



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2023 – 11:46 PM EDT

PDB ID : 4V9J
Title : 70S ribosome translocation intermediate GDPNP-II containing elongation factor EFG/GDPNP, mRNA, and tRNA bound in the pe*/E state.
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-23
Resolution : 3.86 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

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>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

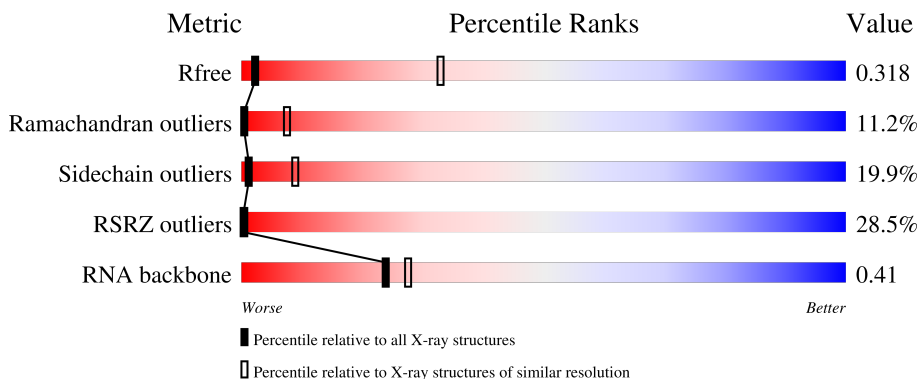
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.86 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	1048 (4.10-3.62)
Ramachandran outliers	138981	1069 (4.10-3.62)
Sidechain outliers	138945	1062 (4.10-3.62)
RSRZ outliers	127900	1206 (4.12-3.60)
RNA backbone	3102	1039 (4.70-3.00)

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 ≥ 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	AB	235	 24% 74% 23%
1	CB	235	 23% 75% 23%
2	AC	207	 26% 73% 26%
2	CC	207	 33% 71% 28%
3	AD	208	 61% 74% 25%

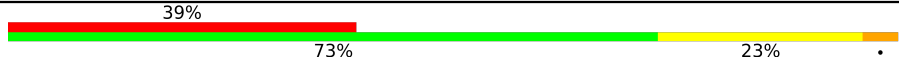

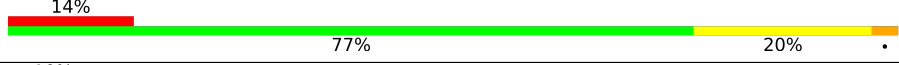


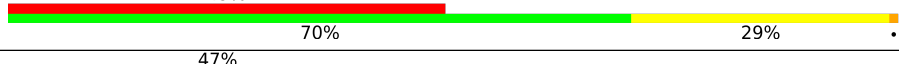

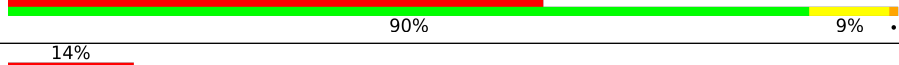
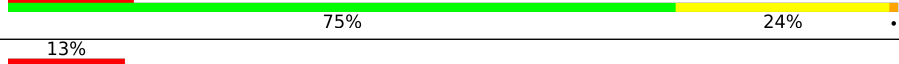


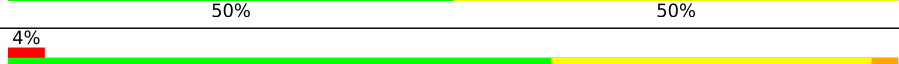
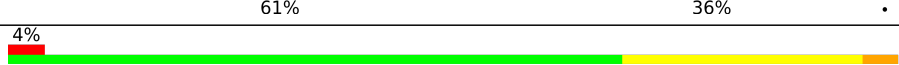
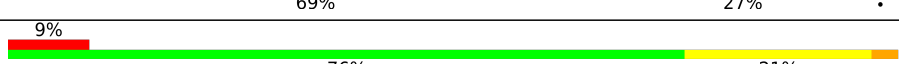

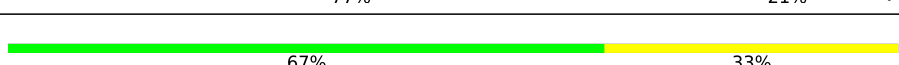
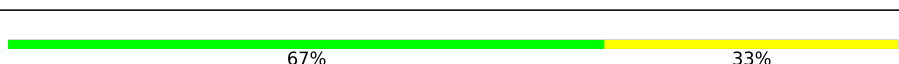




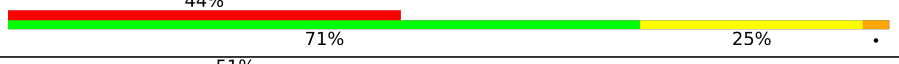
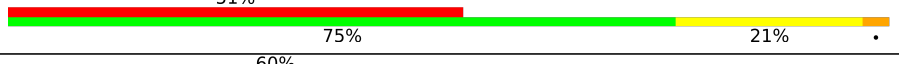


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Mol	Chain	Length	Quality of chain
3	CD	208	61% 80% 17% .
4	AE	151	34% 79% 20% .
4	CE	151	41% 80% 19% .
5	AF	101	% 80% 19% .
5	CF	101	% 78% 20% .
6	AG	155	29% 81% 19%
6	CG	155	17% 79% 20% .
7	AH	138	22% 70% 28% .
7	CH	138	25% 74% 25% .
8	AI	127	77% 77% 21% .
8	CI	127	78% 81% 17% .
9	AJ	99	39% 78% 21% .
9	CJ	99	49% 79% 21%
10	AK	119	13% 79% 19% .
10	CK	119	20% 82% 14% .
11	AL	125	31% 60% 38% ..
11	CL	125	42% 59% 35% 5% .
12	AM	125	30% 76% 21% .
12	CM	125	38% 75% 22% .
13	AN	60	73% 72% 28%
13	CN	60	70% 77% 23%
14	AO	88	22% 75% 24% .
14	CO	88	30% 75% 24% .
15	AP	84	75% 73% 27%
15	CP	84	79% 83% 15% .

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Mol	Chain	Length	Quality of chain
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AA	1511	
20	CA	1511	
21	AV	18	
21	CV	18	
22	AW	77	
22	CW	77	
23	AY	687	
23	CY	687	
24	AU	6	
24	CU	6	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	
27	DE	205	
28	BF	208	

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Mol	Chain	Length	Quality of chain
28	DF	208	53% 69% 28%
29	BG	181	49% 71% 25%
29	DG	181	40% 74% 23%
30	BH	167	18% 76% 23%
30	DH	167	18% 78% 21%
31	BJ	170	99%
31	DJ	170	99%
32	BK	140	20% 84% 16%
32	DK	140	33% 80% 19%
33	BO	122	33% 80% 19%
33	DO	122	41% 80% 20%
34	BP	146	51% 67% 29%
34	DP	146	50% 73% 25%
35	BQ	141	43% 70% 28%
35	DQ	141	42% 74% 24%
36	BR	117	64% 68% 28%
36	DR	117	50% 76% 22%
37	BS	99	79% 63% 28% 9%
37	DS	99	77% 67% 25% 8%
38	BT	138	28% 74% 23%
38	DT	138	33% 75% 21%
39	BU	117	58% 82% 18%
39	DU	117	58% 77% 22%
40	BV	101	30% 63% 35%
40	DV	101	44% 64% 35%

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Mol	Chain	Length	Quality of chain
41	BW	113	62% 79% 17%
41	DW	113	66% 74% 24%
42	BX	93	66% 74% 26%
42	DX	93	59% 78% 20%
43	BY	107	74% 64% 33%
43	DY	107	81% 68% 29%
44	BZ	185	26% 74% 26%
44	DZ	185	22% 72% 27%
45	B0	84	74% 77% 23%
45	D0	84	75% 80% 20%
46	B1	93	58% 65% 32%
46	D1	93	68% 56% 38%
47	B4	35	26% 69% 31%
47	D4	35	17% 74% 20% 6%
48	BN	138	43% 78% 21%
48	DN	138	44% 78% 21%
49	B2	71	24% 79% 21%
49	D2	71	20% 83% 17%
50	B3	60	47% 83% 17%
50	D3	60	53% 83% 17%
51	B5	59	49% 75% 19% 7%
51	D5	59	58% 76% 20%
52	B6	50	46% 60% 32% 8%
52	D6	50	62% 62% 30% 8%
53	B7	49	73% 86% 14%

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Mol	Chain	Length	Quality of chain
53	D7	49	73% 84% 12% .
54	B8	64	81% 66% 30% 5%
54	D8	64	78% 70% 25% 5%
55	B9	37	100% 73% 27%
55	D9	37	97% 76% 24%
56	Be	103	6% 87% 10% ..
56	De	103	9% 85% 13% ..
57	Bf	31	100%
57	Bg	31	100%
57	Df	31	100%
57	Dg	31	100%
58	Bh	30	100%
58	Dh	30	100%
59	BB	119	4% 74% 25% .
59	DB	119	8% 80% 20%
60	BA	2879	10% 72% 26% .
60	DA	2879	10% 74% 25% .

2 Entry composition [i](#)

There are 62 unique types of molecules in this entry. The entry contains 308202 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 protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AB	235	Total 1910	C 1218	N 342	O 345	S 5	0	0	0
1	CB	235	Total 1910	C 1218	N 342	O 345	S 5	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AC	207	Total 1621	C 1022	N 315	O 283	S 1	0	0	0
2	CC	207	Total 1621	C 1022	N 315	O 283	S 1	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0
3	CD	208	Total 1703	C 1066	N 339	O 291	S 7	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AE	151	Total 1156	C 729	N 218	O 205	S 4	0	0	0
4	CE	151	Total 1156	C 729	N 218	O 205	S 4	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
5	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
6	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
7	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
8	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			
9	CJ	99	Total	C	N	O	S	0	0	0
			802	504	157	140	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			
11	CL	125	Total	C	N	O	S	0	0	0
			976	614	196	165	1			

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			
12	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
13	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
14	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			
15	CP	84	Total	C	N	O	S	0	0	0
			706	446	140	119	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			
16	CQ	100	Total	C	N	O	S	0	0	0
			835	534	156	143	2			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
17	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			
18	CS	79	Total	C	N	O	S	0	0	0
			634	405	115	112	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			
19	CT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 20 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
20	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 21 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			
21	CV	18	Total	C	N	O	P	0	0	0
			393	177	81	118	17			

- Molecule 22 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			
22	CW	77	Total	C	N	O	P	0	0	0
			1635	732	291	536	76			

- Molecule 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			
23	CY	687	Total	C	N	O	S	0	0	0
			5380	3414	922	1024	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	129	LYS	HIS	conflict	UNP Q72I01
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 24 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	AU	6	Total	C	N	O	0	0	0
			48	25	13	10			
24	CU	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	DC	228	1742	1101	319	319	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	20	VAL	ILE	conflict	UNP Q72GV9
BC	28	ARG	HIS	conflict	UNP Q72GV9
DC	20	VAL	ILE	conflict	UNP Q72GV9
DC	28	ARG	HIS	conflict	UNP Q72GV9

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	BD	275	2145	1353	428	361	3	0	0	0
26	DD	275	2145	1353	428	361	3	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BE	205	1569	991	300	272	6	0	0	0
27	DE	205	1569	991	300	272	6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BF	208	1628	1037	304	284	3	0	0	0
28	DF	208	1628	1037	304	284	3	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BF	2	LYS	-	insertion	UNP Q72I05
BF	3	GLU	-	insertion	UNP Q72I05
BF	4	VAL	-	insertion	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
BF	5	ALA	-	insertion	UNP Q72I05
BF	6	VAL	-	insertion	UNP Q72I05
DF	2	LYS	-	insertion	UNP Q72I05
DF	3	GLU	-	insertion	UNP Q72I05
DF	4	VAL	-	insertion	UNP Q72I05
DF	5	ALA	-	insertion	UNP Q72I05
DF	6	VAL	-	insertion	UNP Q72I05

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BG	181	1474	942	268	260	4	0	0	0
29	DG	181	1474	942	268	260	4	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BG	5	VAL	LEU	conflict	UNP Q72I16
DG	5	VAL	LEU	conflict	UNP Q72I16

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BH	167	1274	806	238	229	1	0	0	0
30	DH	167	1274	806	238	229	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
31	BJ	170	851	510	170	171	0	0	0
31	DJ	170	851	510	170	171	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			
32	DK	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 33 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
33	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BO	69	ILE	VAL	conflict	UNP Q72I14
DO	69	ILE	VAL	conflict	UNP Q72I14

- Molecule 34 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
34	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 35 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
35	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	conflict	UNP Q72I11
DQ	32	TYR	PHE	conflict	UNP Q72I11

- Molecule 36 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
36	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
37	BS	99	Total	C	N	O	0	0	0
			775	488	155	132			
37	DS	99	Total	C	N	O	0	0	0
			775	488	155	132			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			
38	DT	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	123	GLN	LYS	conflict	UNP Q72JU9
BT	135	ALA	VAL	conflict	UNP Q72JU9
DT	123	GLN	LYS	conflict	UNP Q72JU9
DT	135	ALA	VAL	conflict	UNP Q72JU9

- Molecule 39 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			
39	DU	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 40 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	DV	101	Total 779	C 501	N 142	O 135	S 1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0
41	DW	113	Total 900	C 566	N 177	O 155	S 2	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
42	BX	93	Total 734	C 477	N 132	O 125	0	0	0
42	DX	93	Total 734	C 477	N 132	O 125	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	BY	107	Total 818	C 524	N 155	O 134	S 5	0	0	0
43	DY	107	Total 818	C 524	N 155	O 134	S 5	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BZ	185	Total 1473	C 939	N 262	O 270	S 2	0	0	0
44	DZ	185	Total 1473	C 939	N 262	O 270	S 2	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	B0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0
45	D0	84	Total 662	C 410	N 140	O 111	S 1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B0	11	ARG	LYS	conflict	UNP Q72HR3
D0	11	ARG	LYS	conflict	UNP Q72HR3

- Molecule 46 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			
46	D1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	LYS	ARG	conflict	UNP Q72G84
D1	81	LYS	ARG	conflict	UNP Q72G84

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			
47	D4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 48 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			
48	DN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
49	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B3	60	477	303	91	82	1	0	0	0
50	D3	60	477	303	91	82	1	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	B5	59	459	288	90	76	5	0	0	0
51	D5	59	459	288	90	76	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B5	29	THR	ILE	conflict	UNP P62652
D5	29	THR	ILE	conflict	UNP P62652

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B6	50	433	270	88	71	4	0	0	0
52	D6	50	433	270	88	71	4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	B7	49	430	263	108	57	2	0	0	0
53	D7	49	430	263	108	57	2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	B8	64	517	331	102	82	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	D8	64	517	331	102	82	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B9	37	307	188	68	47	4	0	0	0
55	D9	37	307	188	68	47	4	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	Be	102	686	430	119	137	0	0	0
56	De	102	686	430	119	137	0	0	0

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	Bf	31	156	93	31	32	0	0	0
57	Bg	31	156	93	31	32	0	0	0
57	Df	31	156	93	31	32	0	0	0
57	Dg	31	156	93	31	32	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	Bh	30	151	90	30	31	0	0	0
58	Dh	30	151	90	30	31	0	0	0

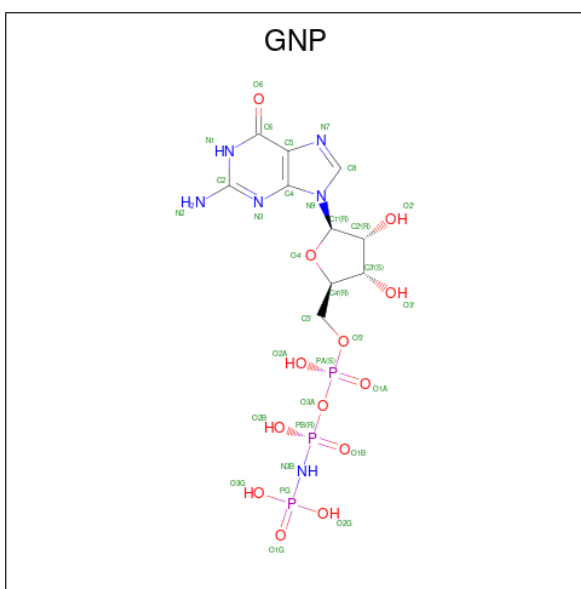
- Molecule 59 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
59	BB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0
59	DB	119	Total 2551	C 1136	N 471	O 826	P 118	0	0	0

- Molecule 60 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
60	BA	2879	Total 61997	C 27594	N 11582	O 19943	P 2878	0	0	0
60	DA	2879	Total 61997	C 27594	N 11582	O 19943	P 2878	0	0	0

- Molecule 61 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
61	AY	1	Total 32	C 10	N 6	O 13	P 3	0	0
61	CY	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
62	AY	1	Total 1	Mg 1	0	0

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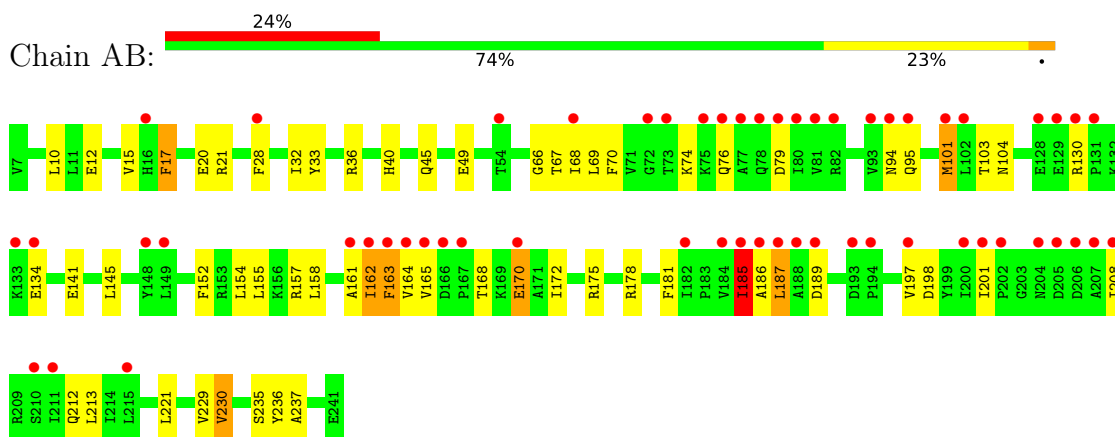
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
62	CY	1	Total	Mg	0	0
			1	1		

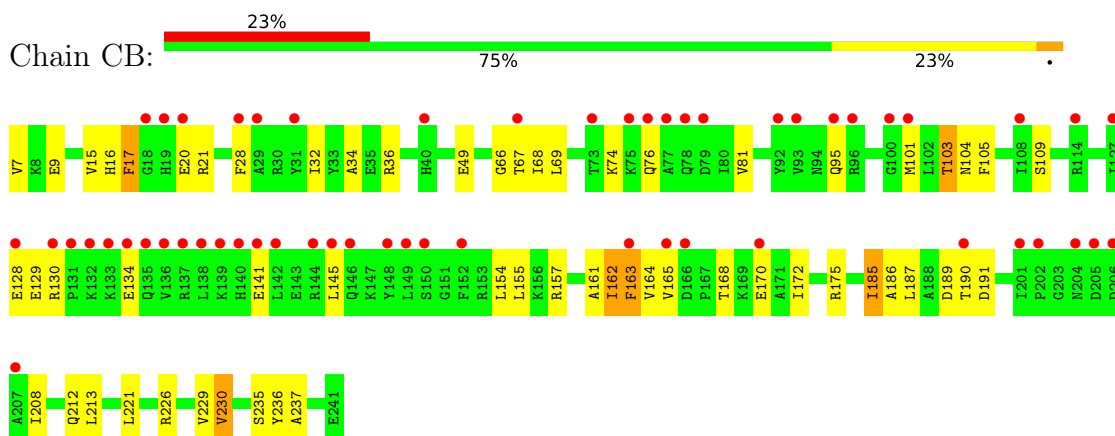
3 Residue-property plots [i](#)

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.

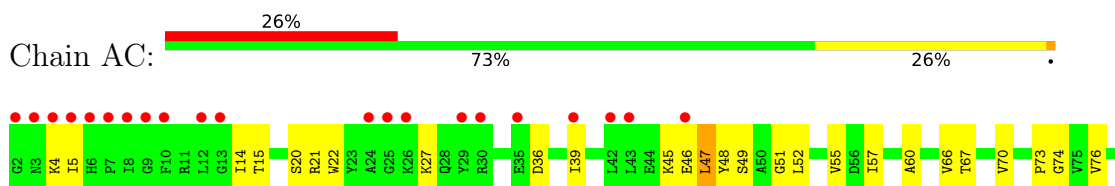
- Molecule 1: 30S ribosomal protein S2

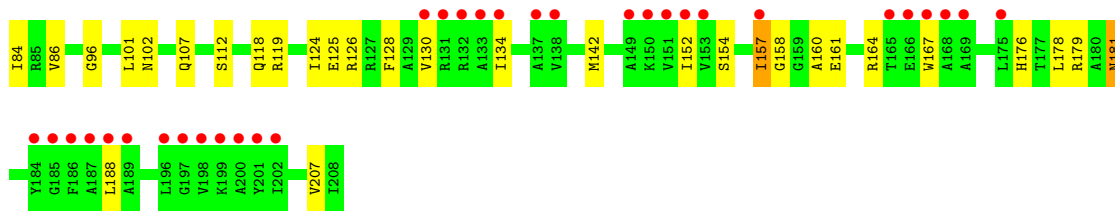


- Molecule 1: 30S ribosomal protein S2

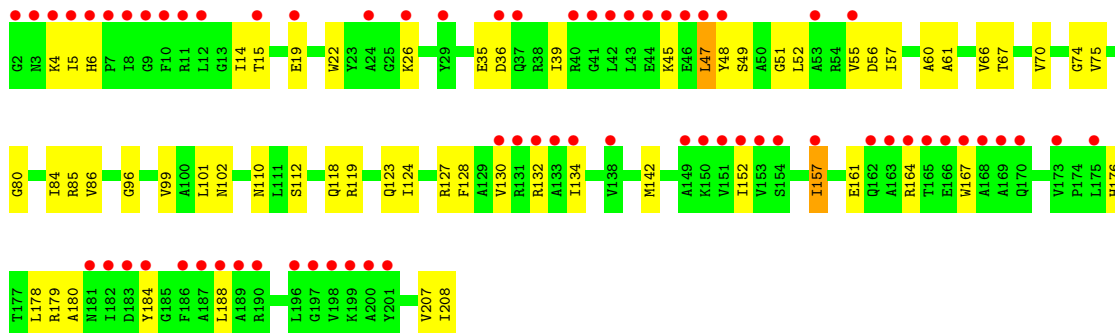
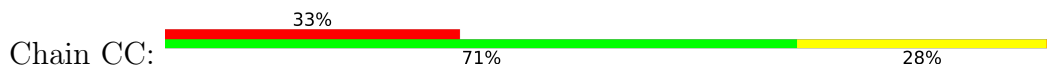


- Molecule 2: 30S ribosomal protein S3

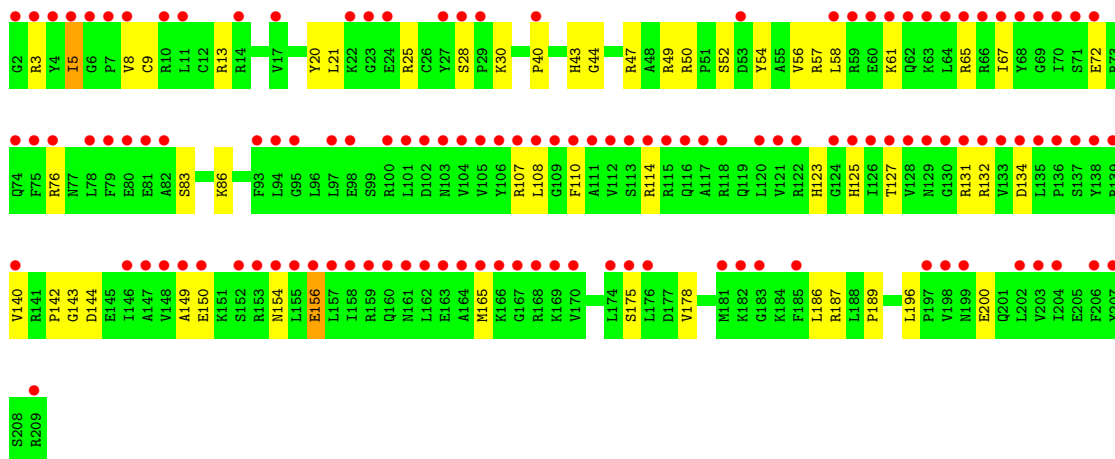
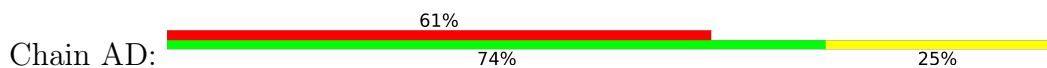




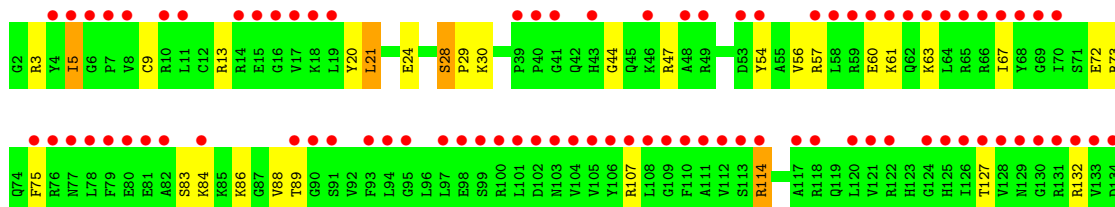
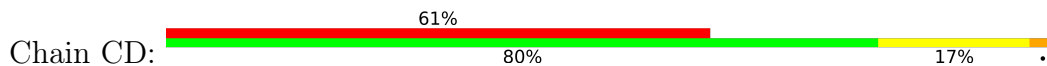
- Molecule 2: 30S ribosomal protein S3

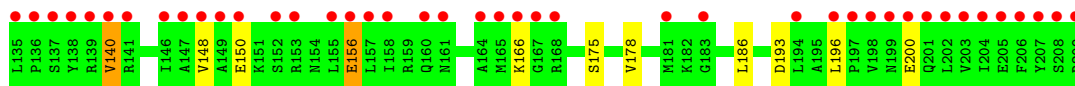


- Molecule 3: 30S ribosomal protein S4

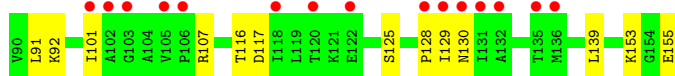
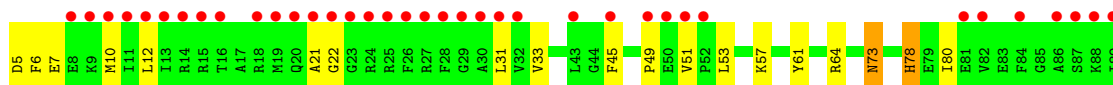
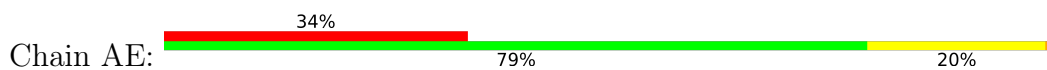


- Molecule 3: 30S ribosomal protein S4

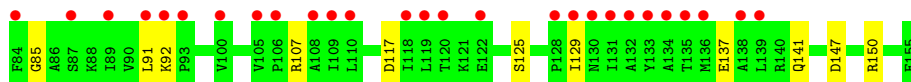
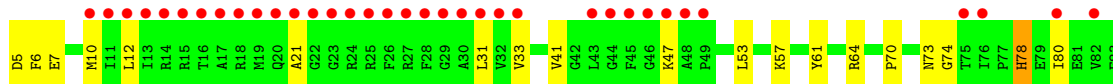
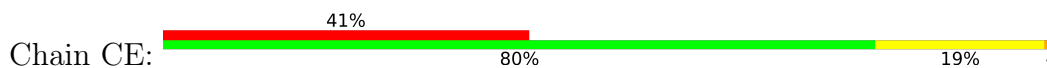




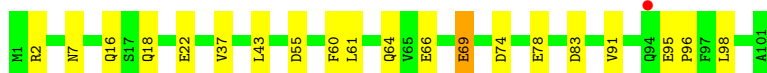
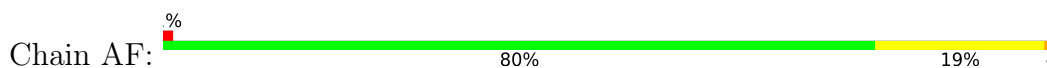
- Molecule 4: 30S ribosomal protein S5



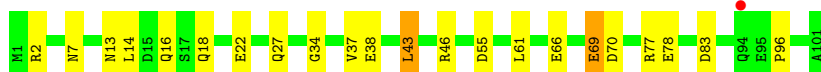
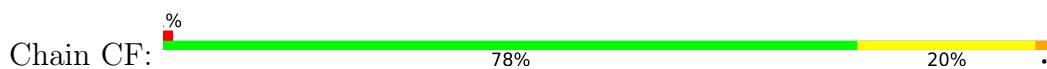
- Molecule 4: 30S ribosomal protein S5



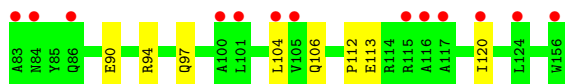
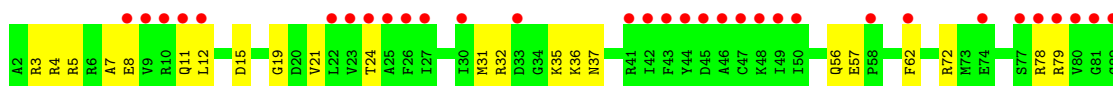
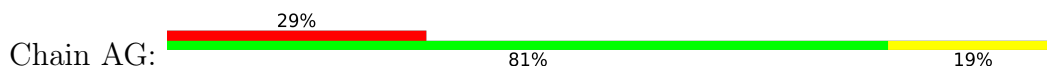
- Molecule 5: 30S ribosomal protein S6



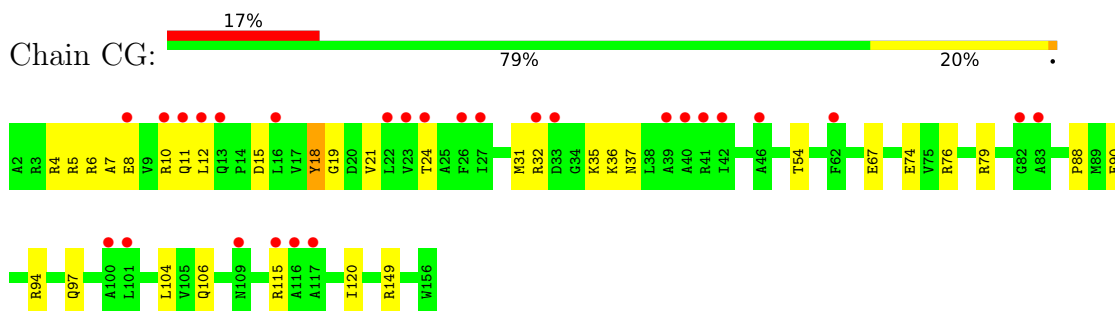
- Molecule 5: 30S ribosomal protein S6



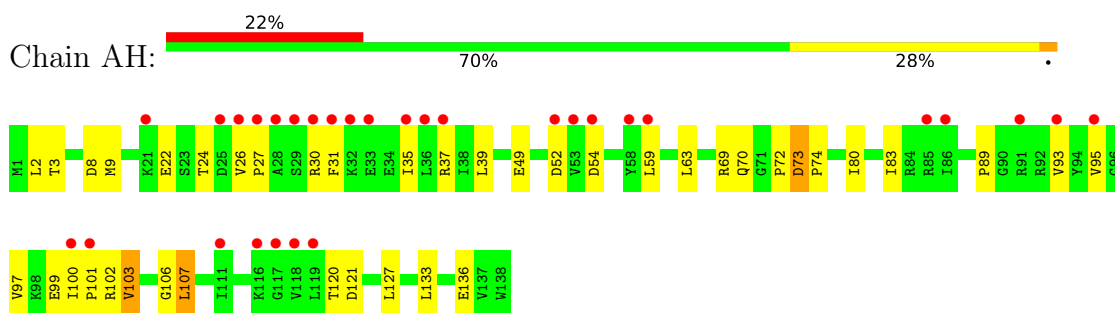
- Molecule 6: 30S ribosomal protein S7



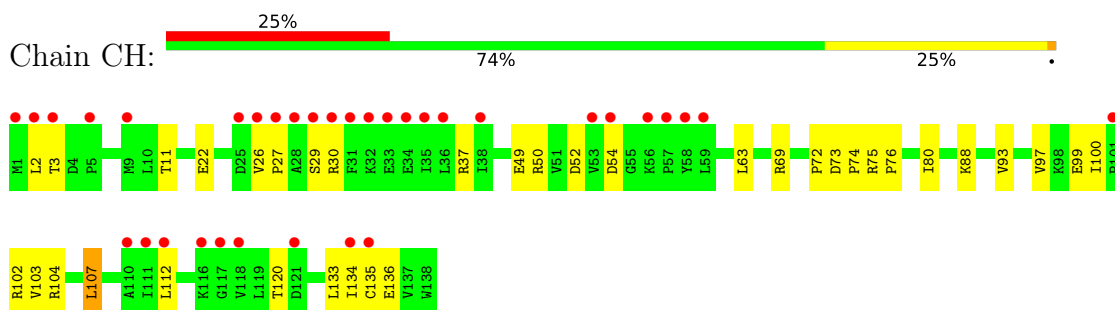
- Molecule 6: 30S ribosomal protein S7



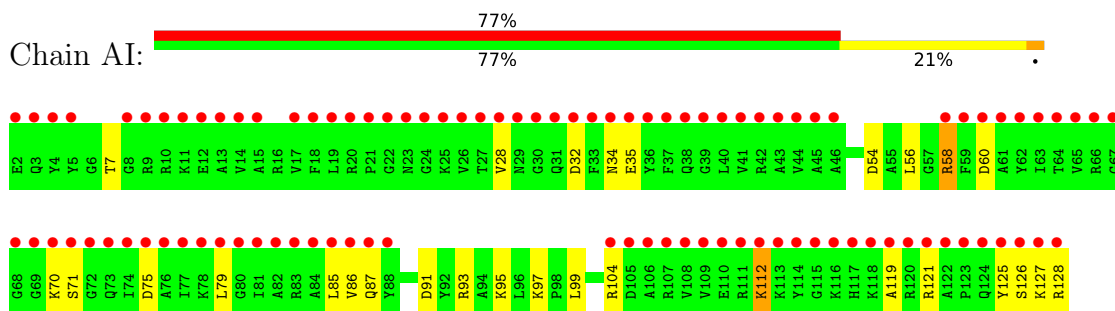
- Molecule 7: 30S ribosomal protein S8



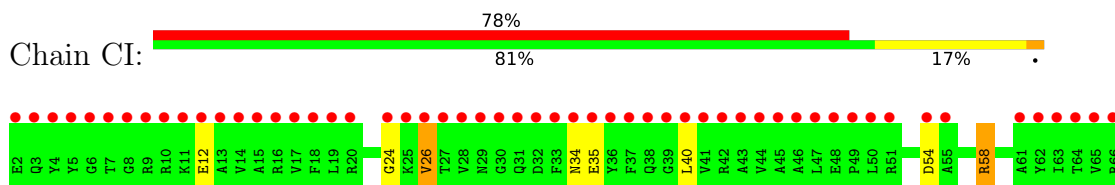
- Molecule 7: 30S ribosomal protein S8

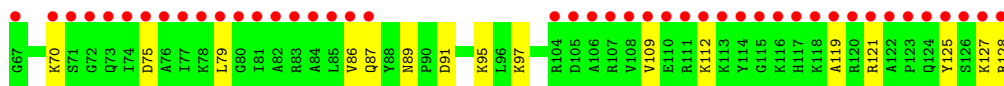


- Molecule 8: 30S ribosomal protein S9

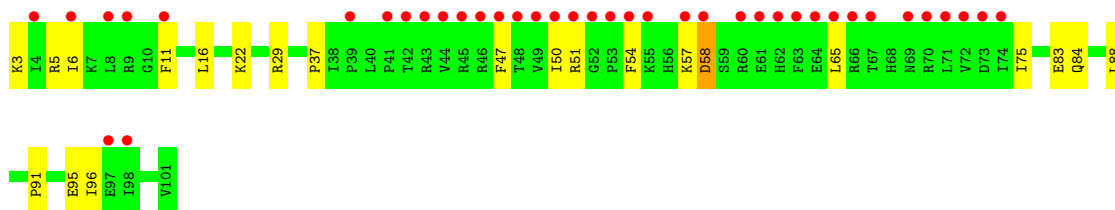
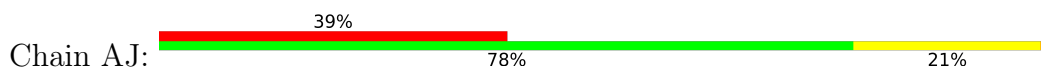


- Molecule 8: 30S ribosomal protein S9

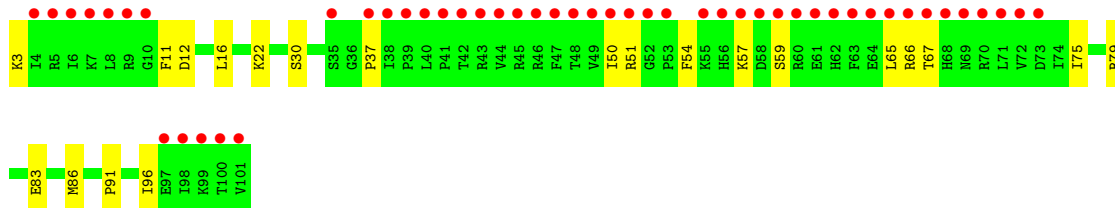
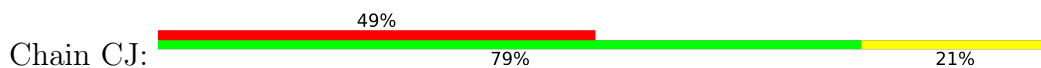




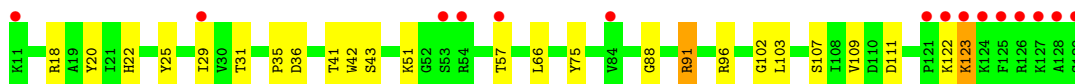
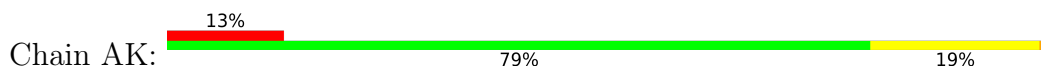
- Molecule 9: 30S ribosomal protein S10



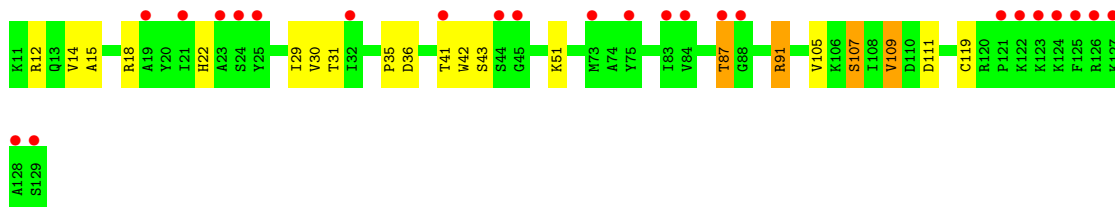
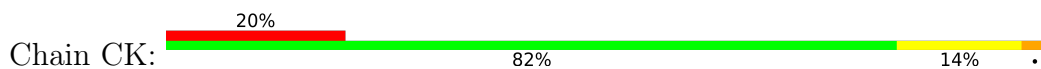
- Molecule 9: 30S ribosomal protein S10



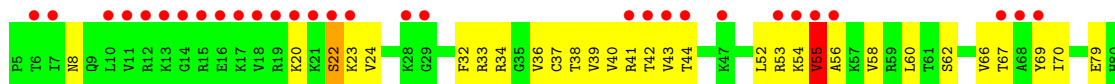
- Molecule 10: 30S ribosomal protein S11

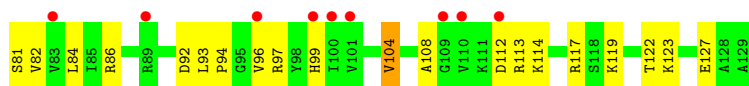


- Molecule 10: 30S ribosomal protein S11

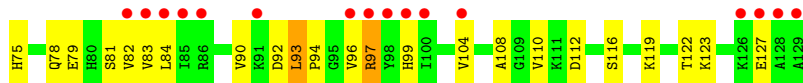
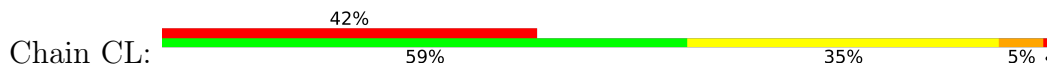


- Molecule 11: 30S ribosomal protein S12

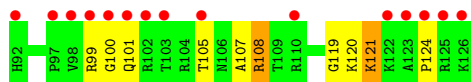
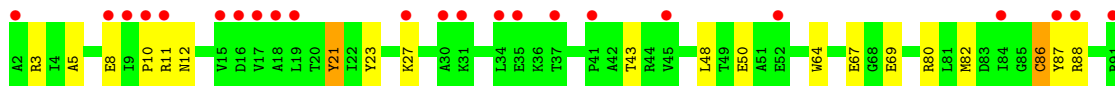
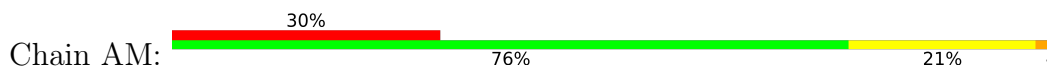




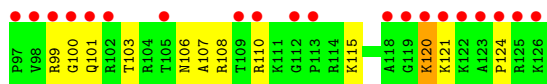
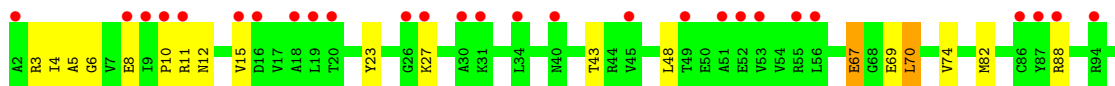
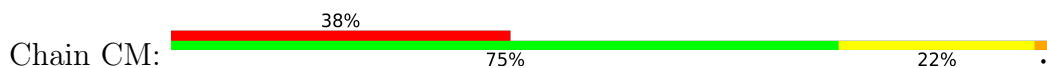
- Molecule 11: 30S ribosomal protein S12



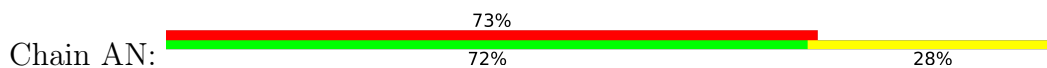
- Molecule 12: 30S ribosomal protein S13



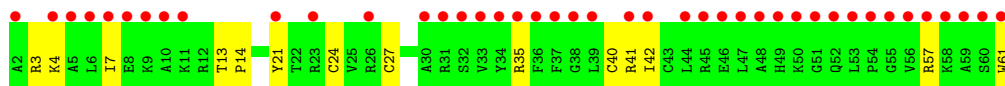
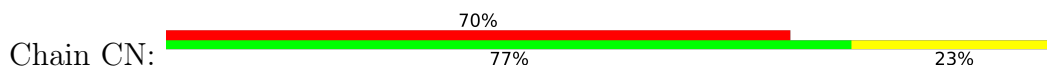
- Molecule 12: 30S ribosomal protein S13



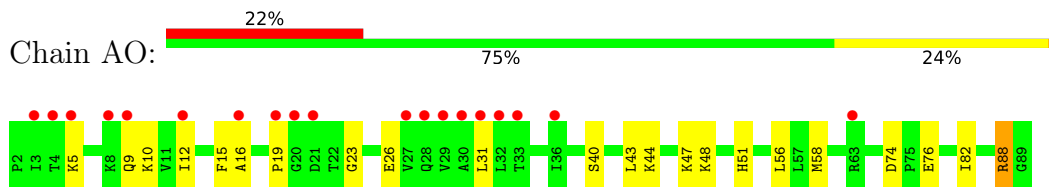
- Molecule 13: 30S ribosomal protein S14 type Z



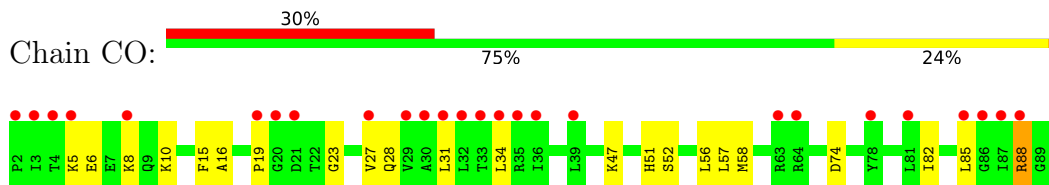
- Molecule 13: 30S ribosomal protein S14 type Z



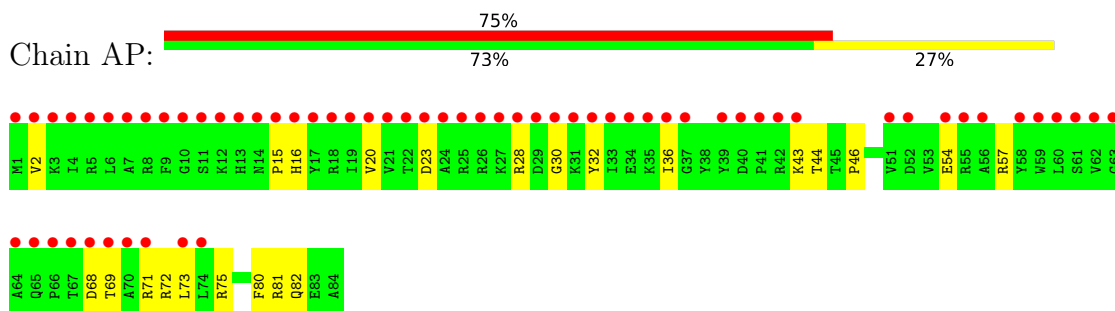
- Molecule 14: 30S ribosomal protein S15



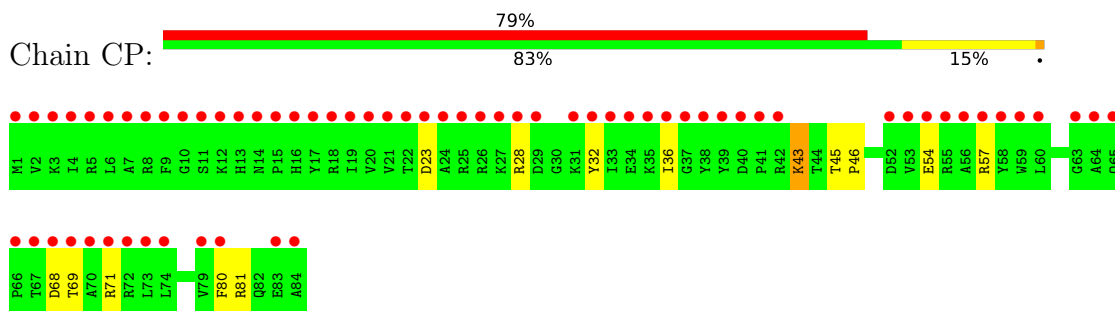
- Molecule 14: 30S ribosomal protein S15



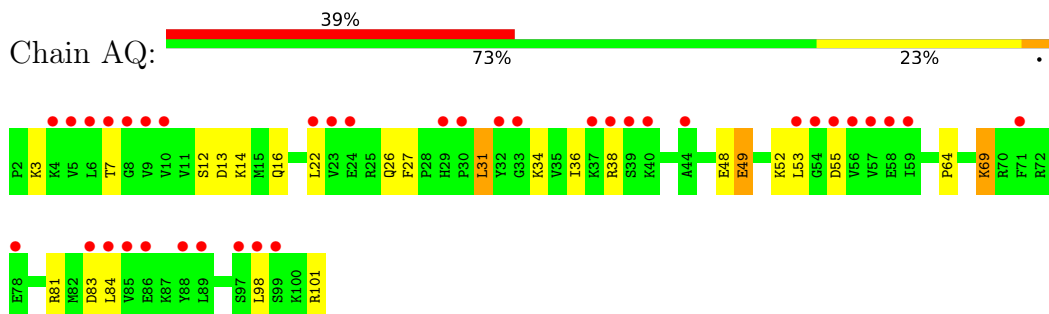
- Molecule 15: 30S ribosomal protein S16



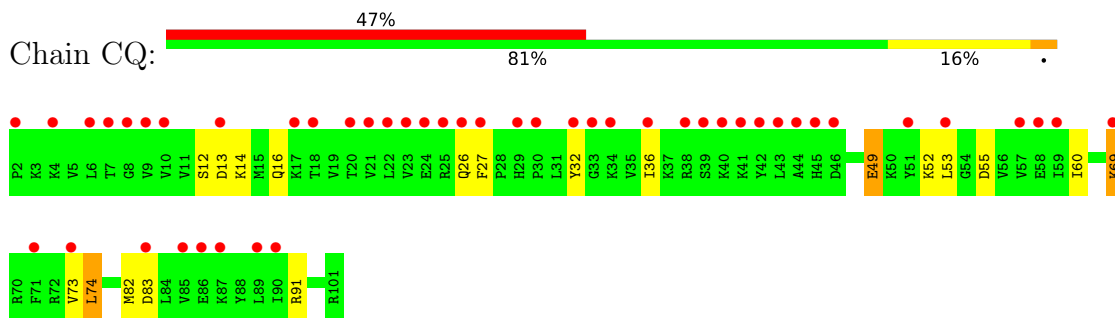
- Molecule 15: 30S ribosomal protein S16



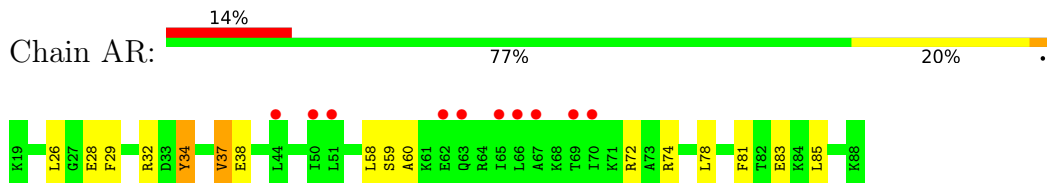
- Molecule 16: 30S ribosomal protein S17



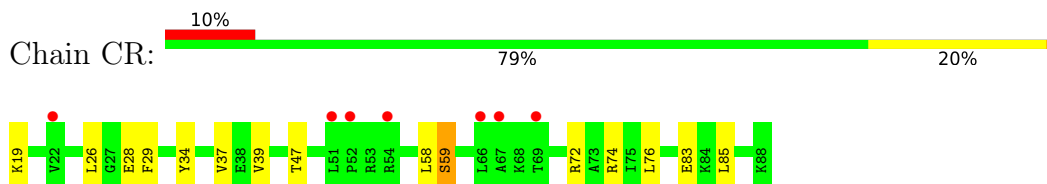
- Molecule 16: 30S ribosomal protein S17



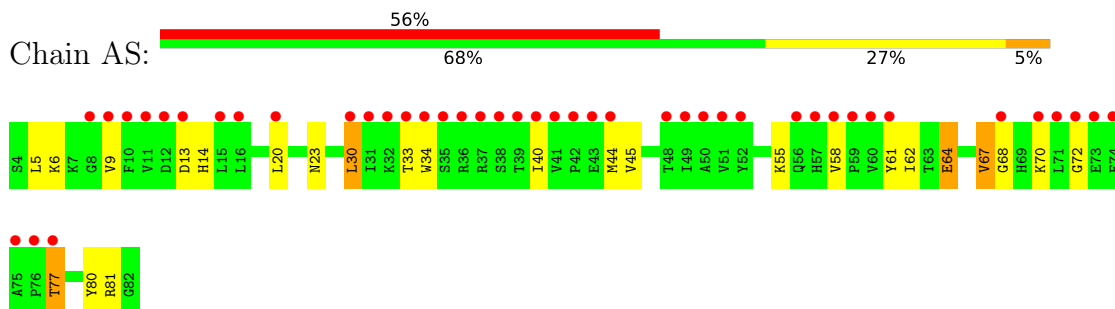
- Molecule 17: 30S ribosomal protein S18



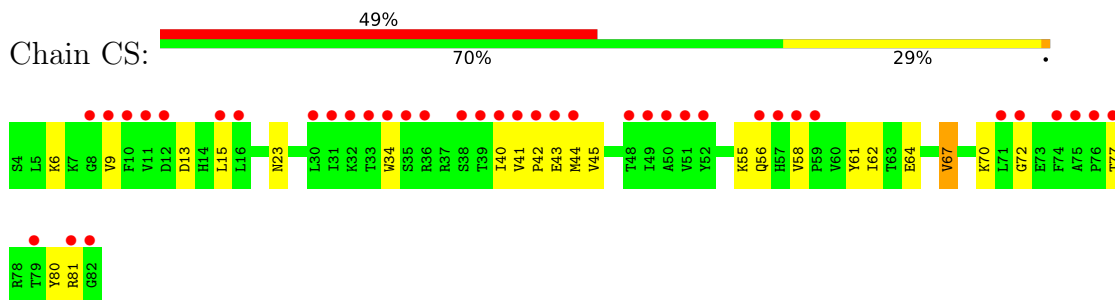
- Molecule 17: 30S ribosomal protein S18



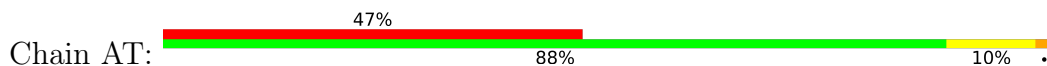
- Molecule 18: 30S ribosomal protein S19

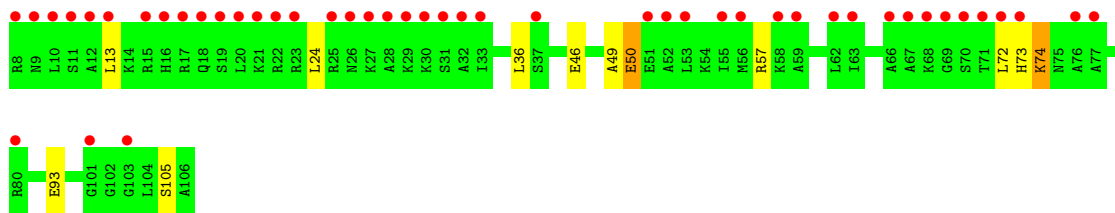


- Molecule 18: 30S ribosomal protein S19

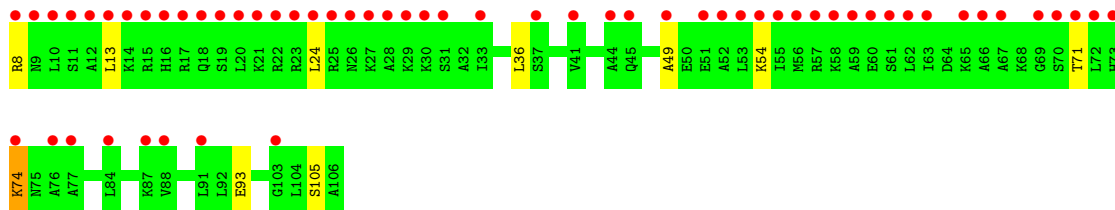


- Molecule 19: 30S ribosomal protein S20

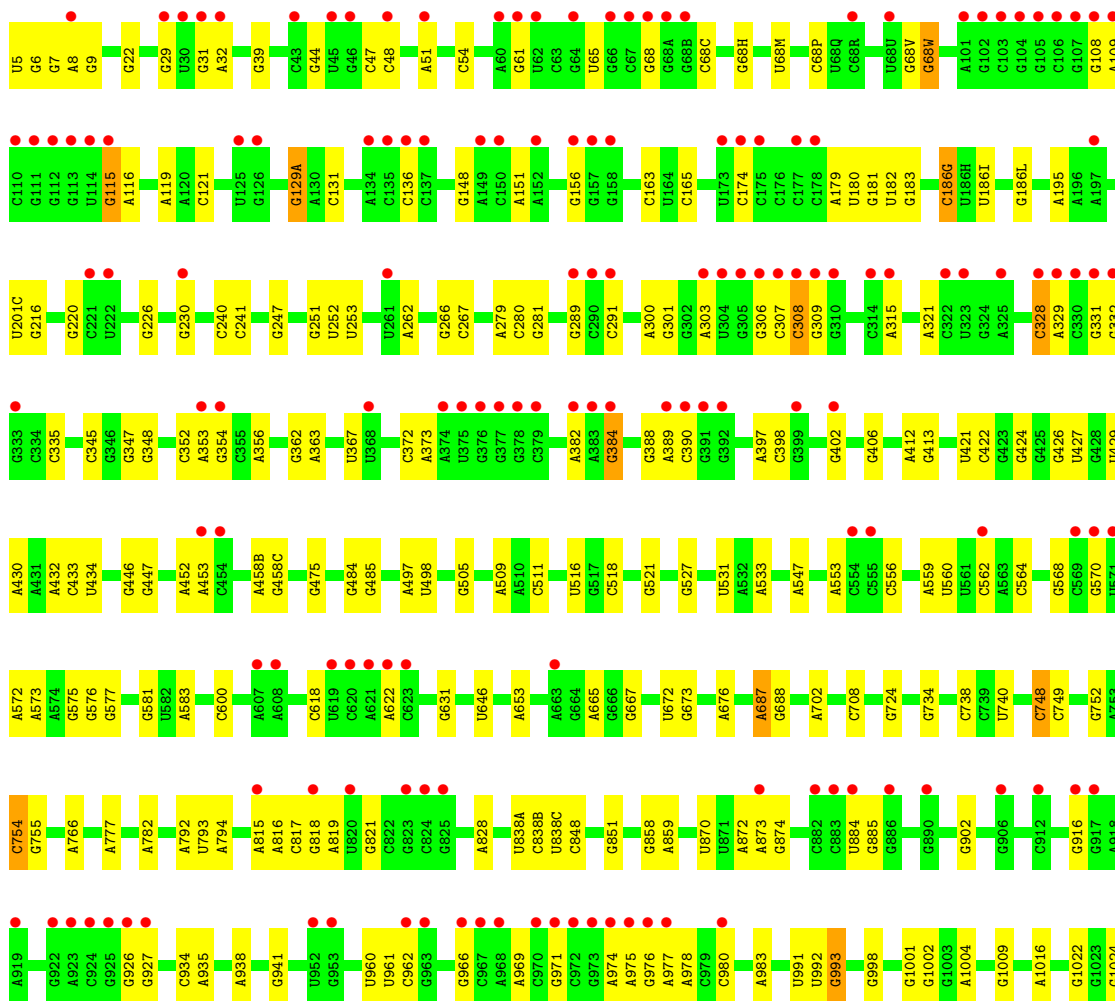
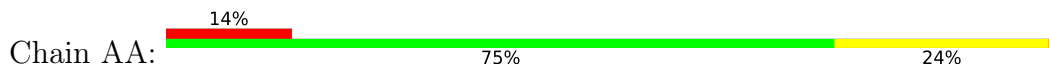


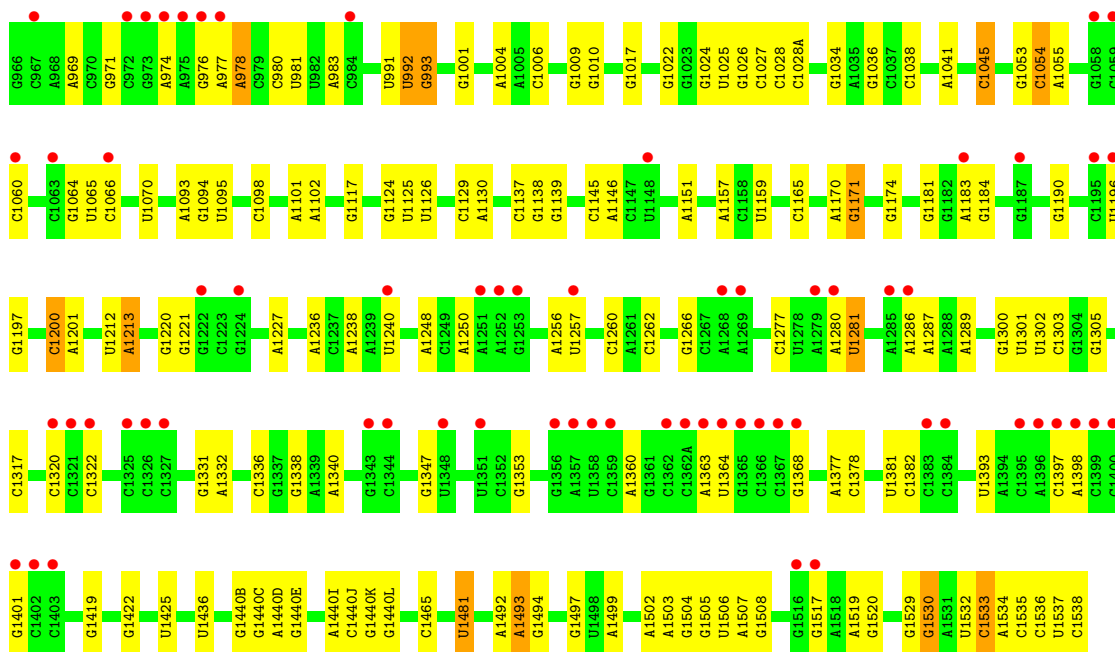


• Molecule 19: 30S ribosomal protein S20

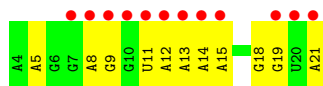


• Molecule 20: 16S ribosomal RNA

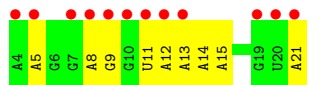




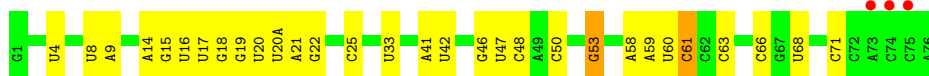
• Molecule 21: messenger RNA



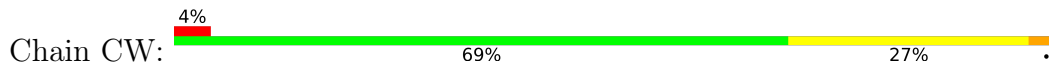
• Molecule 21: messenger RNA



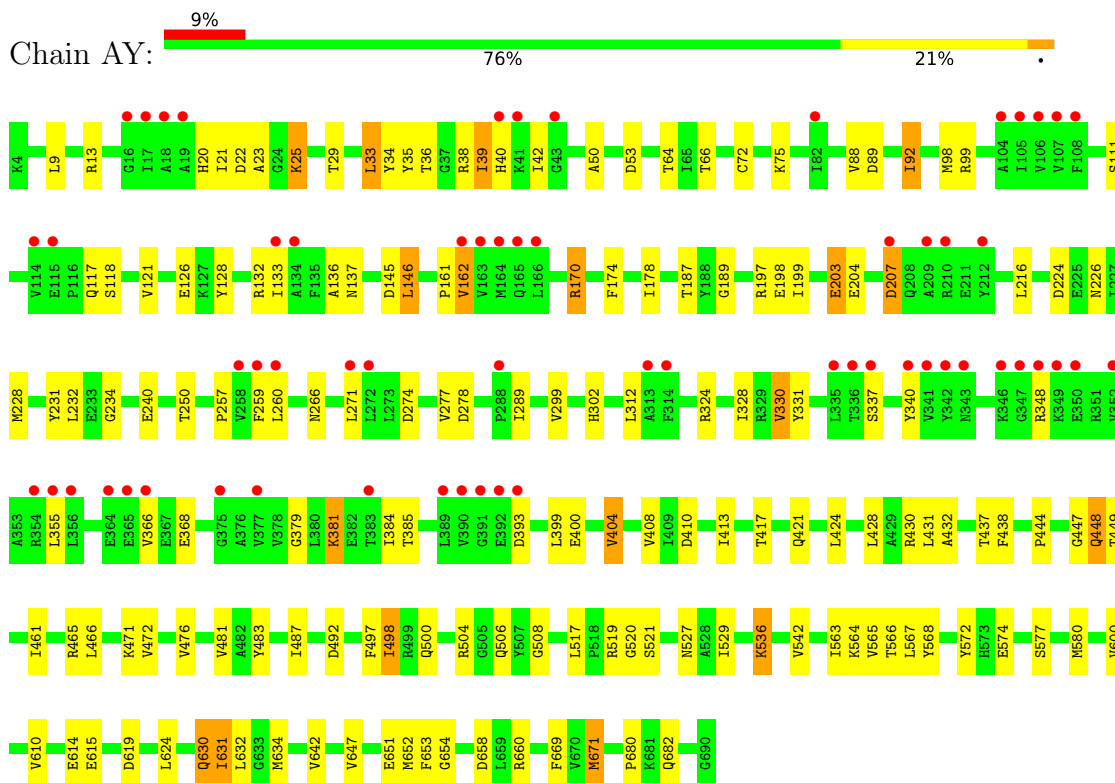
• Molecule 22: tRNA-Met



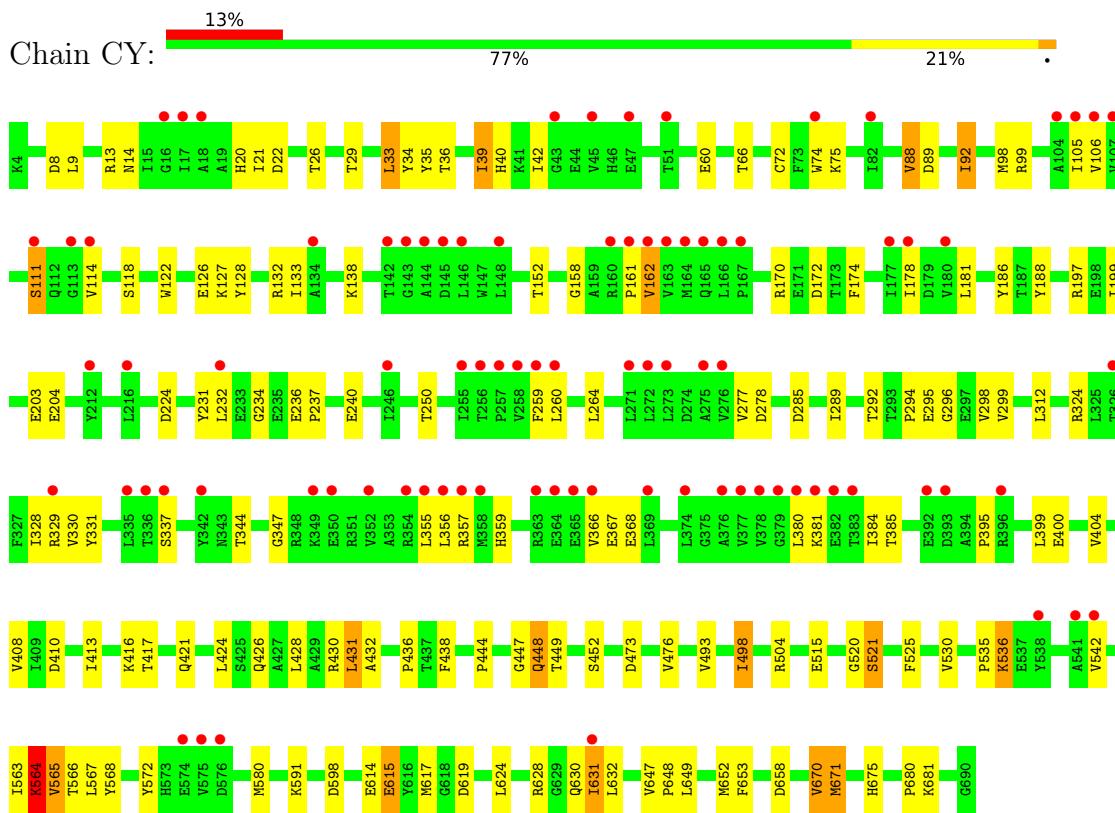
• Molecule 22: tRNA-Met



• Molecule 23: Elongation factor G



• Molecule 23: Elongation factor G



• Molecule 24: Viomycin

Chain AU:  67% 33%



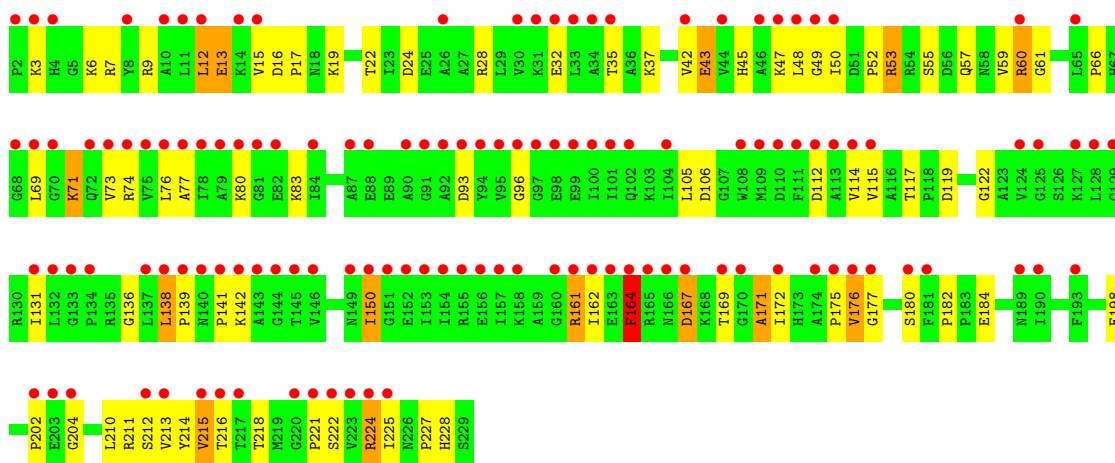
- Molecule 24: Viomycin

Chain CU:  67% 33%



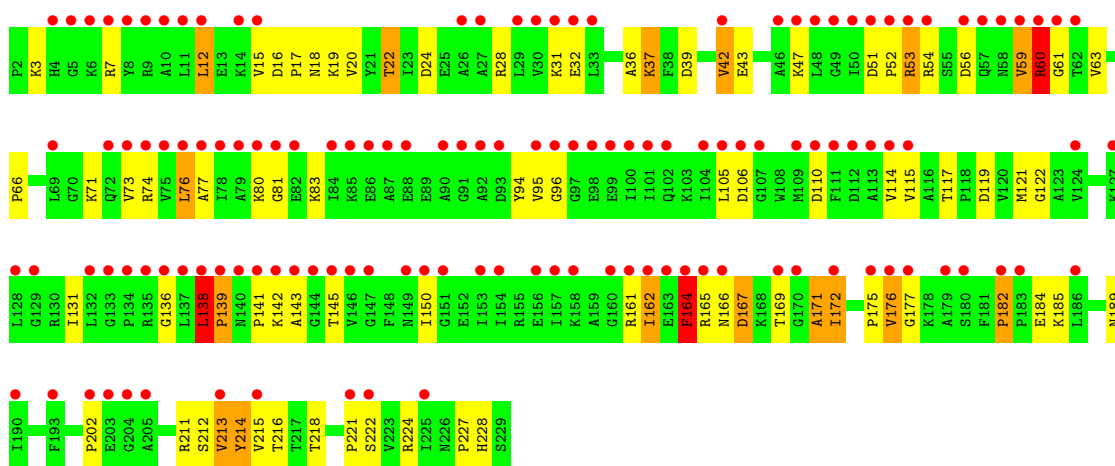
- Molecule 25: 50S ribosomal protein L1

Chain BC:  56% 62% 31% 6%

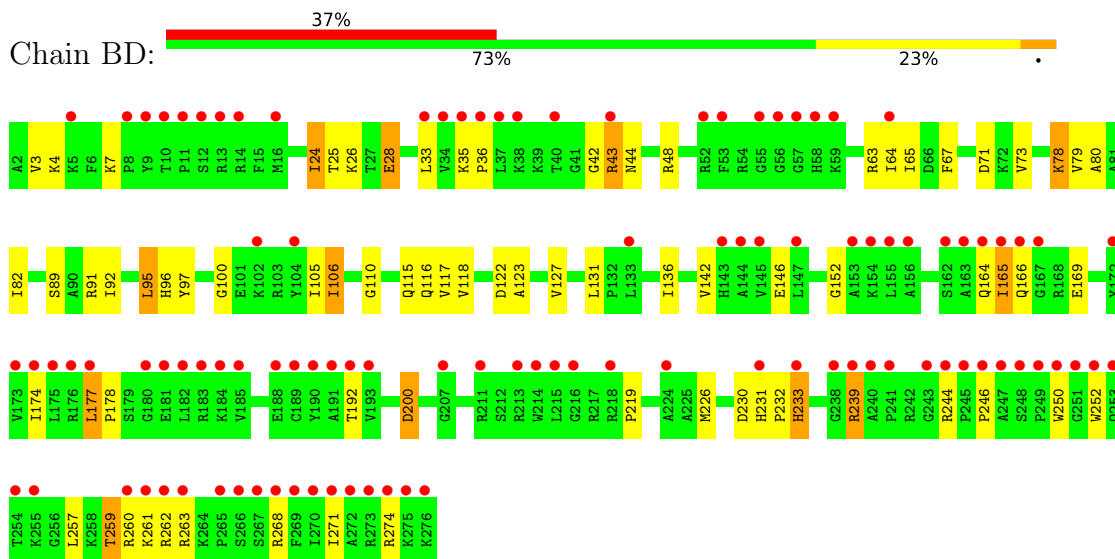


- Molecule 25: 50S ribosomal protein L1

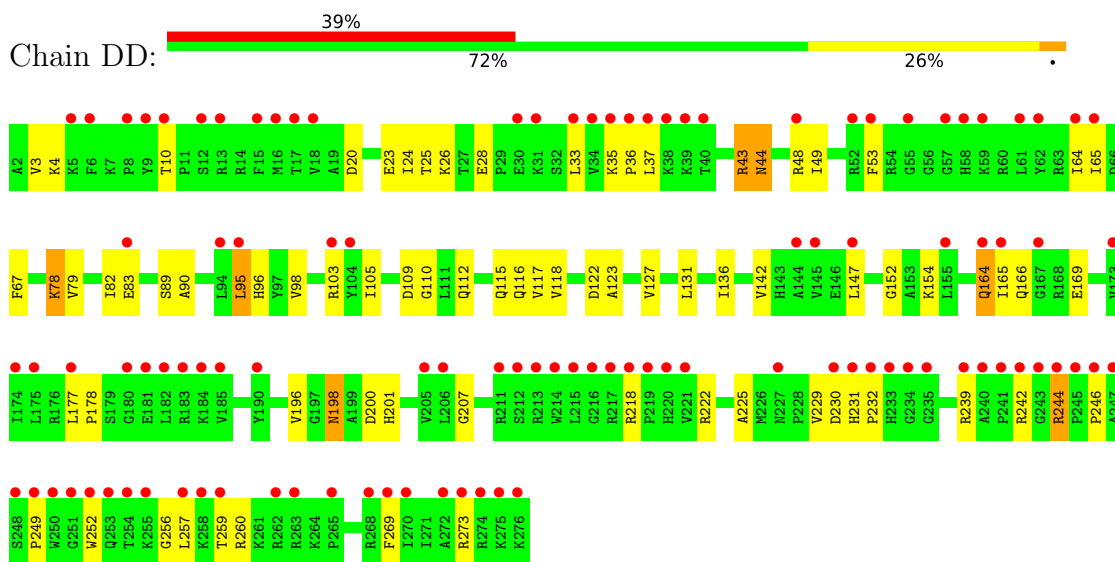
Chain DC:  58% 61% 30% 7%



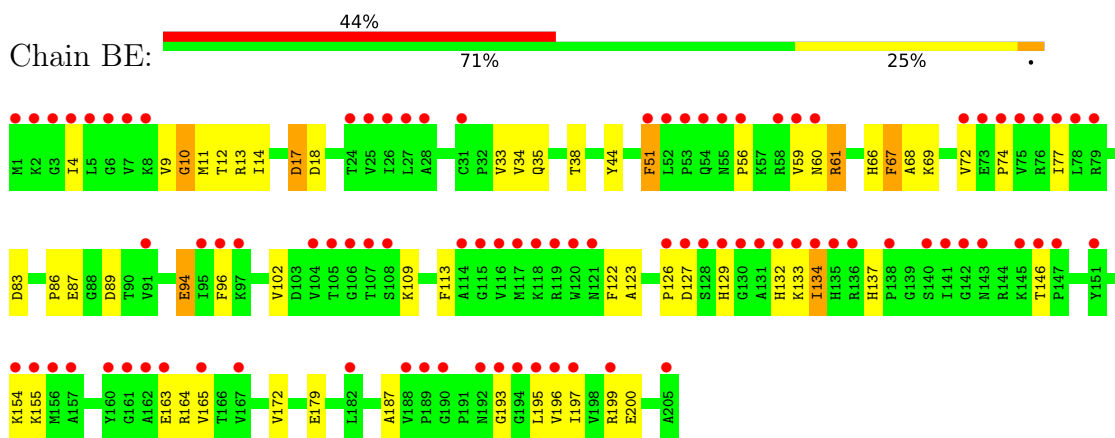
- Molecule 26: 50S ribosomal protein L2



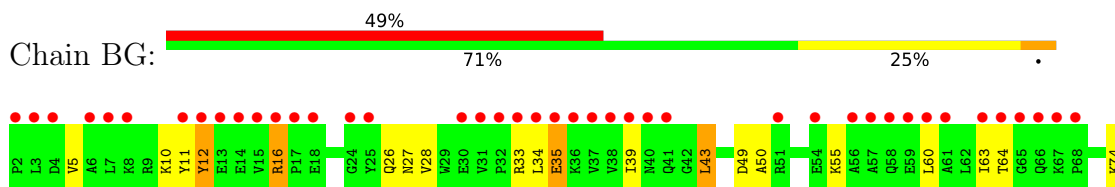
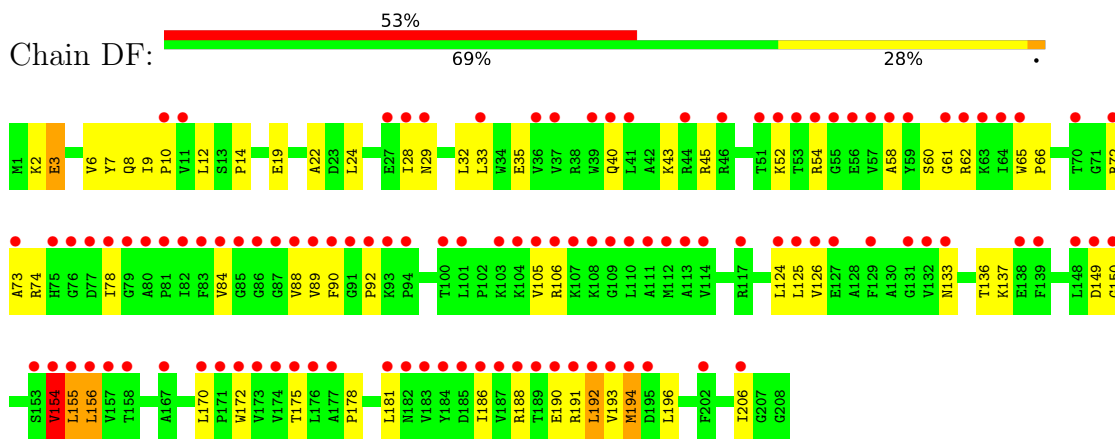
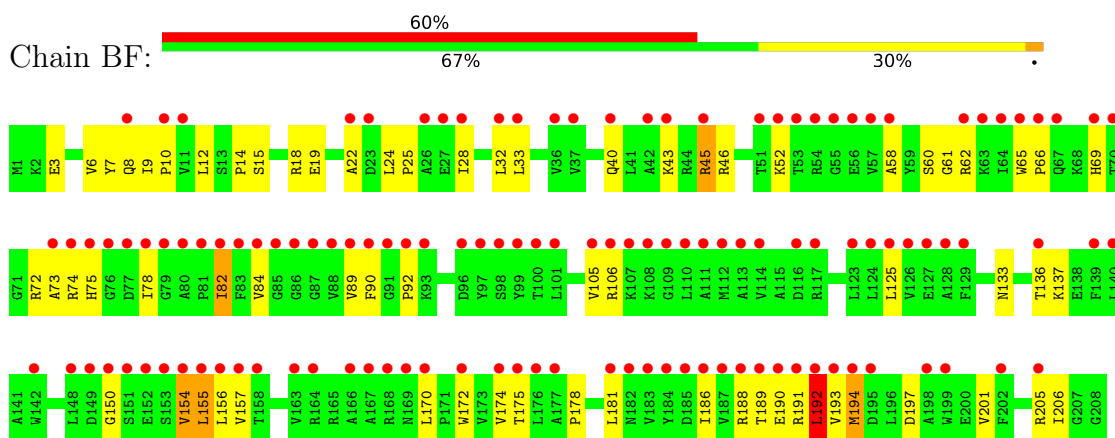
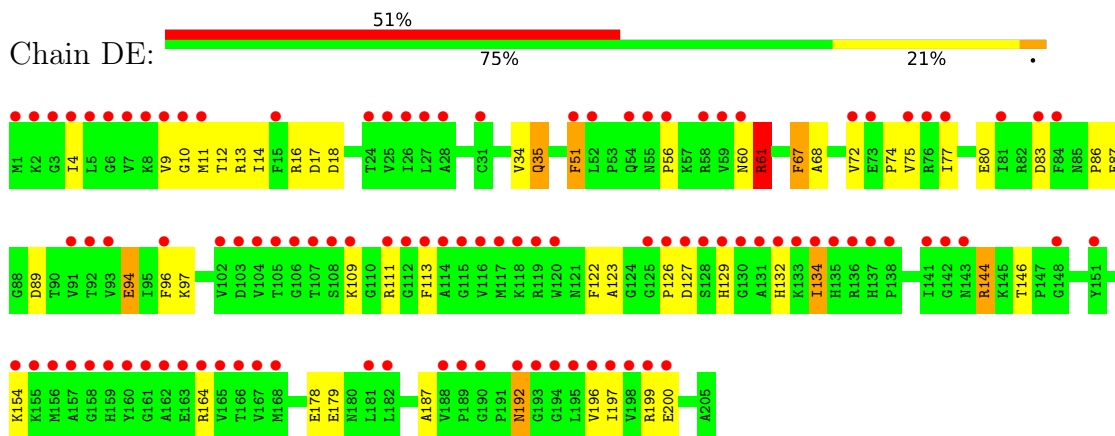
• Molecule 26: 50S ribosomal protein L2

