU
7	m	112	LYS
7	m	115	LEU
7	m	131	LEU
7	m	132	THR
7	m	137	ASP
7	m	140	ARG
7	m	146	LEU
7	m	148	ILE
7	m	151	GLN
7	m	155	THR
7	m	163	LEU
7	m	185	PHE
7	m	213	ASP
7	m	222	LEU
7	m	234	ASP
7	m	257	GLU
7	m	258	LYS
7	m	259	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	m	273	ARG
8	n	5	LYS
8	n	13	GLU
8	n	15	VAL
8	n	52	VAL
8	n	64	LEU
8	n	65	ILE
8	n	84	VAL
8	n	88	SER
8	n	89	THR
8	n	93	VAL
8	n	98	VAL
8	n	129	GLU
8	n	134	ARG
8	n	155	LEU
9	o	24	GLU
9	o	26	VAL
9	o	80	GLN
9	o	82	LYS
9	o	88	ARG
9	o	92	ILE
9	o	93	ASN
9	o	98	LYS
9	o	100	ARG
9	o	109	THR
9	o	121	LYS
9	o	123	THR
9	o	124	LEU
9	o	129	LEU
9	o	168	ILE
9	o	175	LYS
9	o	179	LEU
9	o	180	SER
9	o	182	ASP
9	o	183	ASP
9	o	184	LEU
9	o	239	LEU
10	p	27	THR
10	p	50	VAL
10	p	71	VAL
10	p	74	THR
10	p	79	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	p	81	THR
10	p	84	ARG
10	p	95	ASN
10	p	101	THR
10	p	136	LEU
10	p	150	LEU
10	p	156	ASP
10	p	169	LEU
10	p	173	MET
10	p	190	VAL
10	p	194	THR
10	p	204	ARG
11	q	6	THR
11	q	18	VAL
11	q	19	SER
11	q	33	THR
11	q	41	ILE
11	q	52	LEU
11	q	68	LEU
11	q	69	ARG
11	q	70	THR
11	q	92	TYR
11	q	132	VAL
11	q	138	THR
11	q	146	LEU
11	q	147	SER
11	q	151	VAL
11	q	157	ASN
11	q	161	LEU
11	q	162	GLN
11	q	172	ILE
11	q	173	ARG
11	q	189	GLU
12	r	3	ARG
12	r	7	ARG
12	r	21	ARG
12	r	23	ASN
12	r	24	ARG
12	r	30	LYS
12	r	32	ARG
12	r	35	ASP
12	r	48	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	r	52	LEU
12	r	57	LEU
12	r	62	SER
12	r	63	GLU
12	r	87	LEU
12	r	133	GLN
12	r	138	VAL
12	r	139	ARG
12	r	163	GLN
12	r	165	ILE
12	r	169	LYS
12	r	174	THR
12	r	177	ASP
12	r	190	VAL
12	r	203	LYS
12	r	205	SER
13	s	10	ARG
13	s	13	LYS
13	s	25	GLU
13	s	40	LEU
13	s	44	THR
13	s	46	VAL
13	s	80	LEU
13	s	94	ARG
13	s	95	ASN
13	s	106	ILE
13	s	107	ASP
13	s	112	LEU
13	s	138	VAL
13	s	140	ARG
13	s	142	LYS
13	s	154	THR
14	t	13	HIS
14	t	17	HIS
14	t	23	LYS
14	t	54	LEU
14	t	55	ARG
14	t	58	VAL
14	t	59	ARG
14	t	69	VAL
14	t	70	ARG
14	t	114	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	t	117	LYS
14	t	124	ILE
14	t	165	SER
14	t	168	ARG
15	u	5	SER
15	u	10	SER
15	u	15	VAL
15	u	20	VAL
15	u	38	ILE
15	u	53	VAL
15	u	90	VAL
15	u	91	CYS
15	u	102	LYS
15	u	108	ARG
15	u	135	LEU
16	v	15	GLN
16	v	18	VAL
16	v	22	LEU
16	v	38	ARG
16	v	62	TYR
16	v	68	ARG
16	v	70	ASN
16	v	80	THR
16	v	85	THR
16	v	92	LEU
16	v	101	THR
16	v	117	ASN
16	v	133	ILE
16	v	151	ILE
16	v	153	ASP
16	v	165	THR
16	v	182	ASN
16	v	183	THR
16	v	188	ARG
16	v	195	ASN
16	v	201	ARG
17	w	33	ILE
17	w	41	LEU
17	w	58	LEU
17	w	59	ARG
17	w	78	ARG
17	w	82	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	w	84	LEU
17	w	85	ARG
17	w	94	ARG
17	w	103	LYS
17	w	106	GLU
17	w	108	ILE
17	w	110	PRO
17	w	115	LYS
17	w	117	ARG
17	w	119	VAL
17	w	124	LEU
17	w	126	VAL
17	w	128	ARG
17	w	129	LEU
17	w	137	THR
17	w	143	THR
17	w	184	THR
18	x	7	THR
18	x	8	SER
18	x	23	ARG
18	x	29	THR
18	x	36	ILE
18	x	42	THR
18	x	52	LEU
18	x	53	ASP
18	x	56	ARG
18	x	69	ARG
18	x	112	LEU
18	x	118	GLN
18	x	119	VAL
18	x	120	ASN
18	x	127	ARG
18	x	129	THR
18	x	142	SER
18	x	144	SER
18	x	157	VAL
18	x	168	LEU
18	x	171	ARG
18	x	180	LYS
18	x	181	ARG
19	y	6	THR
19	y	15	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	y	22	ASP
19	y	32	LEU
19	y	41	ASP
19	y	49	LEU
19	y	57	ILE
19	y	69	ARG
19	y	74	GLU
19	y	129	VAL
19	y	135	GLN
19	y	138	LEU
19	y	147	ARG
19	y	150	VAL
19	y	178	ARG
19	y	181	SER
20	z	10	LEU
20	z	29	THR
20	z	41	ILE
20	z	44	LEU
20	z	81	ARG
20	z	103	ARG
20	z	104	ARG
20	z	116	ASP
20	z	130	ASN
20	z	134	HIS
20	z	144	GLN
20	z	175	GLN
20	z	182	ASP
21	0	16	THR
21	0	45	LEU
21	0	49	HIS
21	0	50	LYS
21	0	51	VAL
21	0	61	ILE
21	0	71	LYS
21	0	80	ARG
21	0	97	VAL
21	0	106	LEU
21	0	115	ARG
21	0	122	HIS
21	0	132	THR
21	0	137	ARG
21	0	138	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	0	155	ARG
21	0	157	GLN
21	0	167	ARG
21	0	172	TYR
22	2	12	ARG
22	2	18	ASP
22	2	25	VAL
22	2	27	LEU
22	2	52	MET
22	2	63	VAL
22	2	68	THR
22	2	75	ILE
22	2	78	LYS
22	2	79	MET
22	2	80	VAL
22	2	83	ARG
22	2	96	ILE
22	2	102	ARG
22	2	104	GLU
22	2	126	VAL
22	2	127	GLN
22	2	128	LEU
22	2	131	GLN
22	2	139	ARG
22	2	141	VAL
22	2	149	GLN
22	2	158	THR
23	5	10	LYS
23	5	14	THR
23	5	35	LYS
23	5	39	ASP
23	5	52	ASN
23	5	66	VAL
23	5	75	TYR
23	5	85	LYS
23	5	93	ILE
23	5	100	THR
24	12	14	SER
24	12	32	ARG
24	12	44	SER
24	12	48	ARG
24	12	54	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	12	69	LEU
24	12	72	LYS
24	12	73	VAL
24	12	74	MET
24	12	88	ARG
24	12	102	ILE
24	12	104	ASN
24	12	120	LYS
26	7	4	GLU
26	7	5	ILE
26	7	19	THR
26	7	26	SER
26	7	43	ARG
27	8	27	ARG
27	8	38	LEU
27	8	45	LYS
27	8	49	LYS
27	8	63	ILE
27	8	75	LYS
27	8	109	LYS
27	8	113	LEU
27	8	115	ARG
27	8	117	ASN
27	8	125	ARG
27	8	126	LEU
27	8	133	LEU
27	8	135	ILE
27	8	137	ASN
27	8	139	ILE
27	8	142	ILE
28	9	3	LYS
28	9	5	SER
28	9	17	LYS
28	9	37	LYS
28	9	56	VAL
28	9	74	TYR
28	9	88	GLU
28	9	113	LYS
28	9	115	ARG
28	9	126	LEU
29	AA	14	VAL
29	AA	24	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	AA	37	PRO
29	AA	46	ILE
29	AA	64	LYS
29	AA	81	LEU
29	AA	83	THR
29	AA	90	GLU
29	AA	102	GLU
29	AA	107	ARG
29	AA	134	LEU
30	AB	4	ARG
30	AB	10	LYS
30	AB	22	ILE
30	AB	42	ARG
30	AB	43	ILE
30	AB	56	VAL
30	AB	60	TYR
30	AB	78	LEU
30	AB	88	ASP
30	AB	93	SER
30	AB	98	THR
30	AB	115	LYS
31	AC	18	ARG
31	AC	25	LYS
31	AC	28	LYS
31	AC	31	SER
31	AC	59	LYS
32	AD	16	LEU
32	AD	32	LYS
32	AD	40	LYS
32	AD	43	ILE
32	AD	48	THR
32	AD	54	SER
32	AD	61	MET
32	AD	76	GLU
32	AD	99	ASP
32	AD	101	LEU
32	AD	103	THR
33	AE	6	ASP
33	AE	16	LEU
33	AE	24	SER
33	AE	26	LYS
33	AE	64	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	AE	68	GLU
33	AE	79	ARG
33	AE	84	ASP
33	AE	86	LYS
33	AE	106	THR
33	AE	110	GLU
34	AF	19	ARG
34	AF	33	ARG
34	AF	35	GLN
34	AF	51	SER
34	AF	54	LYS
34	AF	61	LYS
34	AF	62	LYS
34	AF	67	SER
34	AF	73	THR
34	AF	75	LEU
34	AF	78	ASN
34	AF	88	HIS
34	AF	109	LEU
34	AF	128	LEU
35	AG	28	SER
35	AG	37	THR
35	AG	48	ARG
35	AG	59	VAL
35	AG	80	VAL
35	AG	81	VAL
35	AG	98	VAL
36	AH	5	VAL
36	AH	15	THR
36	AH	20	ILE
36	AH	24	LYS
36	AH	29	ILE
36	AH	51	LEU
36	AH	58	ARG
36	AH	65	VAL
36	AH	71	THR
36	AH	74	ARG
37	AI	20	GLN
37	AI	21	LEU
37	AI	27	GLU
37	AI	28	LEU
37	AI	31	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
37	AI	47	VAL
37	AI	71	LYS
37	AI	85	THR
37	AI	89	ARG
37	AI	90	ARG
37	AI	93	THR
37	AI	96	GLU
37	AI	102	GLU
37	AI	119	LYS
38	AJ	13	LYS
38	AJ	17	VAL
38	AJ	25	LYS
38	AJ	26	ILE
38	AJ	43	LEU
38	AJ	45	ARG
38	AJ	57	LEU
38	AJ	68	ARG
38	AJ	84	LYS
38	AJ	88	GLU
38	AJ	90	MET
38	AJ	98	ARG
39	AK	24	ARG
39	AK	25	ARG
39	AK	36	SER
39	AK	44	THR
39	AK	55	ARG
39	AK	59	THR
39	AK	67	LEU
40	AL	24	THR
40	AL	31	LEU
40	AL	50	SER
40	AL	53	THR
40	AL	64	LYS
40	AL	65	LEU
40	AL	67	GLN
40	AL	69	LEU
40	AL	72	THR
40	AL	77	ARG
41	AM	4	GLN
41	AM	5	LYS
41	AM	21	ARG
41	AM	34	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
41	AM	45	ARG
42	AN	78	ILE
42	AN	112	LYS
42	AN	113	ARG
42	AN	114	LYS
42	AN	127	LEU
43	AO	2	ARG
43	AO	4	LYS
43	AO	9	ARG
43	AO	10	THR
43	AO	11	ARG
43	AO	19	LYS
43	AO	21	ARG
44	AP	3	ASN
44	AP	8	ARG
44	AP	21	THR
44	AP	35	LEU
44	AP	38	GLN
44	AP	45	ARG
44	AP	48	SER
44	AP	60	LYS
44	AP	64	THR
44	AP	78	LYS
44	AP	83	LEU
44	AP	84	THR
44	AP	85	LEU
44	AP	93	LEU
44	AP	102	GLN
45	AQ	7	LYS
45	AQ	11	THR
45	AQ	16	VAL
45	AQ	25	GLN
45	AQ	56	THR
45	AQ	59	CYS
45	AQ	78	THR
45	AQ	84	ARG
45	AQ	91	GLU
46	i	34	LYS
46	i	46	LYS
46	i	61	ILE
46	i	64	LYS
46	i	68	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
46	i	84	LYS
46	i	91	THR
46	i	102	THR
46	i	116	GLU
46	i	117	LEU
46	i	126	ASP
46	i	130	GLU
4	CD	44	ILE
4	CD	45	VAL
4	CD	48	ILE
4	CD	62	VAL
4	CD	70	ARG
4	CD	74	GLU
4	CD	82	VAL
4	CD	96	LEU
4	CD	101	VAL
4	CD	109	GLU
4	CD	113	VAL
4	CD	137	ILE
4	CD	149	ARG
4	CD	157	VAL
4	CD	165	VAL
4	CD	180	LEU
4	CD	190	ARG
4	CD	191	LEU
4	CD	199	THR
4	CD	204	MET
4	CD	205	ASN
4	CD	207	VAL
4	CD	217	GLN
4	CD	218	HIS
4	CD	227	ARG
4	CD	243	THR
4	CD	250	GLN
4	CD	252	THR
5	CE	4	ARG
5	CE	7	GLU
5	CE	25	ILE
5	CE	37	ARG
5	CE	44	THR
5	CE	47	LEU
5	CE	73	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	CE	77	THR
5	CE	81	THR
5	CE	85	VAL
5	CE	95	THR
5	CE	103	THR
5	CE	104	THR
5	CE	110	LEU
5	CE	112	ASP
5	CE	114	VAL
5	CE	121	ASN
5	CE	139	GLN
5	CE	160	VAL
5	CE	169	THR
5	CE	173	GLN
5	CE	183	LEU
5	CE	184	ASN
5	CE	188	ILE
5	CE	192	VAL
5	CE	200	GLU
5	CE	205	VAL
5	CE	211	GLN
5	CE	230	THR
5	CE	232	ARG
5	CE	235	THR
5	CE	238	LEU
5	CE	244	ARG
5	CE	249	VAL
5	CE	274	SER
5	CE	284	ARG
5	CE	301	THR
5	CE	303	LYS
5	CE	305	ILE
5	CE	312	VAL
5	CE	319	ASN
5	CE	324	VAL
5	CE	325	LYS
5	CE	332	ARG
5	CE	348	ARG
5	CE	349	LYS
6	CF	22	LEU
6	CF	25	VAL
6	CF	27	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	CF	47	ARG
6	CF	53	SER
6	CF	55	LYS
6	CF	74	ILE
6	CF	76	ARG
6	CF	93	MET
6	CF	103	THR
6	CF	120	TYR
6	CF	133	SER
6	CF	136	LEU
6	CF	138	ARG
6	CF	148	ILE
6	CF	150	LEU
6	CF	154	THR
6	CF	179	LEU
6	CF	187	LEU
6	CF	193	LYS
6	CF	200	THR
6	CF	203	ARG
6	CF	206	LEU
6	CF	222	VAL
6	CF	230	VAL
6	CF	246	ARG
6	CF	278	SER
6	CF	292	SER
6	CF	316	ASN
6	CF	324	LEU
6	CF	327	LEU
6	CF	333	VAL
6	CF	346	LYS
7	CG	5	LYS
7	CG	13	SER
7	CG	22	ARG
7	CG	23	ARG
7	CG	35	ARG
7	CG	41	LYS
7	CG	69	ILE
7	CG	75	LEU
7	CG	92	LEU
7	CG	93	THR
7	CG	105	ILE
7	CG	112	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	CG	113	LEU
7	CG	118	THR
7	CG	126	GLU
7	CG	131	LEU
7	CG	137	ASP
7	CG	140	ARG
7	CG	146	LEU
7	CG	148	ILE
7	CG	151	GLN
7	CG	154	THR
7	CG	155	THR
7	CG	177	GLU
7	CG	179	ARG
7	CG	185	PHE
7	CG	188	GLU
7	CG	190	ILE
7	CG	194	LEU
7	CG	197	SER
7	CG	220	SER
7	CG	232	ASP
7	CG	258	LYS
7	CG	263	GLU
7	CG	293	LEU
8	CH	12	SER
8	CH	15	VAL
8	CH	21	THR
8	CH	28	GLN
8	CH	31	ARG
8	CH	46	ARG
8	CH	52	VAL
8	CH	64	LEU
8	CH	65	ILE
8	CH	78	ARG
8	CH	89	THR
8	CH	129	GLU
8	CH	134	ARG
8	CH	152	THR
8	CH	155	LEU
9	CI	24	GLU
9	CI	26	VAL
9	CI	60	ARG
9	CI	77	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	CI	83	LEU
9	CI	89	ILE
9	CI	92	ILE
9	CI	129	LEU
9	CI	147	LEU
9	CI	158	LYS
9	CI	173	LEU
9	CI	179	LEU
9	CI	184	LEU
9	CI	196	LYS
9	CI	239	LEU
10	CJ	27	THR
10	CJ	50	VAL
10	CJ	65	LEU
10	CJ	71	VAL
10	CJ	74	THR
10	CJ	79	GLN
10	CJ	81	THR
10	CJ	136	LEU
10	CJ	156	ASP
10	CJ	169	LEU
10	CJ	172	LYS
10	CJ	180	VAL
10	CJ	185	ARG
10	CJ	194	THR
10	CJ	197	VAL
10	CJ	219	ASP
10	CJ	248	LYS
11	CK	1	MET
11	CK	5	GLN
11	CK	17	THR
11	CK	18	VAL
11	CK	19	SER
11	CK	22	SER
11	CK	33	THR
11	CK	39	LYS
11	CK	41	ILE
11	CK	48	VAL
11	CK	52	LEU
11	CK	68	LEU
11	CK	69	ARG
11	CK	70	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	CK	80	THR
11	CK	82	VAL
11	CK	92	TYR
11	CK	107	ASP
11	CK	113	GLU
11	CK	122	LYS
11	CK	129	ARG
11	CK	137	SER
11	CK	151	VAL
11	CK	157	ASN
11	CK	161	LEU
11	CK	164	ILE
11	CK	166	ARG
11	CK	170	LYS
11	CK	172	ILE
11	CK	173	ARG
11	CK	177	ASP
11	CK	182	SER
12	CL	3	ARG
12	CL	21	ARG
12	CL	22	TYR
12	CL	32	ARG
12	CL	40	LYS
12	CL	42	THR
12	CL	48	LEU
12	CL	52	LEU
12	CL	57	LEU
12	CL	63	GLU
12	CL	74	LYS
12	CL	87	LEU
12	CL	90	ARG
12	CL	91	VAL
12	CL	100	ASN
12	CL	139	ARG
12	CL	156	ARG
12	CL	163	GLN
12	CL	165	ILE
12	CL	168	SER
12	CL	177	ASP
12	CL	196	PHE
12	CL	197	VAL
13	CM	10	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	CM	12	LEU
13	CM	13	LYS
13	CM	20	ASN
13	CM	22	SER
13	CM	28	ASP
13	CM	30	LEU
13	CM	46	VAL
13	CM	51	ARG
13	CM	56	THR
13	CM	80	LEU
13	CM	95	ASN
13	CM	106	ILE
13	CM	107	ASP
13	CM	112	LEU
13	CM	115	LYS
13	CM	130	VAL
13	CM	137	ARG
13	CM	140	ARG
13	CM	142	LYS
13	CM	161	SER
13	CM	165	GLN
13	CM	166	LYS
14	CN	11	LYS
14	CN	13	HIS
14	CN	23	LYS
14	CN	24	VAL
14	CN	52	ASP
14	CN	54	LEU
14	CN	55	ARG
14	CN	58	VAL
14	CN	59	ARG
14	CN	67	ARG
14	CN	124	ILE
14	CN	131	LYS
14	CN	134	GLU
14	CN	137	GLN
14	CN	140	SER
14	CN	153	ASP
14	CN	154	VAL
14	CN	164	GLU
14	CN	168	ARG
14	CN	171	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	CO	4	ASP
15	CO	10	SER
15	CO	12	TRP
15	CO	15	VAL
15	CO	16	GLU
15	CO	20	VAL
15	CO	24	LYS
15	CO	38	ILE
15	CO	41	GLN
15	CO	45	LEU
15	CO	53	VAL
15	CO	60	LEU
15	CO	63	VAL
15	CO	66	THR
15	CO	90	VAL
15	CO	91	CYS
15	CO	108	ARG
15	CO	128	ARG
15	CO	135	LEU
16	CP	10	LEU
16	CP	17	ASP
16	CP	22	LEU
16	CP	24	ARG
16	CP	43	THR
16	CP	68	ARG
16	CP	80	THR
16	CP	83	LYS
16	CP	105	ARG
16	CP	106	VAL
16	CP	109	ARG
16	CP	133	ILE
16	CP	138	GLN
16	CP	151	ILE
16	CP	153	ASP
16	CP	155	VAL
16	CP	167	THR
16	CP	171	SER
16	CP	183	THR
16	CP	188	ARG
17	CQ	3	VAL
17	CQ	34	VAL
17	CQ	67	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
17	CQ	78	ARG
17	CQ	84	LEU
17	CQ	85	ARG
17	CQ	92	THR
17	CQ	102	LEU
17	CQ	110	PRO
17	CQ	115	LYS
17	CQ	117	ARG
17	CQ	118	VAL
17	CQ	124	LEU
17	CQ	126	VAL
17	CQ	128	ARG
17	CQ	134	LYS
17	CQ	142	SER
17	CQ	143	THR
17	CQ	180	SER
17	CQ	184	THR
17	CQ	190	VAL
17	CQ	192	LYS
18	CR	8	SER
18	CR	9	THR
18	CR	18	ARG
18	CR	22	LEU
18	CR	23	ARG
18	CR	24	VAL
18	CR	32	THR
18	CR	37	ASN
18	CR	42	THR
18	CR	51	VAL
18	CR	52	LEU
18	CR	55	GLN
18	CR	63	PHE
18	CR	69	ARG
18	CR	89	LYS
18	CR	96	GLN
18	CR	111	LYS
18	CR	114	VAL
18	CR	120	ASN
18	CR	126	ARG
18	CR	142	SER
18	CR	144	SER
18	CR	150	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	CR	168	LEU
18	CR	175	ARG
19	CS	26	LEU
19	CS	32	LEU
19	CS	41	ASP
19	CS	69	ARG
19	CS	81	VAL
19	CS	113	LYS
19	CS	135	GLN
19	CS	138	LEU
19	CS	168	THR
20	CT	10	LEU
20	CT	20	ARG
20	CT	44	LEU
20	CT	49	THR
20	CT	57	VAL
20	CT	60	LYS
20	CT	61	SER
20	CT	74	ARG
20	CT	81	ARG
20	CT	86	GLU
20	CT	98	ARG
20	CT	99	LEU
20	CT	103	ARG
20	CT	104	ARG
20	CT	110	ARG
20	CT	121	HIS
20	CT	148	ASP
20	CT	152	GLU
20	CT	153	LYS
20	CT	158	GLU
20	CT	166	ASN
20	CT	182	ASP
21	CU	16	THR
21	CU	51	VAL
21	CU	61	ILE
21	CU	71	LYS
21	CU	80	ARG
21	CU	87	THR
21	CU	88	HIS
21	CU	89	ASN
21	CU	96	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
21	CU	97	VAL
21	CU	100	VAL
21	CU	105	THR
21	CU	113	ARG
21	CU	117	ARG
21	CU	135	VAL
21	CU	136	LYS
21	CU	137	ARG
21	CU	145	THR
21	CU	149	LYS
21	CU	155	ARG
21	CU	156	VAL
21	CU	157	GLN
21	CU	172	TYR
22	CV	3	LYS
22	CV	12	ARG
22	CV	25	VAL
22	CV	27	LEU
22	CV	75	ILE
22	CV	78	LYS
22	CV	79	MET
22	CV	80	VAL
22	CV	83	ARG
22	CV	88	ARG
22	CV	102	ARG
22	CV	103	GLN
22	CV	104	GLU
22	CV	106	LEU
22	CV	126	VAL
22	CV	127	GLN
22	CV	128	LEU
22	CV	139	ARG
22	CV	143	THR
22	CV	154	VAL
23	CW	10	LYS
23	CW	14	THR
23	CW	37	LEU
23	CW	43	VAL
23	CW	49	ASN
23	CW	52	ASN
23	CW	72	SER
23	CW	75	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
23	CW	88	GLN
23	CW	92	TRP
23	CW	94	ARG
23	CW	100	THR
24	CX	22	ILE
24	CX	32	ARG
24	CX	48	ARG
24	CX	57	MET
24	CX	61	THR
24	CX	81	GLN
24	CX	86	ARG
24	CX	88	ARG
24	CX	102	ILE
24	CX	133	SER
26	CY	1	MET
26	CY	17	ARG
26	CY	26	SER
26	CY	59	HIS
27	CZ	27	ARG
27	CZ	38	LEU
27	CZ	45	LYS
27	CZ	63	ILE
27	CZ	69	SER
27	CZ	71	THR
27	CZ	102	LEU
27	CZ	115	ARG
27	CZ	125	ARG
27	CZ	135	ILE
27	CZ	137	ASN
27	CZ	142	ILE
28	DA	4	GLN
28	DA	13	ARG
28	DA	28	ARG
28	DA	37	LYS
28	DA	45	ILE
28	DA	50	ILE
28	DA	56	VAL
28	DA	67	GLU
28	DA	74	TYR
28	DA	115	ARG
28	DA	125	LYS
29	DB	14	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
29	DB	24	VAL
29	DB	46	ILE
29	DB	81	LEU
29	DB	92	PHE
29	DB	97	SER
29	DB	102	GLU
29	DB	103	GLN
29	DB	132	SER
29	DB	134	LEU
30	DC	7	LYS
30	DC	8	THR
30	DC	10	LYS
30	DC	22	ILE
30	DC	42	ARG
30	DC	46	ASP
30	DC	56	VAL
30	DC	60	TYR
30	DC	85	ASP
30	DC	91	LEU
30	DC	115	LYS
31	DD	5	LYS
31	DD	22	LYS
31	DD	23	LYS
31	DD	25	LYS
31	DD	28	LYS
31	DD	33	LYS
31	DD	59	LYS
32	DE	12	GLN
32	DE	34	LEU
32	DE	41	LEU
32	DE	61	MET
32	DE	83	LYS
32	DE	103	THR
33	DF	8	VAL
33	DF	13	THR
33	DF	16	LEU
33	DF	18	LYS
33	DF	24	SER
33	DF	26	LYS
33	DF	28	ARG
33	DF	31	ARG
33	DF	46	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
33	DF	47	ASP
33	DF	64	VAL
33	DF	76	SER
33	DF	79	ARG
33	DF	86	LYS
33	DF	96	VAL
33	DF	104	LEU
33	DF	106	THR
33	DF	107	VAL
34	DG	4	LEU
34	DG	8	LYS
34	DG	10	VAL
34	DG	19	ARG
34	DG	24	ARG
34	DG	27	ARG
34	DG	33	ARG
34	DG	45	ARG
34	DG	67	SER
34	DG	73	THR
34	DG	75	LEU
34	DG	82	LEU
34	DG	86	THR
34	DG	88	HIS
34	DG	111	ARG
34	DG	125	ARG
35	DH	4	SER
35	DH	21	ARG
35	DH	28	SER
35	DH	59	VAL
35	DH	81	VAL
35	DH	92	LYS
35	DH	98	VAL
36	DI	5	VAL
36	DI	6	THR
36	DI	15	THR
36	DI	29	ILE
36	DI	36	LYS
36	DI	58	ARG
36	DI	60	ARG
36	DI	64	THR
36	DI	65	VAL
36	DI	71	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
36	DI	83	ASN
36	DI	86	LYS
36	DI	102	LYS
37	DJ	11	THR
37	DJ	13	SER
37	DJ	20	GLN
37	DJ	21	LEU
37	DJ	36	LEU
37	DJ	43	LYS
37	DJ	45	LYS
37	DJ	47	VAL
37	DJ	49	LYS
37	DJ	62	GLN
37	DJ	69	LEU
37	DJ	71	LYS
37	DJ	73	LYS
37	DJ	89	ARG
37	DJ	90	ARG
37	DJ	107	LYS
37	DJ	119	LYS
38	DK	12	ASN
38	DK	13	LYS
38	DK	17	VAL
38	DK	21	THR
38	DK	26	ILE
38	DK	30	LYS
38	DK	35	ASN
38	DK	36	ARG
38	DK	43	LEU
38	DK	45	ARG
38	DK	68	ARG
38	DK	76	ARG
38	DK	98	ARG
38	DK	100	HIS
39	DL	12	HIS
39	DL	17	THR
39	DL	25	ARG
39	DL	33	THR
39	DL	36	SER
39	DL	55	ARG
39	DL	64	MET
39	DL	67	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
39	DL	80	THR
40	DM	24	THR
40	DM	32	ASN
40	DM	41	THR
40	DM	45	VAL
40	DM	49	SER
40	DM	53	THR
40	DM	65	LEU
40	DM	77	ARG
41	DN	4	GLN
41	DN	21	ARG
41	DN	51	ILE
42	DO	77	ILE
42	DO	92	ASP
42	DO	112	LYS
42	DO	113	ARG
43	DP	2	ARG
43	DP	4	LYS
43	DP	9	ARG
43	DP	24	SER
44	DQ	7	THR
44	DQ	26	THR
44	DQ	35	LEU
44	DQ	45	ARG
44	DQ	60	LYS
44	DQ	64	THR
44	DQ	71	ARG
44	DQ	83	LEU
44	DQ	84	THR
44	DQ	99	GLN
44	DQ	100	LYS
44	DQ	104	LEU
45	DR	7	LYS
45	DR	11	THR
45	DR	16	VAL
45	DR	25	GLN
45	DR	34	HIS
45	DR	40	SER
45	DR	46	THR
45	DR	54	ILE
45	DR	56	THR
45	DR	62	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
45	DR	70	THR
47	p0	4	ILE
47	p0	5	ARG
47	p0	30	VAL
47	p0	42	ARG
47	p0	48	ARG
47	p0	51	VAL
47	p0	67	LEU
47	p0	69	ASP
47	p0	70	LEU
47	p0	74	GLU
47	p0	76	LEU
47	p0	80	VAL
47	p0	93	LEU
47	p0	97	LYS
47	p0	104	ARG
47	p0	192	ASP
48	sM	30	THR
48	sM	43	ASP
48	sM	49	LYS
48	sM	61	ILE
48	sM	68	ARG
48	sM	77	THR
48	sM	78	ASP
49	B	7	PHE
49	B	50	VAL
49	B	59	LEU
49	B	84	ARG
49	B	87	LEU
49	B	88	LYS
49	B	96	THR
49	B	119	ARG
49	B	170	ILE
49	B	172	LEU
49	B	177	LEU
49	B	185	ARG
49	B	188	LEU
49	B	196	SER
49	B	198	MET
49	B	200	ASP
50	C	21	VAL
50	C	25	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
50	C	29	TRP
50	C	30	PHE
50	C	46	THR
50	C	61	LEU
50	C	70	LEU
50	C	74	GLN
50	C	77	GLU
50	C	78	ASP
50	C	81	PHE
50	C	89	ASP
50	C	97	LEU
50	C	105	PHE
50	C	108	ASP
50	C	176	VAL
50	C	180	THR
50	C	181	LEU
50	C	202	LYS
50	C	215	VAL
50	C	218	LEU
50	C	220	GLN
50	C	222	LYS
50	C	223	PHE
51	D	54	GLU
51	D	58	LEU
51	D	64	LYS
51	D	72	LEU
51	D	76	LEU
51	D	89	GLN
51	D	90	THR
51	D	95	ARG
51	D	97	ARG
51	D	113	LEU
51	D	117	THR
51	D	134	LEU
51	D	137	ILE
51	D	140	ARG
51	D	141	ARG
51	D	148	LEU
51	D	153	SER
51	D	208	GLU
51	D	221	THR
51	D	222	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	D	225	LEU
51	D	226	THR
51	D	235	LEU
51	D	237	VAL
51	D	242	ILE
52	E	4	LEU
52	E	7	LYS
52	E	21	LEU
52	E	23	GLU
52	E	66	ILE
52	E	67	ASN
52	E	76	ARG
52	E	84	ILE
52	E	93	ASP
52	E	103	GLU
52	E	105	MET
52	E	113	LEU
52	E	117	ARG
52	E	124	ARG
52	E	151	LYS
52	E	158	ILE
52	E	172	THR
52	E	175	VAL
52	E	176	LEU
52	E	178	ARG
52	E	182	LEU
52	E	202	LEU
53	F	6	LYS
53	F	7	LYS
53	F	9	LEU
53	F	38	LEU
53	F	54	TYR
53	F	65	LEU
53	F	70	VAL
53	F	77	ARG
53	F	105	VAL
53	F	129	VAL
53	F	131	LEU
53	F	133	LYS
53	F	142	HIS
53	F	146	THR
53	F	160	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	F	176	ASP
53	F	180	LEU
53	F	182	TYR
53	F	187	ARG
53	F	197	HIS
53	F	206	ASP
53	F	215	ASP
53	F	227	VAL
53	F	240	LYS
53	F	242	LYS
53	F	246	LEU
54	G	23	VAL
54	G	25	LEU
54	G	38	THR
54	G	43	PHE
54	G	45	LYS
54	G	65	ARG
54	G	76	ARG
54	G	79	ASN
54	G	94	THR
54	G	112	ARG
54	G	149	VAL
54	G	156	ARG
54	G	194	LEU
54	G	196	GLU
54	G	216	GLU
55	H	6	SER
55	H	7	TYR
55	H	25	ARG
55	H	71	THR
55	H	98	ARG
55	H	125	THR
55	H	126	ASP
55	H	128	THR
55	H	132	ARG
55	H	154	ARG
55	H	155	ASP
55	H	170	THR
55	H	189	HIS
55	H	193	LEU
55	H	211	LEU
55	H	212	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	H	223	LYS
56	I	9	LEU
56	I	28	GLU
56	I	30	SER
56	I	38	LEU
56	I	49	ILE
56	I	50	ASP
56	I	64	VAL
56	I	67	LEU
56	I	85	PHE
56	I	87	ASP
56	I	97	ARG
56	I	114	ARG
56	I	116	ARG
56	I	119	THR
56	I	126	LEU
56	I	133	THR
56	I	147	ASN
56	I	181	ILE
56	I	185	ILE
57	J	7	SER
57	J	8	ARG
57	J	29	LEU
57	J	36	THR
57	J	45	SER
57	J	46	VAL
57	J	48	THR
57	J	58	LEU
57	J	60	ILE
57	J	121	LEU
57	J	137	LYS
57	J	138	ASN
57	J	149	SER
57	J	151	LYS
57	J	152	ILE
57	J	164	ARG
57	J	168	CYS
57	J	196	LEU
58	K	3	ARG
58	K	6	ARG
58	K	7	THR
58	K	21	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
58	K	28	LEU
58	K	49	LEU
58	K	60	LEU
58	K	66	ASP
58	K	78	ARG
58	K	89	ASP
58	K	92	LYS
58	K	93	LEU
58	K	94	ASP
58	K	96	VAL
58	K	97	LEU
58	K	99	LEU
58	K	101	VAL
58	K	126	ARG
58	K	138	LYS
58	K	149	ARG
58	K	157	ASP
58	K	161	THR
58	K	171	ARG
58	K	172	VAL
58	K	174	ARG
58	K	182	GLU
59	L	7	ASP
59	L	20	VAL
59	L	28	ASN
59	L	37	THR
59	L	76	LEU
59	L	81	ASN
60	M	5	LEU
60	M	21	ASN
60	M	37	ASN
60	M	40	LEU
60	M	44	THR
60	M	67	ARG
60	M	80	MET
60	M	83	THR
60	M	105	LYS
61	N	28	LEU
61	N	37	VAL
61	N	43	ARG
61	N	46	ARG
61	N	50	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
61	N	61	VAL
61	N	62	LEU
61	N	66	VAL
61	N	71	ILE
61	N	74	LEU
61	N	85	LYS
61	N	103	LEU
61	N	125	ASN
61	N	126	TRP
61	N	132	GLU
61	N	140	PHE
62	O	3	ARG
62	O	9	LYS
62	O	27	LYS
62	O	39	LYS
62	O	62	GLN
62	O	64	ARG
62	O	102	LEU
62	O	105	ASN
62	O	115	LEU
62	O	125	LEU
62	O	129	TYR
62	O	138	ASN
62	O	149	LEU
63	P	13	VAL
63	P	16	VAL
63	P	26	THR
63	P	29	HIS
63	P	31	THR
63	P	43	THR
63	P	92	LYS
63	P	102	LEU
63	P	114	ARG
63	P	119	THR
63	P	127	ARG
63	P	132	ARG
63	P	136	ARG
63	P	137	LEU
64	Q	11	VAL
64	Q	22	LEU
64	Q	29	SER
64	Q	44	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
64	Q	52	LYS
64	Q	88	GLU
64	Q	92	SER
64	Q	110	GLU
65	R	14	LYS
65	R	19	VAL
65	R	28	LEU
65	R	57	LEU
65	R	66	ARG
65	R	69	VAL
65	R	114	ARG
65	R	116	LEU
65	R	117	LEU
65	R	118	ILE
65	R	121	SER
65	R	123	ARG
65	R	128	LYS
65	R	137	ARG
65	R	141	SER
66	S	5	ARG
66	S	38	ILE
66	S	46	LEU
66	S	54	THR
66	S	62	GLN
66	S	69	ILE
66	S	72	LYS
66	S	78	ARG
66	S	84	TYR
66	S	105	GLN
67	T	3	LEU
67	T	5	VAL
67	T	8	GLN
67	T	11	PHE
67	T	13	HIS
67	T	14	ILE
67	T	15	LEU
67	T	17	LEU
67	T	25	ASN
67	T	28	ILE
67	T	71	GLN
67	T	93	THR
67	T	97	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
67	T	136	GLN
67	T	138	THR
68	U	6	VAL
68	U	18	TYR
68	U	22	LEU
68	U	28	LEU
68	U	35	ASP
68	U	36	ILE
68	U	57	ARG
68	U	64	HIS
68	U	67	MET
68	U	70	GLN
68	U	94	ILE
68	U	95	ASP
68	U	111	ILE
68	U	117	SER
68	U	130	ARG
68	U	131	ASP
68	U	132	LEU
68	U	139	THR
68	U	144	GLU
69	V	27	THR
69	V	31	VAL
69	V	41	ILE
69	V	48	HIS
69	V	51	VAL
69	V	60	THR
69	V	61	LYS
69	V	74	GLU
69	V	81	THR
69	V	103	ILE
69	V	117	VAL
70	W	5	LYS
70	W	10	GLU
70	W	11	LEU
70	W	18	SER
70	W	25	LYS
70	W	68	SER
70	W	69	LEU
70	W	74	GLN
70	W	78	LEU
70	W	80	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
71	X	23	ARG
71	X	24	GLN
71	X	25	VAL
71	X	26	LEU
71	X	53	ILE
71	X	56	HIS
71	X	65	LEU
71	X	86	ILE
71	X	93	LEU
71	X	98	GLN
71	X	103	ILE
71	X	119	LYS
71	X	121	VAL
71	X	126	LEU
72	Y	7	ARG
72	Y	9	LEU
72	Y	16	ARG
72	Y	19	ARG
72	Y	59	ILE
72	Y	72	VAL
72	Y	79	ASN
72	Y	100	ASP
72	Y	107	PHE
72	Y	109	ARG
72	Y	110	LYS
72	Y	114	LYS
72	Y	127	VAL
72	Y	131	SER
72	Y	132	LEU
72	Y	138	GLU
72	Y	144	ARG
73	Z	32	ARG
73	Z	57	VAL
73	Z	62	THR
73	Z	102	LYS
73	Z	104	SER
73	Z	124	ARG
74	a	40	VAL
74	a	42	LEU
74	a	49	ARG
74	a	58	ARG
74	a	60	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
74	a	69	LEU
74	a	70	LYS
74	a	85	LYS
74	a	92	ILE
74	a	95	HIS
74	a	97	LYS
75	b	7	SER
75	b	11	ASN
75	b	12	LYS
75	b	33	ASP
75	b	38	ARG
75	b	41	ILE
75	b	44	ILE
75	b	61	GLU
75	b	64	LEU
75	b	66	LYS
75	b	68	TYR
75	b	74	CYS
75	b	76	SER
75	b	91	ASP
76	c	20	LYS
76	c	33	LEU
76	c	61	THR
76	c	77	THR
77	d	19	THR
77	d	28	VAL
77	d	32	PHE
77	d	35	ASP
77	d	49	ARG
77	d	58	GLU
78	e	8	PHE
78	e	12	ARG
78	e	21	CYS
78	e	30	LEU
78	e	32	ARG
79	f	5	HIS
79	f	17	GLN
79	f	20	LYS
79	f	21	VAL
79	f	28	LYS
79	f	50	VAL
80	g	89	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
80	g	91	ILE
80	g	95	HIS
80	g	97	LYS
80	g	130	VAL
80	g	138	ARG
80	g	147	VAL
81	h	10	ARG
81	h	16	HIS
81	h	50	ASP
81	h	60	SER
81	h	66	HIS
81	h	76	ASP
81	h	106	HIS
81	h	108	SER
81	h	117	LYS
81	h	123	ILE
81	h	136	ILE
81	h	141	LEU
81	h	145	LEU
81	h	193	ILE
81	h	198	ASN
81	h	232	TYR
81	h	238	ASP
81	h	265	LEU
81	h	268	GLN
81	h	300	THR
81	h	308	ASN
81	h	314	GLN
81	h	316	MET
81	h	317	THR
81	h	319	ASN
49	s0	9	LEU
49	s0	12	GLU
49	s0	29	VAL
49	s0	30	GLN
49	s0	41	ARG
49	s0	45	VAL
49	s0	50	VAL
49	s0	59	LEU
49	s0	87	LEU
49	s0	93	THR
49	s0	119	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
49	s0	131	GLN
49	s0	154	GLU
49	s0	157	ASP
49	s0	168	HIS
49	s0	172	LEU
49	s0	179	ARG
49	s0	185	ARG
49	s0	188	LEU
49	s0	191	ARG
49	s0	198	MET
50	s1	21	VAL
50	s1	40	ASN
50	s1	47	LEU
50	s1	51	SER
50	s1	70	LEU
50	s1	73	LEU
50	s1	79	HIS
50	s1	81	PHE
50	s1	96	LEU
50	s1	105	PHE
50	s1	110	LEU
50	s1	122	GLU
50	s1	126	THR
50	s1	131	ASP
50	s1	152	ARG
50	s1	153	HIS
50	s1	173	THR
50	s1	180	THR
50	s1	181	LEU
50	s1	193	ILE
50	s1	203	ASP
50	s1	212	VAL
50	s1	223	PHE
50	s1	225	VAL
50	s1	231	LEU
50	s1	234	GLU
51	s2	53	ILE
51	s2	55	GLU
51	s2	58	LEU
51	s2	82	ASN
51	s2	86	VAL
51	s2	91	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
51	s2	94	GLN
51	s2	95	ARG
51	s2	97	ARG
51	s2	102	VAL
51	s2	106	ASP
51	s2	111	VAL
51	s2	113	LEU
51	s2	117	THR
51	s2	139	ILE
51	s2	141	ARG
51	s2	148	LEU
51	s2	150	GLN
51	s2	159	THR
51	s2	164	SER
51	s2	166	THR
51	s2	170	ILE
51	s2	185	LYS
51	s2	205	ARG
51	s2	207	LEU
51	s2	222	TYR
51	s2	225	LEU
51	s2	237	VAL
51	s2	238	SER
51	s2	246	GLU
52	s3	21	LEU
52	s3	37	VAL
52	s3	40	ARG
52	s3	57	ASP
52	s3	66	ILE
52	s3	84	ILE
52	s3	90	ARG
52	s3	115	ILE
52	s3	120	TYR
52	s3	125	TYR
52	s3	158	ILE
52	s3	162	GLN
52	s3	168	ILE
52	s3	169	ASP
52	s3	181	VAL
53	s4	9	LEU
53	s4	12	LEU
53	s4	21	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
53	s4	30	ARG
53	s4	32	SER
53	s4	38	LEU
53	s4	42	LEU
53	s4	49	ARG
53	s4	51	ARG
53	s4	65	LEU
53	s4	67	GLN
53	s4	104	ASP
53	s4	116	ASP
53	s4	131	LEU
53	s4	148	ARG
53	s4	163	ASP
53	s4	164	LEU
53	s4	170	THR
53	s4	176	ASP
53	s4	180	LEU
53	s4	181	VAL
53	s4	182	TYR
53	s4	191	ARG
53	s4	216	ASN
53	s4	227	VAL
54	s5	25	LEU
54	s5	38	THR
54	s5	41	LYS
54	s5	63	GLN
54	s5	68	ILE
54	s5	76	ARG
54	s5	83	ARG
54	s5	93	LEU
54	s5	119	ASP
54	s5	125	THR
54	s5	126	ASP
54	s5	146	THR
54	s5	194	LEU
54	s5	203	LYS
54	s5	216	GLU
55	s6	9	VAL
55	s6	68	LEU
55	s6	71	THR
55	s6	76	LEU
55	s6	78	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
55	s6	97	VAL
55	s6	98	ARG
55	s6	108	VAL
55	s6	109	LEU
55	s6	112	VAL
55	s6	115	LYS
55	s6	120	GLU
55	s6	121	LEU
55	s6	126	ASP
55	s6	128	THR
55	s6	143	LYS
55	s6	151	ASP
55	s6	153	VAL
55	s6	155	ASP
55	s6	177	ARG
55	s6	193	LEU
55	s6	212	LEU
55	s6	215	ARG
55	s6	216	LEU
56	s7	30	SER
56	s7	33	GLU
56	s7	114	ARG
56	s7	116	ARG
56	s7	117	THR
56	s7	123	ASP
56	s7	143	LEU
56	s7	144	VAL
56	s7	159	VAL
56	s7	185	ILE
57	s8	9	HIS
57	s8	29	LEU
57	s8	36	THR
57	s8	52	ASN
57	s8	74	LYS
57	s8	120	THR
57	s8	138	ASN
57	s8	151	LYS
57	s8	153	GLU
57	s8	155	SER
57	s8	168	CYS
57	s8	179	CYS
57	s8	180	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
57	s8	183	ILE
57	s8	184	LEU
58	s9	3	ARG
58	s9	6	ARG
58	s9	16	LYS
58	s9	25	ASP
58	s9	28	LEU
58	s9	39	LYS
58	s9	54	ARG
58	s9	89	ASP
58	s9	93	LEU
58	s9	96	VAL
58	s9	101	VAL
58	s9	126	ARG
58	s9	130	THR
58	s9	132	ARG
58	s9	134	ILE
58	s9	161	THR
58	s9	168	ARG
58	s9	172	VAL
58	s9	180	LYS
58	s9	182	GLU
59	c0	15	LEU
59	c0	26	ASP
59	c0	55	VAL
59	c0	57	THR
60	c1	4	GLU
60	c1	5	LEU
60	c1	6	THR
60	c1	10	GLU
60	c1	32	LYS
60	c1	40	LEU
60	c1	44	THR
60	c1	56	LYS
60	c1	60	PHE
60	c1	67	ARG
60	c1	71	LEU
60	c1	74	THR
60	c1	83	THR
60	c1	94	ILE
60	c1	104	HIS
60	c1	109	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
60	c1	129	ARG
60	c1	136	ARG
61	c2	28	LEU
61	c2	45	LEU
61	c2	52	LEU
61	c2	54	ARG
61	c2	58	LEU
61	c2	59	LEU
61	c2	61	VAL
61	c2	71	ILE
61	c2	81	ASP
61	c2	83	GLU
61	c2	89	ILE
61	c2	103	LEU
61	c2	131	ASP
61	c2	132	GLU
61	c2	137	MET
61	c2	140	PHE
62	c3	6	SER
62	c3	23	PRO
62	c3	30	SER
62	c3	60	VAL
62	c3	64	ARG
62	c3	66	ILE
62	c3	70	LYS
62	c3	87	ASP
62	c3	93	LYS
62	c3	102	LEU
62	c3	125	LEU
62	c3	138	ASN
62	c3	139	TRP
62	c3	143	SER
63	c4	13	VAL
63	c4	26	THR
63	c4	31	THR
63	c4	79	VAL
63	c4	90	ARG
63	c4	107	ARG
63	c4	118	VAL
63	c4	119	THR
63	c4	124	ASP
63	c4	133	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
63	c4	136	ARG
64	c5	10	ARG
64	c5	12	PHE
64	c5	27	GLU
64	c5	36	LEU
64	c5	52	LYS
64	c5	65	LEU
64	c5	69	GLU
64	c5	110	GLU
64	c5	111	MET
64	c5	127	ARG
64	c5	130	ARG
65	c6	17	THR
65	c6	23	LYS
65	c6	26	LYS
65	c6	28	LEU
65	c6	30	LYS
65	c6	43	ILE
65	c6	53	LEU
65	c6	54	LEU
65	c6	57	LEU
65	c6	63	ILE
65	c6	68	ARG
65	c6	69	VAL
65	c6	114	ARG
65	c6	117	LEU
65	c6	127	LYS
65	c6	128	LYS
65	c6	137	ARG
65	c6	143	ARG
82	c7	25	THR
82	c7	29	GLN
82	c7	34	LEU
82	c7	46	LEU
82	c7	55	THR
82	c7	69	ILE
82	c7	72	LYS
82	c7	82	ASP
82	c7	85	VAL
82	c7	105	GLN
82	c7	108	ASP
82	c7	113	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
67	c8	3	LEU
67	c8	5	VAL
67	c8	12	GLN
67	c8	15	LEU
67	c8	25	ASN
67	c8	28	ILE
67	c8	85	PHE
67	c8	94	ASP
67	c8	112	ASP
67	c8	138	THR
67	c8	143	ARG
68	c9	6	VAL
68	c9	28	LEU
68	c9	29	GLU
68	c9	33	TYR
68	c9	68	ARG
68	c9	124	ILE
68	c9	134	ARG
68	c9	140	LEU
68	c9	141	GLU
69	d0	18	GLN
69	d0	23	ARG
69	d0	27	THR
69	d0	60	THR
69	d0	67	THR
69	d0	70	THR
69	d0	103	ILE
69	d0	107	THR
69	d0	108	ILE
70	d1	2	GLU
70	d1	5	LYS
70	d1	11	LEU
70	d1	25	LYS
70	d1	31	SER
70	d1	32	VAL
70	d1	44	ARG
70	d1	81	ASN
71	d2	7	LEU
71	d2	12	ASN
71	d2	15	ASN
71	d2	23	ARG
71	d2	25	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
71	d2	26	LEU
71	d2	41	MET
71	d2	93	LEU
71	d2	103	ILE
71	d2	107	SER
72	d3	9	LEU
72	d3	16	ARG
72	d3	23	ARG
72	d3	40	SER
72	d3	73	ARG
72	d3	84	THR
72	d3	100	ASP
72	d3	103	LEU
72	d3	107	PHE
72	d3	121	ARG
72	d3	127	VAL
72	d3	133	LEU
73	d4	5	VAL
73	d4	26	ASP
73	d4	43	LYS
73	d4	49	LYS
73	d4	52	LYS
73	d4	58	PHE
73	d4	62	THR
73	d4	88	THR
73	d4	105	ARG
73	d4	114	ARG
74	d5	48	ASP
74	d5	51	LEU
74	d5	57	TYR
74	d5	103	ARG
75	d6	10	ARG
75	d6	12	LYS
75	d6	25	ASN
75	d6	29	SER
75	d6	55	GLU
75	d6	61	GLU
75	d6	82	ARG
75	d6	85	ARG
75	d6	90	GLU
75	d6	91	ASP
76	d7	3	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
76	d7	4	VAL
76	d7	34	ASP
76	d7	43	ILE
76	d7	49	HIS
76	d7	67	THR
76	d7	77	THR
77	d8	22	ARG
77	d8	32	PHE
77	d8	33	LEU
77	d8	36	THR
77	d8	39	THR
77	d8	40	ILE
77	d8	66	LEU
78	d9	6	VAL
78	d9	10	HIS
78	d9	30	LEU
78	d9	32	ARG
78	d9	36	LEU
78	d9	39	CYS
78	d9	54	LYS
79	e0	4	VAL
79	e0	13	LYS
79	e0	22	GLU
79	e0	26	LYS
79	e0	29	LYS
79	e0	36	LYS
79	e0	38	LEU
79	e0	39	LEU
79	e0	44	PHE
79	e0	46	ASN
79	e0	48	THR
79	e0	49	LEU
79	e0	54	ARG
83	e1	103	LEU
83	e1	113	LYS
83	e1	118	ARG
83	e1	119	ARG
83	e1	135	HIS
83	e1	137	ASP
83	e1	147	VAL
83	e1	148	TYR
83	e1	150	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
81	sR	16	HIS
81	sR	21	THR
81	sR	25	THR
81	sR	58	VAL
81	sR	64	HIS
81	sR	66	HIS
81	sR	76	ASP
81	sR	96	THR
81	sR	106	HIS
81	sR	145	LEU
81	sR	149	ASP
81	sR	159	ASN
81	sR	188	ILE
81	sR	228	LYS
81	sR	238	ASP
81	sR	245	PHE
81	sR	275	ARG
81	sR	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	j	216	HIS
6	l	110	ASN
6	l	291	ASN
6	l	296	GLN
7	m	40	HIS
8	n	61	ASN
11	q	50	ASN
13	s	109	HIS
15	u	56	GLN
16	v	87	GLN
18	x	10	ASN
21	0	157	GLN
44	AP	82	GLN
6	CF	316	ASN
6	CF	320	ASN
7	CG	40	HIS
7	CG	111	GLN
10	CJ	59	GLN
10	CJ	192	GLN
16	CP	138	GLN

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Mol	Chain	Res	Type
20	CT	92	GLN
21	CU	114	HIS
29	DB	36	HIS
29	DB	57	HIS
32	DE	47	ASN
37	DJ	59	ASN
41	DN	33	ASN
45	DR	33	GLN
45	DR	34	HIS
62	O	101	HIS
65	R	74	HIS
74	a	95	HIS
81	h	52	GLN
53	s4	142	HIS
56	s7	71	HIS
56	s7	150	GLN
59	c0	32	HIS
62	c3	5	HIS
64	c5	103	ASN
65	c6	103	ASN
82	c7	104	ASN
67	c8	25	ASN
67	c8	89	GLN
71	d2	15	ASN
72	d3	28	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3145/3396 (92%)	563 (17%)	51 (1%)
1	AR	3145/3396 (92%)	581 (18%)	51 (1%)
2	3	120/121 (99%)	16 (13%)	0
2	AS	120/121 (99%)	15 (12%)	2 (1%)
25	6	1780/1800 (98%)	383 (21%)	30 (1%)
25	A	1778/1800 (98%)	409 (23%)	47 (2%)
3	4	157/158 (99%)	32 (20%)	2 (1%)
3	AT	157/158 (99%)	28 (17%)	3 (1%)
All	All	10402/10950 (94%)	2027 (19%)	186 (1%)