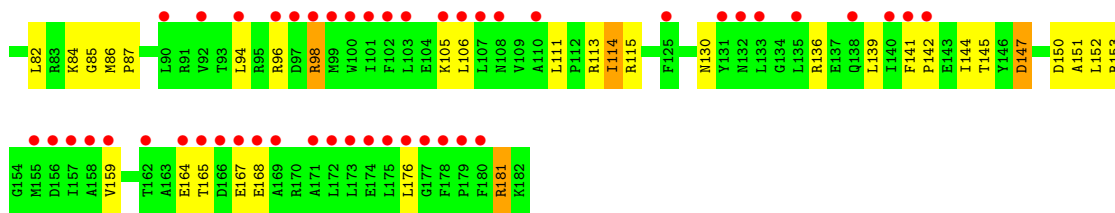


• Molecule 27: 50S ribosomal protein L3

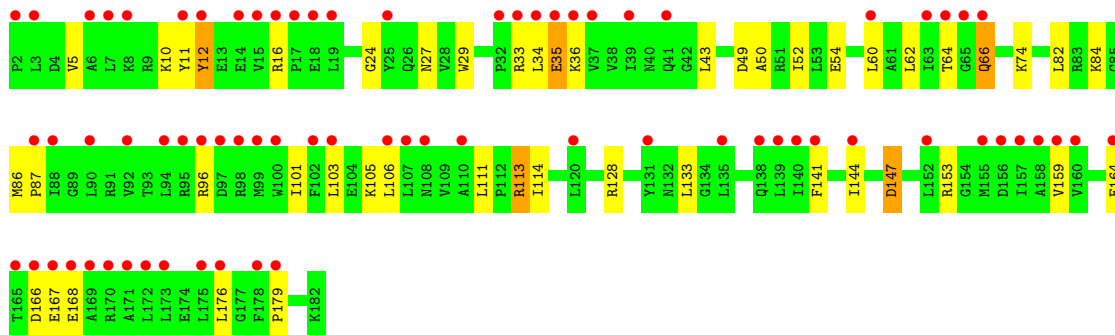
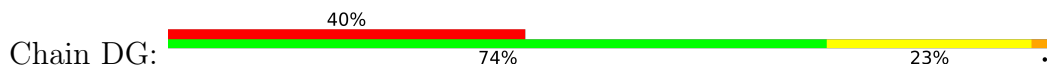


• Molecule 27: 50S ribosomal protein L3

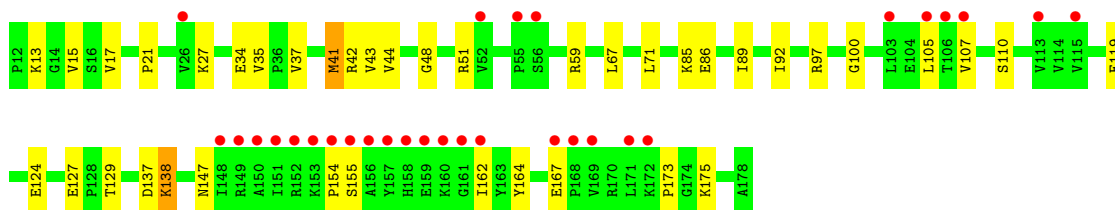
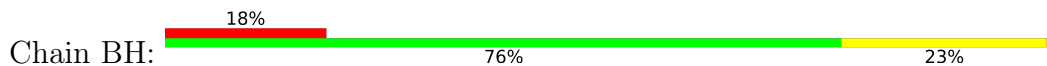




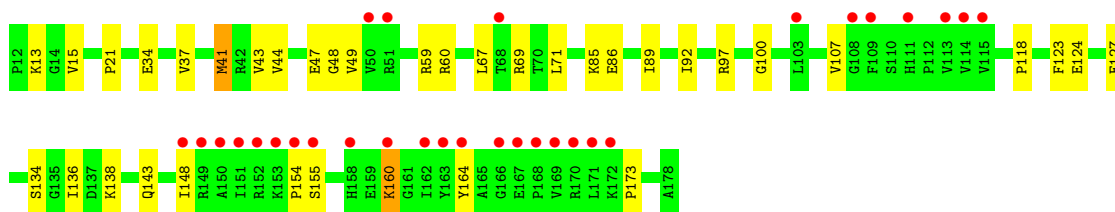
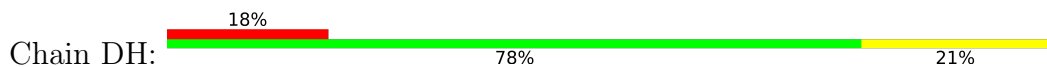
- Molecule 29: 50S ribosomal protein L5



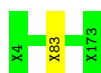
- Molecule 30: 50S ribosomal protein L6



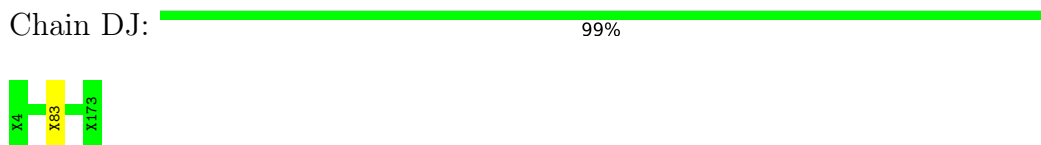
- Molecule 30: 50S ribosomal protein L6



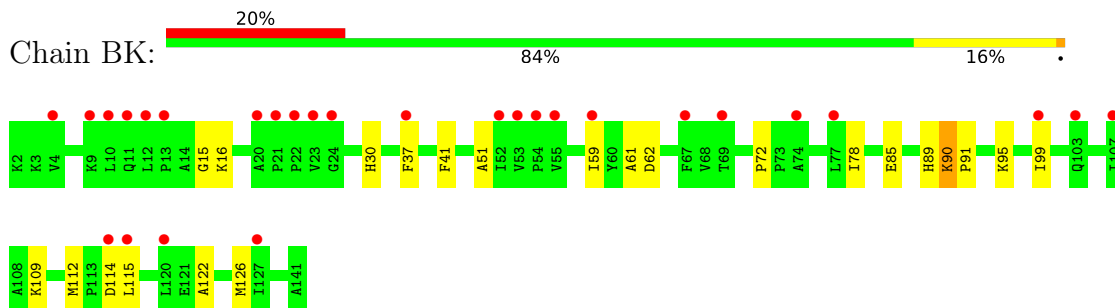
- Molecule 31: 50S ribosomal protein L10



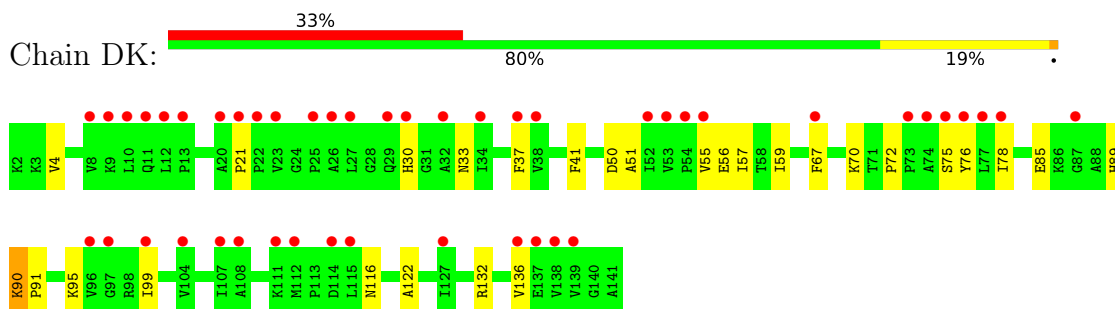
- Molecule 31: 50S ribosomal protein L10



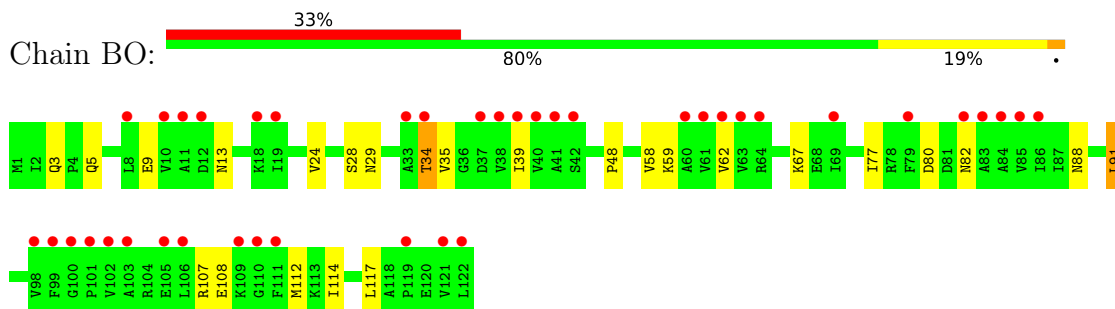
- Molecule 32: 50S ribosomal protein L11



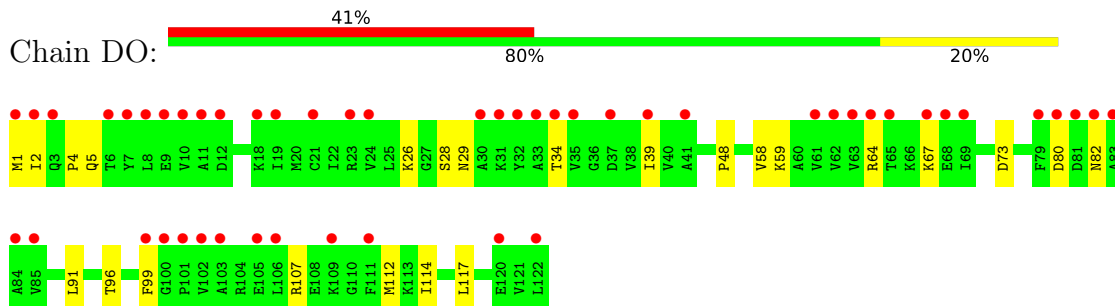
- Molecule 32: 50S ribosomal protein L11



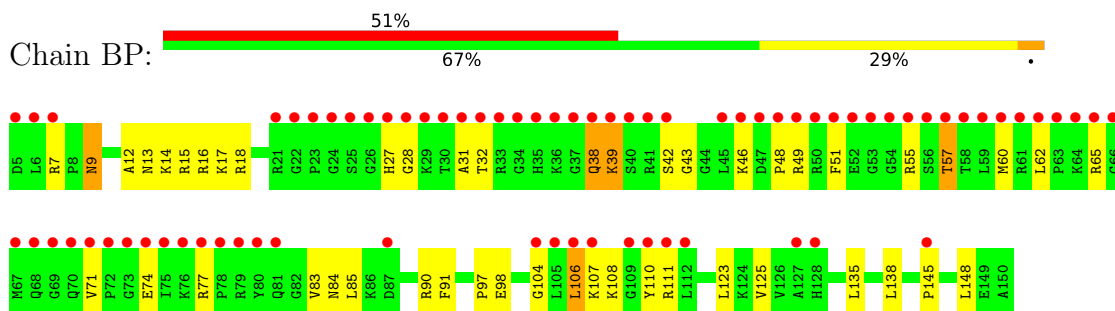
- Molecule 33: 50S ribosomal protein L14



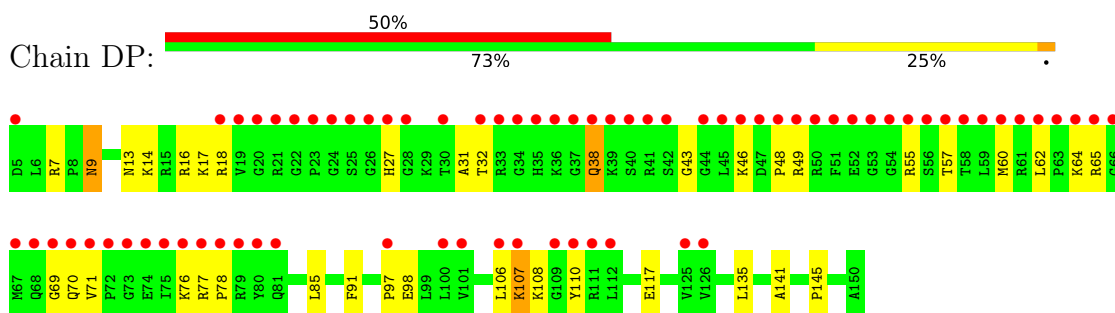
- Molecule 33: 50S ribosomal protein L14



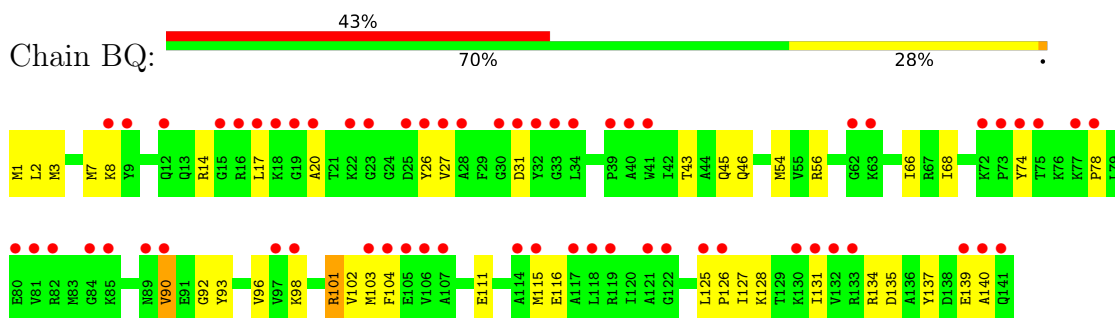
- Molecule 34: 50S ribosomal protein L15



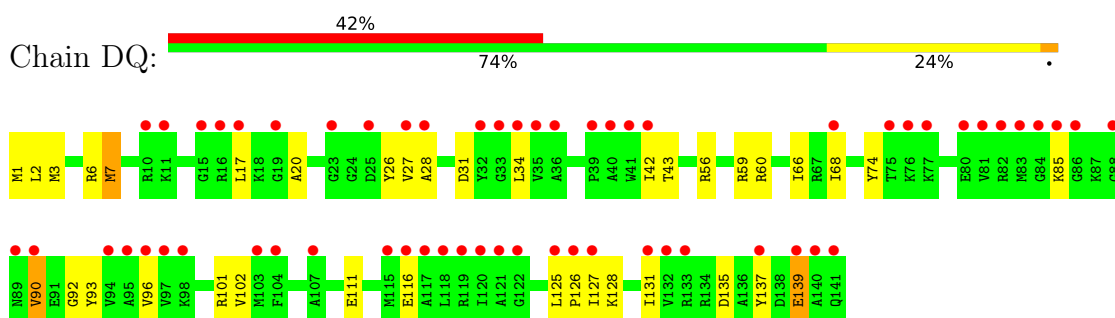
- Molecule 34: 50S ribosomal protein L15



- Molecule 35: 50S ribosomal protein L16

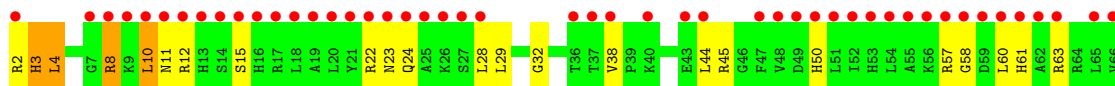


- Molecule 35: 50S ribosomal protein L16

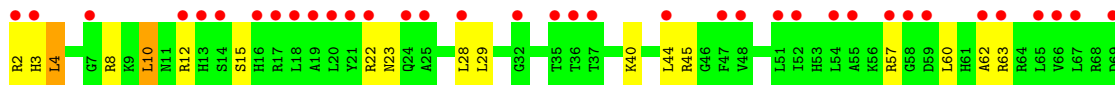
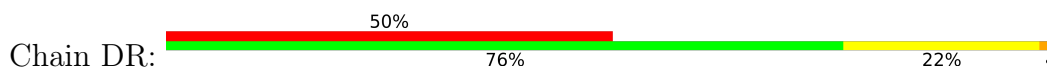


- Molecule 36: 50S ribosomal protein L17

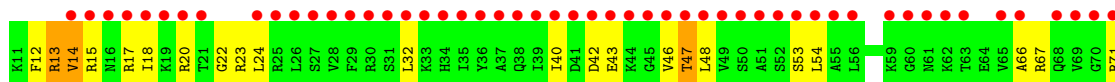
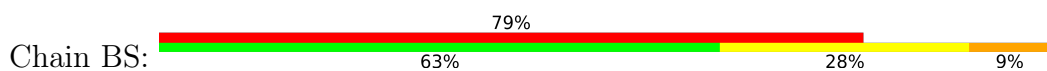




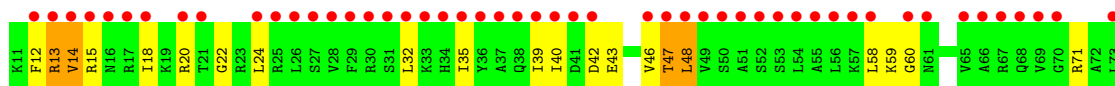
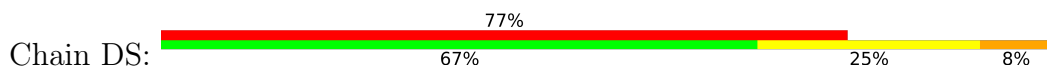
- Molecule 36: 50S ribosomal protein L17



- Molecule 37: 50S ribosomal protein L18



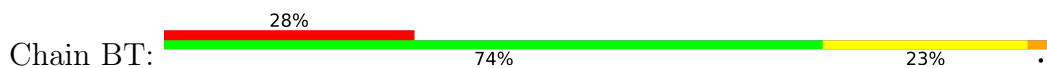
- Molecule 37: 50S ribosomal protein L18



- Molecule 37: 50S ribosomal protein L18



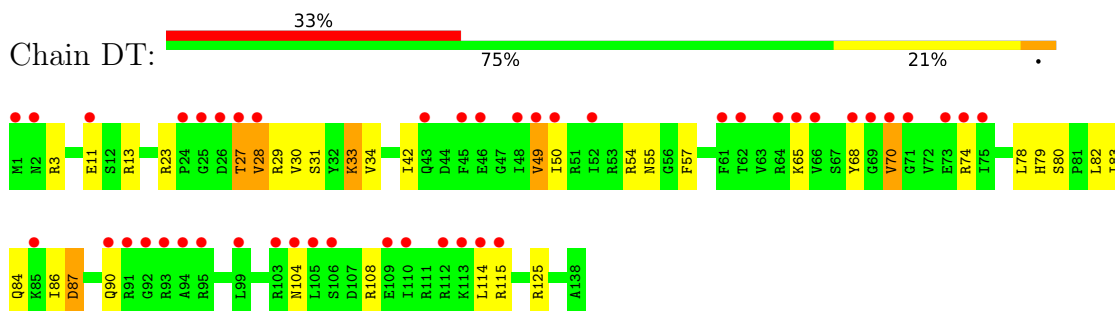
- Molecule 38: 50S ribosomal protein L19



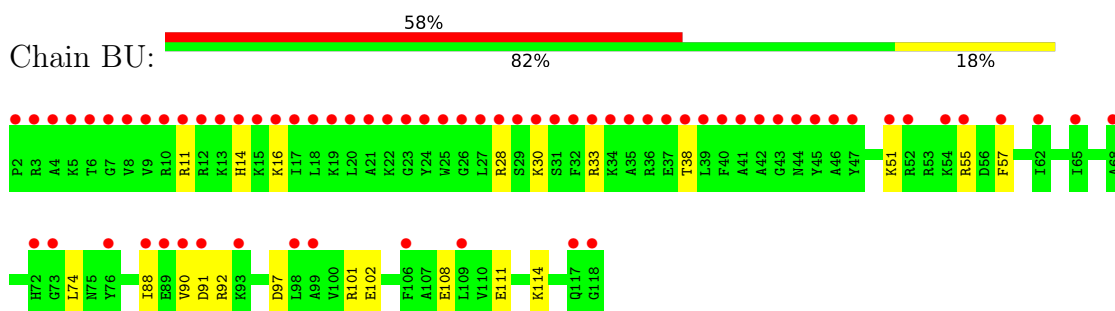
- Molecule 38: 50S ribosomal protein L19



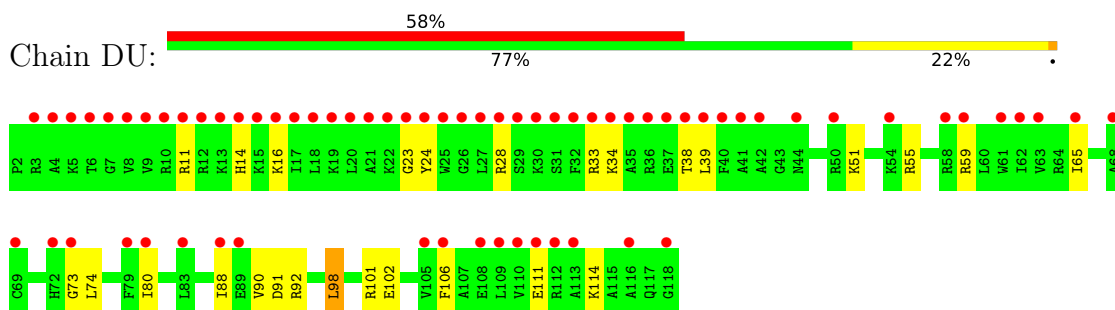
- Molecule 38: 50S ribosomal protein L19



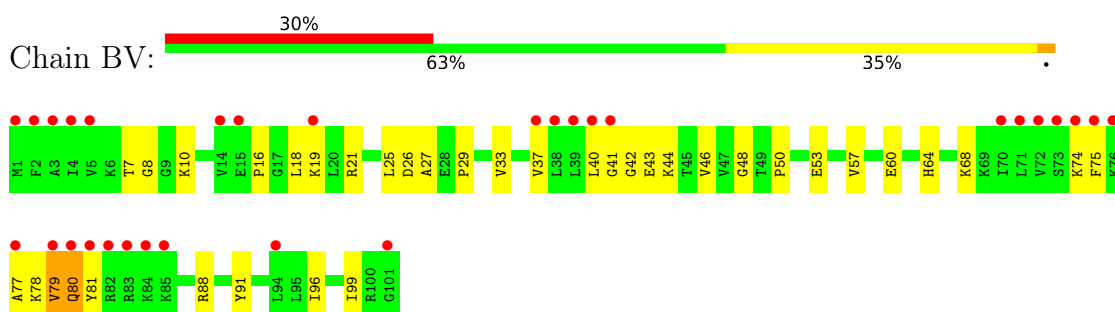
- Molecule 39: 50S ribosomal protein L20



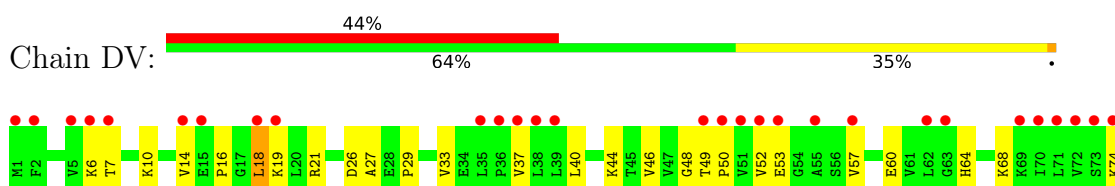
- Molecule 39: 50S ribosomal protein L20

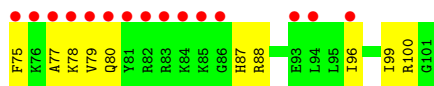


- Molecule 40: 50S ribosomal protein L21

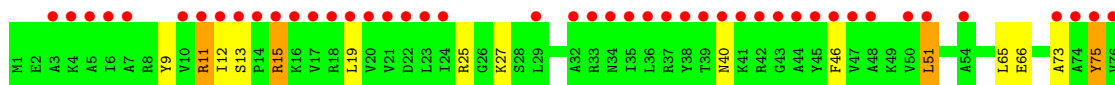
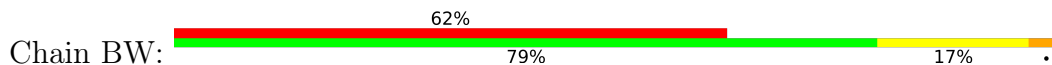


- Molecule 40: 50S ribosomal protein L21

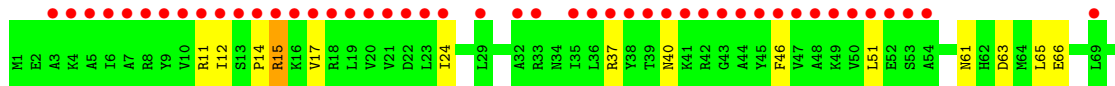
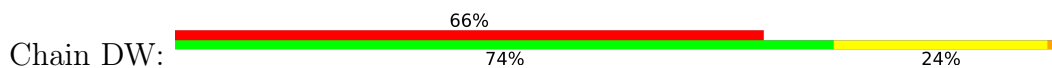




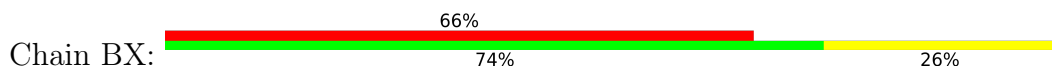
- Molecule 41: 50S ribosomal protein L22



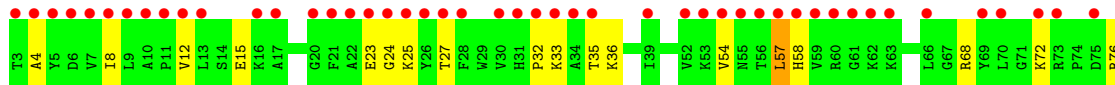
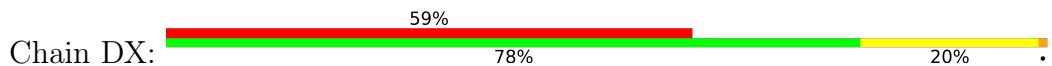
- Molecule 41: 50S ribosomal protein L22



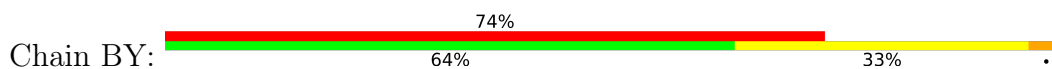
- Molecule 42: 50S ribosomal protein L23

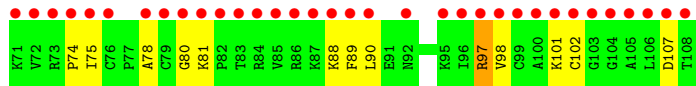
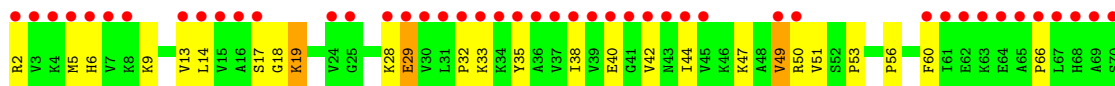


- Molecule 42: 50S ribosomal protein L23

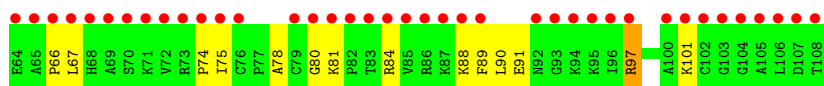
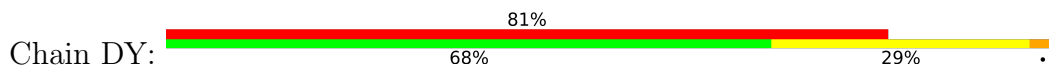


- Molecule 43: 50S ribosomal protein L24

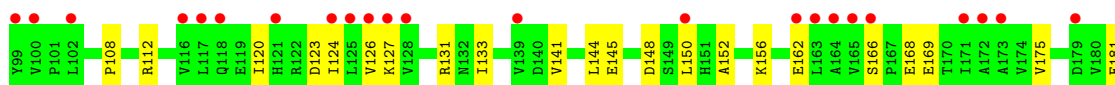
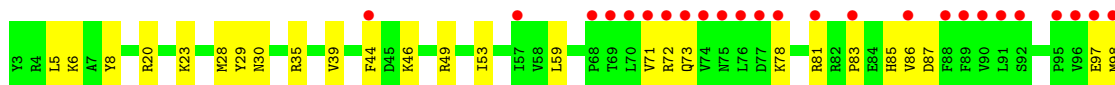
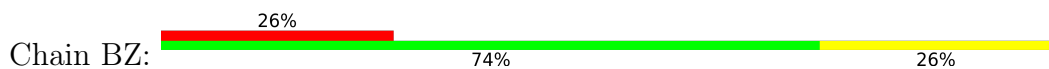




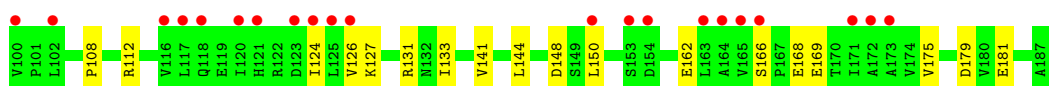
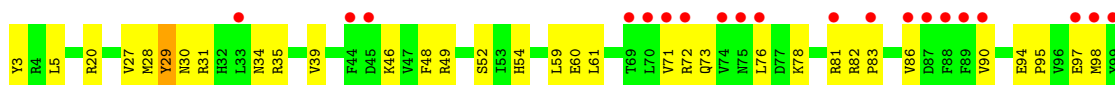
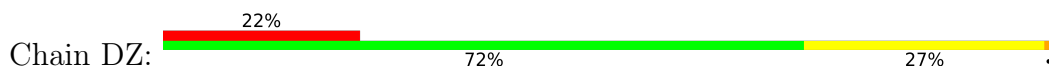
• Molecule 43: 50S ribosomal protein L24



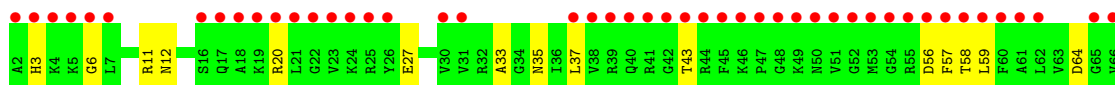
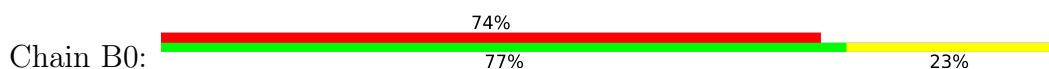
• Molecule 44: 50S ribosomal protein L25



• Molecule 44: 50S ribosomal protein L25

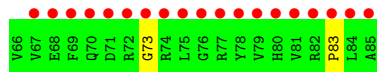
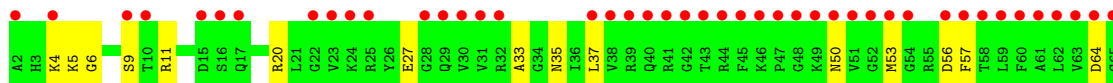
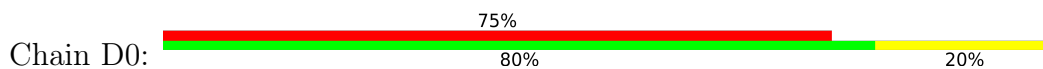


• Molecule 45: 50S ribosomal protein L27

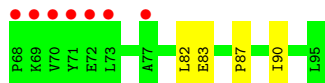




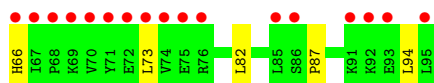
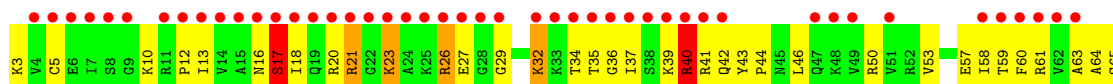
- Molecule 45: 50S ribosomal protein L27



- Molecule 46: 50S ribosomal protein L28



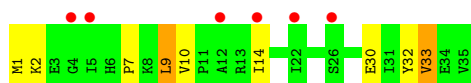
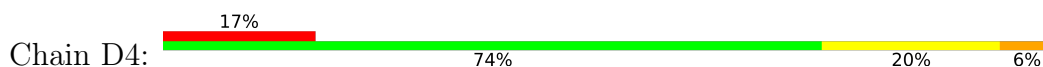
- Molecule 46: 50S ribosomal protein L28



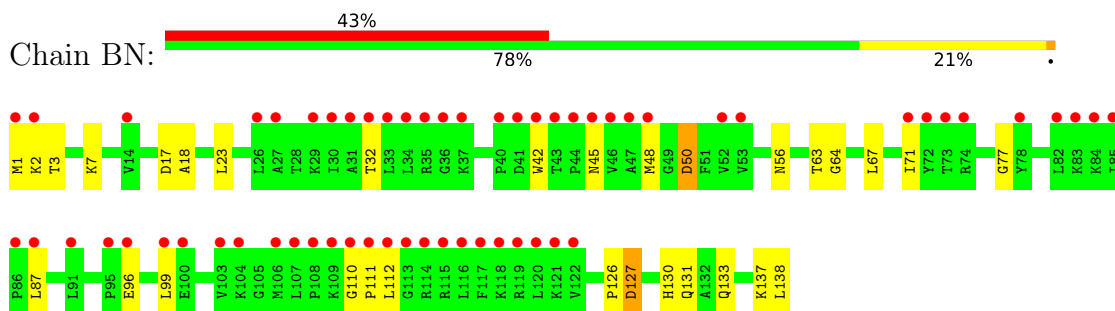
- Molecule 47: 50S ribosomal protein L31



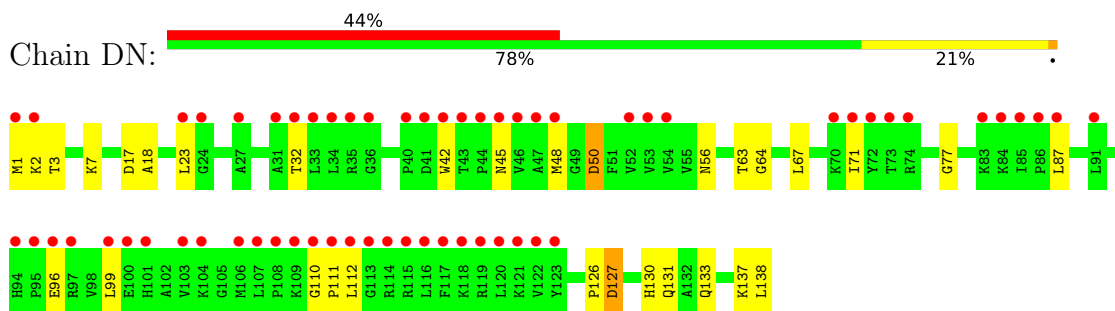
- Molecule 47: 50S ribosomal protein L31



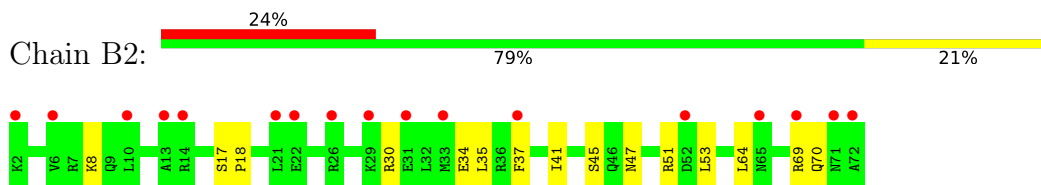
- Molecule 48: 50S ribosomal protein L13



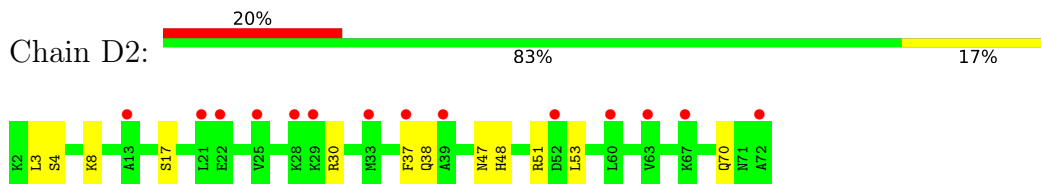
- Molecule 48: 50S ribosomal protein L13



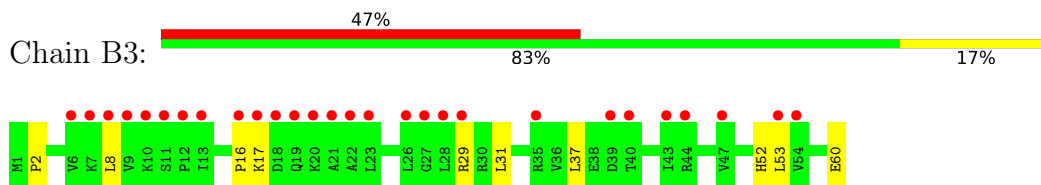
- Molecule 49: 50S ribosomal protein L29



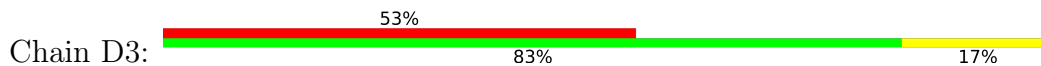
- Molecule 49: 50S ribosomal protein L29

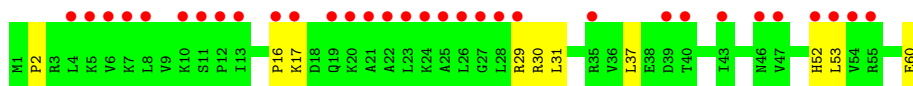


- Molecule 50: 50S ribosomal protein L30

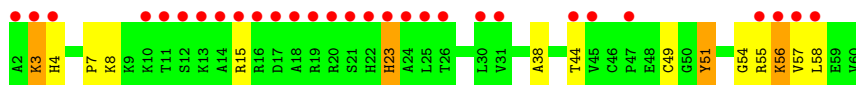
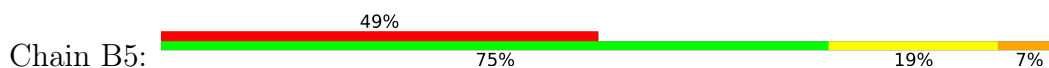


- Molecule 50: 50S ribosomal protein L30

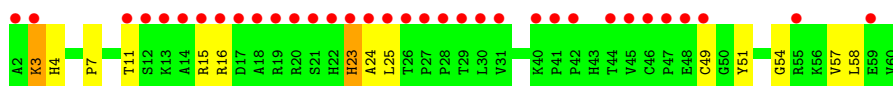
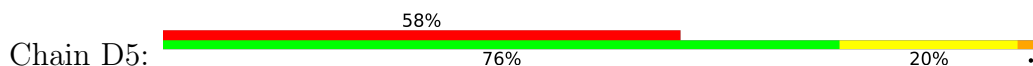




- Molecule 51: 50S ribosomal protein L32



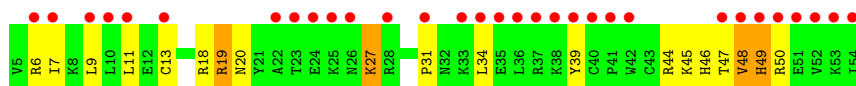
- Molecule 51: 50S ribosomal protein L32



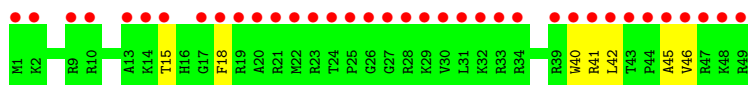
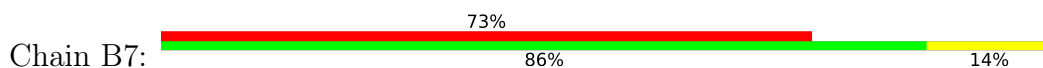
- Molecule 52: 50S ribosomal protein L33



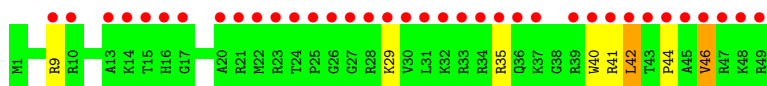
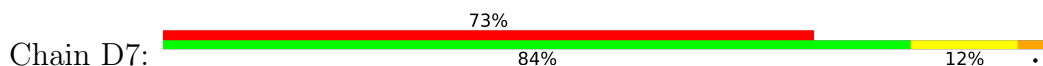
- Molecule 52: 50S ribosomal protein L33




- Molecule 53: 50S ribosomal protein L34

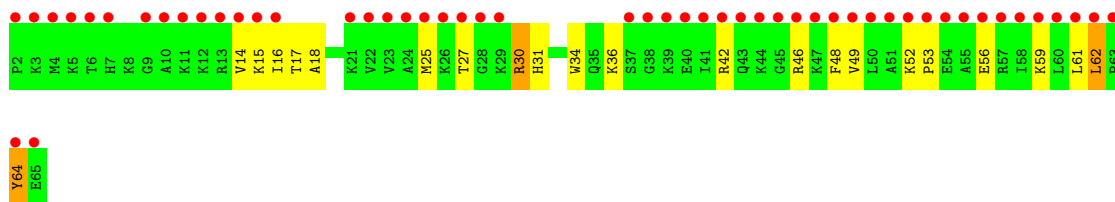


- Molecule 53: 50S ribosomal protein L34




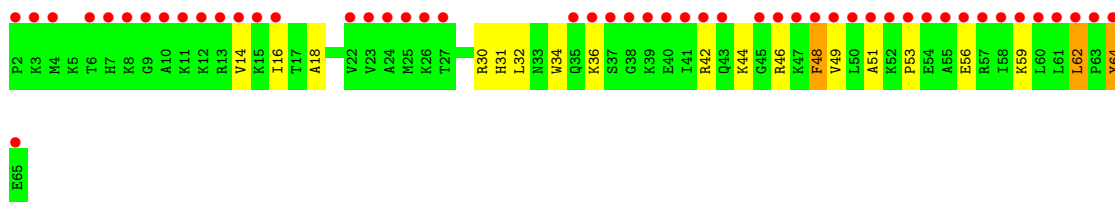
- Molecule 54: 50S ribosomal protein L35

Chain B8: 




- Molecule 54: 50S ribosomal protein L35

Chain D8: 

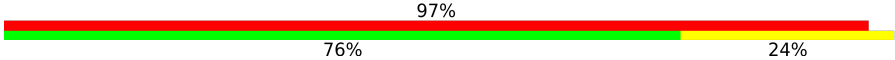


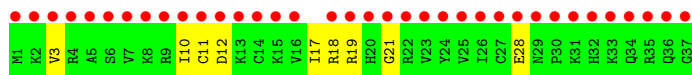
- Molecule 55: 50S ribosomal protein L36

Chain B9: 




- Molecule 55: 50S ribosomal protein L36

Chain D9: 




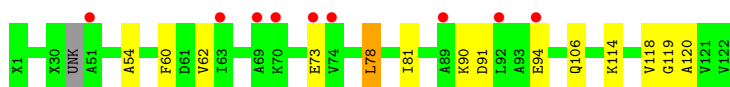
- Molecule 56: 50S ribosomal protein L7/L12

Chain Be: 



- Molecule 56: 50S ribosomal protein L7/L12

Chain De: 



- Molecule 57: 50S ribosomal protein L7/L12

Chain Bf:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Bg:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  100%


There are no outlier residues recorded for this chain.

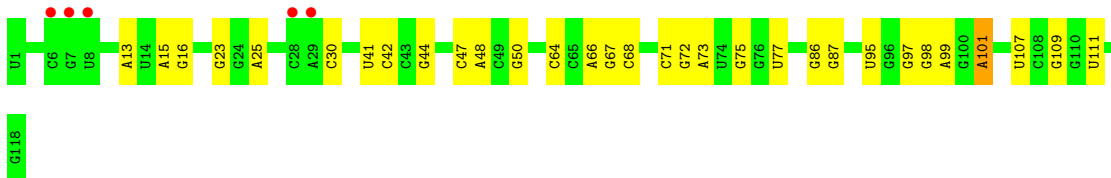
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%


There are no outlier residues recorded for this chain.

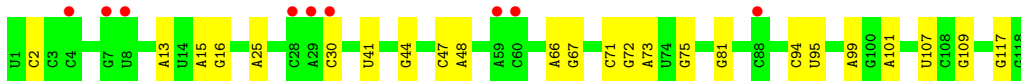
- Molecule 59: 5S ribosomal RNA

Chain BB:  4% 74% 25%

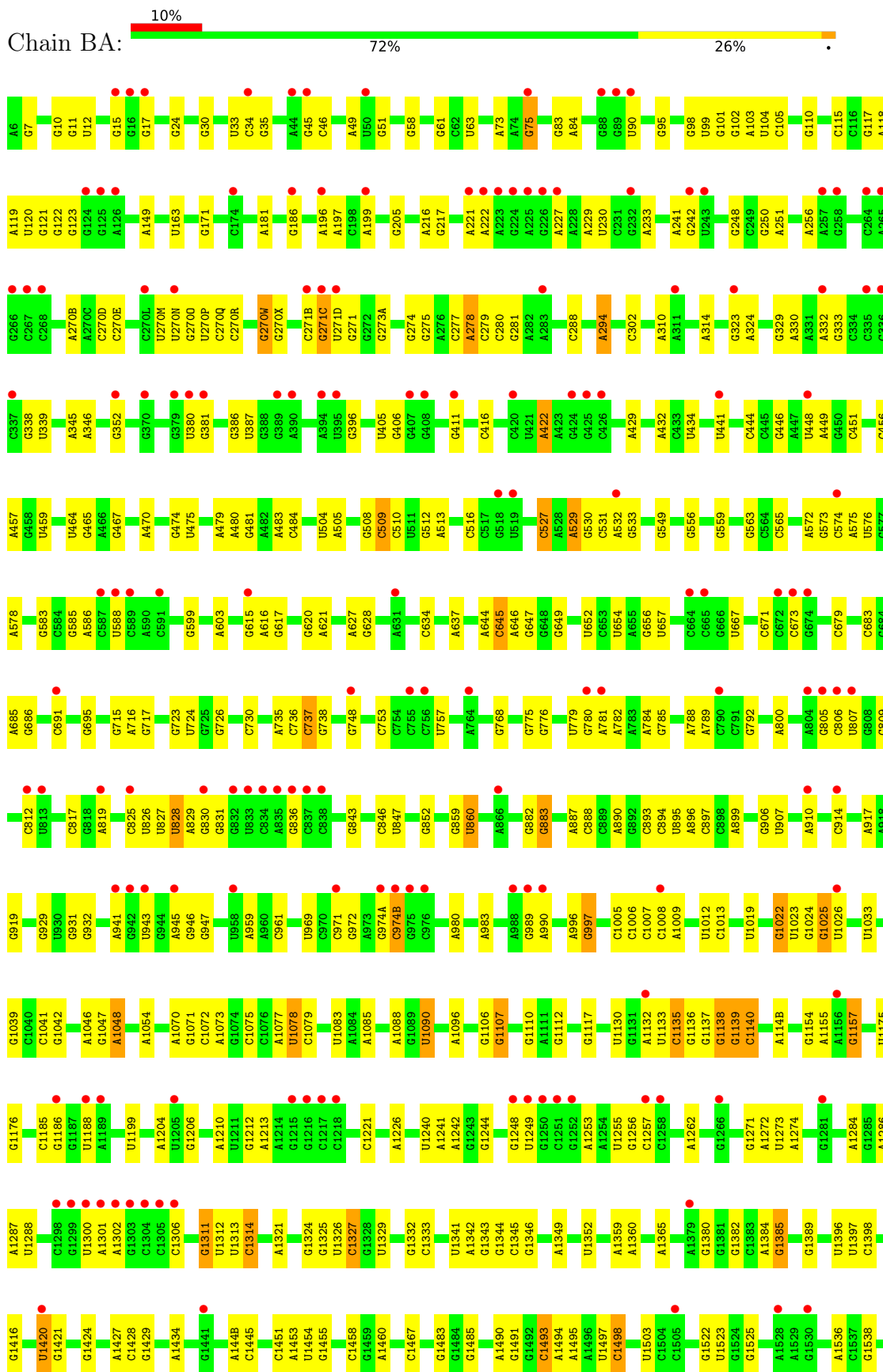


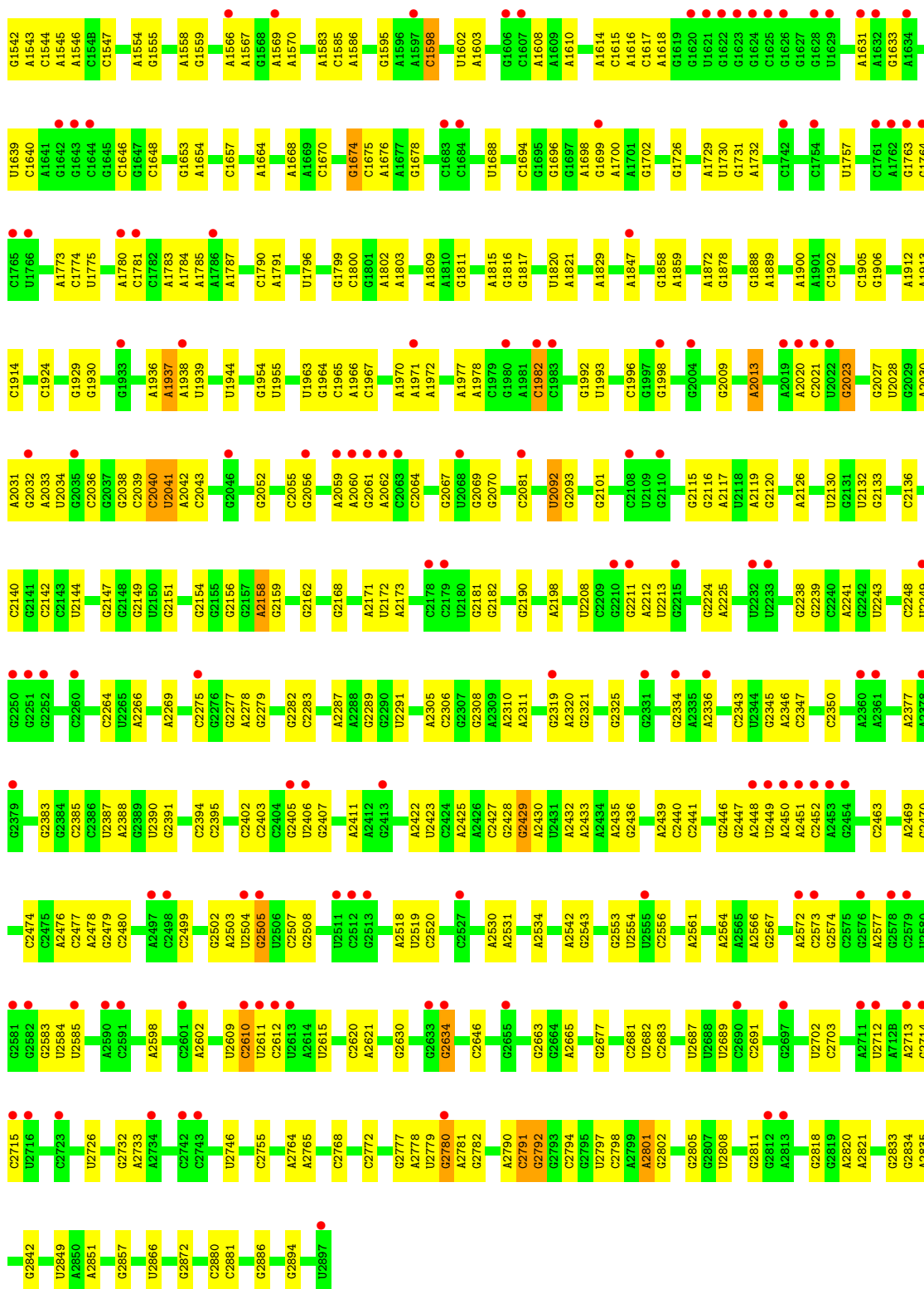
- Molecule 59: 5S ribosomal RNA

Chain DB:  8% 80% 20%

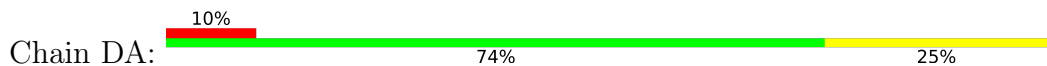


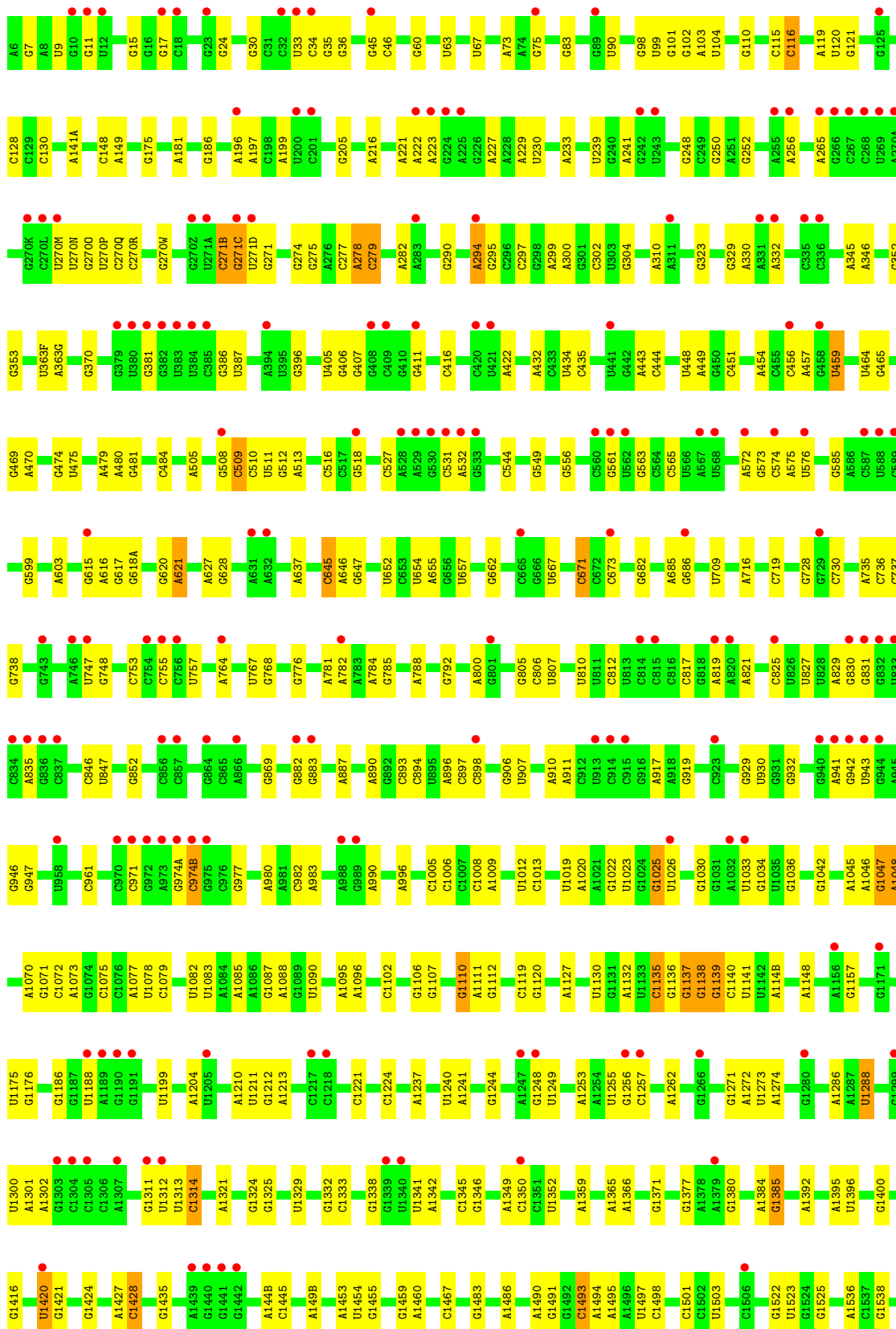
- Molecule 60: 23S ribosomal RNA

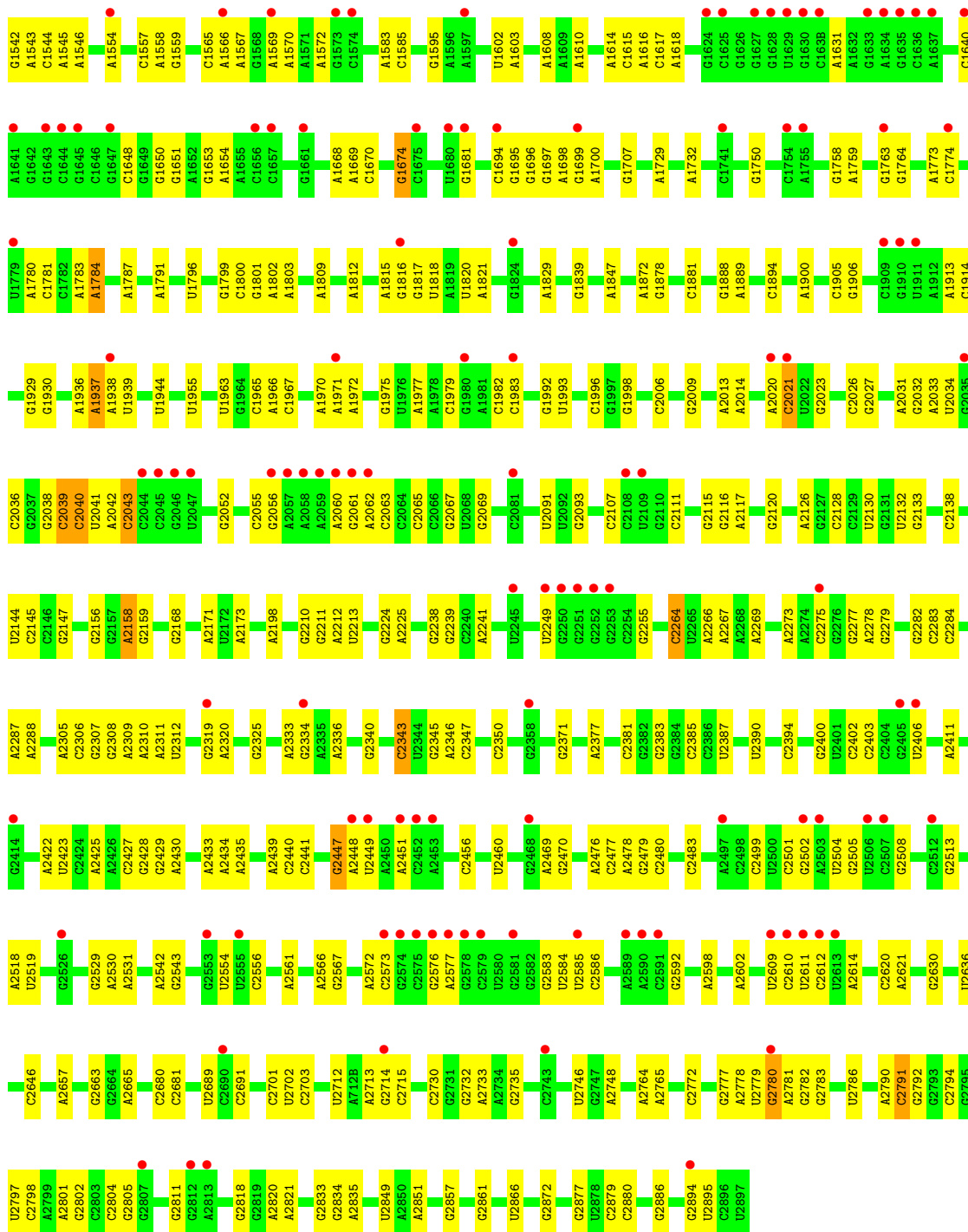




● Molecule 60: 23S ribosomal RNA







4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	302.39Å 683.92Å 356.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.86 182.04 – 3.87	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.86) 64.4 (182.04-3.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.34	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 3.89Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.264 , 0.317 0.271 , 0.318	Depositor DCC
R_{free} test set	21652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	76.3	Xtrriage
Anisotropy	0.322	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 478.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.24$, $\langle L^2 \rangle = 0.09$	Xtrriage
Estimated twinning fraction	0.320 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	308202	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, KBE, DPP, UAL, GNP, 5OH

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	AB	0.46	0/1945	0.80	9/2621 (0.3%)
1	CB	0.43	0/1945	0.80	6/2621 (0.2%)
2	AC	0.30	0/1645	0.60	0/2216
2	CC	0.30	0/1645	0.58	0/2216
3	AD	0.31	0/1733	0.61	0/2318
3	CD	0.30	0/1733	0.59	0/2318
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.58	0/1576
5	AF	0.29	0/856	0.54	0/1154
5	CF	0.28	0/856	0.56	0/1154
6	AG	0.29	0/1276	0.54	0/1709
6	CG	0.29	0/1276	0.53	0/1709
7	AH	0.31	0/1136	0.61	0/1527
7	CH	0.31	0/1136	0.61	0/1527
8	AI	0.33	0/1029	0.56	1/1378 (0.1%)
8	CI	0.32	0/1029	0.56	1/1378 (0.1%)
9	AJ	0.29	0/815	0.56	0/1095
9	CJ	0.30	0/815	0.55	0/1095
10	AK	0.37	0/900	0.71	0/1213
10	CK	0.39	0/900	0.67	0/1213
11	AL	0.49	0/992	0.91	2/1327 (0.2%)
11	CL	0.47	0/992	0.88	2/1327 (0.2%)
12	AM	0.30	0/1008	0.61	0/1347
12	CM	0.27	0/1008	0.59	0/1347
13	AN	0.30	0/501	0.46	0/664
13	CN	0.30	0/501	0.49	0/664
14	AO	0.31	0/745	0.56	0/992
14	CO	0.32	0/745	0.62	0/992
15	AP	0.28	0/722	0.54	0/970
15	CP	0.27	0/722	0.52	0/970
16	AQ	0.40	0/848	0.71	0/1131
16	CQ	0.41	0/848	0.73	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.31	0/579	0.64	0/768
17	CR	0.29	0/579	0.61	0/768
18	AS	0.30	0/647	0.60	0/870
18	CS	0.30	0/647	0.61	0/870
19	AT	0.34	0/764	0.62	0/1006
19	CT	0.33	0/764	0.61	0/1006
20	AA	0.39	0/36351	1.06	104/56736 (0.2%)
20	CA	0.38	2/36351 (0.0%)	1.06	96/56736 (0.2%)
21	AV	0.47	0/443	1.09	5/691 (0.7%)
21	CV	0.29	0/443	0.86	0/691
22	AW	0.42	0/1827	1.14	7/2845 (0.2%)
22	CW	0.37	0/1827	1.06	7/2845 (0.2%)
23	AY	0.37	0/5481	0.68	8/7418 (0.1%)
23	CY	0.41	0/5481	0.69	3/7418 (0.0%)
24	AU	1.08	0/11	1.84	0/13
24	CU	1.09	0/11	1.84	0/13
25	BC	0.52	0/1774	0.84	3/2391 (0.1%)
25	DC	0.55	1/1774 (0.1%)	0.93	7/2391 (0.3%)
26	BD	0.34	0/2195	0.65	2/2955 (0.1%)
26	DD	0.34	0/2195	0.64	2/2955 (0.1%)
27	BE	0.37	0/1602	0.68	2/2160 (0.1%)
27	DE	0.34	0/1602	0.65	1/2160 (0.0%)
28	BF	0.47	1/1663 (0.1%)	0.87	6/2249 (0.3%)
28	DF	0.43	0/1663	0.87	6/2249 (0.3%)
29	BG	0.42	1/1499 (0.1%)	1.33	5/2016 (0.2%)
29	DG	0.39	1/1499 (0.1%)	0.63	0/2016
30	BH	0.30	0/1298	0.56	0/1751
30	DH	0.30	0/1298	0.56	0/1751
32	BK	0.28	0/1054	0.55	0/1427
32	DK	0.27	0/1054	0.52	0/1427
33	BO	0.29	0/943	0.58	0/1269
33	DO	0.29	0/943	0.55	0/1269
34	BP	0.32	0/1131	0.68	0/1504
34	DP	0.30	0/1131	0.62	0/1504
35	BQ	0.33	0/1143	0.60	0/1527
35	DQ	0.32	0/1143	0.63	0/1527
36	BR	0.31	0/974	0.63	0/1302
36	DR	0.32	0/974	0.63	0/1302
37	BS	0.36	0/783	0.69	0/1041
37	DS	0.36	0/783	0.68	0/1041
38	BT	0.34	0/1161	0.67	0/1549
38	DT	0.32	0/1161	0.65	0/1549
39	BU	0.38	0/982	0.59	0/1306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DU	0.38	0/982	0.61	0/1306
40	BV	0.38	0/790	0.73	0/1057
40	DV	0.34	0/790	0.66	1/1057 (0.1%)
41	BW	0.35	0/911	0.66	2/1220 (0.2%)
41	DW	0.34	0/911	0.63	0/1220
42	BX	0.31	0/748	0.57	0/1004
42	DX	0.29	0/748	0.55	1/1004 (0.1%)
43	BY	0.32	0/831	0.61	0/1108
43	DY	0.31	0/831	0.58	0/1108
44	BZ	0.30	0/1505	0.60	0/2042
44	DZ	0.31	0/1505	0.60	0/2042
45	B0	0.27	0/671	0.54	0/892
45	D0	0.27	0/671	0.53	0/892
46	B1	0.48	0/739	0.77	2/981 (0.2%)
46	D1	0.50	0/739	0.82	3/981 (0.3%)
47	B4	0.40	0/276	0.62	0/372
47	D4	0.36	0/276	0.59	0/372
48	BN	0.34	0/1131	0.66	0/1525
48	DN	0.34	0/1131	0.66	0/1525
49	B2	0.36	0/600	0.62	0/793
49	D2	0.34	0/600	0.58	0/793
50	B3	0.29	0/482	0.53	0/646
50	D3	0.29	0/482	0.53	0/646
51	B5	0.33	0/473	0.65	0/639
51	D5	0.31	0/473	0.58	0/639
52	B6	0.32	0/440	0.67	0/586
52	D6	0.34	0/440	0.66	0/586
53	B7	0.31	0/438	0.56	0/575
53	D7	0.32	0/438	0.55	0/575
54	B8	0.33	0/525	0.66	0/691
54	D8	0.32	0/525	0.63	0/691
55	B9	0.43	0/310	0.69	0/407
55	D9	0.30	0/310	0.63	0/407
56	Be	0.33	0/538	0.56	0/715
56	De	0.31	0/538	0.56	0/715
59	BB	0.39	0/2853	1.12	15/4451 (0.3%)
59	DB	0.38	0/2853	1.07	10/4451 (0.2%)
60	BA	0.39	0/69437	1.09	229/108401 (0.2%)
60	DA	0.38	3/69437 (0.0%)	1.06	187/108401 (0.2%)
All	All	0.38	9/330652 (0.0%)	0.97	735/492274 (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
1	AB	0	3
1	CB	0	3
11	AL	0	1
11	CL	0	2
23	AY	0	4
23	CY	0	4
25	BC	0	5
25	DC	0	3
26	BD	0	2
26	DD	0	2
28	BF	0	1
28	DF	0	1
29	BG	0	2
29	DG	0	2
31	BJ	0	1
31	DJ	0	1
37	BS	0	3
37	DS	0	3
38	DT	0	1
41	BW	0	1
41	DW	0	2
46	B1	0	2
46	D1	0	2
All	All	0	51

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	BG	114	ILE	C-N	10.70	1.58	1.34
20	CA	1393	U	N1-C2	9.25	1.46	1.38
29	DG	114	ILE	N-CA	-7.54	1.31	1.46
25	DC	214	TYR	CD1-CE1	6.83	1.49	1.39
28	BF	157	VAL	CB-CG1	-5.60	1.41	1.52
60	DA	1020	A	N9-C8	-5.47	1.33	1.37
60	DA	1137	G	N9-C4	5.46	1.42	1.38
20	CA	1393	U	C2-O2	5.28	1.27	1.22
60	DA	1006	C	N1-C2	5.06	1.45	1.40