All (2027) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	26	A
1	1	40	A
1	1	49	A
1	1	57	A
1	1	59	G
1	1	60	A
1	1	65	A
1	1	66	A
1	1	73	C
1	1	83	U
1	1	85	A
1	1	93	C
1	1	99	A
1	1	103	G
1	1	109	A
1	1	110	G
1	1	111	C
1	1	116	A
1	1	121	A
1	1	122	A
1	1	133	U
1	1	135	C
1	1	136	G
1	1	156	G
1	1	157	A
1	1	166	C
1	1	170	G
1	1	187	A
1	1	190	U
1	1	191	U
1	1	192	C
1	1	200	C
1	1	206	G
1	1	210	U
1	1	213	A
1	1	218	G
1	1	219	A
1	1	237	G
1	1	240	U
1	1	241	G
1	1	243	G
1	1	249	U
1	1	250	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	251	G
1	1	252	U
1	1	253	A
1	1	266	A
1	1	269	G
1	1	282	G
1	1	283	G
1	1	286	U
1	1	295	A
1	1	298	U
1	1	311	C
1	1	315	C
1	1	323	A
1	1	329	U
1	1	338	A
1	1	339	C
1	1	349	A
1	1	350	C
1	1	373	A
1	1	374	A
1	1	376	G
1	1	393	U
1	1	398	A
1	1	399	A
1	1	401	U
1	1	402	A
1	1	403	C
1	1	404	G
1	1	412	G
1	1	421	G
1	1	422	A
1	1	438	A
1	1	440	A
1	1	495	G
1	1	498	A
1	1	520	U
1	1	521	A
1	1	523	A
1	1	531	G
1	1	535	G
1	1	536	U
1	1	546	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	547	G
1	1	548	G
1	1	552	G
1	1	555	U
1	1	557	A
1	1	559	A
1	1	578	A
1	1	579	G
1	1	589	A
1	1	590	G
1	1	592	A
1	1	604	G
1	1	609	G
1	1	611	A
1	1	620	U
1	1	621	A
1	1	636	C
1	1	649	A
1	1	660	A
1	1	677	A
1	1	681	U
1	1	684	G
1	1	691	A
1	1	705	A
1	1	709	A
1	1	712	G
1	1	715	A
1	1	716	A
1	1	727	G
1	1	764	U
1	1	766	U
1	1	767	U
1	1	776	U
1	1	777	U
1	1	781	G
1	1	785	G
1	1	806	A
1	1	817	A
1	1	830	A
1	1	849	C
1	1	861	C
1	1	874	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	879	U
1	1	890	C
1	1	896	A
1	1	907	G
1	1	908	G
1	1	909	G
1	1	914	A
1	1	916	G
1	1	917	A
1	1	921	A
1	1	923	C
1	1	924	G
1	1	937	G
1	1	943	U
1	1	944	C
1	1	959	C
1	1	960	U
1	1	974	G
1	1	979	U
1	1	980	A
1	1	981	U
1	1	982	C
1	1	993	G
1	1	994	G
1	1	1001	G
1	1	1002	A
1	1	1006	A
1	1	1010	G
1	1	1017	C
1	1	1018	G
1	1	1020	G
1	1	1024	G
1	1	1025	A
1	1	1029	G
1	1	1036	A
1	1	1037	C
1	1	1041	U
1	1	1047	A
1	1	1049	C
1	1	1064	A
1	1	1065	A
1	1	1072	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	1081	U
1	1	1087	G
1	1	1093	A
1	1	1094	U
1	1	1095	U
1	1	1097	G
1	1	1098	A
1	1	1103	A
1	1	1104	G
1	1	1117	G
1	1	1131	G
1	1	1153	A
1	1	1159	A
1	1	1160	C
1	1	1180	A
1	1	1181	U
1	1	1186	G
1	1	1191	U
1	1	1192	C
1	1	1201	C
1	1	1205	A
1	1	1209	G
1	1	1216	C
1	1	1217	A
1	1	1222	G
1	1	1227	C
1	1	1232	C
1	1	1235	U
1	1	1236	G
1	1	1237	G
1	1	1241	U
1	1	1243	G
1	1	1245	A
1	1	1246	G
1	1	1248	C
1	1	1249	G
1	1	1258	U
1	1	1262	G
1	1	1263	A
1	1	1264	G
1	1	1269	U
1	1	1270	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	1271	A
1	1	1274	A
1	1	1278	A
1	1	1279	C
1	1	1285	G
1	1	1286	A
1	1	1287	A
1	1	1308	A
1	1	1309	U
1	1	1313	G
1	1	1318	A
1	1	1330	A
1	1	1348	U
1	1	1349	G
1	1	1351	U
1	1	1352	A
1	1	1353	U
1	1	1355	A
1	1	1356	U
1	1	1357	G
1	1	1386	A
1	1	1391	C
1	1	1392	G
1	1	1399	A
1	1	1400	G
1	1	1417	G
1	1	1418	A
1	1	1419	A
1	1	1421	G
1	1	1431	G
1	1	1433	A
1	1	1434	G
1	1	1437	C
1	1	1446	A
1	1	1481	A
1	1	1482	A
1	1	1493	G
1	1	1508	C
1	1	1527	C
1	1	1528	G
1	1	1555	U
1	1	1556	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	1560	G
1	1	1561	G
1	1	1562	C
1	1	1563	C
1	1	1567	U
1	1	1568	U
1	1	1569	U
1	1	1570	U
1	1	1576	G
1	1	1580	A
1	1	1583	A
1	1	1587	A
1	1	1589	A
1	1	1593	A
1	1	1605	A
1	1	1607	U
1	1	1620	U
1	1	1629	U
1	1	1639	C
1	1	1643	A
1	1	1657	C
1	1	1658	G
1	1	1683	A
1	1	1716	U
1	1	1717	U
1	1	1724	U
1	1	1725	C
1	1	1736	G
1	1	1741	A
1	1	1742	U
1	1	1746	U
1	1	1750	A
1	1	1751	G
1	1	1760	A
1	1	1762	C
1	1	1765	U
1	1	1766	G
1	1	1769	G
1	1	1770	G
1	1	1780	G
1	1	1795	U
1	1	1797	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	1814	A
1	1	1815	U
1	1	1816	A
1	1	1817	G
1	1	1819	U
1	1	1820	U
1	1	1821	U
1	1	1835	A
1	1	1839	A
1	1	1841	A
1	1	1842	A
1	1	1846	C
1	1	1849	C
1	1	1850	A
1	1	1858	A
1	1	1866	C
1	1	1879	A
1	1	1880	U
1	1	1886	A
1	1	1901	A
1	1	1906	G
1	1	1927	G
1	1	1951	C
1	1	1952	G
1	1	1953	G
1	1	1954	G
1	1	2094	C
1	1	2101	C
1	1	2102	U
1	1	2111	G
1	1	2113	A
1	1	2114	C
1	1	2121	G
1	1	2122	G
1	1	2131	A
1	1	2139	A
1	1	2140	U
1	1	2144	A
1	1	2149	A
1	1	2158	A
1	1	2169	G
1	1	2187	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	2188	A
1	1	2205	U
1	1	2208	A
1	1	2210	G
1	1	2223	A
1	1	2228	A
1	1	2244	A
1	1	2246	G
1	1	2249	G
1	1	2250	G
1	1	2255	A
1	1	2256	A
1	1	2272	G
1	1	2273	G
1	1	2281	A
1	1	2282	U
1	1	2288	G
1	1	2307	G
1	1	2310	U
1	1	2313	A
1	1	2314	U
1	1	2315	G
1	1	2334	U
1	1	2336	U
1	1	2345	A
1	1	2365	C
1	1	2372	A
1	1	2373	A
1	1	2374	C
1	1	2375	G
1	1	2383	C
1	1	2385	G
1	1	2388	U
1	1	2393	G
1	1	2397	A
1	1	2402	A
1	1	2403	G
1	1	2404	A
1	1	2411	U
1	1	2418	G
1	1	2419	A
1	1	2422	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	2435	G
1	1	2444	C
1	1	2445	A
1	1	2502	A
1	1	2503	G
1	1	2514	U
1	1	2515	A
1	1	2522	G
1	1	2523	A
1	1	2526	C
1	1	2532	U
1	1	2533	G
1	1	2537	U
1	1	2538	U
1	1	2539	C
1	1	2540	A
1	1	2541	U
1	1	2542	U
1	1	2543	U
1	1	2544	U
1	1	2547	A
1	1	2548	C
1	1	2549	G
1	1	2552	C
1	1	2555	G
1	1	2560	C
1	1	2561	A
1	1	2568	C
1	1	2569	A
1	1	2570	U
1	1	2571	U
1	1	2572	C
1	1	2573	G
1	1	2581	U
1	1	2585	G
1	1	2593	A
1	1	2594	C
1	1	2606	G
1	1	2607	G
1	1	2609	A
1	1	2614	G
1	1	2615	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	2638	C
1	1	2652	U
1	1	2656	A
1	1	2657	A
1	1	2658	G
1	1	2674	A
1	1	2677	G
1	1	2689	A
1	1	2690	G
1	1	2691	A
1	1	2694	A
1	1	2696	A
1	1	2714	G
1	1	2719	U
1	1	2728	G
1	1	2729	U
1	1	2737	C
1	1	2752	U
1	1	2753	G
1	1	2772	C
1	1	2777	G
1	1	2778	G
1	1	2780	A
1	1	2787	G
1	1	2796	G
1	1	2800	G
1	1	2801	A
1	1	2802	A
1	1	2803	A
1	1	2810	C
1	1	2814	G
1	1	2817	A
1	1	2818	U
1	1	2842	U
1	1	2843	U
1	1	2845	A
1	1	2853	A
1	1	2860	U
1	1	2867	C
1	1	2871	G
1	1	2872	A
1	1	2876	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	2887	A
1	1	2889	C
1	1	2899	C
1	1	2923	U
1	1	2935	U
1	1	2936	A
1	1	2942	C
1	1	2945	G
1	1	2947	G
1	1	2954	U
1	1	2955	U
1	1	2971	A
1	1	2979	U
1	1	2983	C
1	1	2990	G
1	1	2996	U
1	1	2997	G
1	1	3012	A
1	1	3028	G
1	1	3030	G
1	1	3059	G
1	1	3074	G
1	1	3078	U
1	1	3079	U
1	1	3080	G
1	1	3086	A
1	1	3092	C
1	1	3104	U
1	1	3113	A
1	1	3119	U
1	1	3122	A
1	1	3128	G
1	1	3130	A
1	1	3131	U
1	1	3142	A
1	1	3143	C
1	1	3151	U
1	1	3153	U
1	1	3154	C
1	1	3155	U
1	1	3156	U
1	1	3157	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	3164	C
1	1	3165	A
1	1	3168	A
1	1	3170	A
1	1	3171	U
1	1	3173	G
1	1	3174	A
1	1	3176	G
1	1	3180	A
1	1	3181	C
1	1	3187	A
1	1	3196	U
1	1	3198	U
1	1	3207	U
1	1	3210	A
1	1	3217	C
1	1	3218	A
1	1	3219	G
1	1	3229	G
1	1	3243	A
1	1	3245	A
1	1	3247	G
1	1	3259	U
1	1	3262	U
1	1	3269	U
1	1	3270	U
1	1	3272	C
1	1	3273	A
1	1	3276	G
1	1	3277	U
1	1	3281	U
1	1	3286	G
1	1	3287	U
1	1	3288	G
1	1	3289	G
1	1	3294	A
1	1	3304	U
1	1	3313	U
1	1	3316	A
1	1	3318	G
1	1	3319	U
1	1	3320	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	3341	U
1	1	3345	G
1	1	3347	A
1	1	3351	U
1	1	3352	U
1	1	3353	G
1	1	3354	U
1	1	3355	U
1	1	3369	G
1	1	3370	A
1	1	3375	A
1	1	3378	C
1	1	3383	G
1	1	3389	U
1	1	3390	G
1	1	3396	U
2	3	7	G
2	3	13	A
2	3	22	A
2	3	23	A
2	3	41	G
2	3	42	A
2	3	54	U
2	3	55	A
2	3	65	G
2	3	74	C
2	3	76	A
2	3	78	U
2	3	91	G
2	3	102	A
2	3	112	G
2	3	121	U
3	4	2	A
3	4	16	G
3	4	34	U
3	4	35	C
3	4	48	A
3	4	53	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	4	81	U
3	4	82	U
3	4	83	C
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	102	U
3	4	104	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	128	U
3	4	138	A
3	4	148	G
3	4	152	G
3	4	155	A
3	4	158	U
25	6	2	A
25	6	4	C
25	6	17	C
25	6	25	C
25	6	26	A
25	6	27	U
25	6	34	G
25	6	45	U
25	6	47	A
25	6	50	C
25	6	57	G
25	6	60	U
25	6	61	A
25	6	63	G
25	6	68	A
25	6	73	U
25	6	75	U
25	6	76	A
25	6	77	U
25	6	78	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	104	A
25	6	114	C
25	6	126	A
25	6	132	U
25	6	137	U
25	6	138	A
25	6	140	A
25	6	141	U
25	6	144	U
25	6	145	A
25	6	146	U
25	6	153	G
25	6	159	U
25	6	166	C
25	6	178	U
25	6	188	A
25	6	191	C
25	6	192	U
25	6	193	U
25	6	195	G
25	6	196	G
25	6	197	A
25	6	200	A
25	6	215	A
25	6	216	U
25	6	218	A
25	6	219	A
25	6	220	A
25	6	227	U
25	6	228	G
25	6	230	C
25	6	232	U
25	6	233	C
25	6	240	U
25	6	241	U
25	6	250	C
25	6	260	U
25	6	261	U
25	6	265	A
25	6	271	A
25	6	272	U
25	6	273	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	278	U
25	6	280	U
25	6	299	A
25	6	302	U
25	6	308	C
25	6	314	C
25	6	316	A
25	6	319	U
25	6	320	U
25	6	321	C
25	6	322	G
25	6	337	G
25	6	338	C
25	6	352	A
25	6	359	A
25	6	360	A
25	6	361	C
25	6	393	C
25	6	400	A
25	6	401	A
25	6	402	C
25	6	404	G
25	6	416	A
25	6	418	G
25	6	419	G
25	6	423	G
25	6	424	C
25	6	425	A
25	6	426	G
25	6	428	A
25	6	434	G
25	6	437	A
25	6	439	U
25	6	444	C
25	6	445	A
25	6	448	C
25	6	454	U
25	6	468	A
25	6	469	C
25	6	475	A
25	6	486	G
25	6	487	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	488	G
25	6	489	C
25	6	490	C
25	6	492	A
25	6	493	U
25	6	496	G
25	6	497	G
25	6	500	C
25	6	501	U
25	6	504	U
25	6	505	A
25	6	506	A
25	6	507	U
25	6	510	G
25	6	511	A
25	6	513	U
25	6	516	G
25	6	519	C
25	6	527	A
25	6	535	A
25	6	538	A
25	6	539	G
25	6	540	G
25	6	541	A
25	6	542	A
25	6	543	C
25	6	548	G
25	6	554	C
25	6	556	A
25	6	557	G
25	6	558	U
25	6	559	C
25	6	565	C
25	6	570	A
25	6	574	G
25	6	578	U
25	6	580	A
25	6	582	U
25	6	594	A
25	6	595	G
25	6	597	G
25	6	606	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	610	G
25	6	611	U
25	6	619	A
25	6	620	A
25	6	621	A
25	6	622	A
25	6	623	A
25	6	624	G
25	6	640	U
25	6	650	U
25	6	652	G
25	6	653	C
25	6	658	C
25	6	676	G
25	6	679	U
25	6	680	U
25	6	681	U
25	6	682	C
25	6	683	C
25	6	684	A
25	6	685	A
25	6	691	C
25	6	696	C
25	6	710	U
25	6	711	U
25	6	718	U
25	6	719	U
25	6	720	G
25	6	721	U
25	6	722	G
25	6	723	G
25	6	730	G
25	6	742	U
25	6	743	U
25	6	745	U
25	6	754	A
25	6	755	A
25	6	756	A
25	6	765	G
25	6	766	U
25	6	771	A
25	6	774	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	775	G
25	6	780	A
25	6	781	U
25	6	782	U
25	6	783	G
25	6	787	G
25	6	789	A
25	6	793	A
25	6	794	U
25	6	811	A
25	6	812	A
25	6	814	A
25	6	815	G
25	6	821	U
25	6	823	G
25	6	825	U
25	6	826	U
25	6	829	A
25	6	830	U
25	6	831	U
25	6	832	U
25	6	834	G
25	6	835	U
25	6	856	A
25	6	862	A
25	6	863	A
25	6	864	U
25	6	873	U
25	6	886	U
25	6	898	A
25	6	906	A
25	6	912	U
25	6	913	G
25	6	914	G
25	6	933	A
25	6	935	U
25	6	942	G
25	6	945	U
25	6	959	U
25	6	960	U
25	6	966	A
25	6	969	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	971	A
25	6	992	A
25	6	993	A
25	6	1003	A
25	6	1004	U
25	6	1005	A
25	6	1021	C
25	6	1026	A
25	6	1028	C
25	6	1029	U
25	6	1039	A
25	6	1040	G
25	6	1052	U
25	6	1053	G
25	6	1057	U
25	6	1058	U
25	6	1059	U
25	6	1060	U
25	6	1061	A
25	6	1072	C
25	6	1073	G
25	6	1075	C
25	6	1082	C
25	6	1092	A
25	6	1096	C
25	6	1097	U
25	6	1098	U
25	6	1100	G
25	6	1101	G
25	6	1138	A
25	6	1140	G
25	6	1155	G
25	6	1158	C
25	6	1159	C
25	6	1160	A
25	6	1167	G
25	6	1185	U
25	6	1186	U
25	6	1194	A
25	6	1196	A
25	6	1199	G
25	6	1200	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	1202	A
25	6	1217	A
25	6	1218	G
25	6	1220	C
25	6	1228	G
25	6	1229	G
25	6	1230	A
25	6	1231	U
25	6	1241	G
25	6	1243	G
25	6	1245	G
25	6	1246	C
25	6	1255	G
25	6	1256	A
25	6	1257	U
25	6	1258	U
25	6	1275	A
25	6	1286	U
25	6	1291	G
25	6	1306	C
25	6	1314	U
25	6	1315	U
25	6	1316	G
25	6	1321	A
25	6	1341	A
25	6	1344	A
25	6	1345	A
25	6	1346	A
25	6	1354	G
25	6	1361	U
25	6	1363	U
25	6	1364	G
25	6	1367	G
25	6	1371	A
25	6	1372	U
25	6	1383	G
25	6	1388	A
25	6	1390	U
25	6	1398	U
25	6	1400	A
25	6	1402	G
25	6	1413	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	1414	U
25	6	1415	U
25	6	1427	A
25	6	1428	G
25	6	1429	G
25	6	1445	G
25	6	1446	A
25	6	1448	G
25	6	1458	G
25	6	1459	C
25	6	1461	C
25	6	1471	A
25	6	1482	C
25	6	1490	C
25	6	1491	U
25	6	1492	A
25	6	1493	A
25	6	1506	G
25	6	1514	U
25	6	1516	A
25	6	1521	G
25	6	1523	G
25	6	1524	A
25	6	1535	U
25	6	1536	G
25	6	1537	C
25	6	1538	U
25	6	1540	G
25	6	1554	U
25	6	1557	U
25	6	1559	A
25	6	1569	A
25	6	1573	A
25	6	1574	G
25	6	1575	G
25	6	1584	G
25	6	1601	G
25	6	1603	U
25	6	1616	G
25	6	1621	U
25	6	1634	C
25	6	1657	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	1658	G
25	6	1696	G
25	6	1698	G
25	6	1699	G
25	6	1700	C
25	6	1701	A
25	6	1702	A
25	6	1703	C
25	6	1712	A
25	6	1713	G
25	6	1717	G
25	6	1731	A
25	6	1742	U
25	6	1760	G
25	6	1762	A
25	6	1766	A
25	6	1767	G
25	6	1769	U
25	6	1780	G
25	6	1782	A
25	6	1783	C
25	6	1792	G
25	6	1793	G
25	6	1794	A
25	6	1796	C
25	6	1799	U
25	6	1800	A
1	AR	26	A
1	AR	40	A
1	AR	43	A
1	AR	49	A
1	AR	57	A
1	AR	59	G
1	AR	60	A
1	AR	65	A
1	AR	66	A
1	AR	76	G
1	AR	92	G
1	AR	93	C
1	AR	99	A
1	AR	109	A
1	AR	110	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	116	A
1	AR	120	G
1	AR	121	A
1	AR	122	A
1	AR	133	U
1	AR	135	C
1	AR	136	G
1	AR	156	G
1	AR	157	A
1	AR	165	A
1	AR	166	C
1	AR	172	G
1	AR	173	G
1	AR	182	U
1	AR	187	A
1	AR	190	U
1	AR	191	U
1	AR	192	C
1	AR	200	C
1	AR	210	U
1	AR	211	A
1	AR	213	A
1	AR	218	G
1	AR	219	A
1	AR	224	C
1	AR	231	G
1	AR	234	G
1	AR	240	U
1	AR	241	G
1	AR	243	G
1	AR	245	U
1	AR	249	U
1	AR	250	U
1	AR	251	G
1	AR	252	U
1	AR	253	A
1	AR	269	G
1	AR	286	U
1	AR	295	A
1	AR	298	U
1	AR	315	C
1	AR	316	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	323	A
1	AR	329	U
1	AR	339	C
1	AR	349	A
1	AR	350	C
1	AR	351	A
1	AR	370	U
1	AR	376	G
1	AR	390	G
1	AR	398	A
1	AR	399	A
1	AR	401	U
1	AR	402	A
1	AR	403	C
1	AR	404	G
1	AR	421	G
1	AR	422	A
1	AR	436	A
1	AR	439	C
1	AR	440	A
1	AR	495	G
1	AR	503	C
1	AR	516	A
1	AR	520	U
1	AR	521	A
1	AR	523	A
1	AR	535	G
1	AR	543	C
1	AR	544	C
1	AR	546	C
1	AR	549	U
1	AR	551	A
1	AR	552	G
1	AR	555	U
1	AR	557	A
1	AR	559	A
1	AR	578	A
1	AR	579	G
1	AR	588	G
1	AR	589	A
1	AR	592	A
1	AR	600	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	604	G
1	AR	609	G
1	AR	611	A
1	AR	612	U
1	AR	620	U
1	AR	621	A
1	AR	623	U
1	AR	637	C
1	AR	638	C
1	AR	649	A
1	AR	660	A
1	AR	677	A
1	AR	681	U
1	AR	683	U
1	AR	691	A
1	AR	705	A
1	AR	712	G
1	AR	715	A
1	AR	716	A
1	AR	726	G
1	AR	727	G
1	AR	764	U
1	AR	766	U
1	AR	767	U
1	AR	776	U
1	AR	777	U
1	AR	780	A
1	AR	781	G
1	AR	785	G
1	AR	799	G
1	AR	800	G
1	AR	806	A
1	AR	816	A
1	AR	817	A
1	AR	830	A
1	AR	849	C
1	AR	861	C
1	AR	869	G
1	AR	874	U
1	AR	879	U
1	AR	890	C
1	AR	894	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	896	A
1	AR	907	G
1	AR	908	G
1	AR	910	G
1	AR	914	A
1	AR	916	G
1	AR	917	A
1	AR	921	A
1	AR	923	C
1	AR	937	G
1	AR	944	C
1	AR	959	C
1	AR	960	U
1	AR	964	G
1	AR	974	G
1	AR	979	U
1	AR	980	A
1	AR	981	U
1	AR	982	C
1	AR	994	G
1	AR	1000	C
1	AR	1002	A
1	AR	1006	A
1	AR	1010	G
1	AR	1015	U
1	AR	1017	C
1	AR	1018	G
1	AR	1020	G
1	AR	1021	G
1	AR	1024	G
1	AR	1029	G
1	AR	1036	A
1	AR	1047	A
1	AR	1049	C
1	AR	1064	A
1	AR	1065	A
1	AR	1072	G
1	AR	1081	U
1	AR	1082	U
1	AR	1093	A
1	AR	1094	U
1	AR	1095	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	1096	U
1	AR	1097	G
1	AR	1098	A
1	AR	1103	A
1	AR	1104	G
1	AR	1117	G
1	AR	1131	G
1	AR	1134	G
1	AR	1153	A
1	AR	1159	A
1	AR	1160	C
1	AR	1180	A
1	AR	1181	U
1	AR	1191	U
1	AR	1192	C
1	AR	1201	C
1	AR	1202	A
1	AR	1209	G
1	AR	1217	A
1	AR	1222	G
1	AR	1235	U
1	AR	1236	G
1	AR	1237	G
1	AR	1239	C
1	AR	1241	U
1	AR	1242	G
1	AR	1245	A
1	AR	1246	G
1	AR	1258	U
1	AR	1262	G
1	AR	1263	A
1	AR	1264	G
1	AR	1266	G
1	AR	1285	G
1	AR	1292	C
1	AR	1294	A
1	AR	1307	G
1	AR	1308	A
1	AR	1309	U
1	AR	1313	G
1	AR	1330	A
1	AR	1332	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	1348	U
1	AR	1349	G
1	AR	1351	U
1	AR	1352	A
1	AR	1353	U
1	AR	1355	A
1	AR	1356	U
1	AR	1357	G
1	AR	1385	C
1	AR	1386	A
1	AR	1391	C
1	AR	1392	G
1	AR	1399	A
1	AR	1400	G
1	AR	1419	A
1	AR	1428	A
1	AR	1431	G
1	AR	1432	C
1	AR	1434	G
1	AR	1437	C
1	AR	1438	U
1	AR	1446	A
1	AR	1450	G
1	AR	1455	U
1	AR	1468	A
1	AR	1481	A
1	AR	1482	A
1	AR	1488	G
1	AR	1490	A
1	AR	1496	C
1	AR	1508	C
1	AR	1527	C
1	AR	1533	U
1	AR	1536	G
1	AR	1549	U
1	AR	1555	U
1	AR	1556	C
1	AR	1560	G
1	AR	1562	C
1	AR	1563	C
1	AR	1567	U
1	AR	1568	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	1569	U
1	AR	1570	U
1	AR	1572	U
1	AR	1576	G
1	AR	1579	C
1	AR	1580	A
1	AR	1581	C
1	AR	1582	C
1	AR	1583	A
1	AR	1584	U
1	AR	1587	A
1	AR	1589	A
1	AR	1607	U
1	AR	1620	U
1	AR	1629	U
1	AR	1639	C
1	AR	1643	A
1	AR	1645	U
1	AR	1657	C
1	AR	1683	A
1	AR	1717	U
1	AR	1724	U
1	AR	1725	C
1	AR	1736	G
1	AR	1741	A
1	AR	1750	A
1	AR	1751	G
1	AR	1762	C
1	AR	1765	U
1	AR	1766	G
1	AR	1769	G
1	AR	1770	G
1	AR	1780	G
1	AR	1793	C
1	AR	1795	U
1	AR	1797	A
1	AR	1810	A
1	AR	1812	G
1	AR	1814	A
1	AR	1815	U
1	AR	1816	A
1	AR	1817	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	1819	U
1	AR	1820	U
1	AR	1821	U
1	AR	1835	A
1	AR	1839	A
1	AR	1841	A
1	AR	1842	A
1	AR	1846	C
1	AR	1849	C
1	AR	1850	A
1	AR	1878	G
1	AR	1880	U
1	AR	1886	A
1	AR	1895	A
1	AR	1906	G
1	AR	1952	G
1	AR	1953	G
1	AR	1954	G
1	AR	2094	C
1	AR	2101	C
1	AR	2102	U
1	AR	2112	U
1	AR	2113	A
1	AR	2114	C
1	AR	2121	G
1	AR	2122	G
1	AR	2126	A
1	AR	2131	A
1	AR	2144	A
1	AR	2149	A
1	AR	2155	G
1	AR	2158	A
1	AR	2169	G
1	AR	2174	G
1	AR	2187	G
1	AR	2188	A
1	AR	2205	U
1	AR	2210	G
1	AR	2223	A
1	AR	2225	U
1	AR	2228	A
1	AR	2244	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	2252	A
1	AR	2253	G
1	AR	2254	U
1	AR	2255	A
1	AR	2256	A
1	AR	2261	G
1	AR	2264	U
1	AR	2269	U
1	AR	2270	A
1	AR	2273	G
1	AR	2279	A
1	AR	2281	A
1	AR	2282	U
1	AR	2283	G
1	AR	2288	G
1	AR	2298	U
1	AR	2307	G
1	AR	2310	U
1	AR	2313	A
1	AR	2314	U
1	AR	2315	G
1	AR	2334	U
1	AR	2336	U
1	AR	2372	A
1	AR	2373	A
1	AR	2374	C
1	AR	2375	G
1	AR	2385	G
1	AR	2393	G
1	AR	2394	G
1	AR	2397	A
1	AR	2401	A
1	AR	2402	A
1	AR	2403	G
1	AR	2404	A
1	AR	2411	U
1	AR	2418	G
1	AR	2419	A
1	AR	2443	A
1	AR	2444	C
1	AR	2445	A
1	AR	2502	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	2503	G
1	AR	2504	U
1	AR	2508	U
1	AR	2511	A
1	AR	2514	U
1	AR	2515	A
1	AR	2522	G
1	AR	2523	A
1	AR	2530	G
1	AR	2531	C
1	AR	2532	U
1	AR	2533	G
1	AR	2536	A
1	AR	2537	U
1	AR	2538	U
1	AR	2539	C
1	AR	2540	A
1	AR	2541	U
1	AR	2542	U
1	AR	2543	U
1	AR	2547	A
1	AR	2549	G
1	AR	2552	C
1	AR	2554	A
1	AR	2555	G
1	AR	2561	A
1	AR	2569	A
1	AR	2570	U
1	AR	2571	U
1	AR	2572	C
1	AR	2573	G
1	AR	2581	U
1	AR	2585	G
1	AR	2589	G
1	AR	2593	A
1	AR	2594	C
1	AR	2606	G
1	AR	2607	G
1	AR	2614	G
1	AR	2619	G
1	AR	2638	C
1	AR	2652	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	2656	A
1	AR	2657	A
1	AR	2674	A
1	AR	2677	G
1	AR	2689	A
1	AR	2691	A
1	AR	2694	A
1	AR	2696	A
1	AR	2705	A
1	AR	2714	G
1	AR	2727	A
1	AR	2728	G
1	AR	2729	U
1	AR	2740	A
1	AR	2752	U
1	AR	2753	G
1	AR	2762	A
1	AR	2771	U
1	AR	2772	C
1	AR	2777	G
1	AR	2778	G
1	AR	2791	G
1	AR	2796	G
1	AR	2800	G
1	AR	2801	A
1	AR	2810	C
1	AR	2814	G
1	AR	2816	G
1	AR	2817	A
1	AR	2818	U
1	AR	2829	U
1	AR	2842	U
1	AR	2843	U
1	AR	2845	A
1	AR	2859	U
1	AR	2860	U
1	AR	2867	C
1	AR	2871	G
1	AR	2872	A
1	AR	2873	U
1	AR	2880	U
1	AR	2887	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	2896	A
1	AR	2899	C
1	AR	2923	U
1	AR	2929	C
1	AR	2935	U
1	AR	2936	A
1	AR	2945	G
1	AR	2947	G
1	AR	2951	G
1	AR	2954	U
1	AR	2957	G
1	AR	2971	A
1	AR	2983	C
1	AR	2990	G
1	AR	2996	U
1	AR	2997	G
1	AR	3012	A
1	AR	3049	A
1	AR	3055	U
1	AR	3056	U
1	AR	3059	G
1	AR	3078	U
1	AR	3079	U
1	AR	3081	C
1	AR	3086	A
1	AR	3092	C
1	AR	3100	U
1	AR	3104	U
1	AR	3122	A
1	AR	3130	A
1	AR	3131	U
1	AR	3142	A
1	AR	3143	C
1	AR	3151	U
1	AR	3153	U
1	AR	3154	C
1	AR	3155	U
1	AR	3156	U
1	AR	3157	U
1	AR	3165	A
1	AR	3167	A
1	AR	3168	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	3170	A
1	AR	3173	G
1	AR	3174	A
1	AR	3176	G
1	AR	3179	U
1	AR	3181	C
1	AR	3187	A
1	AR	3195	U
1	AR	3197	G
1	AR	3198	U
1	AR	3199	G
1	AR	3207	U
1	AR	3210	A
1	AR	3217	C
1	AR	3218	A
1	AR	3219	G
1	AR	3223	A
1	AR	3224	G
1	AR	3228	C
1	AR	3229	G
1	AR	3235	C
1	AR	3245	A
1	AR	3246	G
1	AR	3247	G
1	AR	3253	G
1	AR	3259	U
1	AR	3269	U
1	AR	3270	U
1	AR	3276	G
1	AR	3277	U
1	AR	3281	U
1	AR	3286	G
1	AR	3289	G
1	AR	3294	A
1	AR	3295	A
1	AR	3304	U
1	AR	3313	U
1	AR	3316	A
1	AR	3317	U
1	AR	3318	G
1	AR	3319	U
1	AR	3320	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	3330	A
1	AR	3333	G
1	AR	3341	U
1	AR	3345	G
1	AR	3347	A
1	AR	3350	C
1	AR	3351	U
1	AR	3352	U
1	AR	3353	G
1	AR	3354	U
1	AR	3355	U
1	AR	3356	G
1	AR	3359	A
1	AR	3369	G
1	AR	3375	A
1	AR	3376	A
1	AR	3378	C
1	AR	3389	U
1	AR	3390	G
1	AR	3396	U
2	AS	18	C
2	AS	22	A
2	AS	26	C
2	AS	33	U
2	AS	41	G
2	AS	53	U
2	AS	54	U
2	AS	60	G
2	AS	65	G
2	AS	73	C
2	AS	74	C
2	AS	99	G
2	AS	102	A
2	AS	112	G
2	AS	121	U
3	AT	2	A
3	AT	21	C
3	AT	34	U
3	AT	35	C
3	AT	48	A
3	AT	59	A
3	AT	62	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	AT	63	G
3	AT	80	A
3	AT	81	U
3	AT	82	U
3	AT	83	C
3	AT	85	G
3	AT	86	U
3	AT	87	G
3	AT	90	U
3	AT	95	G
3	AT	97	A
3	AT	99	C
3	AT	104	A
3	AT	106	C
3	AT	111	A
3	AT	113	U
3	AT	125	U
3	AT	126	A
3	AT	151	C
3	AT	152	G
3	AT	155	A
25	A	2	A
25	A	4	C
25	A	25	C
25	A	26	A
25	A	27	U
25	A	34	G
25	A	45	U
25	A	46	A
25	A	47	A
25	A	57	G
25	A	60	U
25	A	67	A
25	A	68	A
25	A	69	G
25	A	72	A
25	A	73	U
25	A	74	U
25	A	75	U
25	A	95	G
25	A	104	A
25	A	111	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	114	C
25	A	116	U
25	A	130	C
25	A	131	C
25	A	132	U
25	A	133	U
25	A	134	U
25	A	135	A
25	A	136	C
25	A	137	U
25	A	140	A
25	A	141	U
25	A	144	U
25	A	145	A
25	A	146	U
25	A	153	G
25	A	158	U
25	A	159	U
25	A	176	C
25	A	178	U
25	A	185	U
25	A	186	C
25	A	187	G
25	A	188	A
25	A	190	C
25	A	191	C
25	A	192	U
25	A	193	U
25	A	194	U
25	A	195	G
25	A	196	G
25	A	197	A
25	A	200	A
25	A	215	A
25	A	218	A
25	A	219	A
25	A	220	A
25	A	226	A
25	A	228	G
25	A	229	U
25	A	233	C
25	A	234	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	235	G
25	A	238	U
25	A	239	C
25	A	240	U
25	A	241	U
25	A	242	U
25	A	250	C
25	A	260	U
25	A	261	U
25	A	262	U
25	A	265	A
25	A	271	A
25	A	272	U
25	A	277	U
25	A	278	U
25	A	279	G
25	A	280	U
25	A	281	G
25	A	288	A
25	A	290	G
25	A	299	A
25	A	302	U
25	A	308	C
25	A	309	C
25	A	314	C
25	A	316	A
25	A	319	U
25	A	321	C
25	A	333	A
25	A	337	G
25	A	338	C
25	A	352	A
25	A	359	A
25	A	360	A
25	A	361	C
25	A	378	A
25	A	390	G
25	A	400	A
25	A	401	A
25	A	402	C
25	A	404	G
25	A	416	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	418	G
25	A	424	C
25	A	425	A
25	A	426	G
25	A	434	G
25	A	437	A
25	A	439	U
25	A	440	U
25	A	444	C
25	A	448	C
25	A	468	A
25	A	469	C
25	A	477	A
25	A	484	C
25	A	485	A
25	A	488	G
25	A	493	U
25	A	494	U
25	A	495	C
25	A	496	G
25	A	497	G
25	A	498	G
25	A	499	U
25	A	500	C
25	A	502	U
25	A	504	U
25	A	505	A
25	A	506	A
25	A	507	U
25	A	510	G
25	A	511	A
25	A	512	A
25	A	513	U
25	A	514	G
25	A	515	A
25	A	527	A
25	A	532	U
25	A	536	C
25	A	537	G
25	A	538	A
25	A	539	G
25	A	540	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	541	A
25	A	542	A
25	A	543	C
25	A	544	A
25	A	555	A
25	A	556	A
25	A	557	G
25	A	558	U
25	A	565	C
25	A	579	A
25	A	580	A
25	A	594	A
25	A	595	G
25	A	596	C
25	A	611	U
25	A	619	A
25	A	620	A
25	A	621	A
25	A	622	A
25	A	623	A
25	A	624	G
25	A	639	U
25	A	650	U
25	A	653	C
25	A	654	C
25	A	656	G
25	A	658	C
25	A	677	G
25	A	680	U
25	A	684	A
25	A	685	A
25	A	686	C
25	A	694	U
25	A	696	C
25	A	697	C
25	A	700	C
25	A	702	G
25	A	703	G
25	A	704	C
25	A	705	U
25	A	707	A
25	A	708	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	709	C
25	A	710	U
25	A	711	U
25	A	712	G
25	A	714	G
25	A	717	C
25	A	718	U
25	A	719	U
25	A	720	G
25	A	721	U
25	A	722	G
25	A	723	G
25	A	725	U
25	A	727	U
25	A	730	G
25	A	731	C
25	A	732	G
25	A	733	A
25	A	734	A
25	A	735	C
25	A	736	C
25	A	737	A
25	A	738	G
25	A	742	U
25	A	743	U
25	A	754	A
25	A	755	A
25	A	756	A
25	A	765	G
25	A	766	U
25	A	774	A
25	A	775	G
25	A	778	G
25	A	781	U
25	A	782	U
25	A	783	G
25	A	784	C
25	A	787	G
25	A	789	A
25	A	794	U
25	A	812	A
25	A	815	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	816	G
25	A	818	C
25	A	819	G
25	A	820	U
25	A	821	U
25	A	824	G
25	A	830	U
25	A	831	U
25	A	833	U
25	A	856	A
25	A	860	U
25	A	863	A
25	A	864	U
25	A	886	U
25	A	898	A
25	A	912	U
25	A	913	G
25	A	914	G
25	A	915	A
25	A	916	U
25	A	933	A
25	A	935	U
25	A	942	G
25	A	951	A
25	A	960	U
25	A	966	A
25	A	988	A
25	A	992	A
25	A	993	A
25	A	1003	A
25	A	1004	U
25	A	1005	A
25	A	1025	A
25	A	1026	A
25	A	1028	C
25	A	1039	A
25	A	1040	G
25	A	1052	U
25	A	1053	G
25	A	1058	U
25	A	1060	U
25	A	1061	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	1074	G
25	A	1079	U
25	A	1082	C
25	A	1086	A
25	A	1091	A
25	A	1092	A
25	A	1093	A
25	A	1096	C
25	A	1097	U
25	A	1100	G
25	A	1101	G
25	A	1109	G
25	A	1138	A
25	A	1139	A
25	A	1146	G
25	A	1151	A
25	A	1157	A
25	A	1158	C
25	A	1160	A
25	A	1167	G
25	A	1185	U
25	A	1191	U
25	A	1194	A
25	A	1196	A
25	A	1197	C
25	A	1199	G
25	A	1200	G
25	A	1202	A
25	A	1207	C
25	A	1208	A
25	A	1217	A
25	A	1218	G
25	A	1227	A
25	A	1229	G
25	A	1243	G
25	A	1244	A
25	A	1245	G
25	A	1251	U
25	A	1252	C
25	A	1275	A
25	A	1286	U
25	A	1314	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	1315	U
25	A	1316	G
25	A	1321	A
25	A	1339	C
25	A	1340	U
25	A	1341	A
25	A	1344	A
25	A	1345	A
25	A	1357	A
25	A	1362	U
25	A	1363	U
25	A	1364	G
25	A	1370	U
25	A	1371	A
25	A	1383	G
25	A	1390	U
25	A	1398	U
25	A	1399	C
25	A	1400	A
25	A	1412	G
25	A	1413	U
25	A	1414	U
25	A	1415	U
25	A	1418	G
25	A	1427	A
25	A	1428	G
25	A	1431	C
25	A	1446	A
25	A	1459	C
25	A	1461	C
25	A	1471	A
25	A	1473	U
25	A	1474	G
25	A	1475	A
25	A	1482	C
25	A	1486	G
25	A	1489	U
25	A	1490	C
25	A	1491	U
25	A	1492	A
25	A	1493	A
25	A	1506	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	1516	A
25	A	1517	U
25	A	1521	G
25	A	1523	G
25	A	1524	A
25	A	1535	U
25	A	1536	G
25	A	1537	C
25	A	1538	U
25	A	1542	G
25	A	1557	U
25	A	1559	A
25	A	1569	A
25	A	1572	G
25	A	1574	G
25	A	1584	G
25	A	1601	G
25	A	1614	A
25	A	1616	G
25	A	1619	C
25	A	1626	U
25	A	1631	A
25	A	1634	C
25	A	1635	A
25	A	1657	U
25	A	1658	G
25	A	1683	C
25	A	1684	U
25	A	1698	G
25	A	1699	G
25	A	1700	C
25	A	1701	A
25	A	1702	A
25	A	1703	C
25	A	1711	C
25	A	1712	A
25	A	1713	G
25	A	1715	G
25	A	1731	A
25	A	1732	A
25	A	1760	G
25	A	1762	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	A	1766	A
25	A	1769	U
25	A	1780	G
25	A	1782	A
25	A	1783	C
25	A	1792	G
25	A	1793	G
25	A	1794	A
25	A	1795	U
25	A	1796	C

All (186) RNA pucker outliers are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	43	A
1	1	65	A
1	1	210	U
1	1	239	G
1	1	282	G
1	1	547	G
1	1	588	G
1	1	763	G
1	1	873	C
1	1	916	G
1	1	979	U
1	1	981	U
1	1	993	G
1	1	1064	A
1	1	1094	U
1	1	1097	G
1	1	1103	A
1	1	1273	A
1	1	1307	G
1	1	1329	U
1	1	1352	A
1	1	1355	A
1	1	1554	U
1	1	1562	C
1	1	1568	U
1	1	1716	U
1	1	1816	A
1	1	1820	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	2101	C
1	1	2112	U
1	1	2209	U
1	1	2227	C
1	1	2249	G
1	1	2372	A
1	1	2418	G
1	1	2525	G
1	1	2537	U
1	1	2541	U
1	1	2593	A
1	1	2801	A
1	1	2818	U
1	1	3078	U
1	1	3121	U
1	1	3218	A
1	1	3228	C
1	1	3269	U
1	1	3275	U
1	1	3319	U
1	1	3350	C
1	1	3351	U
1	1	3353	G
3	4	85	G
3	4	125	U
25	6	25	C
25	6	114	C
25	6	139	C
25	6	158	U
25	6	187	G
25	6	217	A
25	6	272	U
25	6	400	A
25	6	417	A
25	6	512	A
25	6	542	A
25	6	558	U
25	6	755	A
25	6	829	A
25	6	834	G
25	6	913	G
25	6	1051	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
25	6	1058	U
25	6	1081	A
25	6	1097	U
25	6	1244	A
25	6	1255	G
25	6	1344	A
25	6	1481	C
25	6	1489	U
25	6	1535	U
25	6	1568	C
25	6	1573	A
25	6	1620	C
25	6	1657	U
1	AR	210	U
1	AR	588	G
1	AR	637	C
1	AR	715	A
1	AR	873	C
1	AR	916	G
1	AR	979	U
1	AR	981	U
1	AR	993	G
1	AR	1064	A
1	AR	1097	G
1	AR	1103	A
1	AR	1190	A
1	AR	1238	C
1	AR	1241	U
1	AR	1284	C
1	AR	1307	G
1	AR	1329	U
1	AR	1331	U
1	AR	1352	A
1	AR	1355	A
1	AR	1481	A
1	AR	1514	G
1	AR	1554	U
1	AR	1562	C
1	AR	1792	C
1	AR	1815	U
1	AR	1816	A
1	AR	1820	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AR	1846	C
1	AR	2101	C
1	AR	2112	U
1	AR	2209	U
1	AR	2252	A
1	AR	2255	A
1	AR	2260	U
1	AR	2269	U
1	AR	2418	G
1	AR	2537	U
1	AR	2541	U
1	AR	2801	A
1	AR	2818	U
1	AR	3078	U
1	AR	3121	U
1	AR	3218	A
1	AR	3228	C
1	AR	3269	U
1	AR	3276	G
1	AR	3319	U
1	AR	3350	C
1	AR	3375	A
2	AS	52	G
2	AS	111	U
3	AT	82	U
3	AT	85	G
3	AT	125	U
25	A	25	C
25	A	45	U
25	A	68	A
25	A	73	U
25	A	130	C
25	A	131	C
25	A	139	C
25	A	158	U
25	A	187	G
25	A	218	A
25	A	240	U
25	A	278	U
25	A	280	U
25	A	417	A
25	A	497	G

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Mol	Chain	Res	Type
25	A	499	U
25	A	501	U
25	A	503	G
25	A	512	A
25	A	555	A
25	A	685	A
25	A	704	C
25	A	720	G
25	A	721	U
25	A	755	A
25	A	782	U
25	A	811	A
25	A	829	A
25	A	913	G
25	A	1051	G
25	A	1081	A
25	A	1157	A
25	A	1196	A
25	A	1207	C
25	A	1226	A
25	A	1244	A
25	A	1250	U
25	A	1339	C
25	A	1344	A
25	A	1370	U
25	A	1481	C
25	A	1568	C
25	A	1573	A
25	A	1615	C
25	A	1657	U
25	A	1698	G
25	A	1761	U

#### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2494 ligands modelled in this entry, 1422 are monoatomic - leaving 1072 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AP	502	-	0,6,6	-	-	-	-	-
84	OHX	1	3699	-	0,6,6	-	-	-	-	-
84	OHX	AR	3582	-	0,6,6	-	-	-	-	-
84	OHX	1	3426	-	0,6,6	-	-	-	-	-
84	OHX	6	1905	-	0,6,6	-	-	-	-	-
84	OHX	1	3671	-	0,6,6	-	-	-	-	-
84	OHX	6	1915	-	0,6,6	-	-	-	-	-
84	OHX	A	2001	-	0,6,6	-	-	-	-	-
84	OHX	1	3421	-	0,6,6	-	-	-	-	-
84	OHX	6	2003	-	0,6,6	-	-	-	-	-
84	OHX	1	3669	-	0,6,6	-	-	-	-	-
84	OHX	6	2057	-	0,6,6	-	-	-	-	-
84	OHX	AR	3636	-	0,6,6	-	-	-	-	-
84	OHX	AS	204	-	0,6,6	-	-	-	-	-
84	OHX	6	1936	-	0,6,6	-	-	-	-	-
84	OHX	AR	3545	-	0,6,6	-	-	-	-	-
84	OHX	1	3423	-	0,6,6	-	-	-	-	-
84	OHX	1	3657	-	0,6,6	-	-	-	-	-
84	OHX	6	2017	-	0,6,6	-	-	-	-	-
84	OHX	1	3452	-	0,6,6	-	-	-	-	-
84	OHX	1	3505	-	0,6,6	-	-	-	-	-
84	OHX	1	3475	-	0,6,6	-	-	-	-	-
84	OHX	1	3593	-	0,6,6	-	-	-	-	-
84	OHX	6	1932	-	0,6,6	-	-	-	-	-
84	OHX	AR	3612	-	0,6,6	-	-	-	-	-
84	OHX	A	1997	-	0,6,6	-	-	-	-	-
84	OHX	AS	205	-	0,6,6	-	-	-	-	-
84	OHX	1	3704	-	0,6,6	-	-	-	-	-
84	OHX	A	1933	-	0,6,6	-	-	-	-	-
84	OHX	1	3493	-	0,6,6	-	-	-	-	-
84	OHX	1	3726	-	0,6,6	-	-	-	-	-
84	OHX	6	1950	-	0,6,6	-	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3579	-	0,6,6	-	-	-		
84	OHX	6	1945	-	0,6,6	-	-	-		
84	OHX	A	2021	-	0,6,6	-	-	-		
84	OHX	6	2034	-	0,6,6	-	-	-		
84	OHX	1	3451	-	0,6,6	-	-	-		
84	OHX	AR	3566	-	0,6,6	-	-	-		
84	OHX	1	3422	-	0,6,6	-	-	-		
84	OHX	1	3638	-	0,6,6	-	-	-		
84	OHX	6	1999	-	0,6,6	-	-	-		
84	OHX	6	2020	-	0,6,6	-	-	-		
84	OHX	AR	3716	-	0,6,6	-	-	-		
84	OHX	1	3450	-	0,6,6	-	-	-		
84	OHX	AR	3565	-	0,6,6	-	-	-		
84	OHX	6	1929	-	0,6,6	-	-	-		
84	OHX	1	3682	-	0,6,6	-	-	-		
84	OHX	A	2033	-	0,6,6	-	-	-		
84	OHX	AR	3462	-	0,6,6	-	-	-		
84	OHX	AR	3540	-	0,6,6	-	-	-		
84	OHX	1	3402	-	0,6,6	-	-	-		
84	OHX	1	3690	-	0,6,6	-	-	-		
84	OHX	AR	3603	-	0,6,6	-	-	-		
84	OHX	AR	3647	-	0,6,6	-	-	-		
84	OHX	3	208	-	0,6,6	-	-	-		
84	OHX	AR	3648	-	0,6,6	-	-	-		
84	OHX	AR	3722	-	0,6,6	-	-	-		
84	OHX	A	1986	-	0,6,6	-	-	-		
84	OHX	A	2019	-	0,6,6	-	-	-		
84	OHX	AR	3504	-	0,6,6	-	-	-		
84	OHX	1	3589	-	0,6,6	-	-	-		
84	OHX	1	3660	-	0,6,6	-	-	-		
84	OHX	AR	3630	-	0,6,6	-	-	-		
84	OHX	d9	101	-	0,6,6	-	-	-		
84	OHX	A	1950	-	0,6,6	-	-	-		
84	OHX	AR	3699	-	0,6,6	-	-	-		
84	OHX	1	3471	-	0,6,6	-	-	-		
84	OHX	1	3549	-	0,6,6	-	-	-		
84	OHX	AR	3446	-	0,6,6	-	-	-		
84	OHX	AR	3721	-	0,6,6	-	-	-		
84	OHX	6	1985	-	0,6,6	-	-	-		
84	OHX	AR	3500	-	0,6,6	-	-	-		
84	OHX	AR	3602	-	0,6,6	-	-	-		
84	OHX	A	1934	-	0,6,6	-	-	-		
84	OHX	A	1960	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3595	-	0,6,6	-	-	-	-	-
84	OHX	A	1971	-	0,6,6	-	-	-	-	-
84	OHX	AR	3418	-	0,6,6	-	-	-	-	-
84	OHX	AR	3425	-	0,6,6	-	-	-	-	-
84	OHX	DI	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3504	-	0,6,6	-	-	-	-	-
84	OHX	AR	3642	-	0,6,6	-	-	-	-	-
84	OHX	AR	3563	-	0,6,6	-	-	-	-	-
84	OHX	1	3409	-	0,6,6	-	-	-	-	-
84	OHX	AE	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3466	-	0,6,6	-	-	-	-	-
84	OHX	1	3634	-	0,6,6	-	-	-	-	-
84	OHX	4	210	-	0,6,6	-	-	-	-	-
84	OHX	6	2029	-	0,6,6	-	-	-	-	-
84	OHX	A	2009	-	0,6,6	-	-	-	-	-
84	OHX	AT	215	-	0,6,6	-	-	-	-	-
84	OHX	1	3558	-	0,6,6	-	-	-	-	-
84	OHX	AR	3730	-	0,6,6	-	-	-	-	-
84	OHX	1	3562	-	0,6,6	-	-	-	-	-
84	OHX	6	1975	-	0,6,6	-	-	-	-	-
84	OHX	6	2028	-	0,6,6	-	-	-	-	-
84	OHX	AK	103	-	0,6,6	-	-	-	-	-
84	OHX	1	3461	-	0,6,6	-	-	-	-	-
84	OHX	AR	3616	-	0,6,6	-	-	-	-	-
84	OHX	1	3480	-	0,6,6	-	-	-	-	-
84	OHX	1	3715	-	0,6,6	-	-	-	-	-
84	OHX	AR	3675	-	0,6,6	-	-	-	-	-
84	OHX	AR	3723	-	0,6,6	-	-	-	-	-
84	OHX	AR	3620	-	0,6,6	-	-	-	-	-
84	OHX	AT	205	-	0,6,6	-	-	-	-	-
84	OHX	AT	208	-	0,6,6	-	-	-	-	-
84	OHX	3	204	-	0,6,6	-	-	-	-	-
84	OHX	1	3601	-	0,6,6	-	-	-	-	-
84	OHX	6	1919	-	0,6,6	-	-	-	-	-
84	OHX	A	1949	-	0,6,6	-	-	-	-	-
84	OHX	AR	3527	-	0,6,6	-	-	-	-	-
84	OHX	AR	3560	-	0,6,6	-	-	-	-	-
84	OHX	A	1957	-	0,6,6	-	-	-	-	-
84	OHX	AR	3530	-	0,6,6	-	-	-	-	-
84	OHX	AR	3738	-	0,6,6	-	-	-	-	-
84	OHX	1	3541	-	0,6,6	-	-	-	-	-
84	OHX	AR	3415	-	0,6,6	-	-	-	-	-
84	OHX	A	1941	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	1947	-	0,6,6	-	-	-	-	-
84	OHX	1	3544	-	0,6,6	-	-	-	-	-
84	OHX	1	3679	-	0,6,6	-	-	-	-	-
84	OHX	AR	3578	-	0,6,6	-	-	-	-	-
84	OHX	AR	3687	-	0,6,6	-	-	-	-	-
84	OHX	AR	3510	-	0,6,6	-	-	-	-	-
84	OHX	AR	3585	-	0,6,6	-	-	-	-	-
84	OHX	1	3706	-	0,6,6	-	-	-	-	-
84	OHX	6	1908	-	0,6,6	-	-	-	-	-
84	OHX	AR	3613	-	0,6,6	-	-	-	-	-
84	OHX	A	2025	-	0,6,6	-	-	-	-	-
84	OHX	6	1933	-	0,6,6	-	-	-	-	-
84	OHX	6	1935	-	0,6,6	-	-	-	-	-
84	OHX	A	1948	-	0,6,6	-	-	-	-	-
84	OHX	1	3465	-	0,6,6	-	-	-	-	-
84	OHX	6	1930	-	0,6,6	-	-	-	-	-
84	OHX	A	2010	-	0,6,6	-	-	-	-	-
84	OHX	AR	3431	-	0,6,6	-	-	-	-	-
84	OHX	1	3667	-	0,6,6	-	-	-	-	-
84	OHX	6	2026	-	0,6,6	-	-	-	-	-
84	OHX	AR	3469	-	0,6,6	-	-	-	-	-
84	OHX	1	3559	-	0,6,6	-	-	-	-	-
84	OHX	6	2013	-	0,6,6	-	-	-	-	-
84	OHX	1	3420	-	0,6,6	-	-	-	-	-
84	OHX	6	2033	-	0,6,6	-	-	-	-	-
84	OHX	6	1911	-	0,6,6	-	-	-	-	-
84	OHX	1	3633	-	0,6,6	-	-	-	-	-
84	OHX	AR	3447	-	0,6,6	-	-	-	-	-
84	OHX	1	3572	-	0,6,6	-	-	-	-	-
84	OHX	AT	204	-	0,6,6	-	-	-	-	-
84	OHX	AR	3513	-	0,6,6	-	-	-	-	-
84	OHX	6	2046	-	0,6,6	-	-	-	-	-
84	OHX	AR	3711	-	0,6,6	-	-	-	-	-
84	OHX	1	3604	-	0,6,6	-	-	-	-	-
84	OHX	A	1945	-	0,6,6	-	-	-	-	-
84	OHX	6	1973	-	0,6,6	-	-	-	-	-
84	OHX	1	3566	-	0,6,6	-	-	-	-	-
84	OHX	AR	3408	-	0,6,6	-	-	-	-	-
84	OHX	1	3497	-	0,6,6	-	-	-	-	-
84	OHX	CG	301	-	0,6,6	-	-	-	-	-
84	OHX	1	3456	-	0,6,6	-	-	-	-	-
84	OHX	A	2007	-	0,6,6	-	-	-	-	-
84	OHX	AR	3445	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	2	201	-	0,6,6	-	-	-		
84	OHX	AR	3518	-	0,6,6	-	-	-		
84	OHX	AR	3529	-	0,6,6	-	-	-		
84	OHX	AR	3543	-	0,6,6	-	-	-		
84	OHX	AR	3646	-	0,6,6	-	-	-		
84	OHX	A	1993	-	0,6,6	-	-	-		
84	OHX	AR	3556	-	0,6,6	-	-	-		
84	OHX	1	3635	-	0,6,6	-	-	-		
84	OHX	1	3650	-	0,6,6	-	-	-		
84	OHX	AR	3658	-	0,6,6	-	-	-		
84	OHX	AR	3639	-	0,6,6	-	-	-		
84	OHX	A	2036	-	0,6,6	-	-	-		
84	OHX	4	209	-	0,6,6	-	-	-		
84	OHX	1	3672	-	0,6,6	-	-	-		
84	OHX	6	1978	-	0,6,6	-	-	-		
84	OHX	AR	3405	-	0,6,6	-	-	-		
84	OHX	AR	3411	-	0,6,6	-	-	-		
84	OHX	1	3499	-	0,6,6	-	-	-		
84	OHX	1	3513	-	0,6,6	-	-	-		
84	OHX	AR	3424	-	0,6,6	-	-	-		
84	OHX	6	1916	-	0,6,6	-	-	-		
84	OHX	AT	213	-	0,6,6	-	-	-		
84	OHX	1	3419	-	0,6,6	-	-	-		
84	OHX	AR	3460	-	0,6,6	-	-	-		
84	OHX	A	1917	-	0,6,6	-	-	-		
84	OHX	c3	201	-	0,6,6	-	-	-		
84	OHX	1	3605	-	0,6,6	-	-	-		
84	OHX	6	2001	-	0,6,6	-	-	-		
84	OHX	6	2053	-	0,6,6	-	-	-		
84	OHX	A	1952	-	0,6,6	-	-	-		
84	OHX	O	201	-	0,6,6	-	-	-		
84	OHX	6	1994	-	0,6,6	-	-	-		
84	OHX	6	1938	-	0,6,6	-	-	-		
84	OHX	6	2018	-	0,6,6	-	-	-		
84	OHX	1	3627	-	0,6,6	-	-	-		
84	OHX	6	1998	-	0,6,6	-	-	-		
84	OHX	1	3496	-	0,6,6	-	-	-		
84	OHX	1	3575	-	0,6,6	-	-	-		
84	OHX	AR	3581	-	0,6,6	-	-	-		
84	OHX	6	1957	-	0,6,6	-	-	-		
84	OHX	A	1958	-	0,6,6	-	-	-		
84	OHX	A	2024	-	0,6,6	-	-	-		
84	OHX	6	2040	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3685	-	0,6,6	-	-	-	-	-
84	OHX	A	1909	-	0,6,6	-	-	-	-	-
84	OHX	1	3581	-	0,6,6	-	-	-	-	-
84	OHX	AR	3521	-	0,6,6	-	-	-	-	-
84	OHX	AR	3672	-	0,6,6	-	-	-	-	-
84	OHX	1	3676	-	0,6,6	-	-	-	-	-
84	OHX	AR	3677	-	0,6,6	-	-	-	-	-
84	OHX	1	3522	-	0,6,6	-	-	-	-	-
84	OHX	A	2017	-	0,6,6	-	-	-	-	-
84	OHX	A	2035	-	0,6,6	-	-	-	-	-
84	OHX	4	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3696	-	0,6,6	-	-	-	-	-
84	OHX	AR	3508	-	0,6,6	-	-	-	-	-
84	OHX	6	1924	-	0,6,6	-	-	-	-	-
84	OHX	A	2042	-	0,6,6	-	-	-	-	-
84	OHX	AS	208	-	0,6,6	-	-	-	-	-
84	OHX	AR	3534	-	0,6,6	-	-	-	-	-
84	OHX	1	3610	-	0,6,6	-	-	-	-	-
84	OHX	6	1962	-	0,6,6	-	-	-	-	-
84	OHX	6	2024	-	0,6,6	-	-	-	-	-
84	OHX	AR	3417	-	0,6,6	-	-	-	-	-
84	OHX	AR	3591	-	0,6,6	-	-	-	-	-
84	OHX	AR	3600	-	0,6,6	-	-	-	-	-
84	OHX	A	1998	-	0,6,6	-	-	-	-	-
84	OHX	AT	210	-	0,6,6	-	-	-	-	-
84	OHX	A	2037	-	0,6,6	-	-	-	-	-
84	OHX	1	3490	-	0,6,6	-	-	-	-	-
84	OHX	1	3649	-	0,6,6	-	-	-	-	-
84	OHX	AR	3458	-	0,6,6	-	-	-	-	-
84	OHX	AR	3573	-	0,6,6	-	-	-	-	-
84	OHX	A	1995	-	0,6,6	-	-	-	-	-
84	OHX	1	3680	-	0,6,6	-	-	-	-	-
84	OHX	A	1943	-	0,6,6	-	-	-	-	-
84	OHX	AR	3533	-	0,6,6	-	-	-	-	-
84	OHX	A	2034	-	0,6,6	-	-	-	-	-
84	OHX	1	3722	-	0,6,6	-	-	-	-	-
84	OHX	A	1999	-	0,6,6	-	-	-	-	-
84	OHX	AR	3512	-	0,6,6	-	-	-	-	-
84	OHX	AR	3548	-	0,6,6	-	-	-	-	-
84	OHX	M	201	-	0,6,6	-	-	-	-	-
84	OHX	AR	3624	-	0,6,6	-	-	-	-	-
84	OHX	6	2015	-	0,6,6	-	-	-	-	-
84	OHX	AR	3414	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3413	-	0,6,6	-	-	-	-	-
84	OHX	AR	3479	-	0,6,6	-	-	-	-	-
84	OHX	1	3644	-	0,6,6	-	-	-	-	-
84	OHX	1	3401	-	0,6,6	-	-	-	-	-
84	OHX	6	1959	-	0,6,6	-	-	-	-	-
84	OHX	AR	3498	-	0,6,6	-	-	-	-	-
84	OHX	1	3598	-	0,6,6	-	-	-	-	-
84	OHX	1	3632	-	0,6,6	-	-	-	-	-
84	OHX	A	2006	-	0,6,6	-	-	-	-	-
84	OHX	6	1931	-	0,6,6	-	-	-	-	-
84	OHX	AR	3410	-	0,6,6	-	-	-	-	-
84	OHX	AR	3464	-	0,6,6	-	-	-	-	-
84	OHX	6	1993	-	0,6,6	-	-	-	-	-
84	OHX	6	1967	-	0,6,6	-	-	-	-	-
84	OHX	6	2009	-	0,6,6	-	-	-	-	-
84	OHX	AR	3412	-	0,6,6	-	-	-	-	-
84	OHX	AR	3725	-	0,6,6	-	-	-	-	-
84	OHX	A	1991	-	0,6,6	-	-	-	-	-
84	OHX	CV	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3556	-	0,6,6	-	-	-	-	-
84	OHX	1	3582	-	0,6,6	-	-	-	-	-
84	OHX	AR	3656	-	0,6,6	-	-	-	-	-
84	OHX	A	1915	-	0,6,6	-	-	-	-	-
84	OHX	1	3583	-	0,6,6	-	-	-	-	-
84	OHX	6	1901	-	0,6,6	-	-	-	-	-
84	OHX	AR	3737	-	0,6,6	-	-	-	-	-
84	OHX	1	3531	-	0,6,6	-	-	-	-	-
84	OHX	1	3483	-	0,6,6	-	-	-	-	-
84	OHX	A	1936	-	0,6,6	-	-	-	-	-
84	OHX	A	1974	-	0,6,6	-	-	-	-	-
84	OHX	6	1949	-	0,6,6	-	-	-	-	-
84	OHX	6	1927	-	0,6,6	-	-	-	-	-
84	OHX	AR	3474	-	0,6,6	-	-	-	-	-
84	OHX	1	3662	-	0,6,6	-	-	-	-	-
84	OHX	1	3417	-	0,6,6	-	-	-	-	-
84	OHX	AR	3482	-	0,6,6	-	-	-	-	-
84	OHX	AR	3507	-	0,6,6	-	-	-	-	-
84	OHX	AR	3520	-	0,6,6	-	-	-	-	-
84	OHX	AR	3629	-	0,6,6	-	-	-	-	-
84	OHX	AR	3663	-	0,6,6	-	-	-	-	-
84	OHX	A	1932	-	0,6,6	-	-	-	-	-
84	OHX	1	3532	-	0,6,6	-	-	-	-	-
84	OHX	1	3723	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3494	-	0,6,6	-	-	-	-	-
84	OHX	A	1975	-	0,6,6	-	-	-	-	-
84	OHX	1	3492	-	0,6,6	-	-	-	-	-
84	OHX	1	3520	-	0,6,6	-	-	-	-	-
84	OHX	A	1916	-	0,6,6	-	-	-	-	-
84	OHX	6	2014	-	0,6,6	-	-	-	-	-
84	OHX	1	3623	-	0,6,6	-	-	-	-	-
84	OHX	1	3670	-	0,6,6	-	-	-	-	-
84	OHX	AR	3470	-	0,6,6	-	-	-	-	-
84	OHX	1	3594	-	0,6,6	-	-	-	-	-
84	OHX	6	1928	-	0,6,6	-	-	-	-	-
84	OHX	1	3443	-	0,6,6	-	-	-	-	-
84	OHX	6	1948	-	0,6,6	-	-	-	-	-
84	OHX	AR	3712	-	0,6,6	-	-	-	-	-
84	OHX	AR	3707	-	0,6,6	-	-	-	-	-
84	OHX	AR	3586	-	0,6,6	-	-	-	-	-
84	OHX	h	401	-	0,6,6	-	-	-	-	-
84	OHX	1	3570	-	0,6,6	-	-	-	-	-
84	OHX	e	101	-	0,6,6	-	-	-	-	-
84	OHX	1	3568	-	0,6,6	-	-	-	-	-
84	OHX	1	3702	-	0,6,6	-	-	-	-	-
84	OHX	A	1987	-	0,6,6	-	-	-	-	-
84	OHX	1	3525	-	0,6,6	-	-	-	-	-
84	OHX	6	1909	-	0,6,6	-	-	-	-	-
84	OHX	AR	3471	-	0,6,6	-	-	-	-	-
84	OHX	AR	3718	-	0,6,6	-	-	-	-	-
84	OHX	AR	3466	-	0,6,6	-	-	-	-	-
84	OHX	r	301	-	0,6,6	-	-	-	-	-
84	OHX	AR	3596	-	0,6,6	-	-	-	-	-
84	OHX	6	1963	-	0,6,6	-	-	-	-	-
84	OHX	AR	3685	-	0,6,6	-	-	-	-	-
84	OHX	1	3665	-	0,6,6	-	-	-	-	-
84	OHX	AR	3615	-	0,6,6	-	-	-	-	-
84	OHX	J	301	-	0,6,6	-	-	-	-	-
84	OHX	3	201	-	0,6,6	-	-	-	-	-
84	OHX	AR	3700	-	0,6,6	-	-	-	-	-
84	OHX	AR	3623	-	0,6,6	-	-	-	-	-
84	OHX	A	1913	-	0,6,6	-	-	-	-	-
84	OHX	1	3542	-	0,6,6	-	-	-	-	-
84	OHX	AR	3501	-	0,6,6	-	-	-	-	-
84	OHX	1	3553	-	0,6,6	-	-	-	-	-
84	OHX	1	3591	-	0,6,6	-	-	-	-	-
84	OHX	1	3406	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3697	-	0,6,6	-	-	-	-	-
84	OHX	AR	3489	-	0,6,6	-	-	-	-	-
84	OHX	A	2000	-	0,6,6	-	-	-	-	-
84	OHX	1	3641	-	0,6,6	-	-	-	-	-
84	OHX	AK	102	-	0,6,6	-	-	-	-	-
84	OHX	AS	206	-	0,6,6	-	-	-	-	-
84	OHX	CX	201	-	0,6,6	-	-	-	-	-
84	OHX	6	2049	-	0,6,6	-	-	-	-	-
84	OHX	6	1992	-	0,6,6	-	-	-	-	-
84	OHX	1	3546	-	0,6,6	-	-	-	-	-
84	OHX	6	1997	-	0,6,6	-	-	-	-	-
84	OHX	A	1938	-	0,6,6	-	-	-	-	-
84	OHX	DG	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3403	-	0,6,6	-	-	-	-	-
84	OHX	1	3538	-	0,6,6	-	-	-	-	-
84	OHX	1	3429	-	0,6,6	-	-	-	-	-
84	OHX	1	3577	-	0,6,6	-	-	-	-	-
84	OHX	AR	3421	-	0,6,6	-	-	-	-	-
84	OHX	1	3404	-	0,6,6	-	-	-	-	-
84	OHX	1	3713	-	0,6,6	-	-	-	-	-
84	OHX	AR	3457	-	0,6,6	-	-	-	-	-
84	OHX	6	1979	-	0,6,6	-	-	-	-	-
84	OHX	AR	3580	-	0,6,6	-	-	-	-	-
84	OHX	AR	3618	-	0,6,6	-	-	-	-	-
84	OHX	1	3688	-	0,6,6	-	-	-	-	-
84	OHX	6	2039	-	0,6,6	-	-	-	-	-
84	OHX	AR	3715	-	0,6,6	-	-	-	-	-
84	OHX	AT	202	-	0,6,6	-	-	-	-	-
84	OHX	z	201	-	0,6,6	-	-	-	-	-
84	OHX	A	1931	-	0,6,6	-	-	-	-	-
84	OHX	1	3433	-	0,6,6	-	-	-	-	-
84	OHX	AR	3477	-	0,6,6	-	-	-	-	-
84	OHX	AR	3561	-	0,6,6	-	-	-	-	-
84	OHX	AR	3488	-	0,6,6	-	-	-	-	-
84	OHX	AR	3526	-	0,6,6	-	-	-	-	-
84	OHX	1	3606	-	0,6,6	-	-	-	-	-
84	OHX	AR	3640	-	0,6,6	-	-	-	-	-
84	OHX	1	3714	-	0,6,6	-	-	-	-	-
84	OHX	1	3617	-	0,6,6	-	-	-	-	-
84	OHX	1	3447	-	0,6,6	-	-	-	-	-
84	OHX	1	3501	-	0,6,6	-	-	-	-	-
84	OHX	1	3708	-	0,6,6	-	-	-	-	-
84	OHX	1	3485	-	0,6,6	-	-	-	-	-



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	4	206	-	0,6,6	-	-	-		
84	OHX	AR	3439	-	0,6,6	-	-	-		
84	OHX	1	3555	-	0,6,6	-	-	-		
84	OHX	AR	3628	-	0,6,6	-	-	-		
84	OHX	DL	102	-	0,6,6	-	-	-		
84	OHX	6	2056	-	0,6,6	-	-	-		
84	OHX	AR	3435	-	0,6,6	-	-	-		
84	OHX	A	1926	-	0,6,6	-	-	-		
84	OHX	AR	3592	-	0,6,6	-	-	-		
84	OHX	1	3664	-	0,6,6	-	-	-		
84	OHX	AR	3444	-	0,6,6	-	-	-		
84	OHX	AR	3694	-	0,6,6	-	-	-		
84	OHX	1	3599	-	0,6,6	-	-	-		
84	OHX	A	1976	-	0,6,6	-	-	-		
84	OHX	A	1966	-	0,6,6	-	-	-		
84	OHX	AR	3459	-	0,6,6	-	-	-		
84	OHX	A	1964	-	0,6,6	-	-	-		
84	OHX	6	1977	-	0,6,6	-	-	-		
84	OHX	6	1996	-	0,6,6	-	-	-		
84	OHX	1	3430	-	0,6,6	-	-	-		
84	OHX	A	2014	-	0,6,6	-	-	-		
84	OHX	1	3437	-	0,6,6	-	-	-		
84	OHX	1	3580	-	0,6,6	-	-	-		
84	OHX	6	1920	-	0,6,6	-	-	-		
84	OHX	AR	3619	-	0,6,6	-	-	-		
84	OHX	1	3476	-	0,6,6	-	-	-		
84	OHX	1	3689	-	0,6,6	-	-	-		
84	OHX	6	1970	-	0,6,6	-	-	-		
84	OHX	1	3487	-	0,6,6	-	-	-		
84	OHX	A	1962	-	0,6,6	-	-	-		
84	OHX	1	3408	-	0,6,6	-	-	-		
84	OHX	6	1914	-	0,6,6	-	-	-		
84	OHX	AR	3567	-	0,6,6	-	-	-		
84	OHX	1	3472	-	0,6,6	-	-	-		
84	OHX	AR	3682	-	0,6,6	-	-	-		
84	OHX	6	1913	-	0,6,6	-	-	-		
84	OHX	1	3438	-	0,6,6	-	-	-		
84	OHX	AR	3684	-	0,6,6	-	-	-		
84	OHX	6	1984	-	0,6,6	-	-	-		
84	OHX	6	2051	-	0,6,6	-	-	-		
84	OHX	6	1991	-	0,6,6	-	-	-		
84	OHX	1	3597	-	0,6,6	-	-	-		
84	OHX	AR	3571	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	CK	201	-	0,6,6	-	-	-	-	-
84	OHX	6	1939	-	0,6,6	-	-	-	-	-
84	OHX	1	3498	-	0,6,6	-	-	-	-	-
84	OHX	1	3612	-	0,6,6	-	-	-	-	-
84	OHX	AS	209	-	0,6,6	-	-	-	-	-
84	OHX	4	202	-	0,6,6	-	-	-	-	-
84	OHX	s8	301	-	0,6,6	-	-	-	-	-
84	OHX	A	2018	-	0,6,6	-	-	-	-	-
84	OHX	1	3468	-	0,6,6	-	-	-	-	-
84	OHX	AR	3643	-	0,6,6	-	-	-	-	-
84	OHX	AR	3609	-	0,6,6	-	-	-	-	-
84	OHX	AR	3413	-	0,6,6	-	-	-	-	-
84	OHX	1	3514	-	0,6,6	-	-	-	-	-
84	OHX	AR	3626	-	0,6,6	-	-	-	-	-
84	OHX	1	3545	-	0,6,6	-	-	-	-	-
84	OHX	AR	3614	-	0,6,6	-	-	-	-	-
84	OHX	AR	3487	-	0,6,6	-	-	-	-	-
84	OHX	AR	3635	-	0,6,6	-	-	-	-	-
84	OHX	A	1954	-	0,6,6	-	-	-	-	-
84	OHX	AR	3541	-	0,6,6	-	-	-	-	-
84	OHX	AR	3681	-	0,6,6	-	-	-	-	-
84	OHX	A	1937	-	0,6,6	-	-	-	-	-
84	OHX	3	207	-	0,6,6	-	-	-	-	-
84	OHX	AR	3584	-	0,6,6	-	-	-	-	-
84	OHX	1	3540	-	0,6,6	-	-	-	-	-
84	OHX	AR	3705	-	0,6,6	-	-	-	-	-
84	OHX	AR	3733	-	0,6,6	-	-	-	-	-
84	OHX	AS	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3539	-	0,6,6	-	-	-	-	-
84	OHX	AR	3631	-	0,6,6	-	-	-	-	-
84	OHX	1	3663	-	0,6,6	-	-	-	-	-
84	OHX	A	1985	-	0,6,6	-	-	-	-	-
84	OHX	CE	403	-	0,6,6	-	-	-	-	-
84	OHX	AR	3437	-	0,6,6	-	-	-	-	-
84	OHX	AT	217	-	0,6,6	-	-	-	-	-
84	OHX	1	3489	-	0,6,6	-	-	-	-	-
84	OHX	6	1922	-	0,6,6	-	-	-	-	-
84	OHX	AR	3622	-	0,6,6	-	-	-	-	-
84	OHX	1	3565	-	0,6,6	-	-	-	-	-
84	OHX	A	1981	-	0,6,6	-	-	-	-	-
84	OHX	1	3488	-	0,6,6	-	-	-	-	-
84	OHX	1	3462	-	0,6,6	-	-	-	-	-
84	OHX	AR	3679	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3686	-	0,6,6	-	-	-	-	-
84	OHX	1	3720	-	0,6,6	-	-	-	-	-
84	OHX	6	1964	-	0,6,6	-	-	-	-	-
84	OHX	AR	3604	-	0,6,6	-	-	-	-	-
84	OHX	AR	3463	-	0,6,6	-	-	-	-	-
84	OHX	AR	3605	-	0,6,6	-	-	-	-	-
84	OHX	1	3648	-	0,6,6	-	-	-	-	-
84	OHX	6	2038	-	0,6,6	-	-	-	-	-
84	OHX	AR	3519	-	0,6,6	-	-	-	-	-
84	OHX	AR	3497	-	0,6,6	-	-	-	-	-
84	OHX	1	3630	-	0,6,6	-	-	-	-	-
84	OHX	AT	206	-	0,6,6	-	-	-	-	-
84	OHX	AR	3537	-	0,6,6	-	-	-	-	-
84	OHX	1	3550	-	0,6,6	-	-	-	-	-
84	OHX	AT	218	-	0,6,6	-	-	-	-	-
84	OHX	1	3453	-	0,6,6	-	-	-	-	-
84	OHX	1	3608	-	0,6,6	-	-	-	-	-
84	OHX	6	1906	-	0,6,6	-	-	-	-	-
84	OHX	1	3506	-	0,6,6	-	-	-	-	-
84	OHX	6	1952	-	0,6,6	-	-	-	-	-
84	OHX	6	1980	-	0,6,6	-	-	-	-	-
84	OHX	1	3595	-	0,6,6	-	-	-	-	-
84	OHX	AR	3655	-	0,6,6	-	-	-	-	-
84	OHX	AR	3509	-	0,6,6	-	-	-	-	-
84	OHX	AR	3726	-	0,6,6	-	-	-	-	-
84	OHX	AS	203	-	0,6,6	-	-	-	-	-
84	OHX	1	3459	-	0,6,6	-	-	-	-	-
84	OHX	6	2004	-	0,6,6	-	-	-	-	-
84	OHX	1	3434	-	0,6,6	-	-	-	-	-
84	OHX	AR	3401	-	0,6,6	-	-	-	-	-
84	OHX	6	2012	-	0,6,6	-	-	-	-	-
84	OHX	A	1996	-	0,6,6	-	-	-	-	-
84	OHX	6	1974	-	0,6,6	-	-	-	-	-
84	OHX	AR	3554	-	0,6,6	-	-	-	-	-
84	OHX	A	1989	-	0,6,6	-	-	-	-	-
84	OHX	1	3415	-	0,6,6	-	-	-	-	-
84	OHX	1	3656	-	0,6,6	-	-	-	-	-
84	OHX	v	301	-	0,6,6	-	-	-	-	-
84	OHX	6	1965	-	0,6,6	-	-	-	-	-
84	OHX	AR	3576	-	0,6,6	-	-	-	-	-
84	OHX	DH	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3719	-	0,6,6	-	-	-	-	-
84	OHX	A	2027	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3521	-	0,6,6	-	-	-		
84	OHX	AR	3528	-	0,6,6	-	-	-		
84	OHX	AR	3587	-	0,6,6	-	-	-		
86	7MB	1	4216	-	16,23,23	1.32	3 (18%)	8,38,38	1.59	2 (25%)
84	OHX	1	3503	-	0,6,6	-	-	-		
84	OHX	1	3620	-	0,6,6	-	-	-		
84	OHX	AR	3486	-	0,6,6	-	-	-		
84	OHX	1	3645	-	0,6,6	-	-	-		
84	OHX	CL	301	-	0,6,6	-	-	-		
84	OHX	1	3560	-	0,6,6	-	-	-		
84	OHX	A	1944	-	0,6,6	-	-	-		
84	OHX	1	3416	-	0,6,6	-	-	-		
84	OHX	4	205	-	0,6,6	-	-	-		
84	OHX	AR	3660	-	0,6,6	-	-	-		
84	OHX	AR	3644	-	0,6,6	-	-	-		
84	OHX	A	2030	-	0,6,6	-	-	-		
84	OHX	1	3463	-	0,6,6	-	-	-		
84	OHX	1	3530	-	0,6,6	-	-	-		
84	OHX	1	3574	-	0,6,6	-	-	-		
84	OHX	6	1986	-	0,6,6	-	-	-		
84	OHX	1	3621	-	0,6,6	-	-	-		
84	OHX	AR	3627	-	0,6,6	-	-	-		
84	OHX	AR	3710	-	0,6,6	-	-	-		
84	OHX	AR	3729	-	0,6,6	-	-	-		
84	OHX	A	1929	-	0,6,6	-	-	-		
84	OHX	1	3585	-	0,6,6	-	-	-		
84	OHX	AR	3676	-	0,6,6	-	-	-		
84	OHX	AR	3683	-	0,6,6	-	-	-		
84	OHX	AT	212	-	0,6,6	-	-	-		
84	OHX	AR	3577	-	0,6,6	-	-	-		
84	OHX	6	2048	-	0,6,6	-	-	-		
84	OHX	1	3446	-	0,6,6	-	-	-		
84	OHX	1	3431	-	0,6,6	-	-	-		
84	OHX	6	2021	-	0,6,6	-	-	-		
84	OHX	AR	3610	-	0,6,6	-	-	-		
84	OHX	1	3640	-	0,6,6	-	-	-		
84	OHX	4	207	-	0,6,6	-	-	-		
84	OHX	AR	3484	-	0,6,6	-	-	-		
84	OHX	1	3628	-	0,6,6	-	-	-		
84	OHX	1	3666	-	0,6,6	-	-	-		
84	OHX	1	3718	-	0,6,6	-	-	-		
84	OHX	k	402	-	0,6,6	-	-	-		
84	OHX	6	1961	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3680	-	0,6,6	-	-	-		
84	OHX	AR	3611	-	0,6,6	-	-	-		
84	OHX	6	1942	-	0,6,6	-	-	-		
84	OHX	1	3692	-	0,6,6	-	-	-		
84	OHX	4	204	-	0,6,6	-	-	-		
84	OHX	A	1903	-	0,6,6	-	-	-		
84	OHX	AR	3673	-	0,6,6	-	-	-		
84	OHX	1	3547	-	0,6,6	-	-	-		
84	OHX	1	3639	-	0,6,6	-	-	-		
84	OHX	6	1988	-	0,6,6	-	-	-		
84	OHX	AT	203	-	0,6,6	-	-	-		
84	OHX	A	1922	-	0,6,6	-	-	-		
84	OHX	A	2023	-	0,6,6	-	-	-		
84	OHX	AR	3516	-	0,6,6	-	-	-		
84	OHX	6	1976	-	0,6,6	-	-	-		
84	OHX	1	3578	-	0,6,6	-	-	-		
84	OHX	1	3590	-	0,6,6	-	-	-		
84	OHX	AR	3455	-	0,6,6	-	-	-		
84	OHX	AR	3659	-	0,6,6	-	-	-		
84	OHX	A	1969	-	0,6,6	-	-	-		
84	OHX	A	2016	-	0,6,6	-	-	-		
84	OHX	1	3432	-	0,6,6	-	-	-		
84	OHX	A	2031	-	0,6,6	-	-	-		
84	OHX	AR	3423	-	0,6,6	-	-	-		
84	OHX	A	1951	-	0,6,6	-	-	-		
84	OHX	AR	3536	-	0,6,6	-	-	-		
84	OHX	1	3516	-	0,6,6	-	-	-		
84	OHX	AR	3491	-	0,6,6	-	-	-		
84	OHX	1	3543	-	0,6,6	-	-	-		
84	OHX	1	3440	-	0,6,6	-	-	-		
84	OHX	1	3655	-	0,6,6	-	-	-		
84	OHX	6	1982	-	0,6,6	-	-	-		
84	OHX	A	1920	-	0,6,6	-	-	-		
84	OHX	AR	3558	-	0,6,6	-	-	-		
84	OHX	1	3469	-	0,6,6	-	-	-		
84	OHX	CO	201	-	0,6,6	-	-	-		
84	OHX	A	1970	-	0,6,6	-	-	-		
84	OHX	AR	3461	-	0,6,6	-	-	-		
84	OHX	AR	3674	-	0,6,6	-	-	-		
84	OHX	A	1955	-	0,6,6	-	-	-		
84	OHX	1	3460	-	0,6,6	-	-	-		
84	OHX	1	3510	-	0,6,6	-	-	-		
84	OHX	6	2019	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3708	-	0,6,6	-	-	-	-	-
84	OHX	A	2039	-	0,6,6	-	-	-	-	-
84	OHX	AR	3436	-	0,6,6	-	-	-	-	-
84	OHX	AR	3483	-	0,6,6	-	-	-	-	-
84	OHX	AR	3552	-	0,6,6	-	-	-	-	-
84	OHX	1	3603	-	0,6,6	-	-	-	-	-
84	OHX	AR	3551	-	0,6,6	-	-	-	-	-
84	OHX	AR	3420	-	0,6,6	-	-	-	-	-
84	OHX	1	3418	-	0,6,6	-	-	-	-	-
84	OHX	1	3727	-	0,6,6	-	-	-	-	-
84	OHX	AR	3688	-	0,6,6	-	-	-	-	-
84	OHX	1	3557	-	0,6,6	-	-	-	-	-
84	OHX	A	1901	-	0,6,6	-	-	-	-	-
84	OHX	AR	3709	-	0,6,6	-	-	-	-	-
84	OHX	CL	302	-	0,6,6	-	-	-	-	-
84	OHX	1	3481	-	0,6,6	-	-	-	-	-
84	OHX	AR	3492	-	0,6,6	-	-	-	-	-
84	OHX	DL	101	-	0,6,6	-	-	-	-	-
84	OHX	1	3534	-	0,6,6	-	-	-	-	-
84	OHX	A	1935	-	0,6,6	-	-	-	-	-
84	OHX	1	3584	-	0,6,6	-	-	-	-	-
84	OHX	AR	3555	-	0,6,6	-	-	-	-	-
84	OHX	1	3724	-	0,6,6	-	-	-	-	-
84	OHX	AR	3517	-	0,6,6	-	-	-	-	-
84	OHX	AR	3428	-	0,6,6	-	-	-	-	-
84	OHX	1	3533	-	0,6,6	-	-	-	-	-
84	OHX	1	3502	-	0,6,6	-	-	-	-	-
84	OHX	AR	3441	-	0,6,6	-	-	-	-	-
84	OHX	AR	3402	-	0,6,6	-	-	-	-	-
84	OHX	AR	3442	-	0,6,6	-	-	-	-	-
84	OHX	1	3427	-	0,6,6	-	-	-	-	-
84	OHX	AR	3448	-	0,6,6	-	-	-	-	-
84	OHX	AR	3535	-	0,6,6	-	-	-	-	-
84	OHX	AR	3678	-	0,6,6	-	-	-	-	-
84	OHX	A	1990	-	0,6,6	-	-	-	-	-
84	OHX	AR	3495	-	0,6,6	-	-	-	-	-
84	OHX	A	1924	-	0,6,6	-	-	-	-	-
84	OHX	1	3473	-	0,6,6	-	-	-	-	-
84	OHX	AR	3664	-	0,6,6	-	-	-	-	-
84	OHX	1	3442	-	0,6,6	-	-	-	-	-
84	OHX	6	1960	-	0,6,6	-	-	-	-	-
84	OHX	A	1904	-	0,6,6	-	-	-	-	-
84	OHX	6	1971	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	A	2011	-	0,6,6	-	-	-		
84	OHX	AR	3452	-	0,6,6	-	-	-		
84	OHX	1	3625	-	0,6,6	-	-	-		
84	OHX	AR	3668	-	0,6,6	-	-	-		
84	OHX	A	2040	-	0,6,6	-	-	-		
84	OHX	6	2025	-	0,6,6	-	-	-		
84	OHX	AR	3632	-	0,6,6	-	-	-		
84	OHX	6	2041	-	0,6,6	-	-	-		
84	OHX	A	1905	-	0,6,6	-	-	-		
84	OHX	A	1963	-	0,6,6	-	-	-		
84	OHX	1	3618	-	0,6,6	-	-	-		
84	OHX	A	1930	-	0,6,6	-	-	-		
84	OHX	AR	3553	-	0,6,6	-	-	-		
84	OHX	CF	401	-	0,6,6	-	-	-		
84	OHX	A	2026	-	0,6,6	-	-	-		
84	OHX	A	2038	-	0,6,6	-	-	-		
84	OHX	AR	3499	-	0,6,6	-	-	-		
84	OHX	6	1958	-	0,6,6	-	-	-		
84	OHX	AR	3727	-	0,6,6	-	-	-		
84	OHX	AR	3450	-	0,6,6	-	-	-		
84	OHX	A	2020	-	0,6,6	-	-	-		
84	OHX	1	3412	-	0,6,6	-	-	-		
84	OHX	1	3725	-	0,6,6	-	-	-		
84	OHX	3	203	-	0,6,6	-	-	-		
84	OHX	A	1983	-	0,6,6	-	-	-		
84	OHX	A	2041	-	0,6,6	-	-	-		
84	OHX	AR	3493	-	0,6,6	-	-	-		
84	OHX	AR	3496	-	0,6,6	-	-	-		
84	OHX	A	1906	-	0,6,6	-	-	-		
84	OHX	AR	3662	-	0,6,6	-	-	-		
84	OHX	AR	3713	-	0,6,6	-	-	-		
84	OHX	AR	3524	-	0,6,6	-	-	-		
84	OHX	AC	101	-	0,6,6	-	-	-		
84	OHX	1	3643	-	0,6,6	-	-	-		
84	OHX	AR	3569	-	0,6,6	-	-	-		
84	OHX	CZ	201	-	0,6,6	-	-	-		
84	OHX	1	3507	-	0,6,6	-	-	-		
84	OHX	6	2042	-	0,6,6	-	-	-		
84	OHX	AG	201	-	0,6,6	-	-	-		
84	OHX	A	1953	-	0,6,6	-	-	-		
84	OHX	A	2008	-	0,6,6	-	-	-		
84	OHX	AR	3671	-	0,6,6	-	-	-		
84	OHX	6	1940	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3473	-	0,6,6	-	-	-		
84	OHX	1	3730	-	0,6,6	-	-	-		
84	OHX	A	2013	-	0,6,6	-	-	-		
84	OHX	1	3511	-	0,6,6	-	-	-		
84	OHX	6	2036	-	0,6,6	-	-	-		
84	OHX	1	3631	-	0,6,6	-	-	-		
84	OHX	1	3675	-	0,6,6	-	-	-		
84	OHX	1	3569	-	0,6,6	-	-	-		
84	OHX	AR	3522	-	0,6,6	-	-	-		
84	OHX	AR	3735	-	0,6,6	-	-	-		
84	OHX	AT	214	-	0,6,6	-	-	-		
84	OHX	A	1973	-	0,6,6	-	-	-		
84	OHX	1	3470	-	0,6,6	-	-	-		
84	OHX	A	2012	-	0,6,6	-	-	-		
84	OHX	AR	3485	-	0,6,6	-	-	-		
84	OHX	AR	3426	-	0,6,6	-	-	-		
84	OHX	1	3661	-	0,6,6	-	-	-		
84	OHX	AR	3523	-	0,6,6	-	-	-		
84	OHX	AR	3621	-	0,6,6	-	-	-		
84	OHX	1	3712	-	0,6,6	-	-	-		
84	OHX	1	3674	-	0,6,6	-	-	-		
84	OHX	k	401	-	0,6,6	-	-	-		
84	OHX	AR	3704	-	0,6,6	-	-	-		
84	OHX	6	2055	-	0,6,6	-	-	-		
84	OHX	A	1946	-	0,6,6	-	-	-		
84	OHX	A	2015	-	0,6,6	-	-	-		
84	OHX	A	2029	-	0,6,6	-	-	-		
84	OHX	6	1925	-	0,6,6	-	-	-		
84	OHX	A	1928	-	0,6,6	-	-	-		
84	OHX	1	3678	-	0,6,6	-	-	-		
84	OHX	AR	3724	-	0,6,6	-	-	-		
84	OHX	1	3651	-	0,6,6	-	-	-		
84	OHX	AR	3416	-	0,6,6	-	-	-		
84	OHX	AR	3451	-	0,6,6	-	-	-		
84	OHX	1	3695	-	0,6,6	-	-	-		
84	OHX	AR	3638	-	0,6,6	-	-	-		
84	OHX	6	2005	-	0,6,6	-	-	-		
84	OHX	A	1921	-	0,6,6	-	-	-		
84	OHX	1	3482	-	0,6,6	-	-	-		
84	OHX	1	3654	-	0,6,6	-	-	-		
84	OHX	1	3519	-	0,6,6	-	-	-		
84	OHX	AR	3657	-	0,6,6	-	-	-		
84	OHX	AR	3468	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AR	3506	-	0,6,6	-	-	-	-	-
84	OHX	1	3624	-	0,6,6	-	-	-	-	-
84	OHX	1	3615	-	0,6,6	-	-	-	-	-
84	OHX	AR	3531	-	0,6,6	-	-	-	-	-
84	OHX	AR	3544	-	0,6,6	-	-	-	-	-
84	OHX	AR	3689	-	0,6,6	-	-	-	-	-
84	OHX	AR	3728	-	0,6,6	-	-	-	-	-
84	OHX	6	2031	-	0,6,6	-	-	-	-	-
84	OHX	AR	3690	-	0,6,6	-	-	-	-	-
84	OHX	AR	3502	-	0,6,6	-	-	-	-	-
84	OHX	AR	3550	-	0,6,6	-	-	-	-	-
84	OHX	AR	3572	-	0,6,6	-	-	-	-	-
84	OHX	AR	3706	-	0,6,6	-	-	-	-	-
84	OHX	1	3691	-	0,6,6	-	-	-	-	-
84	OHX	AR	3422	-	0,6,6	-	-	-	-	-
84	OHX	AR	3589	-	0,6,6	-	-	-	-	-
84	OHX	1	3728	-	0,6,6	-	-	-	-	-
84	OHX	AT	216	-	0,6,6	-	-	-	-	-
84	OHX	AR	3549	-	0,6,6	-	-	-	-	-
84	OHX	1	3707	-	0,6,6	-	-	-	-	-
84	OHX	AR	3574	-	0,6,6	-	-	-	-	-
84	OHX	A	2022	-	0,6,6	-	-	-	-	-
84	OHX	1	3717	-	0,6,6	-	-	-	-	-
84	OHX	AR	3434	-	0,6,6	-	-	-	-	-
84	OHX	A	1988	-	0,6,6	-	-	-	-	-
84	OHX	A	1914	-	0,6,6	-	-	-	-	-
84	OHX	6	1955	-	0,6,6	-	-	-	-	-
84	OHX	1	3705	-	0,6,6	-	-	-	-	-
84	OHX	6	1983	-	0,6,6	-	-	-	-	-
84	OHX	AR	3443	-	0,6,6	-	-	-	-	-
84	OHX	AR	3703	-	0,6,6	-	-	-	-	-
84	OHX	4	208	-	0,6,6	-	-	-	-	-
84	OHX	AR	3409	-	0,6,6	-	-	-	-	-
84	OHX	A	1968	-	0,6,6	-	-	-	-	-
84	OHX	1	3646	-	0,6,6	-	-	-	-	-
84	OHX	4	211	-	0,6,6	-	-	-	-	-
84	OHX	1	3587	-	0,6,6	-	-	-	-	-
84	OHX	A	1982	-	0,6,6	-	-	-	-	-
84	OHX	AS	210	-	0,6,6	-	-	-	-	-
84	OHX	AT	220	-	0,6,6	-	-	-	-	-
84	OHX	1	3586	-	0,6,6	-	-	-	-	-
84	OHX	AR	3456	-	0,6,6	-	-	-	-	-
84	OHX	6	2032	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1953	-	0,6,6	-	-	-		
84	OHX	1	3425	-	0,6,6	-	-	-		
84	OHX	1	3424	-	0,6,6	-	-	-		
84	OHX	1	3703	-	0,6,6	-	-	-		
84	OHX	AR	3480	-	0,6,6	-	-	-		
84	OHX	H	301	-	0,6,6	-	-	-		
84	OHX	AR	3714	-	0,6,6	-	-	-		
84	OHX	6	1923	-	0,6,6	-	-	-		
84	OHX	1	3526	-	0,6,6	-	-	-		
84	OHX	1	3552	-	0,6,6	-	-	-		
84	OHX	3	206	-	0,6,6	-	-	-		
84	OHX	AR	3608	-	0,6,6	-	-	-		
84	OHX	AR	3736	-	0,6,6	-	-	-		
84	OHX	1	3439	-	0,6,6	-	-	-		
84	OHX	AR	3653	-	0,6,6	-	-	-		
84	OHX	CG	303	-	0,6,6	-	-	-		
84	OHX	1	3435	-	0,6,6	-	-	-		
84	OHX	A	1978	-	0,6,6	-	-	-		
84	OHX	1	3592	-	0,6,6	-	-	-		
84	OHX	6	2023	-	0,6,6	-	-	-		
84	OHX	AR	3601	-	0,6,6	-	-	-		
84	OHX	A	1961	-	0,6,6	-	-	-		
84	OHX	AR	3465	-	0,6,6	-	-	-		
84	OHX	1	3684	-	0,6,6	-	-	-		
84	OHX	CE	402	-	0,6,6	-	-	-		
84	OHX	1	3449	-	0,6,6	-	-	-		
84	OHX	6	1904	-	0,6,6	-	-	-		
84	OHX	6	2011	-	0,6,6	-	-	-		
84	OHX	AR	3720	-	0,6,6	-	-	-		
84	OHX	A	1994	-	0,6,6	-	-	-		
84	OHX	1	3716	-	0,6,6	-	-	-		
84	OHX	4	212	-	0,6,6	-	-	-		
84	OHX	AR	3666	-	0,6,6	-	-	-		
84	OHX	AR	3667	-	0,6,6	-	-	-		
84	OHX	AR	3732	-	0,6,6	-	-	-		
84	OHX	DD	102	-	0,6,6	-	-	-		
84	OHX	AR	3559	-	0,6,6	-	-	-		
84	OHX	6	1918	-	0,6,6	-	-	-		
84	OHX	AR	3633	-	0,6,6	-	-	-		
84	OHX	A	1910	-	0,6,6	-	-	-		
84	OHX	AR	3453	-	0,6,6	-	-	-		
84	OHX	AR	3438	-	0,6,6	-	-	-		
84	OHX	A	1925	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3607	-	0,6,6	-	-	-	-	-
84	OHX	1	3647	-	0,6,6	-	-	-	-	-
84	OHX	6	1934	-	0,6,6	-	-	-	-	-
84	OHX	CG	302	-	0,6,6	-	-	-	-	-
84	OHX	1	3457	-	0,6,6	-	-	-	-	-
84	OHX	AR	3432	-	0,6,6	-	-	-	-	-
84	OHX	AR	3494	-	0,6,6	-	-	-	-	-
84	OHX	1	3609	-	0,6,6	-	-	-	-	-
84	OHX	AR	3478	-	0,6,6	-	-	-	-	-
84	OHX	AR	3546	-	0,6,6	-	-	-	-	-
84	OHX	AR	3696	-	0,6,6	-	-	-	-	-
84	OHX	1	3477	-	0,6,6	-	-	-	-	-
84	OHX	1	3500	-	0,6,6	-	-	-	-	-
84	OHX	1	3571	-	0,6,6	-	-	-	-	-
84	OHX	1	3602	-	0,6,6	-	-	-	-	-
84	OHX	AR	3538	-	0,6,6	-	-	-	-	-
84	OHX	AR	3652	-	0,6,6	-	-	-	-	-
84	OHX	AR	3617	-	0,6,6	-	-	-	-	-
84	OHX	AR	3701	-	0,6,6	-	-	-	-	-
84	OHX	AR	3625	-	0,6,6	-	-	-	-	-
84	OHX	AS	207	-	0,6,6	-	-	-	-	-
84	OHX	1	3642	-	0,6,6	-	-	-	-	-
84	OHX	6	1926	-	0,6,6	-	-	-	-	-
84	OHX	AR	3467	-	0,6,6	-	-	-	-	-
84	OHX	AR	3650	-	0,6,6	-	-	-	-	-
84	OHX	CF	402	-	0,6,6	-	-	-	-	-
84	OHX	AR	3645	-	0,6,6	-	-	-	-	-
84	OHX	AR	3419	-	0,6,6	-	-	-	-	-
84	OHX	1	3464	-	0,6,6	-	-	-	-	-
84	OHX	1	3561	-	0,6,6	-	-	-	-	-
84	OHX	c8	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3614	-	0,6,6	-	-	-	-	-
84	OHX	6	1912	-	0,6,6	-	-	-	-	-
84	OHX	A	1939	-	0,6,6	-	-	-	-	-
84	OHX	1	3636	-	0,6,6	-	-	-	-	-
84	OHX	1	3567	-	0,6,6	-	-	-	-	-
84	OHX	6	2037	-	0,6,6	-	-	-	-	-
84	OHX	1	3681	-	0,6,6	-	-	-	-	-
84	OHX	AR	3557	-	0,6,6	-	-	-	-	-
84	OHX	AR	3649	-	0,6,6	-	-	-	-	-
84	OHX	6	1943	-	0,6,6	-	-	-	-	-
84	OHX	1	3527	-	0,6,6	-	-	-	-	-
84	OHX	6	1987	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	2000	-	0,6,6	-	-	-		
84	OHX	AR	3590	-	0,6,6	-	-	-		
84	OHX	1	3441	-	0,6,6	-	-	-		
84	OHX	6	2008	-	0,6,6	-	-	-		
84	OHX	6	1903	-	0,6,6	-	-	-		
84	OHX	6	1946	-	0,6,6	-	-	-		
84	OHX	AR	3475	-	0,6,6	-	-	-		
84	OHX	AR	3593	-	0,6,6	-	-	-		
84	OHX	Q	201	-	0,6,6	-	-	-		
84	OHX	6	1907	-	0,6,6	-	-	-		
84	OHX	A	2028	-	0,6,6	-	-	-		
84	OHX	1	3564	-	0,6,6	-	-	-		
84	OHX	1	3622	-	0,6,6	-	-	-		
84	OHX	AR	3562	-	0,6,6	-	-	-		
84	OHX	A	1967	-	0,6,6	-	-	-		
84	OHX	AR	3731	-	0,6,6	-	-	-		
84	OHX	A	1979	-	0,6,6	-	-	-		
84	OHX	AR	3669	-	0,6,6	-	-	-		
84	OHX	6	2006	-	0,6,6	-	-	-		
84	OHX	AR	3670	-	0,6,6	-	-	-		
84	OHX	A	1919	-	0,6,6	-	-	-		
84	OHX	6	2002	-	0,6,6	-	-	-		
84	OHX	A	1927	-	0,6,6	-	-	-		
84	OHX	AR	3407	-	0,6,6	-	-	-		
84	OHX	AR	3692	-	0,6,6	-	-	-		
84	OHX	1	3563	-	0,6,6	-	-	-		
84	OHX	1	3668	-	0,6,6	-	-	-		
84	OHX	AR	3515	-	0,6,6	-	-	-		
84	OHX	AR	3472	-	0,6,6	-	-	-		
84	OHX	6	1921	-	0,6,6	-	-	-		
84	OHX	1	3537	-	0,6,6	-	-	-		
84	OHX	3	202	-	0,6,6	-	-	-		
84	OHX	1	3711	-	0,6,6	-	-	-		
84	OHX	6	1910	-	0,6,6	-	-	-		
84	OHX	T	201	-	0,6,6	-	-	-		
84	OHX	A	1942	-	0,6,6	-	-	-		
84	OHX	1	3444	-	0,6,6	-	-	-		
84	OHX	AR	3693	-	0,6,6	-	-	-		
84	OHX	A	1902	-	0,6,6	-	-	-		
84	OHX	6	1951	-	0,6,6	-	-	-		
84	OHX	y	201	-	0,6,6	-	-	-		
84	OHX	x	201	-	0,6,6	-	-	-		
84	OHX	1	3509	-	0,6,6	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3486	-	0,6,6	-	-	-	-	-
84	OHX	6	2047	-	0,6,6	-	-	-	-	-
84	OHX	sR	401	-	0,6,6	-	-	-	-	-
84	OHX	AR	3570	-	0,6,6	-	-	-	-	-
84	OHX	6	1981	-	0,6,6	-	-	-	-	-
84	OHX	AR	3539	-	0,6,6	-	-	-	-	-
84	OHX	3	205	-	0,6,6	-	-	-	-	-
84	OHX	A	1918	-	0,6,6	-	-	-	-	-
84	OHX	AR	3598	-	0,6,6	-	-	-	-	-
84	OHX	1	3576	-	0,6,6	-	-	-	-	-
84	OHX	1	3700	-	0,6,6	-	-	-	-	-
84	OHX	AR	3525	-	0,6,6	-	-	-	-	-
84	OHX	1	3445	-	0,6,6	-	-	-	-	-
84	OHX	1	3721	-	0,6,6	-	-	-	-	-
84	OHX	AR	3634	-	0,6,6	-	-	-	-	-
84	OHX	A	1977	-	0,6,6	-	-	-	-	-
84	OHX	AR	3661	-	0,6,6	-	-	-	-	-
84	OHX	A	1992	-	0,6,6	-	-	-	-	-
84	OHX	1	3405	-	0,6,6	-	-	-	-	-
84	OHX	AR	3641	-	0,6,6	-	-	-	-	-
84	OHX	AR	3583	-	0,6,6	-	-	-	-	-
84	OHX	CM	201	-	0,6,6	-	-	-	-	-
84	OHX	1	3407	-	0,6,6	-	-	-	-	-
84	OHX	AR	3568	-	0,6,6	-	-	-	-	-
84	OHX	AR	3403	-	0,6,6	-	-	-	-	-
84	OHX	A	2003	-	0,6,6	-	-	-	-	-
84	OHX	A	1984	-	0,6,6	-	-	-	-	-
84	OHX	1	3710	-	0,6,6	-	-	-	-	-
84	OHX	1	3729	-	0,6,6	-	-	-	-	-
84	OHX	A	2032	-	0,6,6	-	-	-	-	-
84	OHX	1	3478	-	0,6,6	-	-	-	-	-
84	OHX	1	3701	-	0,6,6	-	-	-	-	-
84	OHX	1	3523	-	0,6,6	-	-	-	-	-
84	OHX	1	3467	-	0,6,6	-	-	-	-	-
84	OHX	6	1966	-	0,6,6	-	-	-	-	-
84	OHX	1	3455	-	0,6,6	-	-	-	-	-
84	OHX	1	3454	-	0,6,6	-	-	-	-	-
84	OHX	1	3698	-	0,6,6	-	-	-	-	-
84	OHX	1	3626	-	0,6,6	-	-	-	-	-
84	OHX	6	2045	-	0,6,6	-	-	-	-	-
84	OHX	1	3653	-	0,6,6	-	-	-	-	-
84	OHX	AR	3429	-	0,6,6	-	-	-	-	-
84	OHX	1	401	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3528	-	0,6,6	-	-	-	-	-
84	OHX	6	1956	-	0,6,6	-	-	-	-	-
84	OHX	AR	3594	-	0,6,6	-	-	-	-	-
84	OHX	AR	3404	-	0,6,6	-	-	-	-	-
84	OHX	AR	3607	-	0,6,6	-	-	-	-	-
84	OHX	A	1923	-	0,6,6	-	-	-	-	-
84	OHX	A	1959	-	0,6,6	-	-	-	-	-
84	OHX	A	2005	-	0,6,6	-	-	-	-	-
84	OHX	6	2043	-	0,6,6	-	-	-	-	-
84	OHX	AR	3406	-	0,6,6	-	-	-	-	-
84	OHX	6	1954	-	0,6,6	-	-	-	-	-
84	OHX	AR	3695	-	0,6,6	-	-	-	-	-
84	OHX	1	3611	-	0,6,6	-	-	-	-	-
84	OHX	AR	3433	-	0,6,6	-	-	-	-	-
84	OHX	1	3508	-	0,6,6	-	-	-	-	-
84	OHX	1	3554	-	0,6,6	-	-	-	-	-
84	OHX	AR	3702	-	0,6,6	-	-	-	-	-
84	OHX	A	1956	-	0,6,6	-	-	-	-	-
84	OHX	AR	3734	-	0,6,6	-	-	-	-	-
84	OHX	1	3600	-	0,6,6	-	-	-	-	-
84	OHX	1	3694	-	0,6,6	-	-	-	-	-
84	OHX	AT	211	-	0,6,6	-	-	-	-	-
84	OHX	1	3573	-	0,6,6	-	-	-	-	-
84	OHX	1	3659	-	0,6,6	-	-	-	-	-
84	OHX	6	2054	-	0,6,6	-	-	-	-	-
84	OHX	4	203	-	0,6,6	-	-	-	-	-
84	OHX	AR	3665	-	0,6,6	-	-	-	-	-
84	OHX	AT	207	-	0,6,6	-	-	-	-	-
84	OHX	1	3731	-	0,6,6	-	-	-	-	-
84	OHX	6	1902	-	0,6,6	-	-	-	-	-
84	OHX	1	3512	-	0,6,6	-	-	-	-	-
84	OHX	AR	3564	-	0,6,6	-	-	-	-	-
84	OHX	1	3479	-	0,6,6	-	-	-	-	-
84	OHX	6	2044	-	0,6,6	-	-	-	-	-
84	OHX	6	1990	-	0,6,6	-	-	-	-	-
84	OHX	1	3414	-	0,6,6	-	-	-	-	-
84	OHX	1	3619	-	0,6,6	-	-	-	-	-
84	OHX	AR	3599	-	0,6,6	-	-	-	-	-
84	OHX	1	3529	-	0,6,6	-	-	-	-	-
84	OHX	AR	3717	-	0,6,6	-	-	-	-	-
84	OHX	6	2007	-	0,6,6	-	-	-	-	-
84	OHX	1	3484	-	0,6,6	-	-	-	-	-
84	OHX	6	1937	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	6	1917	-	0,6,6	-	-	-	-	-
84	OHX	1	3658	-	0,6,6	-	-	-	-	-
84	OHX	AT	209	-	0,6,6	-	-	-	-	-
84	OHX	AR	3697	-	0,6,6	-	-	-	-	-
84	OHX	1	3411	-	0,6,6	-	-	-	-	-
84	OHX	1	3686	-	0,6,6	-	-	-	-	-
84	OHX	AR	3588	-	0,6,6	-	-	-	-	-
84	OHX	6	2050	-	0,6,6	-	-	-	-	-
84	OHX	1	3683	-	0,6,6	-	-	-	-	-
84	OHX	1	3693	-	0,6,6	-	-	-	-	-
84	OHX	1	3458	-	0,6,6	-	-	-	-	-
84	OHX	1	3551	-	0,6,6	-	-	-	-	-
84	OHX	AR	3481	-	0,6,6	-	-	-	-	-
84	OHX	x	202	-	0,6,6	-	-	-	-	-
84	OHX	1	3588	-	0,6,6	-	-	-	-	-
84	OHX	AR	3542	-	0,6,6	-	-	-	-	-
84	OHX	CP	501	-	0,6,6	-	-	-	-	-
84	OHX	A	1912	-	0,6,6	-	-	-	-	-
84	OHX	AR	3449	-	0,6,6	-	-	-	-	-
84	OHX	A	2004	-	0,6,6	-	-	-	-	-
84	OHX	c5	201	-	0,6,6	-	-	-	-	-
84	OHX	AR	3532	-	0,6,6	-	-	-	-	-
84	OHX	1	3474	-	0,6,6	-	-	-	-	-
84	OHX	1	3629	-	0,6,6	-	-	-	-	-
84	OHX	1	3536	-	0,6,6	-	-	-	-	-
84	OHX	1	3579	-	0,6,6	-	-	-	-	-
84	OHX	6	1969	-	0,6,6	-	-	-	-	-
84	OHX	6	2030	-	0,6,6	-	-	-	-	-
84	OHX	AR	3511	-	0,6,6	-	-	-	-	-
84	OHX	1	3517	-	0,6,6	-	-	-	-	-
84	OHX	6	1989	-	0,6,6	-	-	-	-	-
84	OHX	6	1947	-	0,6,6	-	-	-	-	-
84	OHX	1	3428	-	0,6,6	-	-	-	-	-
84	OHX	6	2010	-	0,6,6	-	-	-	-	-
84	OHX	6	2027	-	0,6,6	-	-	-	-	-
84	OHX	AR	3427	-	0,6,6	-	-	-	-	-
84	OHX	1	3673	-	0,6,6	-	-	-	-	-
84	OHX	AR	3575	-	0,6,6	-	-	-	-	-
84	OHX	AR	3691	-	0,6,6	-	-	-	-	-
84	OHX	A	1972	-	0,6,6	-	-	-	-	-
84	OHX	1	3410	-	0,6,6	-	-	-	-	-
84	OHX	6	2016	-	0,6,6	-	-	-	-	-
84	OHX	AT	219	-	0,6,6	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	1	3535	-	0,6,6	-	-	-		
86	7MB	AR	4239	-	16,23,23	0.85	0	8,38,38	0.87	0
84	OHX	1	3495	-	0,6,6	-	-	-		
84	OHX	AR	3606	-	0,6,6	-	-	-		
84	OHX	1	3677	-	0,6,6	-	-	-		
84	OHX	1	3596	-	0,6,6	-	-	-		
84	OHX	AR	3651	-	0,6,6	-	-	-		
84	OHX	A	1908	-	0,6,6	-	-	-		
84	OHX	AR	3637	-	0,6,6	-	-	-		
84	OHX	6	1944	-	0,6,6	-	-	-		
84	OHX	AR	3514	-	0,6,6	-	-	-		
84	OHX	AR	3547	-	0,6,6	-	-	-		
84	OHX	A	1980	-	0,6,6	-	-	-		
84	OHX	A	1965	-	0,6,6	-	-	-		
84	OHX	AR	3654	-	0,6,6	-	-	-		
84	OHX	AR	3719	-	0,6,6	-	-	-		
84	OHX	6	2022	-	0,6,6	-	-	-		
84	OHX	A	1907	-	0,6,6	-	-	-		
84	OHX	1	3518	-	0,6,6	-	-	-		
84	OHX	6	2035	-	0,6,6	-	-	-		
84	OHX	1	3436	-	0,6,6	-	-	-		
84	OHX	6	2052	-	0,6,6	-	-	-		
84	OHX	1	3709	-	0,6,6	-	-	-		
84	OHX	AR	3503	-	0,6,6	-	-	-		
84	OHX	A	1911	-	0,6,6	-	-	-		
84	OHX	6	1972	-	0,6,6	-	-	-		
84	OHX	AR	3430	-	0,6,6	-	-	-		
84	OHX	AR	3490	-	0,6,6	-	-	-		
84	OHX	1	3491	-	0,6,6	-	-	-		
84	OHX	AR	3440	-	0,6,6	-	-	-		
84	OHX	AR	3505	-	0,6,6	-	-	-		
84	OHX	6	1995	-	0,6,6	-	-	-		
84	OHX	1	3548	-	0,6,6	-	-	-		
84	OHX	6	1968	-	0,6,6	-	-	-		
84	OHX	1	3613	-	0,6,6	-	-	-		
84	OHX	A	2002	-	0,6,6	-	-	-		
84	OHX	1	3515	-	0,6,6	-	-	-		
84	OHX	1	3524	-	0,6,6	-	-	-		
84	OHX	AR	3454	-	0,6,6	-	-	-		
84	OHX	AR	3476	-	0,6,6	-	-	-		
84	OHX	AR	3739	-	0,6,6	-	-	-		
84	OHX	1	3637	-	0,6,6	-	-	-		
84	OHX	1	3652	-	0,6,6	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
84	OHX	AS	202	-	0,6,6	-	-	-		
84	OHX	AR	3698	-	0,6,6	-	-	-		
84	OHX	A	1940	-	0,6,6	-	-	-		
84	OHX	1	3687	-	0,6,6	-	-	-		
84	OHX	1	3616	-	0,6,6	-	-	-		
84	OHX	1	3448	-	0,6,6	-	-	-		
84	OHX	AR	3597	-	0,6,6	-	-	-		
84	OHX	6	1941	-	0,6,6	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	7MB	AR	4239	-	-	-	0/3/4/4
86	7MB	1	4216	-	-	-	0/3/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
86	1	4216	7MB	C9-C8	-2.54	1.35	1.40
86	1	4216	7MB	O-C1	-2.22	1.19	1.23
86	1	4216	7MB	C10-C11	-2.11	1.36	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
86	1	4216	7MB	C6-C2-N1	-2.82	108.36	113.23
86	1	4216	7MB	C2-N1-C1	-2.34	108.64	113.67

There are no chirality outliers.