All (735) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	BG	114	ILE	O-C-N	-51.93	39.62	122.70
60	BA	1006	C	C6-N1-C2	-15.70	114.02	120.30
60	BA	1006	C	N3-C2-O2	-13.26	112.62	121.90
20	AA	1535	C	P-O3'-C3'	12.55	134.76	119.70
60	BA	2505	G	N1-C6-O6	12.54	127.43	119.90
20	CA	1393	U	N1-C2-O2	12.43	131.50	122.80
60	DA	1006	C	N1-C2-O2	12.16	126.20	118.90
60	DA	1006	C	N3-C2-O2	-11.85	113.61	121.90
20	AA	1535	C	O3'-P-O5'	-11.58	82.00	104.00
20	CA	815	A	C5-C6-N6	11.09	132.57	123.70
20	AA	815	A	N1-C6-N6	-11.01	112.00	118.60
60	BA	1006	C	N1-C2-O2	10.83	125.40	118.90
20	CA	815	A	N1-C6-N6	-10.71	112.17	118.60
20	CA	1393	U	N3-C4-C5	10.67	121.00	114.60
60	BA	2505	G	C5-C6-O6	-10.28	122.43	128.60
60	DA	1137	G	N3-C4-C5	-10.22	123.49	128.60
20	AA	815	A	C5-C6-N6	10.11	131.79	123.70
60	DA	1006	C	C6-N1-C2	-9.95	116.32	120.30
60	DA	2040	C	C6-N1-C2	-9.65	116.44	120.30
23	CY	33	LEU	CA-CB-CG	9.39	136.91	115.30
20	CA	1465	C	C2-N3-C4	-9.22	115.29	119.90
60	BA	2040	C	C2-N1-C1'	9.12	128.83	118.80
60	BA	1135	C	C2-N1-C1'	9.12	128.83	118.80
60	DA	1137	G	O4'-C1'-N9	9.04	115.44	108.20
60	DA	2039	C	N3-C2-O2	-9.04	115.57	121.90
20	AA	1465	C	C2-N3-C4	-8.95	115.43	119.90
1	AB	162	ILE	CB-CA-C	8.93	129.46	111.60
60	BA	1137	G	C6-N1-C2	-8.89	119.77	125.10
60	DA	2039	C	N1-C2-O2	8.76	124.16	118.90
60	BA	1137	G	O4'-C1'-N9	8.68	115.14	108.20
28	BF	155	LEU	N-CA-C	-8.61	87.76	111.00
60	BA	1493	C	N1-C2-O2	8.60	124.06	118.90
20	CA	815	A	N9-C4-C5	8.55	109.22	105.80
60	BA	1135	C	C6-N1-C1'	-8.54	110.56	120.80
1	CB	162	ILE	CB-CA-C	8.50	128.61	111.60
59	DB	75	G	N3-C4-C5	-8.46	124.37	128.60
20	AA	1034	G	N3-C4-N9	-8.45	120.93	126.00
60	BA	1048	A	N1-C6-N6	8.42	123.65	118.60
28	DF	155	LEU	N-CA-C	-8.29	88.61	111.00
59	BB	101	A	C6-N1-C2	-8.24	113.65	118.60
20	CA	1393	U	C5-C4-O4	-8.24	120.96	125.90
60	DA	1493	C	C2-N1-C1'	8.23	127.85	118.80
60	BA	1493	C	C2-N1-C1'	8.21	127.83	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	1020	A	C5-N7-C8	8.20	108.00	103.90
60	DA	2794	C	C2-N1-C1'	8.20	127.82	118.80
60	BA	645	C	C2-N1-C1'	8.18	127.79	118.80
60	DA	1493	C	N1-C2-O2	8.11	123.77	118.90
23	AY	33	LEU	CA-CB-CG	8.09	133.90	115.30
60	BA	1313	U	C2-N1-C1'	8.09	127.40	117.70
60	BA	645	C	N1-C2-O2	8.07	123.74	118.90
60	BA	30	G	N3-C4-N9	8.05	130.83	126.00
59	DB	101	A	C6-N1-C2	-8.03	113.78	118.60
20	CA	1436	U	C2-N3-C4	-7.91	122.25	127.00
60	DA	1138	G	O4'-C1'-N9	7.87	114.49	108.20
60	DA	1006	C	C2-N1-C1'	7.84	127.43	118.80
60	BA	271(B)	C	C2-N1-C1'	7.84	127.43	118.80
59	DB	75	G	C6-N1-C2	-7.84	120.40	125.10
59	DB	75	G	N3-C4-N9	7.81	130.69	126.00
20	CA	115	G	N3-C4-N9	7.76	130.66	126.00
60	DA	479	A	N1-C6-N6	-7.75	113.95	118.60
60	DA	1107	G	N3-C4-N9	-7.75	121.35	126.00
20	AA	1332	A	N1-C6-N6	7.74	123.24	118.60
60	BA	1137	G	N3-C4-C5	-7.72	124.74	128.60
20	CA	687	A	P-O3'-C3'	7.70	128.93	119.70
20	CA	754	C	C2-N1-C1'	7.68	127.25	118.80
60	DA	271(B)	C	C2-N1-C1'	7.67	127.24	118.80
22	AW	68	U	C2-N1-C1'	-7.61	108.57	117.70
20	AA	1213	A	N9-C4-C5	7.56	108.83	105.80
60	BA	2009	G	N3-C4-N9	-7.56	121.46	126.00
60	DA	1314	C	C2-N1-C1'	7.55	127.11	118.80
60	DA	1135	C	C2-N1-C1'	7.52	127.07	118.80
60	BA	1006	C	C2-N1-C1'	7.50	127.05	118.80
60	BA	1774	C	C6-N1-C2	-7.50	117.30	120.30
60	DA	459	U	C6-N1-C2	7.49	125.49	121.00
20	CA	115	G	P-O3'-C3'	7.48	128.68	119.70
60	BA	271(B)	C	N1-C2-O2	7.47	123.38	118.90
60	DA	673	C	C2-N3-C4	-7.46	116.17	119.90
20	CA	1034	G	N3-C4-N9	-7.43	121.54	126.00
60	BA	1006	C	C5-C6-N1	7.43	124.72	121.00
60	DA	1137	G	C8-N9-C4	-7.41	103.44	106.40
60	BA	1420	U	C2-N1-C1'	7.40	126.58	117.70
60	BA	673	C	C5-C4-N4	-7.40	115.02	120.20
20	CA	815	A	N3-C4-N9	-7.39	121.48	127.40
60	BA	1327	C	C2-N1-C1'	7.38	126.92	118.80
59	DB	95	U	C5-C4-O4	7.37	130.32	125.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	1493	C	C6-N1-C2	-7.37	117.35	120.30
60	DA	1020	A	N7-C8-N9	-7.34	110.13	113.80
60	BA	860	U	C2-N1-C1'	7.30	126.46	117.70
20	CA	115	G	N3-C4-C5	-7.29	124.95	128.60
11	AL	55	VAL	CB-CA-C	-7.26	97.60	111.40
60	DA	30	G	N3-C4-N9	7.26	130.36	126.00
60	DA	621	A	N1-C6-N6	-7.25	114.25	118.60
60	BA	95	G	N3-C4-N9	-7.25	121.65	126.00
60	BA	103	A	N1-C6-N6	7.22	122.93	118.60
25	DC	12	LEU	CA-CB-CG	7.20	131.85	115.30
20	CA	115	G	C4-N9-C1'	7.16	135.81	126.50
60	BA	103	A	N9-C4-C5	-7.15	102.94	105.80
60	DA	1313	U	C2-N1-C1'	7.13	126.26	117.70
60	BA	1048	A	C4-C5-C6	7.13	120.56	117.00
60	BA	2780	G	O4'-C1'-N9	7.09	113.87	108.20
60	DA	1774	C	C6-N1-C2	-7.09	117.47	120.30
20	AA	115	G	N3-C4-N9	7.08	130.25	126.00
60	DA	807	U	C2-N3-C4	-7.08	122.75	127.00
20	AA	186(L)	G	N3-C4-N9	-7.07	121.76	126.00
20	CA	815	A	C6-C5-N7	7.06	137.24	132.30
60	DA	294	A	N1-C6-N6	7.06	122.83	118.60
60	BA	1107	G	N3-C4-N9	-7.05	121.77	126.00
20	CA	1465	C	N3-C4-C5	7.02	124.71	121.90
59	BB	75	G	C6-N1-C2	-7.01	120.89	125.10
60	BA	673	C	C2-N3-C4	-7.00	116.40	119.90
1	AB	163	PHE	N-CA-C	-7.00	92.10	111.00
60	DA	1137	G	N3-C4-N9	6.98	130.19	126.00
60	DA	1048	A	N1-C6-N6	6.96	122.78	118.60
11	AL	60	LEU	CA-CB-CG	6.93	131.24	115.30
20	CA	1393	U	N3-C2-O2	-6.92	117.36	122.20
20	CA	1393	U	C6-N1-C2	6.91	125.15	121.00
20	CA	68(E)	G	C5-C6-O6	6.91	132.75	128.60
23	CY	33	LEU	N-CA-C	-6.91	92.35	111.00
60	DA	1020	A	C4-C5-N7	-6.91	107.25	110.70
60	DA	2794	C	N1-C2-O2	6.91	123.04	118.90
60	DA	2158	A	P-O3'-C3'	6.90	127.98	119.70
60	BA	2794	C	C2-N1-C1'	6.89	126.38	118.80
59	BB	95	U	C5-C4-O4	6.87	130.02	125.90
20	CA	328	C	N1-C2-O2	6.87	123.02	118.90
27	BE	61	ARG	C-N-CD	6.86	142.80	128.40
23	AY	567	LEU	CA-CB-CG	6.84	131.03	115.30
20	AA	1028(F)	A	C4-C5-C6	6.84	120.42	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	2794	C	N1-C2-O2	6.83	123.00	118.90
60	BA	1525	G	N3-C4-N9	-6.83	121.90	126.00
60	DA	1137	G	C6-N1-C2	-6.83	121.00	125.10
20	AA	115	G	N3-C4-C5	-6.83	125.19	128.60
60	DA	459	U	N1-C2-N3	-6.83	110.81	114.90
60	DA	576	U	C5-C4-O4	-6.82	121.81	125.90
20	AA	1028(F)	A	N1-C6-N6	6.81	122.69	118.60
20	CA	618	C	C5-C4-N4	6.81	124.97	120.20
23	CY	33	LEU	CB-CG-CD2	6.81	122.57	111.00
22	CW	61	C	N1-C2-O2	6.80	122.98	118.90
60	BA	2585	U	C2-N1-C1'	6.80	125.86	117.70
60	DA	1048	A	C4-C5-C6	6.79	120.39	117.00
60	BA	1774	C	C2-N1-C1'	6.78	126.26	118.80
22	CW	61	C	C2-N1-C1'	6.78	126.26	118.80
60	BA	807	U	C2-N3-C4	-6.77	122.94	127.00
8	AI	58	ARG	NE-CZ-NH1	6.77	123.68	120.30
23	AY	33	LEU	CB-CG-CD2	6.77	122.50	111.00
25	DC	214	TYR	N-CA-C	-6.75	92.76	111.00
60	BA	997	G	O5'-P-OP1	-6.75	99.63	105.70
60	DA	121	G	N3-C4-N9	6.75	130.05	126.00
60	BA	1140	C	C6-N1-C2	-6.74	117.61	120.30
59	BB	101	A	C5-C6-N1	6.73	121.06	117.70
60	BA	1138	G	O4'-C1'-N9	6.73	113.58	108.20
28	BF	192	LEU	CA-CB-CG	6.72	130.76	115.30
60	BA	1598	C	C2-N1-C1'	6.72	126.19	118.80
20	AA	1213	A	N1-C6-N6	-6.72	114.57	118.60
60	DA	1139	G	O5'-P-OP1	-6.70	99.67	105.70
21	AV	19	G	N3-C4-N9	-6.69	121.98	126.00
20	AA	1465	C	N3-C4-C5	6.68	124.57	121.90
60	DA	894	C	C2-N1-C1'	-6.68	111.45	118.80
60	DA	2794	C	C6-N1-C1'	-6.68	112.79	120.80
11	CL	55	VAL	CB-CA-C	-6.66	98.75	111.40
20	CA	1248	A	N1-C6-N6	-6.66	114.61	118.60
60	DA	271(B)	C	N1-C2-O2	6.64	122.89	118.90
60	BA	527	C	C6-N1-C2	-6.64	117.64	120.30
20	AA	754	C	C2-N1-C1'	6.63	126.09	118.80
60	DA	1019	U	C5-C6-N1	6.63	126.01	122.70
60	BA	2792	G	N9-C4-C5	6.62	108.05	105.40
60	DA	2780	G	OP2-P-O3'	6.62	119.77	105.20
60	BA	1226	A	N1-C6-N6	6.62	122.57	118.60
20	CA	1436	U	C5-C4-O4	-6.62	121.93	125.90
60	BA	2343	C	C2-N1-C1'	6.60	126.06	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	103	A	N9-C4-C5	-6.60	103.16	105.80
59	BB	101	A	C5-C6-N6	-6.59	118.43	123.70
8	CI	58	ARG	NE-CZ-NH1	6.59	123.59	120.30
60	BA	1048	A	C6-C5-N7	-6.58	127.69	132.30
60	BA	2040	C	C6-N1-C1'	-6.58	112.90	120.80
60	DA	2895	U	O4'-C1'-N1	6.58	113.47	108.20
60	BA	2009	G	N3-C2-N2	-6.57	115.30	119.90
20	AA	1436	U	C2-N3-C4	-6.56	123.06	127.00
60	BA	1314	C	C2-N1-C1'	6.55	126.01	118.80
20	AA	1305	G	C2-N3-C4	-6.54	108.63	111.90
60	DA	1020	A	C8-N9-C4	6.54	108.42	105.80
60	BA	2040	C	N1-C2-O2	6.52	122.81	118.90
20	AA	115	G	P-O3'-C3'	6.51	127.51	119.70
20	AA	815	A	N9-C4-C5	6.49	108.39	105.80
20	AA	156	G	N3-C2-N2	-6.48	115.36	119.90
60	DA	1213	A	N1-C6-N6	6.46	122.48	118.60
1	CB	163	PHE	N-CA-C	-6.46	93.55	111.00
60	BA	2040	C	N3-C2-O2	-6.45	117.39	121.90
60	BA	1493	C	C5-C6-N1	6.44	124.22	121.00
60	DA	1140	C	C5-C6-N1	6.43	124.22	121.00
60	DA	1493	C	C5-C6-N1	6.43	124.22	121.00
60	DA	1139	G	O4'-C1'-N9	6.43	113.34	108.20
60	DA	1493	C	N3-C2-O2	-6.43	117.40	121.90
22	AW	68	U	C6-N1-C1'	6.43	130.20	121.20
60	BA	1493	C	C6-N1-C2	-6.42	117.73	120.30
60	BA	1226	A	C4-C5-C6	6.42	120.21	117.00
60	DA	1025	G	C5-C6-O6	-6.41	124.75	128.60
60	DA	2264	C	C2-N1-C1'	6.41	125.85	118.80
20	CA	1213	A	N1-C6-N6	-6.37	114.78	118.60
1	AB	164	VAL	CB-CA-C	-6.37	99.31	111.40
59	BB	75	G	N3-C4-C5	-6.37	125.42	128.60
20	AA	815	A	C6-C5-N7	6.36	136.75	132.30
60	BA	1048	A	C4-N9-C1'	6.36	137.74	126.30
60	DA	1137	G	C4-N9-C1'	6.36	134.76	126.50
60	BA	2040	C	OP1-P-OP2	-6.35	110.07	119.60
27	DE	61	ARG	C-N-CD	6.35	141.73	128.40
60	DA	103	A	N1-C6-N6	6.34	122.41	118.60
60	BA	645	C	N3-C2-O2	-6.33	117.47	121.90
60	BA	621	A	N1-C6-N6	-6.33	114.80	118.60
20	AA	1213	A	C5-C6-N6	6.33	128.76	123.70
20	CA	754	C	C6-N1-C2	-6.32	117.77	120.30
20	CA	1009	G	O4'-C1'-N9	6.32	113.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	DF	156	LEU	N-CA-C	-6.32	93.94	111.00
60	BA	1493	C	N3-C2-O2	-6.32	117.48	121.90
60	BA	1314	C	C5-C6-N1	6.31	124.16	121.00
60	BA	509	C	C6-N1-C2	-6.30	117.78	120.30
59	DB	75	G	C5-C6-N1	6.30	114.65	111.50
60	BA	1389	G	N3-C4-N9	6.30	129.78	126.00
60	DA	1019	U	C6-N1-C2	-6.29	117.22	121.00
20	AA	622	A	N1-C6-N6	-6.29	114.83	118.60
11	CL	60	LEU	CA-CB-CG	6.29	129.76	115.30
60	BA	860	U	N3-C2-O2	-6.28	117.81	122.20
20	CA	1393	U	N1-C2-N3	-6.28	111.13	114.90
20	AA	1170	A	N1-C6-N6	6.27	122.36	118.60
29	BG	139	LEU	CA-CB-CG	6.27	129.71	115.30
60	DA	459	U	N3-C4-C5	6.26	118.36	114.60
60	DA	1674	G	N9-C4-C5	-6.26	102.90	105.40
20	CA	115	G	C8-N9-C1'	-6.25	118.88	127.00
60	DA	647	G	N3-C4-N9	6.25	129.75	126.00
60	BA	1675	C	C2-N1-C1'	6.23	125.66	118.80
60	BA	647	G	N3-C4-N9	6.23	129.74	126.00
60	BA	673	C	N3-C4-C5	6.22	124.39	121.90
60	DA	1377	G	N3-C4-N9	6.22	129.73	126.00
60	DA	30	G	N9-C4-C5	-6.21	102.91	105.40
60	DA	294	A	C4-C5-C6	6.21	120.11	117.00
60	DA	1006	C	C5-C6-N1	6.21	124.10	121.00
60	DA	2598	A	N1-C6-N6	6.21	122.32	118.60
20	CA	68(W)	G	N3-C4-N9	-6.20	122.28	126.00
1	AB	187	LEU	CA-CB-CG	6.20	129.56	115.30
20	AA	1034	G	N3-C2-N2	-6.20	115.56	119.90
20	AA	618	C	C5-C4-N4	6.20	124.54	120.20
60	BA	1048	A	C8-N9-C1'	-6.20	116.55	127.70
59	BB	75	G	N3-C4-N9	6.19	129.71	126.00
20	CA	68(E)	G	C6-N1-C2	6.19	128.81	125.10
60	DA	673	C	C5-C4-N4	-6.18	115.87	120.20
60	BA	1139	G	N3-C4-N9	-6.17	122.30	126.00
60	DA	1107	G	N9-C4-C5	6.17	107.87	105.40
20	CA	1213	A	N9-C4-C5	6.17	108.27	105.80
60	DA	565	C	C2-N3-C4	-6.15	116.83	119.90
20	CA	815	A	C4-C5-N7	-6.14	107.63	110.70
20	CA	1393	U	O4'-C1'-N1	6.14	113.11	108.20
60	BA	121	G	N3-C4-N9	6.14	129.68	126.00
41	BW	107	LEU	CA-CB-CG	6.13	129.41	115.30
22	AW	61	C	C2-N1-C1'	6.13	125.54	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	2681	C	C2-N1-C1'	6.12	125.53	118.80
60	BA	2023	G	N3-C4-N9	-6.11	122.33	126.00
60	DA	1385	G	N3-C4-N9	-6.11	122.34	126.00
60	BA	103	A	N3-C4-N9	6.10	132.28	127.40
29	BG	98	ARG	NE-CZ-NH1	6.10	123.35	120.30
60	DA	1818	U	C2-N1-C1'	-6.10	110.38	117.70
60	BA	2119	A	C5-C6-N6	6.09	128.57	123.70
60	DA	1937	A	P-O3'-C3'	6.09	127.01	119.70
20	AA	174	C	C2-N1-C1'	6.09	125.50	118.80
60	BA	1982	C	C2-N1-C1'	6.08	125.49	118.80
60	BA	2802	G	N9-C4-C5	-6.08	102.97	105.40
60	BA	2801	A	N1-C6-N6	6.08	122.25	118.60
20	CA	1481	U	N1-C2-O2	-6.08	118.55	122.80
60	BA	83	G	C2-N3-C4	-6.07	108.86	111.90
28	BF	193	VAL	CB-CA-C	6.07	122.93	111.40
20	CA	838(A)	U	C2-N1-C1'	6.06	124.98	117.70
60	BA	1137	G	N1-C2-N3	6.06	127.54	123.90
60	BA	2092	U	P-O3'-C3'	6.05	126.96	119.70
20	AA	1034	G	N1-C2-N2	6.05	121.64	116.20
26	BD	95	LEU	CA-CB-CG	6.04	129.20	115.30
25	DC	214	TYR	CB-CG-CD1	6.04	124.62	121.00
60	DA	2043	C	C2-N1-C1'	6.04	125.44	118.80
60	DA	974(B)	C	N1-C2-O2	6.03	122.52	118.90
20	CA	328	C	C2-N1-C1'	6.03	125.43	118.80
59	DB	81	G	C5-C6-O6	-6.02	124.99	128.60
60	DA	1140	C	C6-N1-C2	-6.02	117.89	120.30
60	DA	882	G	N9-C4-C5	5.99	107.80	105.40
20	CA	1213	A	C5-C6-N6	5.99	128.49	123.70
20	CA	421	U	C2-N1-C1'	5.98	124.88	117.70
60	BA	2248	C	C2-N1-C1'	-5.98	112.22	118.80
23	AY	207	ASP	C-N-CA	-5.98	106.75	121.70
60	BA	103	A	C8-N9-C1'	-5.97	116.96	127.70
60	BA	121	G	C6-C5-N7	-5.97	126.82	130.40
20	CA	1170	A	N1-C6-N6	5.96	122.18	118.60
20	CA	1493	A	O5'-P-OP2	-5.96	100.33	105.70
60	DA	1135	C	C6-N1-C1'	-5.96	113.64	120.80
20	CA	1248	A	C5-C6-N6	5.96	128.47	123.70
60	BA	2343	C	N1-C2-O2	5.96	122.48	118.90
20	AA	815	A	N3-C4-N9	-5.96	122.64	127.40
20	AA	1289	A	N1-C6-N6	-5.95	115.03	118.60
60	BA	2802	G	N3-C4-N9	5.94	129.56	126.00
20	AA	1034	G	N9-C4-C5	5.93	107.77	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	103	A	C8-N9-C1'	-5.93	117.02	127.70
60	BA	529	A	C4-C5-C6	-5.93	114.03	117.00
20	CA	993	G	N3-C4-N9	5.92	129.55	126.00
60	DA	974(B)	C	C2-N1-C1'	5.92	125.31	118.80
20	CA	68(W)	G	N3-C2-N2	-5.90	115.77	119.90
23	AY	33	LEU	N-CA-C	-5.89	95.10	111.00
20	AA	1332	A	N9-C4-C5	-5.88	103.45	105.80
60	BA	907	U	O4'-C1'-N1	5.88	112.91	108.20
20	AA	115	G	C4-N9-C1'	5.87	134.14	126.50
20	AA	1332	A	C4-C5-C6	5.85	119.93	117.00
60	BA	2181	G	N3-C4-N9	-5.85	122.49	126.00
60	BA	1135	C	N1-C2-O2	5.84	122.41	118.90
20	CA	1045	C	C2-N1-C1'	5.84	125.23	118.80
20	AA	1045	C	N1-C2-O2	5.84	122.40	118.90
60	DA	893	C	C6-N1-C1'	5.84	127.81	120.80
60	DA	1818	U	O4'-C1'-N1	5.83	112.86	108.20
20	AA	1028(C)	G	N1-C2-N2	-5.83	110.95	116.20
60	BA	2802	G	C4-C5-N7	5.83	113.13	110.80
59	BB	75	G	C5-C6-N1	5.83	114.41	111.50
60	BA	1327	C	C6-N1-C2	-5.83	117.97	120.30
60	DA	673	C	N3-C4-C5	5.83	124.23	121.90
60	DA	1420	U	C2-N1-C1'	5.82	124.69	117.70
60	BA	2792	G	O4'-C1'-N9	5.82	112.85	108.20
60	BA	2343	C	C6-N1-C1'	-5.81	113.83	120.80
60	DA	1570	A	N1-C6-N6	5.81	122.09	118.60
28	DF	125	LEU	CA-CB-CG	5.81	128.65	115.30
60	BA	2794	C	C6-N1-C1'	-5.80	113.84	120.80
22	CW	61	C	C6-N1-C1'	-5.79	113.85	120.80
60	BA	737	C	C2-N1-C1'	5.79	125.16	118.80
60	BA	974(B)	C	C2-N1-C1'	5.79	125.16	118.80
60	DA	83	G	C2-N3-C4	-5.79	109.01	111.90
60	DA	1784	A	N1-C6-N6	-5.78	115.13	118.60
60	BA	30	G	N3-C4-C5	-5.78	125.71	128.60
20	CA	68(W)	G	N9-C4-C5	5.78	107.71	105.40
60	BA	1048	A	N3-C4-N9	5.78	132.02	127.40
46	D1	40	ARG	N-CA-C	5.78	126.59	111.00
60	BA	2505	G	C4-C5-N7	5.77	113.11	110.80
60	BA	2289	G	C6-C5-N7	-5.77	126.94	130.40
60	BA	271(B)	C	C6-N1-C1'	-5.76	113.89	120.80
60	DA	882	G	C5-C6-O6	5.76	132.06	128.60
60	DA	1048	A	C6-C5-N7	-5.76	128.27	132.30
60	BA	2714	G	N3-C4-N9	5.75	129.45	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	1982	C	N1-C2-O2	5.75	122.35	118.90
20	AA	754	C	C6-N1-C2	-5.75	118.00	120.30
60	BA	565	C	C2-N3-C4	-5.75	117.03	119.90
60	BA	529	A	N1-C6-N6	-5.74	115.16	118.60
60	BA	45	G	N3-C4-N9	-5.74	122.56	126.00
20	CA	1034	G	N3-C2-N2	-5.74	115.88	119.90
60	DA	2794	C	C5-C6-N1	5.74	123.87	121.00
60	BA	1774	C	N3-C2-O2	-5.73	117.89	121.90
60	DA	2791	C	C2-N1-C1'	5.73	125.10	118.80
60	BA	2009	G	N9-C4-C5	5.73	107.69	105.40
60	BA	2792	G	C8-N9-C4	-5.73	104.11	106.40
20	CA	993	G	N9-C4-C5	-5.73	103.11	105.40
60	DA	271(B)	C	C6-N1-C1'	-5.72	113.93	120.80
20	AA	1045	C	C6-N1-C1'	-5.72	113.94	120.80
60	BA	1385	G	N3-C4-N9	-5.71	122.57	126.00
22	CW	20(A)	U	P-O3'-C3'	5.71	126.56	119.70
20	AA	748	C	P-O3'-C3'	5.71	126.55	119.70
60	BA	24	G	N3-C4-N9	-5.71	122.58	126.00
60	BA	2023	G	N3-C2-N2	-5.70	115.91	119.90
60	DA	2802	G	N3-C4-N9	5.70	129.42	126.00
28	BF	156	LEU	N-CA-C	-5.70	95.61	111.00
60	DA	1377	G	C4-N9-C1'	5.70	133.91	126.50
60	DA	2804	C	C6-N1-C1'	5.70	127.64	120.80
60	BA	1078	U	C2-N1-C1'	5.70	124.53	117.70
20	CA	1508	G	N1-C2-N3	5.70	127.32	123.90
60	BA	1110	G	C2-N3-C4	-5.68	109.06	111.90
60	BA	1872	A	N1-C6-N6	5.68	122.01	118.60
60	DA	645	C	C2-N1-C1'	5.68	125.04	118.80
60	DA	893	C	C2-N1-C1'	-5.67	112.56	118.80
20	AA	553	A	C8-N9-C4	5.67	108.07	105.80
20	AA	1001	G	N3-C4-N9	-5.67	122.60	126.00
60	BA	2101	G	N9-C4-C5	5.67	107.67	105.40
20	CA	1009	G	C8-N9-C1'	5.67	134.37	127.00
20	AA	421	U	C2-N1-C1'	5.66	124.49	117.70
60	BA	860	U	N1-C2-O2	5.66	126.76	122.80
20	AA	68(W)	G	N3-C4-N9	-5.65	122.61	126.00
60	BA	24	G	C8-N9-C1'	5.65	134.35	127.00
20	CA	687	A	OP2-P-O3'	5.65	117.63	105.20
20	AA	1436	U	C5-C4-O4	-5.65	122.51	125.90
60	BA	95	G	N3-C4-C5	5.64	131.42	128.60
20	AA	1425	U	N1-C2-O2	5.63	126.74	122.80
60	BA	1226	A	C6-C5-N7	-5.63	128.36	132.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	894	C	C6-N1-C1'	5.63	127.56	120.80
20	CA	1045	C	C6-N1-C1'	-5.63	114.04	120.80
60	DA	1818	U	C6-N1-C1'	5.63	129.08	121.20
60	DA	271(B)	C	C5-C6-N1	5.62	123.81	121.00
20	CA	1281	U	N3-C2-O2	-5.62	118.27	122.20
60	DA	2681	C	C6-N1-C1'	-5.62	114.06	120.80
60	DA	278	A	P-O3'-C3'	5.61	126.43	119.70
20	AA	1166	G	N1-C2-N2	-5.61	111.15	116.20
20	AA	1200	C	C2-N1-C1'	-5.61	112.63	118.80
20	CA	1009	G	C4-N9-C1'	-5.61	119.21	126.50
60	DA	1120	G	C5-C6-O6	5.61	131.96	128.60
60	BA	645	C	C6-N1-C1'	-5.61	114.07	120.80
20	CA	1248	A	N9-C4-C5	5.60	108.04	105.80
60	DA	2264	C	C6-N1-C1'	-5.60	114.08	120.80
22	AW	61	C	N1-C2-O2	5.60	122.26	118.90
60	DA	1314	C	N1-C2-O2	5.60	122.26	118.90
25	DC	214	TYR	CZ-CE2-CD2	5.60	124.84	119.80
1	CB	161	ALA	C-N-CA	-5.59	107.72	121.70
60	BA	278	A	P-O3'-C3'	5.59	126.41	119.70
20	CA	165	C	N1-C2-O2	-5.58	115.55	118.90
60	DA	116	C	C6-N1-C2	-5.58	118.07	120.30
26	DD	177	LEU	CA-CB-CG	5.58	128.13	115.30
60	DA	1424	G	N3-C4-N9	-5.58	122.65	126.00
20	AA	1034	G	C8-N9-C1'	5.58	134.25	127.00
20	AA	308	C	N3-C2-O2	-5.57	118.00	121.90
60	DA	645	C	N3-C2-O2	-5.57	118.00	121.90
60	BA	2248	C	C6-N1-C1'	5.57	127.48	120.80
20	CA	1054	C	N1-C2-O2	5.56	122.24	118.90
60	BA	2101	G	C4-C5-N7	-5.55	108.58	110.80
20	AA	1508	G	N1-C2-N3	5.55	127.23	123.90
20	CA	1001	G	N9-C4-C5	5.55	107.62	105.40
60	BA	251	A	N3-C4-C5	-5.54	122.92	126.80
60	BA	509	C	C5-C6-N1	5.54	123.77	121.00
60	BA	1998	G	N3-C4-N9	5.54	129.33	126.00
60	DA	1872	A	N1-C6-N6	5.54	121.93	118.60
60	DA	2804	C	C2-N1-C1'	-5.54	112.70	118.80
20	AA	1016	A	N1-C6-N6	5.54	121.92	118.60
60	BA	1774	C	N1-C2-O2	5.54	122.22	118.90
60	BA	1090	U	O4'-C1'-N1	5.54	112.63	108.20
1	AB	172	ILE	N-CA-C	-5.53	96.07	111.00
20	CA	665	A	N1-C6-N6	-5.52	115.29	118.60
60	DA	1377	G	C6-C5-N7	-5.52	127.09	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	1937	A	P-O3'-C3'	5.51	126.32	119.70
26	BD	177	LEU	CA-CB-CG	5.51	127.97	115.30
20	AA	1028(F)	A	C6-C5-N7	-5.51	128.44	132.30
22	AW	66	C	N1-C2-O2	5.51	122.20	118.90
20	AA	553	A	N9-C4-C5	-5.51	103.60	105.80
20	AA	1248	A	N1-C6-N6	-5.51	115.30	118.60
22	CW	68	U	C2-N1-C1'	-5.51	111.09	117.70
20	AA	1034	G	C6-C5-N7	5.50	133.70	130.40
60	BA	2023	G	N1-C2-N2	5.50	121.15	116.20
60	DA	510	C	N1-C2-O2	5.50	122.20	118.90
1	AB	161	ALA	C-N-CA	-5.50	107.96	121.70
27	BE	10	GLY	N-CA-C	5.50	126.84	113.10
20	CA	1010	G	N3-C4-N9	5.50	129.30	126.00
20	AA	1248	A	C5-C6-N6	5.50	128.10	123.70
20	CA	1171	G	N3-C4-N9	-5.49	122.70	126.00
20	AA	1001	G	C8-N9-C1'	5.49	134.14	127.00
20	CA	186(L)	G	N3-C4-N9	-5.49	122.71	126.00
20	CA	1054	C	C2-N1-C1'	5.49	124.84	118.80
22	AW	68	U	N1-C2-O2	-5.49	118.96	122.80
20	CA	186(G)	C	N3-C2-O2	-5.48	118.06	121.90
60	BA	1083	U	O4'-C1'-N1	5.48	112.58	108.20
28	DF	191	ARG	N-CA-C	5.48	125.80	111.00
60	DA	1428	C	C5-C4-N4	-5.48	116.36	120.20
28	DF	193	VAL	CB-CA-C	5.48	121.81	111.40
60	BA	510	C	N1-C2-O2	5.48	122.19	118.90
60	BA	2119	A	N1-C6-N6	-5.47	115.31	118.60
60	DA	1377	G	C8-N9-C1'	-5.47	119.88	127.00
60	BA	894	C	C2-N1-C1'	-5.47	112.78	118.80
60	DA	544	C	C2-N1-C1'	5.47	124.82	118.80
59	DB	101	A	C5-C6-N1	5.47	120.43	117.70
60	BA	251	A	C6-N1-C2	-5.47	115.32	118.60
20	AA	1002	G	N3-C4-N9	-5.47	122.72	126.00
60	DA	2111	C	O4'-C1'-N1	5.47	112.57	108.20
60	BA	645	C	C6-N1-C2	-5.46	118.11	120.30
60	BA	30	G	C8-N9-C1'	-5.46	119.91	127.00
21	AV	18	G	N3-C4-C5	-5.46	125.87	128.60
20	CA	243	A	N1-C6-N6	-5.46	115.33	118.60
59	BB	95	U	C2-N1-C1'	-5.45	111.16	117.70
20	AA	872	A	O4'-C1'-N9	5.45	112.56	108.20
60	BA	1022	G	P-O3'-C3'	5.45	126.23	119.70
60	DA	363(F)	U	N1-C2-O2	5.45	126.61	122.80
29	BG	114	ILE	C-N-CA	5.44	135.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	2802	G	N3-C2-N2	5.44	123.71	119.90
25	DC	164	PHE	N-CA-CB	5.44	120.40	110.60
59	BB	23	G	N3-C4-N9	5.44	129.26	126.00
60	BA	1420	U	C6-N1-C1'	-5.44	113.58	121.20
60	BA	882	G	N9-C4-C5	5.44	107.58	105.40
46	B1	17	SER	N-CA-C	-5.44	96.32	111.00
59	BB	95	U	O4'-C1'-N1	5.43	112.55	108.20
60	BA	1674	G	C6-C5-N7	-5.43	127.14	130.40
26	DD	95	LEU	CA-CB-CG	5.43	127.80	115.30
20	AA	421	U	N1-C2-O2	5.43	126.60	122.80
60	BA	1306	C	O4'-C1'-N1	5.43	112.54	108.20
60	DA	103	A	N3-C4-N9	5.42	131.74	127.40
20	AA	1028(C)	G	N3-C2-N2	5.42	123.69	119.90
21	AV	18	G	C4-N9-C1'	5.42	133.54	126.50
60	BA	737	C	C6-N1-C2	-5.41	118.14	120.30
60	DA	1025	G	N1-C6-O6	5.41	123.15	119.90
60	BA	270(W)	G	N3-C4-N9	-5.41	122.75	126.00
60	DA	2786	U	C2-N1-C1'	5.40	124.19	117.70
60	BA	882	G	C5-C6-O6	5.40	131.84	128.60
60	DA	645	C	N1-C2-O2	5.40	122.14	118.90
60	DA	930	U	C2-N1-C1'	5.40	124.18	117.70
20	CA	312	C	N3-C2-O2	-5.40	118.12	121.90
20	AA	156	G	N1-C2-N2	5.39	121.06	116.20
23	AY	23	ALA	N-CA-CB	-5.39	102.55	110.10
60	BA	1420	U	C5-C6-N1	5.39	125.40	122.70
20	CA	475	G	N3-C4-N9	-5.39	122.76	126.00
60	DA	1048	A	N3-C4-N9	5.39	131.72	127.40
60	BA	1313	U	C6-N1-C1'	-5.39	113.65	121.20
60	BA	2791	C	C6-N1-C2	-5.39	118.14	120.30
60	DA	1525	G	N3-C4-N9	-5.39	122.77	126.00
60	DA	1314	C	C6-N1-C1'	-5.39	114.34	120.80
60	DA	45	G	N3-C4-N9	-5.38	122.77	126.00
20	AA	1034	G	N3-C4-C5	5.38	131.29	128.60
60	DA	1674	G	C6-C5-N7	-5.38	127.17	130.40
20	AA	1332	A	C6-C5-N7	-5.37	128.54	132.30
60	BA	893	C	C5-C4-N4	5.37	123.96	120.20
60	DA	9	U	N1-C2-O2	5.37	126.56	122.80
60	BA	271(C)	G	P-O3'-C3'	5.37	126.14	119.70
60	BA	1420	U	N1-C2-O2	5.37	126.56	122.80
59	BB	95	U	C6-N1-C1'	5.37	128.71	121.20
60	DA	2598	A	C4-C5-C6	5.37	119.68	117.00
21	AV	19	G	N3-C4-C5	5.36	131.28	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	24	G	N3-C4-N9	-5.36	122.78	126.00
60	BA	95	G	N3-C2-N2	-5.36	116.15	119.90
60	DA	459	U	C4-C5-C6	-5.36	116.48	119.70
60	BA	270(E)	C	C6-N1-C1'	5.36	127.23	120.80
60	BA	2791	C	C2-N1-C1'	5.36	124.70	118.80
60	BA	1138	G	C4-N9-C1'	-5.36	119.53	126.50
46	D1	17	SER	N-CA-C	-5.36	96.54	111.00
60	DA	1784	A	C8-N9-C4	-5.36	103.66	105.80
60	DA	454	A	C5-C6-N6	5.35	127.98	123.70
60	DA	1110	G	C2-N3-C4	-5.35	109.22	111.90
20	AA	1027	C	C6-N1-C2	-5.35	118.16	120.30
59	BB	101	A	N3-C4-N9	5.34	131.68	127.40
60	BA	1398	C	N1-C2-O2	5.34	122.11	118.90
1	CB	164	VAL	CB-CA-C	-5.34	101.24	111.40
60	BA	1157	G	N3-C4-N9	5.34	129.21	126.00
20	AA	307	C	N1-C2-O2	5.34	122.11	118.90
60	DA	30	G	C8-N9-C1'	-5.34	120.06	127.00
60	DA	2780	G	P-O3'-C3'	5.34	126.11	119.70
25	DC	138	LEU	N-CA-C	5.34	125.41	111.00
60	BA	2321	G	C8-N9-C4	-5.34	104.27	106.40
20	CA	1001	G	N3-C4-N9	-5.34	122.80	126.00
1	AB	163	PHE	O-C-N	5.33	131.23	122.70
22	CW	68	U	C6-N1-C1'	5.33	128.66	121.20
60	BA	1676	A	C5-C6-N1	5.33	120.36	117.70
60	BA	1570	A	N1-C6-N6	5.32	121.79	118.60
60	DA	1288	U	N3-C2-O2	-5.32	118.48	122.20
60	BA	504	U	N1-C2-O2	5.32	126.52	122.80
60	BA	2610	C	C4-C5-C6	-5.31	114.74	117.40
60	DA	647	G	C8-N9-C1'	-5.31	120.10	127.00
60	DA	1048	A	C8-N9-C1'	-5.31	118.14	127.70
60	BA	1493	C	C6-N1-C1'	-5.30	114.44	120.80
60	DA	1188	U	C2-N1-C1'	5.30	124.06	117.70
60	BA	422	A	C8-N9-C4	-5.30	103.68	105.80
60	DA	510	C	C2-N1-C1'	5.30	124.63	118.80
20	AA	1535	C	OP1-P-O3'	5.30	116.85	105.20
20	CA	115	G	OP2-P-O3'	5.29	116.85	105.20
60	DA	2009	G	N3-C4-N9	-5.29	122.82	126.00
60	DA	1083	U	O4'-C1'-N1	5.29	112.43	108.20
60	BA	1327	C	C5-C6-N1	5.29	123.64	121.00
20	CA	1465	C	C5-C4-N4	-5.29	116.50	120.20
25	DC	213	VAL	N-CA-C	-5.29	96.73	111.00
20	AA	1071	C	C2-N1-C1'	5.28	124.61	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	AA	186(L)	G	C4-N9-C1'	-5.28	119.64	126.50
60	BA	1139	G	N3-C4-C5	5.28	131.24	128.60
60	DA	121	G	C6-C5-N7	-5.28	127.23	130.40
20	AA	1002	G	N9-C4-C5	5.27	107.51	105.40
60	DA	121	G	C4-N9-C1'	5.27	133.35	126.50
20	AA	1527	C	C6-N1-C2	-5.27	118.19	120.30
20	AA	68(C)	C	C6-N1-C1'	5.27	127.12	120.80
20	AA	1200	C	C6-N1-C1'	5.27	127.12	120.80
60	DA	1420	U	OP1-P-O3'	5.27	116.79	105.20
60	DA	1784	A	C2-N3-C4	5.26	113.23	110.60
20	CA	1200	C	C6-N1-C1'	5.26	127.11	120.80
20	AA	618	C	N3-C4-C5	-5.26	119.80	121.90
40	DV	18	LEU	CA-CB-CG	5.26	127.40	115.30
60	DA	422	A	C8-N9-C4	-5.26	103.70	105.80
20	CA	567	G	N3-C4-N9	5.26	129.15	126.00
60	DA	1047	G	O4'-C1'-N9	5.26	112.40	108.20
20	AA	998	G	N3-C4-N9	-5.25	122.85	126.00
60	BA	2634	G	N3-C4-N9	-5.25	122.85	126.00
60	DA	647	G	C6-C5-N7	-5.25	127.25	130.40
60	DA	647	G	C4-N9-C1'	5.25	133.32	126.50
28	DF	154	VAL	CG1-CB-CG2	-5.25	102.50	110.90
60	DA	1139	G	N3-C4-N9	-5.25	122.85	126.00
60	DA	2804	C	O4'-C1'-N1	5.25	112.40	108.20
60	BA	894	C	C6-N1-C1'	5.25	127.09	120.80
41	BW	51	LEU	CA-CB-CG	5.24	127.36	115.30
60	BA	1107	G	N3-C2-N2	-5.24	116.23	119.90
60	DA	671	C	C2-N1-C1'	5.24	124.56	118.80
20	AA	186(G)	C	N3-C2-O2	-5.24	118.23	121.90
60	DA	883	G	N3-C4-N9	-5.24	122.86	126.00
28	BF	191	ARG	N-CA-C	5.23	125.13	111.00
20	AA	1045	C	C2-N1-C1'	5.23	124.55	118.80
46	B1	40	ARG	N-CA-C	5.23	125.11	111.00
20	AA	1071	C	C5-C6-N1	5.22	123.61	121.00
20	AA	1265	G	N3-C4-N9	-5.22	122.87	126.00
60	BA	883	G	N9-C4-C5	5.22	107.49	105.40
20	AA	1508	G	N3-C4-N9	5.22	129.13	126.00
60	BA	1048	A	N9-C4-C5	-5.21	103.71	105.80
20	CA	1332	A	C4-C5-C6	5.21	119.61	117.00
60	BA	974(B)	C	C5-C6-N1	5.21	123.61	121.00
60	DA	2038	G	C6-C5-N7	-5.21	127.27	130.40
60	BA	1726	G	N3-C4-N9	-5.21	122.87	126.00
60	DA	1313	U	C6-N1-C1'	-5.21	113.91	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	2585	U	N1-C2-O2	5.21	126.44	122.80
60	BA	2505	G	N3-C4-C5	5.20	131.20	128.60
60	BA	1774	C	C5-C6-N1	5.20	123.60	121.00
20	CA	312	C	N1-C2-O2	5.20	122.02	118.90
20	CA	328	C	P-O3'-C3'	5.20	125.94	119.70
60	DA	907	U	O4'-C1'-N1	5.20	112.36	108.20
60	DA	2794	C	C5-C4-N4	-5.19	116.56	120.20
42	DX	57	LEU	CA-CB-CG	5.19	127.24	115.30
60	BA	576	U	C5-C4-O4	-5.19	122.79	125.90
60	BA	1311	G	N9-C4-C5	-5.19	103.32	105.40
20	AA	129(A)	G	N3-C4-N9	5.18	129.11	126.00
20	AA	308	C	N1-C2-O2	5.18	122.01	118.90
60	BA	2151	G	N3-C4-N9	-5.18	122.89	126.00
20	AA	646	U	N1-C2-O2	5.17	126.42	122.80
60	DA	294	A	C6-C5-N7	-5.17	128.68	132.30
60	BA	1019	U	C2-N3-C4	5.17	130.10	127.00
60	BA	1139	G	C4-N9-C1'	-5.17	119.78	126.50
60	BA	1525	G	N9-C4-C5	5.16	107.47	105.40
60	BA	270(X)	G	N3-C4-N9	-5.16	122.91	126.00
60	BA	1213	A	N1-C6-N6	5.16	121.69	118.60
60	BA	24	G	C4-N9-C1'	-5.16	119.80	126.50
60	BA	2040	C	C6-N1-C2	-5.16	118.24	120.30
21	AV	18	G	N3-C4-N9	5.15	129.09	126.00
60	BA	75	G	C6-N1-C2	5.15	128.19	125.10
60	BA	1598	C	C5-C6-N1	5.15	123.58	121.00
20	CA	1034	G	N3-C4-C5	5.15	131.18	128.60
1	CB	163	PHE	O-C-N	5.15	130.93	122.70
20	CA	978	A	N1-C6-N6	-5.15	115.51	118.60
60	BA	895	U	C2-N3-C4	5.14	130.09	127.00
22	CW	20	U	C2-N1-C1'	5.14	123.87	117.70
59	BB	50	G	N3-C4-N9	-5.14	122.91	126.00
20	CA	993	G	C8-N9-C1'	-5.14	120.31	127.00
60	DA	130	C	C2-N1-C1'	5.14	124.46	118.80
60	BA	893	C	C6-N1-C1'	5.14	126.97	120.80
20	AA	61	G	N3-C4-N9	-5.14	122.92	126.00
20	AA	186(L)	G	N3-C2-N2	-5.14	116.30	119.90
60	DA	1107	G	N3-C2-N2	-5.14	116.30	119.90
20	AA	186(L)	G	N3-C4-C5	5.13	131.17	128.60
59	DB	101	A	C5-C6-N6	-5.13	119.59	123.70
60	DA	271(C)	G	P-O3'-C3'	5.13	125.86	119.70
1	AB	185	ILE	O-C-N	5.13	130.91	122.70
20	AA	475	G	N3-C4-N9	-5.13	122.92	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	CA	68(N)	U	O4'-C1'-N1	5.13	112.30	108.20
60	BA	895	U	C5-C6-N1	5.13	125.26	122.70
60	DA	103	A	C4-N9-C1'	5.13	135.53	126.30
25	BC	12	LEU	CA-CB-CG	5.12	127.09	115.30
20	CA	201	C	O4'-C1'-N1	5.12	112.30	108.20
25	BC	225	ILE	CB-CA-C	-5.12	101.36	111.60
60	DA	907	U	C5-C4-O4	5.12	128.97	125.90
20	AA	1001	G	N9-C4-C5	5.12	107.45	105.40
60	BA	103	A	C4-N9-C1'	5.12	135.51	126.30
20	AA	1290	G	C4-N9-C1'	5.12	133.15	126.50
29	BG	43	LEU	CA-CB-CG	5.11	127.06	115.30
20	AA	384	G	N3-C4-N9	-5.11	122.93	126.00
60	BA	2794	C	C5-C6-N1	5.11	123.55	121.00
60	BA	1872	A	C4-C5-C6	5.10	119.55	117.00
20	AA	1009	G	C4-N9-C1'	-5.10	119.87	126.50
20	CA	421	U	N1-C2-O2	5.10	126.37	122.80
28	BF	174	VAL	N-CA-C	-5.10	97.24	111.00
20	AA	300	A	N1-C6-N6	5.09	121.66	118.60
60	BA	1498	C	C6-N1-C2	-5.09	118.26	120.30
60	BA	2429	G	O4'-C1'-N9	5.09	112.27	108.20
60	BA	2681	C	C2-N1-C1'	5.09	124.40	118.80
60	DA	2343	C	C2-N1-C1'	5.09	124.40	118.80
20	AA	426	G	N3-C4-N9	-5.09	122.95	126.00
60	BA	527	C	N3-C2-O2	-5.09	118.34	121.90
60	BA	645	C	C5-C6-N1	5.09	123.55	121.00
60	DA	2014	A	N1-C6-N6	-5.09	115.55	118.60
22	AW	53	G	N3-C4-N9	5.09	129.05	126.00
20	CA	1419	G	C6-N1-C2	5.09	128.15	125.10
20	AA	328	C	P-O3'-C3'	5.08	125.80	119.70
20	AA	815	A	C6-N1-C2	5.08	121.65	118.60
60	BA	251	A	N3-C4-N9	5.08	131.47	127.40
20	CA	992	U	P-O3'-C3'	5.08	125.80	119.70
20	CA	1530	G	O4'-C1'-N9	5.08	112.27	108.20
60	DA	2714	G	N3-C4-N9	5.08	129.05	126.00
60	BA	1639	U	C2-N1-C1'	5.08	123.79	117.70
60	BA	294	A	N1-C6-N6	5.08	121.64	118.60
60	DA	1036	G	N3-C4-N9	-5.08	122.95	126.00
60	DA	1338	G	N3-C4-N9	5.08	129.04	126.00
20	CA	186(L)	G	N3-C2-N2	-5.07	116.35	119.90
20	AA	1034	G	C4-N9-C1'	-5.07	119.91	126.50
60	BA	529	A	C5-C6-N1	5.07	120.23	117.70
60	BA	1675	C	C6-N1-C1'	-5.07	114.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	DA	2447	G	P-O3'-C3'	5.07	125.78	119.70
60	BA	2013	A	N1-C6-N6	-5.07	115.56	118.60
25	BC	164	PHE	N-CA-CB	5.07	119.72	110.60
60	BA	2808	U	N1-C2-O2	5.07	126.34	122.80
20	CA	1508	G	C2-N3-C4	-5.06	109.37	111.90
60	DA	103	A	C4-C5-C6	5.06	119.53	117.00
60	BA	2158	A	P-O3'-C3'	5.06	125.77	119.70
20	CA	1393	U	C4-C5-C6	-5.06	116.66	119.70
60	DA	1048	A	C4-N9-C1'	5.06	135.41	126.30
60	DA	1998	G	N3-C4-N9	5.06	129.04	126.00
60	DA	509	C	C6-N1-C2	-5.06	118.28	120.30
60	DA	2147	G	C6-C5-N7	-5.06	127.37	130.40
60	DA	2040	C	N3-C4-C5	-5.05	119.88	121.90
60	BA	509	C	N1-C2-O2	5.05	121.93	118.90
20	CA	328	C	N3-C2-O2	-5.05	118.36	121.90
20	CA	475	G	N3-C2-N2	-5.05	116.36	119.90
46	D1	13	ILE	CB-CA-C	5.05	121.69	111.60
60	DA	2794	C	N3-C4-N4	5.04	121.53	118.00
60	BA	2041	U	C5-C6-N1	5.04	125.22	122.70
60	BA	974(B)	C	C6-N1-C2	-5.04	118.28	120.30
20	CA	815	A	C8-N9-C1'	5.04	136.77	127.70
20	CA	1533	C	O5'-P-OP1	-5.04	101.17	105.70
20	AA	1002	G	C8-N9-C1'	5.04	133.55	127.00
60	BA	270(X)	G	N9-C4-C5	5.04	107.41	105.40
60	DA	1138	G	C5-C6-O6	-5.03	125.58	128.60
20	AA	186(L)	G	C6-C5-N7	5.03	133.42	130.40
60	BA	30	G	C4-N9-C1'	5.03	133.04	126.50
20	CA	618	C	N3-C4-C5	-5.03	119.89	121.90
20	CA	1289	A	N1-C6-N6	-5.03	115.58	118.60
60	DA	130	C	N1-C2-O2	5.03	121.92	118.90
60	DA	279	C	N1-C2-O2	-5.03	115.88	118.90
20	AA	1281	U	N3-C2-O2	-5.03	118.68	122.20
60	BA	271(B)	C	N3-C2-O2	-5.03	118.38	121.90
60	DA	270(W)	G	N3-C4-N9	-5.03	122.98	126.00
20	AA	687	A	P-O3'-C3'	5.03	125.73	119.70
60	BA	2248	C	N1-C2-O2	-5.03	115.89	118.90
20	CA	1034	G	C6-C5-N7	5.03	133.42	130.40
60	BA	95	G	C4-N9-C1'	-5.02	119.97	126.50
20	CA	1027	C	C6-N1-C2	-5.02	118.29	120.30
60	BA	894	C	N3-C4-C5	-5.02	119.89	121.90
23	AY	146	LEU	CA-CB-CG	5.02	126.85	115.30
23	AY	466	LEU	CA-CB-CG	5.02	126.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	809	G	N3-C4-N9	5.02	129.01	126.00
60	BA	1674	G	C2-N3-C4	-5.02	109.39	111.90
59	DB	95	U	C6-N1-C1'	5.02	128.22	121.20
20	AA	165	C	N1-C2-O2	-5.02	115.89	118.90
60	BA	828	U	C2-N1-C1'	5.02	123.72	117.70
60	DA	2040	C	C5-C6-N1	5.02	123.51	121.00
20	AA	1213	A	C8-N9-C4	-5.01	103.80	105.80
60	BA	103	A	C4-C5-C6	5.01	119.51	117.00
60	BA	1424	G	N3-C2-N2	-5.01	116.39	119.90
60	BA	271(B)	C	C5-C6-N1	5.01	123.50	121.00
1	AB	163	PHE	C-N-CA	5.01	134.22	121.70
59	BB	101	A	N3-C4-C5	-5.01	123.30	126.80
60	DA	2021	C	C6-N1-C2	-5.01	118.30	120.30
60	BA	1025	G	C5-C6-O6	-5.00	125.60	128.60
60	BA	2792	G	N3-C2-N2	-5.00	116.40	119.90
60	DA	2043	C	C6-N1-C1'	-5.00	114.80	120.80
20	AA	993	G	N3-C4-N9	5.00	129.00	126.00
60	BA	2792	G	N1-C2-N2	5.00	120.70	116.20
1	CB	162	ILE	N-CA-C	-5.00	97.50	111.00
60	DA	1493	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	170	GLU	Peptide
1	AB	185	ILE	Peptide
1	AB	68	ILE	Peptide
11	AL	32	PHE	Peptide
23	AY	162	VAL	Peptide
23	AY	207	ASP	Mainchain
23	AY	34	TYR	Peptide
23	AY	630	GLN	Peptide
46	B1	16	ASN	Peptide
46	B1	17	SER	Peptide
25	BC	161	ARG	Peptide
25	BC	171	ALA	Peptide
25	BC	210	LEU	Peptide
25	BC	211	ARG	Peptide
25	BC	213	VAL	Peptide
26	BD	164	GLN	Peptide
26	BD	78	LYS	Peptide

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Mol	Chain	Res	Type	Group
28	BF	154	VAL	Peptide
29	BG	111	LEU	Mainchain
29	BG	114	ILE	Mainchain
31	BJ	83	UNK	Peptide
37	BS	14	VAL	Peptide
37	BS	46	VAL	Peptide
37	BS	98	VAL	Peptide
41	BW	75	TYR	Peptide
1	CB	170	GLU	Peptide
1	CB	185	ILE	Peptide
1	CB	68	ILE	Peptide
11	CL	32	PHE	Peptide
11	CL	57	LYS	Peptide
23	CY	162	VAL	Peptide
23	CY	329	ARG	Peptide
23	CY	34	TYR	Peptide
23	CY	564	LYS	Peptide
46	D1	16	ASN	Peptide
46	D1	17	SER	Peptide
25	DC	171	ALA	Peptide
25	DC	211	ARG	Peptide
25	DC	60	ARG	Peptide
26	DD	164	GLN	Peptide
26	DD	78	LYS	Peptide
28	DF	154	VAL	Peptide
29	DG	111	LEU	Mainchain
29	DG	113	ARG	Peptide
31	DJ	83	UNK	Peptide
37	DS	14	VAL	Peptide
37	DS	46	VAL	Peptide
37	DS	98	VAL	Peptide
38	DT	28	VAL	Peptide
41	DW	73	ALA	Peptide
41	DW	75	TYR	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

5.3.1 Protein backbone

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	
1	AB	233/235 (99%)	154 (66%)	60 (26%)	19 (8%)	1	13
1	CB	233/235 (99%)	164 (70%)	49 (21%)	20 (9%)	1	13
2	AC	205/207 (99%)	140 (68%)	43 (21%)	22 (11%)	0	8
2	CC	205/207 (99%)	136 (66%)	47 (23%)	22 (11%)	0	8
3	AD	206/208 (99%)	146 (71%)	46 (22%)	14 (7%)	1	17
3	CD	206/208 (99%)	140 (68%)	49 (24%)	17 (8%)	1	13
4	AE	149/151 (99%)	118 (79%)	22 (15%)	9 (6%)	1	20
4	CE	149/151 (99%)	125 (84%)	16 (11%)	8 (5%)	2	22
5	AF	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	4	32
5	CF	99/101 (98%)	81 (82%)	10 (10%)	8 (8%)	1	14
6	AG	153/155 (99%)	113 (74%)	27 (18%)	13 (8%)	1	13
6	CG	153/155 (99%)	116 (76%)	24 (16%)	13 (8%)	1	13
7	AH	136/138 (99%)	98 (72%)	21 (15%)	17 (12%)	0	5
7	CH	136/138 (99%)	90 (66%)	29 (21%)	17 (12%)	0	5
8	AI	125/127 (98%)	98 (78%)	16 (13%)	11 (9%)	1	12
8	CI	125/127 (98%)	100 (80%)	16 (13%)	9 (7%)	1	16
9	AJ	97/99 (98%)	69 (71%)	22 (23%)	6 (6%)	1	19
9	CJ	97/99 (98%)	71 (73%)	20 (21%)	6 (6%)	1	19
10	AK	117/119 (98%)	81 (69%)	23 (20%)	13 (11%)	0	8
10	CK	117/119 (98%)	82 (70%)	22 (19%)	13 (11%)	0	8
11	AL	123/125 (98%)	55 (45%)	38 (31%)	30 (24%)	0	1
11	CL	123/125 (98%)	54 (44%)	41 (33%)	28 (23%)	0	1
12	AM	123/125 (98%)	85 (69%)	21 (17%)	17 (14%)	0	4
12	CM	123/125 (98%)	85 (69%)	22 (18%)	16 (13%)	0	5
13	AN	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	CN	58/60 (97%)	45 (78%)	8 (14%)	5 (9%)	1	13
14	AO	86/88 (98%)	59 (69%)	20 (23%)	7 (8%)	1	14
14	CO	86/88 (98%)	60 (70%)	20 (23%)	6 (7%)	1	17
15	AP	82/84 (98%)	61 (74%)	14 (17%)	7 (8%)	1	13
15	CP	82/84 (98%)	59 (72%)	20 (24%)	3 (4%)	3	28
16	AQ	98/100 (98%)	71 (72%)	14 (14%)	13 (13%)	0	4
16	CQ	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	12
17	AR	68/70 (97%)	43 (63%)	17 (25%)	8 (12%)	0	6
17	CR	68/70 (97%)	49 (72%)	16 (24%)	3 (4%)	2	25
18	AS	77/79 (98%)	45 (58%)	21 (27%)	11 (14%)	0	4
18	CS	77/79 (98%)	38 (49%)	29 (38%)	10 (13%)	0	5
19	AT	97/99 (98%)	77 (79%)	16 (16%)	4 (4%)	3	26
19	CT	97/99 (98%)	79 (81%)	14 (14%)	4 (4%)	3	26
23	AY	685/687 (100%)	474 (69%)	144 (21%)	67 (10%)	0	10
23	CY	685/687 (100%)	476 (70%)	143 (21%)	66 (10%)	0	10
24	AU	2/6 (33%)	2 (100%)	0	0	100	100
24	CU	2/6 (33%)	2 (100%)	0	0	100	100
25	BC	226/228 (99%)	109 (48%)	65 (29%)	52 (23%)	0	1
25	DC	226/228 (99%)	108 (48%)	66 (29%)	52 (23%)	0	1
26	BD	273/275 (99%)	177 (65%)	66 (24%)	30 (11%)	0	8
26	DD	273/275 (99%)	179 (66%)	57 (21%)	37 (14%)	0	4
27	BE	203/205 (99%)	123 (61%)	50 (25%)	30 (15%)	0	4
27	DE	203/205 (99%)	133 (66%)	41 (20%)	29 (14%)	0	4
28	BF	206/208 (99%)	130 (63%)	47 (23%)	29 (14%)	0	4
28	DF	206/208 (99%)	126 (61%)	55 (27%)	25 (12%)	0	6
29	BG	179/181 (99%)	116 (65%)	45 (25%)	18 (10%)	0	10
29	DG	179/181 (99%)	121 (68%)	43 (24%)	15 (8%)	1	13
30	BH	165/167 (99%)	115 (70%)	35 (21%)	15 (9%)	1	12
30	DH	165/167 (99%)	121 (73%)	26 (16%)	18 (11%)	0	8
32	BK	138/140 (99%)	97 (70%)	28 (20%)	13 (9%)	0	11
32	DK	138/140 (99%)	91 (66%)	35 (25%)	12 (9%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	BO	120/122 (98%)	88 (73%)	25 (21%)	7 (6%)	1	20
33	DO	120/122 (98%)	90 (75%)	22 (18%)	8 (7%)	1	18
34	BP	144/146 (99%)	82 (57%)	41 (28%)	21 (15%)	0	4
34	DP	144/146 (99%)	88 (61%)	35 (24%)	21 (15%)	0	4
35	BQ	139/141 (99%)	93 (67%)	32 (23%)	14 (10%)	0	10
35	DQ	139/141 (99%)	99 (71%)	26 (19%)	14 (10%)	0	10
36	BR	115/117 (98%)	72 (63%)	28 (24%)	15 (13%)	0	5
36	DR	115/117 (98%)	78 (68%)	26 (23%)	11 (10%)	0	10
37	BS	97/99 (98%)	54 (56%)	22 (23%)	21 (22%)	0	1
37	DS	97/99 (98%)	52 (54%)	24 (25%)	21 (22%)	0	1
38	BT	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	4
38	DT	136/138 (99%)	89 (65%)	28 (21%)	19 (14%)	0	4
39	BU	115/117 (98%)	89 (77%)	21 (18%)	5 (4%)	2	25
39	DU	115/117 (98%)	84 (73%)	20 (17%)	11 (10%)	0	10
40	BV	99/101 (98%)	59 (60%)	22 (22%)	18 (18%)	0	2
40	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	4
41	BW	111/113 (98%)	88 (79%)	16 (14%)	7 (6%)	1	19
41	DW	111/113 (98%)	90 (81%)	10 (9%)	11 (10%)	0	10
42	BX	91/93 (98%)	71 (78%)	12 (13%)	8 (9%)	1	12
42	DX	91/93 (98%)	69 (76%)	17 (19%)	5 (6%)	2	21
43	BY	105/107 (98%)	48 (46%)	33 (31%)	24 (23%)	0	1
43	DY	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	2
44	BZ	183/185 (99%)	126 (69%)	42 (23%)	15 (8%)	1	13
44	DZ	183/185 (99%)	120 (66%)	45 (25%)	18 (10%)	0	10
45	B0	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	0	10
45	D0	82/84 (98%)	55 (67%)	20 (24%)	7 (8%)	1	13
46	B1	91/93 (98%)	55 (60%)	19 (21%)	17 (19%)	0	2
46	D1	91/93 (98%)	55 (60%)	17 (19%)	19 (21%)	0	2
47	B4	33/35 (94%)	17 (52%)	13 (39%)	3 (9%)	1	12
47	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	3
48	BN	136/138 (99%)	95 (70%)	25 (18%)	16 (12%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	DN	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	6
49	B2	69/71 (97%)	52 (75%)	13 (19%)	4 (6%)	1	20
49	D2	69/71 (97%)	51 (74%)	14 (20%)	4 (6%)	1	20
50	B3	58/60 (97%)	48 (83%)	7 (12%)	3 (5%)	2	22
50	D3	58/60 (97%)	45 (78%)	10 (17%)	3 (5%)	2	22
51	B5	57/59 (97%)	37 (65%)	10 (18%)	10 (18%)	0	3
51	D5	57/59 (97%)	37 (65%)	13 (23%)	7 (12%)	0	6
52	B6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
52	D6	48/50 (96%)	26 (54%)	11 (23%)	11 (23%)	0	1
53	B7	47/49 (96%)	32 (68%)	11 (23%)	4 (8%)	1	13
53	D7	47/49 (96%)	34 (72%)	9 (19%)	4 (8%)	1	13
54	B8	62/64 (97%)	38 (61%)	18 (29%)	6 (10%)	0	10
54	D8	62/64 (97%)	37 (60%)	17 (27%)	8 (13%)	0	5
55	B9	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	4
55	D9	35/37 (95%)	19 (54%)	12 (34%)	4 (11%)	0	7
56	Be	70/103 (68%)	38 (54%)	25 (36%)	7 (10%)	0	10
56	De	70/103 (68%)	40 (57%)	23 (33%)	7 (10%)	0	10
All	All	13304/13578 (98%)	8936 (67%)	2877 (22%)	1491 (11%)	0	7

All (1491) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	GLU
1	AB	67	THR
1	AB	76	GLN
1	AB	103	THR
1	AB	157	ARG
1	AB	237	ALA
2	AC	45	LYS
2	AC	49	SER
2	AC	107	GLN
2	AC	157	ILE
2	AC	161	GLU
2	AC	207	VAL
3	AD	5	ILE
3	AD	21	LEU

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Mol	Chain	Res	Type
4	AE	6	PHE
4	AE	49	PRO
5	AF	69	GLU
6	AG	8	GLU
6	AG	15	ASP
7	AH	22	GLU
7	AH	74	PRO
7	AH	93	VAL
7	AH	99	GLU
7	AH	100	ILE
7	AH	101	PRO
8	AI	54	ASP
8	AI	56	LEU
8	AI	104	ARG
8	AI	119	ALA
9	AJ	51	ARG
9	AJ	57	LYS
9	AJ	83	GLU
10	AK	41	THR
10	AK	42	TRP
10	AK	43	SER
10	AK	91	ARG
10	AK	109	VAL
10	AK	111	ASP
10	AK	122	LYS
11	AL	34	ARG
11	AL	37	CYS
11	AL	39	VAL
11	AL	43	VAL
11	AL	55	VAL
11	AL	66	VAL
11	AL	81	SER
11	AL	94	PRO
11	AL	96	VAL
11	AL	104	VAL
11	AL	108	ALA
11	AL	123	LYS
12	AM	3	ARG
12	AM	11	ARG
12	AM	12	ASN
12	AM	87	TYR
12	AM	107	ALA

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Mol	Chain	Res	Type
13	AN	14	PRO
15	AP	15	PRO
16	AQ	3	LYS
16	AQ	31	LEU
16	AQ	34	LYS
16	AQ	49	GLU
16	AQ	74	LEU
17	AR	37	VAL
17	AR	81	PHE
18	AS	45	VAL
18	AS	70	LYS
19	AT	74	LYS
23	AY	25	LYS
23	AY	35	TYR
23	AY	39	ILE
23	AY	88	VAL
23	AY	92	ILE
23	AY	146	LEU
23	AY	170	ARG
23	AY	204	GLU
23	AY	324	ARG
23	AY	330	VAL
23	AY	331	TYR
23	AY	400	GLU
23	AY	432	ALA
23	AY	448	GLN
23	AY	472	VAL
23	AY	498	ILE
23	AY	536	LYS
23	AY	564	LYS
23	AY	565	VAL
23	AY	614	GLU
23	AY	631	ILE
23	AY	652	MET
25	BC	17	PRO
25	BC	52	PRO
25	BC	57	GLN
25	BC	66	PRO
25	BC	80	LYS
25	BC	96	GLY
25	BC	114	VAL
25	BC	115	VAL

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Mol	Chain	Res	Type
25	BC	141	PRO
25	BC	162	ILE
25	BC	182	PRO
25	BC	221	PRO
25	BC	222	SER
25	BC	227	PRO
26	BD	36	PRO
26	BD	79	VAL
26	BD	89	SER
26	BD	152	GLY
26	BD	165	ILE
26	BD	231	HIS
26	BD	274	ARG
27	BE	10	GLY
27	BE	12	THR
27	BE	56	PRO
27	BE	60	ASN
27	BE	61	ARG
27	BE	66	HIS
27	BE	67	PHE
27	BE	74	PRO
27	BE	133	LYS
27	BE	134	ILE
28	BF	3	GLU
28	BF	10	PRO
28	BF	15	SER
28	BF	22	ALA
28	BF	69	HIS
28	BF	82	ILE
28	BF	192	LEU
29	BG	12	TYR
29	BG	26	GLN
29	BG	43	LEU
29	BG	96	ARG
29	BG	115	ARG
30	BH	21	PRO
30	BH	41	MET
30	BH	107	VAL
30	BH	164	TYR
32	BK	61	ALA
33	BO	29	ASN
33	BO	48	PRO

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Mol	Chain	Res	Type
34	BP	13	ASN
34	BP	39	LYS
34	BP	51	PHE
34	BP	57	THR
34	BP	65	ARG
34	BP	71	VAL
34	BP	106	LEU
35	BQ	20	ALA
35	BQ	90	VAL
36	BR	3	HIS
36	BR	12	ARG
37	BS	13	ARG
37	BS	14	VAL
37	BS	43	GLU
37	BS	48	LEU
37	BS	98	VAL
37	BS	100	ALA
37	BS	101	LEU
38	BT	28	VAL
38	BT	30	VAL
38	BT	49	VAL
38	BT	50	ILE
38	BT	68	TYR
38	BT	78	LEU
38	BT	83	ILE
40	BV	16	PRO
40	BV	29	PRO
40	BV	46	VAL
40	BV	50	PRO
40	BV	77	ALA
40	BV	78	LYS
40	BV	79	VAL
40	BV	96	ILE
41	BW	73	ALA
41	BW	77	ASP
42	BX	13	LEU
42	BX	32	PRO
43	BY	19	LYS
43	BY	32	PRO
43	BY	40	GLU
43	BY	51	VAL
43	BY	56	PRO

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Mol	Chain	Res	Type
43	BY	97	ARG
43	BY	107	ASP
44	BZ	71	VAL
44	BZ	72	ARG
45	B0	56	ASP
45	B0	73	GLY
46	B1	20	ARG
48	BN	17	ASP
48	BN	18	ALA
48	BN	50	ASP
48	BN	56	ASN
48	BN	63	THR
48	BN	64	GLY
48	BN	130	HIS
48	BN	133	GLN
50	B3	52	HIS
51	B5	23	HIS
51	B5	38	ALA
52	B6	8	LYS
52	B6	13	CYS
52	B6	19	ARG
52	B6	27	LYS
52	B6	44	ARG
53	B7	18	PHE
54	B8	49	VAL
54	B8	62	LEU
55	B9	8	LYS
55	B9	10	ILE
55	B9	18	ARG
56	Be	78	LEU
56	Be	81	ILE
1	CB	20	GLU
1	CB	34	ALA
1	CB	67	THR
1	CB	76	GLN
1	CB	103	THR
1	CB	157	ARG
1	CB	186	ALA
2	CC	36	ASP
2	CC	49	SER
2	CC	60	ALA
2	CC	161	GLU

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Mol	Chain	Res	Type
2	CC	207	VAL
3	CD	5	ILE
3	CD	84	LYS
3	CD	89	THR
3	CD	114	ARG
3	CD	156	GLU
3	CD	166	LYS
4	CE	6	PHE
4	CE	7	GLU
4	CE	21	ALA
5	CF	13	ASN
5	CF	69	GLU
6	CG	6	ARG
6	CG	8	GLU
6	CG	15	ASP
7	CH	22	GLU
7	CH	26	VAL
7	CH	27	PRO
7	CH	93	VAL
7	CH	99	GLU
7	CH	100	ILE
8	CI	54	ASP
8	CI	119	ALA
9	CJ	51	ARG
9	CJ	57	LYS
9	CJ	83	GLU
9	CJ	91	PRO
10	CK	12	ARG
10	CK	42	TRP
10	CK	87	THR
10	CK	91	ARG
10	CK	107	SER
10	CK	109	VAL
10	CK	111	ASP
11	CL	34	ARG
11	CL	37	CYS
11	CL	39	VAL
11	CL	55	VAL
11	CL	66	VAL
11	CL	81	SER
11	CL	104	VAL
11	CL	108	ALA

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Mol	Chain	Res	Type
11	CL	123	LYS
12	CM	12	ASN
12	CM	67	GLU
13	CN	14	PRO
13	CN	27	CYS
16	CQ	53	LEU
16	CQ	74	LEU
17	CR	37	VAL
18	CS	70	LYS
19	CT	74	LYS
23	CY	35	TYR
23	CY	39	ILE
23	CY	88	VAL
23	CY	92	ILE
23	CY	331	TYR
23	CY	347	GLY
23	CY	380	LEU
23	CY	400	GLU
23	CY	431	LEU
23	CY	432	ALA
23	CY	498	ILE
23	CY	536	LYS
23	CY	564	LYS
23	CY	631	ILE
23	CY	671	MET
25	DC	17	PRO
25	DC	43	GLU
25	DC	52	PRO
25	DC	54	ARG
25	DC	59	VAL
25	DC	66	PRO
25	DC	114	VAL
25	DC	115	VAL
25	DC	138	LEU
25	DC	141	PRO
25	DC	162	ILE
25	DC	167	ASP
25	DC	172	ILE
25	DC	175	PRO
25	DC	176	VAL
25	DC	177	GLY
25	DC	182	PRO

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Mol	Chain	Res	Type
25	DC	212	SER
25	DC	213	VAL
25	DC	214	TYR
25	DC	221	PRO
25	DC	222	SER
25	DC	227	PRO
26	DD	3	VAL
26	DD	36	PRO
26	DD	118	VAL
26	DD	166	GLN
26	DD	178	PRO
26	DD	207	GLY
26	DD	231	HIS
27	DE	11	MET
27	DE	12	THR
27	DE	13	ARG
27	DE	56	PRO
27	DE	60	ASN
27	DE	61	ARG
27	DE	72	VAL
27	DE	74	PRO
27	DE	94	GLU
27	DE	126	PRO
27	DE	144	ARG
27	DE	187	ALA
28	DF	3	GLU
28	DF	10	PRO
28	DF	22	ALA
28	DF	90	PHE
28	DF	105	VAL
28	DF	192	LEU
29	DG	12	TYR
29	DG	50	ALA
29	DG	96	ARG
30	DH	13	LYS
30	DH	21	PRO
30	DH	124	GLU
30	DH	164	TYR
30	DH	173	PRO
33	DO	48	PRO
34	DP	38	GLN
34	DP	57	THR

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Mol	Chain	Res	Type
34	DP	65	ARG
34	DP	71	VAL
34	DP	145	PRO
35	DQ	20	ALA
35	DQ	85	LYS
36	DR	57	ARG
37	DS	14	VAL
37	DS	43	GLU
37	DS	47	THR
37	DS	48	LEU
37	DS	98	VAL
37	DS	101	LEU
38	DT	28	VAL
38	DT	30	VAL
38	DT	49	VAL
38	DT	50	ILE
38	DT	68	TYR
38	DT	83	ILE
40	DV	16	PRO
40	DV	46	VAL
40	DV	50	PRO
40	DV	68	LYS
40	DV	77	ALA
40	DV	96	ILE
41	DW	73	ALA
41	DW	77	ASP
41	DW	110	LYS
43	DY	19	LYS
43	DY	32	PRO
43	DY	53	PRO
43	DY	56	PRO
43	DY	66	PRO
43	DY	67	LEU
43	DY	78	ALA
43	DY	97	ARG
44	DZ	71	VAL
44	DZ	72	ARG
44	DZ	168	GLU
44	DZ	169	GLU
45	D0	56	ASP
45	D0	73	GLY
46	D1	26	ARG

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Mol	Chain	Res	Type
46	D1	32	LYS
46	D1	35	THR
46	D1	53	VAL
46	D1	64	ALA
47	D4	14	ILE
48	DN	17	ASP
48	DN	18	ALA
48	DN	50	ASP
48	DN	56	ASN
48	DN	63	THR
48	DN	64	GLY
48	DN	130	HIS
48	DN	133	GLN
52	D6	13	CYS
52	D6	19	ARG
52	D6	44	ARG
52	D6	49	HIS
53	D7	44	PRO
54	D8	49	VAL
54	D8	62	LEU
55	D9	10	ILE
55	D9	18	ARG
56	De	54	ALA
56	De	81	ILE
1	AB	17	PHE
1	AB	165	VAL
1	AB	186	ALA
2	AC	14	ILE
2	AC	36	ASP
2	AC	47	LEU
2	AC	51	GLY
2	AC	60	ALA
2	AC	66	VAL
2	AC	74	GLY
2	AC	178	LEU
3	AD	43	HIS
3	AD	44	GLY
3	AD	114	ARG
4	AE	73	ASN
4	AE	128	PRO
6	AG	57	GLU
6	AG	90	GLU

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Mol	Chain	Res	Type
6	AG	113	GLU
7	AH	27	PRO
8	AI	58	ARG
8	AI	60	ASP
8	AI	87	GLN
10	AK	35	PRO
11	AL	33	ARG
11	AL	36	VAL
12	AM	99	ARG
12	AM	101	GLN
12	AM	119	GLY
12	AM	120	LYS
12	AM	121	LYS
13	AN	27	CYS
14	AO	23	GLY
14	AO	44	LYS
14	AO	48	LYS
15	AP	30	GLY
16	AQ	55	ASP
16	AQ	69	LYS
18	AS	64	GLU
18	AS	67	VAL
18	AS	77	THR
19	AT	49	ALA
19	AT	50	GLU
23	AY	21	ILE
23	AY	36	THR
23	AY	136	ALA
23	AY	161	PRO
23	AY	162	VAL
23	AY	447	GLY
23	AY	471	LYS
23	AY	521	SER
23	AY	527	ASN
23	AY	566	THR
23	AY	568	TYR
23	AY	654	GLY
25	BC	3	LYS
25	BC	35	THR
25	BC	42	VAL
25	BC	43	GLU
25	BC	50	ILE

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Mol	Chain	Res	Type
25	BC	53	ARG
25	BC	55	SER
25	BC	59	VAL
25	BC	60	ARG
25	BC	61	GLY
25	BC	138	LEU
25	BC	142	LYS
25	BC	164	PHE
25	BC	175	PRO
25	BC	176	VAL
25	BC	177	GLY
25	BC	184	GLU
25	BC	218	THR
25	BC	228	HIS
26	BD	3	VAL
26	BD	43	ARG
26	BD	118	VAL
26	BD	123	ALA
26	BD	127	VAL
26	BD	166	GLN
26	BD	178	PRO
26	BD	219	PRO
26	BD	239	ARG
27	BE	13	ARG
27	BE	51	PHE
27	BE	68	ALA
27	BE	72	VAL
27	BE	77	ILE
27	BE	86	PRO
27	BE	94	GLU
27	BE	126	PRO
27	BE	179	GLU
27	BE	187	ALA
28	BF	7	TYR
28	BF	14	PRO
28	BF	73	ALA
28	BF	84	VAL
28	BF	90	PHE
28	BF	92	PRO
28	BF	133	ASN
28	BF	181	LEU
28	BF	194	MET

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Mol	Chain	Res	Type
28	BF	206	ILE
29	BG	27	ASN
29	BG	50	ALA
29	BG	87	PRO
29	BG	147	ASP
29	BG	181	ARG
30	BH	13	LYS
30	BH	100	GLY
30	BH	138	LYS
30	BH	154	PRO
30	BH	173	PRO
32	BK	85	GLU
32	BK	91	PRO
32	BK	114	ASP
32	BK	115	LEU
33	BO	5	GLN
34	BP	14	LYS
34	BP	31	ALA
34	BP	104	GLY
34	BP	145	PRO
35	BQ	78	PRO
35	BQ	92	GLY
35	BQ	102	VAL
35	BQ	126	PRO
35	BQ	127	ILE
35	BQ	140	ALA
36	BR	11	ASN
36	BR	93	GLY
36	BR	108	GLY
37	BS	22	GLY
37	BS	32	LEU
37	BS	96	GLY
38	BT	33	LYS
38	BT	48	ILE
39	BU	88	ILE
40	BV	8	GLY
40	BV	68	LYS
41	BW	11	ARG
43	BY	28	LYS
43	BY	42	VAL
43	BY	53	PRO
43	BY	78	ALA