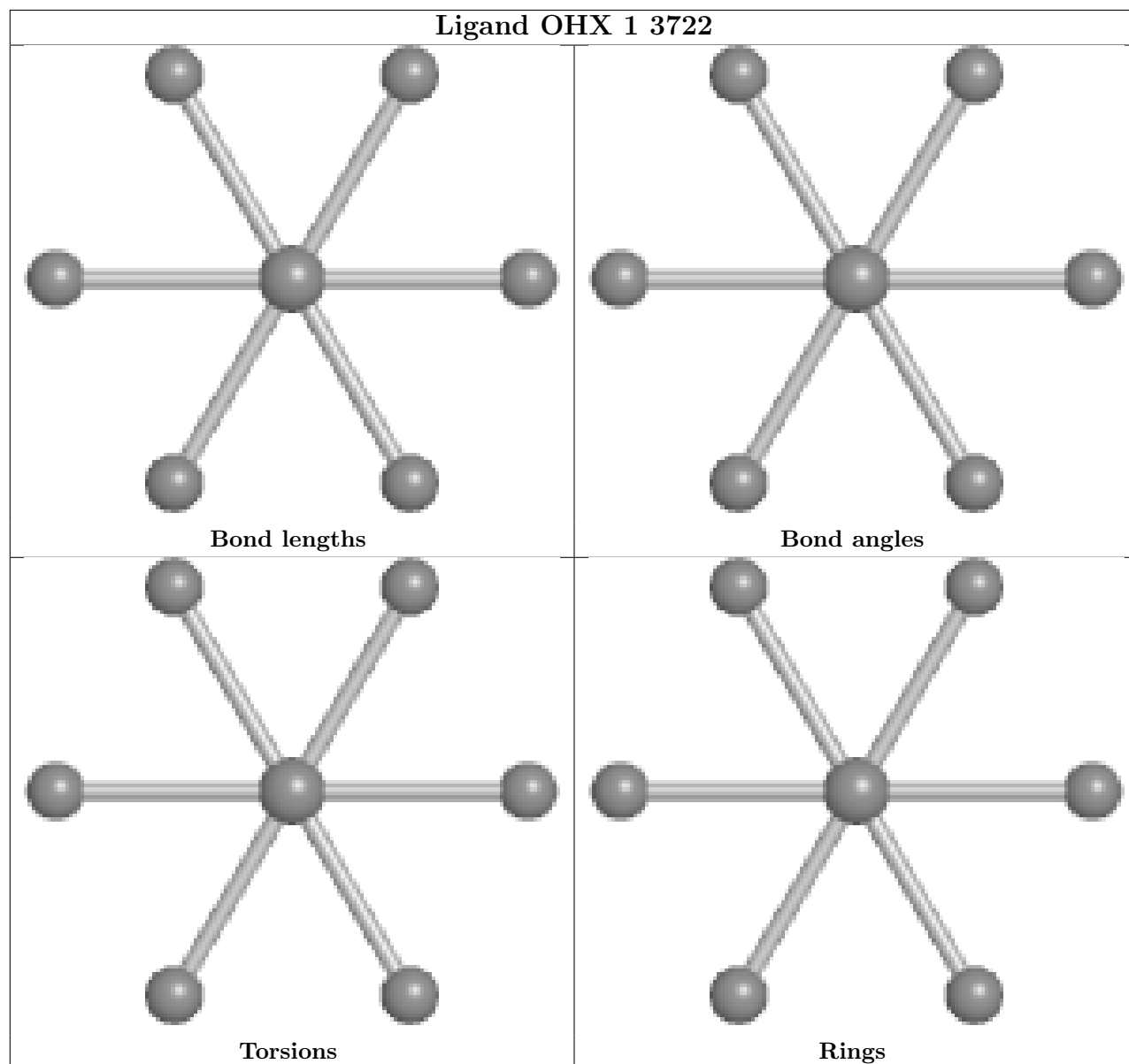
There are no torsion outliers.

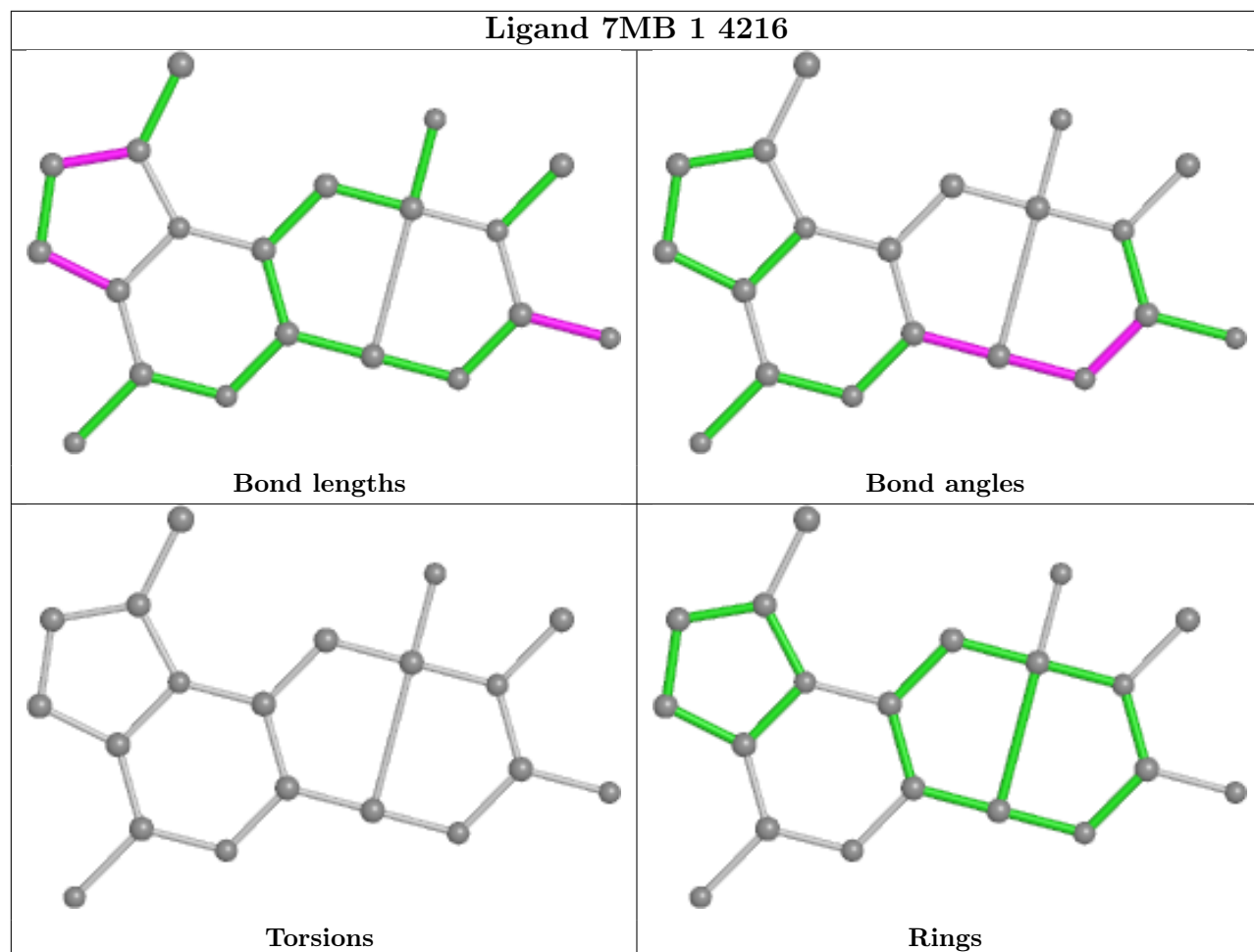
There are no ring outliers.

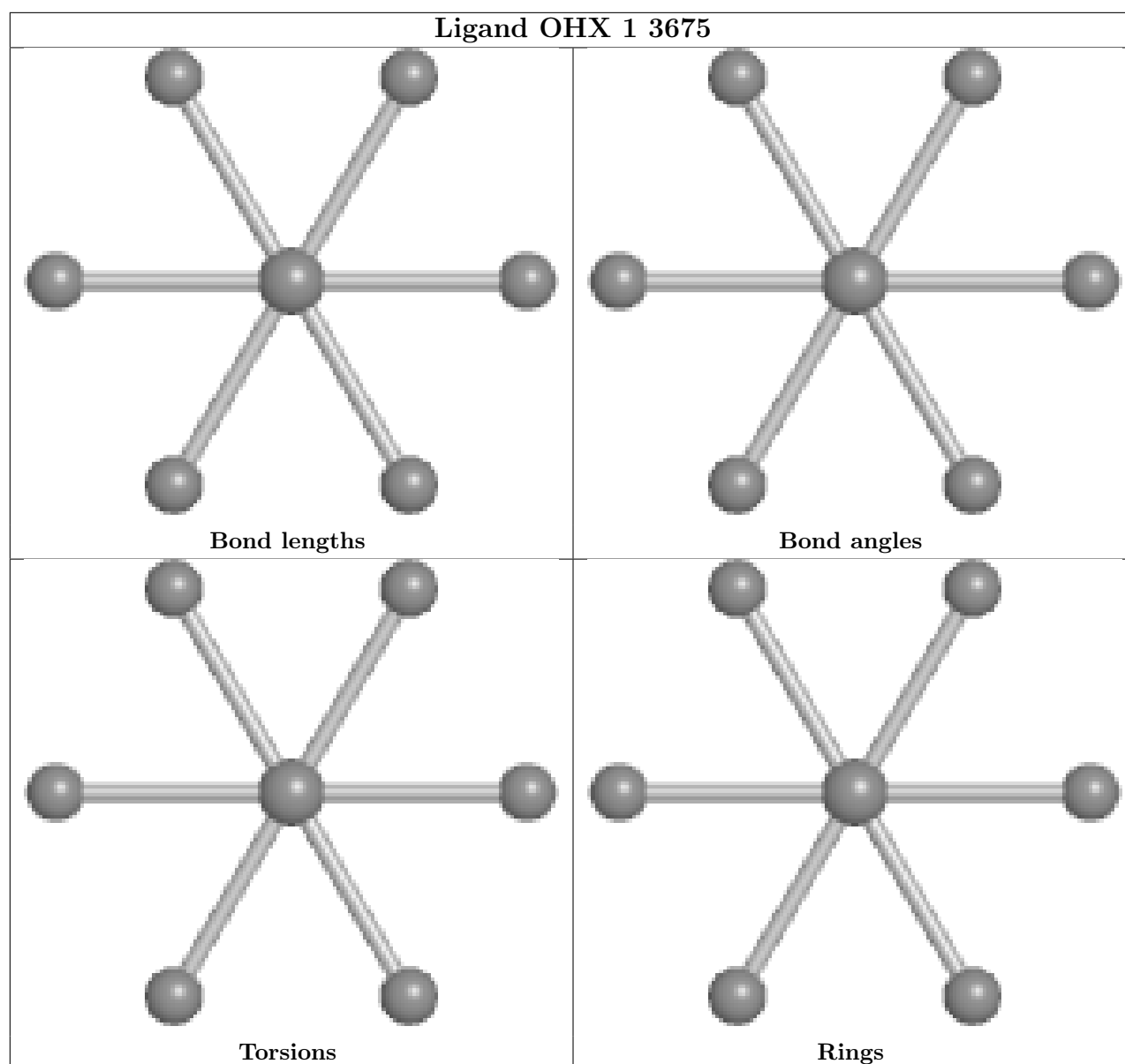
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	sM	2
25	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	sM	85:SER	C	119:UNK	N	44.36
1	sM	139:UNK	C	155:UNK	N	36.85
1	A	1716:C	O3'	1717:G	P	4.45

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	1	3149/3396 (92%)	-0.20	55 (1%) 70 64	22, 53, 169, 269	0
1	AR	3149/3396 (92%)	-0.18	58 (1%) 68 62	22, 51, 152, 280	0
2	3	121/121 (100%)	-0.45	0 100 100	33, 69, 92, 108	0
2	AS	121/121 (100%)	-0.51	1 (0%) 86 81	28, 56, 73, 112	0
3	4	158/158 (100%)	-0.18	1 (0%) 89 86	34, 58, 115, 203	0
3	AT	158/158 (100%)	-0.22	1 (0%) 89 86	35, 62, 125, 189	0
4	CD	252/252 (100%)	-0.39	0 100 100	30, 51, 83, 119	0
4	j	252/252 (100%)	-0.39	0 100 100	29, 54, 76, 118	0
5	CE	386/386 (100%)	-0.48	2 (0%) 91 88	21, 40, 65, 139	0
5	k	386/386 (100%)	-0.32	1 (0%) 94 91	28, 54, 77, 122	0
6	CF	361/361 (100%)	-0.37	0 100 100	30, 50, 79, 110	0
6	l	361/361 (100%)	-0.41	0 100 100	28, 49, 82, 101	0
7	CG	296/296 (100%)	-0.22	4 (1%) 75 69	36, 58, 99, 128	0
7	m	296/296 (100%)	0.03	1 (0%) 94 91	46, 78, 115, 168	0
8	CH	156/175 (89%)	-0.30	0 100 100	35, 49, 88, 129	0
8	n	156/175 (89%)	-0.36	0 100 100	35, 46, 79, 132	0
9	CI	222/222 (100%)	-0.49	2 (0%) 84 79	25, 37, 91, 176	0
9	o	222/222 (100%)	-0.42	0 100 100	28, 40, 80, 161	0
10	CJ	233/233 (100%)	0.65	17 (7%) 15 15	64, 87, 146, 191	0
10	p	233/233 (100%)	0.16	3 (1%) 77 71	54, 82, 138, 160	0
11	CK	191/191 (100%)	-0.36	3 (1%) 72 66	33, 46, 77, 143	0
11	q	191/191 (100%)	-0.28	1 (0%) 91 88	46, 62, 84, 149	0
12	CL	211/220 (95%)	-0.06	4 (1%) 66 61	32, 57, 100, 169	0
12	r	211/220 (95%)	-0.36	0 100 100	35, 53, 108, 127	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	CM	169/169 (100%)	-0.32	0 100 100	45, 61, 83, 105	0
13	s	169/169 (100%)	-0.00	0 100 100	61, 80, 102, 115	0
14	CN	193/193 (100%)	-0.07	1 (0%) 91 88	33, 67, 131, 148	0
14	t	193/193 (100%)	-0.34	1 (0%) 91 88	30, 60, 113, 144	0
15	CO	136/136 (100%)	-0.57	0 100 100	30, 44, 72, 97	0
15	u	136/136 (100%)	-0.42	0 100 100	42, 52, 77, 105	0
16	CP	203/203 (100%)	-0.32	0 100 100	37, 55, 71, 75	0
16	v	203/203 (100%)	-0.45	0 100 100	30, 51, 64, 74	0
17	CQ	197/197 (100%)	-0.53	1 (0%) 91 88	22, 33, 79, 88	0
17	w	197/197 (100%)	-0.51	0 100 100	27, 41, 75, 85	0
18	CR	183/183 (100%)	0.61	25 (13%) 3 4	25, 40, 181, 234	0
18	x	183/183 (100%)	-0.18	8 (4%) 34 30	33, 42, 124, 165	0
19	CS	185/185 (100%)	-0.40	0 100 100	36, 50, 65, 84	0
19	y	185/185 (100%)	-0.43	0 100 100	36, 48, 84, 123	0
20	CT	188/188 (100%)	-0.13	3 (1%) 72 66	42, 61, 148, 170	0
20	z	188/188 (100%)	0.04	3 (1%) 72 66	53, 73, 158, 171	0
21	0	172/172 (100%)	-0.24	1 (0%) 89 86	37, 46, 72, 91	0
21	CU	172/172 (100%)	-0.54	0 100 100	28, 38, 66, 86	0
22	2	159/159 (100%)	-0.25	0 100 100	31, 48, 111, 126	0
22	CV	159/159 (100%)	-0.37	0 100 100	25, 42, 94, 108	0
23	5	100/100 (100%)	0.55	7 (7%) 16 16	86, 108, 135, 159	0
23	CW	100/100 (100%)	0.69	7 (7%) 16 16	70, 94, 120, 162	0
24	CX	136/136 (100%)	-0.12	0 100 100	21, 37, 66, 96	0
24	l2	136/136 (100%)	-0.06	0 100 100	37, 51, 78, 114	0
25	6	1783/1800 (99%)	-0.05	71 (3%) 38 33	34, 76, 201, 266	0
25	A	1781/1800 (98%)	0.09	82 (4%) 32 28	49, 93, 235, 311	0
26	7	98/98 (100%)	1.65	33 (33%) 0 0	52, 69, 199, 216	0
26	CY	98/98 (100%)	0.57	12 (12%) 4 5	35, 52, 188, 226	0
27	8	121/121 (100%)	-0.04	0 100 100	48, 67, 91, 130	0
27	CZ	121/121 (100%)	-0.07	2 (1%) 70 64	48, 67, 91, 132	0
28	9	126/126 (100%)	-0.06	1 (0%) 86 81	42, 58, 80, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	DA	126/126 (100%)	-0.05	1 (0%) 86 81	43, 61, 87, 103	0
29	AA	135/135 (100%)	0.70	4 (2%) 50 44	76, 100, 124, 133	0
29	DB	135/135 (100%)	0.50	4 (2%) 50 44	77, 99, 124, 136	0
30	AB	148/148 (100%)	-0.30	0 100 100	25, 48, 89, 106	0
30	DC	148/148 (100%)	-0.32	0 100 100	26, 52, 87, 95	0
31	AC	58/58 (100%)	-0.41	0 100 100	31, 55, 111, 132	0
31	DD	58/58 (100%)	-0.54	0 100 100	30, 56, 92, 112	0
32	AD	97/97 (100%)	0.42	4 (4%) 37 33	77, 92, 122, 140	0
32	DE	97/97 (100%)	0.16	1 (1%) 82 77	66, 82, 112, 135	0
33	AE	109/109 (100%)	-0.03	2 (1%) 68 62	46, 67, 123, 146	0
33	DF	109/109 (100%)	-0.16	0 100 100	35, 52, 119, 142	0
34	AF	127/127 (100%)	-0.32	2 (1%) 72 66	24, 40, 59, 133	0
34	DG	127/127 (100%)	-0.18	1 (0%) 86 81	24, 46, 66, 132	0
35	AG	106/106 (100%)	-0.58	0 100 100	28, 37, 62, 89	0
35	DH	106/106 (100%)	-0.43	0 100 100	27, 36, 82, 124	0
36	AH	112/112 (100%)	-0.09	0 100 100	53, 73, 130, 149	0
36	DI	112/112 (100%)	-0.20	0 100 100	48, 70, 134, 155	0
37	AI	119/119 (100%)	-0.15	1 (0%) 86 81	45, 68, 85, 92	0
37	DJ	119/119 (100%)	-0.10	2 (1%) 70 64	51, 75, 94, 113	0
38	AJ	99/99 (100%)	0.02	2 (2%) 65 60	50, 69, 116, 148	0
38	DK	99/99 (100%)	0.18	2 (2%) 65 60	59, 74, 118, 154	0
39	AK	87/87 (100%)	-0.46	0 100 100	34, 44, 77, 128	0
39	DL	87/87 (100%)	-0.41	2 (2%) 60 54	33, 47, 88, 167	0
40	AL	77/77 (100%)	0.41	1 (1%) 77 71	78, 94, 120, 130	0
40	DM	77/77 (100%)	1.04	10 (12%) 3 4	75, 94, 120, 129	0
41	AM	50/50 (100%)	-0.44	0 100 100	44, 53, 64, 76	0
41	DN	50/50 (100%)	-0.40	0 100 100	48, 56, 69, 89	0
42	AN	52/52 (100%)	-0.14	0 100 100	43, 53, 80, 108	0
42	DO	52/52 (100%)	-0.49	0 100 100	32, 39, 54, 81	0
43	AO	25/25 (100%)	-0.20	0 100 100	54, 61, 69, 75	0
43	DP	25/25 (100%)	-0.37	0 100 100	42, 50, 62, 68	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	AP	105/105 (100%)	0.21	2 (1%) 66 61	36, 58, 96, 156	0
44	DQ	105/105 (100%)	0.08	0 100 100	42, 59, 96, 138	0
45	AQ	91/91 (100%)	-0.37	0 100 100	38, 62, 91, 121	0
45	DR	91/91 (100%)	-0.44	0 100 100	32, 55, 78, 88	0
46	i	159/168 (94%)	0.59	18 (11%) 5 6	56, 101, 165, 178	0
47	p0	143/220 (65%)	1.20	24 (16%) 1 2	100, 113, 177, 185	0
48	sM	63/104 (60%)	0.38	4 (6%) 20 18	54, 106, 129, 136	0
49	B	206/206 (100%)	0.37	10 (4%) 29 26	92, 115, 139, 176	0
49	s0	206/206 (100%)	0.01	1 (0%) 91 88	72, 95, 124, 136	0
50	C	214/216 (99%)	0.87	32 (14%) 2 3	101, 141, 172, 181	0
50	s1	216/216 (100%)	0.34	3 (1%) 75 69	68, 87, 117, 144	0
51	D	217/217 (100%)	0.04	5 (2%) 60 54	69, 91, 118, 142	0
51	s2	217/217 (100%)	0.03	1 (0%) 91 88	55, 75, 97, 121	0
52	E	223/223 (100%)	0.21	7 (3%) 49 43	78, 95, 131, 155	0
52	s3	223/223 (100%)	0.33	10 (4%) 33 29	74, 111, 145, 158	0
53	F	260/260 (100%)	0.37	4 (1%) 73 68	73, 95, 113, 153	0
53	s4	260/260 (100%)	0.02	1 (0%) 92 90	51, 79, 100, 150	0
54	G	206/206 (100%)	0.73	22 (10%) 6 6	98, 121, 152, 179	0
54	s5	206/206 (100%)	0.35	12 (5%) 23 20	71, 92, 124, 157	0
55	H	226/226 (100%)	0.38	6 (2%) 54 48	66, 105, 142, 160	0
55	s6	218/226 (96%)	0.18	6 (2%) 53 47	51, 83, 123, 148	0
56	I	184/186 (98%)	0.58	9 (4%) 29 26	85, 126, 160, 187	0
56	s7	186/186 (100%)	0.32	8 (4%) 35 31	69, 105, 156, 173	0
57	J	188/199 (94%)	0.32	9 (4%) 30 27	58, 77, 128, 150	0
57	s8	188/199 (94%)	0.17	5 (2%) 54 48	43, 68, 121, 138	0
58	K	185/185 (100%)	0.66	16 (8%) 10 11	87, 107, 149, 185	0
58	s9	185/185 (100%)	0.18	3 (1%) 72 66	63, 80, 128, 169	0
59	L	96/105 (91%)	0.41	2 (2%) 63 58	80, 111, 141, 172	0
59	c0	96/105 (91%)	1.29	27 (28%) 0 0	104, 137, 155, 185	0
60	M	155/155 (100%)	0.50	15 (9%) 7 8	60, 76, 162, 194	0
60	c1	146/155 (94%)	0.07	7 (4%) 30 27	42, 64, 118, 151	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
61	N	124/124 (100%)	1.26	24 (19%) 1 1	140, 159, 203, 214	0
61	c2	124/124 (100%)	1.71	46 (37%) 0 0	159, 186, 216, 234	0
62	O	150/150 (100%)	0.14	3 (2%) 65 60	60, 90, 112, 129	0
62	c3	150/150 (100%)	-0.23	0 100 100	53, 76, 100, 121	0
63	P	127/128 (99%)	0.67	16 (12%) 3 5	65, 128, 158, 165	0
63	c4	128/128 (100%)	0.61	10 (7%) 13 13	55, 84, 100, 130	0
64	Q	124/141 (87%)	0.36	5 (4%) 38 33	80, 103, 150, 165	0
64	c5	135/141 (95%)	0.41	11 (8%) 12 12	75, 102, 144, 168	0
65	R	141/142 (99%)	0.74	17 (12%) 4 5	83, 110, 129, 132	0
65	c6	142/142 (100%)	0.17	2 (1%) 75 69	62, 88, 109, 141	0
66	S	120/125 (96%)	0.02	2 (1%) 70 64	77, 111, 159, 170	0
67	T	145/145 (100%)	0.42	10 (6%) 16 16	71, 111, 145, 160	0
67	c8	145/145 (100%)	0.01	1 (0%) 87 83	71, 88, 121, 137	0
68	U	143/143 (100%)	0.26	7 (4%) 29 26	89, 112, 136, 148	0
68	c9	143/143 (100%)	0.03	1 (0%) 87 83	66, 85, 109, 139	0
69	V	107/110 (97%)	0.49	8 (7%) 14 14	75, 110, 157, 169	0
69	d0	110/110 (100%)	1.03	23 (20%) 1 1	70, 113, 170, 190	0
70	W	87/87 (100%)	0.42	4 (4%) 32 28	91, 105, 126, 148	0
70	d1	87/87 (100%)	0.18	0 100 100	68, 83, 119, 146	0
71	X	129/129 (100%)	0.01	0 100 100	68, 84, 96, 102	0
71	d2	129/129 (100%)	-0.31	0 100 100	50, 64, 77, 88	0
72	Y	144/144 (100%)	0.03	1 (0%) 87 83	57, 67, 88, 124	0
72	d3	144/144 (100%)	-0.24	0 100 100	40, 49, 73, 108	0
73	Z	134/134 (100%)	0.49	5 (3%) 41 37	82, 111, 137, 155	0
73	d4	134/134 (100%)	0.14	3 (2%) 62 56	59, 89, 117, 159	0
74	a	70/70 (100%)	1.00	10 (14%) 2 3	117, 134, 148, 160	0
74	d5	69/70 (98%)	0.61	3 (4%) 35 31	84, 111, 136, 147	0
75	b	97/97 (100%)	0.38	8 (8%) 11 12	69, 95, 165, 171	0
75	d6	97/97 (100%)	-0.10	0 100 100	54, 68, 110, 126	0
76	c	81/81 (100%)	0.67	9 (11%) 5 6	84, 107, 161, 171	0
76	d7	81/81 (100%)	0.22	5 (6%) 20 18	67, 88, 144, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
77	d	63/63 (100%)	1.19	13 (20%) 1 1	103, 124, 146, 159	0
77	d8	63/63 (100%)	0.94	8 (12%) 3 4	82, 104, 132, 141	0
78	d9	53/53 (100%)	0.21	1 (1%) 66 61	73, 84, 133, 153	0
78	e	53/53 (100%)	-0.24	1 (1%) 66 61	72, 82, 116, 137	0
79	e0	62/62 (100%)	0.27	2 (3%) 47 42	58, 81, 140, 161	0
79	f	60/62 (96%)	0.82	6 (10%) 7 8	65, 98, 158, 164	0
80	g	71/71 (100%)	0.84	12 (16%) 1 2	96, 149, 167, 187	0
81	h	318/318 (100%)	0.85	40 (12%) 3 5	100, 124, 161, 200	0
81	sR	318/318 (100%)	0.79	40 (12%) 3 5	92, 119, 148, 191	0
82	c7	117/121 (96%)	-0.15	1 (0%) 84 79	72, 93, 130, 139	0
83	e1	51/51 (100%)	1.02	10 (19%) 1 1	143, 176, 188, 200	0
All	All	33004/33818 (97%)	0.02	1088 (3%) 46 41	21, 72, 152, 311	0

All (1088) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	A	1709	C	16.0
25	A	1711	C	15.6
25	A	1694	A	14.5
26	7	75	THR	14.4
26	7	76	VAL	13.3
18	CR	162	GLU	12.9
18	CR	161	ALA	12.8
25	A	1693	A	12.6
25	A	1702	A	12.1
18	CR	160	ALA	11.8
18	CR	179	GLN	11.5
18	CR	178	ALA	11.0
18	CR	159	LYS	10.9
1	1	1569	U	10.6
25	A	1699	G	10.5
25	A	1703	C	10.4
25	A	1708	U	10.3
25	A	1692	G	10.2
18	CR	158	ALA	9.9
26	7	86	SER	9.7
1	AR	1569	U	9.7
25	A	1695	G	9.7

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Mol	Chain	Res	Type	RSRZ
60	M	3	THR	9.5
46	i	16	ASP	9.5
1	1	1568	U	9.0
25	A	238	U	8.9
26	CY	96	LEU	8.9
26	7	77	LYS	8.8
26	7	88	ASP	8.6
25	A	1700	C	8.6
1	AR	1570	U	8.5
25	A	1698	G	8.4
18	CR	176	ILE	8.3
25	A	1704	U	8.3
18	CR	177	ALA	8.0
25	A	719	U	8.0
18	CR	168	LEU	8.0
1	1	1570	U	8.0
25	A	1710	U	7.9
25	A	1701	A	7.8
18	CR	163	LYS	7.7
1	AR	1351	U	7.7
26	7	69	LYS	7.6
25	6	1700	C	7.5
26	CY	98	PRO	7.3
26	CY	68	ALA	7.3
26	CY	97	LYS	7.3
60	M	2	SER	7.2
26	7	85	ALA	7.2
64	c5	135	THR	7.2
69	d0	121	ASN	7.1
26	CY	66	GLU	7.1
64	c5	134	THR	7.1
26	7	84	GLY	7.0
25	A	1712	A	6.9
46	i	19	VAL	6.8
18	x	161	ALA	6.8
25	6	1701	A	6.8
26	7	68	ALA	6.8
25	A	913	G	6.7
25	A	1697	G	6.7
1	1	1571	A	6.7
18	CR	184	ALA	6.6
25	A	1696	G	6.5

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Mol	Chain	Res	Type	RSRZ
18	CR	165	VAL	6.5
25	A	1705	C	6.5
76	c	38	PRO	6.5
69	d0	98	GLN	6.4
26	7	95	SER	6.4
25	A	715	U	6.4
1	AR	2445	A	6.4
25	6	1693	A	6.3
1	AR	1352	A	6.3
26	CY	67	VAL	6.3
18	CR	164	LYS	6.3
46	i	18	VAL	6.3
25	A	1707	A	6.2
26	CY	95	SER	6.2
1	AR	2539	C	6.1
25	A	1686	C	6.1
25	A	1690	G	6.1
18	CR	170	SER	6.1
64	c5	133	ALA	6.1
60	M	146	ALA	6.1
25	6	1710	U	6.0
61	c2	20	ALA	6.0
38	DK	100	HIS	6.0
25	6	718	U	6.0
54	G	151	GLY	6.0
1	1	2539	C	6.0
25	6	1694	A	5.9
18	CR	175	ARG	5.9
10	CJ	254	ASP	5.8
60	c1	3	THR	5.8
1	1	1955	U	5.7
3	4	158	U	5.7
25	6	194	U	5.7
25	6	493	U	5.7
46	i	173	GLU	5.7
60	M	147	GLY	5.7
54	G	37	GLN	5.7
37	DJ	120	ALA	5.6
26	7	74	LYS	5.6
25	A	1691	A	5.6
25	A	658	C	5.5
25	A	1687	U	5.4

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Mol	Chain	Res	Type	RSRZ
26	CY	69	LYS	5.4
1	1	1567	U	5.4
79	f	61	SER	5.4
18	CR	157	VAL	5.4
26	CY	65	GLU	5.4
34	AF	128	LEU	5.4
18	CR	174	GLY	5.4
69	d0	18	GLN	5.3
18	CR	167	ARG	5.2
46	i	87	THR	5.2
25	A	239	C	5.2
18	CR	180	LYS	5.2
61	N	62	LEU	5.2
1	AR	2506	U	5.2
25	A	1059	U	5.1
25	6	1695	G	5.1
25	A	232	U	5.1
25	6	239	C	5.0
1	AR	1568	U	5.0
25	6	1711	C	5.0
81	sR	121	MET	5.0
59	c0	98	THR	5.0
25	A	717	C	5.0
1	1	1352	A	4.9
1	AR	1571	A	4.9
57	s8	200	LYS	4.9
59	c0	45	ALA	4.9
25	6	1709	C	4.9
44	AP	106	PHE	4.9
25	A	1713	G	4.8
26	7	98	PRO	4.8
61	N	112	ALA	4.8
1	AR	2504	U	4.8
1	1	1351	U	4.8
26	7	71	ARG	4.7
1	1	1572	U	4.7
26	7	89	LEU	4.7
46	i	88	ARG	4.7
10	CJ	256	ALA	4.7
25	A	656	G	4.7
26	7	90	ILE	4.7
75	b	64	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
25	A	718	U	4.7
26	7	78	ALA	4.7
1	1	1349	G	4.7
59	c0	65	TYR	4.7
25	6	719	U	4.7
25	6	1699	G	4.6
18	CR	169	THR	4.6
69	d0	14	GLN	4.6
1	AR	2505	U	4.6
1	1	1952	G	4.6
1	AR	3157	U	4.6
25	6	1712	A	4.6
26	7	81	PRO	4.5
54	G	41	LYS	4.5
81	h	79	TYR	4.5
25	6	75	U	4.5
54	G	150	GLY	4.5
54	G	152	GLY	4.5
23	5	9	GLN	4.5
26	7	92	GLU	4.5
25	A	1688	U	4.5
50	C	55	LYS	4.5
25	A	494	U	4.4
69	d0	100	VAL	4.4
26	7	70	LYS	4.4
18	x	160	ALA	4.4
25	6	678	A	4.4
25	A	491	C	4.4
60	M	152	GLN	4.3
18	x	162	GLU	4.3
56	s7	3	ALA	4.3
81	sR	72	THR	4.3
25	6	232	U	4.3
25	A	493	U	4.3
1	1	1762	C	4.3
60	c1	4	GLU	4.3
65	R	20	ALA	4.3
25	A	716	C	4.3
64	c5	136	SER	4.3
17	CQ	182	ASN	4.3
69	d0	97	VAL	4.3
25	6	506	A	4.2

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Mol	Chain	Res	Type	RSRZ
18	x	163	LYS	4.2
1	AR	2502	A	4.2
26	7	87	LEU	4.2
50	C	130	SER	4.2
18	CR	166	VAL	4.2
58	K	181	ALA	4.2
54	s5	153	GLY	4.2
83	e1	124	PRO	4.1
1	1	1238	C	4.1
25	A	230	C	4.1
26	7	73	ARG	4.1
25	A	492	A	4.1
25	6	494	U	4.1
25	A	1706	C	4.1
1	AR	1567	U	4.1
63	P	15	GLY	4.1
54	G	71	ALA	4.1
65	R	26	LYS	4.1
25	6	1696	G	4.1
1	AR	1350	A	4.1
25	A	714	G	4.0
25	6	229	U	4.0
61	N	85	LYS	4.0
18	CR	172	GLN	4.0
46	i	20	LEU	4.0
59	c0	95	ARG	4.0
1	AR	2503	G	4.0
10	CJ	253	SER	4.0
25	6	1692	G	4.0
61	c2	59	LEU	4.0
25	6	658	C	4.0
50	C	93	GLY	4.0
56	I	74	GLN	4.0
26	7	83	THR	3.9
47	p0	192	ASP	3.9
1	1	1240	A	3.9
25	6	1707	A	3.9
50	C	20	VAL	3.9
64	c5	132	GLY	3.9
61	c2	28	LEU	3.9
68	U	5	SER	3.9
25	A	134	U	3.9

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Mol	Chain	Res	Type	RSRZ
25	A	194	U	3.9
26	CY	81	PRO	3.9
1	AR	2535	A	3.9
75	b	65	PRO	3.9
1	AR	3156	U	3.9
75	b	62	TYR	3.9
1	1	1566	A	3.9
1	1	1763	U	3.9
1	1	3351	U	3.9
26	7	72	SER	3.9
46	i	85	SER	3.9
65	R	66	ARG	3.8
25	6	1228	G	3.8
60	c1	2	SER	3.8
77	d	44	VAL	3.8
38	AJ	99	ARG	3.8
61	c2	80	ASN	3.8
60	M	153	PHE	3.8
34	DG	128	LEU	3.7
54	s5	154	ALA	3.7
74	d5	37	GLN	3.7
66	S	86	PRO	3.7
46	i	172	VAL	3.7
1	AR	3275	U	3.7
18	CR	173	ARG	3.7
60	M	156	PHE	3.7
60	M	145	ALA	3.7
51	D	145	GLY	3.7
58	K	185	GLY	3.7
81	sR	48	THR	3.7
81	sR	314	GLN	3.7
69	d0	19	ILE	3.7
12	CL	219	ALA	3.7
25	6	1702	A	3.7
5	CE	140	ASP	3.7
5	k	387	LEU	3.7
65	R	21	HIS	3.7
60	M	4	GLU	3.7
60	c1	147	GLY	3.7
25	6	1698	G	3.7
61	c2	64	SER	3.6
46	i	22	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
61	c2	123	VAL	3.6
49	B	166	GLY	3.6
54	s5	151	GLY	3.6
80	g	146	SER	3.6
52	E	44	THR	3.6
1	1	1242	G	3.6
25	A	135	A	3.6
58	K	182	GLU	3.6
58	K	106	GLU	3.6
59	c0	48	SER	3.6
61	c2	76	GLU	3.6
50	C	100	PHE	3.6
60	M	155	LYS	3.6
1	AR	1815	U	3.6
56	s7	2	SER	3.6
25	6	1059	U	3.6
54	G	36	ALA	3.5
81	sR	212	ALA	3.5
26	7	96	LEU	3.5
61	N	41	LEU	3.5
25	A	231	U	3.5
61	c2	125	ASN	3.5
81	h	7	LEU	3.5
25	6	1371	A	3.5
25	A	506	A	3.5
46	i	84	LYS	3.5
1	1	1243	G	3.5
28	DA	127	GLU	3.5
61	c2	126	TRP	3.5
78	d9	4	GLU	3.5
1	AR	1025	A	3.5
54	G	38	THR	3.4
25	6	1491	U	3.4
77	d	66	LEU	3.4
61	c2	58	LEU	3.4
1	1	1025	A	3.4
28	9	127	GLU	3.4
81	h	52	GLN	3.4
67	T	146	ALA	3.4
11	CK	189	GLU	3.4
32	DE	105	ALA	3.4
76	c	41	LEU	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
81	sR	124	SER	3.4
73	Z	6	THR	3.4
69	d0	94	GLU	3.4
69	d0	17	GLN	3.4
61	N	111	ASN	3.4
26	7	97	LYS	3.4
77	d	21	SER	3.4
81	h	261	LYS	3.4
59	L	94	GLU	3.4
1	AR	2538	U	3.4
25	A	261	U	3.4
18	CR	183	ALA	3.4
25	A	720	G	3.4
47	p0	87	VAL	3.4
10	CJ	255	SER	3.4
20	CT	189	ALA	3.4
59	c0	70	GLU	3.4
25	A	914	G	3.3
65	R	92	TYR	3.3
26	7	65	GLU	3.3
46	i	83	LYS	3.3
81	sR	253	ALA	3.3
54	G	161	ASP	3.3
60	M	154	ALA	3.3
50	C	91	VAL	3.3
69	V	105	GLN	3.3
51	s2	105	GLY	3.3
79	e0	63	GLN	3.3
81	h	212	ALA	3.3
61	c2	23	THR	3.3
54	s5	155	ALA	3.3
61	c2	84	ASN	3.3
81	sR	214	ALA	3.3
20	CT	182	ASP	3.3
61	c2	82	PRO	3.3
50	C	28	GLU	3.3
61	N	28	LEU	3.3
54	G	155	ALA	3.3
79	f	2	ALA	3.3
18	x	158	ALA	3.2
83	e1	122	SER	3.2
18	x	184	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
10	CJ	121	SER	3.2
25	A	1689	A	3.2
81	sR	61	PHE	3.2
25	A	1716	C	3.2
65	R	62	ASN	3.2
69	d0	102	ARG	3.2
47	p0	217	VAL	3.2
40	DM	69	LEU	3.2
46	i	174	LEU	3.2
73	d4	26	ASP	3.2
25	6	1800	A	3.2
60	c1	146	ALA	3.2
67	T	2	SER	3.2
20	CT	183	ALA	3.2
50	C	94	LYS	3.2
1	1	1350	A	3.2
83	e1	112	GLY	3.2
25	A	820	U	3.2
49	B	28	ASN	3.2
54	s5	37	GLN	3.2
80	g	152	ALA	3.2
55	s6	218	GLU	3.2
59	c0	23	ALA	3.2
61	c2	85	LYS	3.2
50	C	54	LEU	3.2
62	O	61	THR	3.2
46	i	89	ARG	3.2
1	1	2445	A	3.1
25	6	225	A	3.1
55	s6	217	SER	3.1
60	c1	5	LEU	3.1
25	A	1362	U	3.1
29	DB	11	ALA	3.1
10	CJ	182	GLY	3.1
25	6	1703	C	3.1
25	A	912	U	3.1
64	c5	4	ALA	3.1
63	P	16	VAL	3.1
47	p0	104	ARG	3.1
49	B	23	HIS	3.1
59	c0	94	GLU	3.1
50	C	47	LEU	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
23	5	10	LYS	3.1
69	d0	107	THR	3.1
75	b	46	GLU	3.1
81	sR	165	ASP	3.1
26	CY	64	THR	3.1
77	d	5	THR	3.1
69	V	48	HIS	3.1
81	h	33	LEU	3.1
54	s5	156	ARG	3.1
1	AR	1572	U	3.1
1	AR	3352	U	3.1
25	6	1227	A	3.1
53	F	123	LEU	3.1
81	h	252	LEU	3.1
1	1	1239	C	3.1
57	J	200	LYS	3.1
77	d	8	THR	3.1
1	1	1581	C	3.0
25	A	489	C	3.0
61	N	86	VAL	3.0
61	c2	124	LYS	3.0
21	0	1	MET	3.0
25	6	198	A	3.0
25	6	235	G	3.0
81	sR	252	LEU	3.0
52	s3	44	THR	3.0
1	1	2502	A	3.0
39	DL	88	ALA	3.0
25	A	235	G	3.0
58	K	186	GLU	3.0
79	f	42	ARG	3.0
12	CL	220	GLN	3.0
59	c0	71	GLU	3.0
60	M	150	ASN	3.0
65	c6	11	GLY	3.0
67	T	8	GLN	3.0
23	5	27	VAL	3.0
61	c2	63	VAL	3.0
50	C	95	ASN	3.0
1	1	1574	C	3.0
1	1	1954	G	3.0
80	g	124	PRO	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
40	DM	34	ALA	3.0
63	P	41	ARG	3.0
68	U	6	VAL	3.0
69	d0	106	ILE	3.0
1	1	2207	A	3.0
54	G	25	LEU	3.0
49	B	39	ASN	3.0
79	e0	62	VAL	3.0
1	AR	3154	C	3.0
25	6	1708	U	3.0
25	A	488	G	3.0
74	a	65	LEU	3.0
79	f	60	PRO	3.0
80	g	151	ASN	3.0
81	sR	303	ALA	3.0
52	E	45	LYS	3.0
48	sM	85	SER	3.0
46	i	17	VAL	3.0
61	c2	56	GLU	3.0
1	1	1095	U	3.0
69	d0	109	GLU	2.9
1	AR	1016	C	2.9
49	B	198	MET	2.9
77	d	59	SER	2.9
81	h	24	ALA	2.9
40	AL	5	ILE	2.9
1	1	1573	G	2.9
26	7	80	ARG	2.9
50	C	29	TRP	2.9
77	d	9	LEU	2.9
55	s6	169	TYR	2.9
63	P	14	PHE	2.9
25	6	721	U	2.9
54	G	54	LYS	2.9
58	K	113	VAL	2.9
23	5	93	ILE	2.9
25	6	676	G	2.9
44	AP	104	LEU	2.9
63	P	40	ALA	2.9
47	p0	212	HIS	2.9
47	p0	103	ASN	2.9
63	c4	47	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
25	6	234	G	2.9
32	AD	104	LEU	2.9
81	h	32	LEU	2.9
81	sR	134	TRP	2.9
23	CW	52	ASN	2.9
46	i	86	ASN	2.9
26	7	79	GLN	2.9
58	K	112	GLN	2.9
52	E	88	ALA	2.9
61	c2	92	ALA	2.9
81	h	115	ILE	2.9
65	R	114	ARG	2.8
65	R	57	LEU	2.8
81	h	314	GLN	2.8
25	6	238	U	2.8
58	K	138	LYS	2.8
61	c2	112	ALA	2.8
65	R	56	GLY	2.8
20	z	187	GLU	2.8
69	d0	93	LEU	2.8
1	AR	1354	G	2.8
25	6	1690	G	2.8
70	W	34	ILE	2.8
53	F	124	GLY	2.8
25	6	227	U	2.8
25	6	1687	U	2.8
49	B	24	LEU	2.8
69	d0	99	ILE	2.8
25	A	490	C	2.8
64	c5	10	ARG	2.8
26	CY	70	LYS	2.8
56	I	38	LEU	2.8
1	AR	2444	C	2.8
25	6	233	C	2.8
25	6	1686	C	2.8
81	sR	27	ALA	2.8
1	AR	1353	U	2.8
25	6	240	U	2.8
25	6	496	G	2.8
81	sR	167	VAL	2.8
11	CK	191	LEU	2.8
76	c	44	THR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
81	h	72	THR	2.8
48	sM	84	LYS	2.8
81	sR	319	ASN	2.8
1	AR	1764	U	2.8
32	AD	105	ALA	2.8
25	6	722	G	2.8
63	P	96	PRO	2.8
25	6	495	C	2.8
54	s5	152	GLY	2.8
58	K	116	LEU	2.8
50	C	92	GLN	2.7
9	CI	27	ALA	2.7
1	AR	546	C	2.7
20	z	188	ASP	2.7
53	s4	261	LEU	2.7
69	d0	105	GLN	2.7
76	c	33	LEU	2.7
9	CI	26	VAL	2.7
25	A	228	G	2.7
25	A	1685	G	2.7
63	P	29	HIS	2.7
70	W	53	TYR	2.7
61	c2	113	ARG	2.7
74	a	88	ILE	2.7
81	sR	51	ASP	2.7
61	N	88	LEU	2.7
59	c0	96	ASN	2.7
61	N	80	ASN	2.7
1	1	2205	U	2.7
73	d4	2	SER	2.7
80	g	87	THR	2.7
80	g	149	LYS	2.7
74	a	36	ALA	2.7
50	C	25	THR	2.7
69	V	98	GLN	2.7
1	AR	2507	C	2.7
73	Z	2	SER	2.7
77	d	67	ARG	2.7
25	A	495	C	2.7
61	c2	60	VAL	2.7
61	c2	121	VAL	2.7
1	1	2569	A	2.7

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Mol	Chain	Res	Type	RSRZ
29	DB	7	ALA	2.7
38	DK	96	ALA	2.7
74	d5	86	GLU	2.7
54	G	24	VAL	2.7
58	K	95	TYR	2.7
61	c2	115	VAL	2.7
72	Y	51	GLY	2.7
74	d5	88	ILE	2.7
1	AR	1028	U	2.7
39	DL	87	SER	2.7
81	sR	166	SER	2.7
32	AD	24	THR	2.7
40	DM	72	THR	2.7
12	CL	221	ALA	2.7
47	p0	81	LYS	2.7
77	d	45	LYS	2.7
67	T	10	SER	2.6
25	6	491	C	2.6
50	C	230	ALA	2.6
81	h	284	ALA	2.6
81	h	310	ILE	2.6
10	CJ	197	VAL	2.6
33	AE	82	GLU	2.6
10	CJ	119	GLY	2.6
60	M	149	ALA	2.6
61	c2	128	ALA	2.6
55	s6	216	LEU	2.6
61	c2	143	GLN	2.6
81	h	81	LEU	2.6
81	sR	301	LEU	2.6
3	AT	158	U	2.6
68	U	4	VAL	2.6
1	1	3349	C	2.6
77	d	60	GLU	2.6
25	A	1681	A	2.6
81	h	211	ILE	2.6
64	c5	7	ALA	2.6
20	z	186	LYS	2.6
76	c	45	THR	2.6
26	7	82	ILE	2.6
62	O	151	ASN	2.6
1	1	2507	C	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
61	c2	86	VAL	2.6
12	CL	186	GLU	2.6
59	c0	79	TYR	2.6
81	sR	125	GLY	2.6
76	d7	57	GLU	2.6
23	5	89	LEU	2.6
25	A	657	U	2.6
25	6	228	G	2.6
25	6	717	C	2.6
47	p0	47	GLY	2.6
59	c0	13	GLN	2.6
58	s9	148	VAL	2.6
69	V	121	ASN	2.6
33	AE	79	ARG	2.6
81	h	102	ARG	2.6
25	A	1370	U	2.6
81	h	36	ALA	2.6
79	f	49	LEU	2.6
61	N	20	ALA	2.6
1	AR	1349	G	2.6
47	p0	69	ASP	2.6
52	s3	152	PHE	2.6
64	c5	137	ARG	2.6
52	E	87	TYR	2.6
81	sR	130	THR	2.6
68	c9	112	GLY	2.6
69	V	99	ILE	2.5
59	c0	21	VAL	2.5
1	AR	3155	U	2.5
52	s3	176	LEU	2.5
59	c0	35	ILE	2.5
81	h	202	LEU	2.5
47	p0	88	PHE	2.5
56	s7	52	ALA	2.5
75	b	47	ALA	2.5
77	d8	65	ARG	2.5
59	c0	68	LEU	2.5
63	P	19	ILE	2.5
74	a	94	LYS	2.5
1	1	3154	C	2.5
61	c2	57	ALA	2.5
81	h	313	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
52	s3	43	PRO	2.5
37	AI	120	ALA	2.5
25	6	492	A	2.5
73	Z	98	GLU	2.5
81	h	309	VAL	2.5
61	c2	119	SER	2.5
74	a	67	ASP	2.5
54	G	70	VAL	2.5
83	e1	102	VAL	2.5
1	AR	246	U	2.5
50	C	53	GLY	2.5
25	6	484	C	2.5
25	A	237	C	2.5
47	p0	188	VAL	2.5
78	e	4	GLU	2.5
1	AR	240	U	2.5
50	s1	89	ASP	2.5
50	C	233	GLY	2.5
59	c0	42	VAL	2.5
10	CJ	161	GLU	2.5
81	h	307	ASP	2.5
50	s1	235	GLY	2.5
81	sR	180	ALA	2.5
1	AR	1103	A	2.5
81	h	71	CYS	2.5
50	C	46	THR	2.5
25	A	781	U	2.5
67	T	22	VAL	2.5
1	AR	544	C	2.5
1	AR	1762	C	2.5
10	CJ	137	ASN	2.5
46	i	21	PRO	2.5
25	A	240	U	2.5
61	c2	110	GLY	2.5
65	R	143	ARG	2.5
74	a	68	ARG	2.5
61	c2	34	THR	2.5
81	sR	46	LYS	2.5
5	CE	387	LEU	2.5
59	c0	22	VAL	2.5
61	c2	55	GLY	2.5
56	s7	44	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
48	sM	78	ASP	2.4
62	O	26	PHE	2.5
77	d8	31	GLU	2.4
81	h	306	THR	2.4
50	C	121	ILE	2.4
69	V	93	LEU	2.4
60	c1	145	ALA	2.4
61	c2	65	SER	2.4
81	h	283	LYS	2.4
77	d8	10	ALA	2.4
25	A	131	C	2.4
25	A	197	A	2.4
63	c4	62	LEU	2.4
58	K	141	VAL	2.4
83	e1	113	LYS	2.4
1	1	1353	U	2.4
7	CG	296	GLN	2.4
1	1	1951	C	2.4
25	6	230	C	2.4
25	6	679	U	2.4
26	7	64	THR	2.4
40	DM	25	VAL	2.4
59	c0	64	TYR	2.4
81	h	305	TYR	2.4
10	p	256	ALA	2.4
1	1	1815	U	2.4
69	d0	115	GLU	2.4
1	1	1016	C	2.4
25	6	656	G	2.4
59	c0	36	ASP	2.4
67	T	16	ARG	2.4
50	C	90	GLU	2.4
68	U	21	PHE	2.4
47	p0	25	LEU	2.4
76	c	36	LYS	2.4
76	d7	33	LEU	2.4
81	h	45	TRP	2.4
80	g	145	HIS	2.4
77	d	7	VAL	2.4
58	K	87	SER	2.4
81	sR	49	GLY	2.4
54	G	154	ALA	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
57	s8	116	HIS	2.4
68	U	104	VAL	2.4
54	s5	68	ILE	2.4
1	1	1237	G	2.4
80	g	109	ASP	2.4
29	AA	65	ARG	2.4
49	B	41	ARG	2.4
65	R	55	VAL	2.4
1	AR	621	A	2.4
69	d0	95	ALA	2.4
81	sR	292	LEU	2.4
10	CJ	130	TYR	2.4
83	e1	145	HIS	2.4
1	AR	1955	U	2.4
25	6	231	U	2.4
63	c4	45	GLY	2.4
83	e1	127	GLY	2.4
54	G	162	VAL	2.4
61	N	67	THR	2.4
73	Z	100	VAL	2.4
57	J	104	ILE	2.4
74	a	82	HIS	2.4
61	N	119	SER	2.4
56	I	75	THR	2.4
59	L	67	THR	2.4
10	CJ	107	GLU	2.4
25	6	1713	G	2.4
27	CZ	22	LYS	2.4
47	p0	191	TYR	2.4
76	c	32	PHE	2.4
61	c2	78	LEU	2.4
25	A	280	U	2.3
47	p0	60	ARG	2.3
25	6	712	G	2.3
29	AA	46	ILE	2.3
47	p0	205	THR	2.3
68	U	105	LEU	2.3
2	AS	73	C	2.3
1	AR	1763	U	2.3
51	D	146	THR	2.3
61	c2	30	VAL	2.3
65	R	5	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
55	s6	214	LYS	2.3
61	c2	105	LYS	2.3
64	Q	51	SER	2.3
26	7	67	VAL	2.3
51	D	144	TRP	2.3
67	T	3	LEU	2.3
63	P	94	PRO	2.3
69	d0	114	VAL	2.3
81	sR	50	ASP	2.3
80	g	107	LYS	2.3
54	s5	130	ILE	2.3
65	R	96	TYR	2.3
59	c0	55	VAL	2.3
69	V	15	GLN	2.3
76	c	34	ASP	2.3
1	1	1576	G	2.3
49	B	203	PHE	2.3
81	sR	82	SER	2.3
7	CG	4	GLN	2.3
34	AF	127	ALA	2.3
47	p0	26	PHE	2.3
61	c2	136	ILE	2.3
63	P	18	ARG	2.3
80	g	85	TYR	2.3
61	N	52	LEU	2.3
61	N	59	LEU	2.3
77	d8	43	ASN	2.3
1	1	2570	U	2.3
63	c4	63	ALA	2.3
81	sR	3	SER	2.3
52	E	54	ARG	2.3
63	c4	117	ASP	2.3
73	d4	18	LEU	2.3
81	sR	244	ALA	2.3
1	AR	545	U	2.3
1	1	2096	A	2.3
25	6	226	A	2.3
1	AR	243	G	2.3
57	J	167	ALA	2.3
58	K	184	SER	2.3
81	h	213	SER	2.3
81	sR	120	SER	2.3

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Mol	Chain	Res	Type	RSRZ
58	s9	182	GLU	2.3
54	G	20	PHE	2.3
57	J	136	SER	2.3
76	d7	38	PRO	2.3
10	CJ	198	ALA	2.3
52	s3	174	HIS	2.3
23	CW	9	GLN	2.3
49	B	201	LEU	2.3
56	s7	187	SER	2.3
63	P	75	GLY	2.3
52	s3	42	THR	2.3
55	H	147	LEU	2.3
57	J	123	LYS	2.3
61	N	32	LEU	2.3
64	c5	109	PRO	2.3
76	d7	5	GLN	2.3
55	H	145	PHE	2.3
25	A	195	G	2.3
47	p0	221	ALA	2.3
1	1	1094	U	2.3
48	sM	83	LYS	2.3
80	g	86	THR	2.3
50	C	41	ARG	2.3
61	N	21	GLU	2.3
61	c2	21	GLU	2.3
52	E	217	ILE	2.3
18	x	157	VAL	2.3
23	CW	89	LEU	2.3
63	P	103	ARG	2.2
63	P	102	LEU	2.2
10	p	156	ASP	2.2
52	s3	128	GLU	2.2
10	CJ	199	ALA	2.2
50	C	96	LEU	2.2
1	1	1764	U	2.2
1	AR	117	U	2.2
59	c0	37	THR	2.2
55	H	165	GLY	2.2
54	s5	58	LEU	2.2
54	s5	129	PRO	2.2
65	R	3	ALA	2.2
81	h	263	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	AR	1563	C	2.2
11	CK	190	ASP	2.2
14	CN	136	GLU	2.2
25	6	74	U	2.2
61	c2	77	GLY	2.2
74	a	98	GLN	2.2
40	DM	31	LEU	2.2
61	c2	75	VAL	2.2
63	c4	48	VAL	2.2
57	s8	67	TRP	2.2
61	c2	29	LYS	2.2
1	1	3155	U	2.2
25	6	490	C	2.2
7	CG	297	GLN	2.2
56	I	98	ILE	2.2
74	a	69	LEU	2.2
23	CW	14	THR	2.2
51	D	71	THR	2.2
57	J	145	ALA	2.2
18	x	164	LYS	2.2
60	M	148	LYS	2.2
66	S	125	SER	2.2
69	V	94	GLU	2.2
65	R	28	LEU	2.2
70	W	55	LEU	2.2
1	AR	2572	C	2.2
25	A	136	C	2.2
40	DM	26	LYS	2.2
50	C	86	LEU	2.2
55	H	50	PHE	2.2
81	sR	83	ALA	2.2
1	AR	3276	G	2.2
83	e1	123	ASN	2.2
29	DB	96	VAL	2.2
50	C	140	ILE	2.2
83	e1	114	VAL	2.2
49	B	22	THR	2.2
1	1	545	U	2.2
10	CJ	97	TYR	2.2
52	s3	34	TYR	2.2
10	CJ	234	GLY	2.2
47	p0	100	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
56	I	134	GLU	2.2
56	s7	93	LEU	2.2
59	c0	78	GLU	2.2
81	h	262	VAL	2.2
57	J	168	CYS	2.2
58	s9	183	ALA	2.2
25	A	1060	U	2.2
27	CZ	142	ILE	2.2
63	P	27	PHE	2.2
81	h	308	ASN	2.2
61	c2	62	LEU	2.2
51	D	34	GLY	2.2
63	c4	44	GLY	2.2
1	1	2506	U	2.2
55	H	1	MET	2.2
47	p0	218	SER	2.2
65	c6	141	SER	2.2
1	AR	1566	A	2.2
61	c2	114	LYS	2.2
81	h	146	GLY	2.2
81	sR	14	GLU	2.2
25	6	237	C	2.2
63	c4	26	THR	2.2
1	AR	3277	U	2.2
81	h	14	GLU	2.2
56	s7	4	PRO	2.1
47	p0	102	SER	2.1
50	C	99	ASN	2.1
58	K	180	LYS	2.1
81	h	203	THR	2.1
54	s5	35	GLN	2.1
61	N	110	GLY	2.1
32	AD	95	ALA	2.1
74	a	51	LEU	2.1
77	d8	9	LEU	2.1
47	p0	89	THR	2.1
23	CW	34	ALA	2.1
47	p0	216	ALA	2.1
53	F	252	ARG	2.1
59	c0	10	LYS	2.1
1	1	3350	C	2.1
40	DM	43	PHE	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	1	1241	U	2.1
25	6	192	U	2.1
55	H	34	GLN	2.1
56	I	80	GLU	2.1
69	d0	104	THR	2.1
26	7	91	LYS	2.1
50	C	23	PRO	2.1
61	N	60	VAL	2.1
81	h	113	VAL	2.1
77	d8	32	PHE	2.1
25	A	132	U	2.1
61	N	82	PRO	2.1
63	c4	110	LEU	2.1
67	T	17	LEU	2.1
81	sR	103	PHE	2.1
50	C	50	LYS	2.1
77	d8	45	LYS	2.1
47	p0	50	VAL	2.1
23	CW	33	TYR	2.1
25	6	1691	A	2.1
81	sR	122	ILE	2.1
61	N	124	LYS	2.1
69	d0	52	LYS	2.1
82	c7	87	GLU	2.1
40	DM	78	LEU	2.1
56	I	77	LEU	2.1
77	d	55	VAL	2.1
23	5	49	ASN	2.1
54	G	209	TYR	2.1
59	c0	97	PRO	2.1
29	DB	6	LYS	2.1
37	DJ	119	LYS	2.1
61	c2	47	GLU	2.1
38	AJ	98	ARG	2.1
65	R	88	GLY	2.1
81	h	121	MET	2.1
7	CG	5	LYS	2.1
7	m	161	GLY	2.1
47	p0	48	ARG	2.1
81	sR	311	ARG	2.1
64	Q	104	GLN	2.1
79	f	48	THR	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
81	h	295	SER	2.1
56	I	87	ASP	2.1
52	s3	178	ARG	2.1
54	G	26	ALA	2.1
61	N	79	ALA	2.1
67	T	101	LEU	2.1
25	A	233	C	2.1
50	s1	74	GLN	2.1
54	G	96	SER	2.1
57	J	135	LYS	2.1
65	R	29	ILE	2.1
54	G	181	GLU	2.1
56	s7	54	GLY	2.1
61	N	125	ASN	2.1
67	c8	22	VAL	2.1
81	sR	138	GLY	2.1
64	Q	89	MET	2.1
81	sR	80	ALA	2.1
81	h	53	LYS	2.1
1	AR	2537	U	2.1
75	b	60	PRO	2.1
52	E	25	PHE	2.1
61	N	140	PHE	2.1
63	c4	27	PHE	2.1
73	Z	34	ASN	2.1
40	DM	73	LEU	2.1
58	K	118	LEU	2.1
83	e1	111	GLU	2.1
1	1	1103	A	2.1
1	1	1580	A	2.1
1	1	2503	G	2.1
25	6	1256	A	2.1
25	6	1714	A	2.1
81	h	253	ALA	2.1
75	b	69	ASN	2.1
68	U	71	VAL	2.1
81	h	265	LEU	2.1
29	AA	92	PHE	2.1
81	sR	235	SER	2.1
14	t	135	ALA	2.1
50	C	60	ALA	2.1
57	J	62	THR	2.1