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Mol	Chain	Res	Type
44	BZ	73	GLN
44	BZ	78	LYS
44	BZ	120	ILE
45	B0	35	ASN
45	B0	75	LEU
45	B0	83	PRO
46	B1	18	ILE
46	B1	34	THR
46	B1	36	GLY
46	B1	53	VAL
46	B1	64	ALA
47	B4	33	VAL
48	BN	2	LYS
49	B2	41	ILE
50	B3	2	PRO
51	B5	3	LYS
51	B5	8	LYS
51	B5	54	GLY
54	B8	18	ALA
55	B9	12	ASP
56	Be	62	VAL
56	Be	79	ARG
56	Be	120	ALA
1	CB	17	PHE
1	CB	95	GLN
1	CB	105	PHE
1	CB	165	VAL
2	CC	14	ILE
2	CC	45	LYS
2	CC	47	LEU
2	CC	66	VAL
2	CC	130	VAL
2	CC	157	ILE
2	CC	178	LEU
3	CD	20	TYR
3	CD	21	LEU
3	CD	44	GLY
3	CD	186	LEU
5	CF	34	GLY
6	CG	4	ARG
6	CG	5	ARG
6	CG	90	GLU

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Mol	Chain	Res	Type
6	CG	120	ILE
7	CH	74	PRO
7	CH	97	VAL
7	CH	134	ILE
8	CI	24	GLY
8	CI	26	VAL
10	CK	43	SER
11	CL	43	VAL
11	CL	94	PRO
11	CL	96	VAL
11	CL	97	ARG
11	CL	99	HIS
11	CL	119	LYS
12	CM	3	ARG
12	CM	6	GLY
12	CM	10	PRO
12	CM	99	ARG
12	CM	101	GLN
12	CM	107	ALA
12	CM	120	LYS
14	CO	19	PRO
16	CQ	49	GLU
16	CQ	55	ASP
16	CQ	69	LYS
16	CQ	73	VAL
17	CR	28	GLU
18	CS	9	VAL
18	CS	42	PRO
18	CS	45	VAL
19	CT	71	THR
19	CT	105	SER
23	CY	21	ILE
23	CY	22	ASP
23	CY	36	THR
23	CY	75	LYS
23	CY	111	SER
23	CY	161	PRO
23	CY	162	VAL
23	CY	292	THR
23	CY	324	ARG
23	CY	330	VAL
23	CY	395	PRO

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Mol	Chain	Res	Type
23	CY	416	LYS
23	CY	447	GLY
23	CY	448	GLN
23	CY	565	VAL
23	CY	566	THR
23	CY	568	TYR
23	CY	614	GLU
23	CY	652	MET
25	DC	36	ALA
25	DC	61	GLY
25	DC	80	LYS
25	DC	94	TYR
25	DC	96	GLY
25	DC	119	ASP
25	DC	142	LYS
25	DC	184	GLU
25	DC	218	THR
25	DC	228	HIS
26	DD	79	VAL
26	DD	127	VAL
26	DD	152	GLY
26	DD	165	ILE
26	DD	200	ASP
26	DD	273	ARG
27	DE	10	GLY
27	DE	18	ASP
27	DE	34	VAL
27	DE	51	PHE
27	DE	68	ALA
27	DE	77	ILE
28	DF	58	ALA
28	DF	73	ALA
28	DF	84	VAL
28	DF	181	LEU
28	DF	194	MET
28	DF	206	ILE
29	DG	82	LEU
29	DG	87	PRO
29	DG	179	PRO
30	DH	41	MET
30	DH	48	GLY
30	DH	92	ILE

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Mol	Chain	Res	Type
30	DH	100	GLY
30	DH	123	PHE
30	DH	154	PRO
33	DO	4	PRO
33	DO	29	ASN
33	DO	96	THR
34	DP	14	LYS
34	DP	70	GLN
35	DQ	7	MET
35	DQ	90	VAL
35	DQ	92	GLY
35	DQ	111	GLU
35	DQ	127	ILE
35	DQ	139	GLU
36	DR	4	LEU
36	DR	12	ARG
36	DR	63	ARG
36	DR	108	GLY
37	DS	13	ARG
37	DS	22	GLY
37	DS	32	LEU
37	DS	59	LYS
37	DS	96	GLY
37	DS	100	ALA
38	DT	33	LYS
38	DT	80	SER
38	DT	86	ILE
38	DT	104	ASN
39	DU	11	ARG
39	DU	90	VAL
40	DV	44	LYS
40	DV	49	THR
41	DW	40	ASN
42	DX	12	VAL
43	DY	39	VAL
43	DY	51	VAL
43	DY	80	GLY
43	DY	101	LYS
44	DZ	52	SER
44	DZ	73	GLN
44	DZ	78	LYS
44	DZ	95	PRO

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Mol	Chain	Res	Type
44	DZ	108	PRO
45	D0	6	GLY
45	D0	11	ARG
45	D0	83	PRO
47	D4	7	PRO
47	D4	9	LEU
47	D4	33	VAL
48	DN	2	LYS
49	D2	48	HIS
49	D2	70	GLN
50	D3	2	PRO
50	D3	52	HIS
51	D5	23	HIS
51	D5	54	GLY
52	D6	27	LYS
52	D6	46	HIS
54	D8	53	PRO
56	De	62	VAL
56	De	114	LYS
56	De	120	ALA
1	AB	229	VAL
1	AB	230	VAL
1	AB	235	SER
2	AC	112	SER
3	AD	20	TYR
3	AD	40	PRO
3	AD	47	ARG
3	AD	156	GLU
3	AD	186	LEU
3	AD	189	PRO
4	AE	7	GLU
4	AE	21	ALA
4	AE	78	HIS
4	AE	153	LYS
5	AF	43	LEU
6	AG	31	MET
6	AG	37	ASN
7	AH	2	LEU
7	AH	107	LEU
8	AI	70	LYS
9	AJ	37	PRO
9	AJ	58	ASP

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Mol	Chain	Res	Type
10	AK	25	TYR
11	AL	56	ALA
11	AL	79	GLU
11	AL	99	HIS
11	AL	117	ARG
11	AL	127	GLU
12	AM	5	ALA
12	AM	86	CYS
12	AM	124	PRO
13	AN	3	ARG
14	AO	19	PRO
14	AO	40	SER
15	AP	28	ARG
15	AP	43	LYS
15	AP	46	PRO
16	AQ	14	LYS
16	AQ	53	LEU
17	AR	34	TYR
17	AR	60	ALA
17	AR	78	LEU
18	AS	55	LYS
18	AS	72	GLY
23	AY	111	SER
23	AY	203	GLU
23	AY	266	ASN
23	AY	381	LYS
23	AY	417	THR
23	AY	497	PHE
23	AY	577	SER
23	AY	653	PHE
25	BC	69	LEU
25	BC	77	ALA
25	BC	119	ASP
26	BD	48	ARG
26	BD	100	GLY
26	BD	110	GLY
26	BD	200	ASP
26	BD	260	ARG
27	BE	18	ASP
27	BE	123	ALA
27	BE	193	GLY
28	BF	52	LYS

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Mol	Chain	Res	Type
28	BF	58	ALA
28	BF	66	PRO
28	BF	105	VAL
29	BG	82	LEU
29	BG	84	LYS
30	BH	92	ILE
30	BH	137	ASP
32	BK	15	GLY
32	BK	89	HIS
33	BO	28	SER
33	BO	91	LEU
34	BP	17	LYS
34	BP	28	GLY
34	BP	148	LEU
35	BQ	2	LEU
35	BQ	101	ARG
35	BQ	111	GLU
35	BQ	134	ARG
37	BS	47	THR
37	BS	94	TYR
38	BT	2	ASN
38	BT	3	ARG
38	BT	29	ARG
38	BT	70	VAL
38	BT	137	LYS
39	BU	30	LYS
40	BV	27	ALA
40	BV	42	GLY
40	BV	44	LYS
41	BW	12	ILE
42	BX	4	ALA
42	BX	12	VAL
42	BX	33	LYS
43	BY	17	SER
43	BY	18	GLY
43	BY	29	GLU
43	BY	60	PHE
43	BY	80	GLY
44	BZ	53	ILE
44	BZ	108	PRO
44	BZ	152	ALA
44	BZ	166	SER

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Mol	Chain	Res	Type
44	BZ	168	GLU
44	BZ	169	GLU
45	B0	33	ALA
46	B1	10	LYS
46	B1	15	ALA
46	B1	19	GLN
46	B1	23	LYS
46	B1	28	GLY
46	B1	40	ARG
46	B1	87	PRO
47	B4	7	PRO
48	BN	67	LEU
48	BN	127	ASP
50	B3	16	PRO
53	B7	45	ALA
54	B8	30	ARG
54	B8	64	TYR
56	Be	114	LYS
1	CB	191	ASP
1	CB	230	VAL
1	CB	235	SER
1	CB	237	ALA
2	CC	85	ARG
2	CC	96	GLY
2	CC	112	SER
2	CC	180	ALA
3	CD	28	SER
4	CE	73	ASN
4	CE	78	HIS
5	CF	70	ASP
5	CF	96	PRO
6	CG	7	ALA
6	CG	19	GLY
6	CG	37	ASN
7	CH	2	LEU
7	CH	72	PRO
7	CH	76	PRO
7	CH	107	LEU
8	CI	35	GLU
8	CI	58	ARG
9	CJ	37	PRO
10	CK	15	ALA

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Mol	Chain	Res	Type
11	CL	23	LYS
11	CL	36	VAL
11	CL	51	ALA
11	CL	56	ALA
11	CL	79	GLU
13	CN	13	THR
14	CO	16	ALA
14	CO	23	GLY
15	CP	28	ARG
15	CP	43	LYS
16	CQ	12	SER
18	CS	15	LEU
18	CS	55	LYS
18	CS	67	VAL
18	CS	80	TYR
23	CY	74	TRP
23	CY	138	LYS
23	CY	204	GLU
23	CY	234	GLY
23	CY	359	HIS
23	CY	417	THR
23	CY	520	GLY
23	CY	521	SER
23	CY	525	PHE
23	CY	632	LEU
23	CY	653	PHE
23	CY	680	PRO
23	CY	681	LYS
25	DC	3	LYS
25	DC	139	PRO
25	DC	164	PHE
26	DD	43	ARG
26	DD	48	ARG
26	DD	89	SER
26	DD	123	ALA
26	DD	147	LEU
26	DD	222	ARG
26	DD	246	PRO
27	DE	67	PHE
27	DE	75	VAL
27	DE	86	PRO
27	DE	122	PHE

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Mol	Chain	Res	Type
27	DE	179	GLU
27	DE	192	ASN
28	DF	7	TYR
28	DF	14	PRO
28	DF	60	SER
28	DF	133	ASN
28	DF	150	GLY
29	DG	27	ASN
29	DG	35	GLU
29	DG	43	LEU
29	DG	66	GLN
29	DG	84	LYS
29	DG	147	ASP
29	DG	166	ASP
30	DH	47	GLU
30	DH	118	PRO
30	DH	155	SER
30	DH	160	LYS
32	DK	116	ASN
33	DO	5	GLN
33	DO	26	LYS
33	DO	64	ARG
34	DP	31	ALA
34	DP	43	GLY
34	DP	49	ARG
35	DQ	2	LEU
35	DQ	102	VAL
35	DQ	135	ASP
36	DR	40	LYS
36	DR	62	ALA
37	DS	24	LEU
37	DS	83	LYS
37	DS	94	TYR
38	DT	3	ARG
38	DT	27	THR
39	DU	23	GLY
40	DV	27	ALA
40	DV	29	PRO
40	DV	78	LYS
41	DW	12	ILE
42	DX	4	ALA
42	DX	32	PRO

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Mol	Chain	Res	Type
42	DX	33	LYS
43	DY	29	GLU
43	DY	88	LYS
44	DZ	29	TYR
44	DZ	166	SER
46	D1	10	LYS
46	D1	20	ARG
46	D1	23	LYS
46	D1	34	THR
46	D1	65	SER
46	D1	87	PRO
47	D4	2	LYS
48	DN	67	LEU
48	DN	127	ASP
49	D2	3	LEU
49	D2	17	SER
51	D5	3	LYS
52	D6	48	VAL
53	D7	9	ARG
53	D7	42	LEU
54	D8	18	ALA
54	D8	30	ARG
54	D8	48	PHE
54	D8	51	ALA
54	D8	64	TYR
56	De	119	GLY
1	AB	66	GLY
1	AB	70	PHE
1	AB	95	GLN
1	AB	158	LEU
1	AB	170	GLU
2	AC	158	GLY
2	AC	160	ALA
3	AD	142	PRO
3	AD	143	GLY
3	AD	149	ALA
5	AF	96	PRO
6	AG	112	PRO
7	AH	80	ILE
7	AH	103	VAL
7	AH	127	LEU
8	AI	35	GLU

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Mol	Chain	Res	Type
8	AI	127	LYS
9	AJ	91	PRO
10	AK	36	ASP
10	AK	102	GLY
10	AK	123	LYS
11	AL	22	SER
11	AL	40	VAL
11	AL	41	ARG
11	AL	69	TYR
11	AL	112	ASP
11	AL	119	LYS
13	AN	13	THR
14	AO	16	ALA
16	AQ	7	THR
16	AQ	12	SER
17	AR	32	ARG
17	AR	59	SER
19	AT	105	SER
23	AY	38	ARG
23	AY	50	ALA
23	AY	89	ASP
23	AY	234	GLY
23	AY	366	VAL
23	AY	519	ARG
23	AY	682	GLN
25	BC	167	ASP
25	BC	202	PRO
25	BC	212	SER
26	BD	24	ILE
26	BD	28	GLU
26	BD	80	ALA
27	BE	17	ASP
27	BE	33	VAL
27	BE	34	VAL
27	BE	69	LYS
28	BF	45	ARG
28	BF	60	SER
28	BF	178	PRO
29	BG	16	ARG
29	BG	35	GLU
29	BG	142	PRO
30	BH	124	GLU

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Mol	Chain	Res	Type
30	BH	155	SER
32	BK	30	HIS
32	BK	109	LYS
33	BO	13	ASN
34	BP	9	ASN
34	BP	43	GLY
35	BQ	54	MET
36	BR	8	ARG
36	BR	10	LEU
36	BR	57	ARG
36	BR	102	GLU
37	BS	24	LEU
37	BS	66	ALA
37	BS	67	ARG
37	BS	83	LYS
37	BS	93	LYS
37	BS	106	ARG
38	BT	80	SER
38	BT	86	ILE
38	BT	107	ASP
39	BU	90	VAL
39	BU	92	ARG
40	BV	53	GLU
40	BV	80	GLN
41	BW	75	TYR
43	BY	35	TYR
43	BY	81	LYS
43	BY	88	LYS
43	BY	101	LYS
44	BZ	23	LYS
44	BZ	30	ASN
46	B1	25	LYS
48	BN	23	LEU
49	B2	18	PRO
51	B5	51	TYR
51	B5	56	LYS
52	B6	31	PRO
52	B6	49	HIS
53	B7	15	THR
54	B8	53	PRO
1	CB	129	GLU
1	CB	229	VAL

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Mol	Chain	Res	Type
2	CC	26	LYS
2	CC	35	GLU
2	CC	51	GLY
3	CD	47	ARG
3	CD	73	ARG
4	CE	70	PRO
8	CI	87	GLN
8	CI	127	LYS
9	CJ	59	SER
10	CK	36	ASP
10	CK	105	VAL
11	CL	22	SER
12	CM	5	ALA
12	CM	11	ARG
12	CM	70	LEU
13	CN	24	CYS
16	CQ	82	MET
17	CR	59	SER
18	CS	40	ILE
19	CT	49	ALA
23	CY	89	ASP
23	CY	181	LEU
23	CY	615	GLU
23	CY	628	ARG
23	CY	648	PRO
23	CY	649	LEU
23	CY	670	VAL
25	DC	37	LYS
25	DC	53	ARG
25	DC	77	ALA
25	DC	143	ALA
25	DC	171	ALA
26	DD	28	GLU
26	DD	44	ASN
26	DD	110	GLY
26	DD	122	ASP
26	DD	260	ARG
27	DE	35	GLN
27	DE	123	ALA
28	DF	52	LYS
28	DF	66	PRO
28	DF	78	ILE

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Mol	Chain	Res	Type
28	DF	92	PRO
30	DH	59	ARG
30	DH	107	VAL
32	DK	30	HIS
32	DK	51	ALA
32	DK	85	GLU
32	DK	122	ALA
33	DO	28	SER
34	DP	46	LYS
34	DP	48	PRO
34	DP	76	LYS
34	DP	97	PRO
34	DP	107	LYS
34	DP	141	ALA
35	DQ	28	ALA
35	DQ	126	PRO
37	DS	58	LEU
37	DS	82	ILE
37	DS	93	LYS
37	DS	106	ARG
38	DT	55	ASN
38	DT	78	LEU
39	DU	24	TYR
39	DU	88	ILE
39	DU	98	LEU
40	DV	53	GLU
41	DW	15	ARG
41	DW	61	ASN
42	DX	24	GLY
43	DY	18	GLY
43	DY	81	LYS
44	DZ	30	ASN
44	DZ	34	ASN
45	D0	35	ASN
46	D1	12	PRO
46	D1	36	GLY
46	D1	40	ARG
46	D1	44	PRO
46	D1	63	ALA
46	D1	94	LEU
48	DN	23	LEU
50	D3	16	PRO

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Mol	Chain	Res	Type
51	D5	7	PRO
51	D5	24	ALA
55	D9	3	VAL
56	De	78	LEU
1	AB	101	MET
2	AC	130	VAL
2	AC	181	ASN
6	AG	4	ARG
6	AG	5	ARG
7	AH	26	VAL
7	AH	72	PRO
7	AH	106	GLY
8	AI	112	LYS
11	AL	8	ASN
11	AL	23	LYS
11	AL	93	LEU
12	AM	10	PRO
12	AM	21	TYR
12	AM	108	ARG
15	AP	16	HIS
15	AP	82	GLN
16	AQ	73	VAL
18	AS	80	TYR
23	AY	145	ASP
23	AY	228	MET
23	AY	379	GLY
23	AY	404	VAL
23	AY	632	LEU
23	AY	660	ARG
23	AY	671	MET
25	BC	71	LYS
25	BC	136	GLY
25	BC	139	PRO
25	BC	180	SER
25	BC	224	ARG
26	BD	233	HIS
26	BD	259	THR
27	BE	122	PHE
28	BF	25	PRO
30	BH	59	ARG
32	BK	51	ALA
32	BK	90	LYS

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Mol	Chain	Res	Type
32	BK	122	ALA
33	BO	34	THR
34	BP	12	ALA
34	BP	38	GLN
34	BP	49	ARG
36	BR	4	LEU
36	BR	32	GLY
36	BR	38	VAL
36	BR	61	HIS
37	BS	82	ILE
38	BT	55	ASN
39	BU	102	GLU
40	BV	48	GLY
40	BV	81	TYR
41	BW	15	ARG
41	BW	65	LEU
42	BX	23	GLU
44	BZ	83	PRO
45	B0	6	GLY
45	B0	11	ARG
46	B1	22	GLY
46	B1	63	ALA
48	BN	3	THR
49	B2	17	SER
49	B2	70	GLN
52	B6	6	ARG
52	B6	20	ASN
1	CB	128	GLU
1	CB	130	ARG
2	CC	61	ALA
4	CE	74	GLY
5	CF	38	GLU
6	CG	31	MET
7	CH	80	ILE
7	CH	103	VAL
7	CH	120	THR
11	CL	12	ARG
11	CL	93	LEU
11	CL	112	ASP
11	CL	127	GLU
12	CM	124	PRO
13	CN	3	ARG

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Mol	Chain	Res	Type
14	CO	6	GLU
14	CO	88	ARG
15	CP	46	PRO
16	CQ	14	LYS
23	CY	14	ASN
23	CY	294	PRO
25	DC	22	THR
25	DC	60	ARG
25	DC	76	LEU
25	DC	122	GLY
25	DC	202	PRO
26	DD	53	PHE
26	DD	90	ALA
26	DD	109	ASP
26	DD	198	ASN
26	DD	225	ALA
26	DD	242	ARG
27	DE	178	GLU
28	DF	24	LEU
32	DK	33	ASN
32	DK	89	HIS
32	DK	90	LYS
34	DP	9	ASN
34	DP	13	ASN
34	DP	17	LYS
36	DR	93	GLY
36	DR	101	ALA
36	DR	103	ARG
37	DS	85	VAL
38	DT	31	SER
38	DT	70	VAL
38	DT	87	ASP
38	DT	90	GLN
39	DU	92	ARG
39	DU	106	PHE
41	DW	65	LEU
43	DY	50	ARG
43	DY	60	PHE
43	DY	91	GLU
44	DZ	31	ARG
44	DZ	82	ARG
44	DZ	83	PRO

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Mol	Chain	Res	Type
45	D0	33	ALA
48	DN	3	THR
51	D5	49	CYS
52	D6	6	ARG
52	D6	20	ASN
52	D6	31	PRO
55	D9	21	GLY
2	AC	46	GLU
4	AE	22	GLY
6	AG	7	ALA
14	AO	88	ARG
16	AQ	64	PRO
17	AR	28	GLU
18	AS	30	LEU
18	AS	40	ILE
23	AY	121	VAL
23	AY	506	GLN
25	BC	13	GLU
25	BC	22	THR
25	BC	122	GLY
25	BC	171	ALA
25	BC	204	GLY
27	BE	155	LYS
28	BF	78	ILE
29	BG	151	ALA
30	BH	48	GLY
36	BR	63	ARG
37	BS	85	VAL
37	BS	108	GLY
38	BT	31	SER
46	B1	12	PRO
48	BN	110	GLY
51	B5	49	CYS
52	B6	26	ASN
55	B9	3	VAL
56	Be	82	THR
3	CD	75	PHE
5	CF	14	LEU
5	CF	43	LEU
6	CG	18	TYR
6	CG	88	PRO
8	CI	89	ASN

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Mol	Chain	Res	Type
11	CL	69	TYR
12	CM	74	VAL
23	CY	296	GLY
23	CY	493	VAL
25	DC	18	ASN
25	DC	150	ILE
26	DD	98	VAL
26	DD	154	LYS
26	DD	232	PRO
32	DK	21	PRO
32	DK	91	PRO
36	DR	10	LEU
39	DU	59	ARG
40	DV	80	GLN
41	DW	63	ASP
41	DW	80	PRO
44	DZ	39	VAL
46	D1	21	ARG
48	DN	110	GLY
51	D5	57	VAL
1	AB	130	ARG
2	AC	96	GLY
6	AG	120	ILE
11	AL	82	VAL
23	AY	257	PRO
23	AY	384	ILE
23	AY	444	PRO
23	AY	487	ILE
25	BC	215	VAL
26	BD	42	GLY
27	BE	14	ILE
32	BK	72	PRO
35	BQ	27	VAL
36	BR	58	GLY
44	BZ	39	VAL
48	BN	77	GLY
51	B5	7	PRO
53	B7	46	VAL
2	CC	74	GLY
3	CD	29	PRO
12	CM	100	GLY
14	CO	27	VAL

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Mol	Chain	Res	Type
23	CY	158	GLY
23	CY	384	ILE
23	CY	535	PRO
25	DC	136	GLY
26	DD	256	GLY
32	DK	72	PRO
34	DP	69	GLY
35	DQ	27	VAL
41	DW	14	PRO
43	DY	42	VAL
48	DN	77	GLY
52	D6	7	ILE
53	D7	46	VAL
7	AH	73	ASP
10	AK	88	GLY
18	AS	68	GLY
23	AY	42	ILE
23	AY	189	GLY
23	AY	520	GLY
26	BD	106	ILE
26	BD	232	PRO
28	BF	24	LEU
40	BV	41	GLY
43	BY	74	PRO
2	CC	80	GLY
3	CD	88	VAL
3	CD	140	VAL
7	CH	75	ARG
12	CM	4	ILE
23	CY	444	PRO
25	DC	42	VAL
25	DC	81	GLY
27	DE	14	ILE
28	DF	88	VAL
29	DG	24	GLY
30	DH	49	VAL
40	DV	48	GLY
2	AC	73	PRO
6	AG	19	GLY
7	AH	97	VAL
23	AY	508	GLY
29	BG	28	VAL

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Mol	Chain	Res	Type
29	BG	85	GLY
43	BY	49	VAL
43	BY	66	PRO
52	B6	48	VAL
1	CB	66	GLY
10	CK	14	VAL
10	CK	35	PRO
18	CS	72	GLY
23	CY	366	VAL
26	DD	244	ARG
26	DD	249	PRO
27	DE	134	ILE
28	DF	178	PRO
32	DK	55	VAL
34	DP	78	PRO
38	DT	34	VAL
39	DU	73	GLY
43	DY	74	PRO
44	DZ	90	VAL
11	AL	58	VAL
12	AM	100	GLY
23	AY	680	PRO
25	BC	49	GLY
25	BC	150	ILE
26	BD	246	PRO
28	BF	61	GLY
28	BF	150	GLY
34	BP	97	PRO
42	BX	7	VAL
42	BX	52	VAL
47	B4	5	ILE
51	B5	57	VAL
4	CE	85	GLY
11	CL	82	VAL
11	CL	83	VAL
23	CY	42	ILE
23	CY	530	VAL
25	DC	20	VAL
28	DF	61	GLY
29	DG	16	ARG
37	DS	60	GLY
39	DU	102	GLU

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Mol	Chain	Res	Type
13	AN	18	VAL
43	BY	98	VAL
23	CY	436	PRO
46	D1	29	GLY
48	BN	126	PRO
48	DN	126	PRO
34	BP	48	PRO

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	
1	AB	203/203 (100%)	161 (79%)	42 (21%)	1	8
1	CB	203/203 (100%)	165 (81%)	38 (19%)	1	11
2	AC	161/161 (100%)	124 (77%)	37 (23%)	1	6
2	CC	161/161 (100%)	121 (75%)	40 (25%)	0	5
3	AD	180/180 (100%)	138 (77%)	42 (23%)	1	6
3	CD	180/180 (100%)	149 (83%)	31 (17%)	2	14
4	AE	116/116 (100%)	91 (78%)	25 (22%)	1	7
4	CE	116/116 (100%)	93 (80%)	23 (20%)	1	9
5	AF	90/90 (100%)	72 (80%)	18 (20%)	1	9
5	CF	90/90 (100%)	74 (82%)	16 (18%)	2	13
6	AG	126/126 (100%)	109 (86%)	17 (14%)	4	22
6	CG	126/126 (100%)	106 (84%)	20 (16%)	2	17
7	AH	119/119 (100%)	92 (77%)	27 (23%)	1	6
7	CH	119/119 (100%)	99 (83%)	20 (17%)	2	15
8	AI	98/98 (100%)	79 (81%)	19 (19%)	1	10
8	CI	98/98 (100%)	82 (84%)	16 (16%)	2	16
9	AJ	89/89 (100%)	72 (81%)	17 (19%)	1	10
9	CJ	89/89 (100%)	74 (83%)	15 (17%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	AK	90/90 (100%)	76 (84%)	14 (16%)	2	17
10	CK	90/90 (100%)	78 (87%)	12 (13%)	4	22
11	AL	104/104 (100%)	83 (80%)	21 (20%)	1	8
11	CL	104/104 (100%)	77 (74%)	27 (26%)	0	4
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	14
12	CM	100/100 (100%)	82 (82%)	18 (18%)	1	12
13	AN	49/49 (100%)	37 (76%)	12 (24%)	0	5
13	CN	49/49 (100%)	40 (82%)	9 (18%)	1	11
14	AO	79/79 (100%)	63 (80%)	16 (20%)	1	8
14	CO	79/79 (100%)	62 (78%)	17 (22%)	1	7
15	AP	72/72 (100%)	56 (78%)	16 (22%)	1	6
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	15
16	AQ	95/95 (100%)	77 (81%)	18 (19%)	1	10
16	CQ	95/95 (100%)	82 (86%)	13 (14%)	3	21
17	AR	61/61 (100%)	51 (84%)	10 (16%)	2	15
17	CR	61/61 (100%)	48 (79%)	13 (21%)	1	7
18	AS	69/69 (100%)	51 (74%)	18 (26%)	0	4
18	CS	69/69 (100%)	54 (78%)	15 (22%)	1	7
19	AT	76/76 (100%)	66 (87%)	10 (13%)	4	22
19	CT	76/76 (100%)	69 (91%)	7 (9%)	9	34
23	AY	579/579 (100%)	475 (82%)	104 (18%)	1	12
23	CY	579/579 (100%)	472 (82%)	107 (18%)	1	11
24	AU	2/2 (100%)	2 (100%)	0	100	100
24	CU	2/2 (100%)	2 (100%)	0	100	100
25	BC	180/180 (100%)	138 (77%)	42 (23%)	1	6
25	DC	180/180 (100%)	130 (72%)	50 (28%)	0	3
26	BD	217/217 (100%)	164 (76%)	53 (24%)	0	5
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	8
27	BE	165/165 (100%)	131 (79%)	34 (21%)	1	8
27	DE	165/165 (100%)	134 (81%)	31 (19%)	1	11
28	BF	165/165 (100%)	127 (77%)	38 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	DF	165/165 (100%)	126 (76%)	39 (24%)	1	5
29	BG	155/155 (100%)	118 (76%)	37 (24%)	0	5
29	DG	155/155 (100%)	121 (78%)	34 (22%)	1	7
30	BH	136/136 (100%)	109 (80%)	27 (20%)	1	9
30	DH	136/136 (100%)	115 (85%)	21 (15%)	2	17
32	BK	105/105 (100%)	94 (90%)	11 (10%)	7	29
32	DK	105/105 (100%)	88 (84%)	17 (16%)	2	16
33	BO	100/100 (100%)	80 (80%)	20 (20%)	1	9
33	DO	100/100 (100%)	84 (84%)	16 (16%)	2	16
34	BP	112/112 (100%)	80 (71%)	32 (29%)	0	2
34	DP	112/112 (100%)	91 (81%)	21 (19%)	1	11
35	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	4
35	DQ	111/111 (100%)	85 (77%)	26 (23%)	1	5
36	BR	100/100 (100%)	72 (72%)	28 (28%)	0	3
36	DR	100/100 (100%)	81 (81%)	19 (19%)	1	10
37	BS	77/77 (100%)	55 (71%)	22 (29%)	0	2
37	DS	77/77 (100%)	60 (78%)	17 (22%)	1	6
38	BT	120/120 (100%)	99 (82%)	21 (18%)	2	13
38	DT	120/120 (100%)	99 (82%)	21 (18%)	2	13
39	BU	93/93 (100%)	77 (83%)	16 (17%)	2	14
39	DU	93/93 (100%)	76 (82%)	17 (18%)	1	11
40	BV	82/82 (100%)	61 (74%)	21 (26%)	0	5
40	DV	82/82 (100%)	60 (73%)	22 (27%)	0	4
41	BW	92/92 (100%)	73 (79%)	19 (21%)	1	8
41	DW	92/92 (100%)	74 (80%)	18 (20%)	1	9
42	BX	75/75 (100%)	59 (79%)	16 (21%)	1	7
42	DX	75/75 (100%)	60 (80%)	15 (20%)	1	9
43	BY	88/88 (100%)	69 (78%)	19 (22%)	1	7
43	DY	88/88 (100%)	72 (82%)	16 (18%)	1	11
44	BZ	162/162 (100%)	129 (80%)	33 (20%)	1	8
44	DZ	162/162 (100%)	128 (79%)	34 (21%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	B0	66/66 (100%)	55 (83%)	11 (17%)	2	15
45	D0	66/66 (100%)	56 (85%)	10 (15%)	3	18
46	B1	78/78 (100%)	61 (78%)	17 (22%)	1	7
46	D1	78/78 (100%)	53 (68%)	25 (32%)	0	2
47	B4	31/31 (100%)	23 (74%)	8 (26%)	0	4
47	D4	31/31 (100%)	25 (81%)	6 (19%)	1	10
48	BN	117/117 (100%)	100 (86%)	17 (14%)	3	19
48	DN	117/117 (100%)	100 (86%)	17 (14%)	3	19
49	B2	66/66 (100%)	55 (83%)	11 (17%)	2	15
49	D2	66/66 (100%)	58 (88%)	8 (12%)	5	24
50	B3	52/52 (100%)	45 (86%)	7 (14%)	4	22
50	D3	52/52 (100%)	45 (86%)	7 (14%)	4	22
51	B5	51/51 (100%)	42 (82%)	9 (18%)	2	13
51	D5	51/51 (100%)	42 (82%)	9 (18%)	2	13
52	B6	49/49 (100%)	36 (74%)	13 (26%)	0	4
52	D6	49/49 (100%)	37 (76%)	12 (24%)	0	5
53	B7	42/42 (100%)	39 (93%)	3 (7%)	14	44
53	D7	42/42 (100%)	36 (86%)	6 (14%)	3	20
54	B8	54/54 (100%)	35 (65%)	19 (35%)	0	1
54	D8	54/54 (100%)	40 (74%)	14 (26%)	0	4
55	B9	34/34 (100%)	29 (85%)	5 (15%)	3	19
55	D9	34/34 (100%)	29 (85%)	5 (15%)	3	19
56	Be	54/54 (100%)	47 (87%)	7 (13%)	4	23
56	De	54/54 (100%)	46 (85%)	8 (15%)	3	18
All	All	11174/11174 (100%)	8954 (80%)	2220 (20%)	1	9

All (2220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AB	10	LEU
1	AB	12	GLU
1	AB	15	VAL
1	AB	17	PHE
1	AB	21	ARG

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Mol	Chain	Res	Type
1	AB	28	PHE
1	AB	32	ILE
1	AB	33	TYR
1	AB	36	ARG
1	AB	40	HIS
1	AB	45	GLN
1	AB	49	GLU
1	AB	69	LEU
1	AB	74	LYS
1	AB	79	ASP
1	AB	94	ASN
1	AB	101	MET
1	AB	104	ASN
1	AB	134	GLU
1	AB	141	GLU
1	AB	145	LEU
1	AB	152	PHE
1	AB	154	LEU
1	AB	155	LEU
1	AB	162	ILE
1	AB	163	PHE
1	AB	168	THR
1	AB	175	ARG
1	AB	178	ARG
1	AB	181	PHE
1	AB	185	ILE
1	AB	187	LEU
1	AB	189	ASP
1	AB	197	VAL
1	AB	198	ASP
1	AB	201	ILE
1	AB	208	ILE
1	AB	212	GLN
1	AB	213	LEU
1	AB	221	LEU
1	AB	230	VAL
1	AB	236	TYR
2	AC	4	LYS
2	AC	5	ILE
2	AC	15	THR
2	AC	20	SER
2	AC	21	ARG

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Mol	Chain	Res	Type
2	AC	22	TRP
2	AC	27	LYS
2	AC	39	ILE
2	AC	47	LEU
2	AC	48	TYR
2	AC	52	LEU
2	AC	55	VAL
2	AC	57	ILE
2	AC	67	THR
2	AC	70	VAL
2	AC	76	VAL
2	AC	84	ILE
2	AC	86	VAL
2	AC	101	LEU
2	AC	102	ASN
2	AC	118	GLN
2	AC	119	ARG
2	AC	124	ILE
2	AC	125	GLU
2	AC	126	ARG
2	AC	128	PHE
2	AC	134	ILE
2	AC	142	MET
2	AC	152	ILE
2	AC	154	SER
2	AC	157	ILE
2	AC	164	ARG
2	AC	167	TRP
2	AC	176	HIS
2	AC	179	ARG
2	AC	181	ASN
2	AC	188	LEU
3	AD	3	ARG
3	AD	5	ILE
3	AD	8	VAL
3	AD	9	CYS
3	AD	13	ARG
3	AD	25	ARG
3	AD	28	SER
3	AD	30	LYS
3	AD	49	ARG
3	AD	50	ARG

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Mol	Chain	Res	Type
3	AD	52	SER
3	AD	54	TYR
3	AD	56	VAL
3	AD	57	ARG
3	AD	58	LEU
3	AD	61	LYS
3	AD	65	ARG
3	AD	67	ILE
3	AD	72	GLU
3	AD	76	ARG
3	AD	83	SER
3	AD	86	LYS
3	AD	107	ARG
3	AD	108	LEU
3	AD	110	PHE
3	AD	123	HIS
3	AD	125	HIS
3	AD	127	THR
3	AD	131	ARG
3	AD	132	ARG
3	AD	134	ASP
3	AD	140	VAL
3	AD	144	ASP
3	AD	150	GLU
3	AD	154	ASN
3	AD	156	GLU
3	AD	165	MET
3	AD	175	SER
3	AD	178	VAL
3	AD	187	ARG
3	AD	196	LEU
3	AD	200	GLU
4	AE	5	ASP
4	AE	10	MET
4	AE	12	LEU
4	AE	31	LEU
4	AE	33	VAL
4	AE	45	PHE
4	AE	51	VAL
4	AE	53	LEU
4	AE	57	LYS
4	AE	61	TYR

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Mol	Chain	Res	Type
4	AE	64	ARG
4	AE	73	ASN
4	AE	78	HIS
4	AE	80	ILE
4	AE	91	LEU
4	AE	92	LYS
4	AE	101	ILE
4	AE	107	ARG
4	AE	116	THR
4	AE	117	ASP
4	AE	125	SER
4	AE	129	ILE
4	AE	130	ASN
4	AE	139	LEU
4	AE	155	GLU
5	AF	2	ARG
5	AF	7	ASN
5	AF	16	GLN
5	AF	18	GLN
5	AF	22	GLU
5	AF	37	VAL
5	AF	55	ASP
5	AF	60	PHE
5	AF	61	LEU
5	AF	64	GLN
5	AF	66	GLU
5	AF	69	GLU
5	AF	74	ASP
5	AF	78	GLU
5	AF	83	ASP
5	AF	91	VAL
5	AF	95	GLU
5	AF	98	LEU
6	AG	3	ARG
6	AG	11	GLN
6	AG	12	LEU
6	AG	21	VAL
6	AG	24	THR
6	AG	32	ARG
6	AG	35	LYS
6	AG	36	LYS
6	AG	56	GLN

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Mol	Chain	Res	Type
6	AG	62	PHE
6	AG	72	ARG
6	AG	78	ARG
6	AG	79	ARG
6	AG	94	ARG
6	AG	97	GLN
6	AG	104	LEU
6	AG	106	GLN
7	AH	3	THR
7	AH	8	ASP
7	AH	9	MET
7	AH	24	THR
7	AH	30	ARG
7	AH	31	PHE
7	AH	35	ILE
7	AH	37	ARG
7	AH	39	LEU
7	AH	49	GLU
7	AH	52	ASP
7	AH	54	ASP
7	AH	59	LEU
7	AH	63	LEU
7	AH	69	ARG
7	AH	70	GLN
7	AH	73	ASP
7	AH	83	ILE
7	AH	89	PRO
7	AH	95	VAL
7	AH	102	ARG
7	AH	103	VAL
7	AH	107	LEU
7	AH	120	THR
7	AH	121	ASP
7	AH	133	LEU
7	AH	136	GLU
8	AI	7	THR
8	AI	28	VAL
8	AI	32	ASP
8	AI	34	ASN
8	AI	71	SER
8	AI	75	ASP
8	AI	79	LEU

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Mol	Chain	Res	Type
8	AI	85	LEU
8	AI	86	VAL
8	AI	91	ASP
8	AI	93	ARG
8	AI	95	LYS
8	AI	97	LYS
8	AI	99	LEU
8	AI	112	LYS
8	AI	121	ARG
8	AI	125	TYR
8	AI	126	SER
8	AI	128	ARG
9	AJ	3	LYS
9	AJ	5	ARG
9	AJ	6	ILE
9	AJ	11	PHE
9	AJ	16	LEU
9	AJ	22	LYS
9	AJ	29	ARG
9	AJ	47	PHE
9	AJ	50	ILE
9	AJ	54	PHE
9	AJ	58	ASP
9	AJ	65	LEU
9	AJ	75	ILE
9	AJ	84	GLN
9	AJ	88	LEU
9	AJ	95	GLU
9	AJ	96	ILE
10	AK	18	ARG
10	AK	20	TYR
10	AK	22	HIS
10	AK	29	ILE
10	AK	31	THR
10	AK	51	LYS
10	AK	57	THR
10	AK	66	LEU
10	AK	75	TYR
10	AK	91	ARG
10	AK	96	ARG
10	AK	103	LEU
10	AK	107	SER

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Mol	Chain	Res	Type
10	AK	123	LYS
11	AL	20	LYS
11	AL	22	SER
11	AL	24	VAL
11	AL	38	THR
11	AL	42	THR
11	AL	44	THR
11	AL	52	LEU
11	AL	53	ARG
11	AL	54	LYS
11	AL	55	VAL
11	AL	62	SER
11	AL	67	THR
11	AL	70	ILE
11	AL	84	LEU
11	AL	86	ARG
11	AL	92	ASP
11	AL	97	ARG
11	AL	104	VAL
11	AL	113	ARG
11	AL	114	LYS
11	AL	122	THR
12	AM	8	GLU
12	AM	21	TYR
12	AM	23	TYR
12	AM	27	LYS
12	AM	43	THR
12	AM	48	LEU
12	AM	50	GLU
12	AM	64	TRP
12	AM	67	GLU
12	AM	69	GLU
12	AM	80	ARG
12	AM	82	MET
12	AM	86	CYS
12	AM	88	ARG
12	AM	105	THR
12	AM	108	ARG
12	AM	121	LYS
13	AN	4	LYS
13	AN	7	ILE
13	AN	21	TYR

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Mol	Chain	Res	Type
13	AN	22	THR
13	AN	35	ARG
13	AN	40	CYS
13	AN	41	ARG
13	AN	42	ILE
13	AN	56	VAL
13	AN	57	ARG
13	AN	60	SER
13	AN	61	TRP
14	AO	5	LYS
14	AO	9	GLN
14	AO	10	LYS
14	AO	12	ILE
14	AO	15	PHE
14	AO	26	GLU
14	AO	31	LEU
14	AO	43	LEU
14	AO	47	LYS
14	AO	51	HIS
14	AO	56	LEU
14	AO	58	MET
14	AO	74	ASP
14	AO	76	GLU
14	AO	82	ILE
14	AO	88	ARG
15	AP	2	VAL
15	AP	20	VAL
15	AP	23	ASP
15	AP	32	TYR
15	AP	36	ILE
15	AP	44	THR
15	AP	54	GLU
15	AP	57	ARG
15	AP	68	ASP
15	AP	69	THR
15	AP	71	ARG
15	AP	72	ARG
15	AP	73	LEU
15	AP	75	ARG
15	AP	80	PHE
15	AP	81	ARG
16	AQ	13	ASP

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Mol	Chain	Res	Type
16	AQ	16	GLN
16	AQ	22	LEU
16	AQ	26	GLN
16	AQ	27	PHE
16	AQ	31	LEU
16	AQ	36	ILE
16	AQ	38	ARG
16	AQ	48	GLU
16	AQ	49	GLU
16	AQ	52	LYS
16	AQ	69	LYS
16	AQ	74	LEU
16	AQ	81	ARG
16	AQ	83	ASP
16	AQ	84	LEU
16	AQ	98	LEU
16	AQ	101	ARG
17	AR	26	LEU
17	AR	29	PHE
17	AR	34	TYR
17	AR	37	VAL
17	AR	38	GLU
17	AR	58	LEU
17	AR	72	ARG
17	AR	74	ARG
17	AR	83	GLU
17	AR	85	LEU
18	AS	5	LEU
18	AS	6	LYS
18	AS	9	VAL
18	AS	13	ASP
18	AS	14	HIS
18	AS	20	LEU
18	AS	23	ASN
18	AS	30	LEU
18	AS	33	THR
18	AS	34	TRP
18	AS	44	MET
18	AS	58	VAL
18	AS	61	TYR
18	AS	62	ILE
18	AS	64	GLU

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Mol	Chain	Res	Type
18	AS	67	VAL
18	AS	77	THR
18	AS	81	ARG
19	AT	13	LEU
19	AT	24	LEU
19	AT	36	LEU
19	AT	46	GLU
19	AT	50	GLU
19	AT	57	ARG
19	AT	72	LEU
19	AT	73	HIS
19	AT	74	LYS
19	AT	93	GLU
23	AY	9	LEU
23	AY	13	ARG
23	AY	20	HIS
23	AY	22	ASP
23	AY	25	LYS
23	AY	29	THR
23	AY	33	LEU
23	AY	39	ILE
23	AY	40	HIS
23	AY	53	ASP
23	AY	64	THR
23	AY	66	THR
23	AY	72	CYS
23	AY	75	LYS
23	AY	92	ILE
23	AY	98	MET
23	AY	99	ARG
23	AY	117	GLN
23	AY	118	SER
23	AY	126	GLU
23	AY	128	TYR
23	AY	132	ARG
23	AY	133	ILE
23	AY	137	ASN
23	AY	170	ARG
23	AY	174	PHE
23	AY	178	ILE
23	AY	187	THR
23	AY	197	ARG

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Mol	Chain	Res	Type
23	AY	198	GLU
23	AY	199	ILE
23	AY	203	GLU
23	AY	216	LEU
23	AY	224	ASP
23	AY	226	ASN
23	AY	231	TYR
23	AY	232	LEU
23	AY	240	GLU
23	AY	250	THR
23	AY	259	PHE
23	AY	260	LEU
23	AY	271	LEU
23	AY	274	ASP
23	AY	277	VAL
23	AY	278	ASP
23	AY	289	ILE
23	AY	299	VAL
23	AY	302	HIS
23	AY	312	LEU
23	AY	328	ILE
23	AY	330	VAL
23	AY	337	SER
23	AY	340	TYR
23	AY	348	ARG
23	AY	355	LEU
23	AY	368	GLU
23	AY	381	LYS
23	AY	385	THR
23	AY	393	ASP
23	AY	399	LEU
23	AY	404	VAL
23	AY	408	VAL
23	AY	410	ASP
23	AY	413	ILE
23	AY	421	GLN
23	AY	424	LEU
23	AY	428	LEU
23	AY	430	ARG
23	AY	431	LEU
23	AY	437	THR
23	AY	438	PHE

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Mol	Chain	Res	Type
23	AY	448	GLN
23	AY	449	THR
23	AY	461	ILE
23	AY	465	ARG
23	AY	476	VAL
23	AY	481	VAL
23	AY	483	TYR
23	AY	492	ASP
23	AY	498	ILE
23	AY	500	GLN
23	AY	504	ARG
23	AY	517	LEU
23	AY	529	ILE
23	AY	536	LYS
23	AY	542	VAL
23	AY	563	ILE
23	AY	572	TYR
23	AY	574	GLU
23	AY	580	MET
23	AY	600	VAL
23	AY	610	VAL
23	AY	615	GLU
23	AY	619	ASP
23	AY	624	LEU
23	AY	630	GLN
23	AY	631	ILE
23	AY	634	MET
23	AY	642	VAL
23	AY	647	VAL
23	AY	651	GLU
23	AY	658	ASP
23	AY	669	PHE
23	AY	671	MET
25	BC	6	LYS
25	BC	7	ARG
25	BC	9	ARG
25	BC	12	LEU
25	BC	13	GLU
25	BC	15	VAL
25	BC	16	ASP
25	BC	19	LYS
25	BC	24	ASP

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Mol	Chain	Res	Type
25	BC	28	ARG
25	BC	32	GLU
25	BC	37	LYS
25	BC	43	GLU
25	BC	45	HIS
25	BC	47	LYS
25	BC	48	LEU
25	BC	53	ARG
25	BC	60	ARG
25	BC	71	LYS
25	BC	73	VAL
25	BC	74	ARG
25	BC	76	LEU
25	BC	83	LYS
25	BC	93	ASP
25	BC	105	LEU
25	BC	106	ASP
25	BC	112	ASP
25	BC	117	THR
25	BC	131	ILE
25	BC	138	LEU
25	BC	150	ILE
25	BC	161	ARG
25	BC	164	PHE
25	BC	167	ASP
25	BC	169	THR
25	BC	172	ILE
25	BC	176	VAL
25	BC	198	GLU
25	BC	214	TYR
25	BC	215	VAL
25	BC	216	THR
25	BC	224	ARG
26	BD	4	LYS
26	BD	7	LYS
26	BD	24	ILE
26	BD	25	THR
26	BD	26	LYS
26	BD	28	GLU
26	BD	33	LEU
26	BD	35	LYS
26	BD	43	ARG

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Mol	Chain	Res	Type
26	BD	44	ASN
26	BD	63	ARG
26	BD	64	ILE
26	BD	65	ILE
26	BD	67	PHE
26	BD	71	ASP
26	BD	73	VAL
26	BD	78	LYS
26	BD	82	ILE
26	BD	91	ARG
26	BD	92	ILE
26	BD	95	LEU
26	BD	96	HIS
26	BD	97	TYR
26	BD	105	ILE
26	BD	106	ILE
26	BD	115	GLN
26	BD	116	GLN
26	BD	117	VAL
26	BD	122	ASP
26	BD	131	LEU
26	BD	136	ILE
26	BD	142	VAL
26	BD	146	GLU
26	BD	165	ILE
26	BD	169	GLU
26	BD	174	ILE
26	BD	177	LEU
26	BD	192	THR
26	BD	200	ASP
26	BD	226	MET
26	BD	230	ASP
26	BD	233	HIS
26	BD	239	ARG
26	BD	244	ARG
26	BD	250	TRP
26	BD	252	TRP
26	BD	257	LEU
26	BD	259	THR
26	BD	261	LYS
26	BD	262	ARG
26	BD	263	ARG

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Mol	Chain	Res	Type
26	BD	268	ARG
26	BD	271	ILE
27	BE	4	ILE
27	BE	9	VAL
27	BE	11	MET
27	BE	17	ASP
27	BE	35	GLN
27	BE	38	THR
27	BE	44	TYR
27	BE	51	PHE
27	BE	59	VAL
27	BE	67	PHE
27	BE	83	ASP
27	BE	87	GLU
27	BE	89	ASP
27	BE	94	GLU
27	BE	96	PHE
27	BE	102	VAL
27	BE	109	LYS
27	BE	113	PHE
27	BE	127	ASP
27	BE	129	HIS
27	BE	132	HIS
27	BE	134	ILE
27	BE	137	HIS
27	BE	146	THR
27	BE	154	LYS
27	BE	163	GLU
27	BE	164	ARG
27	BE	165	VAL
27	BE	172	VAL
27	BE	195	LEU
27	BE	196	VAL
27	BE	197	ILE
27	BE	199	ARG
27	BE	200	GLU
28	BF	6	VAL
28	BF	8	GLN
28	BF	9	ILE
28	BF	12	LEU
28	BF	18	ARG
28	BF	19	GLU

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Mol	Chain	Res	Type
28	BF	28	ILE
28	BF	32	LEU
28	BF	33	LEU
28	BF	40	GLN
28	BF	43	LYS
28	BF	45	ARG
28	BF	46	ARG
28	BF	62	ARG
28	BF	65	TRP
28	BF	72	ARG
28	BF	74	ARG
28	BF	75	HIS
28	BF	82	ILE
28	BF	89	VAL
28	BF	106	ARG
28	BF	125	LEU
28	BF	136	THR
28	BF	137	LYS
28	BF	154	VAL
28	BF	155	LEU
28	BF	170	LEU
28	BF	172	TRP
28	BF	175	THR
28	BF	186	ILE
28	BF	188	ARG
28	BF	189	THR
28	BF	190	GLU
28	BF	192	LEU
28	BF	194	MET
28	BF	197	ASP
28	BF	201	VAL
28	BF	205	ARG
29	BG	5	VAL
29	BG	10	LYS
29	BG	11	TYR
29	BG	12	TYR
29	BG	16	ARG
29	BG	33	ARG
29	BG	34	LEU
29	BG	35	GLU
29	BG	39	ILE
29	BG	49	ASP

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Mol	Chain	Res	Type
29	BG	55	LYS
29	BG	60	LEU
29	BG	63	ILE
29	BG	64	THR
29	BG	74	LYS
29	BG	86	MET
29	BG	94	LEU
29	BG	98	ARG
29	BG	105	LYS
29	BG	106	LEU
29	BG	113	ARG
29	BG	130	ASN
29	BG	136	ARG
29	BG	141	PHE
29	BG	144	ILE
29	BG	145	THR
29	BG	147	ASP
29	BG	150	ASP
29	BG	152	LEU
29	BG	153	ARG
29	BG	159	VAL
29	BG	164	GLU
29	BG	165	THR
29	BG	167	GLU
29	BG	168	GLU
29	BG	176	LEU
29	BG	181	ARG
30	BH	15	VAL
30	BH	17	VAL
30	BH	27	LYS
30	BH	34	GLU
30	BH	35	VAL
30	BH	37	VAL
30	BH	41	MET
30	BH	42	ARG
30	BH	43	VAL
30	BH	44	VAL
30	BH	51	ARG
30	BH	67	LEU
30	BH	71	LEU
30	BH	85	LYS
30	BH	86	GLU

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Mol	Chain	Res	Type
30	BH	89	ILE
30	BH	97	ARG
30	BH	105	LEU
30	BH	110	SER
30	BH	119	GLU
30	BH	127	GLU
30	BH	129	THR
30	BH	138	LYS
30	BH	147	ASN
30	BH	162	ILE
30	BH	167	GLU
30	BH	175	LYS
32	BK	16	LYS
32	BK	37	PHE
32	BK	41	PHE
32	BK	59	ILE
32	BK	62	ASP
32	BK	78	ILE
32	BK	90	LYS
32	BK	95	LYS
32	BK	99	ILE
32	BK	112	MET
32	BK	126	MET
33	BO	3	GLN
33	BO	9	GLU
33	BO	24	VAL
33	BO	34	THR
33	BO	35	VAL
33	BO	39	ILE
33	BO	58	VAL
33	BO	59	LYS
33	BO	62	VAL
33	BO	67	LYS
33	BO	77	ILE
33	BO	80	ASP
33	BO	82	ASN
33	BO	88	ASN
33	BO	91	LEU
33	BO	107	ARG
33	BO	108	GLU
33	BO	112	MET
33	BO	114	ILE

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Mol	Chain	Res	Type
33	BO	117	LEU
34	BP	7	ARG
34	BP	9	ASN
34	BP	15	ARG
34	BP	16	ARG
34	BP	18	ARG
34	BP	27	HIS
34	BP	32	THR
34	BP	38	GLN
34	BP	39	LYS
34	BP	42	SER
34	BP	46	LYS
34	BP	55	ARG
34	BP	57	THR
34	BP	60	MET
34	BP	62	LEU
34	BP	74	GLU
34	BP	77	ARG
34	BP	83	VAL
34	BP	84	ASN
34	BP	85	LEU
34	BP	90	ARG
34	BP	91	PHE
34	BP	98	GLU
34	BP	106	LEU
34	BP	107	LYS
34	BP	108	LYS
34	BP	110	TYR
34	BP	111	ARG
34	BP	123	LEU
34	BP	125	VAL
34	BP	135	LEU
34	BP	138	LEU
35	BQ	1	MET
35	BQ	3	MET
35	BQ	7	MET
35	BQ	8	LYS
35	BQ	14	ARG
35	BQ	17	LEU
35	BQ	26	TYR
35	BQ	31	ASP
35	BQ	43	THR

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Mol	Chain	Res	Type
35	BQ	45	GLN
35	BQ	46	GLN
35	BQ	56	ARG
35	BQ	66	ILE
35	BQ	68	ILE
35	BQ	74	TYR
35	BQ	90	VAL
35	BQ	93	TYR
35	BQ	96	VAL
35	BQ	98	LYS
35	BQ	101	ARG
35	BQ	103	MET
35	BQ	104	PHE
35	BQ	115	MET
35	BQ	116	GLU
35	BQ	125	LEU
35	BQ	128	LYS
35	BQ	131	ILE
35	BQ	135	ASP
35	BQ	137	TYR
35	BQ	139	GLU
36	BR	2	ARG
36	BR	3	HIS
36	BR	4	LEU
36	BR	8	ARG
36	BR	10	LEU
36	BR	15	SER
36	BR	22	ARG
36	BR	23	ASN
36	BR	24	GLN
36	BR	28	LEU
36	BR	29	LEU
36	BR	44	LEU
36	BR	45	ARG
36	BR	50	HIS
36	BR	60	LEU
36	BR	68	ARG
36	BR	69	ASP
36	BR	71	GLN
36	BR	76	VAL
36	BR	80	PHE
36	BR	81	ASP

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Mol	Chain	Res	Type
36	BR	99	LYS
36	BR	100	LEU
36	BR	102	GLU
36	BR	107	ASP
36	BR	111	LEU
36	BR	113	LEU
36	BR	115	GLU
37	BS	12	PHE
37	BS	13	ARG
37	BS	15	ARG
37	BS	17	ARG
37	BS	18	ILE
37	BS	20	ARG
37	BS	23	ARG
37	BS	40	ILE
37	BS	42	ASP
37	BS	47	THR
37	BS	53	SER
37	BS	54	LEU
37	BS	71	ARG
37	BS	82	ILE
37	BS	85	VAL
37	BS	89	ARG
37	BS	93	LYS
37	BS	97	ARG
37	BS	99	LYS
37	BS	101	LEU
37	BS	103	GLU
37	BS	106	ARG
38	BT	11	GLU
38	BT	13	ARG
38	BT	23	ARG
38	BT	27	THR
38	BT	30	VAL
38	BT	33	LYS
38	BT	46	GLU
38	BT	57	PHE
38	BT	61	PHE
38	BT	65	LYS
38	BT	70	VAL
38	BT	74	ARG
38	BT	78	LEU

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Mol	Chain	Res	Type
38	BT	82	LEU
38	BT	84	GLN
38	BT	90	GLN
38	BT	110	ILE
38	BT	114	LEU
38	BT	115	ARG
38	BT	118	ARG
38	BT	125	ARG
39	BU	11	ARG
39	BU	14	HIS
39	BU	16	LYS
39	BU	28	ARG
39	BU	33	ARG
39	BU	38	THR
39	BU	51	LYS
39	BU	55	ARG
39	BU	57	PHE
39	BU	74	LEU
39	BU	91	ASP
39	BU	97	ASP
39	BU	101	ARG
39	BU	108	GLU
39	BU	111	GLU
39	BU	114	LYS
40	BV	7	THR
40	BV	10	LYS
40	BV	18	LEU
40	BV	19	LYS
40	BV	21	ARG
40	BV	25	LEU
40	BV	26	ASP
40	BV	33	VAL
40	BV	37	VAL
40	BV	40	LEU
40	BV	43	GLU
40	BV	57	VAL
40	BV	60	GLU
40	BV	64	HIS
40	BV	74	LYS
40	BV	75	PHE
40	BV	79	VAL
40	BV	80	GLN

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Mol	Chain	Res	Type
40	BV	88	ARG
40	BV	91	TYR
40	BV	99	ILE
41	BW	9	TYR
41	BW	11	ARG
41	BW	13	SER
41	BW	15	ARG
41	BW	19	LEU
41	BW	25	ARG
41	BW	27	LYS
41	BW	40	ASN
41	BW	46	PHE
41	BW	51	LEU
41	BW	66	GLU
41	BW	86	LEU
41	BW	88	ARG
41	BW	94	ASP
41	BW	95	ILE
41	BW	96	ILE
41	BW	100	THR
41	BW	107	LEU
41	BW	113	LYS
42	BX	6	ASP
42	BX	8	ILE
42	BX	27	THR
42	BX	28	PHE
42	BX	35	THR
42	BX	55	ASN
42	BX	57	LEU
42	BX	58	HIS
42	BX	63	LYS
42	BX	68	ARG
42	BX	70	LEU
42	BX	75	ASP
42	BX	76	ARG
42	BX	82	GLN
42	BX	88	LYS
42	BX	95	LEU
43	BY	2	ARG
43	BY	5	MET
43	BY	6	HIS
43	BY	9	LYS

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Mol	Chain	Res	Type
43	BY	13	VAL
43	BY	14	LEU
43	BY	19	LYS
43	BY	29	GLU
43	BY	33	LYS
43	BY	38	ILE
43	BY	44	ILE
43	BY	47	LYS
43	BY	49	VAL
43	BY	50	ARG
43	BY	75	ILE
43	BY	89	PHE
43	BY	90	LEU
43	BY	97	ARG
43	BY	102	CYS
44	BZ	5	LEU
44	BZ	6	LYS
44	BZ	8	TYR
44	BZ	20	ARG
44	BZ	28	MET
44	BZ	29	TYR
44	BZ	35	ARG
44	BZ	44	PHE
44	BZ	46	LYS
44	BZ	49	ARG
44	BZ	59	LEU
44	BZ	81	ARG
44	BZ	85	HIS
44	BZ	86	VAL
44	BZ	87	ASP
44	BZ	97	GLU
44	BZ	98	MET
44	BZ	112	ARG
44	BZ	123	ASP
44	BZ	124	ILE
44	BZ	126	VAL
44	BZ	127	LYS
44	BZ	131	ARG
44	BZ	133	ILE
44	BZ	141	VAL
44	BZ	144	LEU
44	BZ	145	GLU

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Mol	Chain	Res	Type
44	BZ	148	ASP
44	BZ	150	LEU
44	BZ	156	LYS
44	BZ	162	GLU
44	BZ	175	VAL
44	BZ	181	GLU
45	B0	3	HIS
45	B0	12	ASN
45	B0	20	ARG
45	B0	27	GLU
45	B0	37	LEU
45	B0	43	THR
45	B0	57	PHE
45	B0	58	THR
45	B0	59	LEU
45	B0	64	ASP
45	B0	68	GLU
46	B1	5	CYS
46	B1	17	SER
46	B1	23	LYS
46	B1	26	ARG
46	B1	32	LYS
46	B1	40	ARG
46	B1	41	ARG
46	B1	42	GLN
46	B1	43	TYR
46	B1	46	LEU
46	B1	50	ARG
46	B1	57	GLU
46	B1	58	ILE
46	B1	61	ARG
46	B1	82	LEU
46	B1	83	GLU
46	B1	90	ILE
47	B4	6	HIS
47	B4	9	LEU
47	B4	13	ARG
47	B4	23	GLU
47	B4	28	LYS
47	B4	30	GLU
47	B4	31	ILE
47	B4	32	TYR

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Mol	Chain	Res	Type
48	BN	1	MET
48	BN	7	LYS
48	BN	32	THR
48	BN	42	TRP
48	BN	45	ASN
48	BN	48	MET
48	BN	50	ASP
48	BN	71	ILE
48	BN	87	LEU
48	BN	96	GLU
48	BN	99	LEU
48	BN	111	PRO
48	BN	112	LEU
48	BN	127	ASP
48	BN	131	GLN
48	BN	137	LYS
48	BN	138	LEU
49	B2	8	LYS
49	B2	30	ARG
49	B2	34	GLU
49	B2	35	LEU
49	B2	37	PHE
49	B2	45	SER
49	B2	47	ASN
49	B2	51	ARG
49	B2	53	LEU
49	B2	64	LEU
49	B2	69	ARG
50	B3	8	LEU
50	B3	17	LYS
50	B3	29	ARG
50	B3	31	LEU
50	B3	37	LEU
50	B3	53	LEU
50	B3	60	GLU
51	B5	3	LYS
51	B5	4	HIS
51	B5	15	ARG
51	B5	23	HIS
51	B5	44	THR
51	B5	51	TYR
51	B5	55	ARG

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Mol	Chain	Res	Type
51	B5	56	LYS
51	B5	58	LEU
52	B6	6	ARG
52	B6	9	LEU
52	B6	11	LEU
52	B6	15	GLU
52	B6	18	ARG
52	B6	19	ARG
52	B6	29	ASN
52	B6	34	LEU
52	B6	37	ARG
52	B6	39	TYR
52	B6	47	THR
52	B6	48	VAL
52	B6	49	HIS
53	B7	40	TRP
53	B7	41	ARG
53	B7	42	LEU
54	B8	14	VAL
54	B8	15	LYS
54	B8	16	ILE
54	B8	17	THR
54	B8	25	MET
54	B8	27	THR
54	B8	30	ARG
54	B8	31	HIS
54	B8	34	TRP
54	B8	36	LYS
54	B8	42	ARG
54	B8	46	ARG
54	B8	48	PHE
54	B8	52	LYS
54	B8	56	GLU
54	B8	59	LYS
54	B8	61	LEU
54	B8	62	LEU
54	B8	64	TYR
55	B9	14	CYS
55	B9	19	ARG
55	B9	24	TYR
55	B9	28	GLU
55	B9	35	ARG

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Mol	Chain	Res	Type
56	Be	62	VAL
56	Be	77	GLU
56	Be	78	LEU
56	Be	90	LYS
56	Be	91	ASP
56	Be	94	GLU
56	Be	106	GLN
1	CB	7	VAL
1	CB	9	GLU
1	CB	15	VAL
1	CB	16	HIS
1	CB	17	PHE
1	CB	21	ARG
1	CB	28	PHE
1	CB	32	ILE
1	CB	36	ARG
1	CB	49	GLU
1	CB	69	LEU
1	CB	74	LYS
1	CB	81	VAL
1	CB	101	MET
1	CB	103	THR
1	CB	104	ASN
1	CB	109	SER
1	CB	134	GLU
1	CB	141	GLU
1	CB	145	LEU
1	CB	154	LEU
1	CB	155	LEU
1	CB	162	ILE
1	CB	163	PHE
1	CB	168	THR
1	CB	172	ILE
1	CB	175	ARG
1	CB	185	ILE
1	CB	187	LEU
1	CB	189	ASP
1	CB	190	THR
1	CB	208	ILE
1	CB	212	GLN
1	CB	213	LEU
1	CB	221	LEU

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Mol	Chain	Res	Type
1	CB	226	ARG
1	CB	230	VAL
1	CB	236	TYR
2	CC	4	LYS
2	CC	5	ILE
2	CC	6	HIS
2	CC	15	THR
2	CC	19	GLU
2	CC	22	TRP
2	CC	39	ILE
2	CC	47	LEU
2	CC	48	TYR
2	CC	52	LEU
2	CC	55	VAL
2	CC	56	ASP
2	CC	57	ILE
2	CC	67	THR
2	CC	70	VAL
2	CC	75	VAL
2	CC	84	ILE
2	CC	86	VAL
2	CC	99	VAL
2	CC	101	LEU
2	CC	102	ASN
2	CC	110	ASN
2	CC	118	GLN
2	CC	119	ARG
2	CC	123	GLN
2	CC	124	ILE
2	CC	127	ARG
2	CC	128	PHE
2	CC	132	ARG
2	CC	134	ILE
2	CC	142	MET
2	CC	152	ILE
2	CC	157	ILE
2	CC	164	ARG
2	CC	167	TRP
2	CC	176	HIS
2	CC	179	ARG
2	CC	184	TYR
2	CC	188	LEU

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Mol	Chain	Res	Type
2	CC	208	ILE
3	CD	3	ARG
3	CD	5	ILE
3	CD	9	CYS
3	CD	13	ARG
3	CD	21	LEU
3	CD	24	GLU
3	CD	28	SER
3	CD	30	LYS
3	CD	54	TYR
3	CD	56	VAL
3	CD	57	ARG
3	CD	60	GLU
3	CD	61	LYS
3	CD	63	LYS
3	CD	67	ILE
3	CD	72	GLU
3	CD	83	SER
3	CD	86	LYS
3	CD	107	ARG
3	CD	114	ARG
3	CD	127	THR
3	CD	132	ARG
3	CD	140	VAL
3	CD	148	VAL
3	CD	150	GLU
3	CD	156	GLU
3	CD	175	SER
3	CD	178	VAL
3	CD	193	ASP
3	CD	196	LEU
3	CD	200	GLU
4	CE	5	ASP
4	CE	10	MET
4	CE	12	LEU
4	CE	31	LEU
4	CE	33	VAL
4	CE	41	VAL
4	CE	47	LYS
4	CE	53	LEU
4	CE	57	LYS
4	CE	61	TYR

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Mol	Chain	Res	Type
4	CE	64	ARG
4	CE	78	HIS
4	CE	80	ILE
4	CE	91	LEU
4	CE	92	LYS
4	CE	107	ARG
4	CE	117	ASP
4	CE	125	SER
4	CE	129	ILE
4	CE	137	GLU
4	CE	141	GLN
4	CE	147	ASP
4	CE	150	ARG
5	CF	2	ARG
5	CF	7	ASN
5	CF	16	GLN
5	CF	18	GLN
5	CF	22	GLU
5	CF	27	GLN
5	CF	37	VAL
5	CF	43	LEU
5	CF	46	ARG
5	CF	55	ASP
5	CF	61	LEU
5	CF	66	GLU
5	CF	69	GLU
5	CF	77	ARG
5	CF	78	GLU
5	CF	83	ASP
6	CG	10	ARG
6	CG	11	GLN
6	CG	12	LEU
6	CG	18	TYR
6	CG	21	VAL
6	CG	24	THR
6	CG	32	ARG
6	CG	35	LYS
6	CG	36	LYS
6	CG	54	THR
6	CG	67	GLU
6	CG	74	GLU
6	CG	76	ARG

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Mol	Chain	Res	Type
6	CG	79	ARG
6	CG	94	ARG
6	CG	97	GLN
6	CG	104	LEU
6	CG	106	GLN
6	CG	115	ARG
6	CG	149	ARG
7	CH	3	THR
7	CH	11	THR
7	CH	29	SER
7	CH	30	ARG
7	CH	37	ARG
7	CH	49	GLU
7	CH	50	ARG
7	CH	52	ASP
7	CH	54	ASP
7	CH	63	LEU
7	CH	69	ARG
7	CH	73	ASP
7	CH	88	LYS
7	CH	102	ARG
7	CH	104	ARG
7	CH	107	LEU
7	CH	112	LEU
7	CH	133	LEU
7	CH	135	CYS
7	CH	136	GLU
8	CI	12	GLU
8	CI	26	VAL
8	CI	34	ASN
8	CI	40	LEU
8	CI	70	LYS
8	CI	75	ASP
8	CI	79	LEU
8	CI	86	VAL
8	CI	91	ASP
8	CI	95	LYS
8	CI	97	LYS
8	CI	109	VAL
8	CI	112	LYS
8	CI	121	ARG
8	CI	125	TYR

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Mol	Chain	Res	Type
8	CI	128	ARG
9	CJ	3	LYS
9	CJ	11	PHE
9	CJ	12	ASP
9	CJ	16	LEU
9	CJ	22	LYS
9	CJ	30	SER
9	CJ	50	ILE
9	CJ	54	PHE
9	CJ	65	LEU
9	CJ	66	ARG
9	CJ	67	THR
9	CJ	75	ILE
9	CJ	79	ARG
9	CJ	86	MET
9	CJ	96	ILE
10	CK	18	ARG
10	CK	22	HIS
10	CK	29	ILE
10	CK	30	VAL
10	CK	31	THR
10	CK	41	THR
10	CK	51	LYS
10	CK	87	THR
10	CK	91	ARG
10	CK	107	SER
10	CK	109	VAL
10	CK	119	CYS
11	CL	20	LYS
11	CL	22	SER
11	CL	24	VAL
11	CL	33	ARG
11	CL	38	THR
11	CL	44	THR
11	CL	49	ASN
11	CL	52	LEU
11	CL	53	ARG
11	CL	54	LYS
11	CL	55	VAL
11	CL	57	LYS
11	CL	59	ARG
11	CL	60	LEU

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Mol	Chain	Res	Type
11	CL	66	VAL
11	CL	67	THR
11	CL	70	ILE
11	CL	75	HIS
11	CL	78	GLN
11	CL	84	LEU
11	CL	90	VAL
11	CL	92	ASP
11	CL	93	LEU
11	CL	97	ARG
11	CL	110	VAL
11	CL	116	SER
11	CL	122	THR
12	CM	8	GLU
12	CM	15	VAL
12	CM	23	TYR
12	CM	27	LYS
12	CM	43	THR
12	CM	48	LEU
12	CM	67	GLU
12	CM	69	GLU
12	CM	70	LEU
12	CM	82	MET
12	CM	88	ARG
12	CM	103	THR
12	CM	106	ASN
12	CM	108	ARG
12	CM	110	ARG
12	CM	115	LYS
12	CM	120	LYS
12	CM	121	LYS
13	CN	4	LYS
13	CN	7	ILE
13	CN	21	TYR
13	CN	35	ARG
13	CN	40	CYS
13	CN	41	ARG
13	CN	42	ILE
13	CN	57	ARG
13	CN	61	TRP
14	CO	5	LYS
14	CO	8	LYS

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Mol	Chain	Res	Type
14	CO	10	LYS
14	CO	15	PHE
14	CO	28	GLN
14	CO	31	LEU
14	CO	34	LEU
14	CO	47	LYS
14	CO	51	HIS
14	CO	52	SER
14	CO	56	LEU
14	CO	57	LEU
14	CO	58	MET
14	CO	74	ASP
14	CO	82	ILE
14	CO	85	LEU
14	CO	88	ARG
15	CP	23	ASP
15	CP	32	TYR
15	CP	36	ILE
15	CP	43	LYS
15	CP	45	THR
15	CP	54	GLU
15	CP	57	ARG
15	CP	68	ASP
15	CP	69	THR
15	CP	71	ARG
15	CP	80	PHE
15	CP	81	ARG
16	CQ	13	ASP
16	CQ	16	GLN
16	CQ	26	GLN
16	CQ	27	PHE
16	CQ	32	TYR
16	CQ	36	ILE
16	CQ	49	GLU
16	CQ	52	LYS
16	CQ	60	ILE
16	CQ	69	LYS
16	CQ	74	LEU
16	CQ	83	ASP
16	CQ	91	ARG
17	CR	19	LYS
17	CR	26	LEU

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Mol	Chain	Res	Type
17	CR	29	PHE
17	CR	34	TYR
17	CR	39	VAL
17	CR	47	THR
17	CR	58	LEU
17	CR	59	SER
17	CR	72	ARG
17	CR	74	ARG
17	CR	76	LEU
17	CR	83	GLU
17	CR	85	LEU
18	CS	6	LYS
18	CS	13	ASP
18	CS	23	ASN
18	CS	34	TRP
18	CS	41	VAL
18	CS	43	GLU
18	CS	44	MET
18	CS	56	GLN
18	CS	58	VAL
18	CS	61	TYR
18	CS	62	ILE
18	CS	64	GLU
18	CS	67	VAL
18	CS	77	THR
18	CS	81	ARG
19	CT	8	ARG
19	CT	13	LEU
19	CT	24	LEU
19	CT	36	LEU
19	CT	54	LYS
19	CT	74	LYS
19	CT	93	GLU
23	CY	8	ASP
23	CY	9	LEU
23	CY	13	ARG
23	CY	20	HIS
23	CY	26	THR
23	CY	29	THR
23	CY	33	LEU
23	CY	39	ILE
23	CY	40	HIS

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Mol	Chain	Res	Type
23	CY	60	GLU
23	CY	66	THR
23	CY	72	CYS
23	CY	88	VAL
23	CY	92	ILE
23	CY	98	MET
23	CY	99	ARG
23	CY	105	ILE
23	CY	106	VAL
23	CY	111	SER
23	CY	114	VAL
23	CY	118	SER
23	CY	122	TRP
23	CY	126	GLU
23	CY	127	LYS
23	CY	128	TYR
23	CY	132	ARG
23	CY	133	ILE
23	CY	152	THR
23	CY	170	ARG
23	CY	172	ASP
23	CY	174	PHE
23	CY	178	ILE
23	CY	186	TYR
23	CY	188	TYR
23	CY	197	ARG
23	CY	199	ILE
23	CY	203	GLU
23	CY	224	ASP
23	CY	231	TYR
23	CY	232	LEU
23	CY	236	GLU
23	CY	237	PRO
23	CY	240	GLU
23	CY	250	THR
23	CY	259	PHE
23	CY	260	LEU
23	CY	264	LEU
23	CY	277	VAL
23	CY	278	ASP
23	CY	285	ASP
23	CY	289	ILE

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Mol	Chain	Res	Type
23	CY	295	GLU
23	CY	298	VAL
23	CY	299	VAL
23	CY	312	LEU
23	CY	328	ILE
23	CY	337	SER
23	CY	344	THR
23	CY	355	LEU
23	CY	356	LEU
23	CY	357	ARG
23	CY	367	GLU
23	CY	368	GLU
23	CY	381	LYS
23	CY	385	THR
23	CY	399	LEU
23	CY	404	VAL
23	CY	408	VAL
23	CY	410	ASP
23	CY	413	ILE
23	CY	421	GLN
23	CY	424	LEU
23	CY	426	GLN
23	CY	428	LEU
23	CY	430	ARG
23	CY	431	LEU
23	CY	438	PHE
23	CY	448	GLN
23	CY	449	THR
23	CY	452	SER
23	CY	473	ASP
23	CY	476	VAL
23	CY	498	ILE
23	CY	504	ARG
23	CY	515	GLU
23	CY	521	SER
23	CY	536	LYS
23	CY	542	VAL
23	CY	563	ILE
23	CY	564	LYS
23	CY	565	VAL
23	CY	567	LEU
23	CY	572	TYR

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Mol	Chain	Res	Type
23	CY	580	MET
23	CY	591	LYS
23	CY	598	ASP
23	CY	615	GLU
23	CY	617	MET
23	CY	619	ASP
23	CY	624	LEU
23	CY	630	GLN
23	CY	631	ILE
23	CY	647	VAL
23	CY	658	ASP
23	CY	670	VAL
23	CY	671	MET
23	CY	675	HIS
25	DC	7	ARG
25	DC	12	LEU
25	DC	15	VAL
25	DC	16	ASP
25	DC	19	LYS
25	DC	22	THR
25	DC	24	ASP
25	DC	28	ARG
25	DC	31	LYS
25	DC	32	GLU
25	DC	37	LYS
25	DC	39	ASP
25	DC	42	VAL
25	DC	47	LYS
25	DC	51	ASP
25	DC	53	ARG
25	DC	56	ASP
25	DC	59	VAL
25	DC	60	ARG
25	DC	63	VAL
25	DC	71	LYS
25	DC	73	VAL
25	DC	74	ARG
25	DC	76	LEU
25	DC	83	LYS
25	DC	95	VAL
25	DC	105	LEU
25	DC	106	ASP