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Mol	Chain	Res	Type	RSRZ
77	d	43	ASN	2.1
55	s6	119	GLN	2.1
1	1	1251	A	2.0
1	AR	2540	A	2.0
25	6	1226	A	2.0
59	c0	74	GLU	2.1
63	P	95	GLY	2.1
25	A	1717	G	2.0
64	Q	73	PRO	2.0
49	s0	185	ARG	2.0
60	M	82	ARG	2.0
53	F	190	GLY	2.0
61	N	56	GLU	2.0
69	d0	103	ILE	2.0
80	g	115	THR	2.0
64	c5	5	VAL	2.0
54	G	48	PHE	2.0
10	CJ	148	ALA	2.0
23	CW	97	SER	2.0
50	C	24	PHE	2.0
50	C	131	ASP	2.0
56	I	15	GLU	2.0
57	s8	199	LYS	2.0
61	c2	74	LEU	2.0
69	d0	50	LEU	2.0
76	d7	82	LYS	2.0
67	T	6	GLN	2.0
26	7	94	ARG	2.0
50	C	103	MET	2.0
75	b	63	ALA	2.0
81	sR	123	ILE	2.0
1	AR	2536	A	2.0
23	5	28	PHE	2.0
40	DM	54	LEU	2.0
58	K	111	THR	2.0
64	Q	12	PHE	2.0
1	AR	1032	C	2.0
25	A	189	C	2.0
25	A	196	G	2.0
46	i	175	ASP	2.0
57	s8	111	GLN	2.0
52	s3	3	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
29	AA	5	LEU	2.0
61	c2	61	VAL	2.0
1	AR	1816	A	2.0
59	c0	26	ASP	2.0
63	P	114	ARG	2.0
77	d8	54	LEU	2.0
1	AR	1630	U	2.0
1	AR	1954	G	2.0
11	q	189	GLU	2.0
61	c2	40	GLY	2.0
50	C	84	ILE	2.0
59	c0	67	THR	2.0
76	c	50	ALA	2.0
81	sR	136	ILE	2.0
70	W	69	LEU	2.0
10	p	202	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	6	2193	1/1	0.19	0.90	76,76,76,76	0
85	MG	1	3982	1/1	0.38	0.26	98,98,98,98	0
85	MG	AR	4241	1/1	0.42	0.56	59,59,59,59	0
85	MG	6	2185	1/1	0.50	0.59	60,60,60,60	0
85	MG	6	2181	1/1	0.52	0.49	78,78,78,78	0
85	MG	A	2118	1/1	0.52	0.95	75,75,75,75	0
85	MG	AR	3958	1/1	0.55	0.59	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4010	1/1	0.56	0.61	44,44,44,44	0
85	MG	6	2148	1/1	0.59	0.21	69,69,69,69	0
85	MG	1	3968	1/1	0.59	0.28	50,50,50,50	0
85	MG	CK	202	1/1	0.59	0.64	52,52,52,52	0
85	MG	A	2046	1/1	0.59	0.20	56,56,56,56	0
85	MG	A	2110	1/1	0.59	0.39	108,108,108,108	0
85	MG	AR	3746	1/1	0.59	0.29	39,39,39,39	0
85	MG	1	4107	1/1	0.60	0.28	66,66,66,66	0
85	MG	A	2073	1/1	0.61	0.41	65,65,65,65	0
85	MG	AP	503	1/1	0.61	0.20	61,61,61,61	0
85	MG	A	2112	1/1	0.61	0.41	77,77,77,77	0
85	MG	1	3966	1/1	0.61	0.21	62,62,62,62	0
85	MG	AR	3812	1/1	0.62	0.41	46,46,46,46	0
85	MG	A	2094	1/1	0.63	0.28	110,110,110,110	0
85	MG	AR	4173	1/1	0.64	0.47	38,38,38,38	0
85	MG	1	402	1/1	0.65	0.45	32,32,32,32	0
85	MG	1	3824	1/1	0.65	0.26	77,77,77,77	0
85	MG	6	2190	1/1	0.67	0.41	84,84,84,84	0
85	MG	CO	202	1/1	0.67	0.78	57,57,57,57	0
85	MG	1	4124	1/1	0.67	0.22	52,52,52,52	0
85	MG	AS	228	1/1	0.67	0.25	48,48,48,48	0
85	MG	AR	4167	1/1	0.68	0.51	72,72,72,72	0
85	MG	A	2075	1/1	0.68	0.37	48,48,48,48	0
85	MG	DR	503	1/1	0.69	0.33	54,54,54,54	0
85	MG	6	2139	1/1	0.69	0.31	75,75,75,75	0
85	MG	AR	3813	1/1	0.69	0.33	54,54,54,54	0
85	MG	AR	4217	1/1	0.69	0.24	65,65,65,65	0
85	MG	AR	3826	1/1	0.69	0.61	42,42,42,42	0
85	MG	1	4162	1/1	0.69	0.28	118,118,118,118	0
85	MG	AR	3965	1/1	0.69	0.32	54,54,54,54	0
85	MG	AR	4151	1/1	0.69	0.28	30,30,30,30	0
85	MG	A	2129	1/1	0.69	0.45	58,58,58,58	0
85	MG	AR	4101	1/1	0.70	0.45	48,48,48,48	0
85	MG	1	4092	1/1	0.70	0.16	53,53,53,53	0
84	OHX	AR	3720	7/7	0.70	0.34	267,269,269,270	0
85	MG	1	4073	1/1	0.70	0.30	79,79,79,79	0
85	MG	1	4129	1/1	0.70	0.38	51,51,51,51	0
85	MG	1	4140	1/1	0.70	0.48	49,49,49,49	0
85	MG	1	4175	1/1	0.71	0.80	91,91,91,91	0
85	MG	A	2103	1/1	0.71	0.43	64,64,64,64	0
85	MG	1	3759	1/1	0.71	0.34	69,69,69,69	0
85	MG	1	3801	1/1	0.71	0.52	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AT	223	1/1	0.71	0.91	55,55,55,55	0
85	MG	AR	3971	1/1	0.71	0.35	38,38,38,38	0
85	MG	A	2084	1/1	0.72	0.16	53,53,53,53	0
85	MG	1	4135	1/1	0.72	0.33	64,64,64,64	0
85	MG	AR	3804	1/1	0.72	0.45	36,36,36,36	0
85	MG	1	4102	1/1	0.72	0.39	40,40,40,40	0
85	MG	AR	4024	1/1	0.72	0.42	33,33,33,33	0
84	OHX	CZ	201	7/7	0.72	0.34	303,304,305,305	0
85	MG	1	4131	1/1	0.72	0.33	38,38,38,38	0
85	MG	A	2139	1/1	0.72	0.33	86,86,86,86	0
85	MG	AR	4072	1/1	0.73	0.36	71,71,71,71	0
85	MG	A	2086	1/1	0.73	0.30	50,50,50,50	0
85	MG	A	2089	1/1	0.73	0.48	65,65,65,65	0
85	MG	6	2174	1/1	0.73	0.25	66,66,66,66	0
85	MG	AR	4147	1/1	0.73	0.21	62,62,62,62	0
85	MG	AR	3893	1/1	0.73	0.58	40,40,40,40	0
85	MG	1	4008	1/1	0.73	1.06	76,76,76,76	0
85	MG	1	4076	1/1	0.73	0.27	71,71,71,71	0
85	MG	1	4078	1/1	0.73	0.21	44,44,44,44	0
85	MG	A	2135	1/1	0.73	0.61	50,50,50,50	0
84	OHX	H	301	7/7	0.73	0.32	231,233,235,235	0
84	OHX	AR	3664	7/7	0.74	0.30	287,287,288,288	0
85	MG	1	3736	1/1	0.74	0.16	82,82,82,82	0
85	MG	6	2195	1/1	0.74	0.37	64,64,64,64	0
85	MG	AR	4161	1/1	0.74	0.38	56,56,56,56	0
85	MG	6	2097	1/1	0.74	0.30	79,79,79,79	0
85	MG	1	4027	1/1	0.74	0.35	51,51,51,51	0
85	MG	AR	4202	1/1	0.74	0.50	72,72,72,72	0
85	MG	1	4136	1/1	0.75	0.38	49,49,49,49	0
84	OHX	1	3722	7/7	0.75	0.44	268,268,269,269	0
85	MG	AR	4122	1/1	0.75	0.42	70,70,70,70	0
84	OHX	1	3694	7/7	0.75	0.29	251,252,254,254	0
84	OHX	1	3699	7/7	0.75	0.23	304,306,307,308	0
85	MG	1	3955	1/1	0.75	0.28	52,52,52,52	0
85	MG	AR	3996	1/1	0.76	0.33	38,38,38,38	0
85	MG	6	2152	1/1	0.76	0.31	57,57,57,57	0
85	MG	A	2107	1/1	0.76	0.24	69,69,69,69	0
85	MG	AR	3820	1/1	0.76	0.64	55,55,55,55	0
85	MG	6	2170	1/1	0.76	0.45	46,46,46,46	0
85	MG	1	3789	1/1	0.76	0.70	51,51,51,51	0
84	OHX	AR	3718	7/7	0.76	0.33	255,256,257,257	0
85	MG	1	4183	1/1	0.76	0.47	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4192	1/1	0.76	0.44	38,38,38,38	0
85	MG	A	2147	1/1	0.76	0.20	106,106,106,106	0
85	MG	c9	201	1/1	0.76	0.11	73,73,73,73	0
85	MG	AR	4164	1/1	0.77	0.31	30,30,30,30	0
85	MG	DR	502	1/1	0.77	0.36	76,76,76,76	0
85	MG	1	4034	1/1	0.77	0.16	33,33,33,33	0
85	MG	AR	4036	1/1	0.77	0.25	68,68,68,68	0
85	MG	AR	3880	1/1	0.77	0.43	20,20,20,20	0
85	MG	A	2127	1/1	0.77	0.30	55,55,55,55	0
85	MG	1	3949	1/1	0.77	0.44	41,41,41,41	0
85	MG	1	4206	1/1	0.77	0.46	28,28,28,28	0
85	MG	1	3758	1/1	0.77	0.46	31,31,31,31	0
85	MG	6	2168	1/1	0.77	0.40	50,50,50,50	0
85	MG	6	2065	1/1	0.77	0.46	32,32,32,32	0
85	MG	1	4095	1/1	0.78	0.37	53,53,53,53	0
85	MG	A	2098	1/1	0.78	0.44	72,72,72,72	0
85	MG	1	3830	1/1	0.78	0.56	60,60,60,60	0
85	MG	AR	4026	1/1	0.78	0.21	62,62,62,62	0
85	MG	3	218	1/1	0.78	0.31	49,49,49,49	0
85	MG	AR	4059	1/1	0.78	0.15	67,67,67,67	0
84	OHX	AR	3687	7/7	0.78	0.37	244,245,246,247	0
85	MG	AR	4193	1/1	0.78	0.55	62,62,62,62	0
85	MG	1	4014	1/1	0.78	0.16	46,46,46,46	0
85	MG	AR	4214	1/1	0.78	0.42	61,61,61,61	0
85	MG	6	2075	1/1	0.78	0.39	49,49,49,49	0
85	MG	AR	4220	1/1	0.78	0.38	54,54,54,54	0
85	MG	F	301	1/1	0.78	0.34	71,71,71,71	0
85	MG	AR	4128	1/1	0.78	0.17	54,54,54,54	0
84	OHX	6	2028	7/7	0.79	0.29	248,250,252,252	0
85	MG	A	2109	1/1	0.79	0.31	50,50,50,50	0
85	MG	1	4063	1/1	0.79	0.59	55,55,55,55	0
84	OHX	AS	210	7/7	0.79	0.33	235,237,238,238	0
85	MG	AH	201	1/1	0.79	0.32	60,60,60,60	0
85	MG	4	217	1/1	0.79	0.48	44,44,44,44	0
84	OHX	1	3675	7/7	0.79	0.57	229,229,230,230	0
85	MG	x	203	1/1	0.79	0.26	64,64,64,64	0
85	MG	A	2137	1/1	0.79	0.34	40,40,40,40	0
85	MG	AR	4152	1/1	0.79	0.16	152,152,152,152	0
84	OHX	A	1985	7/7	0.79	0.36	221,222,223,224	0
85	MG	6	2071	1/1	0.79	0.20	73,73,73,73	0
85	MG	1	3976	1/1	0.79	0.35	61,61,61,61	0
87	ZN	c	101	1/1	0.79	0.22	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	4025	1/1	0.80	0.22	40,40,40,40	0
84	OHX	6	2051	7/7	0.80	0.36	228,229,230,231	0
84	OHX	AR	3716	7/7	0.80	0.35	292,293,293,294	0
85	MG	6	2166	1/1	0.80	0.16	36,36,36,36	0
85	MG	1	4001	1/1	0.80	0.31	65,65,65,65	0
85	MG	A	2124	1/1	0.80	0.74	57,57,57,57	0
85	MG	AR	3923	1/1	0.80	0.66	32,32,32,32	0
85	MG	AR	4211	1/1	0.80	0.23	86,86,86,86	0
85	MG	6	2081	1/1	0.80	0.31	94,94,94,94	0
84	OHX	AR	3737	7/7	0.80	0.69	260,261,262,262	0
85	MG	6	2179	1/1	0.80	0.30	52,52,52,52	0
85	MG	AR	4233	1/1	0.80	0.40	55,55,55,55	0
85	MG	6	2110	1/1	0.80	0.33	40,40,40,40	0
85	MG	Y	201	1/1	0.80	0.47	51,51,51,51	0
85	MG	AS	216	1/1	0.80	0.68	41,41,41,41	0
85	MG	1	4119	1/1	0.80	0.29	35,35,35,35	0
85	MG	1	3808	1/1	0.81	0.41	54,54,54,54	0
85	MG	AR	4162	1/1	0.81	0.25	54,54,54,54	0
85	MG	AS	229	1/1	0.81	0.29	68,68,68,68	0
84	OHX	1	3693	7/7	0.81	0.45	264,265,266,266	0
85	MG	AT	227	1/1	0.81	0.36	73,73,73,73	0
85	MG	1	4030	1/1	0.81	0.44	45,45,45,45	0
85	MG	AR	4170	1/1	0.81	0.36	128,128,128,128	0
85	MG	AR	3773	1/1	0.81	0.12	113,113,113,113	0
85	MG	AR	4077	1/1	0.81	0.34	49,49,49,49	0
85	MG	AR	4086	1/1	0.81	0.38	28,28,28,28	0
85	MG	6	2182	1/1	0.81	0.28	53,53,53,53	0
84	OHX	CF	401	7/7	0.81	0.27	245,246,247,247	0
85	MG	AR	3990	1/1	0.81	0.41	37,37,37,37	0
85	MG	1	3947	1/1	0.81	0.41	34,34,34,34	0
85	MG	AR	4221	1/1	0.81	0.27	49,49,49,49	0
85	MG	1	4106	1/1	0.81	0.38	30,30,30,30	0
85	MG	1	3974	1/1	0.81	0.40	43,43,43,43	0
87	ZN	e1	501	1/1	0.81	0.09	176,176,176,176	0
85	MG	AR	4209	1/1	0.82	0.27	48,48,48,48	0
84	OHX	A	2002	7/7	0.82	0.30	242,245,246,247	0
85	MG	AR	4093	1/1	0.82	0.34	46,46,46,46	0
84	OHX	AR	3727	7/7	0.82	0.34	277,279,280,280	0
84	OHX	AR	3728	7/7	0.82	0.35	238,238,239,239	0
85	MG	1	3746	1/1	0.82	0.27	59,59,59,59	0
85	MG	1	4031	1/1	0.82	0.42	38,38,38,38	0
85	MG	A	2104	1/1	0.82	0.27	131,131,131,131	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	1	3717	7/7	0.82	0.48	217,218,219,219	0
85	MG	1	4040	1/1	0.82	0.53	42,42,42,42	0
85	MG	AS	220	1/1	0.82	0.21	42,42,42,42	0
85	MG	AR	4156	1/1	0.82	0.49	71,71,71,71	0
85	MG	AR	4159	1/1	0.82	0.22	64,64,64,64	0
85	MG	1	4044	1/1	0.82	0.32	40,40,40,40	0
85	MG	AT	226	1/1	0.82	0.34	44,44,44,44	0
85	MG	AR	4050	1/1	0.82	0.28	46,46,46,46	0
85	MG	CI	301	1/1	0.82	0.31	48,48,48,48	0
85	MG	AR	4055	1/1	0.82	0.39	47,47,47,47	0
85	MG	AR	4058	1/1	0.82	0.18	57,57,57,57	0
85	MG	CP	502	1/1	0.82	0.38	25,25,25,25	0
85	MG	D	301	1/1	0.82	0.58	42,42,42,42	0
85	MG	CR	203	1/1	0.82	0.33	74,74,74,74	0
85	MG	1	3864	1/1	0.82	0.50	33,33,33,33	0
85	MG	AR	4071	1/1	0.82	0.37	32,32,32,32	0
84	OHX	AS	208	7/7	0.82	0.30	226,226,228,228	0
85	MG	1	3775	1/1	0.82	0.14	59,59,59,59	0
85	MG	1	3762	1/1	0.83	0.48	40,40,40,40	0
85	MG	AR	4119	1/1	0.83	0.19	77,77,77,77	0
84	OHX	CL	302	7/7	0.83	0.24	200,201,201,202	0
85	MG	s	300	1/1	0.83	0.13	53,53,53,53	0
85	MG	1	4079	1/1	0.83	0.47	47,47,47,47	0
84	OHX	CO	201	7/7	0.83	0.33	281,282,283,284	0
85	MG	1	3978	1/1	0.83	0.30	32,32,32,32	0
85	MG	1	4100	1/1	0.83	0.31	87,87,87,87	0
85	MG	A	2068	1/1	0.83	0.45	68,68,68,68	0
84	OHX	6	1976	7/7	0.83	0.42	182,182,183,184	0
85	MG	6	2085	1/1	0.83	0.42	40,40,40,40	0
85	MG	A	2076	1/1	0.83	0.26	50,50,50,50	0
84	OHX	1	3711	7/7	0.83	0.25	301,302,304,304	0
84	OHX	6	2042	7/7	0.83	0.55	246,246,248,248	0
85	MG	1	4109	1/1	0.83	0.32	37,37,37,37	0
85	MG	1	4113	1/1	0.83	0.65	54,54,54,54	0
85	MG	AR	3976	1/1	0.83	0.40	42,42,42,42	0
84	OHX	A	2042	7/7	0.83	0.17	240,242,244,245	0
85	MG	1	3840	1/1	0.83	0.18	39,39,39,39	0
85	MG	AR	4021	1/1	0.83	0.33	36,36,36,36	0
84	OHX	1	3707	7/7	0.83	0.25	237,237,239,239	0
85	MG	1	3941	1/1	0.83	0.30	36,36,36,36	0
84	OHX	1	3709	7/7	0.83	0.43	229,231,231,232	0
85	MG	A	2116	1/1	0.83	0.33	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3670	7/7	0.83	0.29	229,230,230,231	0
85	MG	1	4038	1/1	0.83	0.34	33,33,33,33	0
85	MG	A	2125	1/1	0.83	0.54	51,51,51,51	0
85	MG	AR	4223	1/1	0.83	0.35	54,54,54,54	0
84	OHX	1	3726	7/7	0.83	0.42	231,232,233,233	0
85	MG	AR	4056	1/1	0.83	0.29	44,44,44,44	0
85	MG	1	4174	1/1	0.83	0.33	54,54,54,54	0
85	MG	1	4041	1/1	0.83	0.46	38,38,38,38	0
85	MG	1	3963	1/1	0.83	0.16	69,69,69,69	0
85	MG	1	3964	1/1	0.83	0.33	51,51,51,51	0
85	MG	AB	203	1/1	0.83	0.31	37,37,37,37	0
85	MG	1	4070	1/1	0.83	0.29	37,37,37,37	0
84	OHX	4	210	7/7	0.83	0.31	236,236,236,236	0
85	MG	AT	231	1/1	0.83	0.56	46,46,46,46	0
85	MG	CE	406	1/1	0.83	0.59	48,48,48,48	0
85	MG	1	4161	1/1	0.84	0.28	37,37,37,37	0
84	OHX	1	3727	7/7	0.84	0.33	253,254,255,256	0
84	OHX	1	3731	7/7	0.84	0.28	201,202,205,205	0
85	MG	A	2048	1/1	0.84	0.18	42,42,42,42	0
85	MG	AR	4032	1/1	0.84	0.50	47,47,47,47	0
85	MG	AR	4183	1/1	0.84	0.20	93,93,93,93	0
85	MG	AR	3772	1/1	0.84	0.53	81,81,81,81	0
84	OHX	6	2053	7/7	0.84	0.23	250,252,253,254	0
85	MG	AR	3784	1/1	0.84	0.38	29,29,29,29	0
85	MG	AR	3803	1/1	0.84	0.22	54,54,54,54	0
85	MG	A	2088	1/1	0.84	0.27	66,66,66,66	0
85	MG	1	4181	1/1	0.84	0.23	50,50,50,50	0
84	OHX	6	2057	7/7	0.84	0.17	247,247,250,250	0
85	MG	1	4184	1/1	0.84	0.23	55,55,55,55	0
85	MG	1	4185	1/1	0.84	0.57	48,48,48,48	0
85	MG	AR	4074	1/1	0.84	0.31	44,44,44,44	0
85	MG	1	4064	1/1	0.84	0.34	59,59,59,59	0
85	MG	AR	4234	1/1	0.84	0.28	17,17,17,17	0
84	OHX	1	3683	7/7	0.84	0.30	197,198,199,199	0
84	OHX	A	2007	7/7	0.84	0.20	275,277,278,279	0
85	MG	AR	4100	1/1	0.84	0.35	67,67,67,67	0
85	MG	AS	221	1/1	0.84	0.20	36,36,36,36	0
85	MG	4	213	1/1	0.84	0.48	34,34,34,34	0
84	OHX	A	2015	7/7	0.84	0.35	248,250,254,254	0
84	OHX	A	2034	7/7	0.84	0.14	277,279,281,282	0
85	MG	AR	4125	1/1	0.84	0.22	62,62,62,62	0
84	OHX	1	3676	7/7	0.84	0.42	223,223,225,225	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4085	1/1	0.84	0.28	43,43,43,43	0
85	MG	AR	3986	1/1	0.84	0.86	41,41,41,41	0
85	MG	AR	3988	1/1	0.84	0.31	32,32,32,32	0
84	OHX	6	2025	7/7	0.84	0.20	248,249,250,252	0
84	OHX	1	3703	7/7	0.84	0.58	259,259,260,261	0
85	MG	AR	4001	1/1	0.84	0.43	41,41,41,41	0
85	MG	1	4141	1/1	0.84	0.33	36,36,36,36	0
85	MG	CR	205	1/1	0.84	0.44	29,29,29,29	0
85	MG	DC	203	1/1	0.84	0.25	35,35,35,35	0
84	OHX	c5	201	7/7	0.85	0.32	228,229,230,231	0
85	MG	AR	4043	1/1	0.85	0.32	48,48,48,48	0
85	MG	6	2123	1/1	0.85	0.30	60,60,60,60	0
85	MG	6	2134	1/1	0.85	0.21	43,43,43,43	0
85	MG	A	2069	1/1	0.85	0.29	36,36,36,36	0
84	OHX	AR	3669	7/7	0.85	0.16	245,246,247,248	0
84	OHX	6	2054	7/7	0.85	0.24	253,254,256,256	0
85	MG	1	4134	1/1	0.85	0.19	50,50,50,50	0
85	MG	AR	4061	1/1	0.85	0.50	40,40,40,40	0
85	MG	AR	4218	1/1	0.85	0.26	31,31,31,31	0
84	OHX	CG	302	7/7	0.85	0.24	210,211,212,213	0
84	OHX	1	3710	7/7	0.85	0.33	247,248,248,249	0
85	MG	4	222	1/1	0.85	0.44	61,61,61,61	0
85	MG	4	224	1/1	0.85	0.22	51,51,51,51	0
85	MG	AR	3897	1/1	0.85	0.53	18,18,18,18	0
84	OHX	A	2025	7/7	0.85	0.23	249,252,253,253	0
85	MG	AS	214	1/1	0.85	0.26	68,68,68,68	0
85	MG	AR	3950	1/1	0.85	0.25	41,41,41,41	0
84	OHX	AR	3663	7/7	0.85	0.25	208,209,210,210	0
85	MG	t	201	1/1	0.85	0.25	37,37,37,37	0
85	MG	1	4101	1/1	0.85	0.23	37,37,37,37	0
85	MG	x	206	1/1	0.85	0.36	32,32,32,32	0
85	MG	l2	202	1/1	0.85	0.23	48,48,48,48	0
85	MG	AR	4131	1/1	0.85	0.56	59,59,59,59	0
85	MG	6	2194	1/1	0.85	0.44	34,34,34,34	0
84	OHX	6	2045	7/7	0.85	0.39	196,197,198,199	0
85	MG	1	4052	1/1	0.85	0.12	48,48,48,48	0
85	MG	AR	4155	1/1	0.85	0.29	27,27,27,27	0
85	MG	1	3950	1/1	0.85	0.11	70,70,70,70	0
85	MG	AR	4015	1/1	0.85	0.35	43,43,43,43	0
85	MG	1	3795	1/1	0.85	0.32	37,37,37,37	0
85	MG	AR	3743	1/1	0.85	0.18	41,41,41,41	0
84	OHX	A	1971	7/7	0.85	0.17	216,218,220,221	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3759	1/1	0.85	0.29	103,103,103,103	0
85	MG	DE	201	1/1	0.85	0.15	55,55,55,55	0
85	MG	1	4017	1/1	0.85	0.21	59,59,59,59	0
85	MG	6	2145	1/1	0.86	0.18	51,51,51,51	0
85	MG	6	2147	1/1	0.86	0.31	75,75,75,75	0
85	MG	1	4150	1/1	0.86	1.01	73,73,73,73	0
85	MG	AR	4012	1/1	0.86	0.24	50,50,50,50	0
84	OHX	6	2027	7/7	0.86	0.32	187,188,189,190	0
84	OHX	AR	3702	7/7	0.86	0.41	218,219,220,220	0
85	MG	6	2167	1/1	0.86	0.42	52,52,52,52	0
85	MG	1	3960	1/1	0.86	0.30	27,27,27,27	0
85	MG	6	2169	1/1	0.86	0.39	39,39,39,39	0
84	OHX	1	3600	7/7	0.86	0.46	258,258,259,259	0
85	MG	1	4177	1/1	0.86	0.20	45,45,45,45	0
85	MG	1	4180	1/1	0.86	0.45	55,55,55,55	0
84	OHX	AR	3717	7/7	0.86	0.32	281,282,283,283	0
84	OHX	6	2055	7/7	0.86	0.18	234,235,236,236	0
85	MG	1	3786	1/1	0.86	0.42	37,37,37,37	0
84	OHX	6	2029	7/7	0.86	0.45	246,248,249,250	0
84	OHX	1	3658	7/7	0.86	0.22	211,212,212,213	0
85	MG	1	4194	1/1	0.86	0.23	82,82,82,82	0
85	MG	AR	4062	1/1	0.86	0.20	54,54,54,54	0
84	OHX	6	2043	7/7	0.86	0.32	196,196,198,198	0
85	MG	DA	201	1/1	0.86	0.20	29,29,29,29	0
85	MG	3	213	1/1	0.86	0.51	23,23,23,23	0
84	OHX	AR	3732	7/7	0.86	0.53	245,246,247,247	0
85	MG	DO	202	1/1	0.86	0.27	46,46,46,46	0
85	MG	1	3983	1/1	0.86	0.38	59,59,59,59	0
85	MG	1	4096	1/1	0.86	0.57	53,53,53,53	0
85	MG	1	3984	1/1	0.86	0.30	33,33,33,33	0
85	MG	1	3821	1/1	0.86	0.56	37,37,37,37	0
85	MG	A	2065	1/1	0.86	0.34	31,31,31,31	0
85	MG	4	233	1/1	0.86	0.61	61,61,61,61	0
85	MG	1	4003	1/1	0.86	0.41	46,46,46,46	0
84	OHX	AR	3735	7/7	0.86	0.31	246,247,248,248	0
85	MG	AR	3801	1/1	0.86	0.35	30,30,30,30	0
84	OHX	A	2029	7/7	0.86	0.14	261,263,265,265	0
84	OHX	6	2023	7/7	0.86	0.27	201,203,204,205	0
85	MG	AR	4135	1/1	0.86	0.54	66,66,66,66	0
85	MG	AR	3808	1/1	0.86	0.23	33,33,33,33	0
85	MG	1	4111	1/1	0.86	0.65	62,62,62,62	0
85	MG	z	202	1/1	0.86	0.24	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3815	1/1	0.86	0.18	75,75,75,75	0
85	MG	1	4112	1/1	0.86	0.28	41,41,41,41	0
85	MG	1	3853	1/1	0.86	0.51	61,61,61,61	0
85	MG	AR	3849	1/1	0.86	0.59	18,18,18,18	0
84	OHX	AR	3738	7/7	0.86	0.24	270,271,272,272	0
85	MG	AR	3888	1/1	0.86	0.46	33,33,33,33	0
85	MG	1	4029	1/1	0.86	0.49	42,42,42,42	0
85	MG	1	3866	1/1	0.86	0.34	46,46,46,46	0
85	MG	AR	4172	1/1	0.86	0.32	25,25,25,25	0
85	MG	AR	3899	1/1	0.86	0.35	46,46,46,46	0
85	MG	1	3887	1/1	0.86	0.12	49,49,49,49	0
85	MG	6	2092	1/1	0.86	0.30	45,45,45,45	0
85	MG	AR	3955	1/1	0.86	0.25	32,32,32,32	0
85	MG	AR	4206	1/1	0.86	0.40	31,31,31,31	0
85	MG	1	4032	1/1	0.86	0.29	49,49,49,49	0
85	MG	AR	3962	1/1	0.86	0.20	43,43,43,43	0
85	MG	1	3939	1/1	0.86	0.32	29,29,29,29	0
85	MG	AR	3968	1/1	0.86	0.33	29,29,29,29	0
84	OHX	4	209	7/7	0.86	0.36	194,194,195,195	0
85	MG	AR	4219	1/1	0.86	0.33	47,47,47,47	0
84	OHX	AR	3671	7/7	0.86	0.27	166,166,167,167	0
84	OHX	AR	3685	7/7	0.86	0.40	187,187,188,188	0
85	MG	6	2142	1/1	0.86	0.10	72,72,72,72	0
84	OHX	AR	3730	7/7	0.87	0.34	271,272,273,273	0
84	OHX	A	2030	7/7	0.87	0.24	208,209,211,212	0
85	MG	1	3871	1/1	0.87	0.28	27,27,27,27	0
85	MG	A	2054	1/1	0.87	0.21	59,59,59,59	0
85	MG	1	3875	1/1	0.87	0.25	18,18,18,18	0
85	MG	1	3981	1/1	0.87	0.36	59,59,59,59	0
85	MG	AR	3770	1/1	0.87	0.36	36,36,36,36	0
85	MG	1	4163	1/1	0.87	0.40	68,68,68,68	0
85	MG	AR	4095	1/1	0.87	0.34	36,36,36,36	0
85	MG	1	4103	1/1	0.87	0.35	60,60,60,60	0
85	MG	AR	3775	1/1	0.87	0.27	16,16,16,16	0
84	OHX	1	3674	7/7	0.87	0.36	212,212,213,213	0
85	MG	1	3891	1/1	0.87	0.66	16,16,16,16	0
85	MG	AR	4237	1/1	0.87	0.31	26,26,26,26	0
85	MG	AR	3994	1/1	0.87	0.40	44,44,44,44	0
84	OHX	6	2038	7/7	0.87	0.36	213,215,217,217	0
85	MG	z	203	1/1	0.87	0.20	45,45,45,45	0
85	MG	1	4058	1/1	0.87	0.15	37,37,37,37	0
84	OHX	AR	3609	7/7	0.87	0.31	201,201,202,202	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3641	7/7	0.87	0.40	218,219,219,220	0
84	OHX	AR	3726	7/7	0.87	0.42	220,220,221,221	0
85	MG	AR	4153	1/1	0.87	0.26	52,52,52,52	0
84	OHX	1	3705	7/7	0.87	0.42	222,222,223,223	0
85	MG	1	3749	1/1	0.87	0.35	38,38,38,38	0
85	MG	AR	4029	1/1	0.87	0.35	32,32,32,32	0
85	MG	AR	3834	1/1	0.87	0.18	30,30,30,30	0
85	MG	CF	403	1/1	0.87	0.28	30,30,30,30	0
85	MG	AR	3835	1/1	0.87	0.39	41,41,41,41	0
84	OHX	1	3678	7/7	0.87	0.17	228,228,229,230	0
85	MG	AR	4048	1/1	0.87	0.16	33,33,33,33	0
85	MG	1	3833	1/1	0.87	0.30	41,41,41,41	0
84	OHX	AR	3729	7/7	0.87	0.32	214,215,216,216	0
85	MG	A	2148	1/1	0.87	0.43	103,103,103,103	0
85	MG	A	2151	1/1	0.87	0.10	72,72,72,72	0
85	MG	6	2121	1/1	0.87	0.22	71,71,71,71	0
85	MG	AR	4180	1/1	0.87	0.47	93,93,93,93	0
85	MG	6	2197	1/1	0.87	0.32	57,57,57,57	0
85	MG	1	3761	1/1	0.87	0.42	44,44,44,44	0
85	MG	AF	202	1/1	0.87	0.27	32,32,32,32	0
85	MG	AR	4205	1/1	0.87	0.23	30,30,30,30	0
84	OHX	1	3638	7/7	0.88	0.22	245,246,247,248	0
84	OHX	1	3728	7/7	0.88	0.35	233,233,233,234	0
85	MG	AR	4082	1/1	0.88	0.24	48,48,48,48	0
85	MG	6	2093	1/1	0.88	0.33	47,47,47,47	0
85	MG	AR	3818	1/1	0.88	0.27	45,45,45,45	0
84	OHX	AR	3675	7/7	0.88	0.27	210,211,212,212	0
85	MG	AR	3822	1/1	0.88	0.14	52,52,52,52	0
84	OHX	AR	3734	7/7	0.88	0.29	223,224,224,225	0
85	MG	AR	3832	1/1	0.88	0.18	46,46,46,46	0
84	OHX	A	2031	7/7	0.88	0.23	244,246,248,248	0
85	MG	1	4152	1/1	0.88	0.20	40,40,40,40	0
85	MG	AR	4127	1/1	0.88	0.24	67,67,67,67	0
84	OHX	1	3536	7/7	0.88	0.18	221,221,223,224	0
85	MG	DD	101	1/1	0.88	0.23	32,32,32,32	0
84	OHX	A	2036	7/7	0.88	0.12	274,277,278,279	0
84	OHX	A	2039	7/7	0.88	0.28	264,266,268,268	0
85	MG	AR	4146	1/1	0.88	0.41	37,37,37,37	0
84	OHX	A	2040	7/7	0.88	0.24	246,248,249,250	0
84	OHX	1	3666	7/7	0.88	0.39	186,187,188,188	0
84	OHX	AR	3695	7/7	0.88	0.24	225,226,227,227	0
85	MG	1	4179	1/1	0.88	0.15	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	A	2055	1/1	0.88	0.26	48,48,48,48	0
84	OHX	O	201	7/7	0.88	0.17	249,252,253,253	0
84	OHX	1	3719	7/7	0.88	0.38	264,264,265,265	0
85	MG	1	3733	1/1	0.88	0.44	33,33,33,33	0
85	MG	1	3951	1/1	0.88	0.33	43,43,43,43	0
85	MG	AR	3964	1/1	0.88	0.30	28,28,28,28	0
84	OHX	AR	3705	7/7	0.88	0.28	212,213,213,214	0
85	MG	AR	3967	1/1	0.88	0.34	64,64,64,64	0
84	OHX	AR	3711	7/7	0.88	0.20	227,227,228,228	0
85	MG	A	2087	1/1	0.88	0.28	57,57,57,57	0
85	MG	1	3961	1/1	0.88	0.34	26,26,26,26	0
85	MG	1	4199	1/1	0.88	0.62	25,25,25,25	0
85	MG	A	2091	1/1	0.88	0.44	60,60,60,60	0
85	MG	A	2093	1/1	0.88	0.19	93,93,93,93	0
84	OHX	CF	402	7/7	0.88	0.47	254,255,256,256	0
85	MG	1	4217	1/1	0.88	0.29	18,18,18,18	0
85	MG	A	2100	1/1	0.88	0.32	60,60,60,60	0
85	MG	1	4088	1/1	0.88	0.22	28,28,28,28	0
85	MG	1	3751	1/1	0.88	0.16	50,50,50,50	0
84	OHX	AR	3712	7/7	0.88	0.31	183,183,184,184	0
84	OHX	CG	303	7/7	0.88	0.59	212,213,214,214	0
84	OHX	AR	3639	7/7	0.88	0.18	211,212,213,213	0
84	OHX	CM	201	7/7	0.88	0.22	247,248,249,250	0
85	MG	1	3769	1/1	0.88	0.45	61,61,61,61	0
85	MG	1	3774	1/1	0.88	0.21	84,84,84,84	0
85	MG	A	2123	1/1	0.88	0.20	40,40,40,40	0
85	MG	o	303	1/1	0.88	0.21	38,38,38,38	0
85	MG	AR	3740	1/1	0.88	0.45	46,46,46,46	0
84	OHX	AR	3640	7/7	0.88	0.29	197,198,199,199	0
85	MG	1	3779	1/1	0.88	0.31	29,29,29,29	0
84	OHX	6	1960	7/7	0.88	0.21	155,157,157,158	0
85	MG	AR	3762	1/1	0.88	0.19	40,40,40,40	0
85	MG	1	3985	1/1	0.88	0.34	22,22,22,22	0
85	MG	A	2146	1/1	0.88	0.62	29,29,29,29	0
85	MG	AR	3771	1/1	0.88	0.22	24,24,24,24	0
84	OHX	DL	102	7/7	0.88	0.39	212,212,213,213	0
84	OHX	A	1946	7/7	0.88	0.17	212,214,216,217	0
85	MG	A	2153	1/1	0.88	0.31	66,66,66,66	0
84	OHX	AR	3644	7/7	0.88	0.26	197,197,198,199	0
85	MG	6	2064	1/1	0.88	0.31	62,62,62,62	0
84	OHX	1	3606	7/7	0.88	0.28	193,194,194,195	0
85	MG	b	101	1/1	0.88	0.22	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1993	7/7	0.88	0.40	236,237,239,240	0
85	MG	d3	203	1/1	0.88	0.23	29,29,29,29	0
84	OHX	6	1982	7/7	0.88	0.42	171,172,173,174	0
84	OHX	1	3617	7/7	0.88	0.37	201,202,203,204	0
85	MG	4	232	1/1	0.89	0.30	43,43,43,43	0
84	OHX	AR	3646	7/7	0.89	0.30	167,168,169,169	0
84	OHX	x	201	7/7	0.89	0.44	169,169,170,170	0
85	MG	AS	223	1/1	0.89	0.23	59,59,59,59	0
85	MG	AS	224	1/1	0.89	0.26	55,55,55,55	0
85	MG	AR	4042	1/1	0.89	0.26	20,20,20,20	0
84	OHX	x	202	7/7	0.89	0.27	223,224,225,225	0
85	MG	AR	4047	1/1	0.89	0.21	30,30,30,30	0
85	MG	1	3807	1/1	0.89	0.30	37,37,37,37	0
84	OHX	AR	3668	7/7	0.89	0.32	216,216,217,218	0
84	OHX	AR	3733	7/7	0.89	0.52	289,291,292,292	0
85	MG	CD	302	1/1	0.89	0.75	39,39,39,39	0
84	OHX	1	3720	7/7	0.89	0.23	197,197,199,199	0
84	OHX	6	2047	7/7	0.89	0.32	237,239,240,241	0
84	OHX	A	2038	7/7	0.89	0.56	217,217,220,220	0
85	MG	AR	3782	1/1	0.89	0.27	30,30,30,30	0
84	OHX	6	2048	7/7	0.89	0.42	224,224,225,226	0
85	MG	AR	4063	1/1	0.89	0.17	39,39,39,39	0
85	MG	CQ	202	1/1	0.89	0.19	26,26,26,26	0
85	MG	CQ	203	1/1	0.89	0.40	28,28,28,28	0
85	MG	AR	3787	1/1	0.89	0.18	31,31,31,31	0
85	MG	AR	3788	1/1	0.89	0.43	45,45,45,45	0
85	MG	AR	3794	1/1	0.89	0.34	19,19,19,19	0
84	OHX	1	3645	7/7	0.89	0.25	220,221,221,221	0
85	MG	1	4023	1/1	0.89	0.72	44,44,44,44	0
84	OHX	A	2041	7/7	0.89	0.41	201,203,204,204	0
84	OHX	AR	3681	7/7	0.89	0.21	198,199,200,201	0
85	MG	AR	3811	1/1	0.89	0.30	25,25,25,25	0
85	MG	AR	4096	1/1	0.89	0.27	53,53,53,53	0
84	OHX	AR	3682	7/7	0.89	0.42	213,214,214,215	0
85	MG	1	4138	1/1	0.89	0.37	37,37,37,37	0
85	MG	AR	4107	1/1	0.89	0.26	79,79,79,79	0
85	MG	6	2090	1/1	0.89	0.42	45,45,45,45	0
84	OHX	1	3724	7/7	0.89	0.50	243,244,245,246	0
85	MG	1	3877	1/1	0.89	0.13	44,44,44,44	0
85	MG	AR	4126	1/1	0.89	0.29	73,73,73,73	0
85	MG	1	4142	1/1	0.89	0.58	47,47,47,47	0
85	MG	1	4033	1/1	0.89	0.26	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4130	1/1	0.89	0.17	19,19,19,19	0
85	MG	AR	3830	1/1	0.89	0.29	30,30,30,30	0
84	OHX	c3	201	7/7	0.89	0.25	212,213,214,215	0
85	MG	AR	4141	1/1	0.89	0.23	53,53,53,53	0
84	OHX	6	2015	7/7	0.89	0.41	230,231,232,233	0
85	MG	1	3934	1/1	0.89	0.17	61,61,61,61	0
84	OHX	1	3632	7/7	0.89	0.31	202,202,204,204	0
85	MG	1	4169	1/1	0.89	0.22	39,39,39,39	0
85	MG	6	2144	1/1	0.89	0.30	42,42,42,42	0
85	MG	AR	4154	1/1	0.89	0.10	50,50,50,50	0
84	OHX	6	2056	7/7	0.89	0.22	214,215,217,218	0
85	MG	1	4047	1/1	0.89	0.72	39,39,39,39	0
85	MG	1	4050	1/1	0.89	0.30	34,34,34,34	0
85	MG	AR	3913	1/1	0.89	0.35	20,20,20,20	0
84	OHX	1	3698	7/7	0.89	0.46	177,178,178,179	0
85	MG	6	2153	1/1	0.89	0.24	39,39,39,39	0
85	MG	AR	3952	1/1	0.89	0.24	28,28,28,28	0
85	MG	A	2113	1/1	0.89	0.25	35,35,35,35	0
85	MG	AR	3953	1/1	0.89	0.21	35,35,35,35	0
85	MG	A	2117	1/1	0.89	0.20	52,52,52,52	0
85	MG	1	4056	1/1	0.89	0.39	82,82,82,82	0
84	OHX	AE	201	7/7	0.89	0.20	194,195,195,196	0
85	MG	1	4182	1/1	0.89	0.35	49,49,49,49	0
84	OHX	AR	3520	7/7	0.89	0.20	175,175,176,176	0
84	OHX	1	3664	7/7	0.89	0.35	232,233,234,235	0
84	OHX	AR	3638	7/7	0.89	0.41	208,208,209,209	0
84	OHX	1	3715	7/7	0.89	0.43	219,220,222,222	0
84	OHX	AR	3719	7/7	0.89	0.25	220,220,221,221	0
85	MG	1	3766	1/1	0.89	0.29	23,23,23,23	0
84	OHX	1	3597	7/7	0.89	0.13	237,238,240,240	0
85	MG	6	2189	1/1	0.89	0.29	67,67,67,67	0
85	MG	1	4207	1/1	0.89	0.31	44,44,44,44	0
85	MG	AR	3993	1/1	0.89	0.21	62,62,62,62	0
84	OHX	AR	3725	7/7	0.89	0.33	261,263,264,264	0
84	OHX	1	3671	7/7	0.89	0.45	212,213,214,214	0
84	OHX	6	2041	7/7	0.89	0.36	209,209,210,211	0
85	MG	1	3975	1/1	0.89	0.17	43,43,43,43	0
85	MG	9	201	1/1	0.89	0.19	33,33,33,33	0
85	MG	1	3781	1/1	0.89	0.25	24,24,24,24	0
85	MG	1	3977	1/1	0.89	0.35	21,21,21,21	0
84	OHX	A	2012	7/7	0.89	0.20	218,220,220,222	0
85	MG	4	231	1/1	0.89	0.26	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3998	1/1	0.90	0.49	18,18,18,18	0
85	MG	1	3897	1/1	0.90	0.38	13,13,13,13	0
85	MG	1	3933	1/1	0.90	0.23	37,37,37,37	0
84	OHX	AR	3688	7/7	0.90	0.28	199,200,201,201	0
84	OHX	AR	3693	7/7	0.90	0.28	238,239,240,240	0
84	OHX	AR	3632	7/7	0.90	0.14	227,227,228,228	0
85	MG	1	3945	1/1	0.90	0.29	17,17,17,17	0
85	MG	AS	218	1/1	0.90	0.22	52,52,52,52	0
85	MG	AS	219	1/1	0.90	0.30	35,35,35,35	0
84	OHX	Q	201	7/7	0.90	0.25	245,246,248,249	0
85	MG	AR	4028	1/1	0.90	0.24	44,44,44,44	0
84	OHX	AR	3696	7/7	0.90	0.34	176,176,177,178	0
84	OHX	CE	403	7/7	0.90	0.50	237,238,239,240	0
85	MG	AS	226	1/1	0.90	0.46	36,36,36,36	0
85	MG	AR	3747	1/1	0.90	0.22	23,23,23,23	0
85	MG	AR	4037	1/1	0.90	0.29	33,33,33,33	0
85	MG	AR	4041	1/1	0.90	0.12	47,47,47,47	0
85	MG	AR	3753	1/1	0.90	0.16	51,51,51,51	0
84	OHX	AR	3701	7/7	0.90	0.41	207,208,208,208	0
84	OHX	AR	3637	7/7	0.90	0.30	204,205,205,205	0
85	MG	AR	3766	1/1	0.90	0.23	21,21,21,21	0
84	OHX	z	201	7/7	0.90	0.23	257,258,259,259	0
84	OHX	AR	3706	7/7	0.90	0.22	209,210,211,212	0
84	OHX	AR	3707	7/7	0.90	0.27	207,207,207,207	0
84	OHX	AR	3710	7/7	0.90	0.32	213,215,216,216	0
84	OHX	1	3692	7/7	0.90	0.31	189,190,191,191	0
85	MG	CO	203	1/1	0.90	0.20	46,46,46,46	0
85	MG	AR	4060	1/1	0.90	0.27	56,56,56,56	0
85	MG	t	202	1/1	0.90	0.21	64,64,64,64	0
84	OHX	1	3635	7/7	0.90	0.26	219,220,221,222	0
85	MG	1	3969	1/1	0.90	0.12	45,45,45,45	0
84	OHX	DI	201	7/7	0.90	0.59	194,195,195,196	0
85	MG	1	4108	1/1	0.90	0.26	33,33,33,33	0
84	OHX	6	1980	7/7	0.90	0.38	206,206,208,208	0
85	MG	1	4110	1/1	0.90	0.27	37,37,37,37	0
85	MG	1	3767	1/1	0.90	0.12	34,34,34,34	0
85	MG	DI	202	1/1	0.90	0.26	32,32,32,32	0
85	MG	AR	3805	1/1	0.90	0.17	39,39,39,39	0
84	OHX	1	3648	7/7	0.90	0.27	258,259,260,260	0
85	MG	6	2073	1/1	0.90	0.41	57,57,57,57	0
84	OHX	A	1959	7/7	0.90	0.15	180,182,183,184	0
84	OHX	6	2010	7/7	0.90	0.24	213,214,215,216	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3652	7/7	0.90	0.36	196,196,197,197	0
85	MG	1	3780	1/1	0.90	0.26	26,26,26,26	0
84	OHX	6	2049	7/7	0.90	0.27	218,219,220,221	0
84	OHX	A	1996	7/7	0.90	0.27	208,209,211,212	0
85	MG	1	3988	1/1	0.90	0.26	46,46,46,46	0
85	MG	1	3998	1/1	0.90	0.24	65,65,65,65	0
85	MG	6	2120	1/1	0.90	0.17	61,61,61,61	0
84	OHX	AR	3722	7/7	0.90	0.30	200,201,201,202	0
84	OHX	A	2005	7/7	0.90	0.45	204,206,207,207	0
85	MG	AR	3839	1/1	0.90	0.38	30,30,30,30	0
85	MG	6	2128	1/1	0.90	0.28	53,53,53,53	0
85	MG	AR	4140	1/1	0.90	0.26	24,24,24,24	0
85	MG	AR	3855	1/1	0.90	0.14	37,37,37,37	0
85	MG	AR	4142	1/1	0.90	0.42	55,55,55,55	0
85	MG	6	2133	1/1	0.90	0.29	51,51,51,51	0
85	MG	AR	3884	1/1	0.90	0.27	27,27,27,27	0
84	OHX	AR	3723	7/7	0.90	0.19	240,241,242,242	0
85	MG	AR	3889	1/1	0.90	0.25	42,42,42,42	0
84	OHX	1	3695	7/7	0.90	0.23	200,201,202,202	0
84	OHX	6	2052	7/7	0.90	0.25	244,244,246,246	0
85	MG	1	3809	1/1	0.90	0.32	23,23,23,23	0
84	OHX	A	2019	7/7	0.90	0.14	252,253,255,256	0
84	OHX	A	2023	7/7	0.90	0.23	202,204,206,206	0
84	OHX	A	2024	7/7	0.90	0.36	219,222,223,223	0
85	MG	AR	3951	1/1	0.90	0.17	26,26,26,26	0
84	OHX	1	3729	7/7	0.90	0.37	206,207,207,208	0
85	MG	1	4171	1/1	0.90	0.14	26,26,26,26	0
84	OHX	1	3649	7/7	0.90	0.21	247,248,249,250	0
84	OHX	1	3670	7/7	0.90	0.30	215,215,217,217	0
84	OHX	1	3680	7/7	0.90	0.39	212,212,213,213	0
85	MG	AR	4176	1/1	0.90	0.20	52,52,52,52	0
85	MG	AR	4179	1/1	0.90	0.21	58,58,58,58	0
85	MG	1	4178	1/1	0.90	0.20	42,42,42,42	0
85	MG	A	2134	1/1	0.90	0.56	34,34,34,34	0
85	MG	AR	4181	1/1	0.90	0.20	37,37,37,37	0
84	OHX	AR	3731	7/7	0.90	0.37	175,176,177,178	0
84	OHX	1	3704	7/7	0.90	0.40	277,278,278,278	0
85	MG	AR	4201	1/1	0.90	0.37	31,31,31,31	0
84	OHX	6	2032	7/7	0.90	0.35	236,237,238,239	0
85	MG	AR	4203	1/1	0.90	0.35	37,37,37,37	0
84	OHX	6	2034	7/7	0.90	0.26	236,238,239,240	0
85	MG	1	4043	1/1	0.90	0.35	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3980	1/1	0.90	0.21	32,32,32,32	0
85	MG	1	3880	1/1	0.90	0.50	29,29,29,29	0
85	MG	1	3883	1/1	0.90	0.47	17,17,17,17	0
84	OHX	1	3650	7/7	0.90	0.32	179,181,181,182	0
85	MG	s8	302	1/1	0.90	0.27	44,44,44,44	0
84	OHX	AR	3736	7/7	0.90	0.17	184,185,186,187	0
85	MG	1	3895	1/1	0.90	0.27	29,29,29,29	0
85	MG	AR	3995	1/1	0.90	0.11	38,38,38,38	0
85	MG	1	4202	1/1	0.90	0.33	27,27,27,27	0
85	MG	AR	4084	1/1	0.91	0.19	31,31,31,31	0
85	MG	AR	3864	1/1	0.91	0.26	21,21,21,21	0
84	OHX	AR	3598	7/7	0.91	0.17	205,206,207,208	0
85	MG	1	3986	1/1	0.91	0.13	30,30,30,30	0
84	OHX	AR	3605	7/7	0.91	0.14	194,195,196,196	0
85	MG	1	4105	1/1	0.91	0.51	64,64,64,64	0
84	OHX	J	301	7/7	0.91	0.25	244,245,247,247	0
85	MG	AR	4104	1/1	0.91	0.29	55,55,55,55	0
84	OHX	AR	3678	7/7	0.91	0.53	238,238,239,239	0
85	MG	AR	4117	1/1	0.91	0.23	53,53,53,53	0
85	MG	1	4002	1/1	0.91	0.21	104,104,104,104	0
84	OHX	6	2011	7/7	0.91	0.20	205,205,207,207	0
85	MG	AR	4123	1/1	0.91	0.25	39,39,39,39	0
85	MG	1	3876	1/1	0.91	0.38	39,39,39,39	0
84	OHX	1	3656	7/7	0.91	0.26	229,230,231,231	0
84	OHX	AR	3724	7/7	0.91	0.34	203,204,205,205	0
85	MG	1	4015	1/1	0.91	0.17	38,38,38,38	0
84	OHX	d9	101	7/7	0.91	0.33	234,235,236,237	0
85	MG	6	2196	1/1	0.91	0.38	46,46,46,46	0
85	MG	AR	3956	1/1	0.91	0.20	41,41,41,41	0
85	MG	1	4121	1/1	0.91	0.28	32,32,32,32	0
84	OHX	A	1943	7/7	0.91	0.25	161,163,164,165	0
84	OHX	6	2046	7/7	0.91	0.17	244,245,247,248	0
85	MG	1	4028	1/1	0.91	0.28	24,24,24,24	0
85	MG	1	4133	1/1	0.91	0.45	28,28,28,28	0
85	MG	A	2052	1/1	0.91	0.46	27,27,27,27	0
84	OHX	4	211	7/7	0.91	0.24	225,225,226,226	0
84	OHX	r	301	7/7	0.91	0.19	167,168,168,169	0
85	MG	1	3930	1/1	0.91	0.21	19,19,19,19	0
85	MG	6	2060	1/1	0.91	0.67	23,23,23,23	0
85	MG	AR	3982	1/1	0.91	0.26	35,35,35,35	0
85	MG	AR	3984	1/1	0.91	0.34	49,49,49,49	0
84	OHX	AR	3689	7/7	0.91	0.23	195,197,198,198	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1989	7/7	0.91	0.29	253,254,256,256	0
84	OHX	1	3557	7/7	0.91	0.20	186,187,188,188	0
84	OHX	AR	3694	7/7	0.91	0.40	212,212,213,213	0
85	MG	6	2074	1/1	0.91	0.31	37,37,37,37	0
84	OHX	A	2000	7/7	0.91	0.22	194,195,196,197	0
85	MG	1	3764	1/1	0.91	0.54	38,38,38,38	0
85	MG	1	4153	1/1	0.91	0.21	39,39,39,39	0
84	OHX	1	3661	7/7	0.91	0.57	251,252,253,253	0
84	OHX	1	3712	7/7	0.91	0.41	215,215,216,217	0
85	MG	A	2095	1/1	0.91	0.18	94,94,94,94	0
84	OHX	6	2031	7/7	0.91	0.27	210,211,213,213	0
85	MG	AR	4016	1/1	0.91	0.44	104,104,104,104	0
84	OHX	1	3713	7/7	0.91	0.33	217,217,218,218	0
85	MG	1	4051	1/1	0.91	0.37	63,63,63,63	0
85	MG	6	2116	1/1	0.91	0.42	41,41,41,41	0
85	MG	AR	3791	1/1	0.91	0.47	32,32,32,32	0
84	OHX	AR	3704	7/7	0.91	0.37	223,224,225,225	0
85	MG	AR	3795	1/1	0.91	0.20	22,22,22,22	0
84	OHX	A	2016	7/7	0.91	0.19	207,209,210,211	0
85	MG	A	2114	1/1	0.91	0.36	41,41,41,41	0
85	MG	AR	4034	1/1	0.91	0.25	42,42,42,42	0
84	OHX	AR	3655	7/7	0.91	0.36	216,218,218,219	0
84	OHX	AR	3659	7/7	0.91	0.26	195,196,196,197	0
85	MG	AR	4215	1/1	0.91	0.23	72,72,72,72	0
85	MG	AR	4039	1/1	0.91	0.28	37,37,37,37	0
85	MG	AR	4040	1/1	0.91	0.24	27,27,27,27	0
85	MG	6	2130	1/1	0.91	0.26	42,42,42,42	0
85	MG	AR	3807	1/1	0.91	0.24	27,27,27,27	0
85	MG	A	2130	1/1	0.91	0.29	49,49,49,49	0
85	MG	A	2131	1/1	0.91	0.13	88,88,88,88	0
85	MG	A	2132	1/1	0.91	0.27	71,71,71,71	0
84	OHX	1	3633	7/7	0.91	0.17	193,194,195,197	0
84	OHX	AR	3708	7/7	0.91	0.30	228,228,229,229	0
84	OHX	6	2036	7/7	0.91	0.38	172,174,175,176	0
84	OHX	AT	216	7/7	0.91	0.17	193,193,193,193	0
84	OHX	AT	218	7/7	0.91	0.39	223,224,224,224	0
84	OHX	A	2032	7/7	0.91	0.19	234,236,237,239	0
84	OHX	AT	220	7/7	0.91	0.26	197,197,198,198	0
84	OHX	AR	3666	7/7	0.91	0.20	217,218,218,219	0
85	MG	6	2151	1/1	0.91	0.71	87,87,87,87	0
84	OHX	1	3651	7/7	0.91	0.30	207,208,209,209	0
85	MG	AR	3831	1/1	0.91	0.32	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3713	7/7	0.91	0.16	247,247,248,249	0
85	MG	6	2156	1/1	0.91	0.14	50,50,50,50	0
85	MG	6	2157	1/1	0.91	0.26	45,45,45,45	0
85	MG	6	2160	1/1	0.91	0.24	121,121,121,121	0
84	OHX	1	3718	7/7	0.91	0.38	220,221,221,222	0
85	MG	d5	201	1/1	0.91	0.09	67,67,67,67	0
85	MG	d6	101	1/1	0.91	0.24	37,37,37,37	0
85	MG	AR	4081	1/1	0.91	0.31	52,52,52,52	0
84	OHX	1	3667	7/7	0.91	0.35	189,189,190,191	0
85	MG	6	2072	1/1	0.92	0.23	36,36,36,36	0
85	MG	AR	3876	1/1	0.92	0.43	30,30,30,30	0
84	OHX	A	2013	7/7	0.92	0.32	203,205,206,206	0
84	OHX	AR	3603	7/7	0.92	0.13	182,183,184,185	0
85	MG	AR	3887	1/1	0.92	0.72	35,35,35,35	0
84	OHX	6	2002	7/7	0.92	0.19	218,220,221,221	0
85	MG	6	2079	1/1	0.92	0.34	37,37,37,37	0
84	OHX	A	2017	7/7	0.92	0.24	220,223,224,224	0
85	MG	AR	4185	1/1	0.92	0.36	40,40,40,40	0
85	MG	1	4084	1/1	0.92	0.21	44,44,44,44	0
85	MG	AR	4194	1/1	0.92	0.27	47,47,47,47	0
85	MG	6	2087	1/1	0.92	0.39	28,28,28,28	0
84	OHX	6	2006	7/7	0.92	0.21	199,199,201,201	0
84	OHX	AR	3621	7/7	0.92	0.22	208,209,210,211	0
85	MG	AR	3943	1/1	0.92	0.26	73,73,73,73	0
85	MG	AR	3948	1/1	0.92	0.23	16,16,16,16	0
85	MG	AR	4208	1/1	0.92	0.24	62,62,62,62	0
84	OHX	AR	3628	7/7	0.92	0.27	209,210,211,211	0
85	MG	1	4093	1/1	0.92	0.47	16,16,16,16	0
84	OHX	AR	3721	7/7	0.92	0.30	212,213,213,214	0
85	MG	1	3898	1/1	0.92	0.33	22,22,22,22	0
85	MG	1	3912	1/1	0.92	0.34	30,30,30,30	0
84	OHX	A	2026	7/7	0.92	0.32	191,192,194,194	0
84	OHX	AR	3629	7/7	0.92	0.32	209,210,211,212	0
85	MG	6	2124	1/1	0.92	0.12	62,62,62,62	0
85	MG	6	2127	1/1	0.92	0.17	52,52,52,52	0
84	OHX	1	3682	7/7	0.92	0.27	204,206,207,207	0
85	MG	1	3938	1/1	0.92	0.11	41,41,41,41	0
84	OHX	AR	3634	7/7	0.92	0.18	213,214,215,216	0
84	OHX	1	3657	7/7	0.92	0.40	170,171,171,171	0
85	MG	AR	3973	1/1	0.92	0.19	27,27,27,27	0
85	MG	AR	4244	1/1	0.92	0.34	44,44,44,44	0
84	OHX	1	3688	7/7	0.92	0.24	220,221,221,222	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	3977	1/1	0.92	0.54	26,26,26,26	0
85	MG	AR	3979	1/1	0.92	0.24	45,45,45,45	0
84	OHX	6	2022	7/7	0.92	0.11	235,235,238,239	0
84	OHX	1	3601	7/7	0.92	0.33	200,200,201,202	0
84	OHX	1	3556	7/7	0.92	0.19	180,181,182,183	0
84	OHX	1	3721	7/7	0.92	0.39	191,192,193,193	0
85	MG	1	3952	1/1	0.92	0.16	34,34,34,34	0
84	OHX	1	3608	7/7	0.92	0.28	177,177,179,179	0
85	MG	1	4120	1/1	0.92	0.18	46,46,46,46	0
84	OHX	AR	3647	7/7	0.92	0.31	203,204,205,205	0
85	MG	6	2155	1/1	0.92	0.14	61,61,61,61	0
85	MG	AT	225	1/1	0.92	0.17	60,60,60,60	0
85	MG	1	4123	1/1	0.92	0.23	41,41,41,41	0
84	OHX	1	3665	7/7	0.92	0.16	209,210,211,211	0
85	MG	6	2159	1/1	0.92	0.31	39,39,39,39	0
84	OHX	1	3696	7/7	0.92	0.55	240,240,241,242	0
84	OHX	1	3697	7/7	0.92	0.22	238,240,241,241	0
84	OHX	6	2033	7/7	0.92	0.28	199,200,201,202	0
85	MG	AR	4020	1/1	0.92	0.14	69,69,69,69	0
84	OHX	1	3615	7/7	0.92	0.39	185,186,186,187	0
84	OHX	6	2035	7/7	0.92	0.32	157,158,159,159	0
84	OHX	1	3642	7/7	0.92	0.21	193,193,195,195	0
84	OHX	AS	209	7/7	0.92	0.25	175,176,177,177	0
84	OHX	6	2037	7/7	0.92	0.39	203,204,206,206	0
85	MG	1	3738	1/1	0.92	0.28	57,57,57,57	0
85	MG	1	3742	1/1	0.92	0.36	19,19,19,19	0
85	MG	1	4146	1/1	0.92	0.16	39,39,39,39	0
85	MG	AR	4035	1/1	0.92	0.19	39,39,39,39	0
85	MG	1	3979	1/1	0.92	0.29	47,47,47,47	0
84	OHX	1	3700	7/7	0.92	0.26	161,162,163,163	0
84	OHX	6	2039	7/7	0.92	0.18	204,204,206,206	0
85	MG	1	4157	1/1	0.92	0.21	37,37,37,37	0
84	OHX	AT	219	7/7	0.92	0.38	190,190,190,191	0
85	MG	DP	101	1/1	0.92	0.20	43,43,43,43	0
85	MG	1	3753	1/1	0.92	0.32	28,28,28,28	0
85	MG	1	3754	1/1	0.92	0.32	38,38,38,38	0
84	OHX	6	2040	7/7	0.92	0.30	199,200,201,202	0
84	OHX	AR	3677	7/7	0.92	0.36	180,180,181,181	0
84	OHX	3	208	7/7	0.92	0.16	230,231,232,233	0
85	MG	AR	4052	1/1	0.92	0.32	28,28,28,28	0
84	OHX	1	3701	7/7	0.92	0.24	181,182,182,182	0
85	MG	A	2062	1/1	0.92	0.29	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3551	7/7	0.92	0.16	191,192,192,193	0
84	OHX	6	2044	7/7	0.92	0.35	238,238,239,240	0
85	MG	1	4005	1/1	0.92	0.63	37,37,37,37	0
85	MG	A	2072	1/1	0.92	0.28	44,44,44,44	0
85	MG	1	4006	1/1	0.92	0.23	33,33,33,33	0
84	OHX	AR	3686	7/7	0.92	0.47	186,187,187,187	0
84	OHX	1	3618	7/7	0.92	0.35	189,190,191,192	0
85	MG	1	4011	1/1	0.92	0.18	38,38,38,38	0
85	MG	A	2085	1/1	0.92	0.20	47,47,47,47	0
84	OHX	4	212	7/7	0.92	0.24	201,202,202,202	0
85	MG	AR	3764	1/1	0.92	0.18	27,27,27,27	0
84	OHX	1	3672	7/7	0.92	0.39	161,162,164,164	0
85	MG	AR	4075	1/1	0.92	0.33	35,35,35,35	0
84	OHX	1	3619	7/7	0.92	0.39	190,191,192,193	0
85	MG	AR	4079	1/1	0.92	0.33	36,36,36,36	0
85	MG	1	4021	1/1	0.92	0.24	29,29,29,29	0
84	OHX	1	3708	7/7	0.92	0.30	210,211,211,211	0
85	MG	A	2097	1/1	0.92	0.32	55,55,55,55	0
84	OHX	1	3621	7/7	0.92	0.24	221,223,224,224	0
85	MG	AR	3774	1/1	0.92	0.21	23,23,23,23	0
85	MG	A	2101	1/1	0.92	0.24	64,64,64,64	0
85	MG	AR	4092	1/1	0.92	0.20	25,25,25,25	0
84	OHX	6	1955	7/7	0.92	0.16	191,193,195,196	0
85	MG	A	2105	1/1	0.92	0.25	71,71,71,71	0
84	OHX	1	3622	7/7	0.92	0.20	211,212,213,213	0
84	OHX	A	1969	7/7	0.92	0.20	220,222,223,223	0
84	OHX	1	3654	7/7	0.92	0.29	192,194,194,194	0
84	OHX	1	3679	7/7	0.92	0.24	230,231,232,232	0
84	OHX	1	3631	7/7	0.92	0.18	198,199,199,199	0
85	MG	AR	3792	1/1	0.92	0.38	28,28,28,28	0
85	MG	AR	4108	1/1	0.92	0.17	25,25,25,25	0
85	MG	AR	4114	1/1	0.92	0.17	30,30,30,30	0
84	OHX	A	1991	7/7	0.92	0.21	218,220,221,221	0
85	MG	4	218	1/1	0.92	0.52	7,7,7,7	0
85	MG	1	4036	1/1	0.92	0.25	35,35,35,35	0
85	MG	1	3820	1/1	0.92	0.26	30,30,30,30	0
85	MG	4	227	1/1	0.92	0.21	42,42,42,42	0
85	MG	4	230	1/1	0.92	0.18	54,54,54,54	0
85	MG	AR	3806	1/1	0.92	0.22	68,68,68,68	0
85	MG	1	4039	1/1	0.92	0.23	40,40,40,40	0
84	OHX	6	1990	7/7	0.92	0.33	238,238,239,240	0
85	MG	A	2133	1/1	0.92	0.40	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1993	7/7	0.92	0.24	191,192,193,194	0
84	OHX	A	1997	7/7	0.92	0.25	211,214,214,215	0
85	MG	1	3831	1/1	0.92	0.27	42,42,42,42	0
85	MG	1	4045	1/1	0.92	0.11	62,62,62,62	0
85	MG	A	2140	1/1	0.92	0.30	55,55,55,55	0
84	OHX	A	1999	7/7	0.92	0.23	214,215,217,217	0
85	MG	AR	4143	1/1	0.92	0.25	38,38,38,38	0
85	MG	1	3834	1/1	0.92	0.42	18,18,18,18	0
85	MG	A	2149	1/1	0.92	0.36	49,49,49,49	0
84	OHX	6	2000	7/7	0.92	0.16	210,211,212,213	0
85	MG	A	2152	1/1	0.92	0.16	78,78,78,78	0
85	MG	1	3847	1/1	0.92	0.39	23,23,23,23	0
85	MG	AR	3828	1/1	0.92	0.30	47,47,47,47	0
85	MG	1	4055	1/1	0.92	0.24	33,33,33,33	0
84	OHX	AR	3597	7/7	0.92	0.20	176,177,178,178	0
84	OHX	6	2001	7/7	0.92	0.40	211,211,212,213	0
85	MG	1	4062	1/1	0.92	0.19	33,33,33,33	0
85	MG	AR	4158	1/1	0.92	0.30	21,21,21,21	0
84	OHX	A	2006	7/7	0.92	0.25	215,218,219,219	0
84	OHX	AR	3599	7/7	0.92	0.29	201,202,203,203	0
85	MG	AR	3844	1/1	0.92	0.26	25,25,25,25	0
85	MG	6	2069	1/1	0.92	0.59	26,26,26,26	0
84	OHX	AR	3602	7/7	0.92	0.33	192,193,194,194	0
85	MG	6	2125	1/1	0.93	0.26	63,63,63,63	0
85	MG	AR	3933	1/1	0.93	0.53	13,13,13,13	0
85	MG	1	4128	1/1	0.93	0.19	27,27,27,27	0
84	OHX	6	1977	7/7	0.93	0.15	193,194,196,196	0
84	OHX	1	3553	7/7	0.93	0.22	184,185,186,186	0
85	MG	AR	4184	1/1	0.93	0.20	35,35,35,35	0
85	MG	1	3997	1/1	0.93	0.30	37,37,37,37	0
85	MG	AR	4191	1/1	0.93	0.20	38,38,38,38	0
84	OHX	AR	3657	7/7	0.93	0.34	207,207,209,209	0
85	MG	1	4000	1/1	0.93	0.41	36,36,36,36	0
85	MG	AR	4199	1/1	0.93	0.27	64,64,64,64	0
85	MG	6	2140	1/1	0.93	0.23	46,46,46,46	0
84	OHX	1	3564	7/7	0.93	0.18	173,175,175,175	0
85	MG	6	2143	1/1	0.93	0.18	90,90,90,90	0
84	OHX	AR	3660	7/7	0.93	0.35	167,168,169,170	0
84	OHX	6	1989	7/7	0.93	0.29	169,170,172,172	0
85	MG	1	4004	1/1	0.93	0.21	31,31,31,31	0
84	OHX	1	3566	7/7	0.93	0.24	182,182,183,183	0
85	MG	6	2150	1/1	0.93	0.21	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	4212	1/1	0.93	0.12	48,48,48,48	0
85	MG	AR	4213	1/1	0.93	0.21	34,34,34,34	0
85	MG	AR	3970	1/1	0.93	0.22	53,53,53,53	0
84	OHX	1	3723	7/7	0.93	0.19	201,202,203,204	0
85	MG	AR	3972	1/1	0.93	0.30	38,38,38,38	0
85	MG	1	3810	1/1	0.93	0.23	86,86,86,86	0
85	MG	AR	3974	1/1	0.93	0.24	28,28,28,28	0
84	OHX	A	2022	7/7	0.93	0.29	229,230,232,233	0
85	MG	6	2154	1/1	0.93	0.20	38,38,38,38	0
84	OHX	6	1998	7/7	0.93	0.19	239,240,243,244	0
85	MG	AR	4226	1/1	0.93	0.51	16,16,16,16	0
85	MG	AR	4230	1/1	0.93	0.40	68,68,68,68	0
84	OHX	1	3623	7/7	0.93	0.10	224,225,226,226	0
85	MG	1	4158	1/1	0.93	0.15	29,29,29,29	0
85	MG	1	4159	1/1	0.93	0.16	42,42,42,42	0
85	MG	1	4160	1/1	0.93	0.26	40,40,40,40	0
85	MG	AR	4242	1/1	0.93	0.73	56,56,56,56	0
85	MG	6	2164	1/1	0.93	0.19	63,63,63,63	0
85	MG	AR	3989	1/1	0.93	0.32	85,85,85,85	0
84	OHX	1	3625	7/7	0.93	0.24	186,186,187,187	0
84	OHX	1	3628	7/7	0.93	0.20	234,235,236,237	0
84	OHX	A	2027	7/7	0.93	0.18	236,239,240,241	0
84	OHX	A	2028	7/7	0.93	0.23	252,254,254,256	0
85	MG	1	4024	1/1	0.93	0.37	15,15,15,15	0
85	MG	1	4025	1/1	0.93	0.24	34,34,34,34	0
85	MG	6	2175	1/1	0.93	0.19	41,41,41,41	0
85	MG	AR	4003	1/1	0.93	0.35	73,73,73,73	0
85	MG	AR	4010	1/1	0.93	0.43	28,28,28,28	0
84	OHX	6	2004	7/7	0.93	0.17	193,194,195,196	0
85	MG	AT	221	1/1	0.93	0.40	26,26,26,26	0
85	MG	1	4176	1/1	0.93	0.19	27,27,27,27	0
85	MG	AT	224	1/1	0.93	0.54	35,35,35,35	0
85	MG	1	3842	1/1	0.93	0.58	27,27,27,27	0
85	MG	AR	4018	1/1	0.93	0.12	40,40,40,40	0
84	OHX	AR	3676	7/7	0.93	0.29	196,197,198,198	0
84	OHX	1	3653	7/7	0.93	0.41	193,195,196,196	0
85	MG	AR	4023	1/1	0.93	0.10	36,36,36,36	0
85	MG	CE	405	1/1	0.93	0.41	34,34,34,34	0
84	OHX	6	2008	7/7	0.93	0.29	211,213,214,216	0
84	OHX	AR	3680	7/7	0.93	0.41	220,222,222,223	0
84	OHX	1	3630	7/7	0.93	0.19	199,200,200,201	0
84	OHX	A	2037	7/7	0.93	0.28	238,240,241,241	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AT	211	7/7	0.93	0.26	179,179,180,180	0
85	MG	AR	4030	1/1	0.93	0.26	37,37,37,37	0
84	OHX	1	3655	7/7	0.93	0.20	203,204,205,205	0
85	MG	1	3879	1/1	0.93	0.30	47,47,47,47	0
84	OHX	3	205	7/7	0.93	0.13	169,171,171,173	0
85	MG	AF	201	1/1	0.93	0.24	27,27,27,27	0
85	MG	1	4198	1/1	0.93	0.56	36,36,36,36	0
84	OHX	6	2016	7/7	0.93	0.21	194,194,196,196	0
85	MG	DC	202	1/1	0.93	0.21	28,28,28,28	0
84	OHX	AR	3577	7/7	0.93	0.30	201,201,202,202	0
85	MG	1	4203	1/1	0.93	0.52	34,34,34,34	0
85	MG	AR	3742	1/1	0.93	0.34	29,29,29,29	0
84	OHX	AR	3581	7/7	0.93	0.32	205,205,205,205	0
85	MG	AR	4044	1/1	0.93	0.25	51,51,51,51	0
84	OHX	AR	3586	7/7	0.93	0.14	182,184,185,185	0
84	OHX	M	201	7/7	0.93	0.33	202,204,205,206	0
85	MG	AR	3748	1/1	0.93	0.25	41,41,41,41	0
85	MG	A	2045	1/1	0.93	0.42	35,35,35,35	0
84	OHX	AR	3591	7/7	0.93	0.40	168,169,169,169	0
85	MG	3	215	1/1	0.93	0.23	39,39,39,39	0
85	MG	A	2051	1/1	0.93	0.26	62,62,62,62	0
85	MG	1	3903	1/1	0.93	0.32	32,32,32,32	0
84	OHX	CG	301	7/7	0.93	0.13	191,193,193,195	0
85	MG	4	215	1/1	0.93	0.49	23,23,23,23	0
85	MG	AR	3769	1/1	0.93	0.13	35,35,35,35	0
85	MG	1	3914	1/1	0.93	0.54	31,31,31,31	0
85	MG	A	2067	1/1	0.93	0.57	32,32,32,32	0
84	OHX	6	2021	7/7	0.93	0.33	210,210,212,213	0
84	OHX	1	3568	7/7	0.93	0.20	195,196,196,197	0
85	MG	AR	4064	1/1	0.93	0.21	30,30,30,30	0
85	MG	AR	4069	1/1	0.93	0.20	53,53,53,53	0
85	MG	1	4060	1/1	0.93	0.55	16,16,16,16	0
84	OHX	4	206	7/7	0.93	0.27	179,179,180,180	0
85	MG	4	229	1/1	0.93	0.26	57,57,57,57	0
84	OHX	sR	401	7/7	0.93	0.15	215,216,219,219	0
84	OHX	6	2024	7/7	0.93	0.18	207,208,210,211	0
85	MG	1	3940	1/1	0.93	0.21	21,21,21,21	0
85	MG	1	4072	1/1	0.93	0.23	55,55,55,55	0
85	MG	1	3735	1/1	0.93	0.23	39,39,39,39	0
85	MG	1	4075	1/1	0.93	0.23	20,20,20,20	0
84	OHX	1	3681	7/7	0.93	0.28	210,211,212,212	0
85	MG	AR	4090	1/1	0.93	0.27	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3737	1/1	0.93	0.26	36,36,36,36	0
85	MG	AR	3796	1/1	0.93	0.59	32,32,32,32	0
84	OHX	6	2026	7/7	0.93	0.21	218,219,220,222	0
85	MG	v	302	1/1	0.93	0.39	43,43,43,43	0
85	MG	AR	4097	1/1	0.93	0.33	26,26,26,26	0
84	OHX	1	3609	7/7	0.93	0.21	191,193,194,195	0
84	OHX	AR	3616	7/7	0.93	0.35	210,210,211,212	0
85	MG	AR	4103	1/1	0.93	0.16	35,35,35,35	0
85	MG	1	3747	1/1	0.93	0.31	28,28,28,28	0
85	MG	1	4089	1/1	0.93	0.21	30,30,30,30	0
85	MG	1	4090	1/1	0.93	0.10	54,54,54,54	0
85	MG	A	2111	1/1	0.93	0.22	68,68,68,68	0
85	MG	AR	3809	1/1	0.93	0.12	86,86,86,86	0
85	MG	6	2058	1/1	0.93	0.39	33,33,33,33	0
84	OHX	1	3587	7/7	0.93	0.25	188,189,189,190	0
85	MG	AR	4120	1/1	0.93	0.22	32,32,32,32	0
85	MG	AR	4121	1/1	0.93	0.37	42,42,42,42	0
85	MG	1	3957	1/1	0.93	0.42	29,29,29,29	0
85	MG	A	2121	1/1	0.93	0.08	66,66,66,66	0
85	MG	A	2122	1/1	0.93	0.41	42,42,42,42	0
85	MG	1	3958	1/1	0.93	0.20	54,54,54,54	0
85	MG	AR	4124	1/1	0.93	0.17	54,54,54,54	0
84	OHX	1	3686	7/7	0.93	0.33	207,208,209,209	0
85	MG	A	2126	1/1	0.93	0.16	48,48,48,48	0
84	OHX	1	401	7/7	0.93	0.38	208,209,210,210	0
84	OHX	1	3687	7/7	0.93	0.32	196,196,197,197	0
85	MG	AR	3823	1/1	0.93	0.56	15,15,15,15	0
85	MG	1	3757	1/1	0.93	0.13	46,46,46,46	0
84	OHX	1	3659	7/7	0.93	0.14	208,210,211,211	0
84	OHX	1	3714	7/7	0.93	0.17	155,156,157,158	0
84	OHX	AR	3714	7/7	0.93	0.43	192,193,193,194	0
84	OHX	y	201	7/7	0.93	0.26	204,205,207,208	0
85	MG	6	2083	1/1	0.93	0.47	35,35,35,35	0
85	MG	6	2084	1/1	0.93	0.27	35,35,35,35	0
85	MG	AR	4145	1/1	0.93	0.14	38,38,38,38	0
85	MG	A	2143	1/1	0.93	0.21	151,151,151,151	0
84	OHX	1	3634	7/7	0.93	0.21	206,207,207,209	0
85	MG	1	3765	1/1	0.93	0.13	41,41,41,41	0
85	MG	AR	4148	1/1	0.93	0.14	36,36,36,36	0
85	MG	6	2089	1/1	0.93	0.25	34,34,34,34	0
84	OHX	A	1995	7/7	0.93	0.15	206,207,208,209	0
84	OHX	1	3595	7/7	0.93	0.44	190,191,192,192	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3875	1/1	0.93	0.20	48,48,48,48	0
84	OHX	1	3491	7/7	0.93	0.18	138,138,139,139	0
85	MG	6	2095	1/1	0.93	0.58	32,32,32,32	0
85	MG	1	3980	1/1	0.93	0.26	19,19,19,19	0
85	MG	1	3772	1/1	0.93	0.34	32,32,32,32	0
85	MG	6	2111	1/1	0.93	0.16	42,42,42,42	0
84	OHX	6	1964	7/7	0.93	0.20	175,175,177,177	0
85	MG	d3	202	1/1	0.93	0.54	56,56,56,56	0
84	OHX	6	1974	7/7	0.93	0.20	176,176,178,178	0
84	OHX	1	3640	7/7	0.93	0.19	194,195,196,196	0
84	OHX	AR	3648	7/7	0.93	0.39	196,197,198,198	0
85	MG	d9	102	1/1	0.93	0.44	106,106,106,106	0
85	MG	AR	3907	1/1	0.93	0.36	20,20,20,20	0
85	MG	1	4127	1/1	0.93	0.16	58,58,58,58	0
84	OHX	1	3660	7/7	0.94	0.29	208,209,210,210	0
85	MG	1	3743	1/1	0.94	0.39	23,23,23,23	0
84	OHX	6	1978	7/7	0.94	0.13	176,178,180,181	0
84	OHX	1	3605	7/7	0.94	0.31	171,171,172,172	0
84	OHX	AT	214	7/7	0.94	0.26	173,173,174,174	0
85	MG	1	3989	1/1	0.94	0.48	20,20,20,20	0
84	OHX	AR	3656	7/7	0.94	0.20	187,187,189,189	0
85	MG	1	4188	1/1	0.94	0.21	34,34,34,34	0
85	MG	1	4190	1/1	0.94	0.25	26,26,26,26	0
85	MG	AR	3778	1/1	0.94	0.37	42,42,42,42	0
84	OHX	1	3662	7/7	0.94	0.22	178,179,180,180	0
85	MG	AR	4136	1/1	0.94	0.22	41,41,41,41	0
85	MG	1	3999	1/1	0.94	0.29	38,38,38,38	0
84	OHX	AR	3658	7/7	0.94	0.27	177,177,179,179	0
84	OHX	6	1985	7/7	0.94	0.16	191,193,194,195	0
84	OHX	1	3725	7/7	0.94	0.08	203,204,205,206	0
84	OHX	AR	3661	7/7	0.94	0.53	176,177,178,178	0
85	MG	1	3760	1/1	0.94	0.61	26,26,26,26	0
84	OHX	1	3461	7/7	0.94	0.17	136,137,137,138	0
85	MG	1	4213	1/1	0.94	0.21	36,36,36,36	0
84	OHX	6	1992	7/7	0.94	0.22	185,186,187,188	0
85	MG	3	210	1/1	0.94	0.25	41,41,41,41	0
85	MG	1	3763	1/1	0.94	0.31	34,34,34,34	0
84	OHX	1	3542	7/7	0.94	0.28	156,157,158,158	0
85	MG	3	216	1/1	0.94	0.21	35,35,35,35	0
85	MG	3	217	1/1	0.94	0.15	48,48,48,48	0
84	OHX	AR	3667	7/7	0.94	0.23	207,209,210,210	0
85	MG	3	219	1/1	0.94	0.14	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4012	1/1	0.94	0.20	26,26,26,26	0
84	OHX	CK	201	7/7	0.94	0.24	185,185,186,187	0
84	OHX	6	1995	7/7	0.94	0.18	171,173,174,175	0
85	MG	1	4016	1/1	0.94	0.17	11,11,11,11	0
85	MG	AR	4169	1/1	0.94	0.14	34,34,34,34	0
84	OHX	6	1996	7/7	0.94	0.17	190,191,192,193	0
85	MG	AR	4171	1/1	0.94	0.43	59,59,59,59	0
84	OHX	6	1997	7/7	0.94	0.20	198,199,201,201	0
85	MG	4	226	1/1	0.94	0.10	54,54,54,54	0
84	OHX	1	3544	7/7	0.94	0.17	187,188,190,190	0
85	MG	AR	4178	1/1	0.94	0.23	48,48,48,48	0
85	MG	AR	3824	1/1	0.94	0.14	62,62,62,62	0
84	OHX	AR	3673	7/7	0.94	0.20	179,180,180,180	0
85	MG	AR	3827	1/1	0.94	0.45	40,40,40,40	0
85	MG	1	3778	1/1	0.94	0.19	20,20,20,20	0
84	OHX	AR	3674	7/7	0.94	0.41	215,215,216,216	0
84	OHX	A	1932	7/7	0.94	0.17	178,180,182,182	0
84	OHX	A	1934	7/7	0.94	0.14	176,177,179,179	0
85	MG	AR	4192	1/1	0.94	0.18	44,44,44,44	0
85	MG	1	3782	1/1	0.94	0.41	44,44,44,44	0
85	MG	o	301	1/1	0.94	0.25	39,39,39,39	0
85	MG	AR	4196	1/1	0.94	0.22	39,39,39,39	0
85	MG	AR	3838	1/1	0.94	0.61	21,21,21,21	0
85	MG	1	3783	1/1	0.94	0.30	27,27,27,27	0
84	OHX	1	3611	7/7	0.94	0.23	184,185,185,186	0
85	MG	1	3788	1/1	0.94	0.33	34,34,34,34	0
85	MG	AR	4204	1/1	0.94	0.21	31,31,31,31	0
85	MG	AR	3850	1/1	0.94	0.52	11,11,11,11	0
84	OHX	1	3641	7/7	0.94	0.23	195,196,197,197	0
85	MG	AR	3859	1/1	0.94	0.27	28,28,28,28	0
84	OHX	A	1958	7/7	0.94	0.18	206,207,210,210	0
85	MG	1	3796	1/1	0.94	0.19	33,33,33,33	0
85	MG	1	3798	1/1	0.94	0.19	29,29,29,29	0
85	MG	AR	3879	1/1	0.94	0.54	21,21,21,21	0
84	OHX	1	3702	7/7	0.94	0.33	179,180,181,182	0
85	MG	1	3802	1/1	0.94	0.21	32,32,32,32	0
85	MG	AR	4216	1/1	0.94	0.30	67,67,67,67	0
85	MG	AR	3885	1/1	0.94	0.37	38,38,38,38	0
85	MG	1	4042	1/1	0.94	0.16	65,65,65,65	0
85	MG	1	3804	1/1	0.94	0.61	18,18,18,18	0
84	OHX	A	1960	7/7	0.94	0.15	225,226,227,228	0
85	MG	AR	3891	1/1	0.94	0.36	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2062	1/1	0.94	0.36	32,32,32,32	0
85	MG	AR	3896	1/1	0.94	0.43	37,37,37,37	0
84	OHX	3	207	7/7	0.94	0.17	188,189,190,191	0
84	OHX	AR	3679	7/7	0.94	0.24	218,220,221,221	0
84	OHX	A	1977	7/7	0.94	0.17	202,205,207,207	0
85	MG	1	3811	1/1	0.94	0.21	42,42,42,42	0
85	MG	AR	4240	1/1	0.94	0.14	33,33,33,33	0
85	MG	AR	3916	1/1	0.94	0.41	3,3,3,3	0
85	MG	AR	3918	1/1	0.94	0.40	21,21,21,21	0
85	MG	1	3812	1/1	0.94	0.37	29,29,29,29	0
85	MG	AR	3928	1/1	0.94	0.26	10,10,10,10	0
85	MG	AS	215	1/1	0.94	0.67	12,12,12,12	0
84	OHX	A	1978	7/7	0.94	0.14	210,212,214,214	0
85	MG	AR	3936	1/1	0.94	0.32	20,20,20,20	0
85	MG	AR	3938	1/1	0.94	0.52	20,20,20,20	0
85	MG	AR	3941	1/1	0.94	0.08	46,46,46,46	0
85	MG	AR	3942	1/1	0.94	0.10	45,45,45,45	0
84	OHX	A	1980	7/7	0.94	0.26	194,196,197,197	0
85	MG	AR	3946	1/1	0.94	0.19	28,28,28,28	0
84	OHX	A	1981	7/7	0.94	0.10	231,234,235,236	0
85	MG	AS	227	1/1	0.94	0.51	43,43,43,43	0
84	OHX	6	2005	7/7	0.94	0.27	152,153,155,155	0
85	MG	6	2080	1/1	0.94	0.15	53,53,53,53	0
85	MG	AT	201	1/1	0.94	0.29	31,31,31,31	0
85	MG	1	4061	1/1	0.94	0.40	23,23,23,23	0
84	OHX	1	3613	7/7	0.94	0.23	166,166,167,168	0
84	OHX	AR	3530	7/7	0.94	0.20	147,148,148,148	0
84	OHX	AR	3684	7/7	0.94	0.47	181,182,183,183	0
85	MG	1	3839	1/1	0.94	0.60	7,7,7,7	0
85	MG	AR	3959	1/1	0.94	0.22	32,32,32,32	0
85	MG	AR	3960	1/1	0.94	0.15	17,17,17,17	0
85	MG	AR	3961	1/1	0.94	0.19	23,23,23,23	0
85	MG	6	2088	1/1	0.94	0.38	30,30,30,30	0
85	MG	AR	3963	1/1	0.94	0.38	23,23,23,23	0
84	OHX	AR	3539	7/7	0.94	0.12	169,170,172,172	0
84	OHX	AR	3556	7/7	0.94	0.19	138,139,140,140	0
85	MG	6	2091	1/1	0.94	0.33	54,54,54,54	0
84	OHX	AR	3564	7/7	0.94	0.17	189,190,190,190	0
85	MG	AR	3969	1/1	0.94	0.25	38,38,38,38	0
85	MG	1	3851	1/1	0.94	0.24	34,34,34,34	0
85	MG	CP	503	1/1	0.94	0.25	95,95,95,95	0
84	OHX	AR	3565	7/7	0.94	0.16	161,162,163,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3855	1/1	0.94	0.44	26,26,26,26	0
85	MG	CR	201	1/1	0.94	0.44	14,14,14,14	0
85	MG	6	2099	1/1	0.94	0.22	19,19,19,19	0
85	MG	CR	204	1/1	0.94	0.21	46,46,46,46	0
85	MG	6	2102	1/1	0.94	0.31	14,14,14,14	0
85	MG	CR	206	1/1	0.94	0.15	30,30,30,30	0
85	MG	CU	201	1/1	0.94	0.19	44,44,44,44	0
85	MG	CX	203	1/1	0.94	0.15	45,45,45,45	0
85	MG	6	2104	1/1	0.94	0.24	22,22,22,22	0
85	MG	6	2106	1/1	0.94	0.58	32,32,32,32	0
85	MG	1	4080	1/1	0.94	0.33	55,55,55,55	0
85	MG	1	3862	1/1	0.94	0.34	18,18,18,18	0
84	OHX	AR	3573	7/7	0.94	0.19	178,178,179,180	0
85	MG	DF	201	1/1	0.94	0.31	30,30,30,30	0
85	MG	DG	202	1/1	0.94	0.36	21,21,21,21	0
85	MG	DH	202	1/1	0.94	0.16	30,30,30,30	0
84	OHX	A	2001	7/7	0.94	0.18	185,188,189,189	0
85	MG	AR	3985	1/1	0.94	0.23	19,19,19,19	0
84	OHX	AR	3690	7/7	0.94	0.23	179,179,180,181	0
84	OHX	A	2003	7/7	0.94	0.41	196,198,199,199	0
84	OHX	1	3644	7/7	0.94	0.27	170,171,173,173	0
85	MG	sM	201	1/1	0.94	0.10	41,41,41,41	0
84	OHX	1	3547	7/7	0.94	0.20	168,169,170,170	0
85	MG	AR	3992	1/1	0.94	0.50	19,19,19,19	0
85	MG	6	2126	1/1	0.94	0.33	39,39,39,39	0
84	OHX	AR	3582	7/7	0.94	0.21	166,167,167,168	0
84	OHX	A	2011	7/7	0.94	0.17	208,209,211,211	0
85	MG	6	2129	1/1	0.94	0.22	53,53,53,53	0
85	MG	AR	3997	1/1	0.94	0.26	45,45,45,45	0
85	MG	A	2061	1/1	0.94	0.22	27,27,27,27	0
84	OHX	1	3646	7/7	0.94	0.22	182,183,184,185	0
85	MG	6	2132	1/1	0.94	0.23	38,38,38,38	0
84	OHX	AR	3700	7/7	0.94	0.37	174,175,175,176	0
84	OHX	A	2014	7/7	0.94	0.34	198,199,200,200	0
85	MG	6	2138	1/1	0.94	0.58	49,49,49,49	0
85	MG	A	2071	1/1	0.94	0.32	45,45,45,45	0
84	OHX	AR	3589	7/7	0.94	0.19	186,187,188,189	0
84	OHX	6	2012	7/7	0.94	0.11	188,189,190,191	0
84	OHX	AR	3703	7/7	0.94	0.42	214,214,214,214	0
85	MG	1	3900	1/1	0.94	0.74	34,34,34,34	0
84	OHX	AR	3592	7/7	0.94	0.28	151,152,152,153	0
84	OHX	AR	3593	7/7	0.94	0.20	173,174,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	2014	7/7	0.94	0.23	219,220,221,221	0
85	MG	1	3920	1/1	0.94	0.31	29,29,29,29	0
84	OHX	1	3647	7/7	0.94	0.30	203,204,205,206	0
84	OHX	1	3570	7/7	0.94	0.15	202,203,204,205	0
85	MG	1	4116	1/1	0.94	0.12	81,81,81,81	0
84	OHX	AR	3601	7/7	0.94	0.29	171,172,173,173	0
84	OHX	1	3575	7/7	0.94	0.21	187,188,189,189	0
84	OHX	1	3578	7/7	0.94	0.24	168,170,170,171	0
84	OHX	1	3580	7/7	0.94	0.17	162,164,164,165	0
84	OHX	AR	3606	7/7	0.94	0.30	155,156,157,157	0
85	MG	A	2099	1/1	0.94	0.76	64,64,64,64	0
85	MG	1	4125	1/1	0.94	0.20	58,58,58,58	0
84	OHX	1	3548	7/7	0.94	0.20	179,180,181,181	0
84	OHX	AR	3612	7/7	0.94	0.19	182,183,184,184	0
84	OHX	1	3592	7/7	0.94	0.26	166,166,167,167	0
85	MG	1	4130	1/1	0.94	0.28	68,68,68,68	0
84	OHX	AR	3618	7/7	0.94	0.19	195,196,196,196	0
84	OHX	AR	3620	7/7	0.94	0.27	180,182,183,184	0
84	OHX	1	3550	7/7	0.94	0.15	196,197,198,199	0
85	MG	6	2172	1/1	0.94	0.20	32,32,32,32	0
85	MG	1	3953	1/1	0.94	0.29	32,32,32,32	0
84	OHX	AR	3622	7/7	0.94	0.29	203,203,204,205	0
85	MG	AR	4054	1/1	0.94	0.24	33,33,33,33	0
85	MG	6	2177	1/1	0.94	0.23	25,25,25,25	0
84	OHX	AR	3623	7/7	0.94	0.17	186,187,188,188	0
84	OHX	AR	3624	7/7	0.94	0.30	210,211,212,212	0
85	MG	1	3959	1/1	0.94	0.23	54,54,54,54	0
85	MG	6	2184	1/1	0.94	0.27	43,43,43,43	0
84	OHX	AR	3625	7/7	0.94	0.19	216,216,218,219	0
85	MG	6	2186	1/1	0.94	0.15	82,82,82,82	0
85	MG	6	2188	1/1	0.94	0.32	55,55,55,55	0
85	MG	1	4144	1/1	0.94	0.19	59,59,59,59	0
84	OHX	6	1932	7/7	0.94	0.21	129,129,131,131	0
85	MG	A	2128	1/1	0.94	0.26	53,53,53,53	0
85	MG	AR	4070	1/1	0.94	0.12	42,42,42,42	0
85	MG	6	2192	1/1	0.94	0.63	54,54,54,54	0
85	MG	1	4149	1/1	0.94	0.22	45,45,45,45	0
85	MG	1	3962	1/1	0.94	0.25	33,33,33,33	0
84	OHX	6	1941	7/7	0.94	0.17	158,159,160,161	0
84	OHX	1	3504	7/7	0.94	0.12	154,156,157,158	0
85	MG	1	3965	1/1	0.94	0.12	32,32,32,32	0
84	OHX	AR	3633	7/7	0.94	0.32	173,173,174,174	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	1	3967	1/1	0.94	0.16	47,47,47,47	0
84	OHX	1	3511	7/7	0.94	0.17	166,167,168,168	0
85	MG	AR	4085	1/1	0.94	0.30	37,37,37,37	0
84	OHX	6	1962	7/7	0.94	0.21	187,188,189,190	0
85	MG	AR	4088	1/1	0.94	0.15	50,50,50,50	0
84	OHX	1	3691	7/7	0.94	0.30	206,207,208,208	0
84	OHX	c8	201	7/7	0.94	0.15	198,199,200,201	0
85	MG	A	2150	1/1	0.94	0.17	52,52,52,52	0
85	MG	1	4168	1/1	0.94	0.20	51,51,51,51	0
84	OHX	6	1969	7/7	0.94	0.14	163,163,165,165	0
85	MG	1	4170	1/1	0.94	0.22	33,33,33,33	0
85	MG	AR	3744	1/1	0.94	0.47	20,20,20,20	0
85	MG	AR	4099	1/1	0.94	0.15	44,44,44,44	0
84	OHX	6	1971	7/7	0.94	0.18	177,178,179,180	0
84	OHX	6	1972	7/7	0.94	0.34	196,197,198,199	0
85	MG	s2	301	1/1	0.94	0.60	46,46,46,46	0
85	MG	AR	4102	1/1	0.94	0.32	24,24,24,24	0
84	OHX	6	1973	7/7	0.94	0.26	161,162,163,163	0
85	MG	AR	3750	1/1	0.94	0.39	19,19,19,19	0
85	MG	AR	3752	1/1	0.94	0.53	16,16,16,16	0
84	OHX	AR	3645	7/7	0.94	0.25	174,175,176,176	0
85	MG	AR	3755	1/1	0.94	0.18	34,34,34,34	0
85	MG	AR	3757	1/1	0.94	0.28	32,32,32,32	0
86	7MB	1	4216	20/20	0.94	0.20	48,48,48,48	0
84	OHX	1	3531	7/7	0.94	0.17	179,180,181,181	0
87	ZN	d7	101	1/1	0.94	0.29	176,176,176,176	0
84	OHX	1	3602	7/7	0.94	0.29	228,229,229,230	0
85	MG	AR	3837	1/1	0.95	0.17	16,16,16,16	0
84	OHX	1	3594	7/7	0.95	0.26	150,150,151,151	0
84	OHX	A	2009	7/7	0.95	0.32	191,192,194,195	0
84	OHX	A	2010	7/7	0.95	0.14	192,195,197,197	0
85	MG	AR	3846	1/1	0.95	0.57	17,17,17,17	0
85	MG	AR	3847	1/1	0.95	0.29	35,35,35,35	0
85	MG	AR	3848	1/1	0.95	0.25	15,15,15,15	0
85	MG	1	3852	1/1	0.95	0.59	22,22,22,22	0
84	OHX	AR	3600	7/7	0.95	0.13	172,173,173,174	0
84	OHX	1	3555	7/7	0.95	0.11	190,191,192,192	0
85	MG	AR	3857	1/1	0.95	0.14	46,46,46,46	0
85	MG	1	4066	1/1	0.95	0.28	66,66,66,66	0
85	MG	AR	3862	1/1	0.95	0.27	20,20,20,20	0
85	MG	1	4068	1/1	0.95	0.20	39,39,39,39	0
85	MG	1	3860	1/1	0.95	0.47	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4175	1/1	0.95	0.14	27,27,27,27	0
85	MG	6	2076	1/1	0.95	0.32	18,18,18,18	0
85	MG	AR	4177	1/1	0.95	0.23	18,18,18,18	0
85	MG	6	2078	1/1	0.95	0.42	25,25,25,25	0
84	OHX	6	2030	7/7	0.95	0.38	160,161,162,162	0
84	OHX	1	3627	7/7	0.95	0.15	176,176,178,179	0
84	OHX	AR	3709	7/7	0.95	0.18	163,163,164,164	0
85	MG	1	3867	1/1	0.95	0.37	26,26,26,26	0
85	MG	1	4077	1/1	0.95	0.15	42,42,42,42	0
84	OHX	1	3596	7/7	0.95	0.29	183,184,185,185	0
85	MG	AR	4186	1/1	0.95	0.34	33,33,33,33	0
85	MG	AR	4187	1/1	0.95	0.67	27,27,27,27	0
84	OHX	1	3539	7/7	0.95	0.20	169,169,170,170	0
84	OHX	A	2018	7/7	0.95	0.16	214,215,216,217	0
85	MG	1	4081	1/1	0.95	0.11	35,35,35,35	0
84	OHX	1	3599	7/7	0.95	0.11	190,191,192,193	0
84	OHX	A	2020	7/7	0.95	0.17	188,191,192,192	0
85	MG	AR	3902	1/1	0.95	0.69	24,24,24,24	0
84	OHX	A	2021	7/7	0.95	0.34	176,177,179,179	0
84	OHX	6	1979	7/7	0.95	0.29	165,165,166,167	0
84	OHX	AR	3613	7/7	0.95	0.29	165,166,167,167	0
85	MG	1	4091	1/1	0.95	0.15	49,49,49,49	0
85	MG	AR	3919	1/1	0.95	0.56	11,11,11,11	0
85	MG	AR	3921	1/1	0.95	0.27	10,10,10,10	0
85	MG	1	3888	1/1	0.95	0.26	21,21,21,21	0
84	OHX	AR	3615	7/7	0.95	0.23	169,170,171,171	0
85	MG	AR	3930	1/1	0.95	0.39	14,14,14,14	0
84	OHX	1	3540	7/7	0.95	0.24	145,146,146,148	0
84	OHX	6	1981	7/7	0.95	0.34	195,197,199,199	0
85	MG	6	2108	1/1	0.95	0.29	44,44,44,44	0
85	MG	AR	3939	1/1	0.95	0.43	16,16,16,16	0
85	MG	1	4098	1/1	0.95	0.19	33,33,33,33	0
84	OHX	1	3663	7/7	0.95	0.32	214,216,217,217	0
85	MG	6	2114	1/1	0.95	0.36	28,28,28,28	0
85	MG	AR	3944	1/1	0.95	0.38	39,39,39,39	0
85	MG	AR	3945	1/1	0.95	0.43	22,22,22,22	0
84	OHX	6	1983	7/7	0.95	0.35	169,169,170,170	0
85	MG	AR	3947	1/1	0.95	0.18	26,26,26,26	0
84	OHX	1	3559	7/7	0.95	0.16	182,183,184,184	0
85	MG	1	3906	1/1	0.95	0.23	29,29,29,29	0
85	MG	1	3907	1/1	0.95	0.37	13,13,13,13	0
85	MG	1	3910	1/1	0.95	0.20	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1986	7/7	0.95	0.12	157,157,159,159	0
84	OHX	1	3521	7/7	0.95	0.16	144,145,147,147	0
85	MG	1	3915	1/1	0.95	0.55	19,19,19,19	0
85	MG	AR	3957	1/1	0.95	0.55	37,37,37,37	0
85	MG	1	3918	1/1	0.95	0.37	26,26,26,26	0
85	MG	AS	212	1/1	0.95	0.38	13,13,13,13	0
85	MG	1	3919	1/1	0.95	0.65	30,30,30,30	0
84	OHX	1	3565	7/7	0.95	0.16	168,169,170,170	0
85	MG	6	2131	1/1	0.95	0.38	32,32,32,32	0
84	OHX	A	2033	7/7	0.95	0.19	210,212,214,214	0
85	MG	1	4114	1/1	0.95	0.13	33,33,33,33	0
84	OHX	AR	3626	7/7	0.95	0.32	204,205,205,205	0
84	OHX	A	2035	7/7	0.95	0.30	177,178,180,181	0
85	MG	AR	3966	1/1	0.95	0.24	24,24,24,24	0
85	MG	1	3937	1/1	0.95	0.29	58,58,58,58	0
84	OHX	6	1991	7/7	0.95	0.20	184,185,187,187	0
85	MG	1	4122	1/1	0.95	0.50	45,45,45,45	0
84	OHX	1	3636	7/7	0.95	0.36	170,171,172,172	0
84	OHX	AR	3631	7/7	0.95	0.15	153,155,155,155	0
84	OHX	4	203	7/7	0.95	0.25	181,182,183,184	0
84	OHX	6	1994	7/7	0.95	0.26	168,169,171,171	0
85	MG	1	3946	1/1	0.95	0.17	68,68,68,68	0
84	OHX	4	205	7/7	0.95	0.23	172,173,174,174	0
84	OHX	1	3668	7/7	0.95	0.28	179,179,180,181	0
84	OHX	6	2050	7/7	0.95	0.27	190,191,192,193	0
85	MG	1	4132	1/1	0.95	0.38	42,42,42,42	0
85	MG	AT	228	1/1	0.95	0.22	34,34,34,34	0
84	OHX	1	3543	7/7	0.95	0.14	166,166,167,167	0
84	OHX	1	3607	7/7	0.95	0.24	190,192,193,193	0
84	OHX	1	3706	7/7	0.95	0.17	144,145,146,146	0
84	OHX	1	3523	7/7	0.95	0.20	157,158,159,160	0
85	MG	6	2158	1/1	0.95	0.19	64,64,64,64	0
84	OHX	s8	301	7/7	0.95	0.33	214,216,216,218	0
84	OHX	k	402	7/7	0.95	0.20	156,157,158,158	0
85	MG	6	2161	1/1	0.95	0.17	51,51,51,51	0
84	OHX	1	3673	7/7	0.95	0.16	192,193,194,194	0
84	OHX	1	3545	7/7	0.95	0.18	156,157,158,159	0
84	OHX	1	3526	7/7	0.95	0.13	167,168,169,170	0
85	MG	CQ	201	1/1	0.95	0.30	23,23,23,23	0
85	MG	1	4145	1/1	0.95	0.19	48,48,48,48	0
84	OHX	AR	3650	7/7	0.95	0.39	177,177,178,178	0
84	OHX	AR	3651	7/7	0.95	0.23	229,230,231,231	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	6	2171	1/1	0.95	0.23	34,34,34,34	0
85	MG	AR	4002	1/1	0.95	0.41	42,42,42,42	0
85	MG	1	3734	1/1	0.95	0.32	27,27,27,27	0
85	MG	AR	4004	1/1	0.95	0.33	27,27,27,27	0
85	MG	AR	4009	1/1	0.95	0.28	25,25,25,25	0
85	MG	6	2173	1/1	0.95	0.19	69,69,69,69	0
84	OHX	AT	215	7/7	0.95	0.23	212,213,213,213	0
85	MG	AR	4013	1/1	0.95	0.34	38,38,38,38	0
84	OHX	AG	201	7/7	0.95	0.27	186,187,188,188	0
85	MG	1	4154	1/1	0.95	0.20	92,92,92,92	0
85	MG	6	2178	1/1	0.95	0.25	26,26,26,26	0
85	MG	AR	4019	1/1	0.95	0.14	29,29,29,29	0
84	OHX	AR	3653	7/7	0.95	0.31	178,178,179,179	0
84	OHX	AR	3473	7/7	0.95	0.16	121,122,122,122	0
85	MG	AR	4022	1/1	0.95	0.21	41,41,41,41	0
85	MG	1	3740	1/1	0.95	0.41	7,7,7,7	0
84	OHX	AR	3496	7/7	0.95	0.15	147,147,148,149	0
84	OHX	AR	3500	7/7	0.95	0.12	136,138,139,140	0
85	MG	1	3745	1/1	0.95	0.48	20,20,20,20	0
84	OHX	AR	3505	7/7	0.95	0.17	138,140,141,141	0
85	MG	A	2044	1/1	0.95	0.52	25,25,25,25	0
84	OHX	AR	3517	7/7	0.95	0.15	134,135,135,136	0
84	OHX	1	3612	7/7	0.95	0.24	173,174,175,175	0
84	OHX	AR	3524	7/7	0.95	0.23	152,153,154,155	0
85	MG	A	2050	1/1	0.95	0.32	68,68,68,68	0
85	MG	AR	4033	1/1	0.95	0.30	63,63,63,63	0
84	OHX	AR	3526	7/7	0.95	0.21	164,166,167,167	0
85	MG	A	2053	1/1	0.95	0.33	39,39,39,39	0
84	OHX	AR	3529	7/7	0.95	0.18	161,162,163,163	0
85	MG	1	3755	1/1	0.95	0.21	41,41,41,41	0
85	MG	A	2059	1/1	0.95	0.40	25,25,25,25	0
84	OHX	AR	3665	7/7	0.95	0.26	189,189,189,189	0
85	MG	AR	4038	1/1	0.95	0.26	30,30,30,30	0
84	OHX	6	2009	7/7	0.95	0.22	181,181,183,183	0
85	MG	6	2198	1/1	0.95	0.19	53,53,53,53	0
84	OHX	AR	3533	7/7	0.95	0.15	166,166,167,167	0
84	OHX	CP	501	7/7	0.95	0.23	177,178,178,178	0
84	OHX	1	3484	7/7	0.95	0.14	131,131,133,133	0
85	MG	1	3990	1/1	0.95	0.41	36,36,36,36	0
85	MG	1	3995	1/1	0.95	0.28	54,54,54,54	0
85	MG	A	2074	1/1	0.95	0.55	38,38,38,38	0
84	OHX	AR	3546	7/7	0.95	0.17	140,140,141,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	AR	4049	1/1	0.95	0.09	74,74,74,74	0
85	MG	A	2079	1/1	0.95	0.58	46,46,46,46	0
84	OHX	AR	3547	7/7	0.95	0.20	147,147,147,148	0
84	OHX	A	1929	7/7	0.95	0.22	157,159,160,160	0
85	MG	AR	4053	1/1	0.95	0.27	50,50,50,50	0
84	OHX	AR	3554	7/7	0.95	0.29	159,160,161,161	0
84	OHX	AR	3555	7/7	0.95	0.17	148,149,149,150	0
84	OHX	A	1936	7/7	0.95	0.15	160,162,163,163	0
84	OHX	1	3614	7/7	0.95	0.18	199,200,201,203	0
85	MG	A	2092	1/1	0.95	0.37	87,87,87,87	0
85	MG	1	4196	1/1	0.95	0.36	35,35,35,35	0
85	MG	AR	3749	1/1	0.95	0.26	19,19,19,19	0
84	OHX	A	1945	7/7	0.95	0.16	201,203,204,205	0
84	OHX	AR	3558	7/7	0.95	0.22	159,160,160,160	0
84	OHX	A	1947	7/7	0.95	0.30	162,164,165,165	0
85	MG	1	3776	1/1	0.95	0.28	29,29,29,29	0
85	MG	AR	4065	1/1	0.95	0.17	54,54,54,54	0
85	MG	AR	4067	1/1	0.95	0.28	98,98,98,98	0
85	MG	AR	3756	1/1	0.95	0.71	11,11,11,11	0
85	MG	1	4009	1/1	0.95	0.40	41,41,41,41	0
85	MG	AR	3758	1/1	0.95	0.34	81,81,81,81	0
84	OHX	A	1951	7/7	0.95	0.20	203,205,207,207	0
85	MG	1	4210	1/1	0.95	0.31	32,32,32,32	0
84	OHX	AR	3559	7/7	0.95	0.14	177,178,179,179	0
85	MG	1	4214	1/1	0.95	0.17	50,50,50,50	0
84	OHX	1	3534	7/7	0.95	0.18	148,149,149,150	0
84	OHX	1	3581	7/7	0.95	0.24	153,153,154,154	0
85	MG	3	212	1/1	0.95	0.30	27,27,27,27	0
85	MG	A	2115	1/1	0.95	0.27	85,85,85,85	0
84	OHX	A	1966	7/7	0.95	0.14	194,195,196,197	0
84	OHX	AR	3566	7/7	0.95	0.17	205,206,207,207	0
84	OHX	A	1970	7/7	0.95	0.31	178,180,182,182	0
84	OHX	AR	3567	7/7	0.95	0.16	159,159,160,160	0
85	MG	AR	3776	1/1	0.95	0.17	32,32,32,32	0
84	OHX	A	1974	7/7	0.95	0.10	196,198,200,201	0
85	MG	AR	3780	1/1	0.95	0.27	20,20,20,20	0
84	OHX	AR	3570	7/7	0.95	0.17	161,162,163,163	0
85	MG	3	220	1/1	0.95	0.34	31,31,31,31	0
84	OHX	AR	3571	7/7	0.95	0.18	194,194,195,195	0
85	MG	4	214	1/1	0.95	0.46	18,18,18,18	0
85	MG	AR	3789	1/1	0.95	0.24	36,36,36,36	0
85	MG	1	4026	1/1	0.95	0.54	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1954	7/7	0.95	0.11	181,182,184,185	0
85	MG	1	3799	1/1	0.95	0.30	28,28,28,28	0
84	OHX	1	3716	7/7	0.95	0.17	205,206,208,209	0
84	OHX	A	1982	7/7	0.95	0.29	164,166,167,167	0
85	MG	AR	3797	1/1	0.95	0.38	18,18,18,18	0
84	OHX	6	2019	7/7	0.95	0.31	191,192,193,194	0
84	OHX	6	2020	7/7	0.95	0.23	177,178,179,179	0
85	MG	4	228	1/1	0.95	0.59	42,42,42,42	0
84	OHX	AR	3584	7/7	0.95	0.36	169,169,170,171	0
84	OHX	6	1958	7/7	0.95	0.21	153,153,155,156	0
84	OHX	AR	3588	7/7	0.95	0.16	176,177,178,178	0
84	OHX	1	3584	7/7	0.95	0.29	154,155,156,156	0
84	OHX	AR	3590	7/7	0.95	0.19	172,173,173,173	0
85	MG	AR	3810	1/1	0.95	0.29	28,28,28,28	0
85	MG	1	3818	1/1	0.95	0.39	19,19,19,19	0
85	MG	1	403	1/1	0.95	0.26	20,20,20,20	0
84	OHX	A	1998	7/7	0.95	0.19	213,217,219,219	0
85	MG	AR	4129	1/1	0.95	0.32	21,21,21,21	0
84	OHX	1	3512	7/7	0.95	0.12	170,172,172,173	0
84	OHX	1	3620	7/7	0.95	0.28	208,208,209,209	0
85	MG	1	3826	1/1	0.95	0.26	44,44,44,44	0
85	MG	1	3829	1/1	0.95	0.38	25,25,25,25	0
85	MG	s6	301	1/1	0.95	0.26	64,64,64,64	0
85	MG	AR	4137	1/1	0.95	0.16	57,57,57,57	0
84	OHX	AR	3699	7/7	0.95	0.38	194,195,196,196	0
85	MG	w	201	1/1	0.95	0.17	33,33,33,33	0
85	MG	1	4049	1/1	0.95	0.18	36,36,36,36	0
85	MG	x	204	1/1	0.95	0.15	18,18,18,18	0
84	OHX	6	1966	7/7	0.95	0.14	164,165,166,167	0
84	OHX	AR	3594	7/7	0.95	0.17	169,170,171,171	0
84	OHX	A	2004	7/7	0.95	0.22	192,194,196,196	0
85	MG	1	4053	1/1	0.95	0.18	32,32,32,32	0
84	OHX	1	3537	7/7	0.95	0.25	160,161,162,162	0
84	OHX	1	3593	7/7	0.95	0.15	206,207,208,209	0
85	MG	AR	4116	1/1	0.96	0.29	105,105,105,105	0
84	OHX	6	1950	7/7	0.96	0.12	171,171,173,174	0
85	MG	AR	3798	1/1	0.96	0.39	21,21,21,21	0
85	MG	4	216	1/1	0.96	0.20	42,42,42,42	0
85	MG	AR	3802	1/1	0.96	0.58	16,16,16,16	0
84	OHX	6	1952	7/7	0.96	0.13	183,184,185,186	0
84	OHX	A	1941	7/7	0.96	0.17	195,197,198,198	0
85	MG	4	219	1/1	0.96	0.39	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3604	7/7	0.96	0.08	204,205,206,206	0
84	OHX	1	3462	7/7	0.96	0.16	115,116,117,118	0
84	OHX	AR	3560	7/7	0.96	0.12	173,174,175,175	0
85	MG	1	3777	1/1	0.96	0.26	40,40,40,40	0
84	OHX	AR	3561	7/7	0.96	0.19	171,171,172,172	0
85	MG	1	4018	1/1	0.96	0.24	26,26,26,26	0
85	MG	1	4020	1/1	0.96	0.12	38,38,38,38	0
84	OHX	A	1948	7/7	0.96	0.09	166,169,170,170	0
85	MG	1	4022	1/1	0.96	0.18	24,24,24,24	0
84	OHX	A	1949	7/7	0.96	0.11	165,167,169,169	0
85	MG	k	404	1/1	0.96	0.44	71,71,71,71	0
84	OHX	AR	3563	7/7	0.96	0.17	173,173,174,174	0
84	OHX	A	1952	7/7	0.96	0.25	181,183,185,185	0
84	OHX	A	1953	7/7	0.96	0.18	180,182,184,184	0
85	MG	AR	4144	1/1	0.96	0.15	35,35,35,35	0
85	MG	AR	3825	1/1	0.96	0.18	30,30,30,30	0
85	MG	o	302	1/1	0.96	0.23	27,27,27,27	0
84	OHX	A	1954	7/7	0.96	0.20	172,174,175,175	0
84	OHX	1	3466	7/7	0.96	0.18	120,121,122,123	0
84	OHX	1	3677	7/7	0.96	0.14	170,171,171,171	0
85	MG	1	3790	1/1	0.96	0.52	15,15,15,15	0
85	MG	1	3794	1/1	0.96	0.22	31,31,31,31	0
85	MG	AR	3833	1/1	0.96	0.15	37,37,37,37	0
84	OHX	6	1961	7/7	0.96	0.15	152,153,154,155	0
84	OHX	A	1962	7/7	0.96	0.14	175,176,177,178	0
84	OHX	A	1964	7/7	0.96	0.29	168,169,170,170	0
84	OHX	1	3517	7/7	0.96	0.17	141,142,143,143	0
85	MG	1	3800	1/1	0.96	0.40	37,37,37,37	0
84	OHX	A	1967	7/7	0.96	0.14	167,168,169,170	0
85	MG	AR	4163	1/1	0.96	0.12	30,30,30,30	0
84	OHX	A	1968	7/7	0.96	0.20	168,170,171,172	0
85	MG	1	3803	1/1	0.96	0.23	22,22,22,22	0
85	MG	AR	4168	1/1	0.96	0.32	45,45,45,45	0
84	OHX	AR	3568	7/7	0.96	0.17	162,163,164,165	0
85	MG	6	2061	1/1	0.96	0.21	64,64,64,64	0
84	OHX	AR	3569	7/7	0.96	0.10	182,182,183,183	0
85	MG	AR	3853	1/1	0.96	0.58	17,17,17,17	0
85	MG	AR	3854	1/1	0.96	0.21	28,28,28,28	0
84	OHX	1	3643	7/7	0.96	0.14	192,193,194,194	0
84	OHX	A	1973	7/7	0.96	0.15	201,204,206,208	0
84	OHX	1	3567	7/7	0.96	0.23	177,178,178,179	0
85	MG	AR	3860	1/1	0.96	0.47	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3861	1/1	0.96	0.42	16,16,16,16	0
85	MG	6	2070	1/1	0.96	0.56	17,17,17,17	0
85	MG	AR	3863	1/1	0.96	0.60	15,15,15,15	0
85	MG	AR	4182	1/1	0.96	0.47	48,48,48,48	0
84	OHX	A	1976	7/7	0.96	0.16	165,166,167,168	0
85	MG	AR	3867	1/1	0.96	0.50	13,13,13,13	0
85	MG	AR	3868	1/1	0.96	0.13	33,33,33,33	0
85	MG	AR	3869	1/1	0.96	0.40	12,12,12,12	0
85	MG	AR	3871	1/1	0.96	0.50	20,20,20,20	0
85	MG	AR	3873	1/1	0.96	0.31	23,23,23,23	0
84	OHX	AR	3572	7/7	0.96	0.20	174,175,176,176	0
85	MG	1	3813	1/1	0.96	0.18	24,24,24,24	0
84	OHX	6	1967	7/7	0.96	0.13	157,159,160,160	0
84	OHX	A	1979	7/7	0.96	0.15	200,203,204,205	0
85	MG	AR	4198	1/1	0.96	0.24	34,34,34,34	0
84	OHX	AR	3575	7/7	0.96	0.21	156,158,159,159	0
85	MG	1	3823	1/1	0.96	0.20	51,51,51,51	0
84	OHX	AR	3576	7/7	0.96	0.14	168,169,169,170	0
84	OHX	AR	3683	7/7	0.96	0.36	178,179,179,180	0
84	OHX	A	1983	7/7	0.96	0.20	188,190,192,192	0
84	OHX	1	3470	7/7	0.96	0.13	141,142,143,143	0
85	MG	AR	3892	1/1	0.96	0.44	19,19,19,19	0
84	OHX	A	1986	7/7	0.96	0.25	215,218,220,222	0
84	OHX	A	1988	7/7	0.96	0.12	158,160,162,162	0
85	MG	6	2086	1/1	0.96	0.24	49,49,49,49	0
85	MG	AR	3898	1/1	0.96	0.42	16,16,16,16	0
84	OHX	AR	3579	7/7	0.96	0.13	183,184,185,185	0
85	MG	AR	3900	1/1	0.96	0.33	29,29,29,29	0
85	MG	1	4067	1/1	0.96	0.19	24,24,24,24	0
85	MG	1	3835	1/1	0.96	0.29	19,19,19,19	0
85	MG	1	4069	1/1	0.96	0.18	39,39,39,39	0
84	OHX	A	1990	7/7	0.96	0.42	212,215,216,216	0
84	OHX	1	3610	7/7	0.96	0.28	212,212,212,212	0
85	MG	1	3841	1/1	0.96	0.31	19,19,19,19	0
85	MG	AR	3920	1/1	0.96	0.34	19,19,19,19	0
85	MG	1	4074	1/1	0.96	0.15	45,45,45,45	0
85	MG	AR	4224	1/1	0.96	0.25	26,26,26,26	0
85	MG	6	2096	1/1	0.96	0.38	48,48,48,48	0
85	MG	AR	4229	1/1	0.96	0.46	23,23,23,23	0
84	OHX	A	1992	7/7	0.96	0.13	167,169,170,171	0
85	MG	6	2098	1/1	0.96	0.23	38,38,38,38	0
85	MG	1	3844	1/1	0.96	0.44	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3522	7/7	0.96	0.15	133,134,134,135	0
84	OHX	A	1994	7/7	0.96	0.23	200,203,204,205	0
85	MG	6	2105	1/1	0.96	0.34	24,24,24,24	0
84	OHX	1	3685	7/7	0.96	0.16	173,173,175,175	0
85	MG	6	2107	1/1	0.96	0.41	24,24,24,24	0
85	MG	AS	211	1/1	0.96	0.29	22,22,22,22	0
84	OHX	AR	3585	7/7	0.96	0.16	165,166,167,167	0
85	MG	1	3854	1/1	0.96	0.40	13,13,13,13	0
84	OHX	1	3441	7/7	0.96	0.17	168,169,169,170	0
85	MG	6	2112	1/1	0.96	0.54	25,25,25,25	0
84	OHX	AR	3691	7/7	0.96	0.45	170,171,172,172	0
85	MG	6	2115	1/1	0.96	0.36	36,36,36,36	0
85	MG	AR	3949	1/1	0.96	0.38	19,19,19,19	0
84	OHX	AR	3692	7/7	0.96	0.34	184,186,186,187	0
84	OHX	AR	3587	7/7	0.96	0.19	175,176,177,177	0
84	OHX	1	3576	7/7	0.96	0.14	189,189,191,191	0
85	MG	AS	225	1/1	0.96	0.15	67,67,67,67	0
85	MG	6	2122	1/1	0.96	0.18	48,48,48,48	0
84	OHX	1	3546	7/7	0.96	0.19	147,148,149,150	0
84	OHX	1	3690	7/7	0.96	0.28	174,175,176,176	0
84	OHX	1	3458	7/7	0.96	0.14	131,132,133,133	0
84	OHX	1	3616	7/7	0.96	0.22	177,177,178,178	0
84	OHX	1	3528	7/7	0.96	0.14	169,170,171,171	0
85	MG	AT	222	1/1	0.96	0.43	35,35,35,35	0
84	OHX	3	202	7/7	0.96	0.13	176,177,177,178	0
84	OHX	AR	3596	7/7	0.96	0.30	208,209,210,211	0
85	MG	1	3881	1/1	0.96	0.31	35,35,35,35	0
84	OHX	3	203	7/7	0.96	0.14	143,144,145,145	0
84	OHX	1	3549	7/7	0.96	0.13	190,190,191,192	0
84	OHX	3	206	7/7	0.96	0.09	176,177,179,179	0
85	MG	AT	229	1/1	0.96	0.33	30,30,30,30	0
85	MG	1	3890	1/1	0.96	0.39	23,23,23,23	0
85	MG	CD	301	1/1	0.96	0.20	28,28,28,28	0
85	MG	6	2137	1/1	0.96	0.40	82,82,82,82	0
85	MG	CE	401	1/1	0.96	0.14	30,30,30,30	0
84	OHX	6	1987	7/7	0.96	0.15	179,179,180,181	0
85	MG	1	3894	1/1	0.96	0.42	26,26,26,26	0
84	OHX	6	1988	7/7	0.96	0.12	191,193,195,195	0
85	MG	6	2141	1/1	0.96	0.21	56,56,56,56	0
84	OHX	1	3585	7/7	0.96	0.24	173,174,174,175	0
84	OHX	1	3586	7/7	0.96	0.17	182,183,185,186	0
84	OHX	AR	3604	7/7	0.96	0.15	150,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3975	1/1	0.96	0.27	31,31,31,31	0
85	MG	1	3902	1/1	0.96	0.52	4,4,4,4	0
84	OHX	4	201	7/7	0.96	0.16	143,143,144,144	0
85	MG	AR	3978	1/1	0.96	0.26	20,20,20,20	0
85	MG	1	3905	1/1	0.96	0.59	14,14,14,14	0
85	MG	6	2149	1/1	0.96	0.32	75,75,75,75	0
85	MG	AR	3981	1/1	0.96	0.18	17,17,17,17	0
84	OHX	1	3529	7/7	0.96	0.22	143,144,145,146	0
84	OHX	AR	3608	7/7	0.96	0.32	186,187,188,188	0
84	OHX	AR	3715	7/7	0.96	0.21	144,146,147,147	0
85	MG	1	3911	1/1	0.96	0.33	20,20,20,20	0
84	OHX	4	204	7/7	0.96	0.28	160,160,161,161	0
84	OHX	AR	3611	7/7	0.96	0.33	194,196,197,197	0
85	MG	DC	201	1/1	0.96	0.36	16,16,16,16	0
84	OHX	1	3589	7/7	0.96	0.15	179,180,181,181	0
85	MG	1	3916	1/1	0.96	0.50	14,14,14,14	0
84	OHX	1	3492	7/7	0.96	0.15	127,128,128,128	0
84	OHX	4	208	7/7	0.96	0.27	187,187,188,188	0
84	OHX	1	3624	7/7	0.96	0.20	171,172,173,174	0
85	MG	1	3921	1/1	0.96	0.23	45,45,45,45	0
85	MG	6	2162	1/1	0.96	0.31	69,69,69,69	0
85	MG	6	2163	1/1	0.96	0.12	60,60,60,60	0
85	MG	1	3923	1/1	0.96	0.50	7,7,7,7	0
85	MG	6	2165	1/1	0.96	0.28	45,45,45,45	0
85	MG	1	3926	1/1	0.96	0.54	21,21,21,21	0
85	MG	1	3927	1/1	0.96	0.50	6,6,6,6	0
85	MG	AR	4005	1/1	0.96	0.35	24,24,24,24	0
85	MG	A	2043	1/1	0.96	0.26	47,47,47,47	0
85	MG	AR	4008	1/1	0.96	0.16	33,33,33,33	0
85	MG	1	3928	1/1	0.96	0.13	32,32,32,32	0
84	OHX	1	3552	7/7	0.96	0.20	173,174,175,175	0
85	MG	AR	4011	1/1	0.96	0.47	31,31,31,31	0
84	OHX	AR	3619	7/7	0.96	0.28	169,169,170,170	0
85	MG	1	4139	1/1	0.96	0.18	29,29,29,29	0
84	OHX	1	3533	7/7	0.96	0.19	196,197,198,199	0
85	MG	1	3935	1/1	0.96	0.24	24,24,24,24	0
85	MG	AR	4017	1/1	0.96	0.17	27,27,27,27	0
84	OHX	1	3554	7/7	0.96	0.22	167,168,169,169	0
85	MG	A	2058	1/1	0.96	0.48	27,27,27,27	0
84	OHX	AR	3466	7/7	0.96	0.17	114,115,116,116	0
84	OHX	AR	3472	7/7	0.96	0.12	129,130,130,130	0
84	OHX	1	3629	7/7	0.96	0.14	161,162,162,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3477	7/7	0.96	0.18	119,119,119,120	0
84	OHX	AR	3492	7/7	0.96	0.16	134,135,135,135	0
85	MG	1	4151	1/1	0.96	0.15	53,53,53,53	0
84	OHX	AR	3494	7/7	0.96	0.23	144,145,146,146	0
85	MG	A	2070	1/1	0.96	0.49	59,59,59,59	0
84	OHX	AR	3495	7/7	0.96	0.14	163,165,166,166	0
84	OHX	AR	3630	7/7	0.96	0.10	172,173,174,175	0
84	OHX	6	2003	7/7	0.96	0.18	180,182,183,184	0
84	OHX	AR	3499	7/7	0.96	0.14	130,131,133,133	0
85	MG	AR	4031	1/1	0.96	0.25	31,31,31,31	0
84	OHX	1	3501	7/7	0.96	0.16	123,124,125,125	0
85	MG	A	2077	1/1	0.96	0.19	25,25,25,25	0
84	OHX	1	3535	7/7	0.96	0.10	196,198,199,200	0
85	MG	A	2080	1/1	0.96	0.52	45,45,45,45	0
85	MG	A	2081	1/1	0.96	0.41	48,48,48,48	0
85	MG	A	2082	1/1	0.96	0.19	65,65,65,65	0
85	MG	A	2083	1/1	0.96	0.37	62,62,62,62	0
85	MG	1	3954	1/1	0.96	0.16	45,45,45,45	0
84	OHX	AR	3635	7/7	0.96	0.33	173,175,175,175	0
85	MG	1	3956	1/1	0.96	0.22	15,15,15,15	0
85	MG	1	4164	1/1	0.96	0.16	48,48,48,48	0
84	OHX	AR	3739	7/7	0.96	0.37	151,152,152,152	0
84	OHX	AR	3636	7/7	0.96	0.17	187,188,188,189	0
85	MG	A	2090	1/1	0.96	0.28	46,46,46,46	0
84	OHX	AR	3508	7/7	0.96	0.21	139,139,140,140	0
84	OHX	AR	3514	7/7	0.96	0.26	146,147,147,148	0
85	MG	1	4172	1/1	0.96	0.16	76,76,76,76	0
84	OHX	AT	206	7/7	0.96	0.17	155,155,156,156	0
84	OHX	AT	209	7/7	0.96	0.18	163,163,163,163	0
85	MG	AR	4045	1/1	0.96	0.12	33,33,33,33	0
85	MG	AR	4046	1/1	0.96	0.19	45,45,45,45	0
85	MG	AK	104	1/1	0.96	0.39	44,44,44,44	0
84	OHX	AR	3516	7/7	0.96	0.09	174,176,178,178	0
84	OHX	AT	212	7/7	0.96	0.16	160,160,161,161	0
85	MG	AR	3741	1/1	0.96	0.24	14,14,14,14	0
84	OHX	AT	213	7/7	0.96	0.11	175,176,176,177	0
85	MG	1	3732	1/1	0.96	0.31	27,27,27,27	0
84	OHX	1	3598	7/7	0.96	0.13	173,173,174,175	0
85	MG	A	2108	1/1	0.96	0.39	39,39,39,39	0
84	OHX	1	3669	7/7	0.96	0.23	125,126,127,127	0
84	OHX	AR	3642	7/7	0.96	0.28	189,189,191,191	0
85	MG	AR	4057	1/1	0.96	0.17	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3970	1/1	0.96	0.25	59,59,59,59	0
84	OHX	AT	217	7/7	0.96	0.24	184,185,185,186	0
84	OHX	AR	3643	7/7	0.96	0.28	157,158,159,160	0
85	MG	1	4186	1/1	0.96	0.27	51,51,51,51	0
84	OHX	1	3432	7/7	0.96	0.15	131,131,132,132	0
85	MG	1	3739	1/1	0.96	0.46	15,15,15,15	0
84	OHX	1	3558	7/7	0.96	0.19	166,167,168,168	0
85	MG	1	4193	1/1	0.96	0.37	9,9,9,9	0
84	OHX	6	1914	7/7	0.96	0.14	119,120,121,123	0
85	MG	AR	4068	1/1	0.96	0.18	25,25,25,25	0
84	OHX	1	3507	7/7	0.96	0.17	149,149,150,150	0
85	MG	AR	3760	1/1	0.96	0.39	21,21,21,21	0
85	MG	AR	3761	1/1	0.96	0.10	41,41,41,41	0
85	MG	1	3744	1/1	0.96	0.73	43,43,43,43	0
85	MG	AR	4073	1/1	0.96	0.15	33,33,33,33	0
84	OHX	6	1936	7/7	0.96	0.18	145,146,146,146	0
84	OHX	AR	3649	7/7	0.96	0.30	207,208,208,208	0
85	MG	AR	4076	1/1	0.96	0.16	38,38,38,38	0
85	MG	AR	3768	1/1	0.96	0.24	23,23,23,23	0
84	OHX	AR	3535	7/7	0.96	0.14	157,157,158,158	0
85	MG	1	3748	1/1	0.96	0.25	23,23,23,23	0
84	OHX	AR	3538	7/7	0.96	0.20	184,185,186,186	0
85	MG	AR	4083	1/1	0.96	0.35	23,23,23,23	0
85	MG	1	4208	1/1	0.96	0.30	30,30,30,30	0
84	OHX	6	1940	7/7	0.96	0.15	149,151,152,153	0
84	OHX	AR	3540	7/7	0.96	0.16	151,152,153,154	0
85	MG	AR	4087	1/1	0.96	0.35	31,31,31,31	0
84	OHX	AR	3541	7/7	0.96	0.12	170,171,172,174	0
84	OHX	AR	3545	7/7	0.96	0.23	181,182,182,183	0
85	MG	AR	3777	1/1	0.96	0.14	50,50,50,50	0
85	MG	1	4221	1/1	0.96	0.36	22,22,22,22	0
85	MG	AR	4094	1/1	0.96	0.14	38,38,38,38	0
85	MG	1	3756	1/1	0.96	0.15	22,22,22,22	0
85	MG	AR	3781	1/1	0.96	0.34	11,11,11,11	0
84	OHX	1	3561	7/7	0.96	0.14	184,184,185,186	0
85	MG	AR	4098	1/1	0.96	0.18	27,27,27,27	0
84	OHX	6	2018	7/7	0.96	0.27	186,187,188,189	0
84	OHX	DH	201	7/7	0.96	0.13	155,156,157,157	0
84	OHX	AR	3549	7/7	0.96	0.19	156,157,158,158	0
84	OHX	AR	3550	7/7	0.96	0.17	164,164,165,165	0
84	OHX	A	1927	7/7	0.96	0.12	158,160,162,162	0
85	MG	c6	201	1/1	0.96	0.16	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1928	7/7	0.96	0.12	156,158,159,159	0
85	MG	d3	201	1/1	0.96	0.13	48,48,48,48	0
85	MG	AR	4106	1/1	0.96	0.19	55,55,55,55	0
84	OHX	6	1947	7/7	0.96	0.12	142,144,145,145	0
84	OHX	A	1931	7/7	0.96	0.11	166,168,169,169	0
85	MG	AR	4109	1/1	0.96	0.23	42,42,42,42	0
85	MG	AR	4111	1/1	0.96	0.60	48,48,48,48	0
85	MG	AR	4112	1/1	0.96	0.13	70,70,70,70	0
85	MG	AR	4113	1/1	0.96	0.30	17,17,17,17	0
87	ZN	g	501	1/1	0.96	0.04	143,143,143,143	0
84	OHX	AR	3662	7/7	0.96	0.19	168,169,169,170	0
85	MG	AR	4115	1/1	0.96	0.34	64,64,64,64	0
85	MG	AR	4150	1/1	0.97	0.12	49,49,49,49	0
85	MG	1	4087	1/1	0.97	0.13	37,37,37,37	0
85	MG	AR	3874	1/1	0.97	0.31	18,18,18,18	0
84	OHX	AR	3515	7/7	0.97	0.16	159,160,161,162	0
84	OHX	6	2007	7/7	0.97	0.15	148,150,151,151	0
85	MG	AR	3877	1/1	0.97	0.39	14,14,14,14	0
84	OHX	1	3530	7/7	0.97	0.13	151,151,151,152	0
85	MG	6	2100	1/1	0.97	0.44	16,16,16,16	0
85	MG	6	2101	1/1	0.97	0.28	37,37,37,37	0
85	MG	AR	4160	1/1	0.97	0.26	31,31,31,31	0
84	OHX	AR	3518	7/7	0.97	0.16	161,162,163,163	0
84	OHX	AT	207	7/7	0.97	0.10	162,163,164,164	0
84	OHX	AT	208	7/7	0.97	0.12	154,154,155,155	0
84	OHX	6	1933	7/7	0.97	0.14	121,122,123,123	0
85	MG	AR	4165	1/1	0.97	0.07	88,88,88,88	0
85	MG	AR	3890	1/1	0.97	0.50	33,33,33,33	0
84	OHX	AT	210	7/7	0.97	0.11	164,164,165,165	0
84	OHX	AR	3522	7/7	0.97	0.14	134,135,136,136	0
85	MG	6	2109	1/1	0.97	0.24	39,39,39,39	0
85	MG	AR	3894	1/1	0.97	0.50	24,24,24,24	0
84	OHX	AR	3523	7/7	0.97	0.23	175,176,176,177	0
84	OHX	1	3500	7/7	0.97	0.07	156,157,159,159	0
85	MG	AR	4174	1/1	0.97	0.21	23,23,23,23	0
84	OHX	AR	3525	7/7	0.97	0.13	150,151,151,152	0
85	MG	6	2113	1/1	0.97	0.42	23,23,23,23	0
84	OHX	6	1938	7/7	0.97	0.13	145,146,148,148	0
85	MG	AR	3901	1/1	0.97	0.26	17,17,17,17	0
85	MG	1	4104	1/1	0.97	0.22	32,32,32,32	0
85	MG	AR	3904	1/1	0.97	0.73	11,11,11,11	0
85	MG	AR	3905	1/1	0.97	0.52	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	3908	1/1	0.97	0.36	14,14,14,14	0
85	MG	6	2118	1/1	0.97	0.25	54,54,54,54	0
85	MG	6	2119	1/1	0.97	0.36	31,31,31,31	0
85	MG	1	3909	1/1	0.97	0.19	24,24,24,24	0
84	OHX	AR	3528	7/7	0.97	0.11	147,147,148,149	0
84	OHX	1	3477	7/7	0.97	0.13	118,119,120,120	0
84	OHX	6	2013	7/7	0.97	0.20	149,151,152,153	0
85	MG	AR	3922	1/1	0.97	0.36	20,20,20,20	0
84	OHX	1	3503	7/7	0.97	0.19	145,146,147,148	0
85	MG	AR	3924	1/1	0.97	0.47	13,13,13,13	0
85	MG	AR	4195	1/1	0.97	0.17	21,21,21,21	0
85	MG	AR	3925	1/1	0.97	0.38	14,14,14,14	0
84	OHX	AR	3534	7/7	0.97	0.12	162,163,164,165	0
84	OHX	CE	402	7/7	0.97	0.12	142,143,144,144	0
85	MG	AR	4200	1/1	0.97	0.57	30,30,30,30	0
84	OHX	6	1943	7/7	0.97	0.11	147,149,150,150	0
85	MG	AR	3934	1/1	0.97	0.37	14,14,14,14	0
85	MG	AR	3935	1/1	0.97	0.28	22,22,22,22	0
84	OHX	AR	3536	7/7	0.97	0.17	141,141,142,142	0
84	OHX	6	1945	7/7	0.97	0.16	149,150,151,152	0
84	OHX	6	2017	7/7	0.97	0.20	158,159,160,161	0
85	MG	AR	3940	1/1	0.97	0.10	34,34,34,34	0
85	MG	1	3922	1/1	0.97	0.50	15,15,15,15	0
84	OHX	T	201	7/7	0.97	0.13	133,135,137,138	0
84	OHX	e	101	7/7	0.97	0.22	205,208,210,210	0
84	OHX	h	401	7/7	0.97	0.09	203,206,208,210	0
85	MG	6	2136	1/1	0.97	0.25	29,29,29,29	0
84	OHX	6	1946	7/7	0.97	0.12	160,161,163,164	0
85	MG	1	3929	1/1	0.97	0.43	20,20,20,20	0
84	OHX	1	3482	7/7	0.97	0.14	116,116,117,117	0
84	OHX	AR	3543	7/7	0.97	0.17	181,181,182,182	0
84	OHX	CL	301	7/7	0.97	0.10	165,166,167,168	0
84	OHX	AR	3544	7/7	0.97	0.11	177,178,179,179	0
85	MG	1	3936	1/1	0.97	0.13	48,48,48,48	0
84	OHX	6	1949	7/7	0.97	0.13	165,167,168,168	0
85	MG	AR	3954	1/1	0.97	0.34	36,36,36,36	0
85	MG	AR	4225	1/1	0.97	0.25	23,23,23,23	0
84	OHX	1	3467	7/7	0.97	0.13	124,125,126,126	0
85	MG	AR	4227	1/1	0.97	0.53	18,18,18,18	0
85	MG	AR	4228	1/1	0.97	0.31	12,12,12,12	0
84	OHX	6	1951	7/7	0.97	0.14	165,167,169,170	0
84	OHX	1	3637	7/7	0.97	0.21	180,181,181,181	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	4231	1/1	0.97	0.33	9,9,9,9	0
85	MG	AR	4232	1/1	0.97	0.26	33,33,33,33	0
84	OHX	6	1953	7/7	0.97	0.13	154,155,157,158	0
85	MG	1	3942	1/1	0.97	0.37	20,20,20,20	0
85	MG	AR	4235	1/1	0.97	0.40	15,15,15,15	0
85	MG	1	3943	1/1	0.97	0.32	22,22,22,22	0
85	MG	AR	4238	1/1	0.97	0.47	27,27,27,27	0
85	MG	1	3944	1/1	0.97	0.33	33,33,33,33	0
84	OHX	AR	3551	7/7	0.97	0.19	161,162,163,164	0
84	OHX	DL	101	7/7	0.97	0.14	144,144,144,144	0
84	OHX	1	3562	7/7	0.97	0.08	200,200,201,202	0
85	MG	1	3948	1/1	0.97	0.40	46,46,46,46	0
84	OHX	A	1918	7/7	0.97	0.17	120,122,123,123	0
85	MG	AS	213	1/1	0.97	0.23	40,40,40,40	0
85	MG	1	4147	1/1	0.97	0.25	28,28,28,28	0
84	OHX	A	1920	7/7	0.97	0.13	141,142,143,144	0
85	MG	1	3741	1/1	0.97	0.21	40,40,40,40	0
84	OHX	A	1921	7/7	0.97	0.17	139,141,143,143	0
84	OHX	A	1925	7/7	0.97	0.09	171,172,174,175	0
84	OHX	1	3639	7/7	0.97	0.30	201,203,203,204	0
84	OHX	1	3563	7/7	0.97	0.14	151,152,152,152	0
85	MG	1	4155	1/1	0.97	0.48	66,66,66,66	0
84	OHX	1	3485	7/7	0.97	0.19	151,152,153,153	0
84	OHX	A	1930	7/7	0.97	0.16	164,165,166,167	0
84	OHX	1	3486	7/7	0.97	0.12	146,146,147,147	0
84	OHX	1	3603	7/7	0.97	0.34	162,162,164,164	0
85	MG	1	3750	1/1	0.97	0.09	70,70,70,70	0
84	OHX	A	1933	7/7	0.97	0.12	154,155,156,157	0
85	MG	AS	230	1/1	0.97	0.27	67,67,67,67	0
84	OHX	6	1963	7/7	0.97	0.15	159,159,161,161	0
84	OHX	A	1935	7/7	0.97	0.13	191,193,195,195	0
85	MG	AR	3983	1/1	0.97	0.28	24,24,24,24	0
84	OHX	1	3684	7/7	0.97	0.22	170,171,172,173	0
84	OHX	A	1937	7/7	0.97	0.14	152,154,157,157	0
85	MG	6	2176	1/1	0.97	0.16	73,73,73,73	0
84	OHX	A	1940	7/7	0.97	0.16	174,175,177,178	0
84	OHX	6	1965	7/7	0.97	0.27	161,162,163,163	0
84	OHX	1	3513	7/7	0.97	0.13	140,141,142,142	0
85	MG	AR	3991	1/1	0.97	0.26	15,15,15,15	0
85	MG	6	2180	1/1	0.97	0.16	94,94,94,94	0
85	MG	1	4173	1/1	0.97	0.14	33,33,33,33	0
84	OHX	A	1944	7/7	0.97	0.11	161,163,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3672	7/7	0.97	0.32	137,138,138,138	0
85	MG	1	3973	1/1	0.97	0.26	33,33,33,33	0
84	OHX	1	3541	7/7	0.97	0.12	154,155,156,156	0
84	OHX	6	1968	7/7	0.97	0.17	145,146,147,148	0
85	MG	AR	3999	1/1	0.97	0.37	28,28,28,28	0
85	MG	AR	4000	1/1	0.97	0.38	30,30,30,30	0
84	OHX	1	3514	7/7	0.97	0.13	148,148,149,149	0
84	OHX	1	3730	7/7	0.97	0.13	141,142,143,143	0
84	OHX	A	1950	7/7	0.97	0.17	168,169,170,171	0
84	OHX	1	3569	7/7	0.97	0.27	166,166,167,168	0
84	OHX	1	3689	7/7	0.97	0.14	140,141,142,142	0
85	MG	AR	4006	1/1	0.97	0.10	33,33,33,33	0
85	MG	AR	4007	1/1	0.97	0.11	23,23,23,23	0
85	MG	CQ	204	1/1	0.97	0.33	48,48,48,48	0
85	MG	1	3770	1/1	0.97	0.47	11,11,11,11	0
85	MG	CR	202	1/1	0.97	0.20	20,20,20,20	0
84	OHX	1	3515	7/7	0.97	0.13	128,128,129,129	0
84	OHX	6	1975	7/7	0.97	0.16	160,161,162,162	0
84	OHX	A	1955	7/7	0.97	0.11	145,148,150,150	0
84	OHX	A	1956	7/7	0.97	0.13	171,173,174,175	0
84	OHX	A	1957	7/7	0.97	0.18	169,171,172,173	0
85	MG	CU	202	1/1	0.97	0.20	31,31,31,31	0
85	MG	CX	202	1/1	0.97	0.32	6,6,6,6	0
85	MG	AB	204	1/1	0.97	0.27	42,42,42,42	0
84	OHX	AR	3574	7/7	0.97	0.27	171,172,173,173	0
84	OHX	1	3572	7/7	0.97	0.28	168,168,169,170	0
85	MG	1	4195	1/1	0.97	0.37	52,52,52,52	0
84	OHX	1	3573	7/7	0.97	0.10	196,196,197,197	0
85	MG	1	4197	1/1	0.97	0.13	48,48,48,48	0
85	MG	i	201	1/1	0.97	0.06	57,57,57,57	0
85	MG	1	3991	1/1	0.97	0.25	30,30,30,30	0
85	MG	1	3994	1/1	0.97	0.21	32,32,32,32	0
85	MG	1	4200	1/1	0.97	0.34	18,18,18,18	0
84	OHX	A	1961	7/7	0.97	0.13	175,176,179,180	0
84	OHX	1	3574	7/7	0.97	0.20	138,139,140,140	0
85	MG	AR	4027	1/1	0.97	0.27	33,33,33,33	0
85	MG	AR	3745	1/1	0.97	0.19	32,32,32,32	0
85	MG	1	4204	1/1	0.97	0.41	12,12,12,12	0
85	MG	1	4205	1/1	0.97	0.53	26,26,26,26	0
84	OHX	AR	3578	7/7	0.97	0.39	188,188,189,189	0
85	MG	1	3784	1/1	0.97	0.30	30,30,30,30	0
85	MG	1	3785	1/1	0.97	0.33	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3652	7/7	0.97	0.17	173,174,174,174	0
85	MG	1	4211	1/1	0.97	0.37	21,21,21,21	0
84	OHX	1	3516	7/7	0.97	0.23	131,132,133,133	0
84	OHX	4	202	7/7	0.97	0.10	157,158,158,158	0
85	MG	1	4215	1/1	0.97	0.34	28,28,28,28	0
84	OHX	AR	3583	7/7	0.97	0.18	148,149,150,150	0
85	MG	1	4220	1/1	0.97	0.22	25,25,25,25	0
85	MG	1	3791	1/1	0.97	0.44	21,21,21,21	0
85	MG	A	2056	1/1	0.97	0.39	39,39,39,39	0
85	MG	A	2057	1/1	0.97	0.42	50,50,50,50	0
85	MG	1	4222	1/1	0.97	0.14	30,30,30,30	0
85	MG	3	209	1/1	0.97	0.26	46,46,46,46	0
85	MG	AR	3763	1/1	0.97	0.26	18,18,18,18	0
85	MG	1	3792	1/1	0.97	0.26	16,16,16,16	0
85	MG	A	2063	1/1	0.97	0.42	36,36,36,36	0
85	MG	A	2064	1/1	0.97	0.15	49,49,49,49	0
85	MG	3	211	1/1	0.97	0.30	33,33,33,33	0
85	MG	1	4007	1/1	0.97	0.30	16,16,16,16	0
84	OHX	1	3488	7/7	0.97	0.14	140,140,141,141	0
84	OHX	1	3577	7/7	0.97	0.25	177,178,179,179	0
84	OHX	A	1972	7/7	0.97	0.12	195,196,198,199	0
84	OHX	6	1984	7/7	0.97	0.18	198,200,201,201	0
84	OHX	1	3518	7/7	0.97	0.17	134,135,135,136	0
84	OHX	A	1975	7/7	0.97	0.08	190,193,195,195	0
84	OHX	1	3579	7/7	0.97	0.12	175,175,177,177	0
84	OHX	4	207	7/7	0.97	0.10	174,175,175,176	0
84	OHX	1	3475	7/7	0.97	0.17	128,129,130,130	0
84	OHX	AR	3698	7/7	0.97	0.19	166,167,167,168	0
85	MG	A	2078	1/1	0.97	0.51	28,28,28,28	0
85	MG	1	4019	1/1	0.97	0.20	31,31,31,31	0
85	MG	1	3805	1/1	0.97	0.19	60,60,60,60	0
84	OHX	1	3476	7/7	0.97	0.16	121,121,122,123	0
84	OHX	1	3582	7/7	0.97	0.20	152,153,154,155	0
85	MG	AR	3785	1/1	0.97	0.29	29,29,29,29	0
85	MG	AR	3786	1/1	0.97	0.19	16,16,16,16	0
84	OHX	1	3583	7/7	0.97	0.29	144,144,145,145	0
85	MG	AR	4066	1/1	0.97	0.17	35,35,35,35	0
85	MG	4	223	1/1	0.97	0.26	44,44,44,44	0
84	OHX	1	3495	7/7	0.97	0.12	133,134,135,135	0
84	OHX	AR	3595	7/7	0.97	0.20	160,161,161,162	0
84	OHX	AP	502	7/7	0.97	0.14	124,124,126,127	0
85	MG	AR	3793	1/1	0.97	0.55	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1987	7/7	0.97	0.14	172,173,174,175	0
85	MG	1	3815	1/1	0.97	0.18	40,40,40,40	0
85	MG	1	3817	1/1	0.97	0.30	32,32,32,32	0
84	OHX	AR	3430	7/7	0.97	0.15	137,137,138,138	0
84	OHX	AR	3453	7/7	0.97	0.12	127,128,128,128	0
85	MG	AR	3799	1/1	0.97	0.17	83,83,83,83	0
84	OHX	AR	3460	7/7	0.97	0.12	109,109,110,110	0
85	MG	1	3822	1/1	0.97	0.31	22,22,22,22	0
84	OHX	AR	3463	7/7	0.97	0.18	114,114,115,115	0
85	MG	A	2102	1/1	0.97	0.31	52,52,52,52	0
85	MG	1	4035	1/1	0.97	0.18	131,131,131,131	0
84	OHX	AR	3464	7/7	0.97	0.13	117,118,118,118	0
84	OHX	k	401	7/7	0.97	0.24	169,170,170,170	0
85	MG	A	2106	1/1	0.97	0.47	30,30,30,30	0
85	MG	1	3827	1/1	0.97	0.27	21,21,21,21	0
84	OHX	AR	3467	7/7	0.97	0.13	137,138,138,139	0
84	OHX	1	3524	7/7	0.97	0.22	164,164,166,167	0
84	OHX	1	3496	7/7	0.97	0.18	115,116,117,117	0
85	MG	AR	4091	1/1	0.97	0.16	53,53,53,53	0
84	OHX	AR	3474	7/7	0.97	0.15	119,120,121,121	0
84	OHX	AR	3607	7/7	0.97	0.22	166,166,167,167	0
84	OHX	AR	3475	7/7	0.97	0.17	114,115,115,116	0
85	MG	AR	3814	1/1	0.97	0.33	27,27,27,27	0
84	OHX	1	3527	7/7	0.97	0.18	138,139,140,140	0
85	MG	AR	3816	1/1	0.97	0.21	27,27,27,27	0
85	MG	x	205	1/1	0.97	0.48	20,20,20,20	0
85	MG	A	2119	1/1	0.97	0.38	55,55,55,55	0
85	MG	1	4048	1/1	0.97	0.32	27,27,27,27	0
85	MG	x	207	1/1	0.97	0.15	17,17,17,17	0
84	OHX	AR	3610	7/7	0.97	0.13	139,140,140,140	0
84	OHX	AR	3480	7/7	0.97	0.12	132,132,132,133	0
84	OHX	AR	3481	7/7	0.97	0.11	132,132,133,133	0
85	MG	1	3843	1/1	0.97	0.66	11,11,11,11	0
84	OHX	AR	3484	7/7	0.97	0.20	133,134,135,135	0
84	OHX	AR	3614	7/7	0.97	0.15	164,165,165,166	0
84	OHX	AR	3488	7/7	0.97	0.13	129,130,130,131	0
85	MG	1	4057	1/1	0.97	0.17	30,30,30,30	0
84	OHX	AR	3489	7/7	0.97	0.12	149,150,151,152	0
85	MG	6	2067	1/1	0.97	0.34	41,41,41,41	0
85	MG	1	4059	1/1	0.97	0.26	32,32,32,32	0
84	OHX	A	2008	7/7	0.97	0.13	156,158,159,159	0
85	MG	AR	3836	1/1	0.97	0.31	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	A	2136	1/1	0.97	0.08	110,110,110,110	0
84	OHX	AR	3617	7/7	0.97	0.28	158,158,159,159	0
85	MG	A	2138	1/1	0.97	0.29	35,35,35,35	0
84	OHX	v	301	7/7	0.97	0.14	155,155,156,156	0
85	MG	1	3858	1/1	0.97	0.64	12,12,12,12	0
85	MG	A	2142	1/1	0.97	0.28	90,90,90,90	0
85	MG	AR	3842	1/1	0.97	0.38	10,10,10,10	0
85	MG	A	2144	1/1	0.97	0.24	49,49,49,49	0
85	MG	1	3859	1/1	0.97	0.21	33,33,33,33	0
84	OHX	1	3588	7/7	0.97	0.16	168,169,170,170	0
85	MG	1	3861	1/1	0.97	0.15	65,65,65,65	0
84	OHX	1	3497	7/7	0.97	0.12	140,141,142,142	0
85	MG	1	3863	1/1	0.97	0.43	25,25,25,25	0
84	OHX	1	3590	7/7	0.97	0.18	208,209,210,211	0
84	OHX	AR	3497	7/7	0.97	0.22	140,140,141,141	0
85	MG	6	2082	1/1	0.97	0.54	25,25,25,25	0
84	OHX	1	3591	7/7	0.97	0.12	185,186,187,188	0
84	OHX	1	3498	7/7	0.97	0.11	150,150,151,152	0
85	MG	AR	3858	1/1	0.97	0.47	22,22,22,22	0
85	MG	AR	4133	1/1	0.97	0.13	35,35,35,35	0
85	MG	AR	4134	1/1	0.97	0.28	10,10,10,10	0
84	OHX	AR	3503	7/7	0.97	0.33	152,153,154,154	0
84	OHX	6	1919	7/7	0.97	0.14	112,113,114,114	0
84	OHX	AR	3627	7/7	0.97	0.20	173,173,174,174	0
85	MG	AR	4138	1/1	0.97	0.41	44,44,44,44	0
85	MG	AR	4139	1/1	0.97	0.64	37,37,37,37	0
84	OHX	AR	3506	7/7	0.97	0.17	158,159,159,160	0
84	OHX	6	1927	7/7	0.97	0.16	128,128,130,130	0
84	OHX	AR	3510	7/7	0.97	0.09	154,155,156,157	0
85	MG	AR	3866	1/1	0.97	0.26	20,20,20,20	0
84	OHX	6	1931	7/7	0.97	0.12	151,152,153,153	0
85	MG	1	4082	1/1	0.97	0.13	22,22,22,22	0
86	7MB	AR	4239	20/20	0.97	0.19	44,44,44,44	0
87	ZN	AP	501	1/1	0.97	0.26	115,115,115,115	0
87	ZN	AQ	501	1/1	0.97	0.08	77,77,77,77	0
87	ZN	DQ	501	1/1	0.97	0.15	105,105,105,105	0
85	MG	1	3885	1/1	0.97	0.49	10,10,10,10	0
85	MG	AR	3870	1/1	0.97	0.23	14,14,14,14	0
84	OHX	AS	206	7/7	0.97	0.14	146,146,148,148	0
85	MG	AR	4149	1/1	0.97	0.13	28,28,28,28	0
85	MG	AR	4188	1/1	0.98	0.19	35,35,35,35	0
85	MG	AR	4189	1/1	0.98	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	A	1963	7/7	0.98	0.10	185,187,189,190	0
84	OHX	6	1948	7/7	0.98	0.10	145,147,148,148	0
85	MG	1	4165	1/1	0.98	0.19	38,38,38,38	0
84	OHX	A	1965	7/7	0.98	0.19	167,169,170,171	0
84	OHX	1	3435	7/7	0.98	0.15	103,104,105,105	0
84	OHX	AR	3476	7/7	0.98	0.12	127,128,129,130	0
85	MG	AR	4197	1/1	0.98	0.24	29,29,29,29	0
85	MG	1	3971	1/1	0.98	0.18	63,63,63,63	0
85	MG	1	3972	1/1	0.98	0.31	31,31,31,31	0
84	OHX	1	3437	7/7	0.98	0.14	100,101,102,102	0
85	MG	1	3787	1/1	0.98	0.28	15,15,15,15	0
84	OHX	AR	3478	7/7	0.98	0.12	102,103,103,104	0
84	OHX	AR	3479	7/7	0.98	0.15	119,119,120,120	0
84	OHX	3	204	7/7	0.98	0.08	163,164,165,166	0
84	OHX	1	3571	7/7	0.98	0.27	144,145,145,146	0
84	OHX	1	3532	7/7	0.98	0.13	133,133,134,134	0
85	MG	1	3793	1/1	0.98	0.46	12,12,12,12	0
84	OHX	AR	3485	7/7	0.98	0.25	135,136,137,137	0
85	MG	AR	4210	1/1	0.98	0.37	33,33,33,33	0
84	OHX	AR	3487	7/7	0.98	0.12	116,117,117,117	0
84	OHX	1	3493	7/7	0.98	0.16	147,148,148,149	0
85	MG	1	3797	1/1	0.98	0.13	41,41,41,41	0
84	OHX	1	3494	7/7	0.98	0.11	141,142,144,144	0
84	OHX	AR	3491	7/7	0.98	0.10	130,131,132,132	0
84	OHX	6	1956	7/7	0.98	0.09	192,194,195,196	0
85	MG	1	4189	1/1	0.98	0.22	48,48,48,48	0
84	OHX	AR	3493	7/7	0.98	0.12	137,139,139,140	0
85	MG	6	2183	1/1	0.98	0.23	44,44,44,44	0
84	OHX	6	1957	7/7	0.98	0.14	144,145,146,147	0
84	OHX	1	3433	7/7	0.98	0.21	90,90,90,90	0
85	MG	AR	4222	1/1	0.98	0.15	27,27,27,27	0
85	MG	1	3992	1/1	0.98	0.14	53,53,53,53	0
85	MG	6	2187	1/1	0.98	0.12	82,82,82,82	0
85	MG	1	3993	1/1	0.98	0.10	27,27,27,27	0
84	OHX	6	1959	7/7	0.98	0.11	154,155,156,157	0
84	OHX	1	3464	7/7	0.98	0.11	136,137,138,139	0
85	MG	6	2191	1/1	0.98	0.30	47,47,47,47	0
85	MG	1	3996	1/1	0.98	0.26	51,51,51,51	0
84	OHX	AR	3498	7/7	0.98	0.09	143,144,145,146	0
84	OHX	1	3442	7/7	0.98	0.12	98,99,99,100	0
85	MG	1	4201	1/1	0.98	0.53	31,31,31,31	0
84	OHX	1	3538	7/7	0.98	0.14	135,135,137,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3502	7/7	0.98	0.11	131,132,132,133	0
84	OHX	1	3444	7/7	0.98	0.16	103,104,104,105	0
85	MG	AR	4236	1/1	0.98	0.32	22,22,22,22	0
84	OHX	AR	3504	7/7	0.98	0.21	116,117,117,118	0
84	OHX	1	3468	7/7	0.98	0.14	104,104,104,105	0
85	MG	1	3814	1/1	0.98	0.32	39,39,39,39	0
84	OHX	1	3469	7/7	0.98	0.13	118,118,119,120	0
85	MG	1	4209	1/1	0.98	0.40	22,22,22,22	0
85	MG	AR	4243	1/1	0.98	0.43	22,22,22,22	0
85	MG	1	3816	1/1	0.98	0.36	28,28,28,28	0
85	MG	AR	3987	1/1	0.98	0.33	50,50,50,50	0
84	OHX	AR	3507	7/7	0.98	0.16	136,136,137,137	0
84	OHX	1	3445	7/7	0.98	0.14	95,95,95,96	0
85	MG	1	3819	1/1	0.98	0.25	25,25,25,25	0
84	OHX	AR	3509	7/7	0.98	0.14	135,136,136,137	0
84	OHX	1	3471	7/7	0.98	0.13	118,118,121,121	0
85	MG	AS	217	1/1	0.98	0.16	18,18,18,18	0
85	MG	1	4218	1/1	0.98	0.07	84,84,84,84	0
85	MG	1	4219	1/1	0.98	0.34	47,47,47,47	0
84	OHX	AR	3511	7/7	0.98	0.15	96,96,96,97	0
85	MG	1	4013	1/1	0.98	0.22	56,56,56,56	0
85	MG	AS	222	1/1	0.98	0.22	13,13,13,13	0
84	OHX	AR	3512	7/7	0.98	0.10	132,132,132,133	0
84	OHX	AR	3513	7/7	0.98	0.11	152,153,154,154	0
85	MG	1	3825	1/1	0.98	0.17	42,42,42,42	0
84	OHX	1	3505	7/7	0.98	0.13	139,139,140,140	0
84	OHX	1	3506	7/7	0.98	0.08	159,160,161,162	0
85	MG	AR	3751	1/1	0.98	0.21	29,29,29,29	0
85	MG	1	3828	1/1	0.98	0.41	29,29,29,29	0
84	OHX	6	1970	7/7	0.98	0.19	178,179,180,180	0
85	MG	AR	3754	1/1	0.98	0.14	35,35,35,35	0
84	OHX	AS	201	7/7	0.98	0.16	98,99,100,101	0
84	OHX	AS	202	7/7	0.98	0.11	122,123,124,124	0
84	OHX	AS	203	7/7	0.98	0.11	118,119,120,120	0
84	OHX	AS	204	7/7	0.98	0.12	140,141,141,141	0
84	OHX	AS	205	7/7	0.98	0.11	144,146,147,147	0
85	MG	1	3836	1/1	0.98	0.24	17,17,17,17	0
85	MG	1	3838	1/1	0.98	0.36	20,20,20,20	0
84	OHX	1	3626	7/7	0.98	0.16	137,137,138,138	0
85	MG	AR	4014	1/1	0.98	0.35	32,32,32,32	0
85	MG	AT	230	1/1	0.98	0.23	48,48,48,48	0
84	OHX	AS	207	7/7	0.98	0.11	163,165,166,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3473	7/7	0.98	0.12	119,120,121,121	0
85	MG	AR	3765	1/1	0.98	0.44	23,23,23,23	0
84	OHX	AR	3519	7/7	0.98	0.12	135,135,136,136	0
85	MG	CE	404	1/1	0.98	0.27	24,24,24,24	0
84	OHX	1	3508	7/7	0.98	0.12	140,142,143,144	0
85	MG	4	220	1/1	0.98	0.37	37,37,37,37	0
85	MG	4	221	1/1	0.98	0.15	52,52,52,52	0
84	OHX	AT	204	7/7	0.98	0.10	143,143,143,143	0
85	MG	1	3846	1/1	0.98	0.38	16,16,16,16	0
84	OHX	AT	205	7/7	0.98	0.09	151,151,151,151	0
85	MG	4	225	1/1	0.98	0.18	43,43,43,43	0
85	MG	1	3849	1/1	0.98	0.44	21,21,21,21	0
85	MG	1	4037	1/1	0.98	0.19	61,61,61,61	0
84	OHX	AR	3521	7/7	0.98	0.12	160,161,161,162	0
84	OHX	1	3509	7/7	0.98	0.18	155,155,157,157	0
85	MG	AR	3779	1/1	0.98	0.28	20,20,20,20	0
84	OHX	1	3510	7/7	0.98	0.22	148,148,149,149	0
84	OHX	1	3474	7/7	0.98	0.14	131,132,133,133	0
84	OHX	1	3446	7/7	0.98	0.16	107,108,109,110	0
85	MG	AR	3783	1/1	0.98	0.39	15,15,15,15	0
85	MG	1	3857	1/1	0.98	0.39	12,12,12,12	0
85	MG	j	301	1/1	0.98	0.13	26,26,26,26	0
84	OHX	1	3448	7/7	0.98	0.24	104,105,106,106	0
84	OHX	AR	3527	7/7	0.98	0.10	138,139,140,141	0
85	MG	1	4046	1/1	0.98	0.09	54,54,54,54	0
84	OHX	1	3449	7/7	0.98	0.10	119,120,121,121	0
85	MG	AR	3790	1/1	0.98	0.28	17,17,17,17	0
84	OHX	1	3478	7/7	0.98	0.11	133,134,135,135	0
84	OHX	6	1907	7/7	0.98	0.19	100,101,101,101	0
85	MG	r	302	1/1	0.98	0.10	40,40,40,40	0
84	OHX	AR	3531	7/7	0.98	0.10	123,124,124,124	0
84	OHX	AR	3532	7/7	0.98	0.17	129,130,130,131	0
85	MG	1	3865	1/1	0.98	0.47	13,13,13,13	0
84	OHX	1	3479	7/7	0.98	0.15	136,137,138,138	0
84	OHX	6	1915	7/7	0.98	0.12	100,101,102,102	0
85	MG	1	3868	1/1	0.98	0.58	9,9,9,9	0
85	MG	AR	3800	1/1	0.98	0.28	22,22,22,22	0
85	MG	1	3869	1/1	0.98	0.33	33,33,33,33	0
85	MG	1	3870	1/1	0.98	0.51	11,11,11,11	0
84	OHX	1	3480	7/7	0.98	0.13	141,141,142,142	0
85	MG	1	3872	1/1	0.98	0.39	23,23,23,23	0
85	MG	1	3874	1/1	0.98	0.42	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1920	7/7	0.98	0.12	124,126,127,128	0
84	OHX	AR	3537	7/7	0.98	0.11	133,134,135,135	0
84	OHX	6	1921	7/7	0.98	0.14	121,124,124,126	0
85	MG	6	2059	1/1	0.98	0.42	40,40,40,40	0
85	MG	1	3878	1/1	0.98	0.18	36,36,36,36	0
85	MG	A	2049	1/1	0.98	0.34	35,35,35,35	0
84	OHX	6	1924	7/7	0.98	0.12	123,124,126,127	0
84	OHX	1	3481	7/7	0.98	0.11	130,131,132,133	0
85	MG	6	2063	1/1	0.98	0.28	31,31,31,31	0
84	OHX	6	1928	7/7	0.98	0.09	150,151,152,152	0
84	OHX	6	1929	7/7	0.98	0.14	147,148,151,152	0
85	MG	6	2066	1/1	0.98	0.27	87,87,87,87	0
85	MG	AR	3817	1/1	0.98	0.31	20,20,20,20	0
85	MG	1	3884	1/1	0.98	0.38	27,27,27,27	0
85	MG	6	2068	1/1	0.98	0.35	76,76,76,76	0
85	MG	AR	3821	1/1	0.98	0.35	26,26,26,26	0
85	MG	A	2060	1/1	0.98	0.41	20,20,20,20	0
84	OHX	AR	3654	7/7	0.98	0.20	161,162,163,164	0
85	MG	1	3886	1/1	0.98	0.43	24,24,24,24	0
84	OHX	6	1930	7/7	0.98	0.12	114,115,116,117	0
84	OHX	1	3520	7/7	0.98	0.07	149,150,152,152	0
85	MG	1	3889	1/1	0.98	0.28	19,19,19,19	0
85	MG	A	2066	1/1	0.98	0.44	62,62,62,62	0
85	MG	AR	4078	1/1	0.98	0.31	23,23,23,23	0
84	OHX	1	3450	7/7	0.98	0.12	116,117,118,118	0
85	MG	AR	4080	1/1	0.98	0.16	16,16,16,16	0
84	OHX	1	3560	7/7	0.98	0.13	155,156,158,158	0
85	MG	AR	3829	1/1	0.98	0.41	16,16,16,16	0
85	MG	1	3892	1/1	0.98	0.52	14,14,14,14	0
85	MG	6	2077	1/1	0.98	0.56	51,51,51,51	0
85	MG	1	3893	1/1	0.98	0.28	38,38,38,38	0
84	OHX	AR	3548	7/7	0.98	0.18	165,166,166,166	0
85	MG	1	4083	1/1	0.98	0.11	34,34,34,34	0
84	OHX	CX	201	7/7	0.98	0.17	121,122,123,124	0
85	MG	AR	4089	1/1	0.98	0.39	15,15,15,15	0
85	MG	1	3896	1/1	0.98	0.41	10,10,10,10	0
84	OHX	6	1935	7/7	0.98	0.12	136,137,138,139	0
84	OHX	DG	201	7/7	0.98	0.16	132,133,133,134	0
84	OHX	1	3483	7/7	0.98	0.10	118,119,120,121	0
84	OHX	6	1937	7/7	0.98	0.11	140,141,141,141	0
85	MG	AR	3843	1/1	0.98	0.24	13,13,13,13	0
84	OHX	AR	3552	7/7	0.98	0.12	148,148,149,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3845	1/1	0.98	0.23	32,32,32,32	0
85	MG	1	3904	1/1	0.98	0.44	4,4,4,4	0
84	OHX	AR	3553	7/7	0.98	0.12	160,160,161,162	0
84	OHX	A	1908	7/7	0.98	0.16	111,111,113,114	0
84	OHX	A	1909	7/7	0.98	0.13	124,125,128,129	0
84	OHX	A	1910	7/7	0.98	0.11	123,125,127,128	0
84	OHX	A	1911	7/7	0.98	0.13	115,117,118,120	0
85	MG	6	2094	1/1	0.98	0.28	24,24,24,24	0
84	OHX	A	1912	7/7	0.98	0.09	132,133,135,136	0
85	MG	AR	3856	1/1	0.98	0.53	10,10,10,10	0
85	MG	A	2096	1/1	0.98	0.27	51,51,51,51	0
84	OHX	A	1913	7/7	0.98	0.14	121,122,123,124	0
84	OHX	A	1915	7/7	0.98	0.09	149,151,152,154	0
85	MG	1	3913	1/1	0.98	0.27	38,38,38,38	0
84	OHX	A	1916	7/7	0.98	0.11	128,130,131,131	0
84	OHX	1	3452	7/7	0.98	0.14	111,111,112,113	0
84	OHX	AK	102	7/7	0.98	0.10	121,122,122,122	0
85	MG	1	3917	1/1	0.98	0.36	18,18,18,18	0
85	MG	6	2103	1/1	0.98	0.41	40,40,40,40	0
85	MG	AR	3865	1/1	0.98	0.27	23,23,23,23	0
85	MG	AR	4118	1/1	0.98	0.27	29,29,29,29	0
84	OHX	AK	103	7/7	0.98	0.12	145,146,146,146	0
84	OHX	A	1922	7/7	0.98	0.10	138,140,141,141	0
84	OHX	A	1923	7/7	0.98	0.09	137,138,140,140	0
84	OHX	A	1924	7/7	0.98	0.10	153,154,155,156	0
84	OHX	AR	3557	7/7	0.98	0.11	144,145,146,146	0
84	OHX	A	1926	7/7	0.98	0.11	149,150,151,152	0
85	MG	1	4115	1/1	0.98	0.17	97,97,97,97	0
85	MG	1	3925	1/1	0.98	0.38	15,15,15,15	0
85	MG	1	4117	1/1	0.98	0.34	26,26,26,26	0
85	MG	1	4118	1/1	0.98	0.23	87,87,87,87	0
84	OHX	6	1999	7/7	0.98	0.18	177,179,179,181	0
85	MG	AR	3878	1/1	0.98	0.27	12,12,12,12	0
84	OHX	AR	3427	7/7	0.98	0.22	87,87,87,87	0
85	MG	A	2120	1/1	0.98	0.08	74,74,74,74	0
85	MG	AR	4132	1/1	0.98	0.08	36,36,36,36	0
84	OHX	AR	3429	7/7	0.98	0.09	105,105,106,106	0
85	MG	AR	3881	1/1	0.98	0.41	12,12,12,12	0
84	OHX	6	1939	7/7	0.98	0.11	131,133,134,135	0
84	OHX	AR	3562	7/7	0.98	0.07	173,174,175,176	0
85	MG	AR	3886	1/1	0.98	0.25	15,15,15,15	0
85	MG	1	3932	1/1	0.98	0.26	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	OHX	AR	3433	7/7	0.98	0.17	94,94,94,95	0
85	MG	1	4126	1/1	0.98	0.33	30,30,30,30	0
84	OHX	AR	3441	7/7	0.98	0.14	109,110,110,111	0
84	OHX	AR	3442	7/7	0.98	0.15	110,111,111,111	0
84	OHX	AR	3443	7/7	0.98	0.14	98,99,100,101	0
84	OHX	AR	3445	7/7	0.98	0.13	94,94,94,95	0
84	OHX	AR	3448	7/7	0.98	0.12	109,110,110,110	0
85	MG	AR	3895	1/1	0.98	0.39	21,21,21,21	0
84	OHX	A	1938	7/7	0.98	0.14	138,139,140,141	0
84	OHX	AR	3450	7/7	0.98	0.11	109,110,112,113	0
84	OHX	AR	3451	7/7	0.98	0.15	104,105,106,106	0
84	OHX	A	1942	7/7	0.98	0.14	163,165,166,167	0
84	OHX	AR	3452	7/7	0.98	0.11	108,109,110,111	0
85	MG	A	2141	1/1	0.98	0.32	73,73,73,73	0
84	OHX	1	3454	7/7	0.98	0.14	111,112,113,113	0
84	OHX	AR	3454	7/7	0.98	0.12	120,120,121,121	0
85	MG	AR	3903	1/1	0.98	0.41	5,5,5,5	0
84	OHX	AR	3455	7/7	0.98	0.17	106,107,108,108	0
84	OHX	AR	3456	7/7	0.98	0.12	109,110,110,111	0
84	OHX	AR	3457	7/7	0.98	0.13	107,107,108,108	0
85	MG	AR	3908	1/1	0.98	0.46	18,18,18,18	0
85	MG	AR	3911	1/1	0.98	0.43	16,16,16,16	0
85	MG	AR	3912	1/1	0.98	0.54	1,1,1,1	0
84	OHX	AR	3459	7/7	0.98	0.14	97,97,98,99	0
85	MG	AR	3914	1/1	0.98	0.35	13,13,13,13	0
85	MG	AR	3915	1/1	0.98	0.29	20,20,20,20	0
84	OHX	1	3525	7/7	0.98	0.10	151,152,153,154	0
85	MG	AR	4166	1/1	0.98	0.11	58,58,58,58	0
85	MG	AR	3917	1/1	0.98	0.33	29,29,29,29	0
84	OHX	6	1942	7/7	0.98	0.09	142,143,144,145	0
84	OHX	AR	3580	7/7	0.98	0.18	139,139,140,140	0
85	MG	1	4148	1/1	0.98	0.57	35,35,35,35	0
85	MG	1	3768	1/1	0.98	0.30	24,24,24,24	0
84	OHX	1	3455	7/7	0.98	0.13	104,104,105,105	0
84	OHX	6	1944	7/7	0.98	0.12	154,155,157,158	0
85	MG	1	3771	1/1	0.98	0.48	23,23,23,23	0
84	OHX	1	3487	7/7	0.98	0.10	139,140,142,142	0
85	MG	AR	3926	1/1	0.98	0.51	10,10,10,10	0
85	MG	1	3773	1/1	0.98	0.46	15,15,15,15	0
85	MG	AR	3929	1/1	0.98	0.13	75,75,75,75	0
84	OHX	AR	3468	7/7	0.98	0.11	111,112,113,114	0
85	MG	AR	3931	1/1	0.98	0.18	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
85	MG	AR	3932	1/1	0.98	0.38	25,25,25,25	0
84	OHX	AR	3469	7/7	0.98	0.10	122,124,125,125	0
84	OHX	AR	3697	7/7	0.98	0.21	115,116,116,116	0
87	ZN	DR	501	1/1	0.98	0.07	73,73,73,73	0
84	OHX	AR	3470	7/7	0.98	0.09	125,127,127,128	0
84	OHX	AR	3471	7/7	0.98	0.12	127,127,128,128	0
84	OHX	1	3456	7/7	0.98	0.13	114,115,116,117	0
87	ZN	d9	103	1/1	0.98	0.10	86,86,86,86	0
84	OHX	1	3490	7/7	0.98	0.10	134,135,136,136	0
84	OHX	1	3416	7/7	0.99	0.15	86,86,86,86	0
84	OHX	AR	3482	7/7	0.99	0.10	116,117,117,117	0
84	OHX	AR	3483	7/7	0.99	0.16	124,125,125,126	0
84	OHX	1	3417	7/7	0.99	0.19	97,97,97,97	0
84	OHX	1	3457	7/7	0.99	0.14	108,108,109,109	0
84	OHX	AR	3486	7/7	0.99	0.09	118,119,120,121	0
85	MG	1	3931	1/1	0.99	0.12	31,31,31,31	0
84	OHX	1	3418	7/7	0.99	0.13	85,85,85,85	0
84	OHX	1	3459	7/7	0.99	0.09	134,134,135,136	0
85	MG	1	4086	1/1	0.99	0.32	16,16,16,16	0
85	MG	AR	3906	1/1	0.99	0.23	15,15,15,15	0
84	OHX	1	3460	7/7	0.99	0.12	112,114,115,116	0
84	OHX	AR	3490	7/7	0.99	0.09	108,108,109,110	0
85	MG	AR	3909	1/1	0.99	0.37	14,14,14,14	0
85	MG	AR	3910	1/1	0.99	0.32	17,17,17,17	0
85	MG	AB	201	1/1	0.99	0.50	15,15,15,15	0
85	MG	AB	202	1/1	0.99	0.22	34,34,34,34	0
84	OHX	1	3419	7/7	0.99	0.19	93,93,93,93	0
84	OHX	1	3420	7/7	0.99	0.20	91,91,92,92	0
85	MG	j	302	1/1	0.99	0.14	29,29,29,29	0
85	MG	k	403	1/1	0.99	0.21	24,24,24,24	0
84	OHX	1	3463	7/7	0.99	0.08	108,109,109,109	0
84	OHX	1	3421	7/7	0.99	0.11	84,84,84,84	0
84	OHX	1	3465	7/7	0.99	0.10	113,114,114,114	0
85	MG	1	4094	1/1	0.99	0.13	43,43,43,43	0
84	OHX	1	3422	7/7	0.99	0.17	94,94,94,94	0
85	MG	AR	4105	1/1	0.99	0.08	41,41,41,41	0
84	OHX	2	201	7/7	0.99	0.17	94,94,94,94	0
84	OHX	6	1901	7/7	0.99	0.23	92,92,92,92	0
85	MG	1	4099	1/1	0.99	0.31	16,16,16,16	0
84	OHX	A	1984	7/7	0.99	0.12	151,152,153,154	0
84	OHX	6	1902	7/7	0.99	0.24	102,102,102,102	0
85	MG	AR	3927	1/1	0.99	0.64	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	6	1903	7/7	0.99	0.20	89,89,90,90	0
84	OHX	AR	3501	7/7	0.99	0.11	118,118,120,120	0
84	OHX	6	1905	7/7	0.99	0.20	100,100,101,101	0
84	OHX	6	1906	7/7	0.99	0.19	94,94,95,95	0
84	OHX	1	3423	7/7	0.99	0.15	91,92,92,92	0
84	OHX	6	1908	7/7	0.99	0.16	91,91,91,91	0
84	OHX	6	1909	7/7	0.99	0.16	103,104,104,104	0
85	MG	DC	204	1/1	0.99	0.17	45,45,45,45	0
84	OHX	6	1910	7/7	0.99	0.14	93,93,93,93	0
84	OHX	6	1911	7/7	0.99	0.15	99,100,100,100	0
85	MG	AR	3937	1/1	0.99	0.43	9,9,9,9	0
85	MG	l2	201	1/1	0.99	0.28	21,21,21,21	0
85	MG	1	3806	1/1	0.99	0.28	31,31,31,31	0
85	MG	DH	203	1/1	0.99	0.23	41,41,41,41	0
84	OHX	6	1912	7/7	0.99	0.09	107,108,110,110	0
84	OHX	AT	203	7/7	0.99	0.21	83,83,83,83	0
84	OHX	6	1913	7/7	0.99	0.13	105,105,106,107	0
84	OHX	1	3424	7/7	0.99	0.19	92,93,93,93	0
84	OHX	1	3425	7/7	0.99	0.16	93,93,93,93	0
84	OHX	6	1916	7/7	0.99	0.11	102,103,104,104	0
84	OHX	6	1917	7/7	0.99	0.10	113,114,116,117	0
84	OHX	6	1918	7/7	0.99	0.11	103,104,105,105	0
84	OHX	1	3426	7/7	0.99	0.15	93,93,93,94	0
84	OHX	1	3519	7/7	0.99	0.10	112,112,113,113	0
85	MG	A	2047	1/1	0.99	0.39	55,55,55,55	0
84	OHX	1	3427	7/7	0.99	0.15	87,87,87,87	0
84	OHX	6	1922	7/7	0.99	0.10	111,112,113,114	0
84	OHX	AR	3401	7/7	0.99	0.26	93,93,93,93	0
84	OHX	AR	3402	7/7	0.99	0.27	89,89,89,89	0
84	OHX	AR	3403	7/7	0.99	0.19	86,86,86,86	0
84	OHX	AR	3404	7/7	0.99	0.19	88,89,89,89	0
84	OHX	AR	3405	7/7	0.99	0.23	94,94,94,94	0
84	OHX	AR	3406	7/7	0.99	0.23	86,86,86,86	0
84	OHX	AR	3407	7/7	0.99	0.24	88,88,88,88	0
84	OHX	AR	3408	7/7	0.99	0.22	83,83,83,83	0
84	OHX	AR	3409	7/7	0.99	0.20	92,92,92,92	0
84	OHX	AR	3410	7/7	0.99	0.13	86,86,86,86	0
84	OHX	AR	3411	7/7	0.99	0.20	83,83,83,83	0
84	OHX	AR	3412	7/7	0.99	0.16	85,85,85,85	0
84	OHX	AR	3413	7/7	0.99	0.16	84,84,84,84	0
85	MG	1	4137	1/1	0.99	0.20	38,38,38,38	0
85	MG	1	3832	1/1	0.99	0.34	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3414	7/7	0.99	0.18	90,90,90,90	0
84	OHX	AR	3415	7/7	0.99	0.23	86,86,86,87	0
84	OHX	AR	3416	7/7	0.99	0.17	88,88,88,89	0
84	OHX	AR	3417	7/7	0.99	0.14	86,86,86,86	0
85	MG	1	4143	1/1	0.99	0.07	53,53,53,53	0
85	MG	AR	4157	1/1	0.99	0.22	29,29,29,29	0
85	MG	1	3837	1/1	0.99	0.64	25,25,25,25	0
85	MG	1	3987	1/1	0.99	0.24	32,32,32,32	0
84	OHX	AR	3418	7/7	0.99	0.14	92,92,93,93	0
84	OHX	AR	3419	7/7	0.99	0.13	94,94,95,95	0
84	OHX	AR	3420	7/7	0.99	0.16	87,87,87,87	0
84	OHX	CV	201	7/7	0.99	0.21	91,91,91,91	0
84	OHX	AR	3421	7/7	0.99	0.12	89,89,89,89	0
84	OHX	AR	3422	7/7	0.99	0.15	86,86,86,86	0
84	OHX	DD	102	7/7	0.99	0.17	88,89,89,89	0
85	MG	1	3845	1/1	0.99	0.36	14,14,14,14	0
84	OHX	AR	3542	7/7	0.99	0.19	133,134,134,134	0
84	OHX	AR	3423	7/7	0.99	0.14	85,85,85,85	0
85	MG	1	3848	1/1	0.99	0.20	26,26,26,26	0
84	OHX	AR	3424	7/7	0.99	0.19	86,87,87,87	0
84	OHX	AR	3425	7/7	0.99	0.10	85,85,85,85	0
84	OHX	AR	3426	7/7	0.99	0.13	88,88,88,89	0
84	OHX	A	1901	7/7	0.99	0.21	101,101,102,102	0
84	OHX	A	1902	7/7	0.99	0.16	96,97,97,97	0
84	OHX	A	1903	7/7	0.99	0.26	117,118,118,119	0
85	MG	1	3856	1/1	0.99	0.31	15,15,15,15	0
84	OHX	A	1904	7/7	0.99	0.12	107,107,108,108	0
85	MG	1	4167	1/1	0.99	0.15	52,52,52,52	0
84	OHX	A	1905	7/7	0.99	0.18	102,102,103,103	0
84	OHX	A	1906	7/7	0.99	0.17	112,113,113,113	0
84	OHX	A	1907	7/7	0.99	0.09	117,118,120,121	0
84	OHX	6	1923	7/7	0.99	0.14	136,138,139,139	0
84	OHX	AR	3428	7/7	0.99	0.10	97,97,98,98	0
85	MG	6	2117	1/1	0.99	0.41	21,21,21,21	0
84	OHX	1	3472	7/7	0.99	0.12	114,115,115,116	0
85	MG	AR	3819	1/1	0.99	0.49	53,53,53,53	0
84	OHX	6	1925	7/7	0.99	0.12	116,116,118,118	0
84	OHX	AR	3431	7/7	0.99	0.14	86,86,86,86	0
85	MG	AR	4190	1/1	0.99	0.24	107,107,107,107	0
84	OHX	AR	3432	7/7	0.99	0.13	91,91,91,91	0
84	OHX	A	1914	7/7	0.99	0.11	109,110,111,112	0
84	OHX	6	1926	7/7	0.99	0.10	122,123,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	AR	3434	7/7	0.99	0.16	87,87,88,88	0
84	OHX	A	1917	7/7	0.99	0.12	126,128,129,130	0
84	OHX	AR	3435	7/7	0.99	0.11	96,96,96,96	0
84	OHX	A	1919	7/7	0.99	0.10	113,115,116,116	0
85	MG	1	3873	1/1	0.99	0.40	18,18,18,18	0
84	OHX	AR	3436	7/7	0.99	0.16	87,87,87,87	0
84	OHX	AR	3437	7/7	0.99	0.11	89,89,89,89	0
84	OHX	AR	3438	7/7	0.99	0.12	89,89,89,90	0
84	OHX	AR	3439	7/7	0.99	0.16	91,91,92,92	0
84	OHX	AR	3440	7/7	0.99	0.12	98,98,98,99	0
84	OHX	1	3428	7/7	0.99	0.14	96,96,96,96	0
85	MG	6	2135	1/1	0.99	0.22	38,38,38,38	0
85	MG	1	4191	1/1	0.99	0.45	22,22,22,22	0
84	OHX	1	3429	7/7	0.99	0.13	89,89,90,90	0
84	OHX	1	3430	7/7	0.99	0.14	97,97,97,98	0
85	MG	AR	3840	1/1	0.99	0.33	22,22,22,22	0
85	MG	AR	3841	1/1	0.99	0.32	25,25,25,25	0
85	MG	1	3882	1/1	0.99	0.38	11,11,11,11	0
84	OHX	AR	3444	7/7	0.99	0.10	101,102,102,103	0
84	OHX	1	3431	7/7	0.99	0.12	95,95,95,95	0
84	OHX	AR	3446	7/7	0.99	0.09	99,100,100,101	0
84	OHX	AR	3447	7/7	0.99	0.13	88,88,89,89	0
84	OHX	1	3402	7/7	0.99	0.24	90,90,91,91	0
84	OHX	AR	3449	7/7	0.99	0.12	98,99,99,100	0
85	MG	6	2146	1/1	0.99	0.14	44,44,44,44	0
84	OHX	1	3403	7/7	0.99	0.23	90,90,90,90	0
85	MG	AR	3851	1/1	0.99	0.34	29,29,29,29	0
85	MG	AR	3852	1/1	0.99	0.44	18,18,18,18	0
84	OHX	1	3434	7/7	0.99	0.14	94,95,95,95	0
84	OHX	6	1934	7/7	0.99	0.09	141,141,143,144	0
84	OHX	1	3404	7/7	0.99	0.20	93,93,93,93	0
84	OHX	1	3436	7/7	0.99	0.11	101,102,104,104	0
84	OHX	A	1939	7/7	0.99	0.08	153,155,156,157	0
84	OHX	1	3405	7/7	0.99	0.26	97,98,98,98	0
84	OHX	1	3438	7/7	0.99	0.13	91,91,92,92	0
85	MG	1	3752	1/1	0.99	0.29	27,27,27,27	0
84	OHX	1	3439	7/7	0.99	0.11	102,103,103,104	0
85	MG	1	3899	1/1	0.99	0.41	12,12,12,12	0
85	MG	A	2145	1/1	0.99	0.21	83,83,83,83	0
85	MG	1	4212	1/1	0.99	0.32	27,27,27,27	0
84	OHX	AR	3458	7/7	0.99	0.11	100,101,101,102	0
85	MG	1	3901	1/1	0.99	0.49	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	OHX	1	3440	7/7	0.99	0.14	94,95,95,95	0
84	OHX	1	3406	7/7	0.99	0.22	85,85,85,85	0
84	OHX	AR	3461	7/7	0.99	0.11	108,109,109,110	0
85	MG	AR	4051	1/1	0.99	0.12	62,62,62,62	0
85	MG	1	4054	1/1	0.99	0.14	40,40,40,40	0
84	OHX	AR	3462	7/7	0.99	0.11	106,107,108,108	0
84	OHX	3	201	7/7	0.99	0.10	106,107,108,108	0
85	MG	AR	3872	1/1	0.99	0.45	0,0,0,0	0
84	OHX	1	3407	7/7	0.99	0.20	83,83,83,83	0
84	OHX	AR	3465	7/7	0.99	0.12	100,101,102,102	0
84	OHX	1	3443	7/7	0.99	0.12	95,95,95,95	0
84	OHX	1	3489	7/7	0.99	0.11	114,115,116,117	0
84	OHX	1	3408	7/7	0.99	0.12	89,89,89,89	0
84	OHX	1	3409	7/7	0.99	0.21	85,85,85,85	0
85	MG	3	214	1/1	0.99	0.42	12,12,12,12	0
84	OHX	1	3410	7/7	0.99	0.20	88,88,88,88	0
84	OHX	1	3447	7/7	0.99	0.14	95,95,95,95	0
85	MG	AR	3882	1/1	0.99	0.58	11,11,11,11	0
85	MG	AR	3883	1/1	0.99	0.34	12,12,12,12	0
85	MG	1	4065	1/1	0.99	0.26	35,35,35,35	0
84	OHX	1	3411	7/7	0.99	0.19	93,93,93,93	0
84	OHX	1	3412	7/7	0.99	0.22	88,88,88,88	0
87	ZN	AK	101	1/1	0.99	0.13	38,38,38,38	0
84	OHX	1	3413	7/7	0.99	0.18	88,88,89,89	0
84	OHX	1	3451	7/7	0.99	0.10	101,101,102,103	0
84	OHX	1	3414	7/7	0.99	0.17	90,90,90,90	0
85	MG	1	4071	1/1	0.99	0.37	16,16,16,16	0
87	ZN	b	102	1/1	0.99	0.10	68,68,68,68	0
84	OHX	1	3499	7/7	0.99	0.10	124,125,126,126	0
87	ZN	e	102	1/1	0.99	0.06	74,74,74,74	0
84	OHX	1	3453	7/7	0.99	0.09	130,132,133,133	0
87	ZN	d6	102	1/1	0.99	0.10	59,59,59,59	0
84	OHX	1	3415	7/7	0.99	0.15	89,90,90,90	0
84	OHX	1	3502	7/7	0.99	0.10	100,101,102,102	0
85	MG	1	3924	1/1	0.99	0.54	8,8,8,8	0
85	MG	AR	4207	1/1	1.00	0.14	50,50,50,50	0
87	ZN	AN	500	1/1	1.00	0.11	43,43,43,43	0
85	MG	1	4156	1/1	1.00	0.13	65,65,65,65	0
84	OHX	AC	101	7/7	1.00	0.18	89,90,90,90	0
87	ZN	DL	103	1/1	1.00	0.12	37,37,37,37	0
87	ZN	DO	201	1/1	1.00	0.13	31,31,31,31	0
85	MG	AR	4110	1/1	1.00	0.11	45,45,45,45	0

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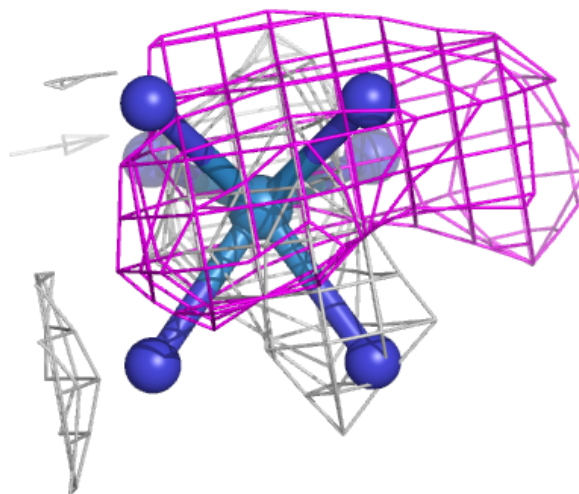
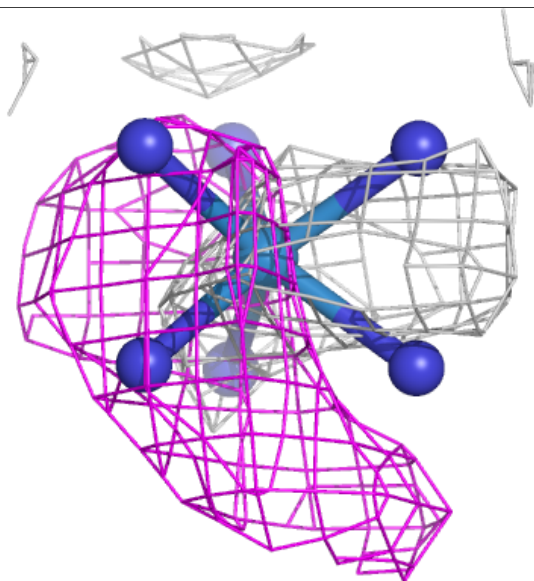
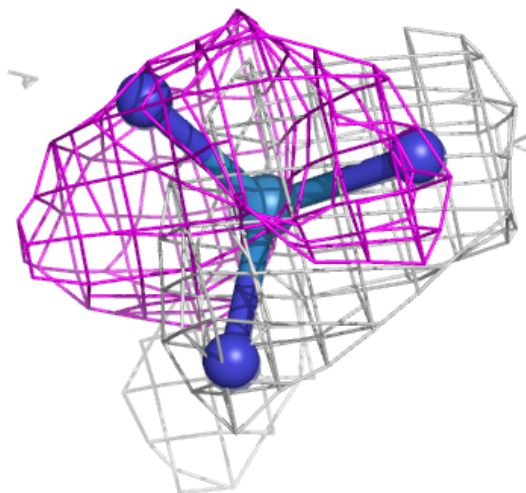
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
85	MG	1	4097	1/1	1.00	0.17	61,61,61,61	0
85	MG	1	4166	1/1	1.00	0.12	30,30,30,30	0
84	OHX	AT	202	7/7	1.00	0.20	86,86,87,87	0
84	OHX	6	1904	7/7	1.00	0.15	96,96,96,96	0
84	OHX	1	3401	7/7	1.00	0.26	89,89,90,90	0
85	MG	1	3850	1/1	1.00	0.12	29,29,29,29	0
85	MG	1	4187	1/1	1.00	0.10	55,55,55,55	0
85	MG	AR	3767	1/1	1.00	0.11	34,34,34,34	0
85	MG	s1	301	1/1	1.00	0.16	67,67,67,67	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