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Mol	Chain	Res	Type
25	DC	110	ASP
25	DC	117	THR
25	DC	121	MET
25	DC	131	ILE
25	DC	138	LEU
25	DC	139	PRO
25	DC	145	THR
25	DC	161	ARG
25	DC	162	ILE
25	DC	164	PHE
25	DC	165	ARG
25	DC	166	ASN
25	DC	167	ASP
25	DC	169	THR
25	DC	172	ILE
25	DC	176	VAL
25	DC	182	PRO
25	DC	185	LYS
25	DC	189	ASN
25	DC	215	VAL
25	DC	216	THR
25	DC	224	ARG
26	DD	4	LYS
26	DD	10	THR
26	DD	20	ASP
26	DD	23	GLU
26	DD	24	ILE
26	DD	25	THR
26	DD	26	LYS
26	DD	33	LEU
26	DD	35	LYS
26	DD	37	LEU
26	DD	43	ARG
26	DD	44	ASN
26	DD	49	ILE
26	DD	64	ILE
26	DD	65	ILE
26	DD	67	PHE
26	DD	78	LYS
26	DD	82	ILE
26	DD	83	GLU
26	DD	95	LEU

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Mol	Chain	Res	Type
26	DD	96	HIS
26	DD	103	ARG
26	DD	105	ILE
26	DD	112	GLN
26	DD	115	GLN
26	DD	116	GLN
26	DD	117	VAL
26	DD	131	LEU
26	DD	136	ILE
26	DD	142	VAL
26	DD	164	GLN
26	DD	169	GLU
26	DD	196	VAL
26	DD	198	ASN
26	DD	201	HIS
26	DD	218	ARG
26	DD	229	VAL
26	DD	230	ASP
26	DD	239	ARG
26	DD	244	ARG
26	DD	252	TRP
26	DD	257	LEU
26	DD	259	THR
26	DD	269	PHE
27	DE	4	ILE
27	DE	9	VAL
27	DE	16	ARG
27	DE	17	ASP
27	DE	35	GLN
27	DE	51	PHE
27	DE	61	ARG
27	DE	67	PHE
27	DE	80	GLU
27	DE	83	ASP
27	DE	87	GLU
27	DE	89	ASP
27	DE	94	GLU
27	DE	96	PHE
27	DE	97	LYS
27	DE	109	LYS
27	DE	111	ARG
27	DE	113	PHE

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Mol	Chain	Res	Type
27	DE	127	ASP
27	DE	129	HIS
27	DE	132	HIS
27	DE	134	ILE
27	DE	144	ARG
27	DE	146	THR
27	DE	154	LYS
27	DE	164	ARG
27	DE	192	ASN
27	DE	196	VAL
27	DE	197	ILE
27	DE	199	ARG
27	DE	200	GLU
28	DF	2	LYS
28	DF	3	GLU
28	DF	6	VAL
28	DF	8	GLN
28	DF	9	ILE
28	DF	12	LEU
28	DF	19	GLU
28	DF	28	ILE
28	DF	29	ASN
28	DF	32	LEU
28	DF	33	LEU
28	DF	35	GLU
28	DF	40	GLN
28	DF	43	LYS
28	DF	45	ARG
28	DF	54	ARG
28	DF	62	ARG
28	DF	65	TRP
28	DF	72	ARG
28	DF	74	ARG
28	DF	89	VAL
28	DF	106	ARG
28	DF	124	LEU
28	DF	126	VAL
28	DF	136	THR
28	DF	137	LYS
28	DF	149	ASP
28	DF	154	VAL
28	DF	155	LEU

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Mol	Chain	Res	Type
28	DF	156	LEU
28	DF	170	LEU
28	DF	172	TRP
28	DF	175	THR
28	DF	186	ILE
28	DF	188	ARG
28	DF	190	GLU
28	DF	192	LEU
28	DF	194	MET
28	DF	196	LEU
29	DG	5	VAL
29	DG	10	LYS
29	DG	11	TYR
29	DG	12	TYR
29	DG	29	TRP
29	DG	33	ARG
29	DG	34	LEU
29	DG	35	GLU
29	DG	36	LYS
29	DG	49	ASP
29	DG	52	ILE
29	DG	54	GLU
29	DG	60	LEU
29	DG	62	LEU
29	DG	64	THR
29	DG	66	GLN
29	DG	74	LYS
29	DG	86	MET
29	DG	101	ILE
29	DG	103	LEU
29	DG	105	LYS
29	DG	106	LEU
29	DG	113	ARG
29	DG	128	ARG
29	DG	133	LEU
29	DG	141	PHE
29	DG	144	ILE
29	DG	147	ASP
29	DG	153	ARG
29	DG	159	VAL
29	DG	164	GLU
29	DG	167	GLU

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Mol	Chain	Res	Type
29	DG	168	GLU
29	DG	176	LEU
30	DH	15	VAL
30	DH	34	GLU
30	DH	37	VAL
30	DH	41	MET
30	DH	43	VAL
30	DH	44	VAL
30	DH	60	ARG
30	DH	67	LEU
30	DH	69	ARG
30	DH	71	LEU
30	DH	85	LYS
30	DH	86	GLU
30	DH	89	ILE
30	DH	97	ARG
30	DH	127	GLU
30	DH	134	SER
30	DH	136	ILE
30	DH	138	LYS
30	DH	143	GLN
30	DH	148	ILE
30	DH	160	LYS
32	DK	4	VAL
32	DK	37	PHE
32	DK	41	PHE
32	DK	50	ASP
32	DK	56	GLU
32	DK	57	ILE
32	DK	59	ILE
32	DK	67	PHE
32	DK	70	LYS
32	DK	75	SER
32	DK	76	TYR
32	DK	78	ILE
32	DK	90	LYS
32	DK	95	LYS
32	DK	99	ILE
32	DK	132	ARG
32	DK	136	VAL
33	DO	1	MET
33	DO	2	ILE

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Mol	Chain	Res	Type
33	DO	34	THR
33	DO	39	ILE
33	DO	58	VAL
33	DO	59	LYS
33	DO	67	LYS
33	DO	73	ASP
33	DO	80	ASP
33	DO	82	ASN
33	DO	91	LEU
33	DO	99	PHE
33	DO	107	ARG
33	DO	112	MET
33	DO	114	ILE
33	DO	117	LEU
34	DP	7	ARG
34	DP	9	ASN
34	DP	16	ARG
34	DP	18	ARG
34	DP	27	HIS
34	DP	32	THR
34	DP	38	GLN
34	DP	55	ARG
34	DP	60	MET
34	DP	62	LEU
34	DP	64	LYS
34	DP	77	ARG
34	DP	85	LEU
34	DP	91	PHE
34	DP	98	GLU
34	DP	106	LEU
34	DP	107	LYS
34	DP	108	LYS
34	DP	110	TYR
34	DP	117	GLU
34	DP	135	LEU
35	DQ	1	MET
35	DQ	3	MET
35	DQ	6	ARG
35	DQ	7	MET
35	DQ	17	LEU
35	DQ	26	TYR
35	DQ	31	ASP

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Mol	Chain	Res	Type
35	DQ	34	LEU
35	DQ	42	ILE
35	DQ	43	THR
35	DQ	56	ARG
35	DQ	59	ARG
35	DQ	60	ARG
35	DQ	66	ILE
35	DQ	68	ILE
35	DQ	74	TYR
35	DQ	90	VAL
35	DQ	93	TYR
35	DQ	96	VAL
35	DQ	101	ARG
35	DQ	116	GLU
35	DQ	125	LEU
35	DQ	128	LYS
35	DQ	131	ILE
35	DQ	137	TYR
35	DQ	139	GLU
36	DR	2	ARG
36	DR	3	HIS
36	DR	4	LEU
36	DR	8	ARG
36	DR	10	LEU
36	DR	15	SER
36	DR	22	ARG
36	DR	23	ASN
36	DR	28	LEU
36	DR	29	LEU
36	DR	44	LEU
36	DR	45	ARG
36	DR	60	LEU
36	DR	75	LEU
36	DR	76	VAL
36	DR	81	ASP
36	DR	94	TYR
36	DR	99	LYS
36	DR	111	LEU
37	DS	12	PHE
37	DS	13	ARG
37	DS	15	ARG
37	DS	18	ILE

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Mol	Chain	Res	Type
37	DS	20	ARG
37	DS	35	ILE
37	DS	39	ILE
37	DS	40	ILE
37	DS	42	ASP
37	DS	47	THR
37	DS	48	LEU
37	DS	71	ARG
37	DS	82	ILE
37	DS	85	VAL
37	DS	99	LYS
37	DS	103	GLU
37	DS	106	ARG
38	DT	11	GLU
38	DT	13	ARG
38	DT	23	ARG
38	DT	27	THR
38	DT	29	ARG
38	DT	33	LYS
38	DT	42	ILE
38	DT	49	VAL
38	DT	54	ARG
38	DT	57	PHE
38	DT	65	LYS
38	DT	70	VAL
38	DT	74	ARG
38	DT	79	HIS
38	DT	82	LEU
38	DT	84	GLN
38	DT	87	ASP
38	DT	108	ARG
38	DT	114	LEU
38	DT	115	ARG
38	DT	125	ARG
39	DU	14	HIS
39	DU	16	LYS
39	DU	28	ARG
39	DU	33	ARG
39	DU	34	LYS
39	DU	38	THR
39	DU	39	LEU
39	DU	51	LYS

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Mol	Chain	Res	Type
39	DU	55	ARG
39	DU	65	ILE
39	DU	74	LEU
39	DU	80	ILE
39	DU	91	ASP
39	DU	98	LEU
39	DU	101	ARG
39	DU	111	GLU
39	DU	114	LYS
40	DV	6	LYS
40	DV	7	THR
40	DV	10	LYS
40	DV	14	VAL
40	DV	18	LEU
40	DV	19	LYS
40	DV	21	ARG
40	DV	26	ASP
40	DV	33	VAL
40	DV	37	VAL
40	DV	40	LEU
40	DV	52	VAL
40	DV	57	VAL
40	DV	60	GLU
40	DV	64	HIS
40	DV	74	LYS
40	DV	75	PHE
40	DV	79	VAL
40	DV	87	HIS
40	DV	88	ARG
40	DV	99	ILE
40	DV	100	ARG
41	DW	11	ARG
41	DW	15	ARG
41	DW	17	VAL
41	DW	24	ILE
41	DW	37	ARG
41	DW	46	PHE
41	DW	51	LEU
41	DW	66	GLU
41	DW	88	ARG
41	DW	92	ARG
41	DW	94	ASP

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Mol	Chain	Res	Type
41	DW	95	ILE
41	DW	96	ILE
41	DW	100	THR
41	DW	103	ILE
41	DW	105	VAL
41	DW	107	LEU
41	DW	113	LYS
42	DX	8	ILE
42	DX	15	GLU
42	DX	23	GLU
42	DX	25	LYS
42	DX	27	THR
42	DX	35	THR
42	DX	36	LYS
42	DX	54	VAL
42	DX	57	LEU
42	DX	58	HIS
42	DX	68	ARG
42	DX	72	LYS
42	DX	76	ARG
42	DX	88	LYS
42	DX	95	LEU
43	DY	2	ARG
43	DY	6	HIS
43	DY	7	VAL
43	DY	9	LYS
43	DY	13	VAL
43	DY	29	GLU
43	DY	31	LEU
43	DY	33	LYS
43	DY	44	ILE
43	DY	47	LYS
43	DY	50	ARG
43	DY	75	ILE
43	DY	84	ARG
43	DY	89	PHE
43	DY	90	LEU
43	DY	97	ARG
44	DZ	3	TYR
44	DZ	5	LEU
44	DZ	20	ARG
44	DZ	27	VAL

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Mol	Chain	Res	Type
44	DZ	28	MET
44	DZ	29	TYR
44	DZ	35	ARG
44	DZ	46	LYS
44	DZ	48	PHE
44	DZ	49	ARG
44	DZ	54	HIS
44	DZ	59	LEU
44	DZ	60	GLU
44	DZ	61	LEU
44	DZ	76	LEU
44	DZ	81	ARG
44	DZ	86	VAL
44	DZ	94	GLU
44	DZ	97	GLU
44	DZ	98	MET
44	DZ	112	ARG
44	DZ	124	ILE
44	DZ	126	VAL
44	DZ	127	LYS
44	DZ	131	ARG
44	DZ	133	ILE
44	DZ	141	VAL
44	DZ	144	LEU
44	DZ	148	ASP
44	DZ	150	LEU
44	DZ	162	GLU
44	DZ	175	VAL
44	DZ	179	ASP
44	DZ	181	GLU
45	D0	4	LYS
45	D0	5	LYS
45	D0	9	SER
45	D0	20	ARG
45	D0	27	GLU
45	D0	37	LEU
45	D0	50	ASN
45	D0	53	MET
45	D0	57	PHE
45	D0	64	ASP
46	D1	3	LYS
46	D1	5	CYS

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Mol	Chain	Res	Type
46	D1	17	SER
46	D1	18	ILE
46	D1	21	ARG
46	D1	23	LYS
46	D1	26	ARG
46	D1	27	GLU
46	D1	32	LYS
46	D1	37	ILE
46	D1	39	LYS
46	D1	40	ARG
46	D1	41	ARG
46	D1	42	GLN
46	D1	43	TYR
46	D1	46	LEU
46	D1	50	ARG
46	D1	57	GLU
46	D1	58	ILE
46	D1	59	THR
46	D1	60	PHE
46	D1	61	ARG
46	D1	66	HIS
46	D1	73	LEU
46	D1	82	LEU
47	D4	1	MET
47	D4	9	LEU
47	D4	10	VAL
47	D4	30	GLU
47	D4	32	TYR
47	D4	33	VAL
48	DN	1	MET
48	DN	7	LYS
48	DN	32	THR
48	DN	42	TRP
48	DN	45	ASN
48	DN	48	MET
48	DN	50	ASP
48	DN	71	ILE
48	DN	87	LEU
48	DN	96	GLU
48	DN	99	LEU
48	DN	111	PRO
48	DN	112	LEU

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Mol	Chain	Res	Type
48	DN	127	ASP
48	DN	131	GLN
48	DN	137	LYS
48	DN	138	LEU
49	D2	4	SER
49	D2	8	LYS
49	D2	30	ARG
49	D2	37	PHE
49	D2	38	GLN
49	D2	47	ASN
49	D2	51	ARG
49	D2	53	LEU
50	D3	17	LYS
50	D3	29	ARG
50	D3	30	ARG
50	D3	31	LEU
50	D3	37	LEU
50	D3	53	LEU
50	D3	60	GLU
51	D5	3	LYS
51	D5	4	HIS
51	D5	11	THR
51	D5	15	ARG
51	D5	16	ARG
51	D5	23	HIS
51	D5	25	LEU
51	D5	51	TYR
51	D5	58	LEU
52	D6	9	LEU
52	D6	11	LEU
52	D6	18	ARG
52	D6	19	ARG
52	D6	27	LYS
52	D6	34	LEU
52	D6	39	TYR
52	D6	45	LYS
52	D6	47	THR
52	D6	48	VAL
52	D6	49	HIS
52	D6	50	ARG
53	D7	29	LYS
53	D7	35	ARG

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Mol	Chain	Res	Type
53	D7	40	TRP
53	D7	41	ARG
53	D7	42	LEU
53	D7	46	VAL
54	D8	14	VAL
54	D8	16	ILE
54	D8	31	HIS
54	D8	32	LEU
54	D8	34	TRP
54	D8	36	LYS
54	D8	42	ARG
54	D8	44	LYS
54	D8	46	ARG
54	D8	48	PHE
54	D8	56	GLU
54	D8	59	LYS
54	D8	62	LEU
54	D8	64	TYR
55	D9	11	CYS
55	D9	12	ASP
55	D9	17	ILE
55	D9	19	ARG
55	D9	28	GLU
56	De	60	PHE
56	De	73	GLU
56	De	78	LEU
56	De	90	LYS
56	De	91	ASP
56	De	94	GLU
56	De	106	GLN
56	De	118	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	AB	135	GLN
2	AC	98	ASN
2	AC	123	GLN
3	AD	74	GLN
6	AG	28	ASN
6	AG	106	GLN
6	AG	148	ASN

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Mol	Chain	Res	Type
7	AH	78	GLN
9	AJ	76	ASN
9	AJ	84	GLN
11	AL	8	ASN
14	AO	42	HIS
15	AP	82	GLN
16	AQ	26	GLN
16	AQ	94	ASN
17	AR	36	ASN
23	AY	14	ASN
23	AY	20	HIS
23	AY	137	ASN
26	BD	115	GLN
26	BD	143	HIS
27	BE	129	HIS
27	BE	135	HIS
27	BE	143	ASN
28	BF	8	GLN
28	BF	40	GLN
28	BF	67	GLN
28	BF	75	HIS
29	BG	130	ASN
34	BP	84	ASN
36	BR	13	HIS
36	BR	23	ASN
39	BU	104	GLN
48	BN	45	ASN
48	BN	69	GLN
48	BN	94	HIS
48	BN	131	GLN
48	BN	133	GLN
50	B3	46	ASN
52	B6	20	ASN
54	B8	33	ASN
2	CC	6	HIS
2	CC	123	GLN
2	CC	136	GLN
2	CC	181	ASN
3	CD	119	GLN
3	CD	123	HIS
3	CD	125	HIS
4	CE	78	HIS

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Mol	Chain	Res	Type
4	CE	127	ASN
5	CF	11	ASN
6	CG	37	ASN
7	CH	78	GLN
8	CI	124	GLN
9	CJ	76	ASN
9	CJ	84	GLN
10	CK	116	HIS
14	CO	42	HIS
16	CQ	26	GLN
17	CR	36	ASN
23	CY	14	ASN
23	CY	20	HIS
23	CY	40	HIS
23	CY	137	ASN
23	CY	362	HIS
23	CY	448	GLN
23	CY	684	GLN
25	DC	58	ASN
26	DD	115	GLN
26	DD	198	ASN
27	DE	143	ASN
27	DE	159	HIS
27	DE	169	ASN
28	DF	8	GLN
28	DF	40	GLN
28	DF	67	GLN
29	DG	58	GLN
32	DK	116	ASN
36	DR	23	ASN
37	DS	34	HIS
37	DS	38	GLN
38	DT	43	GLN
38	DT	58	ASN
40	DV	11	GLN
40	DV	64	HIS
46	D1	45	ASN
46	D1	47	GLN
48	DN	45	ASN
48	DN	94	HIS
48	DN	131	GLN
48	DN	133	GLN

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Mol	Chain	Res	Type
49	D2	9	GLN
49	D2	47	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
20	AA	1511/1511 (100%)	330 (21%)	21 (1%)
20	CA	1511/1511 (100%)	304 (20%)	18 (1%)
21	AV	17/18 (94%)	8 (47%)	1 (5%)
21	CV	17/18 (94%)	8 (47%)	1 (5%)
22	AW	76/77 (98%)	27 (35%)	2 (2%)
22	CW	76/77 (98%)	22 (28%)	2 (2%)
59	BB	118/119 (99%)	26 (22%)	2 (1%)
59	DB	118/119 (99%)	19 (16%)	1 (0%)
60	BA	2878/2879 (99%)	729 (25%)	26 (0%)
60	DA	2878/2879 (99%)	692 (24%)	22 (0%)
All	All	9200/9208 (99%)	2165 (23%)	96 (1%)

All (2165) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
20	AA	6	G
20	AA	7	G
20	AA	8	A
20	AA	9	G
20	AA	22	G
20	AA	29	G
20	AA	31	G
20	AA	32	A
20	AA	39	G
20	AA	44	G
20	AA	47	C
20	AA	48	C
20	AA	51	A
20	AA	54	C
20	AA	65	U
20	AA	68	G
20	AA	68(H)	G
20	AA	68(M)	U
20	AA	68(P)	C
20	AA	68(V)	G

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Mol	Chain	Res	Type
20	AA	68(W)	G
20	AA	108	G
20	AA	109	A
20	AA	115	G
20	AA	116	A
20	AA	119	A
20	AA	121	C
20	AA	129(A)	G
20	AA	131	C
20	AA	136	C
20	AA	148	G
20	AA	151	A
20	AA	163	C
20	AA	179	A
20	AA	180	U
20	AA	182	U
20	AA	183	G
20	AA	186(G)	C
20	AA	186(I)	U
20	AA	195	A
20	AA	201(C)	U
20	AA	216	G
20	AA	220	G
20	AA	226	G
20	AA	230	G
20	AA	240	C
20	AA	241	C
20	AA	247	G
20	AA	251	G
20	AA	252	U
20	AA	253	U
20	AA	262	A
20	AA	267	C
20	AA	279	A
20	AA	280	C
20	AA	281	G
20	AA	289	G
20	AA	291	C
20	AA	301	G
20	AA	303	A
20	AA	306	G
20	AA	308	C

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Mol	Chain	Res	Type
20	AA	309	G
20	AA	315	A
20	AA	321	A
20	AA	328	C
20	AA	329	A
20	AA	331	G
20	AA	332	G
20	AA	335	C
20	AA	345	C
20	AA	347	G
20	AA	348	G
20	AA	352	C
20	AA	353	A
20	AA	354	G
20	AA	356	A
20	AA	362	G
20	AA	363	A
20	AA	367	U
20	AA	372	C
20	AA	373	A
20	AA	382	A
20	AA	384	G
20	AA	388	G
20	AA	389	A
20	AA	390	C
20	AA	397	A
20	AA	398	C
20	AA	402	G
20	AA	406	G
20	AA	412	A
20	AA	413	G
20	AA	422	C
20	AA	424	G
20	AA	427	U
20	AA	430	A
20	AA	432	A
20	AA	433	C
20	AA	434	U
20	AA	446	G
20	AA	447	G
20	AA	452	A
20	AA	453	A

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Mol	Chain	Res	Type
20	AA	458(B)	A
20	AA	458(C)	G
20	AA	485	G
20	AA	497	A
20	AA	498	U
20	AA	505	G
20	AA	509	A
20	AA	511	C
20	AA	516	U
20	AA	518	C
20	AA	521	G
20	AA	527	G
20	AA	531	U
20	AA	533	A
20	AA	547	A
20	AA	556	C
20	AA	559	A
20	AA	560	U
20	AA	562	C
20	AA	564	C
20	AA	568	G
20	AA	570	G
20	AA	572	A
20	AA	573	A
20	AA	575	G
20	AA	576	G
20	AA	577	G
20	AA	581	G
20	AA	583	A
20	AA	600	C
20	AA	631	G
20	AA	653	A
20	AA	665	A
20	AA	667	G
20	AA	673	G
20	AA	676	A
20	AA	688	G
20	AA	702	A
20	AA	708	C
20	AA	724	G
20	AA	734	G
20	AA	738	C

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Mol	Chain	Res	Type
20	AA	740	U
20	AA	749	C
20	AA	752	G
20	AA	754	C
20	AA	755	G
20	AA	766	A
20	AA	777	A
20	AA	782	A
20	AA	793	U
20	AA	794	A
20	AA	816	A
20	AA	817	C
20	AA	818	G
20	AA	819	A
20	AA	821	G
20	AA	828	A
20	AA	838(A)	U
20	AA	838(B)	C
20	AA	838(C)	U
20	AA	848	C
20	AA	851	G
20	AA	858	G
20	AA	859	A
20	AA	870	U
20	AA	873	A
20	AA	874	G
20	AA	884	U
20	AA	885	G
20	AA	902	G
20	AA	916	G
20	AA	926	G
20	AA	927	G
20	AA	934	C
20	AA	935	A
20	AA	938	A
20	AA	941	G
20	AA	960	U
20	AA	961	U
20	AA	962	C
20	AA	966	G
20	AA	969	A
20	AA	971	G

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Mol	Chain	Res	Type
20	AA	974	A
20	AA	975	A
20	AA	976	G
20	AA	977	A
20	AA	978	A
20	AA	980	C
20	AA	983	A
20	AA	991	U
20	AA	992	U
20	AA	993	G
20	AA	1004	A
20	AA	1022	G
20	AA	1024	G
20	AA	1025	U
20	AA	1026	G
20	AA	1027	C
20	AA	1028(A)	C
20	AA	1038	C
20	AA	1045	C
20	AA	1046	A
20	AA	1054	C
20	AA	1055	A
20	AA	1060	C
20	AA	1064	G
20	AA	1065	U
20	AA	1066	C
20	AA	1070	U
20	AA	1084	G
20	AA	1094	G
20	AA	1095	U
20	AA	1098	C
20	AA	1099	G
20	AA	1101	A
20	AA	1102	A
20	AA	1117	G
20	AA	1124	G
20	AA	1125	U
20	AA	1126	U
20	AA	1129	C
20	AA	1130	A
20	AA	1137	C
20	AA	1138	G

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Mol	Chain	Res	Type
20	AA	1139	G
20	AA	1140	C
20	AA	1146	A
20	AA	1151	A
20	AA	1157	A
20	AA	1159	U
20	AA	1171	G
20	AA	1174	G
20	AA	1181	G
20	AA	1191	A
20	AA	1196	U
20	AA	1197	G
20	AA	1200	C
20	AA	1201	A
20	AA	1212	U
20	AA	1213	A
20	AA	1220	G
20	AA	1227	A
20	AA	1238	A
20	AA	1240	U
20	AA	1241	G
20	AA	1256	A
20	AA	1257	U
20	AA	1260	C
20	AA	1270	C
20	AA	1277	C
20	AA	1278	U
20	AA	1280	A
20	AA	1281	U
20	AA	1286	A
20	AA	1287	A
20	AA	1290	G
20	AA	1291	G
20	AA	1297	C
20	AA	1300	G
20	AA	1301	U
20	AA	1302	U
20	AA	1303	C
20	AA	1305	G
20	AA	1317	C
20	AA	1322	C
20	AA	1331	G

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Mol	Chain	Res	Type
20	AA	1336	C
20	AA	1338	G
20	AA	1340	A
20	AA	1345	U
20	AA	1346	A
20	AA	1347	G
20	AA	1348	U
20	AA	1353	G
20	AA	1360	A
20	AA	1362(A)	C
20	AA	1363	A
20	AA	1364	U
20	AA	1378	C
20	AA	1381	U
20	AA	1382	C
20	AA	1397	C
20	AA	1398	A
20	AA	1401	G
20	AA	1402	C
20	AA	1422	G
20	AA	1425	U
20	AA	1440(B)	G
20	AA	1440(C)	G
20	AA	1440(D)	A
20	AA	1440(E)	G
20	AA	1440(H)	U
20	AA	1440(I)	A
20	AA	1440(J)	C
20	AA	1440(K)	G
20	AA	1440(L)	G
20	AA	1461	G
20	AA	1482	G
20	AA	1483	A
20	AA	1487	G
20	AA	1489	G
20	AA	1492	A
20	AA	1493	A
20	AA	1494	G
20	AA	1499	A
20	AA	1502	A
20	AA	1503	A
20	AA	1504	G

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Mol	Chain	Res	Type
20	AA	1505	G
20	AA	1506	U
20	AA	1507	A
20	AA	1515	C
20	AA	1517	G
20	AA	1519	A
20	AA	1520	G
20	AA	1528	U
20	AA	1529	G
20	AA	1530	G
20	AA	1532	U
20	AA	1533	C
20	AA	1534	A
20	AA	1535	C
20	AA	1536	C
20	AA	1538	C
21	AV	5	A
21	AV	9	G
21	AV	11	U
21	AV	12	A
21	AV	13	A
21	AV	14	A
21	AV	15	A
21	AV	21	A
22	AW	4	U
22	AW	8	U
22	AW	9	A
22	AW	14	A
22	AW	15	G
22	AW	16	U
22	AW	17	U
22	AW	18	G
22	AW	19	G
22	AW	20	U
22	AW	20(A)	U
22	AW	21	A
22	AW	22	G
22	AW	25	C
22	AW	33	U
22	AW	42	U
22	AW	46	G
22	AW	47	U

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Mol	Chain	Res	Type
22	AW	48	C
22	AW	50	C
22	AW	53	G
22	AW	58	A
22	AW	59	A
22	AW	60	U
22	AW	61	C
22	AW	63	C
22	AW	71	C
59	BB	13	A
59	BB	15	A
59	BB	16	G
59	BB	25	A
59	BB	30	C
59	BB	41	U
59	BB	42	C
59	BB	44	G
59	BB	47	C
59	BB	48	A
59	BB	64	C
59	BB	67	G
59	BB	68	C
59	BB	71	C
59	BB	72	G
59	BB	73	A
59	BB	77	U
59	BB	86	G
59	BB	87	G
59	BB	97	G
59	BB	98	G
59	BB	99	A
59	BB	101	A
59	BB	107	U
59	BB	109	G
59	BB	111	U
60	BA	7	G
60	BA	10	G
60	BA	11	G
60	BA	12	U
60	BA	15	G
60	BA	17	G
60	BA	33	U

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Mol	Chain	Res	Type
60	BA	34	C
60	BA	35	G
60	BA	46	C
60	BA	49	A
60	BA	51	G
60	BA	58	G
60	BA	61	G
60	BA	63	U
60	BA	73	A
60	BA	75	G
60	BA	84	A
60	BA	90	U
60	BA	98	G
60	BA	99	U
60	BA	101	G
60	BA	102	G
60	BA	104	U
60	BA	105	C
60	BA	110	G
60	BA	115	C
60	BA	117	G
60	BA	118	A
60	BA	119	A
60	BA	120	U
60	BA	122	G
60	BA	123	G
60	BA	149	A
60	BA	163	U
60	BA	171	G
60	BA	181	A
60	BA	186	G
60	BA	196	A
60	BA	197	A
60	BA	199	A
60	BA	205	G
60	BA	216	A
60	BA	217	G
60	BA	221	A
60	BA	222	A
60	BA	227	A
60	BA	229	A
60	BA	230	U

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Mol	Chain	Res	Type
60	BA	233	A
60	BA	241	A
60	BA	242	G
60	BA	248	G
60	BA	250	G
60	BA	256	A
60	BA	270(B)	A
60	BA	270(D)	C
60	BA	270(M)	U
60	BA	270(N)	U
60	BA	270(O)	G
60	BA	270(P)	U
60	BA	270(Q)	C
60	BA	270(R)	C
60	BA	270(W)	G
60	BA	271(D)	U
60	BA	271	G
60	BA	273(A)	G
60	BA	274	G
60	BA	275	G
60	BA	277	C
60	BA	278	A
60	BA	279	C
60	BA	280	C
60	BA	281	G
60	BA	288	C
60	BA	294	A
60	BA	302	C
60	BA	310	A
60	BA	314	A
60	BA	323	G
60	BA	324	A
60	BA	329	G
60	BA	330	A
60	BA	332	A
60	BA	333	G
60	BA	338	G
60	BA	339	U
60	BA	345	A
60	BA	346	A
60	BA	352	G
60	BA	380	U

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Mol	Chain	Res	Type
60	BA	381	G
60	BA	386	G
60	BA	387	U
60	BA	396	G
60	BA	405	U
60	BA	406	G
60	BA	411	G
60	BA	416	C
60	BA	422	A
60	BA	429	A
60	BA	432	A
60	BA	434	U
60	BA	441	U
60	BA	444	C
60	BA	446	G
60	BA	448	U
60	BA	449	A
60	BA	451	C
60	BA	456	C
60	BA	457	A
60	BA	459	U
60	BA	464	U
60	BA	465	G
60	BA	467	G
60	BA	470	A
60	BA	475	U
60	BA	480	A
60	BA	481	G
60	BA	483	A
60	BA	484	C
60	BA	505	A
60	BA	508	G
60	BA	509	C
60	BA	512	G
60	BA	513	A
60	BA	516	C
60	BA	527	C
60	BA	529	A
60	BA	530	G
60	BA	531	C
60	BA	532	A
60	BA	533	G

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Mol	Chain	Res	Type
60	BA	549	G
60	BA	556	G
60	BA	559	G
60	BA	563	G
60	BA	572	A
60	BA	573	G
60	BA	574	C
60	BA	575	A
60	BA	578	A
60	BA	583	G
60	BA	585	G
60	BA	586	A
60	BA	588	U
60	BA	599	G
60	BA	603	A
60	BA	615	G
60	BA	616	A
60	BA	617	G
60	BA	620	G
60	BA	627	A
60	BA	628	G
60	BA	634	C
60	BA	637	A
60	BA	644	A
60	BA	645	C
60	BA	646	A
60	BA	649	G
60	BA	652	U
60	BA	654	U
60	BA	656	G
60	BA	657	U
60	BA	667	U
60	BA	671	C
60	BA	679	C
60	BA	683	C
60	BA	685	A
60	BA	686	G
60	BA	691	C
60	BA	695	G
60	BA	715	G
60	BA	716	A
60	BA	717	G

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Mol	Chain	Res	Type
60	BA	723	G
60	BA	724	U
60	BA	726	G
60	BA	730	C
60	BA	735	A
60	BA	736	C
60	BA	737	C
60	BA	738	G
60	BA	748	G
60	BA	753	C
60	BA	757	U
60	BA	768	G
60	BA	775	G
60	BA	776	G
60	BA	779	U
60	BA	780	G
60	BA	781	A
60	BA	782	A
60	BA	784	A
60	BA	785	G
60	BA	788	A
60	BA	789	A
60	BA	792	G
60	BA	800	A
60	BA	805	G
60	BA	806	C
60	BA	812	C
60	BA	817	C
60	BA	819	A
60	BA	825	C
60	BA	826	U
60	BA	827	U
60	BA	828	U
60	BA	829	A
60	BA	831	G
60	BA	836	G
60	BA	843	G
60	BA	846	C
60	BA	847	U
60	BA	852	G
60	BA	859	G
60	BA	860	U

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Mol	Chain	Res	Type
60	BA	883	G
60	BA	887	A
60	BA	888	C
60	BA	890	A
60	BA	896	A
60	BA	897	C
60	BA	899	A
60	BA	906	G
60	BA	910	A
60	BA	914	C
60	BA	917	A
60	BA	919	G
60	BA	929	G
60	BA	931	G
60	BA	932	G
60	BA	941	A
60	BA	943	U
60	BA	945	A
60	BA	946	G
60	BA	947	G
60	BA	959	A
60	BA	961	C
60	BA	969	U
60	BA	971	C
60	BA	972	G
60	BA	974(A)	G
60	BA	974(B)	C
60	BA	980	A
60	BA	983	A
60	BA	989	G
60	BA	990	A
60	BA	996	A
60	BA	997	G
60	BA	1005	C
60	BA	1007	C
60	BA	1008	C
60	BA	1009	A
60	BA	1012	U
60	BA	1013	C
60	BA	1022	G
60	BA	1023	U
60	BA	1024	G

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Mol	Chain	Res	Type
60	BA	1025	G
60	BA	1026	U
60	BA	1033	U
60	BA	1039	G
60	BA	1041	C
60	BA	1042	G
60	BA	1046	A
60	BA	1047	G
60	BA	1048	A
60	BA	1054	A
60	BA	1070	A
60	BA	1071	G
60	BA	1072	C
60	BA	1073	A
60	BA	1075	C
60	BA	1077	A
60	BA	1078	U
60	BA	1079	C
60	BA	1085	A
60	BA	1088	A
60	BA	1090	U
60	BA	1096	A
60	BA	1106	G
60	BA	1107	G
60	BA	1112	G
60	BA	1117	G
60	BA	1130	U
60	BA	1132	A
60	BA	1133	U
60	BA	1135	C
60	BA	1136	G
60	BA	1138	G
60	BA	1139	G
60	BA	1140	C
60	BA	114(B)	A
60	BA	1154	G
60	BA	1155	A
60	BA	1157	G
60	BA	1175	U
60	BA	1176	G
60	BA	1186	G
60	BA	1188	U

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Mol	Chain	Res	Type
60	BA	1199	U
60	BA	1204	A
60	BA	1206	G
60	BA	1210	A
60	BA	1212	G
60	BA	1221	C
60	BA	1240	U
60	BA	1241	A
60	BA	1242	A
60	BA	1244	G
60	BA	1248	G
60	BA	1249	U
60	BA	1253	A
60	BA	1255	U
60	BA	1256	G
60	BA	1257	C
60	BA	1262	A
60	BA	1271	G
60	BA	1272	A
60	BA	1273	U
60	BA	1274	A
60	BA	1284	A
60	BA	1286	A
60	BA	1287	A
60	BA	1288	U
60	BA	1300	U
60	BA	1301	A
60	BA	1302	A
60	BA	1311	G
60	BA	1312	U
60	BA	1314	C
60	BA	1321	A
60	BA	1324	G
60	BA	1325	G
60	BA	1326	U
60	BA	1327	C
60	BA	1329	U
60	BA	1332	G
60	BA	1333	C
60	BA	1341	U
60	BA	1342	A
60	BA	1343	G

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Mol	Chain	Res	Type
60	BA	1344	G
60	BA	1345	C
60	BA	1346	G
60	BA	1349	A
60	BA	1352	U
60	BA	1359	A
60	BA	1360	A
60	BA	1365	A
60	BA	1380	G
60	BA	1382	G
60	BA	1384	A
60	BA	1385	G
60	BA	1396	U
60	BA	1397	U
60	BA	1416	G
60	BA	1420	U
60	BA	1421	G
60	BA	1427	A
60	BA	1428	C
60	BA	1429	G
60	BA	1434	A
60	BA	144(B)	A
60	BA	1445	C
60	BA	1451	C
60	BA	1453	A
60	BA	1454	U
60	BA	1455	G
60	BA	1458	C
60	BA	1460	A
60	BA	1467	C
60	BA	1483	G
60	BA	1485	G
60	BA	1490	A
60	BA	1491	G
60	BA	1493	C
60	BA	1494	A
60	BA	1495	A
60	BA	1497	U
60	BA	1498	C
60	BA	1503	U
60	BA	1522	G
60	BA	1523	U

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Mol	Chain	Res	Type
60	BA	1536	A
60	BA	1538	G
60	BA	1542	G
60	BA	1543	A
60	BA	1544	C
60	BA	1545	A
60	BA	1546	A
60	BA	1547	C
60	BA	1554	A
60	BA	1555	G
60	BA	1558	A
60	BA	1559	G
60	BA	1566	A
60	BA	1567	A
60	BA	1569	A
60	BA	1583	A
60	BA	1585	C
60	BA	1586	A
60	BA	1595	G
60	BA	1598	C
60	BA	1602	U
60	BA	1603	A
60	BA	1608	A
60	BA	1610	A
60	BA	1614	A
60	BA	1615	C
60	BA	1616	A
60	BA	1617	C
60	BA	1618	A
60	BA	1631	A
60	BA	1633	G
60	BA	1640	C
60	BA	1646	C
60	BA	1648	C
60	BA	1653	G
60	BA	1654	A
60	BA	1657	C
60	BA	1664	A
60	BA	1668	A
60	BA	1670	C
60	BA	1674	G
60	BA	1678	G

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Mol	Chain	Res	Type
60	BA	1688	U
60	BA	1694	C
60	BA	1696	G
60	BA	1698	A
60	BA	1699	G
60	BA	1700	A
60	BA	1702	G
60	BA	1729	A
60	BA	1730	U
60	BA	1731	G
60	BA	1732	A
60	BA	1757	U
60	BA	1763	G
60	BA	1764	G
60	BA	1773	A
60	BA	1775	U
60	BA	1780	A
60	BA	1781	C
60	BA	1783	A
60	BA	1784	A
60	BA	1785	A
60	BA	1787	A
60	BA	1790	C
60	BA	1791	A
60	BA	1796	U
60	BA	1799	G
60	BA	1800	C
60	BA	1802	A
60	BA	1803	A
60	BA	1809	A
60	BA	1811	G
60	BA	1815	A
60	BA	1816	G
60	BA	1817	G
60	BA	1820	U
60	BA	1821	A
60	BA	1829	A
60	BA	1847	A
60	BA	1859	A
60	BA	1878	G
60	BA	1888	G
60	BA	1889	A

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Mol	Chain	Res	Type
60	BA	1900	A
60	BA	1902	C
60	BA	1905	C
60	BA	1906	G
60	BA	1912	A
60	BA	1914	C
60	BA	1924	C
60	BA	1929	G
60	BA	1930	G
60	BA	1936	A
60	BA	1937	A
60	BA	1938	A
60	BA	1939	U
60	BA	1944	U
60	BA	1954	G
60	BA	1955	U
60	BA	1963	U
60	BA	1964	G
60	BA	1965	C
60	BA	1966	A
60	BA	1967	C
60	BA	1970	A
60	BA	1971	A
60	BA	1972	A
60	BA	1977	A
60	BA	1978	A
60	BA	1982	C
60	BA	1992	G
60	BA	1993	U
60	BA	1996	C
60	BA	2013	A
60	BA	2020	A
60	BA	2021	C
60	BA	2023	G
60	BA	2027	G
60	BA	2028	U
60	BA	2030	A
60	BA	2031	A
60	BA	2032	G
60	BA	2033	A
60	BA	2034	U
60	BA	2036	C

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Mol	Chain	Res	Type
60	BA	2038	G
60	BA	2039	C
60	BA	2040	C
60	BA	2041	U
60	BA	2042	A
60	BA	2043	C
60	BA	2052	G
60	BA	2055	C
60	BA	2056	G
60	BA	2059	A
60	BA	2060	A
60	BA	2061	G
60	BA	2062	A
60	BA	2064	C
60	BA	2067	G
60	BA	2069	G
60	BA	2070	G
60	BA	2081	C
60	BA	2092	U
60	BA	2093	G
60	BA	2115	G
60	BA	2116	G
60	BA	2117	A
60	BA	2120	G
60	BA	2126	A
60	BA	2130	U
60	BA	2132	U
60	BA	2133	G
60	BA	2136	C
60	BA	2140	C
60	BA	2142	C
60	BA	2144	U
60	BA	2147	G
60	BA	2149	G
60	BA	2154	G
60	BA	2156	G
60	BA	2159	G
60	BA	2162	G
60	BA	2168	G
60	BA	2171	A
60	BA	2172	U
60	BA	2173	A

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Mol	Chain	Res	Type
60	BA	2182	G
60	BA	2190	G
60	BA	2198	A
60	BA	2208	U
60	BA	2211	G
60	BA	2212	A
60	BA	2213	U
60	BA	2224	G
60	BA	2225	A
60	BA	2238	G
60	BA	2239	G
60	BA	2241	A
60	BA	2243	U
60	BA	2249	U
60	BA	2264	C
60	BA	2266	A
60	BA	2269	A
60	BA	2275	C
60	BA	2277	G
60	BA	2278	A
60	BA	2279	G
60	BA	2282	G
60	BA	2283	C
60	BA	2287	A
60	BA	2291	U
60	BA	2305	A
60	BA	2306	C
60	BA	2308	G
60	BA	2310	A
60	BA	2311	A
60	BA	2319	G
60	BA	2320	A
60	BA	2325	G
60	BA	2334	G
60	BA	2336	A
60	BA	2345	G
60	BA	2346	A
60	BA	2347	C
60	BA	2350	C
60	BA	2377	A
60	BA	2383	G
60	BA	2385	C

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Mol	Chain	Res	Type
60	BA	2387	U
60	BA	2388	A
60	BA	2390	U
60	BA	2391	G
60	BA	2394	C
60	BA	2395	C
60	BA	2402	C
60	BA	2403	C
60	BA	2405	G
60	BA	2406	U
60	BA	2407	G
60	BA	2411	A
60	BA	2422	A
60	BA	2423	U
60	BA	2425	A
60	BA	2427	C
60	BA	2428	G
60	BA	2429	G
60	BA	2430	A
60	BA	2432	A
60	BA	2433	A
60	BA	2435	A
60	BA	2436	G
60	BA	2439	A
60	BA	2440	C
60	BA	2441	C
60	BA	2446	G
60	BA	2447	G
60	BA	2448	A
60	BA	2449	U
60	BA	2450	A
60	BA	2451	A
60	BA	2452	C
60	BA	2463	C
60	BA	2469	A
60	BA	2470	G
60	BA	2474	C
60	BA	2476	A
60	BA	2477	C
60	BA	2478	A
60	BA	2479	G
60	BA	2480	C

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Mol	Chain	Res	Type
60	BA	2499	C
60	BA	2502	G
60	BA	2503	A
60	BA	2504	U
60	BA	2505	G
60	BA	2507	C
60	BA	2508	G
60	BA	2518	A
60	BA	2519	U
60	BA	2520	C
60	BA	2530	A
60	BA	2531	A
60	BA	2534	A
60	BA	2542	A
60	BA	2543	G
60	BA	2553	G
60	BA	2554	U
60	BA	2556	C
60	BA	2561	A
60	BA	2564	A
60	BA	2566	A
60	BA	2567	G
60	BA	2572	A
60	BA	2573	C
60	BA	2574	G
60	BA	2577	A
60	BA	2583	G
60	BA	2584	U
60	BA	2598	A
60	BA	2602	A
60	BA	2609	U
60	BA	2610	C
60	BA	2611	U
60	BA	2612	C
60	BA	2615	U
60	BA	2620	C
60	BA	2621	A
60	BA	2630	G
60	BA	2634	G
60	BA	2646	C
60	BA	2663	G
60	BA	2665	A

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Mol	Chain	Res	Type
60	BA	2677	G
60	BA	2682	U
60	BA	2683	C
60	BA	2687	U
60	BA	2689	U
60	BA	2691	C
60	BA	2702	U
60	BA	2703	C
60	BA	2712	U
60	BA	2713	A
60	BA	2715	C
60	BA	2726	U
60	BA	2732	G
60	BA	2733	A
60	BA	2746	U
60	BA	2755	C
60	BA	2764	A
60	BA	2765	A
60	BA	2768	C
60	BA	2772	C
60	BA	2777	G
60	BA	2778	A
60	BA	2779	U
60	BA	2780	G
60	BA	2781	A
60	BA	2782	G
60	BA	2790	A
60	BA	2791	C
60	BA	2792	G
60	BA	2797	U
60	BA	2798	C
60	BA	2801	A
60	BA	2805	G
60	BA	2811	G
60	BA	2818	G
60	BA	2820	A
60	BA	2821	A
60	BA	2833	G
60	BA	2834	G
60	BA	2835	A
60	BA	2842	G
60	BA	2849	U

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Mol	Chain	Res	Type
60	BA	2851	A
60	BA	2857	G
60	BA	2866	U
60	BA	2872	G
60	BA	2880	C
60	BA	2881	C
60	BA	2886	G
60	BA	2894	G
20	CA	6	G
20	CA	7	G
20	CA	9	G
20	CA	22	G
20	CA	29	G
20	CA	32	A
20	CA	39	G
20	CA	47	C
20	CA	48	C
20	CA	51	A
20	CA	54	C
20	CA	59	A
20	CA	68	G
20	CA	68(H)	G
20	CA	68(I)	G
20	CA	68(L)	U
20	CA	68(M)	U
20	CA	68(P)	C
20	CA	68(V)	G
20	CA	109	A
20	CA	115	G
20	CA	116	A
20	CA	119	A
20	CA	121	C
20	CA	129(A)	G
20	CA	131	C
20	CA	136	C
20	CA	144	G
20	CA	147	G
20	CA	163	C
20	CA	182	U
20	CA	183	G
20	CA	186(G)	C
20	CA	186(I)	U

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Mol	Chain	Res	Type
20	CA	195	A
20	CA	201(C)	U
20	CA	216	G
20	CA	220	G
20	CA	224	C
20	CA	230	G
20	CA	247	G
20	CA	251	G
20	CA	252	U
20	CA	253	U
20	CA	267	C
20	CA	279	A
20	CA	280	C
20	CA	281	G
20	CA	289	G
20	CA	297	G
20	CA	301	G
20	CA	309	G
20	CA	312	C
20	CA	321	A
20	CA	328	C
20	CA	329	A
20	CA	331	G
20	CA	332	G
20	CA	335	C
20	CA	341	C
20	CA	345	C
20	CA	346	G
20	CA	347	G
20	CA	352	C
20	CA	353	A
20	CA	354	G
20	CA	357	G
20	CA	367	U
20	CA	372	C
20	CA	373	A
20	CA	382	A
20	CA	384	G
20	CA	388	G
20	CA	390	C
20	CA	393	A
20	CA	397	A

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Mol	Chain	Res	Type
20	CA	398	C
20	CA	412	A
20	CA	413	G
20	CA	414	A
20	CA	422	C
20	CA	424	G
20	CA	427	U
20	CA	430	A
20	CA	433	C
20	CA	440	A
20	CA	452	A
20	CA	453	A
20	CA	455	C
20	CA	458	C
20	CA	458(B)	A
20	CA	458(D)	G
20	CA	481	G
20	CA	485	G
20	CA	486	U
20	CA	497	A
20	CA	498	U
20	CA	505	G
20	CA	511	C
20	CA	516	U
20	CA	518	C
20	CA	521	G
20	CA	527	G
20	CA	531	U
20	CA	532	A
20	CA	533	A
20	CA	547	A
20	CA	562	C
20	CA	568	G
20	CA	569	C
20	CA	572	A
20	CA	573	A
20	CA	575	G
20	CA	576	G
20	CA	577	G
20	CA	581	G
20	CA	589	C
20	CA	600	C

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Mol	Chain	Res	Type
20	CA	616	G
20	CA	653	A
20	CA	664	G
20	CA	665	A
20	CA	667	G
20	CA	673	G
20	CA	687	A
20	CA	688	G
20	CA	724	G
20	CA	734	G
20	CA	749	C
20	CA	752	G
20	CA	755	G
20	CA	766	A
20	CA	782	A
20	CA	793	U
20	CA	794	A
20	CA	799	G
20	CA	816	A
20	CA	817	C
20	CA	818	G
20	CA	819	A
20	CA	820	U
20	CA	828	A
20	CA	838(A)	U
20	CA	838(B)	C
20	CA	838(C)	U
20	CA	848	C
20	CA	857	C
20	CA	859	A
20	CA	867	G
20	CA	870	U
20	CA	873	A
20	CA	882	C
20	CA	884	U
20	CA	888	G
20	CA	926	G
20	CA	927	G
20	CA	934	C
20	CA	935	A
20	CA	938	A
20	CA	945	G

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Mol	Chain	Res	Type
20	CA	960	U
20	CA	961	U
20	CA	969	A
20	CA	971	G
20	CA	974	A
20	CA	976	G
20	CA	977	A
20	CA	978	A
20	CA	980	C
20	CA	981	U
20	CA	983	A
20	CA	991	U
20	CA	992	U
20	CA	993	G
20	CA	1004	A
20	CA	1006	C
20	CA	1017	G
20	CA	1022	G
20	CA	1024	G
20	CA	1025	U
20	CA	1026	G
20	CA	1028	C
20	CA	1028(A)	C
20	CA	1036	G
20	CA	1038	C
20	CA	1041	A
20	CA	1045	C
20	CA	1053	G
20	CA	1054	C
20	CA	1055	A
20	CA	1060	C
20	CA	1064	G
20	CA	1065	U
20	CA	1066	C
20	CA	1070	U
20	CA	1093	A
20	CA	1094	G
20	CA	1095	U
20	CA	1098	C
20	CA	1101	A
20	CA	1102	A
20	CA	1117	G

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Mol	Chain	Res	Type
20	CA	1124	G
20	CA	1125	U
20	CA	1126	U
20	CA	1129	C
20	CA	1130	A
20	CA	1137	C
20	CA	1138	G
20	CA	1139	G
20	CA	1145	C
20	CA	1146	A
20	CA	1151	A
20	CA	1157	A
20	CA	1159	U
20	CA	1165	C
20	CA	1171	G
20	CA	1174	G
20	CA	1181	G
20	CA	1183	A
20	CA	1184	G
20	CA	1190	G
20	CA	1196	U
20	CA	1197	G
20	CA	1200	C
20	CA	1201	A
20	CA	1212	U
20	CA	1213	A
20	CA	1220	G
20	CA	1221	G
20	CA	1227	A
20	CA	1236	A
20	CA	1238	A
20	CA	1240	U
20	CA	1250	A
20	CA	1256	A
20	CA	1257	U
20	CA	1260	C
20	CA	1262	C
20	CA	1266	G
20	CA	1277	C
20	CA	1280	A
20	CA	1281	U
20	CA	1286	A

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Mol	Chain	Res	Type
20	CA	1287	A
20	CA	1300	G
20	CA	1301	U
20	CA	1302	U
20	CA	1303	C
20	CA	1305	G
20	CA	1317	C
20	CA	1320	C
20	CA	1322	C
20	CA	1331	G
20	CA	1336	C
20	CA	1338	G
20	CA	1340	A
20	CA	1347	G
20	CA	1353	G
20	CA	1360	A
20	CA	1363	A
20	CA	1364	U
20	CA	1368	G
20	CA	1377	A
20	CA	1378	C
20	CA	1381	U
20	CA	1382	C
20	CA	1397	C
20	CA	1398	A
20	CA	1401	G
20	CA	1422	G
20	CA	1425	U
20	CA	1440(B)	G
20	CA	1440(C)	G
20	CA	1440(D)	A
20	CA	1440(E)	G
20	CA	1440(I)	A
20	CA	1440(J)	C
20	CA	1440(K)	G
20	CA	1440(L)	G
20	CA	1481	U
20	CA	1492	A
20	CA	1493	A
20	CA	1494	G
20	CA	1497	G
20	CA	1499	A

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Mol	Chain	Res	Type
20	CA	1502	A
20	CA	1503	A
20	CA	1504	G
20	CA	1505	G
20	CA	1506	U
20	CA	1507	A
20	CA	1517	G
20	CA	1519	A
20	CA	1520	G
20	CA	1529	G
20	CA	1530	G
20	CA	1532	U
20	CA	1533	C
20	CA	1534	A
20	CA	1535	C
20	CA	1536	C
20	CA	1537	U
20	CA	1538	C
21	CV	5	A
21	CV	9	G
21	CV	11	U
21	CV	12	A
21	CV	13	A
21	CV	14	A
21	CV	15	A
21	CV	21	A
22	CW	4	U
22	CW	9	A
22	CW	14	A
22	CW	15	G
22	CW	16	U
22	CW	17	U
22	CW	18	G
22	CW	19	G
22	CW	20	U
22	CW	20(A)	U
22	CW	21	A
22	CW	22	G
22	CW	25	C
22	CW	42	U
22	CW	46	G
22	CW	47	U

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Mol	Chain	Res	Type
22	CW	48	C
22	CW	50	C
22	CW	53	G
22	CW	58	A
22	CW	60	U
22	CW	61	C
59	DB	2	C
59	DB	13	A
59	DB	15	A
59	DB	16	G
59	DB	25	A
59	DB	30	C
59	DB	41	U
59	DB	44	G
59	DB	47	C
59	DB	48	A
59	DB	67	G
59	DB	71	C
59	DB	72	G
59	DB	73	A
59	DB	94	C
59	DB	99	A
59	DB	107	U
59	DB	109	G
59	DB	117	G
60	DA	7	G
60	DA	11	G
60	DA	15	G
60	DA	17	G
60	DA	33	U
60	DA	34	C
60	DA	35	G
60	DA	36	G
60	DA	46	C
60	DA	60	G
60	DA	63	U
60	DA	67	U
60	DA	73	A
60	DA	75	G
60	DA	90	U
60	DA	98	G
60	DA	99	U

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Mol	Chain	Res	Type
60	DA	101	G
60	DA	102	G
60	DA	104	U
60	DA	110	G
60	DA	115	C
60	DA	116	C
60	DA	119	A
60	DA	120	U
60	DA	128	C
60	DA	141(A)	A
60	DA	148	C
60	DA	149	A
60	DA	175	G
60	DA	181	A
60	DA	186	G
60	DA	196	A
60	DA	197	A
60	DA	199	A
60	DA	205	G
60	DA	216	A
60	DA	221	A
60	DA	222	A
60	DA	223	A
60	DA	227	A
60	DA	229	A
60	DA	230	U
60	DA	233	A
60	DA	239	U
60	DA	241	A
60	DA	248	G
60	DA	250	G
60	DA	252	G
60	DA	256	A
60	DA	265	A
60	DA	270(M)	U
60	DA	270(N)	U
60	DA	270(O)	G
60	DA	270(P)	U
60	DA	270(Q)	C
60	DA	270(R)	C
60	DA	271(B)	C
60	DA	271(D)	U

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Mol	Chain	Res	Type
60	DA	271	G
60	DA	274	G
60	DA	275	G
60	DA	277	C
60	DA	279	C
60	DA	282	A
60	DA	290	G
60	DA	294	A
60	DA	295	G
60	DA	297	C
60	DA	299	A
60	DA	300	A
60	DA	302	C
60	DA	304	G
60	DA	310	A
60	DA	323	G
60	DA	329	G
60	DA	330	A
60	DA	332	A
60	DA	345	A
60	DA	346	A
60	DA	352	G
60	DA	353	G
60	DA	363(G)	A
60	DA	370	G
60	DA	381	G
60	DA	386	G
60	DA	387	U
60	DA	396	G
60	DA	405	U
60	DA	406	G
60	DA	407	G
60	DA	411	G
60	DA	416	C
60	DA	432	A
60	DA	434	U
60	DA	435	C
60	DA	443	A
60	DA	444	C
60	DA	448	U
60	DA	449	A
60	DA	451	C

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Mol	Chain	Res	Type
60	DA	456	C
60	DA	457	A
60	DA	459	U
60	DA	464	U
60	DA	465	G
60	DA	469	G
60	DA	470	A
60	DA	475	U
60	DA	480	A
60	DA	481	G
60	DA	484	C
60	DA	505	A
60	DA	508	G
60	DA	509	C
60	DA	511	U
60	DA	512	G
60	DA	513	A
60	DA	516	C
60	DA	518	G
60	DA	527	C
60	DA	531	C
60	DA	532	A
60	DA	549	G
60	DA	556	G
60	DA	561	G
60	DA	563	G
60	DA	572	A
60	DA	573	G
60	DA	574	C
60	DA	575	A
60	DA	585	G
60	DA	599	G
60	DA	603	A
60	DA	615	G
60	DA	616	A
60	DA	617	G
60	DA	618(A)	G
60	DA	620	G
60	DA	621	A
60	DA	627	A
60	DA	628	G
60	DA	637	A

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Mol	Chain	Res	Type
60	DA	645	C
60	DA	646	A
60	DA	652	U
60	DA	654	U
60	DA	655	A
60	DA	657	U
60	DA	662	G
60	DA	667	U
60	DA	671	C
60	DA	682	G
60	DA	685	A
60	DA	686	G
60	DA	709	U
60	DA	716	A
60	DA	719	C
60	DA	728	G
60	DA	730	C
60	DA	735	A
60	DA	736	C
60	DA	737	C
60	DA	738	G
60	DA	747	U
60	DA	748	G
60	DA	753	C
60	DA	755	C
60	DA	757	U
60	DA	764	A
60	DA	767	U
60	DA	768	G
60	DA	776	G
60	DA	781	A
60	DA	782	A
60	DA	784	A
60	DA	785	G
60	DA	788	A
60	DA	792	G
60	DA	800	A
60	DA	805	G
60	DA	806	C
60	DA	810	U
60	DA	812	C
60	DA	817	C

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Mol	Chain	Res	Type
60	DA	819	A
60	DA	821	A
60	DA	825	C
60	DA	827	U
60	DA	829	A
60	DA	831	G
60	DA	835	A
60	DA	846	C
60	DA	847	U
60	DA	852	G
60	DA	869	G
60	DA	887	A
60	DA	890	A
60	DA	896	A
60	DA	897	C
60	DA	898	C
60	DA	906	G
60	DA	910	A
60	DA	911	A
60	DA	917	A
60	DA	919	G
60	DA	929	G
60	DA	932	G
60	DA	941	A
60	DA	942	G
60	DA	943	U
60	DA	946	G
60	DA	947	G
60	DA	961	C
60	DA	971	C
60	DA	974(A)	G
60	DA	974(B)	C
60	DA	977	G
60	DA	980	A
60	DA	982	C
60	DA	983	A
60	DA	990	A
60	DA	996	A
60	DA	1005	C
60	DA	1008	C
60	DA	1009	A
60	DA	1012	U

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Mol	Chain	Res	Type
60	DA	1013	C
60	DA	1022	G
60	DA	1023	U
60	DA	1025	G
60	DA	1026	U
60	DA	1030	G
60	DA	1033	U
60	DA	1034	G
60	DA	1042	G
60	DA	1045	A
60	DA	1046	A
60	DA	1047	G
60	DA	1048	A
60	DA	1070	A
60	DA	1071	G
60	DA	1072	C
60	DA	1073	A
60	DA	1075	C
60	DA	1077	A
60	DA	1078	U
60	DA	1079	C
60	DA	1082	U
60	DA	1085	A
60	DA	1087	G
60	DA	1088	A
60	DA	1090	U
60	DA	1095	A
60	DA	1096	A
60	DA	1102	C
60	DA	1106	G
60	DA	1110	G
60	DA	1111	A
60	DA	1112	G
60	DA	1119	C
60	DA	1127	A
60	DA	1130	U
60	DA	1132	A
60	DA	1135	C
60	DA	1136	G
60	DA	1138	G
60	DA	1139	G
60	DA	1141	U

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Mol	Chain	Res	Type
60	DA	114(B)	A
60	DA	1148	A
60	DA	1157	G
60	DA	1175	U
60	DA	1176	G
60	DA	1186	G
60	DA	1199	U
60	DA	1204	A
60	DA	1210	A
60	DA	1211	U
60	DA	1212	G
60	DA	1221	C
60	DA	1224	C
60	DA	1237	A
60	DA	1241	A
60	DA	1244	G
60	DA	1248	G
60	DA	1249	U
60	DA	1253	A
60	DA	1255	U
60	DA	1256	G
60	DA	1257	C
60	DA	1262	A
60	DA	1271	G
60	DA	1272	A
60	DA	1273	U
60	DA	1274	A
60	DA	1286	A
60	DA	1288	U
60	DA	1300	U
60	DA	1301	A
60	DA	1302	A
60	DA	1311	G
60	DA	1312	U
60	DA	1314	C
60	DA	1321	A
60	DA	1324	G
60	DA	1325	G
60	DA	1329	U
60	DA	1332	G
60	DA	1333	C
60	DA	1341	U

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Mol	Chain	Res	Type
60	DA	1342	A
60	DA	1345	C
60	DA	1346	G
60	DA	1349	A
60	DA	1350	C
60	DA	1352	U
60	DA	1359	A
60	DA	1365	A
60	DA	1366	A
60	DA	1371	G
60	DA	1380	G
60	DA	1384	A
60	DA	1385	G
60	DA	1392	A
60	DA	1395	A
60	DA	1396	U
60	DA	1400	G
60	DA	1416	G
60	DA	1420	U
60	DA	1421	G
60	DA	1427	A
60	DA	1428	C
60	DA	1435	G
60	DA	144(B)	A
60	DA	1445	C
60	DA	149(B)	A
60	DA	1453	A
60	DA	1454	U
60	DA	1455	G
60	DA	1459	G
60	DA	1460	A
60	DA	1467	C
60	DA	1483	G
60	DA	1486	A
60	DA	1490	A
60	DA	1491	G
60	DA	1493	C
60	DA	1494	A
60	DA	1495	A
60	DA	1497	U
60	DA	1498	C
60	DA	1501	C

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Mol	Chain	Res	Type
60	DA	1503	U
60	DA	1522	G
60	DA	1523	U
60	DA	1536	A
60	DA	1538	G
60	DA	1542	G
60	DA	1543	A
60	DA	1544	C
60	DA	1545	A
60	DA	1546	A
60	DA	1554	A
60	DA	1557	C
60	DA	1558	A
60	DA	1559	G
60	DA	1565	C
60	DA	1566	A
60	DA	1567	A
60	DA	1569	A
60	DA	1572	A
60	DA	1583	A
60	DA	1585	C
60	DA	1595	G
60	DA	1602	U
60	DA	1603	A
60	DA	1608	A
60	DA	1610	A
60	DA	1614	A
60	DA	1615	C
60	DA	1616	A
60	DA	1617	C
60	DA	1618	A
60	DA	1631	A
60	DA	1640	C
60	DA	1648	C
60	DA	1650	G
60	DA	1651	G
60	DA	1653	G
60	DA	1654	A
60	DA	1668	A
60	DA	1669	A
60	DA	1670	C
60	DA	1674	G

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Mol	Chain	Res	Type
60	DA	1681	G
60	DA	1694	C
60	DA	1695	G
60	DA	1696	G
60	DA	1697	G
60	DA	1698	A
60	DA	1699	G
60	DA	1700	A
60	DA	1707	G
60	DA	1729	A
60	DA	1732	A
60	DA	1750	G
60	DA	1758	G
60	DA	1759	A
60	DA	1763	G
60	DA	1764	G
60	DA	1773	A
60	DA	1780	A
60	DA	1781	C
60	DA	1783	A
60	DA	1784	A
60	DA	1787	A
60	DA	1791	A
60	DA	1796	U
60	DA	1799	G
60	DA	1800	C
60	DA	1801	G
60	DA	1802	A
60	DA	1803	A
60	DA	1809	A
60	DA	1812	A
60	DA	1815	A
60	DA	1816	G
60	DA	1817	G
60	DA	1820	U
60	DA	1821	A
60	DA	1829	A
60	DA	1839	G
60	DA	1847	A
60	DA	1878	G
60	DA	1881	C
60	DA	1888	G

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Mol	Chain	Res	Type
60	DA	1889	A
60	DA	1894	C
60	DA	1900	A
60	DA	1905	C
60	DA	1906	G
60	DA	1913	A
60	DA	1914	C
60	DA	1929	G
60	DA	1930	G
60	DA	1936	A
60	DA	1938	A
60	DA	1939	U
60	DA	1944	U
60	DA	1955	U
60	DA	1963	U
60	DA	1965	C
60	DA	1966	A
60	DA	1967	C
60	DA	1970	A
60	DA	1971	A
60	DA	1972	A
60	DA	1975	G
60	DA	1977	A
60	DA	1979	C
60	DA	1982	C
60	DA	1983	C
60	DA	1992	G
60	DA	1993	U
60	DA	1996	C
60	DA	2006	C
60	DA	2013	A
60	DA	2020	A
60	DA	2021	C
60	DA	2023	G
60	DA	2026	C
60	DA	2027	G
60	DA	2031	A
60	DA	2032	G
60	DA	2033	A
60	DA	2034	U
60	DA	2036	C
60	DA	2039	C

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Mol	Chain	Res	Type
60	DA	2040	C
60	DA	2041	U
60	DA	2042	A
60	DA	2043	C
60	DA	2052	G
60	DA	2055	C
60	DA	2056	G
60	DA	2060	A
60	DA	2061	G
60	DA	2062	A
60	DA	2063	C
60	DA	2065	C
60	DA	2067	G
60	DA	2069	G
60	DA	2091	U
60	DA	2093	G
60	DA	2107	C
60	DA	2115	G
60	DA	2116	G
60	DA	2117	A
60	DA	2120	G
60	DA	2126	A
60	DA	2128	C
60	DA	2130	U
60	DA	2132	U
60	DA	2133	G
60	DA	2138	C
60	DA	2144	U
60	DA	2145	C
60	DA	2156	G
60	DA	2158	A
60	DA	2159	G
60	DA	2168	G
60	DA	2171	A
60	DA	2173	A
60	DA	2198	A
60	DA	2210	G
60	DA	2211	G
60	DA	2212	A
60	DA	2213	U
60	DA	2224	G
60	DA	2225	A

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Mol	Chain	Res	Type
60	DA	2238	G
60	DA	2239	G
60	DA	2241	A
60	DA	2249	U
60	DA	2255	G
60	DA	2264	C
60	DA	2266	A
60	DA	2267	A
60	DA	2269	A
60	DA	2273	A
60	DA	2275	C
60	DA	2277	G
60	DA	2278	A
60	DA	2279	G
60	DA	2282	G
60	DA	2283	C
60	DA	2284	C
60	DA	2287	A
60	DA	2288	A
60	DA	2305	A
60	DA	2306	C
60	DA	2307	G
60	DA	2308	G
60	DA	2309	A
60	DA	2310	A
60	DA	2311	A
60	DA	2312	U
60	DA	2319	G
60	DA	2320	A
60	DA	2325	G
60	DA	2333	A
60	DA	2334	G
60	DA	2336	A
60	DA	2340	G
60	DA	2343	C
60	DA	2345	G
60	DA	2346	A
60	DA	2347	C
60	DA	2350	C
60	DA	2371	G
60	DA	2377	A
60	DA	2381	C

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Mol	Chain	Res	Type
60	DA	2383	G
60	DA	2385	C
60	DA	2387	U
60	DA	2390	U
60	DA	2394	C
60	DA	2400	G
60	DA	2402	C
60	DA	2403	C
60	DA	2406	U
60	DA	2411	A
60	DA	2422	A
60	DA	2423	U
60	DA	2425	A
60	DA	2427	C
60	DA	2428	G
60	DA	2429	G
60	DA	2430	A
60	DA	2433	A
60	DA	2434	A
60	DA	2435	A
60	DA	2439	A
60	DA	2440	C
60	DA	2441	C
60	DA	2447	G
60	DA	2448	A
60	DA	2449	U
60	DA	2451	A
60	DA	2456	C
60	DA	2460	U
60	DA	2469	A
60	DA	2470	G
60	DA	2476	A
60	DA	2477	C
60	DA	2478	A
60	DA	2479	G
60	DA	2480	C
60	DA	2483	C
60	DA	2499	C
60	DA	2501	C
60	DA	2502	G
60	DA	2504	U
60	DA	2505	G

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Mol	Chain	Res	Type
60	DA	2508	G
60	DA	2513	G
60	DA	2518	A
60	DA	2519	U
60	DA	2529	G
60	DA	2530	A
60	DA	2531	A
60	DA	2542	A
60	DA	2543	G
60	DA	2554	U
60	DA	2556	C
60	DA	2561	A
60	DA	2566	A
60	DA	2567	G
60	DA	2572	A
60	DA	2573	C
60	DA	2576	G
60	DA	2577	A
60	DA	2583	G
60	DA	2584	U
60	DA	2585	U
60	DA	2586	C
60	DA	2592	G
60	DA	2602	A
60	DA	2609	U
60	DA	2610	C
60	DA	2611	U
60	DA	2612	C
60	DA	2614	A
60	DA	2620	C
60	DA	2621	A
60	DA	2630	G
60	DA	2636	U
60	DA	2646	C
60	DA	2657	A
60	DA	2663	G
60	DA	2665	A
60	DA	2680	C
60	DA	2689	U
60	DA	2691	C
60	DA	2701	C
60	DA	2702	U

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Mol	Chain	Res	Type
60	DA	2703	C
60	DA	2712	U
60	DA	2713	A
60	DA	2715	C
60	DA	2730	C
60	DA	2732	G
60	DA	2733	A
60	DA	2735	G
60	DA	2746	U
60	DA	2748	A
60	DA	2764	A
60	DA	2765	A
60	DA	2772	C
60	DA	2777	G
60	DA	2778	A
60	DA	2779	U
60	DA	2780	G
60	DA	2781	A
60	DA	2782	G
60	DA	2783	G
60	DA	2790	A
60	DA	2791	C
60	DA	2792	G
60	DA	2797	U
60	DA	2798	C
60	DA	2801	A
60	DA	2805	G
60	DA	2811	G
60	DA	2818	G
60	DA	2820	A
60	DA	2821	A
60	DA	2833	G
60	DA	2834	G
60	DA	2835	A
60	DA	2849	U
60	DA	2851	A
60	DA	2857	G
60	DA	2861	G
60	DA	2866	U
60	DA	2872	G
60	DA	2877	G
60	DA	2879	C

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Mol	Chain	Res	Type
60	DA	2880	C
60	DA	2886	G
60	DA	2894	G

All (96) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
20	AA	5	U
20	AA	115	G
20	AA	181	G
20	AA	251	G
20	AA	266	G
20	AA	328	C
20	AA	429	U
20	AA	484	G
20	AA	672	U
20	AA	687	A
20	AA	748	C
20	AA	792	A
20	AA	992	U
20	AA	1064	G
20	AA	1101	A
20	AA	1145	C
20	AA	1286	A
20	AA	1504	G
20	AA	1532	U
20	AA	1535	C
20	AA	1537	U
21	AV	8	A
22	AW	20(A)	U
22	AW	41	A
59	BB	66	A
59	BB	98	G
60	BA	221	A
60	BA	271(C)	G
60	BA	278	A
60	BA	474	G
60	BA	479	A
60	BA	616	A
60	BA	735	A
60	BA	830	G
60	BA	1022	G

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Mol	Chain	Res	Type
60	BA	1139	G
60	BA	1154	G
60	BA	1185	C
60	BA	1240	U
60	BA	1542	G
60	BA	1558	A
60	BA	1783	A
60	BA	1858	G
60	BA	1913	A
60	BA	1937	A
60	BA	1992	G
60	BA	2040	C
60	BA	2092	U
60	BA	2158	A
60	BA	2171	A
60	BA	2447	G
60	BA	2791	C
20	CA	5	U
20	CA	115	G
20	CA	251	G
20	CA	266	G
20	CA	328	C
20	CA	429	U
20	CA	484	G
20	CA	531	U
20	CA	687	A
20	CA	748	C
20	CA	992	U
20	CA	1064	G
20	CA	1101	A
20	CA	1145	C
20	CA	1200	C
20	CA	1504	G
20	CA	1532	U
20	CA	1537	U
21	CV	8	A
22	CW	20(A)	U
22	CW	41	A
59	DB	66	A
60	DA	221	A
60	DA	271(C)	G
60	DA	278	A

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Mol	Chain	Res	Type
60	DA	474	G
60	DA	830	G
60	DA	1022	G
60	DA	1110	G
60	DA	1137	G
60	DA	1240	U
60	DA	1420	U
60	DA	1542	G
60	DA	1558	A
60	DA	1815	A
60	DA	1913	A
60	DA	1937	A
60	DA	1992	G
60	DA	2158	A
60	DA	2212	A
60	DA	2447	G
60	DA	2518	A
60	DA	2780	G
60	DA	2791	C

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
24	DPP	AU	2	24	3,5,6	0.50	0	1,5,7	0.26	0
24	DPP	CU	2	24	3,5,6	0.50	0	1,5,7	0.25	0
24	UAL	CU	5	24	7,8,9	2.68	3 (42%)	5,9,11	2.09	1 (20%)
24	5OH	AU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	5OH	CU	6	24	8,12,13	0.75	0	3,16,18	1.07	0
24	KBE	CU	1	24	8,8,9	1.06	0	7,8,10	2.18	1 (14%)
24	UAL	AU	5	24	7,8,9	2.70	3 (42%)	5,9,11	2.08	1 (20%)
24	KBE	AU	1	24	8,8,9	1.05	0	7,8,10	2.18	1 (14%)

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
24	DPP	AU	2	24	-	2/2/4/6	-
24	DPP	CU	2	24	-	2/2/4/6	-
24	UAL	CU	5	24	-	0/3/7/9	-
24	5OH	AU	6	24	-	0/2/18/20	0/1/1/1
24	5OH	CU	6	24	-	0/2/18/20	0/1/1/1
24	KBE	CU	1	24	-	2/7/7/8	-
24	UAL	AU	5	24	-	0/3/7/9	-
24	KBE	AU	1	24	-	2/7/7/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AU	5	UAL	C-CA	5.54	1.54	1.45
24	CU	5	UAL	C-CA	5.50	1.54	1.45
24	AU	5	UAL	C1-N1	-3.43	1.34	1.40
24	CU	5	UAL	C1-N1	-3.40	1.35	1.40
24	AU	5	UAL	CB-N1	-2.23	1.30	1.35
24	CU	5	UAL	CB-N1	-2.23	1.30	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CU	1	KBE	CB-CA-C	5.37	120.16	112.25
24	AU	1	KBE	CB-CA-C	5.36	120.14	112.25
24	CU	5	UAL	O-C-CA	-4.21	120.03	125.39
24	AU	5	UAL	O-C-CA	-4.19	120.06	125.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AU	1	KBE	C-CA-CB-N
24	AU	1	KBE	C-CA-CB-CG
24	CU	1	KBE	C-CA-CB-N
24	CU	1	KBE	C-CA-CB-CG
24	AU	2	DPP	N-CA-CB-NG
24	CU	2	DPP	N-CA-CB-NG

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Mol	Chain	Res	Type	Atoms
24	AU	2	DPP	C-CA-CB-NG
24	CU	2	DPP	C-CA-CB-NG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
61	GNP	AY	701	62	29,34,34	1.56	4 (13%)	33,54,54	2.68	13 (39%)
61	GNP	CY	702	62	29,34,34	1.56	4 (13%)	33,54,54	2.68	13 (39%)

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
61	GNP	AY	701	62	-	7/14/38/38	0/3/3/3
61	GNP	CY	702	62	-	7/14/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	CY	702	GNP	PG-O1G	4.78	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	AY	701	GNP	PG-O1G	4.76	1.53	1.46
61	CY	702	GNP	C6-N1	3.62	1.39	1.33
61	AY	701	GNP	C6-N1	3.60	1.39	1.33
61	AY	701	GNP	PB-O3A	-2.52	1.55	1.59
61	CY	702	GNP	PB-O3A	-2.52	1.55	1.59
61	AY	701	GNP	PA-O2A	-2.12	1.45	1.55
61	CY	702	GNP	PA-O2A	-2.11	1.45	1.55

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	702	GNP	C5-C6-N1	-8.58	111.69	123.43
61	AY	701	GNP	C5-C6-N1	-8.56	111.72	123.43
61	CY	702	GNP	C2-N1-C6	5.77	125.09	115.93
61	AY	701	GNP	C2-N1-C6	5.76	125.08	115.93
61	AY	701	GNP	C2-N3-C4	-4.87	109.80	115.36
61	CY	702	GNP	C2-N3-C4	-4.85	109.82	115.36
61	AY	701	GNP	PB-O3A-PA	-4.70	116.08	132.62
61	CY	702	GNP	PB-O3A-PA	-4.69	116.10	132.62
61	CY	702	GNP	O2B-PB-O1B	3.48	117.21	109.92
61	AY	701	GNP	O2B-PB-O1B	3.46	117.18	109.92
61	AY	701	GNP	O2G-PG-O3G	3.31	116.47	107.64
61	CY	702	GNP	O2G-PG-O3G	3.31	116.45	107.64
61	AY	701	GNP	C4-C5-N7	3.03	112.56	109.40
61	CY	702	GNP	C4-C5-N7	3.00	112.52	109.40
61	CY	702	GNP	O3G-PG-O1G	-2.99	105.95	113.45
61	AY	701	GNP	O3G-PG-O1G	-2.97	105.98	113.45
61	AY	701	GNP	O1B-PB-N3B	2.85	115.97	111.77
61	CY	702	GNP	O1B-PB-N3B	2.84	115.95	111.77
61	AY	701	GNP	C4-C5-C6	-2.57	118.34	120.80
61	CY	702	GNP	C4-C5-C6	-2.52	118.39	120.80
61	CY	702	GNP	N3-C2-N1	-2.23	124.24	127.22
61	CY	702	GNP	C5'-C4'-C3'	-2.23	106.82	115.18
61	AY	701	GNP	C5'-C4'-C3'	-2.22	106.87	115.18
61	AY	701	GNP	N3-C2-N1	-2.21	124.27	127.22
61	CY	702	GNP	O1G-PG-N3B	-2.17	108.57	111.77
61	AY	701	GNP	O1G-PG-N3B	-2.16	108.59	111.77

There are no chirality outliers.

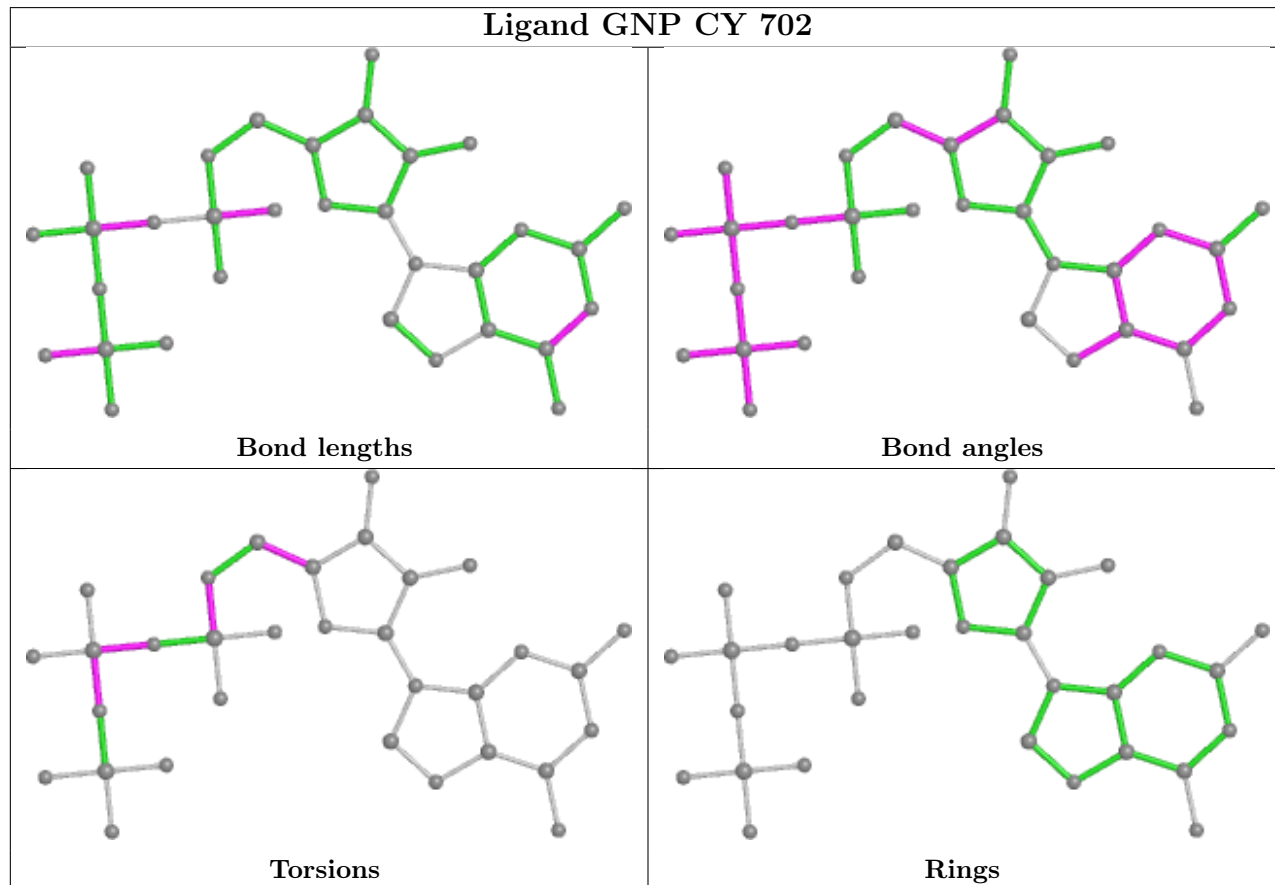
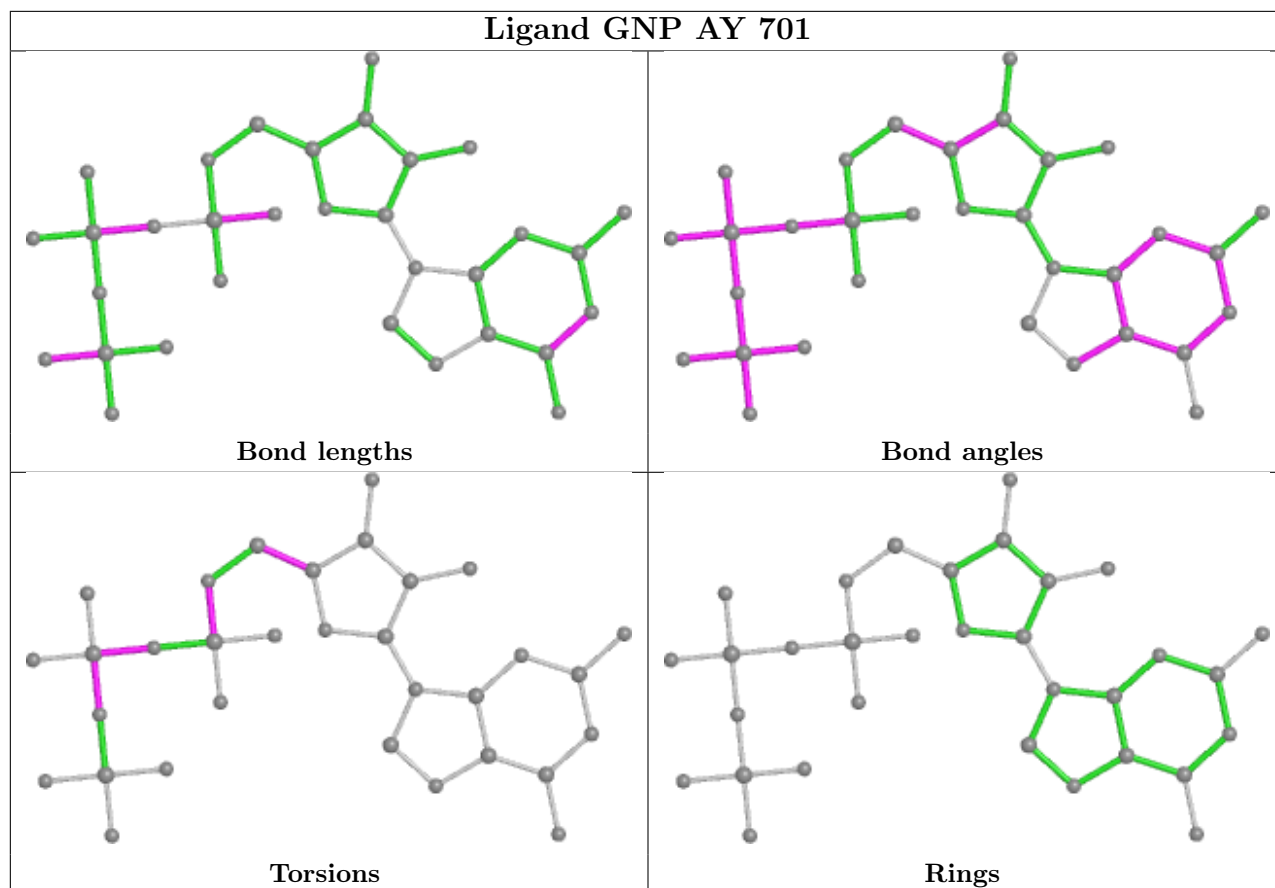
All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	AY	701	GNP	PG-N3B-PB-O1B
61	AY	701	GNP	PG-N3B-PB-O3A
61	AY	701	GNP	PA-O3A-PB-O1B
61	AY	701	GNP	PA-O3A-PB-O2B
61	AY	701	GNP	C5'-O5'-PA-O3A
61	AY	701	GNP	C5'-O5'-PA-O1A
61	CY	702	GNP	PG-N3B-PB-O1B
61	CY	702	GNP	PG-N3B-PB-O3A
61	CY	702	GNP	PA-O3A-PB-O1B
61	CY	702	GNP	PA-O3A-PB-O2B
61	CY	702	GNP	C5'-O5'-PA-O3A
61	CY	702	GNP	C5'-O5'-PA-O1A
61	AY	701	GNP	C3'-C4'-C5'-O5'
61	CY	702	GNP	C3'-C4'-C5'-O5'

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](#)

There are no chain breaks in this entry.

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, 95th 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 ²)	Q<0.9
1	AB	235/235 (100%)	0.81	56 (23%) 0 0	13, 75, 147, 218	0
1	CB	235/235 (100%)	0.71	55 (23%) 0 0	26, 78, 150, 182	0
2	AC	207/207 (100%)	1.30	53 (25%) 0 0	21, 64, 129, 194	0
2	CC	207/207 (100%)	1.20	68 (32%) 0 0	33, 66, 122, 164	0
3	AD	208/208 (100%)	2.77	126 (60%) 0 0	24, 71, 131, 187	0
3	CD	208/208 (100%)	3.03	127 (61%) 0 0	16, 79, 141, 186	0
4	AE	151/151 (100%)	1.12	52 (34%) 0 0	10, 57, 124, 176	0
4	CE	151/151 (100%)	2.07	62 (41%) 0 0	23, 71, 126, 185	0
5	AF	101/101 (100%)	-0.63	1 (0%) 82 75	36, 69, 131, 173	0
5	CF	101/101 (100%)	-0.57	1 (0%) 82 75	29, 64, 127, 176	0
6	AG	155/155 (100%)	0.89	45 (29%) 0 0	20, 84, 135, 192	0
6	CG	155/155 (100%)	0.39	27 (17%) 1 1	39, 86, 144, 209	0
7	AH	138/138 (100%)	0.80	30 (21%) 0 1	21, 64, 118, 145	0
7	CH	138/138 (100%)	0.76	34 (24%) 0 0	33, 67, 126, 179	0
8	AI	127/127 (100%)	4.12	98 (77%) 0 0	13, 74, 122, 146	0
8	CI	127/127 (100%)	4.55	99 (77%) 0 0	16, 69, 128, 177	0
9	AJ	99/99 (100%)	1.80	39 (39%) 0 0	34, 74, 129, 147	0
9	CJ	99/99 (100%)	2.34	49 (49%) 0 0	24, 81, 132, 167	0
10	AK	119/119 (100%)	0.19	15 (12%) 3 4	17, 68, 129, 145	0
10	CK	119/119 (100%)	0.85	24 (20%) 1 1	37, 83, 128, 165	0
11	AL	125/125 (100%)	1.33	39 (31%) 0 0	22, 64, 128, 177	0
11	CL	125/125 (100%)	1.93	53 (42%) 0 0	21, 72, 139, 179	0
12	AM	125/125 (100%)	1.38	38 (30%) 0 0	54, 96, 167, 207	0
12	CM	125/125 (100%)	1.60	47 (37%) 0 0	58, 97, 159, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AN	60/60 (100%)	3.82	44 (73%)	0	0	3, 48, 113, 131	0
13	CN	60/60 (100%)	3.60	42 (70%)	0	0	30, 54, 113, 147	0
14	AO	88/88 (100%)	0.85	19 (21%)	0	1	24, 64, 113, 158	0
14	CO	88/88 (100%)	1.15	26 (29%)	0	0	32, 73, 127, 165	0
15	AP	84/84 (100%)	6.13	63 (75%)	0	0	35, 82, 143, 179	0
15	CP	84/84 (100%)	5.62	66 (78%)	0	0	29, 73, 132, 175	0
16	AQ	100/100 (100%)	1.70	39 (39%)	0	0	24, 66, 120, 137	0
16	CQ	100/100 (100%)	2.14	47 (47%)	0	0	42, 74, 130, 159	0
17	AR	70/70 (100%)	0.26	10 (14%)	2	3	28, 54, 107, 143	0
17	CR	70/70 (100%)	0.38	7 (10%)	7	6	26, 69, 132, 198	0
18	AS	79/79 (100%)	3.21	44 (55%)	0	0	25, 95, 172, 193	0
18	CS	79/79 (100%)	2.40	39 (49%)	0	0	26, 89, 165, 199	0
19	AT	99/99 (100%)	2.19	47 (47%)	0	0	16, 66, 130, 188	0
19	CT	99/99 (100%)	2.69	59 (59%)	0	0	27, 80, 144, 169	0
20	AA	1511/1511 (100%)	0.43	216 (14%)	2	3	11, 79, 165, 273	0
20	CA	1511/1511 (100%)	0.44	194 (12%)	3	4	6, 84, 166, 265	0
21	AV	18/18 (100%)	2.58	12 (66%)	0	0	41, 113, 170, 197	0
21	CV	18/18 (100%)	2.94	12 (66%)	0	0	33, 135, 179, 181	0
22	AW	77/77 (100%)	-0.21	3 (3%)	39	31	24, 109, 168, 243	0
22	CW	77/77 (100%)	-0.01	3 (3%)	39	31	43, 116, 183, 208	0
23	AY	687/687 (100%)	-0.02	61 (8%)	9	7	26, 80, 149, 224	0
23	CY	687/687 (100%)	0.10	87 (12%)	3	4	25, 86, 158, 217	0
24	AU	2/6 (33%)	-0.70	0	100	100	66, 66, 66, 66	0
24	CU	2/6 (33%)	-1.14	0	100	100	66, 66, 66, 66	0
25	BC	228/228 (100%)	2.67	127 (55%)	0	0	77, 137, 202, 235	0
25	DC	228/228 (100%)	2.93	132 (57%)	0	0	73, 140, 196, 228	0
26	BD	275/275 (100%)	1.65	103 (37%)	0	0	12, 58, 126, 156	0
26	DD	275/275 (100%)	1.60	106 (38%)	0	0	18, 59, 122, 191	0
27	BE	205/205 (100%)	2.22	90 (43%)	0	0	16, 58, 123, 159	0
27	DE	205/205 (100%)	2.48	104 (50%)	0	0	20, 74, 138, 209	0
28	BF	208/208 (100%)	2.80	124 (59%)	0	0	41, 78, 145, 195	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
28	DF	208/208 (100%)	2.78	110 (52%)	0	0	26, 76, 155, 199	0
29	BG	181/181 (100%)	2.10	89 (49%)	0	0	24, 87, 153, 191	0
29	DG	181/181 (100%)	1.69	73 (40%)	0	0	40, 94, 165, 199	0
30	BH	167/167 (100%)	0.49	30 (17%)	1	1	7, 68, 133, 171	0
30	DH	167/167 (100%)	0.50	30 (17%)	1	1	11, 67, 139, 168	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	0.85	28 (20%)	1	1	24, 91, 182, 225	0
32	DK	140/140 (100%)	1.29	46 (32%)	0	0	30, 110, 178, 234	0
33	BO	122/122 (100%)	1.43	40 (32%)	0	0	24, 45, 123, 162	0
33	DO	122/122 (100%)	1.75	50 (40%)	0	0	20, 58, 106, 159	0
34	BP	146/146 (100%)	2.88	74 (50%)	0	0	22, 76, 132, 175	0
34	DP	146/146 (100%)	2.59	73 (50%)	0	0	28, 78, 141, 189	0
35	BQ	141/141 (100%)	1.83	61 (43%)	0	0	17, 63, 130, 200	0
35	DQ	141/141 (100%)	2.09	59 (41%)	0	0	22, 68, 140, 174	0
36	BR	117/117 (100%)	2.73	75 (64%)	0	0	15, 57, 119, 178	0
36	DR	117/117 (100%)	2.13	59 (50%)	0	0	18, 69, 143, 195	0
37	BS	99/99 (100%)	5.89	78 (78%)	0	0	22, 104, 172, 208	0
37	DS	99/99 (100%)	4.96	76 (76%)	0	0	18, 106, 167, 216	0
38	BT	138/138 (100%)	1.13	39 (28%)	0	0	22, 71, 133, 179	0
38	DT	138/138 (100%)	1.27	45 (32%)	0	0	19, 75, 153, 238	0
39	BU	117/117 (100%)	3.44	68 (58%)	0	0	40, 57, 131, 184	0
39	DU	117/117 (100%)	3.07	68 (58%)	0	0	24, 61, 118, 158	0
40	BV	101/101 (100%)	1.70	30 (29%)	0	0	13, 54, 114, 146	0
40	DV	101/101 (100%)	2.41	44 (43%)	0	0	20, 72, 127, 200	0
41	BW	113/113 (100%)	2.88	70 (61%)	0	0	16, 55, 121, 147	0
41	DW	113/113 (100%)	3.79	75 (66%)	0	0	5, 65, 136, 178	0
42	BX	93/93 (100%)	3.08	61 (65%)	0	0	18, 60, 114, 149	0
42	DX	93/93 (100%)	2.97	55 (59%)	0	0	34, 63, 128, 170	0
43	BY	107/107 (100%)	4.27	79 (73%)	0	0	8, 86, 151, 180	0
43	DY	107/107 (100%)	4.05	87 (81%)	0	0	35, 76, 151, 176	0
44	BZ	185/185 (100%)	0.87	48 (25%)	0	0	30, 76, 142, 176	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DZ	185/185 (100%)	0.56	41 (22%)	0	0	36, 82, 147, 226	0
45	B0	84/84 (100%)	5.18	62 (73%)	0	0	18, 92, 159, 181	0
45	D0	84/84 (100%)	5.01	63 (75%)	0	0	19, 85, 145, 160	0
46	B1	93/93 (100%)	3.52	54 (58%)	0	0	26, 91, 161, 204	0
46	D1	93/93 (100%)	4.57	63 (67%)	0	0	38, 92, 166, 194	0
47	B4	35/35 (100%)	0.80	9 (25%)	0	0	49, 106, 171, 203	0
47	D4	35/35 (100%)	0.45	6 (17%)	1	1	82, 115, 164, 187	0
48	BN	138/138 (100%)	2.11	60 (43%)	0	0	59, 83, 108, 111	0
48	DN	138/138 (100%)	2.04	61 (44%)	0	0	58, 84, 107, 116	0
49	B2	71/71 (100%)	1.12	17 (23%)	0	0	38, 79, 143, 185	0
49	D2	71/71 (100%)	0.92	14 (19%)	1	1	42, 70, 130, 187	0
50	B3	60/60 (100%)	1.69	28 (46%)	0	0	34, 62, 117, 150	0
50	D3	60/60 (100%)	2.58	32 (53%)	0	0	53, 68, 130, 149	0
51	B5	59/59 (100%)	2.54	29 (49%)	0	0	26, 56, 131, 149	0
51	D5	59/59 (100%)	2.50	34 (57%)	0	0	16, 83, 166, 185	0
52	B6	50/50 (100%)	1.98	23 (46%)	0	0	63, 99, 159, 175	0
52	D6	50/50 (100%)	3.07	31 (62%)	0	0	61, 118, 161, 188	0
53	B7	49/49 (100%)	3.44	36 (73%)	0	0	18, 47, 122, 156	0
53	D7	49/49 (100%)	3.54	36 (73%)	0	0	33, 61, 140, 186	0
54	B8	64/64 (100%)	4.20	52 (81%)	0	0	29, 63, 152, 160	0
54	D8	64/64 (100%)	5.09	50 (78%)	0	0	28, 75, 142, 191	0
55	B9	37/37 (100%)	10.16	37 (100%)	0	0	71, 109, 177, 183	0
55	D9	37/37 (100%)	12.55	36 (97%)	0	0	102, 132, 185, 210	0
56	Be	72/103 (69%)	-0.04	6 (8%)	11	9	40, 109, 188, 239	0
56	De	72/103 (69%)	0.14	9 (12%)	3	4	46, 118, 183, 199	0
57	Bf	0/31	-	-	-	-	-	-
57	Bg	0/31	-	-	-	-	-	-
57	Df	0/31	-	-	-	-	-	-
57	Dg	0/31	-	-	-	-	-	-
58	Bh	0/30	-	-	-	-	-	-
58	Dh	0/30	-	-	-	-	-	-
59	BB	119/119 (100%)	-0.32	5 (4%)	36	30	27, 111, 173, 186	0
59	DB	119/119 (100%)	-0.18	9 (7%)	13	10	35, 118, 182, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
60	BA	2879/2879 (100%)	0.22	290 (10%) 7 6	7, 78, 171, 308	0
60	DA	2879/2879 (100%)	0.23	286 (9%) 7 6	5, 79, 177, 310	0
All	All	22716/23310 (97%)	1.26	6463 (28%) 0 0	3, 79, 161, 310	0

All (6463) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	D9	11	CYS	26.6
55	D9	27	CYS	26.1
60	DA	2250	G	24.1
55	D9	34	GLN	24.1
55	B9	14	CYS	23.5
55	B9	27	CYS	22.2
25	DC	111	PHE	21.7
45	D0	76	GLY	21.6
37	BS	88	ASP	20.4
46	D1	17	SER	19.0
55	D9	26	ILE	18.9
55	D9	36	GLN	18.8
55	D9	25	VAL	18.2
55	D9	32	HIS	18.2
15	AP	23	ASP	17.9
46	D1	38	SER	17.8
37	DS	34	HIS	17.1
55	D9	14	CYS	17.1
37	DS	38	GLN	17.0
9	AJ	48	THR	17.0
15	AP	10	GLY	16.9
60	BA	2250	G	16.9
12	AM	123	ALA	16.5
55	D9	29	ASN	16.4
45	B0	52	GLY	16.3
54	D8	15	LYS	16.2
12	AM	124	PRO	16.0
55	D9	10	ILE	16.0
45	B0	40	GLN	15.9
20	AA	135	C	15.9
46	D1	16	ASN	15.8
45	B0	43	THR	15.8
55	B9	26	ILE	15.5
15	AP	22	THR	15.4

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Mol	Chain	Res	Type	RSRZ
15	AP	11	SER	15.3
46	B1	38	SER	15.3
37	DS	37	ALA	15.2
55	B9	34	GLN	15.0
55	B9	12	ASP	14.9
37	DS	31	SER	14.8
41	DW	5	ALA	14.8
37	BS	53	SER	14.7
55	B9	11	CYS	14.7
37	BS	52	SER	14.7
46	D1	18	ILE	14.6
15	CP	70	ALA	14.6
15	CP	23	ASP	14.5
37	BS	35	ILE	14.5
37	BS	51	ALA	14.3
55	D9	23	VAL	14.2
4	CE	29	GLY	14.2
25	DC	112	ASP	14.1
15	AP	26	ARG	14.1
55	D9	21	GLY	14.0
46	D1	15	ALA	14.0
37	BS	38	GLN	13.9
3	CD	102	ASP	13.9
55	D9	12	ASP	13.9
37	DS	88	ASP	13.8
55	B9	25	VAL	13.8
55	D9	30	PRO	13.8
55	D9	28	GLU	13.8
15	CP	22	THR	13.7
55	D9	7	VAL	13.7
60	DA	2251	G	13.7
37	BS	37	ALA	13.5
39	BU	14	HIS	13.3
15	CP	24	ALA	13.2
15	AP	5	ARG	13.1
55	D9	19	ARG	13.1
46	B1	17	SER	13.1
46	D1	40	ARG	13.1
37	BS	27	SER	13.1
15	AP	8	ARG	13.1
55	D9	22	ARG	13.0
55	B9	28	GLU	12.9

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Mol	Chain	Res	Type	RSRZ
15	AP	7	ALA	12.9
45	B0	42	GLY	12.9
40	BV	83	ARG	12.9
20	AA	31	G	12.9
20	CA	48	C	12.8
34	BP	5	ASP	12.8
55	B9	32	HIS	12.7
8	CI	37	PHE	12.7
55	D9	8	LYS	12.5
37	BS	34	HIS	12.5
54	D8	65	GLU	12.4
55	D9	24	TYR	12.4
55	B9	15	LYS	12.3
18	CS	33	THR	12.3
45	B0	22	GLY	12.3
41	DW	3	ALA	12.2
15	AP	17	TYR	12.2
37	BS	31	SER	12.1
15	AP	69	THR	12.1
60	DA	942	G	12.1
55	D9	37	GLY	12.1
60	DA	224	G	12.0
38	DT	92	GLY	12.0
55	D9	9	ARG	12.0
37	BS	17	ARG	12.0
10	CK	128	ALA	12.0
37	BS	36	TYR	11.9
55	D9	15	LYS	11.9
20	CA	818	G	11.9
15	CP	69	THR	11.9
46	B1	14	VAL	11.8
15	AP	24	ALA	11.8
46	D1	41	ARG	11.8
20	CA	306	G	11.8
45	B0	47	PRO	11.8
15	AP	34	GLU	11.8
45	D0	71	ASP	11.7
37	BS	50	SER	11.7
60	BA	267	C	11.7
20	CA	31	G	11.7
55	B9	4	ARG	11.7
25	BC	109	MET	11.7

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Mol	Chain	Res	Type	RSRZ
8	CI	31	GLN	11.7
28	DF	77	ASP	11.6
54	D8	16	ILE	11.6
37	DS	29	PHE	11.6
55	D9	20	HIS	11.6
46	D1	14	VAL	11.6
15	AP	28	ARG	11.6
15	CP	8	ARG	11.5
43	BY	36	ALA	11.5
41	DW	4	LYS	11.5
13	CN	49	HIS	11.5
46	D1	20	ARG	11.5
4	CE	30	ALA	11.5
46	D1	22	GLY	11.5
40	DV	81	TYR	11.5
51	B5	17	ASP	11.4
52	D6	49	HIS	11.4
55	B9	7	VAL	11.4
37	DS	40	ILE	11.4
37	DS	53	SER	11.4
48	BN	73	THR	11.4
42	DX	80	ILE	11.4
16	CQ	22	LEU	11.4
37	DS	27	SER	11.4
15	AP	29	ASP	11.3
15	CP	9	PHE	11.3
19	CT	16	HIS	11.3
23	CY	165	GLN	11.3
34	BP	51	PHE	11.3
55	B9	29	ASN	11.2
41	DW	10	VAL	11.2
18	AS	33	THR	11.2
45	D0	40	GLN	11.2
54	D8	64	TYR	11.2
28	DF	125	LEU	11.2
46	B1	19	GLN	11.2
55	B9	10	ILE	11.2
10	CK	127	LYS	11.2
25	BC	111	PHE	11.1
29	DG	100	TRP	11.1
55	B9	9	ARG	11.1
15	CP	7	ALA	11.1

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Mol	Chain	Res	Type	RSRZ
15	CP	18	ARG	11.0
3	AD	102	ASP	10.9
37	DS	50	SER	10.9
45	D0	78	TYR	10.9
15	AP	13	HIS	10.9
20	AA	111	G	10.8
45	D0	47	PRO	10.8
37	BS	16	ASN	10.8
8	CI	118	LYS	10.8
29	DG	99	MET	10.8
35	DQ	140	ALA	10.8
15	CP	17	TYR	10.7
37	BS	87	PHE	10.7
37	BS	41	ASP	10.7
25	DC	137	LEU	10.7
25	BC	110	ASP	10.6
15	AP	16	HIS	10.6
60	BA	380	U	10.6
37	BS	101	LEU	10.6
45	D0	73	GLY	10.5
46	B1	15	ALA	10.5
55	D9	18	ARG	10.5
15	CP	34	GLU	10.5
20	CA	1367	C	10.5
46	D1	39	LYS	10.5
55	B9	23	VAL	10.5
45	B0	58	THR	10.5
8	CI	5	TYR	10.5
46	B1	18	ILE	10.5
43	BY	79	CYS	10.4
55	B9	30	PRO	10.4
8	AI	117	HIS	10.4
20	CA	1366	C	10.4
55	B9	6	SER	10.4
60	DA	2506	U	10.4
40	BV	82	ARG	10.4
20	CA	975	A	10.3
37	BS	48	LEU	10.3
15	CP	19	ILE	10.3
2	AC	168	ALA	10.3
15	AP	14	ASN	10.3
15	CP	11	SER	10.3

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Mol	Chain	Res	Type	RSRZ
28	DF	78	ILE	10.2
54	D8	25	MET	10.2
10	CK	129	SER	10.2
37	BS	30	ARG	10.2
4	CE	47	LYS	10.2
46	B1	40	ARG	10.2
4	CE	46	GLY	10.2
37	DS	28	VAL	10.1
45	B0	53	MET	10.1
45	B0	44	ARG	10.1
1	AB	205	ASP	10.1
42	BX	76	ARG	10.1
45	B0	41	ARG	10.1
39	BU	40	PHE	10.1
45	D0	75	LEU	10.1
25	DC	140	ASN	10.1
29	BG	100	TRP	10.1
27	BE	127	ASP	10.1
9	AJ	47	PHE	10.0
3	AD	161	ASN	10.0
45	B0	78	TYR	10.0
55	B9	13	LYS	10.0
8	CI	117	HIS	10.0
60	BA	2448	A	10.0
41	DW	104	THR	10.0
37	DS	25	ARG	10.0
26	DD	246	PRO	10.0
55	D9	33	LYS	10.0
26	DD	36	PRO	10.0
37	BS	29	PHE	10.0
20	CA	391	G	9.9
60	BA	1980	G	9.9
15	AP	25	ARG	9.9
8	CI	15	ALA	9.9
2	AC	6	HIS	9.9
55	D9	35	ARG	9.9
35	BQ	141	GLN	9.9
46	D1	19	GLN	9.9
60	DA	2581	G	9.9
45	B0	45	PHE	9.9
38	DT	93	ARG	9.9
27	BE	115	GLY	9.9

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Mol	Chain	Res	Type	RSRZ
34	BP	63	PRO	9.9
45	B0	57	PHE	9.8
34	BP	50	ARG	9.8
48	DN	73	THR	9.8
3	AD	109	GLY	9.8
53	B7	47	ARG	9.8
40	BV	73	SER	9.8
37	BS	86	ALA	9.8
19	CT	9	ASN	9.8
45	D0	60	PHE	9.8
34	DP	110	TYR	9.8
12	CM	52	GLU	9.8
42	BX	80	ILE	9.8
54	B8	25	MET	9.8
34	DP	65	ARG	9.8
40	BV	81	TYR	9.8
18	CS	32	LYS	9.8
34	DP	42	SER	9.8
12	CM	126	LYS	9.7
15	CP	25	ARG	9.7
55	B9	8	LYS	9.7
45	D0	43	THR	9.7
20	CA	64	G	9.7
15	AP	12	LYS	9.7
25	BC	175	PRO	9.7
60	BA	2449	U	9.7
20	CA	1357	A	9.7
25	DC	143	ALA	9.7
45	D0	61	ALA	9.7
20	AA	134	A	9.6
27	DE	115	GLY	9.6
20	AA	112	G	9.6
34	BP	65	ARG	9.6
34	BP	48	PRO	9.6
54	B8	5	LYS	9.6
40	DV	73	SER	9.6
60	BA	196	A	9.6
15	AP	9	PHE	9.6
8	CI	36	TYR	9.6
40	DV	75	PHE	9.6
39	DU	14	HIS	9.6
19	AT	9	ASN	9.6

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Mol	Chain	Res	Type	RSRZ
15	AP	6	LEU	9.6
25	DC	138	LEU	9.6
32	BK	12	LEU	9.6
37	DS	51	ALA	9.6
45	D0	72	ARG	9.5
28	DF	124	LEU	9.5
48	BN	43	THR	9.5
20	CA	149	A	9.5
20	AA	30	U	9.5
54	B8	6	THR	9.5
1	AB	78	GLN	9.5
60	BA	125	G	9.5
38	BT	92	GLY	9.5
43	DY	108	THR	9.5
54	D8	14	VAL	9.5
60	BA	1971	A	9.5
32	DK	12	LEU	9.5
28	BF	79	GLY	9.5
28	DF	194	MET	9.5
45	D0	80	HIS	9.5
15	AP	27	LYS	9.5
55	B9	33	LYS	9.4
54	D8	23	VAL	9.4
28	BF	124	LEU	9.4
28	DF	186	ILE	9.4
37	DS	36	TYR	9.4
10	CK	125	PHE	9.4
28	DF	185	ASP	9.4
13	AN	49	HIS	9.4
37	DS	89	ARG	9.4
43	DY	6	HIS	9.4
51	D5	17	ASP	9.4
48	BN	72	TYR	9.3
9	CJ	48	THR	9.3
37	DS	30	ARG	9.3
37	BS	49	VAL	9.3
35	BQ	140	ALA	9.3
2	CC	151	VAL	9.3
40	DV	82	ARG	9.3
39	BU	38	THR	9.3
60	BA	379	G	9.3
3	CD	149	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
6	AG	82	GLY	9.3
15	CP	21	VAL	9.3
19	CT	23	ARG	9.3
41	DW	11	ARG	9.3
40	DV	76	LYS	9.3
45	D0	52	GLY	9.3
45	B0	2	ALA	9.3
18	AS	59	PRO	9.2
41	DW	75	TYR	9.2
15	AP	15	PRO	9.2
34	DP	48	PRO	9.2
11	CL	19	ARG	9.2
20	AA	328	C	9.2
27	DE	127	ASP	9.2
43	BY	71	LYS	9.2
8	AI	115	GLY	9.2
37	DS	49	VAL	9.2
40	BV	74	LYS	9.2
8	AI	105	ASP	9.2
8	AI	4	TYR	9.2
28	BF	63	LYS	9.2
48	BN	84	LYS	9.2
43	BY	80	GLY	9.1
34	BP	78	PRO	9.1
60	BA	2062	A	9.1
34	DP	57	THR	9.1
43	BY	75	ILE	9.1
8	CI	73	GLN	9.1
8	CI	119	ALA	9.1
18	AS	58	VAL	9.1
37	BS	47	THR	9.1
45	D0	62	LEU	9.1
3	CD	103	ASN	9.1
38	BT	93	ARG	9.1
37	DS	35	ILE	9.1
25	BC	112	ASP	9.1
9	AJ	49	VAL	9.1
43	DY	71	LYS	9.1
60	DA	2502	G	9.0
15	CP	10	GLY	9.0
29	DG	97	ASP	9.0
51	B5	21	SER	9.0

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Mol	Chain	Res	Type	RSRZ
60	DA	837	C	9.0
37	DS	33	LYS	9.0
37	DS	39	ILE	9.0
15	CP	59	TRP	9.0
3	AD	110	PHE	9.0
37	BS	40	ILE	9.0
36	DR	58	GLY	9.0
19	AT	16	HIS	9.0
55	B9	22	ARG	9.0
54	D8	6	THR	9.0
37	BS	89	ARG	9.0
45	D0	46	LYS	9.0
33	DO	34	THR	9.0
55	B9	1	MET	9.0
34	BP	52	GLU	8.9
39	DU	7	GLY	8.9
7	AH	58	TYR	8.9
11	CL	29	GLY	8.9
27	DE	126	PRO	8.9
37	BS	20	ARG	8.9
18	AS	74	PHE	8.9
54	D8	56	GLU	8.9
15	CP	6	LEU	8.9
26	BD	144	ALA	8.9
43	BY	74	PRO	8.9
45	B0	23	VAL	8.9
3	CD	207	TYR	8.9
37	BS	54	LEU	8.9
8	CI	75	ASP	8.9
39	BU	7	GLY	8.9
43	DY	16	ALA	8.9
15	CP	26	ARG	8.9
43	BY	72	VAL	8.8
45	B0	4	LYS	8.8
8	CI	32	ASP	8.8
55	B9	36	GLN	8.8
8	CI	115	GLY	8.8
25	DC	164	PHE	8.8
34	BP	21	ARG	8.8
25	DC	50	ILE	8.8
46	B1	16	ASN	8.8
8	CI	38	GLN	8.8

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Mol	Chain	Res	Type	RSRZ
4	CE	130	ASN	8.8
20	CA	977	A	8.8
45	B0	59	LEU	8.8
46	D1	28	GLY	8.8
3	CD	69	GLY	8.7
20	AA	331	G	8.7
27	BE	126	PRO	8.7
42	DX	11	PRO	8.7
35	DQ	85	LYS	8.7
45	B0	48	GLY	8.7
27	BE	76	ARG	8.7
46	B1	13	ILE	8.7
29	BG	66	GLN	8.7
39	DU	5	LYS	8.7
8	CI	8	GLY	8.7
26	BD	183	ARG	8.7
36	BR	69	ASP	8.7
43	BY	108	THR	8.7
26	BD	145	VAL	8.7
4	CE	28	PHE	8.7
15	CP	36	ILE	8.7
34	BP	64	LYS	8.7
43	BY	42	VAL	8.7
34	DP	41	ARG	8.7
40	DV	80	GLN	8.7
20	AA	306	G	8.7
34	BP	57	THR	8.7
27	DE	3	GLY	8.7
60	DA	456	C	8.7
60	BA	1634	A	8.6
37	BS	28	VAL	8.6
48	DN	72	TYR	8.6
35	DQ	40	ALA	8.6
27	BE	53	PRO	8.6
41	DW	100	THR	8.6
15	AP	65	GLN	8.6
39	DU	40	PHE	8.6
20	CA	104	G	8.6
37	DS	26	LEU	8.6
15	AP	32	TYR	8.6
25	DC	14	LYS	8.6
60	DA	2059	A	8.6

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Mol	Chain	Res	Type	RSRZ
41	DW	12	ILE	8.6
42	BX	79	ALA	8.6
20	AA	64	G	8.6
34	DP	58	THR	8.6
48	DN	116	LEU	8.6
46	B1	20	ARG	8.5
3	CD	147	ALA	8.5
15	AP	4	ILE	8.5
60	BA	989	G	8.5
60	DA	836	G	8.5
28	BF	194	MET	8.5
60	BA	974(A)	G	8.5
15	CP	35	LYS	8.5
48	BN	85	ILE	8.5
55	B9	37	GLY	8.5
15	AP	31	LYS	8.5
42	BX	77	LYS	8.5
15	AP	66	PRO	8.5
41	DW	101	SER	8.5
42	DX	8	ILE	8.5
45	D0	57	PHE	8.5
37	DS	41	ASP	8.5
9	AJ	45	ARG	8.5
28	DF	192	LEU	8.5
48	DN	85	ILE	8.4
53	B7	27	GLY	8.4
60	DA	1032	A	8.4
34	BP	72	PRO	8.4
9	AJ	64	GLU	8.4
28	DF	79	GLY	8.4
52	D6	37	ARG	8.4
36	DR	102	GLU	8.4
8	CI	122	ALA	8.4
34	DP	36	LYS	8.4
40	DV	74	LYS	8.4
34	BP	40	SER	8.4
54	D8	24	ALA	8.4
8	CI	6	GLY	8.4
46	D1	13	ILE	8.4
8	AI	82	ALA	8.4
34	BP	58	THR	8.4
8	CI	4	TYR	8.4

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Mol	Chain	Res	Type	RSRZ
8	CI	29	ASN	8.4
45	B0	46	LYS	8.4
37	BS	39	ILE	8.4
45	D0	42	GLY	8.4
41	DW	105	VAL	8.4
46	D1	8	SER	8.4
54	D8	46	ARG	8.4
8	AI	73	GLN	8.4
13	AN	48	ALA	8.4
48	BN	83	LYS	8.4
53	B7	41	ARG	8.4
16	CQ	86	GLU	8.4
9	CJ	47	PHE	8.3
11	AL	21	LYS	8.3
15	CP	20	VAL	8.3
20	CA	328	C	8.3
8	AI	83	ARG	8.3
28	DF	76	GLY	8.3
19	CT	72	LEU	8.3
43	DY	11	ASP	8.3
11	AL	20	LYS	8.3
34	DP	51	PHE	8.3
46	B1	39	LYS	8.3
40	DV	83	ARG	8.3
15	CP	1	MET	8.3
44	DZ	121	HIS	8.3
37	DS	87	PHE	8.3
19	AT	72	LEU	8.3
30	BH	152	ARG	8.3
45	D0	58	THR	8.3
26	BD	184	LYS	8.3
35	DQ	89	ASN	8.3
55	D9	1	MET	8.3
42	DX	9	LEU	8.3
39	BU	25	TRP	8.3
42	DX	81	VAL	8.3
20	AA	555	C	8.2
60	DA	755	C	8.2
43	DY	2	ARG	8.2
51	B5	16	ARG	8.2
20	CA	307	C	8.2
45	B0	51	VAL	8.2

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Mol	Chain	Res	Type	RSRZ
38	BT	1	MET	8.2
27	DE	114	ALA	8.2
34	BP	47	ASP	8.2
45	D0	59	LEU	8.2
41	DW	22	ASP	8.2
35	DQ	141	GLN	8.2
39	BU	6	THR	8.2
41	DW	74	ALA	8.2
43	BY	43	ASN	8.2
34	DP	61	ARG	8.2
8	CI	7	THR	8.2
25	DC	134	PRO	8.2
29	BG	97	ASP	8.2
13	AN	35	ARG	8.2
12	AM	125	ARG	8.2
23	AY	17	ILE	8.2
28	BF	57	VAL	8.2
36	DR	69	ASP	8.2
23	CY	164	MET	8.1
28	DF	184	TYR	8.1
28	DF	10	PRO	8.1
44	BZ	70	LEU	8.1
60	BA	942	G	8.1
2	AC	166	GLU	8.1
53	B7	29	LYS	8.1
12	CM	124	PRO	8.1
25	DC	182	PRO	8.1
41	DW	7	ALA	8.1
11	CL	20	LYS	8.1
15	AP	68	ASP	8.1
25	BC	77	ALA	8.1
46	D1	37	ILE	8.1
45	B0	70	GLN	8.1
16	CQ	23	VAL	8.1
8	AI	32	ASP	8.1
21	CV	21	A	8.1
15	CP	33	ILE	8.1
12	AM	122	LYS	8.1
26	DD	243	GLY	8.1
30	BH	150	ALA	8.1
25	DC	8	TYR	8.1
12	AM	126	LYS	8.1

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Mol	Chain	Res	Type	RSRZ
41	BW	22	ASP	8.1
46	D1	21	ARG	8.1
54	B8	65	GLU	8.0
54	D8	37	SER	8.0
4	CE	14	ARG	8.0
8	AI	123	PRO	8.0
27	DE	135	HIS	8.0
46	D1	27	GLU	8.0
20	CA	1363	A	8.0
29	BG	99	MET	8.0
52	D6	42	TRP	8.0
11	CL	13	LYS	8.0
37	BS	70	GLY	8.0
39	DU	35	ALA	8.0
34	BP	46	LYS	8.0
11	CL	67	THR	8.0
19	CT	71	THR	8.0
40	BV	75	PHE	8.0
43	BY	35	TYR	8.0
54	B8	13	ARG	8.0
30	BH	154	PRO	8.0
9	CJ	69	ASN	7.9
15	AP	20	VAL	7.9
54	B8	56	GLU	7.9
39	DU	31	SER	7.9
60	DA	1971	A	7.9
54	D8	7	HIS	7.9
32	BK	21	PRO	7.9
43	BY	69	ALA	7.9
8	CI	124	GLN	7.9
39	DU	29	SER	7.9
20	CA	135	C	7.9
52	D6	48	VAL	7.9
28	BF	78	ILE	7.9
28	BF	176	LEU	7.9
48	BN	44	PRO	7.9
39	BU	36	ARG	7.9
25	BC	2	PRO	7.9
25	DC	102	GLN	7.9
51	D5	23	HIS	7.9
2	CC	168	ALA	7.9
60	BA	2060	A	7.9

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Mol	Chain	Res	Type	RSRZ
34	DP	47	ASP	7.9
43	BY	6	HIS	7.9
8	AI	122	ALA	7.9
33	DO	1	MET	7.9
54	D8	60	LEU	7.9
41	DW	6	ILE	7.9
53	D7	48	LYS	7.9
45	B0	26	TYR	7.9
32	DK	99	ILE	7.9
3	AD	103	ASN	7.8
39	DU	6	THR	7.8
34	DP	38	GLN	7.8
45	D0	79	VAL	7.8
27	BE	118	LYS	7.8
25	BC	128	LEU	7.8
39	BU	15	LYS	7.8
1	AB	166	ASP	7.8
12	CM	123	ALA	7.8
40	DV	84	LYS	7.8
39	BU	32	PHE	7.8
8	AI	23	ASN	7.8
43	DY	7	VAL	7.8
15	CP	55	ARG	7.8
18	AS	72	GLY	7.8
42	DX	61	GLY	7.8
25	BC	11	LEU	7.8
42	DX	5	TYR	7.8
51	B5	11	THR	7.8
51	D5	44	THR	7.8
6	AG	81	GLY	7.8
60	BA	425	G	7.8
8	CI	42	ARG	7.8
28	BF	56	GLU	7.8
30	BH	149	ARG	7.8
25	DC	105	LEU	7.8
45	B0	56	ASP	7.8
54	D8	63	PRO	7.8
28	BF	53	THR	7.8
40	BV	85	LYS	7.7
39	BU	8	VAL	7.7
3	CD	134	ASP	7.7
4	CE	132	ALA	7.7

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Mol	Chain	Res	Type	RSRZ
3	CD	98	GLU	7.7
48	BN	113	GLY	7.7
2	CC	166	GLU	7.7
26	DD	251	GLY	7.7
15	AP	19	ILE	7.7
8	CI	9	ARG	7.7
34	DP	75	ILE	7.7
38	DT	26	ASP	7.7
48	DN	84	LYS	7.7
28	BF	192	LEU	7.7
20	AA	174	C	7.7
18	AS	44	MET	7.7
43	BY	41	GLY	7.7
55	D9	13	LYS	7.7
27	BE	55	ASN	7.7
15	CP	16	HIS	7.7
27	DE	134	ILE	7.7
35	DQ	76	LYS	7.7
46	D1	60	PHE	7.7
41	BW	43	GLY	7.7
25	BC	176	VAL	7.7
23	AY	105	ILE	7.7
25	DC	110	ASP	7.7
54	D8	10	ALA	7.7
29	BG	178	PHE	7.7
28	BF	66	PRO	7.7
15	CP	39	TYR	7.7
34	BP	27	HIS	7.7
15	AP	3	LYS	7.7
53	D7	32	LYS	7.7
15	AP	70	ALA	7.7
20	AA	307	C	7.6
60	BA	833	U	7.6
20	AA	1357	A	7.6
43	BY	68	HIS	7.6
46	B1	21	ARG	7.6
48	DN	113	GLY	7.6
48	DN	117	PHE	7.6
55	B9	24	TYR	7.6
28	DF	183	VAL	7.6
9	CJ	45	ARG	7.6
28	BF	108	LYS	7.6

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Mol	Chain	Res	Type	RSRZ
36	BR	99	LYS	7.6
3	AD	112	VAL	7.6
28	DF	172	TRP	7.6
46	B1	41	ARG	7.6
28	BF	76	GLY	7.6
8	AI	67	GLY	7.6
34	BP	49	ARG	7.6
35	DQ	84	GLY	7.6
53	D7	49	ARG	7.6
37	DS	101	LEU	7.6
25	BC	95	VAL	7.6
2	AC	184	TYR	7.6
26	DD	241	PRO	7.6
33	BO	84	ALA	7.6
33	DO	100	GLY	7.6
3	CD	136	PRO	7.6
28	DF	157	VAL	7.6
36	BR	50	HIS	7.6
8	AI	84	ALA	7.6
20	AA	383	A	7.6
39	DU	25	TRP	7.6
43	DY	72	VAL	7.6
45	B0	38	VAL	7.6
41	BW	18	ARG	7.6
6	AG	80	VAL	7.6
28	BF	186	ILE	7.5
29	BG	156	ASP	7.5
39	DU	39	LEU	7.5
27	DE	131	ALA	7.5
39	DU	36	ARG	7.5
8	AI	124	GLN	7.5
15	CP	28	ARG	7.5
16	CQ	21	VAL	7.5
52	D6	25	LYS	7.5
54	D8	53	PRO	7.5
18	AS	51	VAL	7.5
25	DC	104	ILE	7.5
9	AJ	65	LEU	7.5
13	CN	48	ALA	7.5
45	B0	19	LYS	7.5
54	B8	4	MET	7.5
23	AY	18	ALA	7.5

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Mol	Chain	Res	Type	RSRZ
34	DP	46	LYS	7.5
46	D1	71	TYR	7.5
51	B5	12	SER	7.5
55	B9	21	GLY	7.5
54	B8	60	LEU	7.5
25	BC	101	ILE	7.5
33	DO	33	ALA	7.5
46	B1	35	THR	7.5
43	BY	70	SER	7.5
43	BY	67	LEU	7.5
25	BC	114	VAL	7.5
10	CK	121	PRO	7.4
26	DD	252	TRP	7.4
37	DS	54	LEU	7.4
45	D0	50	ASN	7.4
26	BD	267	SER	7.4
48	DN	71	ILE	7.4
25	DC	139	PRO	7.4
26	DD	248	SER	7.4
45	D0	41	ARG	7.4
27	DE	107	THR	7.4
43	BY	38	ILE	7.4
11	CL	83	VAL	7.4
14	CO	20	GLY	7.4
25	BC	157	ILE	7.4
33	DO	2	ILE	7.4
21	CV	20	U	7.4
34	BP	36	LYS	7.4
45	D0	49	LYS	7.4
3	CD	66	ARG	7.4
25	BC	76	LEU	7.4
28	DF	75	HIS	7.4
42	BX	78	LYS	7.4
10	AK	128	ALA	7.4
2	CC	152	ILE	7.4
9	CJ	64	GLU	7.4
27	BE	52	LEU	7.4
53	D7	42	LEU	7.4
18	AS	39	THR	7.4
25	BC	33	LEU	7.4
54	B8	53	PRO	7.4
15	AP	18	ARG	7.4

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Mol	Chain	Res	Type	RSRZ
38	DT	1	MET	7.4
26	BD	155	LEU	7.4
8	CI	116	LYS	7.4
26	BD	276	LYS	7.4
27	BE	75	VAL	7.4
28	DF	80	ALA	7.4
29	BG	102	PHE	7.4
26	BD	246	PRO	7.4
39	BU	18	LEU	7.4
39	DU	4	ALA	7.4
43	BY	39	VAL	7.4
52	B6	49	HIS	7.3
8	AI	80	GLY	7.3
8	AI	116	LYS	7.3
15	AP	30	GLY	7.3
9	CJ	70	ARG	7.3
37	BS	42	ASP	7.3
40	BV	84	LYS	7.3
18	AS	37	ARG	7.3
53	B7	48	LYS	7.3
4	CE	31	LEU	7.3
25	DC	96	GLY	7.3
45	B0	3	HIS	7.3
15	CP	37	GLY	7.3
27	DE	163	GLU	7.3
23	CY	260	LEU	7.3
27	DE	75	VAL	7.3
28	BF	155	LEU	7.3
34	DP	50	ARG	7.3
48	BN	115	ARG	7.3
37	BS	73	LEU	7.3
45	D0	48	GLY	7.3
8	AI	37	PHE	7.3
43	BY	76	CYS	7.3
34	BP	53	GLY	7.3
19	AT	71	THR	7.3
60	DA	1420	U	7.3
9	AJ	73	ASP	7.3
37	BS	26	LEU	7.3
45	D0	51	VAL	7.3
8	CI	74	ILE	7.3
18	AS	40	ILE	7.3

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Mol	Chain	Res	Type	RSRZ
30	DH	154	PRO	7.3
42	BX	34	ALA	7.3
3	CD	148	VAL	7.3
27	BE	195	LEU	7.3
39	DU	16	LYS	7.3
15	AP	36	ILE	7.3
39	DU	30	LYS	7.3
3	CD	68	TYR	7.3
37	BS	60	GLY	7.3
41	DW	43	GLY	7.3
19	AT	10	LEU	7.2
4	CE	120	THR	7.2
8	CI	65	VAL	7.2
28	DF	193	VAL	7.2
18	AS	32	LYS	7.2
46	D1	69	LYS	7.2
8	CI	40	LEU	7.2
25	DC	157	ILE	7.2
48	BN	116	LEU	7.2
46	D1	70	VAL	7.2
54	B8	59	LYS	7.2
54	B8	14	VAL	7.2
54	B8	64	TYR	7.2
8	AI	127	LYS	7.2
20	CA	134	A	7.2
26	DD	245	PRO	7.2
8	CI	66	ARG	7.2
53	D7	43	THR	7.2
42	DX	7	VAL	7.2
3	CD	60	GLU	7.2
16	AQ	6	LEU	7.2
38	DT	25	GLY	7.2
12	AM	11	ARG	7.2
34	BP	38	GLN	7.2
45	D0	44	ARG	7.2
55	D9	6	SER	7.2
26	BD	175	LEU	7.2
53	D7	31	LEU	7.2
11	AL	16	GLU	7.2
23	AY	165	GLN	7.2
34	BP	74	GLU	7.2
34	BP	61	ARG	7.2

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Mol	Chain	Res	Type	RSRZ
35	DQ	119	ARG	7.2
39	BU	17	ILE	7.2
26	BD	247	ALA	7.2
54	B8	10	ALA	7.2
2	AC	149	ALA	7.2
20	AA	1028(A)	C	7.2
25	DC	133	GLY	7.2
51	D5	16	ARG	7.2
26	DD	249	PRO	7.2
8	CI	128	ARG	7.2
41	DW	46	PHE	7.2
60	DA	1205	U	7.2
2	CC	169	ALA	7.2
9	CJ	58	ASP	7.2
46	D1	42	GLN	7.2
28	BF	77	ASP	7.1
32	BK	13	PRO	7.1
3	CD	93	PHE	7.1
2	CC	150	LYS	7.1
10	CK	126	ARG	7.1
27	DE	195	LEU	7.1
8	AI	74	ILE	7.1
27	BE	117	MET	7.1
43	DY	43	ASN	7.1
46	B1	37	ILE	7.1
19	AT	73	HIS	7.1
39	DU	38	THR	7.1
8	CI	16	ARG	7.1
29	DG	7	LEU	7.1
4	CE	45	PHE	7.1
30	BH	153	LYS	7.1
43	DY	3	VAL	7.1
51	B5	20	ARG	7.1
34	BP	75	ILE	7.1
18	AS	57	HIS	7.1
28	BF	112	MET	7.1
8	AI	13	ALA	7.1
8	CI	17	VAL	7.1
20	CA	1398	A	7.1
34	BP	22	GLY	7.1
39	BU	31	SER	7.1
27	DE	137	HIS	7.1

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Mol	Chain	Res	Type	RSRZ
39	DU	32	PHE	7.1
46	B1	42	GLN	7.1
13	AN	47	LEU	7.1
44	BZ	71	VAL	7.1
50	D3	20	LYS	7.1
13	AN	37	PHE	7.1
48	BN	42	TRP	7.1
3	CD	7	PRO	7.1
20	CA	607	A	7.1
42	DX	79	ALA	7.1
28	DF	189	THR	7.1
13	AN	44	LEU	7.1
36	BR	58	GLY	7.1
39	BU	12	ARG	7.0
46	D1	23	LYS	7.0
42	DX	25	LYS	7.0
8	CI	41	VAL	7.0
15	CP	2	VAL	7.0
8	AI	24	GLY	7.0
15	CP	4	ILE	7.0
26	BD	253	GLN	7.0
39	BU	4	ALA	7.0
19	AT	18	GLN	7.0
20	CA	976	G	7.0
27	BE	51	PHE	7.0
39	BU	3	ARG	7.0
20	AA	110	C	7.0
3	CD	70	ILE	7.0
27	BE	116	VAL	7.0
37	DS	16	ASN	7.0
20	CA	110	C	7.0
39	DU	15	LYS	7.0
41	BW	12	ILE	7.0
28	BF	158	THR	7.0
41	DW	93	ALA	7.0
10	CK	123	LYS	7.0
30	DH	153	LYS	7.0
37	DS	52	SER	7.0
36	DR	103	ARG	7.0
39	BU	29	SER	7.0
1	CB	19	HIS	7.0
46	B1	60	PHE	7.0

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Mol	Chain	Res	Type	RSRZ
3	AD	170	VAL	6.9
26	BD	268	ARG	6.9
55	B9	19	ARG	6.9
55	D9	16	VAL	6.9
12	AM	16	ASP	6.9
41	DW	17	VAL	6.9
19	AT	59	ALA	6.9
10	AK	129	SER	6.9
28	BF	157	VAL	6.9
51	D5	45	VAL	6.9
55	B9	16	VAL	6.9
20	AA	308	C	6.9
27	DE	128	SER	6.9
43	DY	45	VAL	6.9
13	AN	34	TYR	6.9
53	D7	41	ARG	6.9
11	CL	30	ALA	6.9
60	BA	1250	G	6.9
20	AA	1363	A	6.9
34	BP	41	ARG	6.9
25	DC	72	GLN	6.9
26	DD	276	LYS	6.9
48	BN	112	LEU	6.9
8	AI	81	ILE	6.9
32	BK	115	LEU	6.9
8	CI	13	ALA	6.9
8	CI	76	ALA	6.9
25	BC	8	TYR	6.9
46	D1	32	LYS	6.9
8	AI	31	GLN	6.9
43	BY	37	VAL	6.9
7	CH	32	LYS	6.9
27	DE	130	GLY	6.9
15	CP	15	PRO	6.9
32	BK	11	GLN	6.9
39	DU	34	LYS	6.9
20	AA	104	G	6.9
8	AI	12	GLU	6.9
29	BG	157	ILE	6.9
51	B5	19	ARG	6.9
13	AN	38	GLY	6.9
2	AC	198	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
18	CS	50	ALA	6.9
41	DW	76	VAL	6.9
28	DF	176	LEU	6.9
41	DW	16	LYS	6.9
22	CW	74	C	6.9
35	DQ	97	VAL	6.9
8	AI	77	ILE	6.9
34	DP	67	MET	6.8
3	CD	118	ARG	6.8
15	AP	64	ALA	6.8
39	BU	13	LYS	6.8
28	DF	40	GLN	6.8
60	DA	380	U	6.8
15	AP	55	ARG	6.8
2	AC	199	LYS	6.8
3	CD	146	ILE	6.8
25	DC	30	VAL	6.8
34	DP	68	GLN	6.8
53	B7	26	GLY	6.8
27	BE	120	TRP	6.8
28	BF	65	TRP	6.8
3	AD	8	VAL	6.8
18	AS	76	PRO	6.8
54	D8	22	VAL	6.8
12	AM	15	VAL	6.8
12	AM	10	PRO	6.8
54	B8	11	LYS	6.8
41	DW	21	VAL	6.8
43	DY	8	LYS	6.8
43	DY	15	VAL	6.8
3	AD	108	LEU	6.8
4	CE	134	ALA	6.8
15	CP	71	ARG	6.8
3	CD	198	VAL	6.8
20	CA	619	U	6.8
45	D0	70	GLN	6.8
9	AJ	63	PHE	6.8
25	DC	49	GLY	6.8
4	AE	132	ALA	6.8
25	BC	104	ILE	6.8
43	BY	15	VAL	6.8
19	AT	19	SER	6.8

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Mol	Chain	Res	Type	RSRZ
39	BU	24	TYR	6.8
29	BG	155	MET	6.8
8	CI	77	ILE	6.8
11	CL	68	ALA	6.8
45	B0	37	LEU	6.8
42	BX	56	THR	6.8
3	AD	5	ILE	6.8
28	DF	107	LYS	6.8
37	BS	32	LEU	6.8
9	CJ	60	ARG	6.7
3	CD	152	SER	6.7
20	CA	1368	G	6.7
13	CN	47	LEU	6.7
28	DF	182	ASN	6.7
33	BO	100	GLY	6.7
54	D8	12	LYS	6.7
27	BE	128	SER	6.7
38	DT	94	ALA	6.7
38	BT	2	ASN	6.7
9	CJ	57	LYS	6.7
38	BT	91	ARG	6.7
43	BY	32	PRO	6.7
52	D6	24	GLU	6.7
33	DO	65	THR	6.7
13	CN	44	LEU	6.7
28	BF	125	LEU	6.7
8	AI	118	LYS	6.7
15	AP	33	ILE	6.7
23	CY	356	LEU	6.7
2	CC	201	TYR	6.7
3	CD	199	ASN	6.7
8	CI	123	PRO	6.7
16	AQ	98	LEU	6.7
28	DF	155	LEU	6.7
18	AS	36	ARG	6.7
11	CL	28	LYS	6.7
45	B0	79	VAL	6.7
2	AC	150	LYS	6.7
20	AA	330	C	6.7
20	AA	1362(A)	C	6.7
9	CJ	66	ARG	6.7
38	BT	52	ILE	6.7

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Mol	Chain	Res	Type	RSRZ
52	B6	51	GLU	6.7
46	D1	59	THR	6.7
27	DE	76	ARG	6.7
36	BR	101	ALA	6.7
2	CC	186	PHE	6.7
36	BR	100	LEU	6.7
60	DA	2611	U	6.7
28	BF	193	VAL	6.7
44	BZ	96	VAL	6.7
1	CB	131	PRO	6.7
15	CP	27	LYS	6.7
60	DA	1634	A	6.7
23	AY	106	VAL	6.7
41	DW	103	ILE	6.7
25	BC	94	TYR	6.7
14	CO	30	ALA	6.6
1	AB	211	ILE	6.6
40	BV	80	GLN	6.6
9	CJ	50	ILE	6.6
36	BR	95	THR	6.6
60	BA	1982	C	6.6
26	BD	269	PHE	6.6
13	AN	57	ARG	6.6
40	DV	71	LEU	6.6
45	D0	77	ARG	6.6
13	CN	59	ALA	6.6
60	DA	2452	C	6.6
8	CI	64	THR	6.6
54	D8	38	GLY	6.6
3	CD	40	PRO	6.6
53	B7	46	VAL	6.6
39	BU	41	ALA	6.6
43	DY	75	ILE	6.6
39	BU	37	GLU	6.6
2	CC	200	ALA	6.6
30	DH	150	ALA	6.6
37	BS	15	ARG	6.6
35	BQ	139	GLU	6.6
12	CM	125	ARG	6.6
41	DW	20	VAL	6.6
19	AT	55	ILE	6.6
23	CY	144	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
39	BU	42	ALA	6.6
45	B0	25	ARG	6.6
60	DA	943	U	6.6
37	BS	21	THR	6.6
18	AS	73	GLU	6.6
41	BW	21	VAL	6.6
60	BA	805	G	6.6
13	CN	52	GLN	6.6
25	DC	113	ALA	6.6
29	DG	6	ALA	6.6
7	AH	31	PHE	6.6
27	DE	10	GLY	6.6
39	BU	21	ALA	6.6
42	BX	75	ASP	6.6
11	AL	14	GLY	6.6
28	DF	158	THR	6.6
60	BA	975	G	6.6
3	AD	70	ILE	6.6
12	AM	99	ARG	6.6
40	DV	77	ALA	6.6
43	DY	105	ALA	6.6
45	D0	81	VAL	6.6
28	DF	53	THR	6.6
39	BU	39	LEU	6.6
25	BC	34	ALA	6.6
13	AN	54	PRO	6.5
35	BQ	18	LYS	6.5
43	BY	14	LEU	6.6
51	B5	23	HIS	6.5
41	BW	4	LYS	6.5
43	BY	81	LYS	6.5
27	DE	25	VAL	6.5
28	DF	88	VAL	6.5
39	BU	9	VAL	6.5
11	CL	14	GLY	6.5
12	CM	122	LYS	6.5
26	BD	165	ILE	6.5
3	AD	111	ALA	6.5
45	D0	45	PHE	6.5
26	DD	254	THR	6.5
52	D6	40	CYS	6.5
20	AA	67	C	6.5

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Mol	Chain	Res	Type	RSRZ
30	DH	149	ARG	6.5
41	BW	11	ARG	6.5
45	B0	76	GLY	6.5
20	AA	882	C	6.5
42	DX	34	ALA	6.5
8	CI	114	TYR	6.5
14	CO	31	LEU	6.5
60	BA	1217	C	6.5
3	AD	113	SER	6.5
26	DD	183	ARG	6.5
46	B1	59	THR	6.5
4	CE	11	ILE	6.5
25	BC	96	GLY	6.5
43	BY	83	THR	6.5
23	CY	166	LEU	6.5
34	BP	30	THR	6.5
35	BQ	19	GLY	6.5
37	BS	33	LYS	6.5
43	BY	34	LYS	6.5
27	DE	4	ILE	6.5
13	AN	41	ARG	6.5
18	AS	31	ILE	6.5
2	AC	169	ALA	6.5
38	DT	24	PRO	6.5
8	CI	14	VAL	6.5
8	CI	18	PHE	6.5
9	AJ	62	HIS	6.5
34	BP	59	LEU	6.4
48	DN	115	ARG	6.4
45	B0	80	HIS	6.4
10	CK	122	LYS	6.4
13	AN	2	ALA	6.4
20	CA	103	C	6.4
26	DD	35	LYS	6.4
38	BT	94	ALA	6.4
54	B8	15	LYS	6.4
23	CY	258	VAL	6.4
39	DU	37	GLU	6.4
15	CP	3	LYS	6.4
25	DC	87	ALA	6.4
20	AA	48	C	6.4
42	BX	57	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
60	BA	2334	G	6.4
60	DA	561	G	6.4
8	AI	35	GLU	6.4
46	D1	49	VAL	6.4
20	AA	974	A	6.4
20	AA	136	C	6.4
15	AP	35	LYS	6.4
27	BE	154	LYS	6.4
27	BE	194	GLY	6.4
29	BG	177	GLY	6.4
38	BT	114	LEU	6.4
43	BY	3	VAL	6.4
26	DD	38	LYS	6.4
30	DH	152	ARG	6.4
16	AQ	9	VAL	6.4
45	B0	24	LYS	6.4
54	B8	63	PRO	6.4
37	DS	86	ALA	6.4
60	BA	222	A	6.4
54	D8	59	LYS	6.4
39	DU	18	LEU	6.4
45	D0	37	LEU	6.4
53	B7	28	ARG	6.4
1	AB	77	ALA	6.4
16	CQ	43	LEU	6.4
26	BD	239	ARG	6.4
60	DA	941	A	6.4
60	BA	1420	U	6.4
50	D3	22	ALA	6.4
28	DF	110	LEU	6.4
42	BX	9	LEU	6.4
27	DE	116	VAL	6.4
7	CH	117	GLY	6.4
25	DC	98	GLU	6.4
29	DG	37	VAL	6.4
60	DA	269	U	6.3
29	DG	98	ARG	6.3
59	BB	7	G	6.3
15	CP	29	ASP	6.3
60	DA	2081	C	6.3
34	BP	60	MET	6.3
34	DP	49	ARG	6.3

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Mol	Chain	Res	Type	RSRZ
3	CD	110	PHE	6.3
29	BG	41	GLN	6.3
3	CD	67	ILE	6.3
20	AA	873	A	6.3
8	CI	3	GLN	6.3
8	AI	27	THR	6.3
28	DF	112	MET	6.3
8	CI	87	GLN	6.3
18	CS	43	GLU	6.3
27	DE	6	GLY	6.3
34	DP	37	GLY	6.3
60	BA	242	G	6.3
26	BD	248	SER	6.3
34	BP	111	ARG	6.3
41	BW	19	LEU	6.3
44	DZ	70	LEU	6.3
18	CS	12	ASP	6.3
27	BE	7	VAL	6.3
8	AI	126	SER	6.3
8	AI	33	PHE	6.3
27	DE	2	LYS	6.3
51	B5	14	ALA	6.3
3	CD	150	GLU	6.3
44	BZ	83	PRO	6.3
3	AD	169	LYS	6.3
18	CS	31	ILE	6.3
19	CT	55	ILE	6.3
23	AY	16	GLY	6.3
37	DS	32	LEU	6.3
43	DY	106	LEU	6.3
20	CA	390	C	6.3
34	BP	71	VAL	6.3
27	BE	193	GLY	6.3
3	CD	97	LEU	6.3
2	CC	10	PHE	6.3
26	DD	247	ALA	6.3
21	AV	11	U	6.3
42	DX	69	TYR	6.3
39	BU	43	GLY	6.3
46	D1	67	ILE	6.3
19	CT	59	ALA	6.3
39	DU	17	ILE	6.3

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Mol	Chain	Res	Type	RSRZ
20	CA	201(A)	U	6.3
3	AD	162	LEU	6.2
3	AD	10	ARG	6.2
43	BY	44	ILE	6.2
43	DY	41	GLY	6.2
42	DX	10	ALA	6.2
54	D8	11	LYS	6.2
19	CT	20	LEU	6.2
4	CE	26	PHE	6.2
25	DC	97	GLY	6.2
9	CJ	40	LEU	6.2
46	B1	48	LYS	6.2
13	CN	60	SER	6.2
18	AS	75	ALA	6.2
15	AP	67	THR	6.2
37	BS	18	ILE	6.2
10	CK	124	LYS	6.2
18	CS	51	VAL	6.2
41	DW	8	ARG	6.2
15	AP	37	GLY	6.2
15	CP	5	ARG	6.2
28	DF	87	GLY	6.2
43	BY	63	LYS	6.2
46	D1	48	LYS	6.2
19	CT	66	ALA	6.2
28	BF	191	ARG	6.2
27	DE	132	HIS	6.2
25	DC	33	LEU	6.2
52	B6	11	LEU	6.2
60	BA	283	A	6.2
39	BU	20	LEU	6.2
2	AC	200	ALA	6.2
51	B5	18	ALA	6.2
3	CD	127	THR	6.2
4	CE	48	ALA	6.2
37	BS	65	VAL	6.2
40	DV	79	VAL	6.2
8	AI	59	PHE	6.2
45	B0	60	PHE	6.2
51	B5	25	LEU	6.2
26	BD	164	GLN	6.2
48	DN	35	ARG	6.2

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Mol	Chain	Res	Type	RSRZ
35	DQ	88	GLY	6.2
2	AC	7	PRO	6.2
19	CT	56	MET	6.2
25	BC	78	ILE	6.2
27	BE	156	MET	6.2
20	CA	136	C	6.2
40	BV	40	LEU	6.2
21	AV	21	A	6.2
15	CP	14	ASN	6.1
16	CQ	58	GLU	6.1
29	BG	165	THR	6.1
9	CJ	71	LEU	6.1
52	D6	54	ILE	6.1
8	AI	34	ASN	6.1
9	CJ	62	HIS	6.1
60	BA	2581	G	6.1
2	AC	201	TYR	6.1
16	CQ	44	ALA	6.1
4	AE	29	GLY	6.1
25	BC	49	GLY	6.1
38	BT	50	ILE	6.1
42	DX	6	ASP	6.1
13	AN	36	PHE	6.1
38	DT	91	ARG	6.1
1	AB	206	ASP	6.1
26	DD	240	ALA	6.1
3	AD	131	ARG	6.1
13	CN	51	GLY	6.1
2	AC	5	ILE	6.1
45	D0	2	ALA	6.1
60	DA	225	A	6.1
34	DP	59	LEU	6.1
45	B0	21	LEU	6.1
48	DN	114	ARG	6.1
34	DP	60	MET	6.1
50	D3	28	LEU	6.1
54	D8	13	ARG	6.1
3	CD	181	MET	6.1
29	BG	39	ILE	6.1
21	CV	8	A	6.1
3	CD	126	ILE	6.1
48	BN	109	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
27	BE	54	GLN	6.1
8	AI	62	TYR	6.1
9	AJ	46	ARG	6.1
3	AD	115	ARG	6.1
39	BU	35	ALA	6.1
43	DY	107	ASP	6.1
60	DA	528	A	6.1
3	AD	163	GLU	6.1
23	CY	392	GLU	6.1
25	DC	88	GLU	6.1
3	AD	183	GLY	6.1
20	AA	1403	C	6.1
8	CI	120	ARG	6.1
29	DG	2	PRO	6.1
43	DY	74	PRO	6.1
59	DB	29	A	6.1
1	AB	79	ASP	6.1
20	CA	1358	U	6.1
18	CS	15	LEU	6.1
29	DG	96	ARG	6.1
12	CM	10	PRO	6.1
34	BP	76	LYS	6.1
34	DP	39	LYS	6.1
48	DN	100	GLU	6.0
4	CE	133	TYR	6.0
28	DF	113	ALA	6.0
41	BW	20	VAL	6.0
41	BW	47	VAL	6.0
35	DQ	41	TRP	6.0
14	AO	32	LEU	6.0
27	DE	55	ASN	6.0
28	BF	169	ASN	6.0
54	D8	61	LEU	6.0
8	CI	27	THR	6.0
13	CN	37	PHE	6.0
30	DH	151	ILE	6.0
7	AH	32	LYS	6.0
37	BS	92	TYR	6.0
37	DS	17	ARG	6.0
41	DW	106	ILE	6.0
11	AL	13	LYS	6.0
25	BC	138	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
15	CP	32	TYR	6.0
41	BW	44	ALA	6.0
43	DY	31	LEU	6.0
45	B0	18	ALA	6.0
8	CI	63	ILE	6.0
28	DF	11	VAL	6.0
3	CD	202	LEU	6.0
8	AI	18	PHE	6.0
41	BW	82	LEU	6.0
36	DR	104	ARG	6.0
41	BW	45	TYR	6.0
15	AP	52	ASP	6.0
34	BP	62	LEU	6.0
32	BK	22	PRO	6.0
34	DP	63	PRO	6.0
20	AA	1251	A	6.0
33	DO	31	LYS	6.0
34	DP	35	HIS	6.0
3	AD	152	SER	6.0
26	DD	250	TRP	6.0
35	BQ	89	ASN	6.0
43	DY	73	ARG	6.0
4	CE	12	LEU	6.0
4	CE	119	LEU	6.0
18	AS	71	LEU	6.0
50	D3	27	GLY	6.0
52	B6	10	LEU	6.0
46	D1	9	GLY	6.0
27	BE	131	ALA	6.0
27	DE	7	VAL	6.0
9	CJ	61	GLU	6.0
53	B7	9	ARG	6.0
40	BV	72	VAL	5.9
42	DX	24	GLY	5.9
60	DA	631	A	6.0
41	DW	73	ALA	5.9
48	BN	71	ILE	5.9
8	AI	75	ASP	5.9
20	CA	972	C	5.9
60	BA	790	C	5.9
2	AC	167	TRP	5.9
55	B9	20	HIS	5.9

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Mol	Chain	Res	Type	RSRZ
60	DA	2058	A	5.9
9	CJ	67	THR	5.9
38	BT	115	ARG	5.9
3	AD	100	ARG	5.9
34	BP	26	GLY	5.9
1	AB	188	ALA	5.9
35	DQ	33	GLY	5.9
43	DY	70	SER	5.9
48	DN	112	LEU	5.9
20	CA	1362(A)	C	5.9
26	DD	244	ARG	5.9
8	CI	33	PHE	5.9
34	BP	45	LEU	5.9
13	CN	10	ALA	5.9
37	BS	99	LYS	5.9
48	DN	53	VAL	5.9
8	AI	10	ARG	5.9
16	AQ	10	VAL	5.9
33	DO	64	ARG	5.9
27	DE	106	GLY	5.9
39	BU	30	LYS	5.9
50	D3	23	LEU	5.9
27	BE	119	ARG	5.9
27	DE	196	VAL	5.9
4	CE	13	ILE	5.9
20	AA	1531	A	5.9
25	DC	52	PRO	5.9
29	BG	2	PRO	5.9
42	BX	8	ILE	5.9
43	DY	12	THR	5.9
51	B5	13	LYS	5.9
25	BC	221	PRO	5.9
34	BP	23	PRO	5.9
52	B6	13	CYS	5.9
19	CT	24	LEU	5.9
33	DO	84	ALA	5.9
19	CT	21	LYS	5.9
40	BV	71	LEU	5.9
27	BE	114	ALA	5.9
44	DZ	99	TYR	5.9
32	DK	37	PHE	5.9
3	CD	94	LEU	5.9