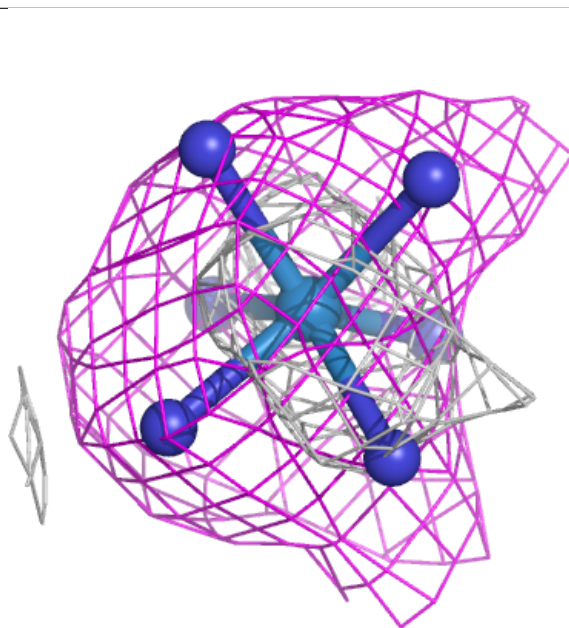
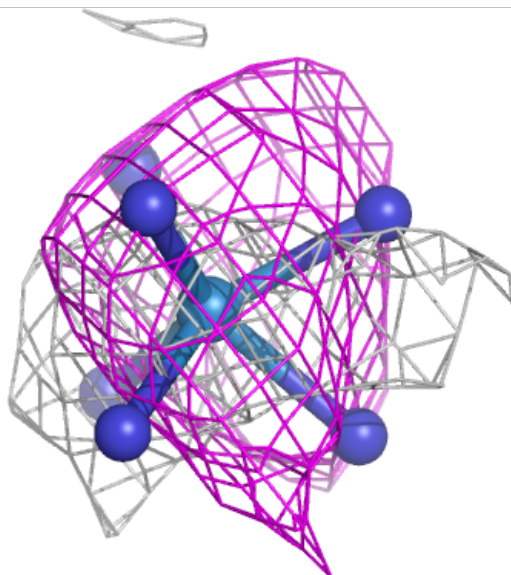
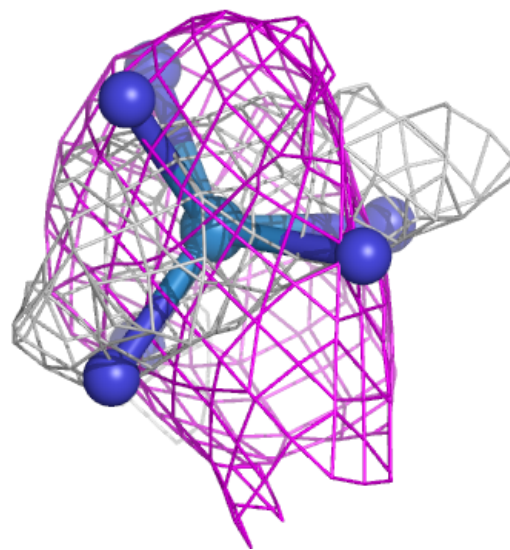
**Electron density around OHX 1 3722:**

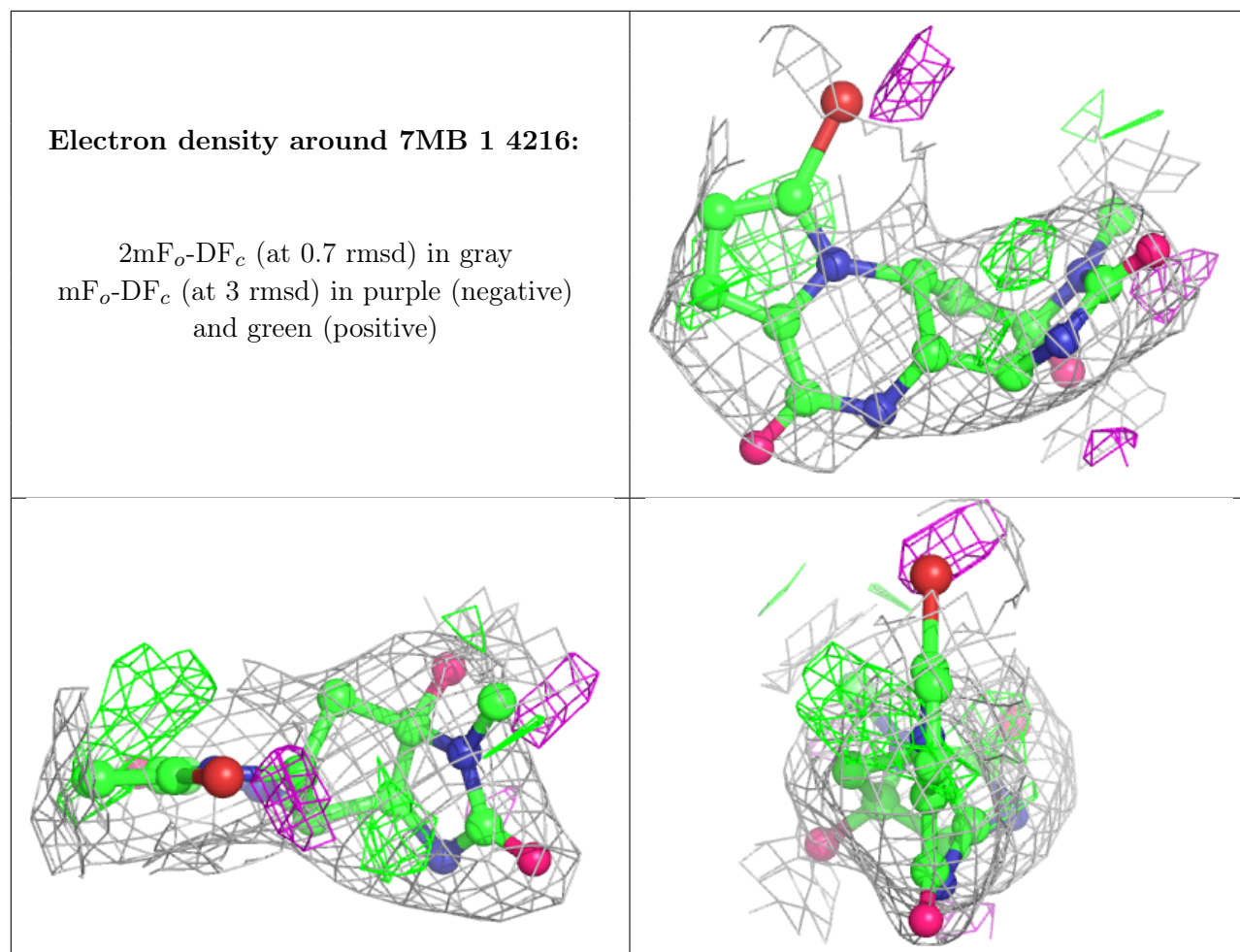
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around OHX 1 3675:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.