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Mol	Chain	Res	Type	RSRZ
36	BR	54	LEU	5.9
48	DN	34	LEU	5.9
4	CE	135	THR	5.9
43	DY	54	LYS	5.9
54	B8	24	ALA	5.9
15	CP	13	HIS	5.9
20	CA	30	U	5.9
20	CA	382	A	5.9
16	AQ	7	THR	5.9
25	BC	79	ALA	5.9
41	BW	104	THR	5.9
15	AP	63	GLY	5.9
20	AA	1365	G	5.9
36	DR	105	ARG	5.8
13	AN	46	GLU	5.8
30	BH	155	SER	5.8
43	DY	17	SER	5.8
43	BY	105	ALA	5.8
48	BN	45	ASN	5.8
19	AT	69	GLY	5.8
43	BY	107	ASP	5.8
4	CE	131	ILE	5.8
18	AS	49	ILE	5.8
36	BR	16	HIS	5.8
41	BW	16	LYS	5.8
3	AD	11	LEU	5.8
27	DE	136	ARG	5.8
32	DK	11	GLN	5.8
51	D5	20	ARG	5.8
60	BA	812	C	5.8
60	DA	268	C	5.8
27	DE	24	THR	5.8
8	AI	78	LYS	5.8
2	CC	6	HIS	5.8
53	D7	39	ARG	5.8
33	BO	101	PRO	5.8
28	DF	90	PHE	5.8
11	CL	129	ALA	5.8
35	BQ	82	ARG	5.8
26	DD	242	ARG	5.8
41	BW	5	ALA	5.8
54	D8	62	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
29	DG	8	LYS	5.8
54	D8	54	GLU	5.8
2	CC	3	ASN	5.8
13	AN	53	LEU	5.8
28	DF	156	LEU	5.8
45	B0	39	ARG	5.8
46	D1	7	ILE	5.8
20	AA	108	G	5.8
29	BG	176	LEU	5.8
37	BS	61	ASN	5.8
39	DU	24	TYR	5.8
1	CB	133	LYS	5.8
3	CD	105	VAL	5.8
43	DY	39	VAL	5.8
34	BP	37	GLY	5.8
13	CN	32	SER	5.8
8	AI	46	ALA	5.8
42	BX	7	VAL	5.8
26	BD	174	ILE	5.8
27	DE	26	ILE	5.8
28	BF	87	GLY	5.8
16	CQ	45	HIS	5.8
3	CD	138	TYR	5.8
8	CI	112	LYS	5.8
20	AA	332	G	5.8
27	DE	165	VAL	5.8
33	DO	80	ASP	5.8
40	BV	76	LYS	5.8
43	BY	28	LYS	5.8
60	DA	223	A	5.8
60	DA	256	A	5.8
28	BF	129	PHE	5.8
27	DE	1	MET	5.8
7	CH	118	VAL	5.8
46	B1	49	VAL	5.8
28	BF	80	ALA	5.8
25	DC	128	LEU	5.8
41	DW	19	LEU	5.8
12	AM	18	ALA	5.8
42	DX	28	PHE	5.8
19	AT	17	ARG	5.8
35	DQ	82	ARG	5.8

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Mol	Chain	Res	Type	RSRZ
15	CP	31	LYS	5.7
27	BE	5	LEU	5.7
43	BY	7	VAL	5.7
55	B9	3	VAL	5.7
9	CJ	63	PHE	5.7
28	BF	139	PHE	5.7
28	BF	189	THR	5.7
42	DX	82	GLN	5.7
60	BA	837	C	5.7
41	BW	17	VAL	5.7
2	AC	165	THR	5.7
13	AN	56	VAL	5.7
3	CD	109	GLY	5.7
35	DQ	42	ILE	5.7
20	AA	377	G	5.7
20	CA	1365	G	5.7
42	DX	26	TYR	5.7
29	BG	65	GLY	5.7
39	BU	16	LYS	5.7
40	DV	85	LYS	5.7
60	DA	1629	U	5.7
25	DC	221	PRO	5.7
49	B2	33	MET	5.7
3	CD	76	ARG	5.7
13	AN	61	TRP	5.7
37	DS	97	ARG	5.7
2	AC	187	ALA	5.7
39	DU	21	ALA	5.7
53	B7	1	MET	5.7
41	BW	46	PHE	5.7
8	AI	25	LYS	5.7
47	B4	12	ALA	5.7
29	BG	98	ARG	5.7
48	BN	117	PHE	5.7
15	CP	64	ALA	5.7
9	CJ	49	VAL	5.7
9	CJ	65	LEU	5.7
26	BD	34	VAL	5.7
28	BF	55	GLY	5.7
36	BR	71	GLN	5.7
54	D8	43	GLN	5.7
33	DO	32	TYR	5.7

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Mol	Chain	Res	Type	RSRZ
15	AP	59	TRP	5.7
20	CA	381	C	5.7
42	DX	70	LEU	5.7
1	AB	94	ASN	5.7
8	AI	29	ASN	5.7
37	DS	92	TYR	5.7
41	DW	45	TYR	5.7
41	BW	83	LYS	5.7
53	D7	28	ARG	5.7
3	AD	116	GLN	5.7
40	BV	4	ILE	5.7
26	BD	245	PRO	5.7
13	AN	55	GLY	5.7
8	CI	83	ARG	5.7
27	DE	199	ARG	5.7
32	DK	75	SER	5.7
44	BZ	75	ASN	5.7
11	AL	68	ALA	5.7
25	BC	75	VAL	5.7
39	DU	11	ARG	5.7
20	AA	1364	U	5.7
36	BR	24	GLN	5.7
39	BU	27	LEU	5.7
3	AD	126	ILE	5.7
8	CI	26	VAL	5.7
32	DK	10	LEU	5.7
8	CI	121	ARG	5.7
44	BZ	163	LEU	5.6
60	DA	914	C	5.6
41	DW	51	LEU	5.6
16	CQ	39	SER	5.6
3	AD	7	PRO	5.6
44	BZ	90	VAL	5.6
46	D1	47	GLN	5.6
3	CD	106	TYR	5.6
3	AD	137	SER	5.6
39	BU	26	GLY	5.6
20	CA	354	G	5.6
29	DG	3	LEU	5.6
54	B8	62	LEU	5.6
60	BA	336	C	5.6
8	CI	10	ARG	5.6

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Mol	Chain	Res	Type	RSRZ
8	AI	19	LEU	5.6
45	B0	17	GLN	5.6
45	D0	53	MET	5.6
20	CA	109	A	5.6
22	CW	73	A	5.6
20	CA	620	C	5.6
41	DW	23	LEU	5.6
4	CE	24	ARG	5.6
18	CS	39	THR	5.6
36	BR	37	THR	5.6
37	BS	100	ALA	5.6
8	AI	79	LEU	5.6
23	AY	260	LEU	5.6
53	D7	27	GLY	5.6
32	DK	34	ILE	5.6
35	DQ	10	ARG	5.6
55	D9	4	ARG	5.6
2	AC	46	GLU	5.6
28	BF	75	HIS	5.6
26	BD	240	ALA	5.6
26	DD	231	HIS	5.6
28	BF	117	ARG	5.6
34	DP	53	GLY	5.6
41	BW	15	ARG	5.6
41	DW	107	LEU	5.6
4	AE	102	ALA	5.6
44	BZ	121	HIS	5.6
27	BE	196	VAL	5.6
25	BC	113	ALA	5.6
34	BP	67	MET	5.6
48	DN	96	GLU	5.6
3	AD	160	GLN	5.6
27	DE	5	LEU	5.6
33	DO	62	VAL	5.6
54	B8	55	ALA	5.6
30	BH	151	ILE	5.6
13	CN	50	LYS	5.6
27	BE	155	LYS	5.6
39	BU	28	ARG	5.6
60	DA	381	G	5.6
16	AQ	24	GLU	5.5
41	BW	93	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
3	AD	158	ILE	5.5
9	CJ	7	LYS	5.5
19	CT	26	ASN	5.5
8	AI	121	ARG	5.5
9	CJ	72	VAL	5.5
25	DC	48	LEU	5.5
2	CC	199	LYS	5.5
25	BC	3	LYS	5.5
25	DC	106	ASP	5.5
25	DC	190	ILE	5.5
26	BD	55	GLY	5.5
43	BY	30	VAL	5.5
2	AC	152	ILE	5.5
3	CD	206	PHE	5.5
26	BD	251	GLY	5.5
25	BC	213	VAL	5.5
33	BO	61	VAL	5.5
37	BS	69	VAL	5.5
54	D8	47	LYS	5.5
60	DA	267	C	5.5
3	CD	64	LEU	5.5
8	AI	26	VAL	5.5
42	DX	60	ARG	5.5
53	B7	30	VAL	5.5
7	CH	31	PHE	5.5
60	DA	1340	U	5.5
60	DA	1554	A	5.5
29	BG	107	LEU	5.5
18	AS	35	SER	5.5
37	BS	102	ALA	5.5
53	D7	47	ARG	5.5
8	CI	113	LYS	5.5
1	AB	76	GLN	5.5
9	AJ	44	VAL	5.5
26	BD	185	VAL	5.5
40	BV	39	LEU	5.5
43	DY	83	THR	5.5
46	D1	73	LEU	5.5
3	CD	63	LYS	5.5
39	BU	22	LYS	5.5
32	DK	22	PRO	5.5
39	BU	73	GLY	5.5

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Mol	Chain	Res	Type	RSRZ
44	DZ	165	VAL	5.5
27	DE	51	PHE	5.5
43	BY	66	PRO	5.5
20	CA	825	G	5.5
60	BA	232	G	5.5
13	CN	58	LYS	5.5
18	CS	57	HIS	5.5
19	AT	56	MET	5.5
8	AI	76	ALA	5.5
12	CM	16	ASP	5.5
28	BF	98	SER	5.5
50	D3	26	LEU	5.5
29	BG	168	GLU	5.5
33	BO	111	PHE	5.5
29	DG	157	ILE	5.5
20	AA	113	G	5.5
60	BA	836	G	5.5
18	AS	16	LEU	5.5
41	BW	85	VAL	5.5
48	DN	122	VAL	5.5
41	BW	33	ARG	5.5
43	BY	86	ARG	5.5
3	AD	127	THR	5.5
3	CD	133	VAL	5.5
46	B1	28	GLY	5.5
54	B8	58	ILE	5.5
20	AA	305	G	5.5
50	B3	20	LYS	5.5
50	D3	21	ALA	5.5
3	CD	101	LEU	5.5
37	BS	106	ARG	5.5
27	DE	27	LEU	5.5
38	BT	62	THR	5.5
60	BA	1257	C	5.5
4	CE	27	ARG	5.4
27	DE	117	MET	5.5
3	AD	166	LYS	5.4
15	CP	56	ALA	5.4
35	BQ	85	LYS	5.4
40	DV	14	VAL	5.4
42	DX	31	HIS	5.4
39	DU	22	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
51	D5	25	LEU	5.4
34	DP	45	LEU	5.4
48	BN	46	VAL	5.4
54	B8	22	VAL	5.4
2	CC	7	PRO	5.4
28	BF	190	GLU	5.4
43	DY	28	LYS	5.4
8	CI	28	VAL	5.4
50	D3	54	VAL	5.4
19	AT	11	SER	5.4
2	CC	44	GLU	5.4
44	BZ	97	GLU	5.4
45	D0	68	GLU	5.4
18	CS	9	VAL	5.4
23	AY	104	ALA	5.4
28	DF	111	ALA	5.4
44	BZ	69	THR	5.4
39	BU	11	ARG	5.4
18	AS	12	ASP	5.4
50	B3	28	LEU	5.4
8	AI	119	ALA	5.4
43	DY	81	LYS	5.4
16	AQ	22	LEU	5.4
27	BE	59	VAL	5.4
42	BX	31	HIS	5.4
60	DA	271(D)	U	5.4
10	AK	124	LYS	5.4
60	DA	2579	C	5.4
18	CS	40	ILE	5.4
41	BW	10	VAL	5.4
15	CP	12	LYS	5.4
43	BY	97	ARG	5.4
48	BN	47	ALA	5.4
60	DA	408	G	5.4
27	DE	108	SER	5.4
3	AD	75	PHE	5.4
28	BF	88	VAL	5.4
9	AJ	53	PRO	5.4
27	DE	198	VAL	5.4
51	D5	46	CYS	5.4
32	BK	54	PRO	5.4
34	DP	27	HIS	5.4

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Mol	Chain	Res	Type	RSRZ
20	CA	66	G	5.4
4	CE	129	ILE	5.4
42	BX	29	TRP	5.4
18	AS	38	SER	5.4
25	DC	144	GLY	5.4
18	CS	59	PRO	5.4
19	CT	29	LYS	5.4
26	BD	147	LEU	5.4
34	DP	64	LYS	5.4
4	CE	136	MET	5.4
20	CA	824	C	5.4
8	AI	36	TYR	5.4
26	BD	35	LYS	5.3
43	DY	30	VAL	5.3
54	B8	47	LYS	5.3
44	BZ	95	PRO	5.3
53	D7	34	ARG	5.3
18	AS	50	ALA	5.3
25	BC	30	VAL	5.3
27	DE	194	GLY	5.3
37	BS	108	GLY	5.3
43	DY	14	LEU	5.3
34	DP	23	PRO	5.3
25	BC	215	VAL	5.3
28	BF	109	GLY	5.3
2	CC	42	LEU	5.3
25	DC	153	ILE	5.3
39	BU	44	ASN	5.3
43	BY	8	LYS	5.3
43	BY	45	VAL	5.3
8	CI	62	TYR	5.3
1	AB	167	PRO	5.3
60	BA	2275	C	5.3
21	CV	19	G	5.3
60	BA	1763	G	5.3
8	AI	17	VAL	5.3
15	AP	2	VAL	5.3
2	AC	186	PHE	5.3
18	AS	15	LEU	5.3
44	BZ	165	VAL	5.3
60	DA	2060	A	5.3
34	DP	76	LYS	5.3

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Mol	Chain	Res	Type	RSRZ
41	BW	23	LEU	5.3
8	AI	114	TYR	5.3
11	CL	21	LYS	5.3
25	DC	203	GLU	5.3
41	DW	13	SER	5.3
59	DB	7	G	5.3
60	BA	2576	G	5.3
9	CJ	42	THR	5.3
29	DG	102	PHE	5.3
34	BP	73	GLY	5.3
39	DU	12	ARG	5.3
13	CN	45	ARG	5.3
41	BW	6	ILE	5.3
46	B1	22	GLY	5.3
26	BD	10	THR	5.3
60	BA	2743	C	5.3
1	AB	170	GLU	5.3
18	AS	13	ASP	5.3
39	BU	19	LYS	5.3
14	CO	87	ILE	5.3
38	BT	97	ALA	5.3
29	DG	103	LEU	5.3
41	DW	47	VAL	5.3
13	CN	36	PHE	5.3
42	BX	21	PHE	5.3
28	BF	182	ASN	5.3
41	BW	14	PRO	5.3
26	DD	275	LYS	5.3
3	AD	125	HIS	5.3
13	CN	53	LEU	5.3
15	CP	73	LEU	5.3
40	BV	38	LEU	5.3
43	BY	62	GLU	5.3
60	BA	866	A	5.3
28	BF	107	LYS	5.3
26	DD	34	VAL	5.3
25	DC	101	ILE	5.3
3	CD	166	LYS	5.3
20	AA	304	U	5.3
39	BU	34	LYS	5.3
40	BV	2	PHE	5.3
11	CL	128	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
25	BC	139	PRO	5.3
15	AP	39	TYR	5.3
34	DP	21	ARG	5.3
34	DP	55	ARG	5.3
34	DP	40	SER	5.3
43	BY	100	ALA	5.3
3	CD	135	LEU	5.3
23	CY	393	ASP	5.3
16	CQ	59	ILE	5.3
20	AA	66	G	5.2
11	CL	55	VAL	5.2
28	DF	106	ARG	5.2
26	DD	253	GLN	5.2
27	DE	103	ASP	5.2
28	DF	56	GLU	5.2
41	DW	97	LYS	5.2
33	BO	41	ALA	5.2
41	DW	42	ARG	5.2
54	B8	42	ARG	5.2
37	DS	99	LYS	5.2
13	CN	61	TRP	5.2
18	CS	44	MET	5.2
35	DQ	103	MET	5.2
3	CD	203	VAL	5.2
34	DP	79	ARG	5.2
39	DU	28	ARG	5.2
8	CI	19	LEU	5.2
8	CI	127	LYS	5.2
9	AJ	71	LEU	5.2
46	D1	6	GLU	5.2
26	BD	252	TRP	5.2
20	AA	975	A	5.2
40	DV	72	VAL	5.2
35	BQ	26	TYR	5.2
54	B8	61	LEU	5.2
26	BD	233	HIS	5.2
43	DY	80	GLY	5.2
60	BA	34	C	5.2
41	DW	94	ASP	5.2
38	DT	62	THR	5.2
11	CL	99	HIS	5.2
43	BY	87	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
36	BR	21	TYR	5.2
20	CA	177	C	5.2
54	D8	4	MET	5.2
29	BG	64	THR	5.2
54	D8	9	GLY	5.2
9	CJ	6	ILE	5.2
20	CA	325	A	5.2
25	DC	51	ASP	5.2
25	DC	222	SER	5.2
3	CD	132	ARG	5.2
15	AP	21	VAL	5.2
48	DN	103	VAL	5.2
27	BE	135	HIS	5.2
7	CH	35	ILE	5.2
25	DC	59	VAL	5.2
25	DC	202	PRO	5.2
29	BG	37	VAL	5.2
34	BP	39	LYS	5.2
4	AE	31	LEU	5.2
25	BC	48	LEU	5.2
33	DO	103	ALA	5.2
20	AA	390	C	5.2
37	DS	91	PRO	5.2
9	AJ	43	ARG	5.2
25	BC	35	THR	5.2
43	DY	69	ALA	5.2
28	DF	62	ARG	5.2
36	BR	18	LEU	5.2
55	B9	5	ALA	5.2
11	CL	98	TYR	5.2
25	DC	84	ILE	5.2
54	D8	42	ARG	5.2
18	AS	41	VAL	5.2
20	CA	1060	C	5.2
28	DF	187	VAL	5.2
35	BQ	17	LEU	5.2
37	DS	70	GLY	5.2
41	BW	39	THR	5.2
46	B1	34	THR	5.2
1	CB	132	LYS	5.2
54	B8	41	ILE	5.2
60	BA	332	A	5.2

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Mol	Chain	Res	Type	RSRZ
9	AJ	61	GLU	5.2
2	AC	197	GLY	5.2
46	B1	36	GLY	5.2
27	DE	105	THR	5.1
60	DA	2573	C	5.1
50	D3	12	PRO	5.1
60	BA	75	G	5.1
23	CY	163	VAL	5.1
43	BY	89	PHE	5.1
3	CD	205	GLU	5.1
20	AA	1366	C	5.1
26	BD	254	THR	5.1
29	DG	94	LEU	5.1
45	D0	16	SER	5.1
46	D1	33	LYS	5.1
20	CA	148	G	5.1
8	AI	38	GLN	5.1
20	AA	1257	U	5.1
27	BE	142	GLY	5.1
32	DK	74	ALA	5.1
48	DN	110	GLY	5.1
60	BA	574	C	5.1
9	AJ	50	ILE	5.1
29	BG	103	LEU	5.1
3	CD	209	ARG	5.1
13	AN	45	ARG	5.1
16	AQ	86	GLU	5.1
3	AD	136	PRO	5.1
60	DA	974(A)	G	5.1
25	BC	154	ILE	5.1
28	BF	183	VAL	5.1
35	DQ	118	LEU	5.1
25	DC	60	ARG	5.1
8	AI	106	ALA	5.1
25	BC	92	ALA	5.1
18	AS	10	PHE	5.1
20	AA	374	A	5.1
28	DF	81	PRO	5.1
27	DE	182	LEU	5.1
11	CL	6	THR	5.1
42	DX	56	THR	5.1
60	DA	1635	G	5.1

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Mol	Chain	Res	Type	RSRZ
3	AD	101	LEU	5.1
15	CP	65	GLN	5.1
34	DP	70	GLN	5.1
54	D8	2	PRO	5.1
34	DP	34	GLY	5.1
2	CC	45	LYS	5.1
52	D6	41	PRO	5.1
20	AA	619	U	5.1
41	BW	94	ASP	5.1
48	BN	41	ASP	5.1
28	BF	174	VAL	5.1
8	AI	11	LYS	5.1
25	BC	212	SER	5.1
42	DX	27	THR	5.1
37	BS	105	ALA	5.1
53	B7	31	LEU	5.1
43	DY	97	ARG	5.1
13	AN	11	LYS	5.1
27	BE	77	ILE	5.1
45	B0	5	LYS	5.1
1	CB	140	HIS	5.1
20	CA	873	A	5.1
41	DW	9	TYR	5.1
50	B3	12	PRO	5.1
3	AD	147	ALA	5.1
25	BC	177	GLY	5.1
50	D3	6	VAL	5.1
4	CE	25	ARG	5.1
55	B9	35	ARG	5.1
7	CH	5	PRO	5.1
60	DA	125	G	5.1
16	AQ	5	VAL	5.1
13	AN	39	LEU	5.1
19	CT	77	ALA	5.1
6	CG	33	ASP	5.1
2	AC	138	VAL	5.1
10	AK	127	LYS	5.1
60	BA	1607	C	5.0
45	D0	15	ASP	5.0
51	B5	24	ALA	5.0
52	B6	54	ILE	5.0
18	CS	74	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
2	CC	149	ALA	5.0
19	AT	33	ILE	5.0
26	BD	56	GLY	5.0
27	BE	106	GLY	5.0
43	DY	82	PRO	5.0
45	B0	72	ARG	5.0
42	BX	53	LYS	5.0
60	DA	1627	G	5.0
6	CG	26	PHE	5.0
26	DD	213	ARG	5.0
19	CT	25	ARG	5.0
28	BF	33	LEU	5.0
33	BO	106	LEU	5.0
60	BA	1621	U	5.0
4	AE	21	ALA	5.0
8	CI	25	LYS	5.0
30	DH	167	GLU	5.0
35	BQ	25	ASP	5.0
45	D0	56	ASP	5.0
51	D5	13	LYS	5.0
3	AD	114	ARG	5.0
8	AI	85	LEU	5.0
46	D1	58	ILE	5.0
4	AE	30	ALA	5.0
33	BO	102	VAL	5.0
26	DD	175	LEU	5.0
27	BE	4	ILE	5.0
36	DR	70	LEU	5.0
25	BC	81	GLY	5.0
29	BG	164	GLU	5.0
20	CA	1397	C	5.0
44	DZ	71	VAL	5.0
60	DA	973	A	5.0
4	AE	10	MET	5.0
16	CQ	4	LYS	5.0
27	DE	154	LYS	5.0
28	DF	86	GLY	5.0
34	DP	56	SER	5.0
38	BT	113	LYS	5.0
48	BN	27	ALA	5.0
11	CL	96	VAL	5.0
3	CD	100	ARG	5.0

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Mol	Chain	Res	Type	RSRZ
4	CE	15	ARG	5.0
34	BP	70	GLN	5.0
8	CI	67	GLY	5.0
20	AA	1320	C	5.0
20	CA	882	C	5.0
59	DB	28	C	5.0
23	AY	390	VAL	5.0
25	BC	42	VAL	5.0
25	DC	215	VAL	5.0
13	CN	31	ARG	5.0
36	BR	94	TYR	5.0
43	BY	31	LEU	5.0
19	AT	58	LYS	5.0
19	CT	18	GLN	5.0
29	BG	175	LEU	5.0
2	CC	190	ARG	5.0
3	CD	121	VAL	5.0
15	AP	40	ASP	5.0
25	DC	11	LEU	5.0
30	BH	105	LEU	5.0
41	DW	98	LYS	5.0
46	D1	68	PRO	5.0
60	DA	833	U	5.0
48	BN	74	ARG	5.0
19	CT	62	LEU	5.0
48	BN	111	PRO	5.0
52	D6	47	THR	5.0
41	BW	3	ALA	5.0
27	DE	52	LEU	5.0
60	DA	2613	U	5.0
33	BO	12	ASP	5.0
2	CC	165	THR	5.0
46	D1	72	GLU	5.0
60	BA	89	G	5.0
20	AA	1395	C	5.0
29	BG	16	ARG	5.0
41	BW	105	VAL	4.9
3	AD	63	LYS	4.9
35	DQ	83	MET	4.9
3	CD	208	SER	4.9
41	BW	13	SER	4.9
51	D5	21	SER	4.9

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Mol	Chain	Res	Type	RSRZ
2	CC	40	ARG	4.9
35	DQ	117	ALA	4.9
8	CI	39	GLY	4.9
19	CT	11	SER	4.9
29	DG	159	VAL	4.9
37	BS	46	VAL	4.9
8	CI	43	ALA	4.9
26	BD	36	PRO	4.9
36	DR	101	ALA	4.9
44	BZ	76	LEU	4.9
44	BZ	150	LEU	4.9
20	CA	351	G	4.9
20	CA	1356	G	4.9
60	DA	242	G	4.9
3	CD	8	VAL	4.9
28	DF	83	PHE	4.9
29	BG	180	PHE	4.9
51	B5	15	ARG	4.9
4	CE	22	GLY	4.9
20	AA	977	A	4.9
25	BC	222	SER	4.9
28	BF	111	ALA	4.9
36	BR	19	ALA	4.9
41	DW	44	ALA	4.9
23	CY	82	ILE	4.9
34	BP	77	ARG	4.9
3	AD	69	GLY	4.9
25	DC	76	LEU	4.9
34	BP	68	GLN	4.9
20	CA	1224	G	4.9
53	D7	44	PRO	4.9
25	BC	189	ASN	4.9
43	BY	2	ARG	4.9
34	BP	56	SER	4.9
25	DC	150	ILE	4.9
46	B1	61	ARG	4.9
3	AD	24	GLU	4.9
20	CA	308	C	4.9
26	BD	191	ALA	4.9
35	BQ	28	ALA	4.9
60	DA	2275	C	4.9
3	AD	132	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
16	AQ	23	VAL	4.9
26	BD	154	LYS	4.9
28	DF	114	VAL	4.9
3	CD	80	GLU	4.9
50	D3	40	THR	4.9
3	AD	149	ALA	4.9
12	CM	102	ARG	4.9
3	CD	43	HIS	4.9
38	BT	26	ASP	4.9
28	DF	109	GLY	4.9
3	CD	164	ALA	4.9
20	CA	332	G	4.9
29	DG	88	ILE	4.9
45	D0	39	ARG	4.9
25	BC	93	ASP	4.9
25	DC	132	LEU	4.9
32	DK	21	PRO	4.9
34	DP	62	LEU	4.9
9	CJ	51	ARG	4.9
27	DE	157	ALA	4.9
60	BA	50	U	4.9
23	CY	105	ILE	4.9
28	DF	133	ASN	4.9
3	CD	62	GLN	4.9
36	BR	72	ASP	4.9
48	BN	110	GLY	4.9
20	AA	890	G	4.9
25	BC	74	ARG	4.9
43	DY	38	ILE	4.9
48	BN	48	MET	4.9
40	DV	38	LEU	4.9
2	CC	9	GLY	4.9
4	CE	21	ALA	4.9
60	BA	2497	A	4.9
33	DO	82	ASN	4.9
3	AD	159	ARG	4.9
25	DC	165	ARG	4.9
55	B9	2	LYS	4.9
25	BC	193	PHE	4.9
28	BF	181	LEU	4.9
45	B0	75	LEU	4.9
48	DN	120	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
9	CJ	52	GLY	4.9
13	CN	11	LYS	4.9
54	B8	54	GLU	4.9
3	AD	164	ALA	4.9
4	AE	25	ARG	4.8
26	DD	216	GLY	4.8
46	D1	61	ARG	4.8
48	BN	35	ARG	4.8
13	CN	2	ALA	4.8
32	BK	99	ILE	4.8
20	AA	1183	A	4.8
46	B1	24	ALA	4.8
53	D7	30	VAL	4.8
8	AI	125	TYR	4.8
41	BW	29	LEU	4.8
25	BC	102	GLN	4.8
25	DC	170	GLY	4.8
13	CN	41	ARG	4.8
60	BA	1379	A	4.8
37	DS	42	ASP	4.8
37	DS	60	GLY	4.8
3	AD	64	LEU	4.8
27	BE	107	THR	4.8
45	B0	55	ARG	4.8
20	AA	1224	G	4.8
11	CL	18	VAL	4.8
23	CY	162	VAL	4.8
27	BE	130	GLY	4.8
35	BQ	33	GLY	4.8
42	BX	69	TYR	4.8
3	AD	168	ARG	4.8
28	DF	89	VAL	4.8
26	BD	153	ALA	4.8
42	DX	72	LYS	4.8
41	DW	80	PRO	4.8
43	BY	73	ARG	4.8
16	CQ	7	THR	4.8
25	DC	114	VAL	4.8
26	DD	58	HIS	4.8
28	BF	152	GLU	4.8
38	DT	2	ASN	4.8
32	DK	27	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
45	D0	17	GLN	4.8
35	DQ	132	VAL	4.8
2	AC	2	GLY	4.8
23	AY	166	LEU	4.8
29	BG	173	LEU	4.8
53	D7	14	LYS	4.8
20	CA	174	C	4.8
60	BA	780	G	4.8
60	BA	988	A	4.8
60	BA	2590	A	4.8
16	AQ	59	ILE	4.8
44	BZ	162	GLU	4.8
1	CB	135	GLN	4.8
15	AP	1	MET	4.8
25	DC	15	VAL	4.8
54	B8	16	ILE	4.8
27	DE	162	ALA	4.8
36	BR	79	LEU	4.8
39	BU	99	ALA	4.8
46	D1	26	ARG	4.8
29	BG	141	PHE	4.8
25	BC	100	ILE	4.8
37	DS	73	LEU	4.8
48	BN	114	ARG	4.8
3	AD	68	TYR	4.8
14	CO	4	THR	4.8
19	CT	30	LYS	4.8
45	D0	31	VAL	4.8
40	DV	70	ILE	4.8
8	AI	43	ALA	4.8
13	CN	46	GLU	4.8
20	CA	1383	C	4.8
20	CA	1403	C	4.8
34	DP	5	ASP	4.8
42	BX	17	ALA	4.8
60	DA	2334	G	4.8
23	CY	378	VAL	4.8
34	BP	42	SER	4.8
35	DQ	77	LYS	4.8
37	BS	85	VAL	4.8
23	CY	396	ARG	4.8
37	DS	48	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
44	BZ	102	LEU	4.8
1	AB	189	ASP	4.8
6	AG	46	ALA	4.8
29	BG	158	ALA	4.8
2	CC	26	LYS	4.8
27	DE	156	MET	4.8
35	DQ	104	PHE	4.8
45	B0	71	ASP	4.8
3	AD	146	ILE	4.8
13	AN	52	GLN	4.8
60	DA	2612	C	4.8
19	CT	13	LEU	4.8
25	DC	81	GLY	4.8
26	DD	233	HIS	4.8
28	BF	156	LEU	4.8
36	DR	20	LEU	4.8
54	B8	38	GLY	4.8
37	BS	74	ALA	4.8
54	D8	55	ALA	4.8
60	BA	2413	G	4.8
2	CC	55	VAL	4.8
4	AE	13	ILE	4.7
29	DG	41	GLN	4.7
54	D8	50	LEU	4.7
13	CN	34	TYR	4.7
33	DO	11	ALA	4.7
44	BZ	164	ALA	4.7
44	DZ	88	PHE	4.7
51	D5	47	PRO	4.7
59	BB	6	C	4.7
11	CL	85	ILE	4.7
39	DU	27	LEU	4.7
20	AA	29	G	4.7
23	AY	259	PHE	4.7
60	DA	2319	G	4.7
27	DE	9	VAL	4.7
48	DN	86	PRO	4.7
28	BF	28	ILE	4.7
3	CD	137	SER	4.7
19	CT	65	LYS	4.7
25	DC	163	GLU	4.7
34	DP	22	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
7	AH	118	VAL	4.7
46	D1	24	ALA	4.7
60	DA	336	C	4.7
42	BX	32	PRO	4.7
2	CC	2	GLY	4.7
15	CP	58	TYR	4.7
25	DC	73	VAL	4.7
32	DK	8	VAL	4.7
25	BC	150	ILE	4.7
48	DN	118	LYS	4.7
60	BA	1301	A	4.7
3	AD	122	ARG	4.7
37	BS	25	ARG	4.7
25	DC	69	LEU	4.7
48	BN	108	PRO	4.7
8	AI	72	GLY	4.7
36	BR	80	PHE	4.7
60	BA	1626	G	4.7
25	BC	44	VAL	4.7
41	BW	7	ALA	4.7
1	AB	194	PRO	4.7
53	B7	42	LEU	4.7
43	DY	89	PHE	4.7
25	BC	203	GLU	4.7
30	BH	167	GLU	4.7
15	AP	71	ARG	4.7
23	CY	363	ARG	4.7
29	DG	138	GLN	4.7
41	DW	92	ARG	4.7
8	AI	69	GLY	4.7
52	D6	52	VAL	4.7
3	AD	165	MET	4.7
60	BA	691	C	4.7
16	AQ	39	SER	4.7
28	BF	172	TRP	4.7
8	AI	109	VAL	4.7
8	CI	30	GLY	4.7
9	CJ	46	ARG	4.7
45	B0	77	ARG	4.7
3	CD	165	MET	4.7
18	AS	56	GLN	4.7
28	BF	123	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
32	DK	111	LYS	4.7
34	BP	110	TYR	4.7
39	DU	20	LEU	4.7
50	D3	46	ASN	4.7
3	AD	107	ARG	4.7
43	DY	32	PRO	4.7
48	DN	119	ARG	4.7
52	D6	23	THR	4.7
35	DQ	95	ALA	4.7
40	DV	78	LYS	4.7
3	AD	62	GLN	4.7
50	D3	13	ILE	4.7
3	AD	105	VAL	4.7
8	CI	104	ARG	4.7
9	CJ	73	ASP	4.7
27	BE	60	ASN	4.7
23	CY	383	THR	4.7
36	BR	65	LEU	4.7
39	DU	106	PHE	4.7
60	BA	1216	G	4.7
60	BA	2585	U	4.7
20	AA	883	C	4.7
50	B3	6	VAL	4.7
4	AE	81	GLU	4.7
8	CI	34	ASN	4.7
23	CY	145	ASP	4.7
32	DK	114	ASP	4.7
43	BY	64	GLU	4.7
2	CC	188	LEU	4.7
9	CJ	41	PRO	4.7
39	DU	68	ALA	4.7
20	CA	201	C	4.7
60	BA	221	A	4.7
38	DT	64	ARG	4.7
43	DY	9	LYS	4.7
27	DE	73	GLU	4.7
2	AC	8	ILE	4.7
25	DC	166	ASN	4.7
27	BE	26	ILE	4.7
29	DG	141	PHE	4.7
4	AE	20	GLN	4.6
45	D0	10	THR	4.6

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Mol	Chain	Res	Type	RSRZ
8	CI	2	GLU	4.6
27	DE	138	PRO	4.6
43	BY	61	ILE	4.6
11	AL	67	THR	4.6
29	DG	64	THR	4.6
3	CD	11	LEU	4.6
15	AP	60	LEU	4.6
43	DY	44	ILE	4.6
41	BW	37	ARG	4.6
2	AC	196	LEU	4.6
26	BD	57	GLY	4.6
26	DD	37	LEU	4.6
40	DV	94	LEU	4.6
60	BA	1302	A	4.6
2	AC	4	LYS	4.6
11	CL	12	ARG	4.6
40	DV	19	LYS	4.6
48	BN	122	VAL	4.6
3	AD	138	TYR	4.6
26	DD	64	ILE	4.6
29	BG	167	GLU	4.6
27	BE	58	ARG	4.6
20	AA	967	C	4.6
60	DA	283	A	4.6
2	CC	43	LEU	4.6
18	AS	34	TRP	4.6
4	AE	28	PHE	4.6
20	CA	46	G	4.6
40	DV	53	GLU	4.6
52	D6	26	ASN	4.6
60	DA	2576	G	4.6
12	CM	99	ARG	4.6
18	CS	41	VAL	4.6
19	CT	17	ARG	4.6
42	BX	30	VAL	4.6
35	BQ	115	MET	4.6
23	CY	167	PRO	4.6
28	DF	171	PRO	4.6
35	DQ	34	LEU	4.6
26	BD	181	GLU	4.6
26	BD	270	ILE	4.6
28	BF	83	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
28	DF	150	GLY	4.6
29	DG	178	PHE	4.6
37	BS	104	GLY	4.6
27	BE	157	ALA	4.6
28	DF	93	LYS	4.6
37	DS	20	ARG	4.6
41	BW	38	TYR	4.6
53	D7	21	ARG	4.6
54	D8	3	LYS	4.6
60	BA	424	G	4.6
60	DA	2578	G	4.6
6	CG	41	ARG	4.6
27	BE	73	GLU	4.6
26	DD	16	MET	4.6
18	CS	16	LEU	4.6
18	CS	36	ARG	4.6
18	CS	82	GLY	4.6
27	DE	164	ARG	4.6
28	DF	57	VAL	4.6
42	DX	30	VAL	4.6
52	D6	51	GLU	4.6
18	AS	48	THR	4.6
28	DF	101	LEU	4.6
3	CD	111	ALA	4.6
27	BE	31	CYS	4.6
29	DG	173	LEU	4.6
20	AA	1359	C	4.6
26	DD	6	PHE	4.6
28	DF	108	LYS	4.6
44	BZ	88	PHE	4.6
25	DC	32	GLU	4.6
27	BE	205	ALA	4.6
28	BF	110	LEU	4.6
38	DT	114	LEU	4.6
52	B6	34	LEU	4.6
23	CY	259	PHE	4.6
27	DE	113	PHE	4.6
3	CD	125	HIS	4.6
39	DU	19	LYS	4.6
9	CJ	39	PRO	4.6
27	BE	189	PRO	4.6
26	BD	9	TYR	4.6

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Mol	Chain	Res	Type	RSRZ
33	DO	83	ALA	4.6
2	AC	188	LEU	4.6
3	CD	58	LEU	4.6
12	CM	121	LYS	4.6
15	CP	79	VAL	4.6
20	AA	353	A	4.6
43	DY	92	ASN	4.6
26	DD	12	SER	4.6
3	AD	134	ASP	4.6
23	CY	355	LEU	4.6
26	BD	241	PRO	4.6
28	DF	181	LEU	4.6
32	BK	10	LEU	4.6
44	DZ	125	LEU	4.6
20	CA	331	G	4.6
60	DA	975	G	4.6
3	CD	99	SER	4.5
33	DO	9	GLU	4.5
25	DC	136	GLY	4.5
42	BX	39	ILE	4.5
48	BN	120	LEU	4.5
39	DU	8	VAL	4.5
60	BA	2059	A	4.5
8	AI	87	GLN	4.5
14	AO	4	THR	4.5
42	BX	27	THR	4.5
43	BY	96	ILE	4.5
18	CS	38	SER	4.5
28	DF	91	GLY	4.5
11	CL	23	LYS	4.5
43	BY	101	LYS	4.5
16	CQ	38	ARG	4.5
18	CS	34	TRP	4.5
37	DS	85	VAL	4.5
42	BX	16	LYS	4.5
8	CI	12	GLU	4.5
9	CJ	59	SER	4.5
20	AA	973	G	4.5
20	CA	376	G	4.5
29	BG	61	ALA	4.5
34	BP	25	SER	4.5
37	BS	19	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
3	AD	209	ARG	4.5
3	CD	153	ARG	4.5
11	CL	56	ALA	4.5
16	CQ	71	PHE	4.5
28	BF	42	ALA	4.5
33	BO	103	ALA	4.5
51	D5	24	ALA	4.5
60	BA	2232	U	4.5
9	AJ	57	LYS	4.5
54	B8	2	PRO	4.5
60	DA	820	A	4.5
25	DC	95	VAL	4.5
35	BQ	132	VAL	4.5
36	BR	66	VAL	4.5
39	BU	5	LYS	4.5
60	DA	2609	U	4.5
29	DG	176	LEU	4.5
41	DW	37	ARG	4.5
1	CB	73	THR	4.5
54	D8	49	VAL	4.5
13	CN	7	ILE	4.5
3	AD	135	LEU	4.5
29	BG	106	LEU	4.5
33	BO	110	GLY	4.5
34	BP	28	GLY	4.5
41	DW	14	PRO	4.5
52	D6	31	PRO	4.5
20	AA	68(A)	G	4.5
46	B1	6	GLU	4.5
26	DD	39	LYS	4.5
36	BR	14	SER	4.5
23	AY	355	LEU	4.5
35	BQ	119	ARG	4.5
2	AC	130	VAL	4.5
3	AD	128	VAL	4.5
28	DF	154	VAL	4.5
39	DU	69	CYS	4.5
42	DX	77	LYS	4.5
25	DC	109	MET	4.5
60	BA	587	C	4.5
60	DA	1625	C	4.5
2	AC	12	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
39	DU	59	ARG	4.5
60	BA	518	G	4.5
60	BA	2035	G	4.5
37	DS	66	ALA	4.5
38	BT	109	GLU	4.5
3	CD	139	ARG	4.5
8	AI	104	ARG	4.5
9	CJ	8	LEU	4.5
18	CS	30	LEU	4.5
27	DE	168	MET	4.5
34	DP	106	LEU	4.5
51	B5	55	ARG	4.5
27	BE	3	GLY	4.5
54	B8	3	LYS	4.5
2	AC	3	ASN	4.5
27	DE	197	ILE	4.5
20	CA	820	U	4.5
33	DO	12	ASP	4.5
37	DS	65	VAL	4.5
45	B0	49	LYS	4.5
54	D8	39	LYS	4.5
13	AN	10	ALA	4.5
26	BD	143	HIS	4.5
27	DE	142	GLY	4.5
33	DO	35	VAL	4.5
35	DQ	90	VAL	4.5
43	DY	42	VAL	4.5
20	AA	323	U	4.5
34	DP	78	PRO	4.5
41	DW	15	ARG	4.5
4	CE	10	MET	4.5
43	DY	5	MET	4.5
44	BZ	98	MET	4.5
28	DF	73	ALA	4.4
6	AG	26	PHE	4.4
28	BF	81	PRO	4.4
33	DO	81	ASP	4.4
42	BX	13	LEU	4.4
48	BN	82	LEU	4.4
20	AA	173	U	4.4
42	BX	20	GLY	4.4
27	BE	132	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
34	BP	35	HIS	4.4
30	BH	148	ILE	4.4
41	BW	42	ARG	4.4
60	DA	1938	A	4.4
43	DY	66	PRO	4.4
60	DA	2108	C	4.4
36	BR	36	THR	4.4
34	BP	66	GLY	4.4
43	DY	37	VAL	4.4
37	BS	94	TYR	4.4
3	CD	61	LYS	4.4
14	CO	32	LEU	4.4
15	CP	74	LEU	4.4
17	AR	66	LEU	4.4
20	CA	375	U	4.4
41	BW	51	LEU	4.4
44	DZ	90	VAL	4.4
39	DU	13	LYS	4.4
41	BW	103	ILE	4.4
60	BA	426	C	4.4
10	AK	123	LYS	4.4
42	DX	21	PHE	4.4
9	AJ	66	ARG	4.4
41	DW	33	ARG	4.4
2	CC	189	ALA	4.4
8	AI	61	ALA	4.4
28	BF	64	ILE	4.4
35	DQ	139	GLU	4.4
55	B9	31	LYS	4.4
42	BX	81	VAL	4.4
1	AB	210	SER	4.4
13	AN	23	ARG	4.4
20	AA	178	C	4.4
43	DY	103	GLY	4.4
60	BA	834	C	4.4
25	DC	12	LEU	4.4
25	DC	92	ALA	4.4
27	DE	28	ALA	4.4
42	BX	89	ILE	4.4
43	BY	33	LYS	4.4
2	CC	164	ARG	4.4
25	DC	4	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
42	BX	55	ASN	4.4
18	CS	10	PHE	4.4
19	AT	66	ALA	4.4
25	BC	164	PHE	4.4
35	BQ	34	LEU	4.4
41	DW	36	LEU	4.4
60	BA	266	G	4.4
20	CA	176	C	4.4
23	AY	107	VAL	4.4
28	BF	85	GLY	4.4
36	BR	11	ASN	4.4
25	BC	153	ILE	4.4
35	BQ	118	LEU	4.4
36	DR	100	LEU	4.4
43	DY	34	LYS	4.4
43	DY	86	ARG	4.4
8	AI	30	GLY	4.4
16	CQ	41	LYS	4.4
3	AD	97	LEU	4.4
28	DF	202	PHE	4.4
13	AN	59	ALA	4.4
23	CY	364	GLU	4.4
50	D3	43	ILE	4.4
45	D0	65	GLY	4.4
18	CS	35	SER	4.4
30	DH	155	SER	4.4
48	DN	109	LYS	4.4
8	CI	80	GLY	4.4
14	CO	3	ILE	4.4
33	DO	99	PHE	4.4
41	BW	81	ALA	4.4
28	BF	54	ARG	4.4
33	DO	3	GLN	4.4
50	B3	19	GLN	4.4
43	BY	88	LYS	4.4
44	DZ	123	ASP	4.4
54	D8	27	THR	4.4
1	CB	31	TYR	4.4
16	CQ	29	HIS	4.4
43	DY	79	CYS	4.4
4	CE	91	LEU	4.4
23	AY	335	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
23	CY	16	GLY	4.4
39	DU	88	ILE	4.4
12	AM	102	ARG	4.4
15	AP	56	ALA	4.4
44	DZ	97	GLU	4.4
48	BN	52	VAL	4.4
42	BX	74	PRO	4.4
13	CN	55	GLY	4.4
16	AQ	99	SER	4.4
8	CI	125	TYR	4.4
27	BE	134	ILE	4.4
34	BP	69	GLY	4.4
60	BA	2020	A	4.4
41	DW	99	ARG	4.4
46	B1	27	GLU	4.4
48	BN	96	GLU	4.4
53	B7	32	LYS	4.4
12	AM	19	LEU	4.4
60	DA	831	G	4.4
60	DA	2894	G	4.4
3	CD	114	ARG	4.3
3	CD	140	VAL	4.3
8	AI	128	ARG	4.3
12	AM	87	TYR	4.3
26	BD	213	ARG	4.3
27	DE	119	ARG	4.3
44	BZ	74	VAL	4.3
17	AR	69	THR	4.3
43	BY	65	ALA	4.3
45	D0	85	ALA	4.3
4	CE	20	GLN	4.3
12	CM	101	GLN	4.3
34	BP	105	LEU	4.3
3	AD	4	TYR	4.3
7	AH	30	ARG	4.3
28	DF	54	ARG	4.3
3	CD	161	ASN	4.3
60	BA	2573	C	4.3
20	AA	971	G	4.3
2	CC	5	ILE	4.3
25	DC	204	GLY	4.3
26	BD	64	ILE	4.3

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Mol	Chain	Res	Type	RSRZ
30	BH	169	VAL	4.3
43	DY	104	GLY	4.3
27	BE	151	TYR	4.3
54	B8	49	VAL	4.3
34	DP	74	GLU	4.3
48	DN	99	LEU	4.3
26	DD	239	ARG	4.3
36	BR	63	ARG	4.3
54	B8	12	LYS	4.3
54	D8	26	LYS	4.3
60	BA	1252	G	4.3
60	DA	75	G	4.3
4	AE	106	PRO	4.3
4	CE	128	PRO	4.3
44	BZ	73	GLN	4.3
34	BP	106	LEU	4.3
8	AI	14	VAL	4.3
8	AI	113	LYS	4.3
20	AA	221	C	4.3
51	D5	19	ARG	4.3
53	D7	45	ALA	4.3
20	CA	570	G	4.3
39	DU	109	LEU	4.3
1	AB	204	ASN	4.3
29	BG	179	PRO	4.3
29	DG	66	GLN	4.3
48	DN	45	ASN	4.3
12	AM	30	ALA	4.3
25	DC	77	ALA	4.3
25	DC	86	GLU	4.3
4	AE	12	LEU	4.3
8	AI	65	VAL	4.3
36	BR	12	ARG	4.3
41	DW	95	ILE	4.3
43	BY	49	VAL	4.3
21	CV	11	U	4.3
26	BD	249	PRO	4.3
12	CM	56	LEU	4.3
44	DZ	150	LEU	4.3
54	B8	52	LYS	4.3
60	BA	830	G	4.3
54	B8	7	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
60	BA	390	A	4.3
60	DA	196	A	4.3
37	BS	96	GLY	4.3
45	B0	54	GLY	4.3
17	AR	63	GLN	4.3
20	CA	150	C	4.3
56	Be	51	ALA	4.3
60	DA	857	C	4.3
36	BR	20	LEU	4.3
50	D3	53	LEU	4.3
3	CD	65	ARG	4.3
13	AN	31	ARG	4.3
20	CA	45	U	4.3
53	D7	22	MET	4.3
33	DO	101	PRO	4.3
35	BQ	20	ALA	4.3
47	D4	12	ALA	4.3
36	DR	48	VAL	4.3
43	DY	102	CYS	4.3
60	BA	1305	C	4.3
1	AB	207	ALA	4.3
33	BO	109	LYS	4.3
35	DQ	121	ALA	4.3
48	DN	111	PRO	4.3
43	DY	4	LYS	4.3
59	BB	29	A	4.3
3	AD	98	GLU	4.3
14	CO	19	PRO	4.3
26	BD	156	ALA	4.3
33	BO	85	VAL	4.3
36	BR	102	GLU	4.3
60	DA	1824	G	4.3
27	DE	91	VAL	4.3
3	CD	158	ILE	4.3
20	AA	177	C	4.3
27	BE	146	THR	4.3
44	BZ	99	TYR	4.3
48	DN	87	LEU	4.3
26	DD	8	PRO	4.3
34	DP	72	PRO	4.3
3	CD	108	LEU	4.3
25	DC	145	THR	4.3

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Mol	Chain	Res	Type	RSRZ
60	BA	748	G	4.3
3	AD	148	VAL	4.3
20	CA	1195	C	4.3
60	DA	974(B)	C	4.3
30	BH	162	ILE	4.3
28	DF	103	LYS	4.3
11	AL	42	THR	4.2
29	BG	13	GLU	4.2
43	DY	100	ALA	4.2
45	D0	38	VAL	4.2
23	AY	349	LYS	4.2
3	AD	124	GLY	4.2
60	DA	335	C	4.2
51	D5	14	ALA	4.2
25	DC	162	ILE	4.2
3	AD	182	LYS	4.2
28	DF	29	ASN	4.2
16	CQ	32	TYR	4.2
41	DW	85	VAL	4.2
3	CD	79	PHE	4.2
23	AY	336	THR	4.2
20	CA	178	C	4.2
28	BF	202	PHE	4.2
8	AI	107	ARG	4.2
34	DP	109	GLY	4.2
46	B1	12	PRO	4.2
47	B4	1	MET	4.2
48	BN	1	MET	4.2
19	AT	12	ALA	4.2
45	B0	68	GLU	4.2
8	AI	8	GLY	4.2
20	AA	375	U	4.2
21	CV	13	A	4.2
42	DX	3	THR	4.2
46	B1	4	VAL	4.2
6	AG	83	ALA	4.2
20	AA	175	C	4.2
1	AB	187	LEU	4.2
18	CS	81	ARG	4.2
19	CT	10	LEU	4.2
28	BF	185	ASP	4.2
29	BG	32	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
36	BR	47	PHE	4.2
60	DA	1189	A	4.2
2	AC	185	GLY	4.2
3	AD	130	GLY	4.2
26	DD	17	THR	4.2
27	BE	147	PRO	4.2
28	BF	195	ASP	4.2
34	DP	19	VAL	4.2
41	DW	39	THR	4.2
46	B1	33	LYS	4.2
43	BY	40	GLU	4.2
15	CP	60	LEU	4.2
20	AA	926	G	4.2
60	BA	2578	G	4.2
37	DS	96	GLY	4.2
25	BC	158	LYS	4.2
34	BP	87	ASP	4.2
35	DQ	25	ASP	4.2
37	BS	76	LYS	4.2
8	AI	15	ALA	4.2
19	AT	70	SER	4.2
19	CT	63	ILE	4.2
29	BG	14	GLU	4.2
46	B1	58	ILE	4.2
49	B2	71	ASN	4.2
26	BD	216	GLY	4.2
30	DH	114	VAL	4.2
48	DN	1	MET	4.2
60	BA	974(B)	C	4.2
60	BA	976	C	4.2
9	AJ	42	THR	4.2
14	AO	19	PRO	4.2
29	DG	35	GLU	4.2
32	BK	103	GLN	4.2
37	BS	72	ALA	4.2
3	AD	157	LEU	4.2
19	AT	20	LEU	4.2
20	CA	374	A	4.2
28	DF	85	GLY	4.2
34	BP	34	GLY	4.2
60	BA	631	A	4.2
8	CI	107	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
14	AO	28	GLN	4.2
41	BW	92	ARG	4.2
7	CH	2	LEU	4.2
42	BX	58	HIS	4.2
23	AY	41	LYS	4.2
1	CB	202	PRO	4.2
4	AE	50	GLU	4.2
36	DR	63	ARG	4.2
44	BZ	72	ARG	4.2
60	DA	1248	G	4.2
6	AG	45	ASP	4.2
15	CP	68	ASP	4.2
42	BX	33	LYS	4.2
51	D5	22	HIS	4.2
8	AI	45	ALA	4.2
8	AI	3	GLN	4.2
11	AL	10	LEU	4.2
8	CI	78	LYS	4.2
15	CP	41	PRO	4.2
7	AH	29	SER	4.2
32	DK	136	VAL	4.2
33	DO	7	TYR	4.2
35	BQ	131	ILE	4.2
3	CD	78	LEU	4.2
4	AE	135	THR	4.2
20	CA	175	C	4.2
25	DC	154	ILE	4.2
27	BE	141	ILE	4.2
41	DW	24	ILE	4.2
60	BA	2611	U	4.2
60	DA	1305	C	4.2
14	AO	8	LYS	4.2
30	BH	172	LYS	4.2
45	D0	84	LEU	4.2
48	DN	70	LYS	4.2
52	D6	35	GLU	4.2
28	DF	105	VAL	4.2
11	AL	22	SER	4.2
53	B7	22	MET	4.2
60	DA	835	A	4.2
29	BG	7	LEU	4.1
36	BR	51	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
7	AH	101	PRO	4.1
6	CG	115	ARG	4.1
25	DC	193	PHE	4.1
35	DQ	86	GLY	4.1
37	DS	12	PHE	4.1
14	CO	88	ARG	4.1
26	DD	219	PRO	4.1
42	BX	11	PRO	4.1
2	AC	133	ALA	4.1
17	CR	51	LEU	4.1
20	AA	391	G	4.1
20	CA	1343	G	4.1
27	DE	155	LYS	4.1
20	CA	65	U	4.1
52	B6	9	LEU	4.1
12	AM	101	GLN	4.1
54	B8	57	ARG	4.1
9	CJ	98	ILE	4.1
47	B4	7	PRO	4.1
35	BQ	41	TRP	4.1
52	D6	11	LEU	4.1
19	CT	12	ALA	4.1
27	DE	129	HIS	4.1
2	CC	131	ARG	4.1
20	CA	922	G	4.1
35	DQ	131	ILE	4.1
43	DY	96	ILE	4.1
38	BT	51	ARG	4.1
2	CC	184	TYR	4.1
27	DE	161	GLY	4.1
29	BG	11	TYR	4.1
60	DA	532	A	4.1
60	DA	819	A	4.1
25	BC	174	ALA	4.1
26	BD	12	SER	4.1
53	B7	23	ARG	4.1
29	BG	172	LEU	4.1
34	BP	80	TYR	4.1
38	BT	110	ILE	4.1
60	BA	674	G	4.1
2	AC	151	VAL	4.1
34	DP	81	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
52	B6	48	VAL	4.1
14	CO	64	ARG	4.1
20	AA	149	A	4.1
46	B1	43	TYR	4.1
60	BA	126	A	4.1
60	BA	1631	A	4.1
60	DA	1247	A	4.1
9	AJ	72	VAL	4.1
11	AL	112	ASP	4.1
27	DE	188	VAL	4.1
32	BK	23	VAL	4.1
25	DC	31	LYS	4.1
33	BO	105	GLU	4.1
2	AC	29	TYR	4.1
25	DC	61	GLY	4.1
29	DG	172	LEU	4.1
37	DS	58	LEU	4.1
60	DA	673	C	4.1
60	DA	1643	G	4.1
1	CB	96	ARG	4.1
13	AN	22	THR	4.1
34	BP	55	ARG	4.1
51	D5	29	THR	4.1
8	CI	46	ALA	4.1
27	BE	138	PRO	4.1
27	DE	133	LYS	4.1
52	D6	10	LEU	4.1
37	DS	83	LYS	4.1
60	DA	2575	C	4.1
60	DA	379	G	4.1
32	DK	104	VAL	4.1
12	CM	11	ARG	4.1
44	DZ	89	PHE	4.1
60	BA	764	A	4.1
4	AE	51	VAL	4.1
14	AO	29	VAL	4.1
15	AP	58	TYR	4.1
25	BC	129	GLY	4.1
19	CT	58	LYS	4.1
26	DD	217	ARG	4.1
11	AL	56	ALA	4.1
26	DD	269	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
36	BR	9	LYS	4.1
42	DX	16	LYS	4.1
48	BN	99	LEU	4.1
20	CA	51	A	4.1
43	DY	35	TYR	4.1
3	AD	60	GLU	4.1
32	DK	108	ALA	4.1
18	AS	60	VAL	4.1
19	AT	62	LEU	4.1
9	CJ	100	THR	4.1
33	DO	85	VAL	4.1
53	B7	25	PRO	4.1
20	CA	67	C	4.1
28	DF	191	ARG	4.1
1	CB	152	PHE	4.1
20	AA	384	G	4.1
3	CD	157	LEU	4.1
18	AS	9	VAL	4.1
25	BC	4	HIS	4.1
45	D0	67	VAL	4.1
26	BD	190	TYR	4.1
4	CE	17	ALA	4.0
45	B0	62	LEU	4.0
56	De	94	GLU	4.0
7	AH	35	ILE	4.0
23	CY	106	VAL	4.0
26	BD	265	PRO	4.0
28	DF	52	LYS	4.0
48	DN	104	LYS	4.0
52	D6	7	ILE	4.0
60	BA	271(B)	C	4.0
60	DA	825	C	4.0
60	DA	834	C	4.0
60	DA	1640	C	4.0
36	DR	2	ARG	4.0
48	DN	108	PRO	4.0
48	DN	123	TYR	4.0
20	AA	325	A	4.0
60	DA	944	G	4.0
60	DA	2062	A	4.0
2	CC	153	VAL	4.0
25	BC	47	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
27	DE	167	VAL	4.0
40	DV	86	GLY	4.0
35	DQ	75	THR	4.0
36	BR	70	LEU	4.0
60	BA	1304	C	4.0
3	AD	76	ARG	4.0
3	CD	46	LYS	4.0
11	AL	43	VAL	4.0
36	DR	21	TYR	4.0
39	BU	106	PHE	4.0
43	BY	104	GLY	4.0
6	AG	79	ARG	4.0
8	AI	64	THR	4.0
12	CM	2	ALA	4.0
15	AP	73	LEU	4.0
35	DQ	16	ARG	4.0
26	DD	212	SER	4.0
60	BA	420	C	4.0
6	CG	40	ALA	4.0
16	AQ	77	VAL	4.0
40	DV	15	GLU	4.0
53	B7	45	ALA	4.0
47	B4	24	THR	4.0
21	AV	8	A	4.0
26	DD	57	GLY	4.0
3	AD	71	SER	4.0
3	CD	197	PRO	4.0
20	AA	376	G	4.0
35	BQ	32	TYR	4.0
14	CO	35	ARG	4.0
48	DN	94	HIS	4.0
45	D0	22	GLY	4.0
9	CJ	44	VAL	4.0
9	CJ	99	LYS	4.0
50	B3	54	VAL	4.0
54	B8	44	LYS	4.0
6	AG	100	ALA	4.0
35	DQ	120	ILE	4.0
36	BR	43	GLU	4.0
51	D5	2	ALA	4.0
20	AA	1398	A	4.0
20	CA	383	A	4.0

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Mol	Chain	Res	Type	RSRZ
60	BA	1847	A	4.0
60	BA	2812	G	4.0
60	DA	2780	G	4.0
27	DE	181	LEU	4.0
39	BU	65	ILE	4.0
60	BA	1983	C	4.0
34	BP	107	LYS	4.0
34	DP	80	TYR	4.0
3	AD	118	ARG	4.0
3	CD	120	LEU	4.0
37	DS	106	ARG	4.0
3	CD	204	ILE	4.0
4	CE	122	GLU	4.0
19	CT	61	SER	4.0
23	AY	392	GLU	4.0
28	BF	10	PRO	4.0
28	BF	27	GLU	4.0
27	BE	6	GLY	4.0
16	CQ	6	LEU	4.0
42	BX	52	VAL	4.0
1	CB	77	ALA	4.0
46	B1	23	LYS	4.0
1	CB	137	ARG	4.0
18	AS	30	LEU	4.0
19	AT	53	LEU	4.0
23	CY	107	VAL	4.0
25	DC	161	ARG	4.0
33	DO	63	VAL	4.0
35	DQ	17	LEU	4.0
35	DQ	115	MET	4.0
19	CT	70	SER	4.0
28	DF	153	SER	4.0
19	CT	84	LEU	4.0
45	B0	7	LEU	4.0
29	DG	39	ILE	4.0
16	CQ	33	GLY	4.0
34	DP	66	GLY	4.0
7	AH	33	GLU	4.0
23	CY	18	ALA	4.0
43	DY	29	GLU	4.0
20	AA	1117	G	4.0
20	CA	384	G	4.0

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Mol	Chain	Res	Type	RSRZ
54	D8	52	LYS	4.0
14	CO	21	ASP	4.0
19	AT	23	ARG	4.0
20	AA	1402	C	4.0
27	DE	125	GLY	4.0
29	DG	107	LEU	4.0
33	BO	121	VAL	4.0
50	B3	11	SER	4.0
1	AB	28	PHE	4.0
2	CC	198	VAL	4.0
8	CI	79	LEU	4.0
9	AJ	67	THR	4.0
12	CM	88	ARG	4.0
29	BG	25	TYR	4.0
8	AI	63	ILE	4.0
32	DK	26	ALA	4.0
8	AI	42	ARG	3.9
37	DS	15	ARG	3.9
60	DA	533	G	3.9
42	DX	57	LEU	3.9
6	CG	24	THR	3.9
7	CH	25	ASP	3.9
20	CA	329	A	3.9
60	DA	270(A)	A	3.9
60	DA	311	A	3.9
37	BS	66	ALA	3.9
16	CQ	53	LEU	3.9
52	D6	33	LYS	3.9
60	BA	2081	C	3.9
23	CY	365	GLU	3.9
50	D3	8	LEU	3.9
54	D8	57	ARG	3.9
20	AA	1286	A	3.9
28	BF	67	GLN	3.9
35	BQ	81	VAL	3.9
15	CP	66	PRO	3.9
44	DZ	44	PHE	3.9
42	DX	35	THR	3.9
39	BU	91	ASP	3.9
18	CS	11	VAL	3.9
26	BD	193	VAL	3.9
29	BG	60	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
46	D1	62	VAL	3.9
20	AA	554	C	3.9
20	CA	43	C	3.9
25	DC	177	GLY	3.9
12	AM	88	ARG	3.9
11	AL	96	VAL	3.9
13	AN	60	SER	3.9
40	DV	5	VAL	3.9
37	DS	84	GLN	3.9
48	DN	83	LYS	3.9
3	AD	65	ARG	3.9
20	AA	884	U	3.9
52	B6	50	ARG	3.9
35	BQ	97	VAL	3.9
37	DS	21	THR	3.9
48	DN	33	LEU	3.9
25	DC	107	GLY	3.9
40	BV	41	GLY	3.9
1	CB	190	THR	3.9
16	CQ	27	PHE	3.9
20	AA	1351	U	3.9
27	DE	193	GLY	3.9
28	DF	61	GLY	3.9
43	BY	17	SER	3.9
11	AL	19	ARG	3.9
34	BP	81	GLN	3.9
32	DK	137	GLU	3.9
35	BQ	107	ALA	3.9
13	AN	50	LYS	3.9
40	DV	36	PRO	3.9
48	BN	107	LEU	3.9
1	CB	148	TYR	3.9
2	CC	29	TYR	3.9
36	DR	36	THR	3.9
60	BA	311	A	3.9
4	CE	118	ILE	3.9
9	CJ	43	ARG	3.9
20	CA	823	G	3.9
27	DE	8	LYS	3.9
29	BG	8	LYS	3.9
60	BA	1300	U	3.9
35	BQ	78	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
36	DR	115	GLU	3.9
20	CA	1066	C	3.9
46	B1	11	ARG	3.9
11	AL	28	LYS	3.9
26	BD	275	LYS	3.9
37	DS	69	VAL	3.9
10	AK	125	PHE	3.9
11	CL	127	GLU	3.9
51	D5	18	ALA	3.9
14	CO	2	PRO	3.9
35	BQ	73	PRO	3.9
45	B0	20	ARG	3.9
25	BC	141	PRO	3.9
13	AN	42	ILE	3.9
13	CN	26	ARG	3.9
26	BD	238	GLY	3.9
60	DA	574	C	3.9
40	BV	70	ILE	3.9
16	CQ	34	LYS	3.9
4	CE	16	THR	3.9
13	CN	8	GLU	3.9
28	DF	58	ALA	3.9
60	BA	2610	C	3.9
2	CC	4	LYS	3.9
27	DE	160	TYR	3.9
38	BT	25	GLY	3.9
48	BN	36	GLY	3.9
25	BC	69	LEU	3.9
29	DG	34	LEU	3.9
60	BA	2406	U	3.9
19	CT	60	GLU	3.9
3	AD	61	LYS	3.9
7	AH	100	ILE	3.9
20	AA	966	G	3.9
28	DF	82	ILE	3.9
28	DF	100	THR	3.9
16	CQ	8	GLY	3.9
26	BD	33	LEU	3.9
28	BF	114	VAL	3.9
2	AC	189	ALA	3.9
20	AA	197	A	3.8
20	CA	49	U	3.8

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Mol	Chain	Res	Type	RSRZ
2	CC	41	GLY	3.8
18	CS	77	THR	3.8
26	DD	173	VAL	3.8
19	AT	67	ALA	3.8
4	AE	11	ILE	3.8
60	BA	1620	G	3.8
3	AD	120	LEU	3.8
4	CE	84	PHE	3.8
18	AS	42	PRO	3.8
29	DG	166	ASP	3.8
27	BE	136	ARG	3.8
41	BW	32	ALA	3.8
35	DQ	125	LEU	3.8
36	BR	113	LEU	3.8
43	BY	106	LEU	3.8
32	BK	37	PHE	3.8
28	BF	23	ASP	3.8
48	DN	41	ASP	3.8
22	AW	75	C	3.8
60	BA	2498	C	3.8
60	DA	271(A)	U	3.8
60	DA	1630	G	3.8
3	CD	6	GLY	3.8
13	AN	51	GLY	3.8
38	DT	99	LEU	3.8
42	BX	5	TYR	3.8
20	AA	1252	A	3.8
6	AG	115	ARG	3.8
13	CN	9	LYS	3.8
15	CP	42	ARG	3.8
27	BE	105	THR	3.8
3	CD	104	VAL	3.8
19	AT	63	ILE	3.8
25	BC	151	GLY	3.8
28	DF	84	VAL	3.8
6	AG	47	CYS	3.8
27	DE	15	PHE	3.8
44	DZ	166	SER	3.8
20	CA	1325	C	3.8
48	BN	95	PRO	3.8
60	DA	1774	C	3.8
1	CB	134	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
49	B2	22	GLU	3.8
7	AH	59	LEU	3.8
18	AS	11	VAL	3.8
20	AA	32	A	3.8
25	BC	204	GLY	3.8
40	DV	37	VAL	3.8
41	DW	50	VAL	3.8
1	AB	101	MET	3.8
8	AI	120	ARG	3.8
13	CN	35	ARG	3.8
36	BR	2	ARG	3.8
45	B0	50	ASN	3.8
55	D9	31	LYS	3.8
52	D6	22	ALA	3.8
7	AH	26	VAL	3.8
48	BN	32	THR	3.8
3	CD	95	GLY	3.8
35	BQ	15	GLY	3.8
20	CA	1395	C	3.8
38	DT	115	ARG	3.8
39	DU	58	ARG	3.8
42	BX	60	ARG	3.8
43	BY	84	ARG	3.8
60	BA	1248	G	3.8
60	BA	2405	G	3.8
1	AB	185	ILE	3.8
8	CI	35	GLU	3.8
21	CV	12	A	3.8
33	BO	38	VAL	3.8
33	DO	61	VAL	3.8
7	CH	3	THR	3.8
3	AD	66	ARG	3.8
26	DD	104	TYR	3.8
44	DZ	72	ARG	3.8
53	D7	16	HIS	3.8
60	DA	200	U	3.8
60	DA	384	U	3.8
60	DA	1188	U	3.8
7	CH	26	VAL	3.8
25	BC	202	PRO	3.8
26	BD	37	LEU	3.8
28	BF	84	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
43	DY	13	VAL	3.8
44	DZ	126	VAL	3.8
8	AI	20	ARG	3.8
8	AI	112	LYS	3.8
20	AA	290	C	3.8
42	BX	61	GLY	3.8
8	AI	60	ASP	3.8
21	AV	10	G	3.8
21	CV	9	G	3.8
28	BF	96	ASP	3.8
45	D0	64	ASP	3.8
4	AE	122	GLU	3.8
29	BG	54	GLU	3.8
42	BX	51	VAL	3.8
4	AE	88	LYS	3.8
54	B8	48	PHE	3.8
60	BA	243	U	3.8
4	AE	120	THR	3.8
30	DH	169	VAL	3.8
32	BK	114	ASP	3.8
36	DR	113	LEU	3.8
9	CJ	5	ARG	3.8
26	DD	13	ARG	3.8
45	D0	82	ARG	3.8
21	AV	12	A	3.8
60	BA	2711	A	3.8
20	AA	46	G	3.8
13	CN	56	VAL	3.8
38	BT	99	LEU	3.8
41	BW	74	ALA	3.8
42	DX	52	VAL	3.8
60	BA	943	U	3.8
60	DA	2406	U	3.8
37	BS	43	GLU	3.8
4	AE	49	PRO	3.8
35	BQ	30	GLY	3.8
2	CC	8	ILE	3.8
26	DD	145	VAL	3.8
6	AG	74	GLU	3.8
26	DD	211	ARG	3.8
20	CA	114	U	3.8
20	CA	1253	G	3.8

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Mol	Chain	Res	Type	RSRZ
60	BA	224	G	3.8
37	DS	105	ALA	3.8
52	B6	47	THR	3.8
4	CE	23	GLY	3.8
6	AG	33	ASP	3.8
26	DD	265	PRO	3.8
19	CT	14	LYS	3.8
25	BC	180	SER	3.8
12	CM	9	ILE	3.8
26	DD	103	ARG	3.8
28	DF	27	GLU	3.8
34	DP	30	THR	3.7
20	AA	1353	G	3.7
20	CA	305	G	3.7
60	BA	352	G	3.7
60	DA	1628	G	3.7
4	CE	110	LEU	3.7
29	BG	3	LEU	3.7
40	BV	14	VAL	3.7
53	D7	35	ARG	3.7
29	DG	11	TYR	3.7
39	BU	76	TYR	3.7
20	CA	1240	U	3.7
60	BA	945	A	3.7
3	AD	153	ARG	3.7
30	BH	168	PRO	3.7
39	DU	3	ARG	3.7
44	DZ	102	LEU	3.7
50	B3	26	LEU	3.7
53	D7	23	ARG	3.7
3	AD	175	SER	3.7
1	CB	170	GLU	3.7
3	AD	106	TYR	3.7
23	CY	379	GLY	3.7
43	DY	25	GLY	3.7
13	AN	58	LYS	3.7
26	DD	5	LYS	3.7
29	BG	36	LYS	3.7
8	AI	9	ARG	3.7
30	BH	113	VAL	3.7
8	CI	81	ILE	3.7
27	BE	96	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
30	DH	162	ILE	3.7
36	BR	53	HIS	3.7
41	DW	102	HIS	3.7
19	CT	19	SER	3.7
20	AA	1367	C	3.7
20	CA	1362	C	3.7
60	DA	409	C	3.7
20	AA	101	A	3.7
20	CA	353	A	3.7
60	DA	2249	U	3.7
28	BF	86	GLY	3.7
39	DU	110	VAL	3.7
3	CD	5	ILE	3.7
20	AA	309	G	3.7
20	AA	399	G	3.7
60	BA	2633	G	3.7
3	AD	176	LEU	3.7
3	AD	199	ASN	3.7
60	BA	1008	C	3.7
60	DA	1656	C	3.7
36	DR	55	ALA	3.7
25	BC	31	LYS	3.7
52	D6	53	LYS	3.7
25	BC	12	LEU	3.7
25	BC	73	VAL	3.7
26	BD	176	ARG	3.7
26	DD	273	ARG	3.7
50	B3	43	ILE	3.7
42	DX	53	LYS	3.7
50	D3	24	LYS	3.7
51	B5	22	HIS	3.7
20	CA	967	C	3.7
60	BA	1218	C	3.7
26	BD	163	ALA	3.7
16	AQ	78	GLU	3.7
37	BS	44	LYS	3.7
50	B3	10	LYS	3.7
51	B5	10	LYS	3.7
29	BG	159	VAL	3.7
50	D3	4	LEU	3.7
38	DT	50	ILE	3.7
48	BN	118	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
60	BA	2252	G	3.7
11	AL	15	ARG	3.7
11	CL	66	VAL	3.7
34	DP	52	GLU	3.7
43	BY	29	GLU	3.7
36	BR	13	HIS	3.7
36	DR	95	THR	3.7
45	D0	23	VAL	3.7
50	B3	27	GLY	3.7
16	CQ	83	ASP	3.7
41	BW	101	SER	3.7
26	BD	224	ALA	3.7
7	CH	58	TYR	3.7
25	DC	176	VAL	3.7
29	BG	31	VAL	3.7
40	DV	50	PRO	3.7
41	BW	36	LEU	3.7
41	BW	76	VAL	3.7
8	CI	70	LYS	3.7
54	B8	26	LYS	3.7
19	CT	52	ALA	3.7
60	BA	389	G	3.7
19	CT	22	ARG	3.7
20	AA	389	A	3.7
20	CA	974	A	3.7
38	DT	112	ARG	3.7
60	DA	2057	A	3.7
2	CC	197	GLY	3.7
23	CY	538	TYR	3.7
28	BF	100	THR	3.7
32	DK	78	ILE	3.7
42	DX	55	ASN	3.7
20	AA	571	U	3.7
11	AL	12	ARG	3.7
12	CM	110	ARG	3.7
54	B8	51	ALA	3.7
16	CQ	9	VAL	3.7
28	BF	36	VAL	3.7
25	DC	129	GLY	3.7
27	BE	190	GLY	3.7
44	BZ	91	LEU	3.7
48	BN	34	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	AB	208	ILE	3.7
6	AG	42	ILE	3.7
38	DT	113	LYS	3.7
6	CG	12	LEU	3.7
15	AP	61	SER	3.7
43	BY	16	ALA	3.7
29	BG	101	ILE	3.7
60	DA	383	U	3.7
60	DA	2585	U	3.7
32	BK	20	ALA	3.7
37	DS	100	ALA	3.7
15	CP	83	GLU	3.7
28	BF	52	LYS	3.7
60	BA	381	G	3.7
60	DA	382	G	3.7
3	CD	17	VAL	3.7
35	BQ	90	VAL	3.7
2	AC	9	GLY	3.6
19	CT	37	SER	3.6
38	BT	100	TYR	3.6
17	CR	52	PRO	3.6
3	AD	104	VAL	3.6
28	DF	188	ARG	3.6
36	DR	66	VAL	3.6
42	DX	4	ALA	3.6
35	BQ	105	GLU	3.6
60	BA	1938	A	3.6
20	AA	818	G	3.6
20	AA	1064	G	3.6
39	DU	65	ILE	3.6
60	BA	1624	G	3.6
4	AE	18	ARG	3.6
36	DR	57	ARG	3.6
25	BC	143	ALA	3.6
28	BF	187	VAL	3.6
35	BQ	40	ALA	3.6
36	BR	48	VAL	3.6
16	CQ	24	GLU	3.6
6	AG	84	ASN	3.6
38	BT	112	ARG	3.6
46	B1	51	VAL	3.6
60	DA	2690	C	3.6

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Mol	Chain	Res	Type	RSRZ
50	B3	23	LEU	3.6
23	CY	357	ARG	3.6
37	DS	13	ARG	3.6
60	DA	271(C)	G	3.6
3	CD	128	VAL	3.6
25	DC	58	ASN	3.6
27	BE	143	ASN	3.6
45	D0	63	VAL	3.6
8	CI	11	LYS	3.6
25	DC	90	ALA	3.6
29	DG	156	ASP	3.6
30	DH	168	PRO	3.6
3	AD	207	TYR	3.6
20	CA	1326	C	3.6
34	DP	111	ARG	3.6
41	BW	111	HIS	3.6
60	BA	1132	A	3.6
60	DA	562	U	3.6
35	BQ	130	LYS	3.6
39	BU	54	LYS	3.6
15	AP	41	PRO	3.6
25	DC	93	ASP	3.6
4	CE	44	GLY	3.6
34	BP	79	ARG	3.6
43	DY	10	GLY	3.6
56	Be	73	GLU	3.6
8	AI	86	VAL	3.6
13	CN	4	LYS	3.6
15	AP	62	VAL	3.6
25	DC	146	VAL	3.6
26	BD	182	LEU	3.6
28	BF	126	VAL	3.6
29	BG	94	LEU	3.6
44	BZ	116	VAL	3.6
1	CB	141	GLU	3.6
7	AH	27	PRO	3.6
26	BD	250	TRP	3.6
26	DD	9	TYR	3.6
29	DG	25	TYR	3.6
12	CM	15	VAL	3.6
46	B1	67	ILE	3.6
21	AV	20	U	3.6

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Mol	Chain	Res	Type	RSRZ
60	DA	1574	C	3.6
28	BF	97	TYR	3.6
44	DZ	124	ILE	3.6
8	AI	108	VAL	3.6
28	BF	11	VAL	3.6
43	DY	95	LYS	3.6
3	AD	181	MET	3.6
29	BG	35	GLU	3.6
43	DY	33	LYS	3.6
55	D9	3	VAL	3.6
6	AG	62	PHE	3.6
3	CD	131	ARG	3.6
2	CC	46	GLU	3.6
12	CM	8	GLU	3.6
25	DC	100	ILE	3.6
28	DF	64	ILE	3.6
38	BT	49	VAL	3.6
15	CP	72	ARG	3.6
4	CE	109	ILE	3.6
3	CD	124	GLY	3.6
28	BF	105	VAL	3.6
33	BO	62	VAL	3.6
35	BQ	74	TYR	3.6
48	DN	42	TRP	3.6
51	D5	48	GLU	3.6
55	D9	2	LYS	3.6
16	CQ	18	THR	3.6
28	BF	116	ASP	3.6
29	BG	6	ALA	3.6
37	BS	55	ALA	3.6
40	DV	1	MET	3.6
42	DX	78	LYS	3.6
2	AC	153	VAL	3.6
3	CD	200	GLU	3.6
20	AA	222	U	3.6
35	BQ	106	VAL	3.6
54	B8	50	LEU	3.6
60	BA	588	U	3.6
20	CA	890	G	3.6
60	DA	458	G	3.6
50	B3	9	VAL	3.6
60	DA	34	C	3.6

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Mol	Chain	Res	Type	RSRZ
26	DD	257	LEU	3.6
28	DF	65	TRP	3.6
28	DF	46	ARG	3.6
38	BT	24	PRO	3.6
4	AE	136	MET	3.6
8	CI	84	ALA	3.6
8	CI	106	ALA	3.6
9	AJ	58	ASP	3.6
19	AT	26	ASN	3.6
23	AY	342	TYR	3.6
23	AY	356	LEU	3.6
29	BG	12	TYR	3.6
30	DH	171	LEU	3.6
42	DX	20	GLY	3.6
2	AC	131	ARG	3.5
20	AA	137	C	3.5
20	CA	219	C	3.5
60	BA	370	G	3.5
9	AJ	54	PHE	3.5
40	DV	51	VAL	3.5
50	D3	39	ASP	3.5
60	BA	519	U	3.5
60	BA	1249	U	3.5
23	CY	366	VAL	3.5
27	BE	72	VAL	3.5
28	DF	129	PHE	3.5
29	BG	57	ALA	3.5
36	DR	80	PHE	3.5
50	D3	25	ALA	3.5
25	BC	91	GLY	3.5
40	DV	35	LEU	3.5
45	B0	6	GLY	3.5
22	AW	73	A	3.5
33	DO	109	LYS	3.5
51	D5	15	ARG	3.5
60	BA	1530	G	3.5
60	BA	1566	A	3.5
60	DA	1304	C	3.5
60	DA	2405	G	3.5
8	CI	61	ALA	3.5
12	AM	98	VAL	3.5
4	CE	43	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
28	BF	113	ALA	3.5
32	DK	53	VAL	3.5
29	DG	60	LEU	3.5
34	BP	31	ALA	3.5
42	BX	10	ALA	3.5
60	DA	1026	U	3.5
28	BF	8	GLN	3.5
39	DU	111	GLU	3.5
32	DK	23	VAL	3.5
43	BY	13	VAL	3.5
28	DF	94	PRO	3.5
42	DX	32	PRO	3.5
10	AK	126	ARG	3.5
16	AQ	97	SER	3.5
3	AD	82	ALA	3.5
4	AE	101	ILE	3.5
11	AL	55	VAL	3.5
23	CY	255	ILE	3.5
44	BZ	89	PHE	3.5
48	DN	52	VAL	3.5
46	D1	85	LEU	3.5
41	BW	91	GLY	3.5
54	D8	8	LYS	3.5
28	BF	82	ILE	3.5
42	DX	39	ILE	3.5
45	B0	81	VAL	3.5
1	AB	186	ALA	3.5
19	AT	32	ALA	3.5
33	BO	37	ASP	3.5
60	BA	1026	U	3.5
60	DA	915	C	3.5
13	CN	54	PRO	3.5
34	DP	20	GLY	3.5
41	BW	87	PRO	3.5
20	CA	108	G	3.5
20	CA	484	G	3.5
60	DA	801	G	3.5
60	DA	1440	G	3.5
23	AY	114	VAL	3.5
35	DQ	96	VAL	3.5
46	B1	62	VAL	3.5
25	DC	26	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
29	DG	106	LEU	3.5
26	BD	261	LYS	3.5
16	AQ	88	TYR	3.5
26	BD	273	ARG	3.5
36	BR	17	ARG	3.5
36	DR	19	ALA	3.5
39	BU	118	GLY	3.5
41	DW	38	TYR	3.5
3	CD	49	ARG	3.5
4	AE	9	LYS	3.5
7	AH	36	LEU	3.5
26	DD	270	ILE	3.5
44	BZ	166	SER	3.5
53	D7	46	VAL	3.5
60	BA	2690	C	3.5
19	AT	21	LYS	3.5
35	DQ	98	LYS	3.5
50	B3	8	LEU	3.5
20	AA	953	G	3.5
36	DR	52	ILE	3.5
40	BV	5	VAL	3.5
26	BD	177	LEU	3.5
25	DC	135	ARG	3.5
36	BR	62	ALA	3.5
60	BA	2108	C	3.5
1	CB	144	ARG	3.5
25	BC	142	LYS	3.5
29	DG	140	ILE	3.5
38	BT	90	GLN	3.5
26	BD	263	ARG	3.5
39	BU	33	ARG	3.5
52	D6	36	LEU	3.5
43	BY	78	ALA	3.5
16	AQ	8	GLY	3.5
20	AA	157	G	3.5
39	DU	26	GLY	3.5
60	DA	615	G	3.5
4	CE	106	PRO	3.5
27	BE	25	VAL	3.5
7	AH	25	ASP	3.5
25	DC	78	ILE	3.5
30	DH	109	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
28	BF	40	GLN	3.5
42	DX	33	LYS	3.5
25	DC	179	ALA	3.5
33	BO	11	ALA	3.5
49	B2	72	ALA	3.5
60	DA	2577	A	3.5
26	BD	38	LYS	3.5
32	DK	9	LYS	3.5
1	AB	95	GLN	3.5
13	AN	5	ALA	3.5
47	B4	6	HIS	3.5
2	CC	130	VAL	3.5
2	CC	187	ALA	3.5
20	CA	1402	C	3.5
8	AI	68	GLY	3.5
35	BQ	27	VAL	3.5
36	BR	15	SER	3.5
39	DU	108	GLU	3.5
6	AG	101	LEU	3.5
52	B6	26	ASN	3.5
60	BA	2712	U	3.5
60	DA	2245	U	3.5
60	BA	2046	G	3.5
60	DA	1624	G	3.5
15	CP	38	TYR	3.5
34	DP	24	GLY	3.5
11	CL	7	ILE	3.4
20	AA	824	C	3.4
27	DE	141	ILE	3.4
34	BP	112	LEU	3.4
47	D4	22	ILE	3.4
48	BN	119	ARG	3.4
50	B3	44	ARG	3.4
60	BA	2572	A	3.5
59	BB	28	C	3.4
4	CE	108	ALA	3.4
40	BV	3	ALA	3.4
23	AY	366	VAL	3.4
28	BF	184	TYR	3.4
39	BU	93	LYS	3.4
8	CI	105	ASP	3.4
49	B2	37	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
13	CN	39	LEU	3.4
14	AO	12	ILE	3.4
30	BH	171	LEU	3.4
36	BR	22	ARG	3.4
37	DS	56	LEU	3.4
26	BD	231	HIS	3.4
60	BA	2582	G	3.4
18	CS	75	ALA	3.4
18	CS	76	PRO	3.4
20	CA	1396	A	3.4
43	BY	82	PRO	3.4
45	D0	83	PRO	3.4
54	D8	51	ALA	3.4
60	DA	222	A	3.4
3	CD	57	ARG	3.4
23	CY	271	LEU	3.4
39	BU	52	ARG	3.4
46	D1	36	GLY	3.4
7	CH	27	PRO	3.4
37	BS	77	ALA	3.4
38	BT	104	ASN	3.4
26	BD	192	THR	3.4
49	D2	25	VAL	3.4
34	DP	69	GLY	3.4
35	DQ	68	ILE	3.4
20	AA	570	G	3.4
54	B8	37	SER	3.4
60	BA	186	G	3.4
60	DA	508	G	3.4
60	DA	572	A	3.4
25	BC	115	VAL	3.4
26	BD	272	ALA	3.4
36	BR	84	ALA	3.4
41	DW	81	ALA	3.4
25	BC	132	LEU	3.4
46	B1	73	LEU	3.4
48	DN	32	THR	3.4
12	AM	27	LYS	3.4
4	AE	14	ARG	3.4
27	DE	104	VAL	3.4
37	DS	95	HIS	3.4
26	BD	133	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
53	B7	34	ARG	3.4
27	DE	60	ASN	3.4
60	BA	2697	G	3.4
60	BA	2713	A	3.4
60	DA	385	C	3.4
60	DA	530	G	3.4
16	CQ	73	VAL	3.4
28	DF	167	ALA	3.4
30	BH	56	SER	3.4
33	DO	111	PHE	3.4
50	D3	55	ARG	3.4
25	DC	99	GLU	3.4
36	BR	110	PRO	3.4
37	BS	59	LYS	3.4
50	D3	5	LYS	3.4
35	BQ	104	PHE	3.4
4	AE	129	ILE	3.4
16	AQ	33	GLY	3.4
20	CA	965	A	3.4
28	BF	151	SER	3.4
55	D9	5	ALA	3.4
60	DA	567	A	3.4
4	CE	49	PRO	3.4
20	CA	398	C	3.4
20	CA	1364	U	3.4
28	DF	92	PRO	3.4
48	DN	121	LYS	3.4
60	BA	1266	G	3.4
43	DY	36	ALA	3.4
53	B7	10	ARG	3.4
53	B7	19	ARG	3.4
29	DG	131	TYR	3.4
27	BE	129	HIS	3.4
37	BS	62	LYS	3.4
28	DF	174	VAL	3.4
45	D0	30	VAL	3.4
1	CB	150	SER	3.4
20	AA	102	G	3.4
20	AA	289	G	3.4
26	DD	165	ILE	3.4
35	BQ	122	GLY	3.4
38	DT	106	SER	3.4

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Mol	Chain	Res	Type	RSRZ
39	DU	118	GLY	3.4
60	BA	2612	C	3.4
4	AE	32	VAL	3.4
15	CP	80	PHE	3.4
19	CT	15	ARG	3.4
26	BD	53	PHE	3.4
41	BW	84	ARG	3.4
45	B0	30	VAL	3.4
2	AC	137	ALA	3.4
7	CH	36	LEU	3.4
23	CY	380	LEU	3.4
33	BO	60	ALA	3.4
42	BX	19	ALA	3.4
23	CY	178	ILE	3.4
27	BE	145	LYS	3.4
3	AD	93	PHE	3.4
27	BE	74	PRO	3.4
36	BR	61	HIS	3.4
45	D0	25	ARG	3.4
60	BA	1629	U	3.4
60	DA	1439	A	3.4
20	AA	620	C	3.4
20	CA	44	G	3.4
23	CY	631	ILE	3.4
25	BC	32	GLU	3.4
60	BA	1628	G	3.4
60	DA	1312	U	3.4
32	BK	53	VAL	3.4
60	BA	2260	C	3.4
11	CL	10	LEU	3.4
18	CS	42	PRO	3.4
25	DC	79	ALA	3.4
43	DY	88	LYS	3.4
20	AA	976	G	3.4
28	DF	39	TRP	3.4
4	AE	82	VAL	3.4
53	D7	9	ARG	3.4
1	CB	76	GLN	3.4
4	AE	87	SER	3.4
6	AG	117	ALA	3.4
38	BT	102	ILE	3.4
40	BV	15	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
43	BY	25	GLY	3.4
43	DY	24	VAL	3.4
60	BA	1625	C	3.4
23	CY	104	ALA	3.3
2	AC	132	ARG	3.3
60	DA	576	U	3.3
17	CR	66	LEU	3.3
28	DF	148	LEU	3.3
28	DF	170	LEU	3.3
60	BA	910	A	3.3
12	CM	49	THR	3.3
15	CP	67	THR	3.3
20	AA	970	C	3.3
25	BC	50	ILE	3.3
39	DU	80	ILE	3.3
59	DB	60	C	3.3
11	CL	35	GLY	3.3
13	CN	23	ARG	3.3
23	AY	365	GLU	3.3
33	DO	105	GLU	3.3
3	CD	18	LYS	3.3
1	AB	201	ILE	3.3
20	AA	378	G	3.3
20	AA	825	G	3.3
41	BW	89	ALA	3.3
60	BA	2251	G	3.3
60	DA	1311	G	3.3
3	AD	129	ASN	3.3
26	DD	190	TYR	3.3
4	CE	32	VAL	3.3
27	DE	200	GLU	3.3
34	DP	73	GLY	3.3
39	DU	9	VAL	3.3
41	DW	79	GLY	3.3
25	DC	186	LEU	3.3
26	DD	147	LEU	3.3
27	BE	27	LEU	3.3
49	D2	28	LYS	3.3
60	BA	2453	A	3.3
60	DA	856	C	3.3
23	CY	17	ILE	3.3
41	DW	32	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
48	DN	47	ALA	3.3
45	D0	4	LYS	3.3
60	DA	747	U	3.3
29	DG	120	LEU	3.3
60	DA	2061	G	3.3
4	AE	131	ILE	3.3
4	CE	138	ALA	3.3
36	BR	55	ALA	3.3
56	De	69	ALA	3.3
25	BC	170	GLY	3.3
25	DC	151	GLY	3.3
28	BF	150	GLY	3.3
38	DT	109	GLU	3.3
42	BX	25	LYS	3.3
42	BX	64	LYS	3.3
17	AR	51	LEU	3.3
60	DA	814	C	3.3
7	CH	111	ILE	3.3
10	CK	23	ALA	3.3
36	BR	83	ILE	3.3
46	D1	11	ARG	3.3
23	CY	349	LYS	3.3
26	BD	173	VAL	3.3
29	DG	155	MET	3.3
30	DH	108	GLY	3.3
50	D3	10	LYS	3.3
53	D7	29	LYS	3.3
3	CD	160	GLN	3.3
16	CQ	2	PRO	3.3
28	BF	170	LEU	3.3
53	D7	15	THR	3.3
60	DA	989	G	3.3
37	DS	82	ILE	3.3
8	AI	41	VAL	3.3
11	CL	43	VAL	3.3
3	CD	15	GLU	3.3
7	AH	117	GLY	3.3
20	CA	221	C	3.3
20	CA	1063	C	3.3
22	AW	74	C	3.3
35	BQ	23	GLY	3.3
53	D7	17	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
60	DA	1754	C	3.3
7	CH	101	PRO	3.3
26	BD	11	PRO	3.3
60	BA	395	U	3.3
60	DA	568	U	3.3
23	AY	343	ASN	3.3
42	BX	59	VAL	3.3
56	De	89	ALA	3.3
12	CM	119	GLY	3.3
23	CY	382	GLU	3.3
51	D5	30	LEU	3.3
26	BD	274	ARG	3.3
35	BQ	16	ARG	3.3
60	BA	2714	G	3.3
60	DA	1573	G	3.3
20	AA	1358	U	3.3
20	CA	1399	C	3.3
28	BF	128	ALA	3.3
36	BR	76	VAL	3.3
8	CI	110	GLU	3.3
25	BC	160	GLY	3.3
40	BV	1	MET	3.3
48	DN	107	LEU	3.3
29	DG	16	ARG	3.3
37	BS	97	ARG	3.3
14	CO	29	VAL	3.3
25	DC	85	LYS	3.3
51	D5	27	PRO	3.3
25	BC	217	THR	3.3
33	BO	63	VAL	3.3
51	B5	2	ALA	3.3
7	CH	59	LEU	3.3
19	AT	8	ARG	3.3
20	AA	925	G	3.3
20	AA	103	C	3.3
28	DF	149	ASP	3.3
38	DT	103	ARG	3.3
29	DG	63	ILE	3.3
30	BH	160	LYS	3.3
33	BO	64	ARG	3.3
41	BW	95	ILE	3.3
60	DA	1644	C	3.3

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Mol	Chain	Res	Type	RSRZ
25	BC	144	GLY	3.3
33	DO	6	THR	3.3
43	DY	93	GLY	3.3
25	BC	155	ARG	3.3
46	D1	76	ARG	3.3
8	AI	21	PRO	3.3
8	CI	49	PRO	3.3
25	BC	87	ALA	3.3
60	BA	44	A	3.3
3	CD	81	GLU	3.3
28	BF	106	ARG	3.3
51	B5	26	THR	3.3
60	DA	2253	G	3.3
1	CB	40	HIS	3.3
2	AC	24	ALA	3.3
37	DS	68	GLN	3.3
51	D5	28	PRO	3.3
48	BN	91	LEU	3.3
26	DD	55	GLY	3.3
6	AG	9	VAL	3.3
20	AA	382	A	3.3
20	AA	952	U	3.3
20	CA	1351	U	3.3
42	BX	28	PHE	3.3
54	B8	23	VAL	3.3
60	BA	2249	U	3.3
60	DA	764	A	3.3
2	CC	36	ASP	3.3
17	CR	67	ALA	3.3
25	BC	46	ALA	3.3
16	AQ	58	GLU	3.3
21	AV	9	G	3.3
27	BE	79	ARG	3.3
30	DH	170	ARG	3.3
35	DQ	133	ARG	3.3
41	DW	78	GLU	3.3
60	BA	411	G	3.3
23	CY	369	LEU	3.2
39	DU	83	LEU	3.2
41	BW	107	LEU	3.2
1	CB	114	ARG	3.2
3	CD	122	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
4	AE	23	GLY	3.2
16	AQ	4	LYS	3.2
21	AV	14	A	3.2
2	AC	134	ILE	3.2
8	AI	28	VAL	3.2
54	D8	58	ILE	3.2
18	CS	79	THR	3.2
60	BA	2021	C	3.2
60	BA	2579	C	3.2
25	BC	134	PRO	3.2
26	DD	263	ARG	3.2
41	DW	54	ALA	3.2
17	CR	22	VAL	3.2
29	BG	38	VAL	3.2
36	DR	98	LEU	3.2
39	BU	98	LEU	3.2
13	AN	26	ARG	3.2
20	CA	1286	A	3.2
35	BQ	133	ARG	3.2
46	D1	35	THR	3.2
50	B3	40	THR	3.2
25	BC	15	VAL	3.2
46	D1	93	GLU	3.2
50	B3	39	ASP	3.2
53	B7	18	PHE	3.2
17	AR	67	ALA	3.2
34	BP	29	LYS	3.2
53	D7	37	LYS	3.2
60	BA	1643	G	3.2
12	CM	112	GLY	3.2
45	B0	69	PHE	3.2
27	BE	197	ILE	3.2
41	DW	77	ASP	3.2
48	BN	30	ILE	3.2
6	AG	48	LYS	3.2
12	AM	110	ARG	3.2
18	AS	70	LYS	3.2
20	AA	815	A	3.2
23	CY	272	LEU	3.2
60	BA	1156	A	3.2
50	D3	52	HIS	3.2
51	B5	47	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
60	DA	1257	C	3.2
42	DX	89	ILE	3.2
3	CD	53	ASP	3.2
6	AG	10	ARG	3.2
13	CN	30	ALA	3.2
21	CV	7	G	3.2
36	BR	103	ARG	3.2
43	DY	84	ARG	3.2
41	BW	73	ALA	3.2
1	AB	184	VAL	3.2
1	CB	78	GLN	3.2
4	CE	19	MET	3.2
4	AE	15	ARG	3.2
8	AI	70	LYS	3.2
12	AM	9	ILE	3.2
25	BC	72	GLN	3.2
35	BQ	103	MET	3.2
33	DO	122	LEU	3.2
35	BQ	125	LEU	3.2
36	DR	3	HIS	3.2
36	DR	99	LYS	3.2
37	BS	95	HIS	3.2
38	DT	95	ARG	3.2
41	BW	98	LYS	3.2
44	BZ	125	LEU	3.2
52	B6	42	TRP	3.2
28	BF	153	SER	3.2
4	CE	89	ILE	3.2
32	BK	107	ILE	3.2
54	B8	40	GLU	3.2
56	De	73	GLU	3.2
26	BD	52	ARG	3.2
32	DK	73	PRO	3.2
3	AD	133	VAL	3.2
8	CI	108	VAL	3.2
25	BC	220	GLY	3.2
26	DD	53	PHE	3.2
29	BG	169	ALA	3.2
48	DN	27	ALA	3.2
60	DA	866	A	3.2
11	CL	22	SER	3.2
50	D3	11	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	CD	168	ARG	3.2
26	DD	33	LEU	3.2
20	CA	1322	C	3.2
53	B7	44	PRO	3.2
20	AA	820	U	3.2
4	AE	45	PHE	3.2
42	BX	72	LYS	3.2
29	DG	90	LEU	3.2
4	CE	93	PRO	3.2
20	AA	354	G	3.2
35	DQ	126	PRO	3.2
60	DA	2252	G	3.2
9	CJ	101	VAL	3.2
44	DZ	173	ALA	3.2
20	AA	261	U	3.2
29	BG	51	ARG	3.2
43	DY	67	LEU	3.2
1	AB	163	PHE	3.2
32	DK	13	PRO	3.2
11	CL	126	LYS	3.2
29	DG	12	TYR	3.2
29	DG	36	LYS	3.2
33	BO	34	THR	3.2
44	BZ	78	LYS	3.2
44	DZ	86	VAL	3.2
17	AR	50	ILE	3.2
26	BD	16	MET	3.2
39	BU	10	ARG	3.2
47	B4	22	ILE	3.2
20	CA	568	G	3.2
42	BX	82	GLN	3.2
8	CI	109	VAL	3.2
36	BR	114	VAL	3.2
2	AC	25	GLY	3.2
13	CN	57	ARG	3.2
23	CY	335	LEU	3.2
27	DE	159	HIS	3.2
19	AT	30	LYS	3.2
26	BD	266	SER	3.2
27	DE	96	PHE	3.2
34	DP	71	VAL	3.2
37	BS	68	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
3	AD	78	LEU	3.2
13	CN	6	LEU	3.2
17	AR	70	ILE	3.2
37	BS	90	GLY	3.2
41	DW	18	ARG	3.2
42	BX	73	ARG	3.2
60	BA	2511	U	3.2
3	AD	74	GLN	3.2
23	CY	114	VAL	3.2
27	DE	93	VAL	3.2
29	DG	160	VAL	3.2
3	AD	23	GLY	3.2
48	DN	95	PRO	3.2
41	DW	35	ILE	3.2
3	AD	156	GLU	3.2
16	CQ	20	THR	3.2
25	BC	82	GLU	3.2
28	DF	51	THR	3.2
16	CQ	87	LYS	3.2
25	DC	115	VAL	3.2
29	BG	125	PHE	3.2
48	BN	104	LYS	3.2
51	B5	56	LYS	3.2
11	AL	89	ARG	3.1
28	BF	74	ARG	3.1
60	BA	2451	A	3.1
27	DE	81	ILE	3.1
20	CA	392	G	3.1
20	CA	973	G	3.1
29	BG	30	GLU	3.1
60	BA	2319	G	3.1
60	DA	1633	G	3.1
60	DA	2056	G	3.1
3	CD	112	VAL	3.1
20	AA	1028(B)	C	3.1
20	CA	1359	C	3.1
60	BA	2512	C	3.1
3	CD	48	ALA	3.1
11	CL	33	ARG	3.1
32	DK	32	ALA	3.1
4	AE	52	PRO	3.1
34	DP	25	SER	3.1

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Mol	Chain	Res	Type	RSRZ
41	BW	24	ILE	3.1
28	BF	127	GLU	3.1
46	B1	32	LYS	3.1
60	BA	835	A	3.1
60	BA	941	A	3.1
25	BC	26	ALA	3.1
25	DC	74	ARG	3.1
6	AG	22	LEU	3.1
32	BK	127	ILE	3.1
35	DQ	28	ALA	3.1
52	D6	9	LEU	3.1
20	CA	115	G	3.1
55	B9	17	ILE	3.1
44	DZ	83	PRO	3.1
23	AY	258	VAL	3.1
26	DD	18	VAL	3.1
32	DK	139	VAL	3.1
36	BR	23	ASN	3.1
3	AD	94	LEU	3.1
8	CI	47	LEU	3.1
13	AN	6	LEU	3.1
30	DH	158	HIS	3.1
38	DT	110	ILE	3.1
41	BW	54	ALA	3.1
42	DX	58	HIS	3.1
49	D2	39	ALA	3.1
25	BC	97	GLY	3.1
39	DU	73	GLY	3.1
1	CB	101	MET	3.1
7	AH	116	LYS	3.1
29	BG	67	LYS	3.1
29	DG	32	PRO	3.1
41	DW	41	LYS	3.1
60	BA	199	A	3.1
60	DA	2451	A	3.1
8	CI	86	VAL	3.1
30	DH	113	VAL	3.1
4	AE	27	ARG	3.1
20	AA	1401	G	3.1
20	AA	1516	G	3.1
26	BD	58	HIS	3.1
29	DG	158	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
29	DG	165	THR	3.1
30	BH	158	HIS	3.1
32	BK	69	THR	3.1
36	BR	10	LEU	3.1
48	BN	26	LEU	3.1
60	DA	743	G	3.1
4	AE	26	PHE	3.1
12	CM	98	VAL	3.1
32	BK	55	VAL	3.1
33	DO	102	VAL	3.1
36	BR	97	VAL	3.1
38	DT	70	VAL	3.1
50	D3	47	VAL	3.1
33	DO	23	ARG	3.1
60	BA	90	U	3.1
1	CB	145	LEU	3.1
1	CB	75	LYS	3.1
35	BQ	117	ALA	3.1
4	AE	22	GLY	3.1
43	DY	46	LYS	3.1
49	D2	67	LYS	3.1
60	BA	1786	A	3.1
19	CT	41	VAL	3.1
23	CY	542	VAL	3.1
29	BG	58	GLN	3.1
44	DZ	98	MET	3.1
46	D1	12	PRO	3.1
20	CA	330	C	3.1
33	DO	21	CYS	3.1
60	BA	2063	C	3.1
9	CJ	38	ILE	3.1
16	AQ	32	TYR	3.1
26	BD	271	ILE	3.1
39	DU	62	ILE	3.1
60	DA	972	G	3.1
1	CB	28	PHE	3.1
23	AY	43	GLY	3.1
3	AD	3	ARG	3.1
39	DU	89	GLU	3.1
50	D3	16	PRO	3.1
13	AN	32	SER	3.1
8	CI	45	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
11	CL	91	LYS	3.1
36	DR	54	LEU	3.1
18	CS	52	TYR	3.1
48	BN	29	LYS	3.1
54	D8	41	ILE	3.1
3	AD	80	GLU	3.1
20	AA	1354	C	3.1
25	BC	145	THR	3.1
27	DE	111	ARG	3.1
60	DA	1675	C	3.1
29	BG	90	LEU	3.1
43	DY	53	PRO	3.1
19	AT	52	ALA	3.1
20	CA	377	G	3.1
29	BG	131	TYR	3.1
60	BA	2634	G	3.1
60	DA	2574	G	3.1
8	CI	24	GLY	3.1
33	DO	37	ASP	3.1
35	BQ	84	GLY	3.1
36	DR	114	VAL	3.1
20	CA	964	A	3.1
49	D2	22	GLU	3.1
25	DC	57	GLN	3.1
3	AD	29	PRO	3.1
32	DK	107	ILE	3.1
39	BU	2	PRO	3.1
13	CN	21	TYR	3.1
37	DS	74	ALA	3.1
38	DT	52	ILE	3.1
3	AD	6	GLY	3.1
2	CC	167	TRP	3.1
2	CC	183	ASP	3.1
34	DP	18	ARG	3.1
52	D6	13	CYS	3.1
19	AT	68	LYS	3.1
37	DS	93	LYS	3.1
3	AD	27	TYR	3.1
6	AG	24	THR	3.1
20	CA	399	G	3.1
60	BA	1606	G	3.1
30	BH	161	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
45	D0	69	PHE	3.1
1	AB	165	VAL	3.1
7	CH	56	LYS	3.1
29	BG	105	LYS	3.1
3	AD	198	VAL	3.1
25	BC	10	ALA	3.1
33	BO	83	ALA	3.1
48	BN	86	PRO	3.1
46	B1	26	ARG	3.1
53	B7	15	THR	3.1
60	BA	673	C	3.1
1	AB	75	LYS	3.1
11	CL	54	LYS	3.1
38	DT	46	GLU	3.1
40	BV	19	LYS	3.1
52	B6	53	LYS	3.1
15	CP	40	ASP	3.1
1	CB	201	ILE	3.1
20	AA	1202	G	3.1
60	BA	2004	G	3.1
1	AB	131	PRO	3.1
10	CK	25	TYR	3.1
20	AA	1534	A	3.1
11	AL	44	THR	3.1
25	BC	90	ALA	3.1
27	DE	59	VAL	3.1
56	De	51	ALA	3.1
1	AB	215	LEU	3.1
43	DY	40	GLU	3.1
6	CG	42	ILE	3.1
20	AA	150	C	3.1
36	DR	59	ASP	3.1
3	AD	197	PRO	3.1
19	CT	73	HIS	3.1
27	BE	165	VAL	3.1
51	D5	55	ARG	3.1
25	DC	91	GLY	3.1
42	BX	67	GLY	3.1
20	CA	625	G	3.1
26	BD	162	SER	3.1
27	BE	108	SER	3.1
49	D2	33	MET	3.1

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Mol	Chain	Res	Type	RSRZ
51	D5	12	SER	3.1
60	DA	1256	G	3.1
14	AO	27	VAL	3.0
28	BF	154	VAL	3.0
46	B1	50	ARG	3.0
46	B1	53	VAL	3.0
36	BR	44	LEU	3.0
60	BA	2723	C	3.0
60	DA	1657	C	3.0
13	AN	7	ILE	3.0
26	BD	260	ARG	3.0
26	DD	274	ARG	3.0
33	DO	24	VAL	3.0
46	D1	5	CYS	3.0
48	BN	37	LYS	3.0
46	D1	75	GLU	3.0
60	BA	2019	A	3.0
60	DA	265	A	3.0
20	CA	963	G	3.0
20	CA	1401	G	3.0
60	DA	1303	G	3.0
60	DA	1339	G	3.0
38	DT	45	PHE	3.0
42	DX	59	VAL	3.0
28	BF	73	ALA	3.0
54	B8	9	GLY	3.0
1	CB	166	ASP	3.0
41	BW	86	LEU	3.0
44	DZ	87	ASP	3.0
10	CK	83	ILE	3.0
25	BC	84	ILE	3.0
26	DD	268	ARG	3.0
38	DT	75	ILE	3.0
11	AL	23	LYS	3.0
3	CD	201	GLN	3.0
48	BN	33	LEU	3.0
1	CB	206	ASP	3.0
11	CL	5	PRO	3.0
12	AM	52	GLU	3.0
48	DN	40	PRO	3.0
60	BA	2032	G	3.0
1	AB	197	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
4	AE	89	ILE	3.0
10	AK	29	ILE	3.0
14	AO	3	ILE	3.0
38	BT	96	ARG	3.0
20	CA	934	C	3.0
26	DD	59	LYS	3.0
48	BN	121	LYS	3.0
60	BA	914	C	3.0
39	DU	44	ASN	3.0
48	BN	31	ALA	3.0
40	BV	94	LEU	3.0
8	AI	66	ARG	3.0
11	CL	16	GLU	3.0
12	CM	113	PRO	3.0
20	CA	68(X)	U	3.0
20	CA	327	A	3.0
25	DC	80	LYS	3.0
60	DA	958	U	3.0
1	AB	148	TYR	3.0
7	AH	119	LEU	3.0
8	CI	82	ALA	3.0
16	CQ	89	LEU	3.0
25	DC	46	ALA	3.0
20	AA	68	G	3.0
26	BD	207	GLY	3.0
28	BF	175	THR	3.0
37	DS	61	ASN	3.0
60	DA	23	G	3.0
11	CL	97	ARG	3.0
20	AA	1066	C	3.0
49	B2	31	GLU	3.0
28	BF	37	VAL	3.0
48	BN	103	VAL	3.0
60	BA	755	C	3.0
60	BA	1298	C	3.0
8	CI	72	GLY	3.0
20	AA	1532	U	3.0
23	AY	134	ALA	3.0
42	BX	18	TYR	3.0
49	D2	13	ALA	3.0
9	CJ	35	SER	3.0
60	BA	2555	U	3.0

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Mol	Chain	Res	Type	RSRZ
1	AB	162	ILE	3.0
16	AQ	85	VAL	3.0
13	CN	38	GLY	3.0
21	AV	19	G	3.0
44	DZ	164	ALA	3.0
9	AJ	55	LYS	3.0
12	CM	105	THR	3.0
20	AA	314	C	3.0
36	DR	22	ARG	3.0
12	AM	97	PRO	3.0
51	D5	42	PRO	3.0
9	CJ	9	ARG	3.0
23	CY	43	GLY	3.0
44	BZ	77	ASP	3.0
35	DQ	11	LYS	3.0
36	BR	40	LYS	3.0
44	BZ	127	LYS	3.0
1	AB	73	THR	3.0
7	AH	53	VAL	3.0
14	AO	9	GLN	3.0
26	DD	65	ILE	3.0
28	DF	132	VAL	3.0
43	DY	85	VAL	3.0
1	CB	29	ALA	3.0
4	AE	43	LEU	3.0
3	CD	130	GLY	3.0
20	AA	322	C	3.0
23	CY	143	GLY	3.0
36	DR	84	ALA	3.0
60	DA	665	C	3.0
54	B8	29	LYS	3.0
59	DB	8	U	3.0
6	AG	49	ILE	3.0
25	DC	180	SER	3.0
20	CA	1285	A	3.0
60	BA	2378	A	3.0
37	DS	67	ARG	3.0
46	B1	69	LYS	3.0
16	CQ	46	ASP	3.0
27	BE	1	MET	3.0
29	DG	168	GLU	3.0
35	BQ	31	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
37	DS	14	VAL	3.0
20	AA	1399	C	3.0
20	AA	1187	G	3.0
33	DO	106	LEU	3.0
35	BQ	72	LYS	3.0
53	B7	39	ARG	3.0
60	BA	124	G	3.0
60	DA	1441	G	3.0
9	AJ	41	PRO	3.0
32	DK	138	VAL	3.0
39	BU	72	HIS	3.0
60	BA	1528	A	3.0
8	CI	50	LEU	3.0
2	CC	163	ALA	3.0
12	AM	2	ALA	3.0
44	BZ	81	ARG	3.0
9	AJ	98	ILE	3.0
20	AA	623	C	3.0
33	BO	39	ILE	3.0
60	BA	1781	C	3.0
60	DA	1741	C	3.0
6	CG	16	LEU	3.0
20	CA	105	G	3.0
25	DC	53	ARG	3.0
27	DE	54	GLN	3.0
32	BK	120	LEU	3.0
60	BA	2655	G	3.0
15	CP	53	VAL	3.0
27	DE	158	GLY	3.0
28	BF	177	ALA	3.0
19	CT	33	ILE	3.0
20	AA	152	A	3.0
20	AA	621	A	3.0
25	BC	98	GLU	3.0
26	DD	61	LEU	3.0
26	DD	227	ASN	3.0
26	DD	255	LYS	3.0
56	De	92	LEU	3.0
26	DD	230	ASP	3.0
38	BT	107	ASP	3.0
49	B2	52	ASP	3.0
27	DE	102	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
35	BQ	121	ALA	2.9
36	DR	32	GLY	2.9
6	AG	8	GLU	2.9
8	AI	2	GLU	2.9
2	CC	47	LEU	2.9
3	AD	202	LEU	2.9
19	AT	80	ARG	2.9
27	DE	109	LYS	2.9
48	DN	2	LYS	2.9
49	D2	29	LYS	2.9
53	B7	49	ARG	2.9
60	DA	2526	G	2.9
10	CK	88	GLY	2.9
16	AQ	56	VAL	2.9
20	CA	1279	A	2.9
33	BO	33	ALA	2.9
37	DS	98	VAL	2.9
40	BV	77	ALA	2.9
60	BA	532	A	2.9
26	DD	174	ILE	2.9
8	CI	48	GLU	2.9
20	CA	304	U	2.9
27	BE	133	LYS	2.9
41	DW	52	GLU	2.9
60	BA	1205	U	2.9
60	DA	2555	U	2.9
41	BW	90	ARG	2.9
19	CT	49	ALA	2.9
34	BP	54	GLY	2.9
49	B2	6	VAL	2.9
37	DS	18	ILE	2.9
1	AB	202	PRO	2.9
1	CB	20	GLU	2.9
7	AH	91	ARG	2.9
11	CL	84	LEU	2.9
19	CT	8	ARG	2.9
35	BQ	80	GLU	2.9
60	BA	615	G	2.9
38	BT	101	PHE	2.9
1	CB	165	VAL	2.9
11	CL	82	VAL	2.9
19	CT	44	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
41	DW	48	ALA	2.9
12	CM	120	LYS	2.9
14	AO	5	LYS	2.9
11	CL	53	ARG	2.9
16	AQ	54	GLY	2.9
28	DF	206	ILE	2.9
35	DQ	107	ALA	2.9
36	DR	112	ALA	2.9
53	B7	14	LYS	2.9
3	CD	59	ARG	2.9
20	CA	102	G	2.9
23	CY	374	LEU	2.9
48	DN	91	LEU	2.9
60	DA	1190	G	2.9
1	AB	54	THR	2.9
3	AD	140	VAL	2.9
41	DW	108	GLY	2.9
26	DD	155	LEU	2.9
32	DK	115	LEU	2.9
48	DN	106	MET	2.9
19	CT	31	SER	2.9
42	DX	12	VAL	2.9
1	CB	18	GLY	2.9
18	AS	77	THR	2.9
19	CT	69	GLY	2.9
21	AV	13	A	2.9
27	BE	24	THR	2.9
27	DE	166	THR	2.9
53	B7	43	THR	2.9
60	DA	1569	A	2.9
8	CI	85	LEU	2.9
20	AA	963	G	2.9
26	DD	52	ARG	2.9
45	D0	74	ARG	2.9
60	BA	2505	G	2.9
28	DF	36	VAL	2.9
35	DQ	81	VAL	2.9
9	AJ	60	ARG	2.9
13	AN	30	ALA	2.9
25	DC	9	ARG	2.9
27	BE	28	ALA	2.9
43	DY	94	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
36	BR	7	GLY	2.9
60	BA	838	C	2.9
19	CT	51	GLU	2.9
20	AA	68(U)	U	2.9
60	DA	746	A	2.9
8	CI	20	ARG	2.9
9	AJ	74	ILE	2.9
48	DN	36	GLY	2.9
50	B3	13	ILE	2.9
39	DU	61	TRP	2.9
60	BA	832	G	2.9
1	CB	95	GLN	2.9
12	CM	109	THR	2.9
29	BG	59	GLU	2.9
56	Be	55	GLU	2.9
11	AL	54	LYS	2.9
32	DK	77	LEU	2.9
53	D7	20	ALA	2.9
53	D7	33	ARG	2.9
20	AA	45	U	2.9
20	AA	1393	U	2.9
10	CK	41	THR	2.9
20	CA	1251	A	2.9
27	BE	91	VAL	2.9
32	BK	4	VAL	2.9
46	D1	91	LYS	2.9
3	AD	28	SER	2.9
7	CH	29	SER	2.9
21	CV	10	G	2.9
29	BG	34	LEU	2.9
29	DG	169	ALA	2.9
29	DG	179	PRO	2.9
28	DF	139	PHE	2.9
12	AM	45	VAL	2.9
20	CA	984	C	2.9
25	BC	108	TRP	2.9
12	CM	31	LYS	2.9
42	DX	63	LYS	2.9
4	AE	16	THR	2.9
53	D7	36	GLN	2.9
9	AJ	39	PRO	2.9
12	CM	30	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
19	AT	77	ALA	2.9
33	DO	8	LEU	2.9
42	BX	91	ALA	2.9
9	CJ	56	HIS	2.9
60	BA	990	A	2.9
44	BZ	92	SER	2.9
43	DY	62	GLU	2.9
9	AJ	9	ARG	2.9
28	BF	99	TYR	2.9
20	AA	924	C	2.9
20	AA	1234	C	2.9
28	DF	55	GLY	2.9
33	DO	79	PHE	2.9
34	BP	104	GLY	2.9
36	DR	62	ALA	2.9
36	DR	67	LEU	2.9
49	D2	37	PHE	2.9
51	B5	58	LEU	2.9
54	D8	45	GLY	2.9
60	BA	1933	G	2.9
60	BA	2210	G	2.9
32	DK	30	HIS	2.9
16	CQ	36	ILE	2.9
20	AA	1285	A	2.9
20	CA	1280	A	2.9
33	DO	39	ILE	2.9
12	CM	118	ALA	2.9
43	DY	65	ALA	2.9
29	BG	15	VAL	2.9
50	B3	7	LYS	2.9
7	CH	34	GLU	2.9
14	CO	63	ARG	2.9
38	BT	95	ARG	2.9
45	B0	16	SER	2.9
6	CG	11	GLN	2.9
6	CG	101	LEU	2.9
15	AP	74	LEU	2.9
20	AA	1385	G	2.9
30	BH	103	LEU	2.9
60	BA	337	C	2.9
60	BA	1766	U	2.9
52	B6	33	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
20	CA	32	A	2.8
60	DA	1566	A	2.8
60	DA	2020	A	2.8
16	CQ	42	TYR	2.8
28	DF	33	LEU	2.8
3	AD	117	ALA	2.8
6	CG	10	ARG	2.8
20	CA	290	C	2.8
20	CA	449	C	2.8
43	BY	99	CYS	2.8
34	BP	6	LEU	2.8
60	BA	1306	C	2.8
25	DC	225	ILE	2.8
21	AV	15	A	2.8
28	DF	173	VAL	2.8
44	DZ	45	ASP	2.8
60	BA	1189	A	2.8
23	AY	288	PRO	2.8
11	CL	100	ILE	2.8
8	CI	126	SER	2.8
12	CM	27	LYS	2.8
26	DD	184	LYS	2.8
30	DH	148	ILE	2.8
8	AI	22	GLY	2.8
28	DF	126	VAL	2.8
7	AH	85	ARG	2.8
20	CA	1320	C	2.8
23	AY	314	PHE	2.8
23	CY	336	THR	2.8
32	DK	25	PRO	2.8
37	BS	56	LEU	2.8
41	BW	96	ILE	2.8
23	CY	377	VAL	2.8
34	DP	26	GLY	2.8
35	DQ	35	VAL	2.8
39	BU	23	GLY	2.8
60	DA	782	A	2.8
26	BD	218	ARG	2.8
29	DG	33	ARG	2.8
34	BP	33	ARG	2.8
9	CJ	53	PRO	2.8
12	CM	97	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
16	CQ	30	PRO	2.8
29	DG	139	LEU	2.8
37	DS	24	LEU	2.8
36	DR	87	TYR	2.8
51	D5	26	THR	2.8
13	CN	5	ALA	2.8
20	CA	1327	C	2.8
42	DX	54	VAL	2.8
53	B7	13	ALA	2.8
60	DA	815	C	2.8
11	AL	17	LYS	2.8
19	CT	54	LYS	2.8
20	CA	15	G	2.8
35	DQ	116	GLU	2.8
54	D8	36	LYS	2.8
33	DO	10	VAL	2.8
46	B1	70	VAL	2.8
29	BG	96	ARG	2.8
50	D3	19	GLN	2.8
27	BE	2	LYS	2.8
60	BA	1258	C	2.8
15	CP	84	ALA	2.8
38	BT	103	ARG	2.8
3	CD	75	PHE	2.8
23	AY	272	LEU	2.8
26	BD	215	LEU	2.8
60	BA	2716	U	2.8
12	CM	87	TYR	2.8
43	DY	55	TYR	2.8
37	BS	71	ARG	2.8
40	BV	37	VAL	2.8
51	D5	41	PRO	2.8
4	AE	130	ASN	2.8
10	AK	11	LYS	2.8
25	DC	127	LYS	2.8
6	AG	77	SER	2.8
13	CN	42	ILE	2.8
20	CA	624	C	2.8
34	DP	112	LEU	2.8
49	D2	21	LEU	2.8
38	DT	74	ARG	2.8
10	AK	121	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
20	AA	608	A	2.8
37	DS	90	GLY	2.8
38	DT	69	GLY	2.8
2	AC	42	LEU	2.8
20	AA	333	G	2.8
21	AV	7	G	2.8
36	DR	44	LEU	2.8
40	DV	7	THR	2.8
60	BA	2331	G	2.8
60	DA	2812	G	2.8
25	BC	146	VAL	2.8
26	BD	13	ARG	2.8
33	BO	98	VAL	2.8
15	CP	63	GLY	2.8
19	AT	27	LYS	2.8
37	DS	77	ALA	2.8
2	CC	175	LEU	2.8
6	AG	43	PHE	2.8
20	AA	379	C	2.8
25	BC	167	ASP	2.8
36	BR	49	ASP	2.8
60	BA	665	C	2.8
3	AD	150	GLU	2.8
7	CH	53	VAL	2.8
25	BC	172	ILE	2.8
28	DF	28	ILE	2.8
28	DF	70	THR	2.8
36	DR	24	GLN	2.8
4	CE	87	SER	2.8
20	AA	1440(I)	A	2.8
43	DY	51	VAL	2.8
39	DU	72	HIS	2.8
9	CJ	10	GLY	2.8
7	CH	121	ASP	2.8
19	CT	53	LEU	2.8
23	AY	271	LEU	2.8
25	BC	137	LEU	2.8
26	DD	94	LEU	2.8
30	BH	55	PRO	2.8
3	CD	89	THR	2.8
54	B8	27	THR	2.8
6	AG	156	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
10	CK	44	SER	2.8
14	AO	30	ALA	2.8
18	AS	68	GLY	2.8
25	DC	5	GLY	2.8
49	D2	72	ALA	2.8
60	BA	825	C	2.8
60	BA	1251	C	2.8
60	DA	2109	U	2.8
20	CA	363	A	2.8
29	DG	167	GLU	2.8
33	BO	40	VAL	2.8
33	DO	69	ILE	2.8
60	DA	2503	A	2.8
23	AY	164	MET	2.8
27	BE	8	LYS	2.8
48	DN	31	ALA	2.8
60	BA	1642	G	2.8
1	AB	128	GLU	2.8
8	AI	111	ARG	2.8
13	CN	33	VAL	2.8
25	DC	75	VAL	2.8
8	CI	54	ASP	2.8
16	AQ	55	ASP	2.8
28	DF	104	LYS	2.8
51	B5	3	LYS	2.8
60	BA	1188	U	2.8
60	DA	33	U	2.8
60	DA	201	C	2.8
11	AL	29	GLY	2.8
26	DD	40	THR	2.8
28	BF	70	THR	2.8
19	AT	31	SER	2.7
20	AA	1092	A	2.8
23	CY	148	LEU	2.8
34	DP	32	THR	2.8
35	BQ	75	THR	2.8
36	BR	112	ALA	2.8
36	DR	37	THR	2.8
44	BZ	117	LEU	2.8
44	BZ	171	ILE	2.7
45	B0	82	ARG	2.7
50	B3	16	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
52	B6	7	ILE	2.7
8	AI	5	TYR	2.7
16	CQ	26	GLN	2.7
1	CB	138	LEU	2.7
26	DD	95	LEU	2.7
27	BE	140	SER	2.7
43	BY	92	ASN	2.7
60	BA	271(D)	U	2.7
60	DA	243	U	2.7
50	D3	17	LYS	2.7
20	AA	1394	A	2.7
6	AG	116	ALA	2.7
26	DD	182	LEU	2.7
15	AP	51	VAL	2.7
25	BC	131	ILE	2.7
28	DF	44	ARG	2.7
38	DT	104	ASN	2.7
41	DW	40	ASN	2.7
45	B0	67	VAL	2.7
1	AB	134	GLU	2.7
23	AY	364	GLU	2.7
27	DE	189	PRO	2.7
2	CC	48	TYR	2.7
20	CA	378	G	2.7
30	DH	103	LEU	2.7
32	BK	74	ALA	2.7
33	BO	122	LEU	2.7
60	BA	323	G	2.7
60	BA	1998	G	2.7
60	DA	2046	G	2.7
9	AJ	52	GLY	2.7
1	CB	93	VAL	2.7
4	CE	100	VAL	2.7
20	AA	912	C	2.7
20	CA	1384	C	2.7
13	AN	9	LYS	2.7
25	BC	14	LYS	2.7
28	BF	45	ARG	2.7
30	BH	107	VAL	2.7
53	B7	21	ARG	2.7
20	CA	1269	A	2.7
51	B5	44	THR	2.7

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Mol	Chain	Res	Type	RSRZ
60	BA	1597	A	2.7
44	DZ	118	GLN	2.7
28	DF	195	ASP	2.7
60	BA	441	U	2.7
60	BA	2022	U	2.7
36	DR	18	LEU	2.7
36	DR	94	TYR	2.7
38	DT	68	TYR	2.7
60	BA	2715	C	2.7
25	BC	125	GLY	2.7
41	BW	35	ILE	2.7
51	B5	45	VAL	2.7
59	DB	59	A	2.7
1	AB	193	ASP	2.7
1	CB	79	ASP	2.7
23	CY	574	GLU	2.7
25	DC	82	GLU	2.7
20	CA	571	U	2.7
23	AY	337	SER	2.7
39	BU	45	TYR	2.7
3	AD	121	VAL	2.7
11	CL	47	LYS	2.7
36	DR	90	ARG	2.7
60	DA	2449	U	2.7
26	BD	166	GLN	2.7
17	AR	62	GLU	2.7
20	AA	1362	C	2.7
60	BA	258	G	2.7
60	BA	2601	C	2.7
60	BA	2780	G	2.7
60	DA	10	G	2.7
60	DA	686	G	2.7
15	CP	57	ARG	2.7
25	BC	127	LYS	2.7
43	BY	102	CYS	2.7
37	DS	55	ALA	2.7
40	DV	49	THR	2.7
52	B6	41	PRO	2.7
53	D7	24	THR	2.7
54	B8	21	LYS	2.7
1	AB	80	ILE	2.7
10	CK	21	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
25	BC	190	ILE	2.7
27	BE	167	VAL	2.7
28	BF	89	VAL	2.7
40	DV	52	VAL	2.7
29	DG	152	LEU	2.7
35	BQ	8	LYS	2.7
42	BX	92	LEU	2.7
11	AL	18	VAL	2.7
14	CO	27	VAL	2.7
33	BO	86	ILE	2.7
48	DN	44	PRO	2.7
1	AB	16	HIS	2.7
20	CA	1400	C	2.7
25	BC	149	ASN	2.7
20	AA	1368	G	2.7
20	AA	1250	A	2.7
27	BE	163	GLU	2.7
33	BO	8	LEU	2.7
60	BA	1303	G	2.7
26	DD	258	LYS	2.7
41	BW	41	LYS	2.7
23	CY	177	ILE	2.7
28	BF	167	ALA	2.7
42	DX	75	ASP	2.7
10	CK	87	THR	2.7
35	DQ	127	ILE	2.7
23	AY	40	HIS	2.7
37	BS	63	THR	2.7
16	CQ	69	LYS	2.7
26	BD	5	LYS	2.7
38	DT	90	GLN	2.7
1	CB	136	VAL	2.7
46	D1	4	VAL	2.7
2	CC	53	ALA	2.7
20	AA	1384	C	2.7
20	CA	47	C	2.7
44	DZ	171	ILE	2.7
60	DA	971	C	2.7
60	DA	1217	C	2.7
23	CY	161	PRO	2.7
2	AC	10	PHE	2.7
18	CS	71	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
20	AA	823	G	2.7
20	AA	916	G	2.7
20	CA	107	G	2.7
16	AQ	38	ARG	2.7
29	BG	33	ARG	2.7
29	DG	175	LEU	2.7
41	DW	49	LYS	2.7
54	B8	43	GLN	2.7
30	DH	50	VAL	2.7
35	BQ	114	ALA	2.7
3	CD	10	ARG	2.7
10	AK	54	ARG	2.7
27	DE	118	LYS	2.7
43	BY	60	PHE	2.7
20	CA	400	C	2.7
27	BE	188	VAL	2.7
60	BA	2450	A	2.7
60	DA	1681	G	2.7
2	CC	11	ARG	2.7
23	AY	348	ARG	2.7
48	DN	74	ARG	2.7
18	CS	56	GLN	2.7
23	CY	45	VAL	2.7
27	DE	151	TYR	2.7
44	BZ	126	VAL	2.7
48	BN	14	VAL	2.7
9	AJ	6	ILE	2.7
26	DD	167	GLY	2.7
26	DD	234	GLY	2.7
43	DY	58	GLY	2.7
43	DY	61	ILE	2.7
44	DZ	172	ALA	2.7
3	CD	39	PRO	2.7
14	AO	31	LEU	2.7
26	DD	48	ARG	2.7
27	DE	84	PHE	2.7
38	BT	33	LYS	2.7
48	BN	40	PRO	2.7
54	B8	46	ARG	2.7
6	CG	8	GLU	2.7
26	DD	181	GLU	2.7
35	DQ	80	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
60	DA	2507	C	2.7
44	BZ	139	VAL	2.7
20	CA	1183	A	2.7
52	D6	39	TYR	2.7
60	BA	257	A	2.7
25	BC	68	GLY	2.7
4	CE	18	ARG	2.6
16	AQ	84	LEU	2.6
20	AA	402	G	2.7
60	BA	45	G	2.7
60	DA	729	G	2.7
60	DA	1910	G	2.7
30	BH	26	VAL	2.6
34	DP	125	VAL	2.6
2	AC	202	ILE	2.6
32	BK	59	ILE	2.6
39	BU	117	GLN	2.6
43	DY	22	GLY	2.6
6	AG	41	ARG	2.6
19	AT	25	ARG	2.6
20	AA	1352	C	2.6
20	AA	1383	C	2.6
45	B0	61	ALA	2.6
36	BR	60	LEU	2.6
39	BU	55	ARG	2.6
3	CD	77	ASN	2.6
20	AA	51	A	2.6
20	AA	607	A	2.6
37	BS	14	VAL	2.6
42	BX	43	VAL	2.6
5	AF	94	GLN	2.6
19	CT	27	LYS	2.6
19	CT	45	GLN	2.6
43	DY	21	LYS	2.6
4	AE	24	ARG	2.6
15	AP	42	ARG	2.6
20	AA	906	G	2.6
25	BC	216	THR	2.6
26	BD	43	ARG	2.6
28	BF	205	ARG	2.6
36	DR	17	ARG	2.6
52	D6	28	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
16	CQ	85	VAL	2.6
20	CA	1257	U	2.6
6	AG	120	ILE	2.6
49	B2	29	LYS	2.6
60	BA	2178	C	2.6
26	DD	177	LEU	2.6
28	DF	177	ALA	2.6
36	DR	51	LEU	2.6
38	BT	64	ARG	2.6
44	BZ	173	ALA	2.6
48	DN	97	ARG	2.6
49	D2	60	LEU	2.6
11	CL	69	TYR	2.6
27	BE	56	PRO	2.6
27	DE	143	ASN	2.6
51	D5	40	LYS	2.6
20	CA	1516	G	2.6
26	DD	272	ALA	2.6
33	BO	79	PHE	2.6
60	BA	2211	G	2.6
23	AY	207	ASP	2.6
28	DF	175	THR	2.6
29	BG	162	THR	2.6
38	DT	27	THR	2.6
39	DU	105	VAL	2.6
48	BN	53	VAL	2.6
3	CD	84	LYS	2.6
60	DA	1636	C	2.6
60	DA	2021	C	2.6
60	DA	2610	C	2.6
21	CV	5	A	2.6
26	BD	244	ARG	2.6
6	AG	11	GLN	2.6
6	AG	86	GLN	2.6
51	B5	30	LEU	2.6
6	CG	27	ILE	2.6
20	AA	61	G	2.6
60	BA	1186	G	2.6
60	DA	2035	G	2.6
1	AB	72	GLY	2.6
8	AI	39	GLY	2.6
16	AQ	89	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	CB	204	ASN	2.6
19	AT	28	ALA	2.6
19	CT	67	ALA	2.6
38	BT	105	LEU	2.6
41	DW	82	LEU	2.6
33	BO	42	SER	2.6
44	DZ	116	VAL	2.6
60	BA	756	C	2.6
60	DA	531	C	2.6
60	DA	1983	C	2.6
16	CQ	51	TYR	2.6
20	CA	448	A	2.6
23	CY	142	THR	2.6
25	BC	161	ARG	2.6
44	DZ	69	THR	2.6
48	DN	48	MET	2.6
3	AD	40	PRO	2.6
18	AS	8	GLY	2.6
28	BF	166	ALA	2.6
39	DU	23	GLY	2.6
35	DQ	27	VAL	2.6
44	DZ	74	VAL	2.6
50	B3	47	VAL	2.6
20	AA	126	G	2.6
23	CY	354	ARG	2.6
28	BF	168	ARG	2.6
39	DU	79	PHE	2.6
6	AG	124	LEU	2.6
46	D1	51	VAL	2.6
20	AA	8	A	2.6
3	AD	58	LEU	2.6
23	CY	358	MET	2.6
39	DU	33	ARG	2.6
6	AG	58	PRO	2.6
12	AM	105	THR	2.6
23	CY	134	ALA	2.6
30	DH	166	GLY	2.6
37	BS	91	PRO	2.6
41	BW	50	VAL	2.6
7	CH	134	ILE	2.6
35	DQ	32	TYR	2.6
38	BT	106	SER	2.6

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Mol	Chain	Res	Type	RSRZ
60	DA	1266	G	2.6
19	AT	13	LEU	2.6
23	CY	232	LEU	2.6
25	DC	29	LEU	2.6
60	BA	2591	C	2.6
60	DA	970	C	2.6
1	AB	93	VAL	2.6
23	AY	163	VAL	2.6
25	DC	6	LYS	2.6
32	BK	9	LYS	2.6
46	B1	63	ALA	2.6
46	D1	74	VAL	2.6
23	AY	383	THR	2.6
29	BG	68	PRO	2.6
50	B3	29	ARG	2.6
2	CC	12	LEU	2.6
38	DT	105	LEU	2.6
10	AK	122	LYS	2.6
46	D1	63	ALA	2.6
49	B2	2	LYS	2.6
53	D7	13	ALA	2.6
20	AA	158	G	2.6
20	AA	1356	G	2.6
20	CA	326	G	2.6
28	BF	188	ARG	2.6
46	D1	34	THR	2.6
18	AS	43	GLU	2.6
27	BE	160	TYR	2.6
36	BR	75	LEU	2.6
42	BX	26	TYR	2.6
60	DA	560	C	2.6
3	AD	2	GLY	2.6
14	CO	86	GLY	2.6
40	DV	63	GLY	2.6
7	CH	135	CYS	2.6
4	CE	76	ILE	2.6
17	AR	65	ILE	2.6
51	D5	11	THR	2.6
14	AO	20	GLY	2.6
23	CY	180	VAL	2.6
32	DK	112	MET	2.6
43	DY	87	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
39	DU	10	ARG	2.6
60	BA	664	C	2.6
20	AA	68(B)	G	2.6
20	CA	653	A	2.6
36	BR	52	ILE	2.6
60	BA	2513	G	2.6
3	CD	54	TYR	2.6
3	CD	196	LEU	2.6
46	D1	25	LYS	2.6
8	CI	44	VAL	2.6
4	AE	8	GLU	2.5
7	CH	38	ILE	2.5
36	BR	67	LEU	2.5
36	BR	115	GLU	2.5
46	D1	95	LEU	2.5
51	D5	3	LYS	2.5
32	DK	29	GLN	2.5
39	DU	63	VAL	2.5
42	BX	12	VAL	2.5
19	CT	28	ALA	2.5
23	AY	210	ARG	2.5
60	BA	2068	U	2.5
60	DA	2044	C	2.5
20	CA	61	G	2.5
60	BA	1623	G	2.5
40	DV	69	LYS	2.5
8	AI	110	GLU	2.5
25	BC	124	VAL	2.5
26	DD	30	GLU	2.5
45	B0	66	VAL	2.5
49	D2	63	VAL	2.5
1	CB	130	ARG	2.5
28	BF	142	TRP	2.5
28	DF	117	ARG	2.5
33	DO	30	ALA	2.5
20	CA	1252	A	2.5
23	CY	257	PRO	2.5
46	B1	44	PRO	2.5
26	DD	218	ARG	2.5
52	D6	50	ARG	2.5
55	B9	18	ARG	2.5
60	BA	1762	A	2.5

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Mol	Chain	Res	Type	RSRZ
60	DA	1755	A	2.5
60	DA	2448	A	2.5
39	BU	46	ALA	2.5
1	AB	133	LYS	2.5
2	AC	157	ILE	2.5
19	CT	91	LEU	2.5
29	BG	135	LEU	2.5
48	BN	87	LEU	2.5
9	CJ	97	GLU	2.5
7	CH	9	MET	2.5
3	AD	167	GLY	2.5
13	AN	19	ARG	2.5
7	AH	28	ALA	2.5
23	CY	113	GLY	2.5
35	DQ	39	PRO	2.5
48	DN	101	HIS	2.5
9	CJ	55	LYS	2.5
20	AA	114	U	2.5
1	CB	108	ILE	2.5
7	CH	33	GLU	2.5
20	AA	60	A	2.5
60	BA	1765	C	2.5
60	BA	2452	C	2.5
8	CI	71	SER	2.5
27	DE	58	ARG	2.5
7	CH	112	LEU	2.5
12	AM	92	HIS	2.5
20	AA	105	G	2.5
60	DA	1980	G	2.5
11	AL	7	ILE	2.5
27	DE	83	ASP	2.5
42	BX	6	ASP	2.5
12	AM	17	VAL	2.5
20	AA	62	U	2.5
25	BC	163	GLU	2.5
12	CM	100	GLY	2.5
16	AQ	37	LYS	2.5
20	AA	68(R)	C	2.5
26	BD	8	PRO	2.5
45	D0	28	GLY	2.5
48	DN	24	GLY	2.5
14	CO	81	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
41	DW	69	LEU	2.5
51	B5	4	HIS	2.5
7	AH	52	ASP	2.5
23	CY	47	GLU	2.5
16	AQ	71	PHE	2.5
20	AA	107	G	2.5
38	DT	85	LYS	2.5
60	DA	266	G	2.5
6	AG	30	ILE	2.5
11	CL	27	LEU	2.5
44	BZ	86	VAL	2.5
3	CD	14	ARG	2.5
28	BF	62	ARG	2.5
39	BU	47	TYR	2.5
20	AA	569	C	2.5
25	DC	62	THR	2.5
60	DA	2512	C	2.5
47	B4	26	SER	2.5
49	B2	10	LEU	2.5
16	AQ	73	VAL	2.5
25	BC	165	ARG	2.5
23	CY	256	THR	2.5
28	BF	136	THR	2.5
34	BP	109	GLY	2.5
53	B7	24	THR	2.5
60	BA	226	G	2.5
60	BA	1441	G	2.5
2	AC	43	LEU	2.5
11	AL	110	VAL	2.5
27	DE	120	TRP	2.5
41	DW	29	LEU	2.5
56	Be	75	ILE	2.5
5	CF	94	GLN	2.5
30	DH	51	ARG	2.5
14	CO	78	TYR	2.5
15	AP	54	GLU	2.5
30	DH	172	LYS	2.5
60	BA	335	C	2.5
60	DA	1156	A	2.5
11	AL	6	THR	2.5
25	DC	169	THR	2.5
26	DD	144	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
36	BR	98	LEU	2.5
37	DS	47	THR	2.5
23	CY	111	SER	2.5
50	D3	35	ARG	2.5
13	AN	21	TYR	2.5
14	CO	5	LYS	2.5
46	B1	72	GLU	2.5
50	D3	7	LYS	2.5
60	BA	2233	U	2.5
20	AA	922	G	2.5
32	DK	67	PHE	2.5
29	DG	108	ASN	2.5
33	BO	19	ILE	2.5
12	AM	41	PRO	2.5
29	BG	174	GLU	2.5
23	AY	19	ALA	2.5
29	BG	24	GLY	2.5
33	BO	10	VAL	2.5
34	BP	24	GLY	2.5
35	BQ	62	GLY	2.5
26	BD	14	ARG	2.5
43	BY	85	VAL	2.5
49	B2	13	ALA	2.5
12	AM	103	THR	2.5
43	BY	95	LYS	2.5
56	De	70	LYS	2.5
20	AA	1392	G	2.5
29	DG	164	GLU	2.5
30	BH	157	TYR	2.5
60	DA	832	G	2.5
50	B3	53	LEU	2.5
4	CE	92	LYS	2.5
6	AG	78	ARG	2.5
20	AA	43	C	2.5
20	AA	315	A	2.5
30	BH	156	ALA	2.5
52	B6	52	VAL	2.5
60	BA	806	C	2.5
60	BA	1683	C	2.5
60	BA	1742	C	2.5
26	BD	255	LYS	2.5
25	DC	56	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
2	CC	19	GLU	2.5
17	CR	69	THR	2.5
28	BF	51	THR	2.5
34	BP	32	THR	2.5
3	CD	91	SER	2.5
26	DD	215	LEU	2.5
45	D0	9	SER	2.5
3	CD	117	ALA	2.5
25	BC	162	ILE	2.5
27	BE	104	VAL	2.5
36	BR	57	ARG	2.5
48	DN	46	VAL	2.5
50	B3	22	ALA	2.5
54	B8	28	GLY	2.5
40	DV	6	LYS	2.5
52	D6	38	LYS	2.5
10	CK	75	TYR	2.4
20	CA	838	G	2.4
60	BA	17	G	2.4
60	DA	1299	G	2.4
1	CB	146	GLN	2.4
23	AY	389	LEU	2.4
25	BC	88	GLU	2.4
33	BO	119	PRO	2.4
60	BA	1761	C	2.4
60	DA	2591	C	2.4
2	AC	39	ILE	2.4
6	CG	32	ARG	2.4
26	DD	31	LYS	2.4
1	AB	102	LEU	2.4
16	AQ	40	LYS	2.4
44	BZ	118	GLN	2.4
45	D0	24	LYS	2.4
28	BF	58	ALA	2.4
20	AA	622	A	2.4
20	AA	663	A	2.4
20	CA	1517	G	2.4
60	BA	271(C)	G	2.4
60	BA	2056	G	2.4
3	AD	59	ARG	2.4
3	CD	155	LEU	2.4
8	AI	40	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
23	CY	146	LEU	2.4
25	BC	152	GLU	2.4
28	DF	190	GLU	2.4
42	DX	92	LEU	2.4
43	BY	90	LEU	2.4
60	BA	2504	U	2.4
4	CE	33	VAL	2.4
28	DF	63	LYS	2.4
54	B8	39	LYS	2.4
39	DU	42	ALA	2.4
41	DW	96	ILE	2.4
50	B3	21	ALA	2.4
28	DF	41	LEU	2.4
6	AG	105	VAL	2.4
36	BR	8	ARG	2.4
29	BG	17	PRO	2.4
35	DQ	122	GLY	2.4
56	De	63	ILE	2.4
6	CG	117	ALA	2.4
14	AO	33	THR	2.4
20	AA	329	A	2.4
20	AA	927	G	2.4
26	BD	40	THR	2.4
27	BE	162	ALA	2.4
36	DR	35	THR	2.4
47	D4	26	SER	2.4
60	BA	223	A	2.4
60	DA	270(M)	U	2.4
60	BA	2110	G	2.4
60	DA	1645	G	2.4
3	AD	139	ARG	2.4
12	AM	35	GLU	2.4
18	CS	58	VAL	2.4
28	BF	163	VAL	2.4
12	AM	84	ILE	2.4
33	DO	19	ILE	2.4
29	BG	171	ALA	2.4
32	DK	20	ALA	2.4
43	DY	60	PHE	2.4
23	CY	326	THR	2.4
50	B3	18	ASP	2.4
20	CA	222	U	2.4

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Mol	Chain	Res	Type	RSRZ
23	AY	354	ARG	2.4
25	BC	80	LYS	2.4
25	DC	54	ARG	2.4
27	BE	78	LEU	2.4
44	BZ	128	VAL	2.4
16	CQ	90	ILE	2.4
20	AA	1254	C	2.4
6	AG	25	ALA	2.4
23	AY	375	GLY	2.4
29	BG	140	ILE	2.4
32	DK	97	GLY	2.4
60	DA	1597	A	2.4
20	AA	917	G	2.4
20	AA	1185	G	2.4
34	BP	145	PRO	2.4
37	DS	102	ALA	2.4
1	CB	139	LYS	2.4
18	AS	61	TYR	2.4
19	AT	22	ARG	2.4
23	CY	337	SER	2.4
33	DO	18	LYS	2.4
12	AM	8	GLU	2.4
19	CT	88	VAL	2.4
34	DP	33	ARG	2.4
39	DU	50	ARG	2.4
42	DX	66	LEU	2.4
23	AY	115	GLU	2.4
32	DK	127	ILE	2.4
34	DP	54	GLY	2.4
2	AC	30	ARG	2.4
8	AI	71	SER	2.4
8	CI	111	ARG	2.4
11	CL	86	ARG	2.4
36	BR	28	LEU	2.4
46	D1	92	LYS	2.4
20	AA	1282	C	2.4
41	BW	78	GLU	2.4
42	BX	35	THR	2.4
60	BA	2527	C	2.4
2	CC	182	ILE	2.4
54	B8	45	GLY	2.4
39	DU	41	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
60	DA	883	G	2.4
44	DZ	76	LEU	2.4
51	D5	49	CYS	2.4
3	CD	4	TYR	2.4
13	AN	25	VAL	2.4
2	CC	157	ILE	2.4
33	DO	120	GLU	2.4
9	AJ	11	PHE	2.4
26	BD	59	LYS	2.4
26	BD	102	LYS	2.4
27	DE	192	ASN	2.4
39	DU	116	ALA	2.4
53	B7	2	LYS	2.4
4	CE	105	VAL	2.4
20	AA	980	C	2.4
23	AY	341	VAL	2.4
26	DD	220	HIS	2.4
60	BA	268	C	2.4
60	BA	1569	A	2.4
35	DQ	137	TYR	2.4
3	AD	53	ASP	2.4
18	CS	49	ILE	2.4
38	DT	11	GLU	2.4
23	AY	393	ASP	2.4
43	DY	101	LYS	2.4
60	BA	2379	G	2.4
10	CK	19	ALA	2.4
6	CG	22	LEU	2.4
7	AH	93	VAL	2.4
20	AA	368	U	2.4
20	CA	1148	U	2.4
60	BA	813	U	2.4
45	D0	29	GLN	2.4
39	BU	57	PHE	2.4
39	BU	62	ILE	2.4
20	AA	923	A	2.4
23	CY	381	LYS	2.4
26	BD	180	GLY	2.4
2	CC	133	ALA	2.4
3	AD	14	ARG	2.4
11	AL	53	ARG	2.4
12	CM	18	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
12	CM	51	ALA	2.4
19	AT	15	ARG	2.4
52	D6	6	ARG	2.4
60	BA	1644	C	2.4
51	B5	57	VAL	2.4
56	Be	74	VAL	2.4
3	AD	72	GLU	2.4
33	BO	69	ILE	2.4
33	DO	68	GLU	2.4
3	CD	41	GLY	2.4
12	AM	100	GLY	2.4
23	AY	347	GLY	2.4
60	BA	2061	G	2.4
2	CC	196	LEU	2.4
6	CG	46	ALA	2.4
15	CP	52	ASP	2.4
16	AQ	57	VAL	2.4
25	BC	65	LEU	2.4
26	DD	185	VAL	2.4
48	DN	43	THR	2.4
27	DE	56	PRO	2.4
29	BG	18	GLU	2.4
3	CD	16	GLY	2.4
45	D0	54	GLY	2.4
60	DA	754	C	2.4
3	CD	107	ARG	2.4
6	CG	116	ALA	2.4
8	CI	55	ALA	2.4
9	AJ	70	ARG	2.4
36	BR	25	ALA	2.4
36	DR	12	ARG	2.4
36	DR	28	LEU	2.4
60	BA	807	U	2.4
60	BA	958	U	2.4
60	DA	913	U	2.4
3	AD	206	PHE	2.4
23	AY	108	PHE	2.4
25	DC	183	PRO	2.4
60	BA	15	G	2.4
36	DR	111	LEU	2.4
37	DS	104	GLY	2.4
43	BY	103	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
38	DT	66	VAL	2.4
44	DZ	117	LEU	2.4
45	B0	31	VAL	2.4
44	DZ	154	ASP	2.4
60	BA	1632	A	2.4
19	CT	87	LYS	2.4
25	DC	172	ILE	2.3
35	BQ	39	PRO	2.3
47	B4	23	GLU	2.3
60	BA	2897	U	2.3
1	AB	200	ILE	2.3
19	AT	29	LYS	2.3
46	D1	86	SER	2.3
12	AM	37	THR	2.3
20	AA	115	G	2.3
23	CY	576	ASP	2.3
38	BT	11	GLU	2.3
60	DA	11	G	2.3
60	DA	518	G	2.3
6	AG	23	VAL	2.3
20	CA	197	A	2.3
29	BG	40	ASN	2.3
36	BR	38	VAL	2.3
43	BY	98	VAL	2.3
60	DA	2497	A	2.3
4	AE	118	ILE	2.3
60	DA	588	U	2.3
14	AO	63	ARG	2.3
26	BD	262	ARG	2.3
6	CG	82	GLY	2.3
27	BE	182	LEU	2.3
29	BG	92	VAL	2.3
29	BG	138	GLN	2.3
29	BG	142	PRO	2.3
29	DG	65	GLY	2.3
29	DG	87	PRO	2.3
53	D7	40	TRP	2.3
38	DT	49	VAL	2.3
41	BW	48	ALA	2.3
11	AL	47	LYS	2.3
11	AL	100	ILE	2.3
23	CY	329	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
60	DA	17	G	2.3
60	DA	864	G	2.3
60	DA	2414	G	2.3
20	AA	109	A	2.3
20	AA	968	A	2.3
49	B2	21	LEU	2.3
60	BA	394	A	2.3
60	DA	294	A	2.3
20	CA	1321	C	2.3
26	DD	180	GLY	2.3
40	BV	79	VAL	2.3
60	DA	2045	C	2.3
3	AD	67	ILE	2.3
23	AY	133	ILE	2.3
32	BK	52	ILE	2.3
46	D1	66	HIS	2.3
23	AY	391	GLY	2.3
27	BE	161	GLY	2.3
38	DT	71	GLY	2.3
25	DC	205	ALA	2.3
29	DG	17	PRO	2.3
44	BZ	179	ASP	2.3
20	AA	230	G	2.3
20	AA	453	A	2.3
20	CA	1222	G	2.3
23	CY	246	ILE	2.3
60	DA	45	G	2.3
60	DA	1641	A	2.3
3	AD	155	LEU	2.3
4	CE	82	VAL	2.3
11	CL	50	SER	2.3
39	BU	68	ALA	2.3
41	DW	72	LYS	2.3
7	AH	54	ASP	2.3
18	CS	48	THR	2.3
25	DC	7	ARG	2.3
29	DG	144	ILE	2.3
38	BT	48	ILE	2.3
1	AB	129	GLU	2.3
11	AL	99	HIS	2.3
26	DD	83	GLU	2.3
42	DX	23	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
43	BY	24	VAL	2.3
2	AC	13	GLY	2.3
25	BC	133	GLY	2.3
27	DE	112	GLY	2.3
3	CD	82	ALA	2.3
7	CH	28	ALA	2.3
20	AA	303	A	2.3
20	CA	908	A	2.3
60	BA	227	A	2.3
60	DA	988	A	2.3
60	DA	1779	U	2.3
26	DD	262	ARG	2.3
60	DA	2453	A	2.3
23	CY	51	THR	2.3
35	BQ	9	TYR	2.3
47	D4	5	ILE	2.3
60	DA	756	C	2.3
60	DA	1218	C	2.3
28	BF	32	LEU	2.3
3	CD	167	GLY	2.3
29	BG	132	ASN	2.3
12	CM	55	ARG	2.3
53	D7	10	ARG	2.3
11	CL	11	VAL	2.3
13	AN	33	VAL	2.3
20	CA	323	U	2.3
23	CY	216	LEU	2.3
32	DK	96	VAL	2.3
51	D5	31	VAL	2.3
60	DA	2047	U	2.3
1	CB	163	PHE	2.3
45	B0	73	GLY	2.3
47	D4	4	GLY	2.3
60	DA	331	A	2.3
12	CM	40	ASN	2.3
20	CA	403	C	2.3
20	CA	711	G	2.3
20	CA	1059	C	2.3
42	BX	22	ALA	2.3
59	DB	30	C	2.3
60	BA	1684	C	2.3
40	DV	62	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
29	DG	171	ALA	2.3
40	DV	55	ALA	2.3
41	BW	99	ARG	2.3
42	BX	68	ARG	2.3
50	D3	29	ARG	2.3
23	AY	162	VAL	2.3
25	DC	149	ASN	2.3
48	DN	23	LEU	2.3
52	D6	34	LEU	2.3
60	DA	332	A	2.3
20	CA	554	C	2.3
60	BA	589	C	2.3
6	CG	83	ALA	2.3
11	AL	41	ARG	2.3
11	CL	26	ALA	2.3
26	DD	214	TRP	2.3
60	BA	1215	G	2.3
3	CD	194	LEU	2.3
6	AG	104	LEU	2.3
34	DP	100	LEU	2.3
19	AT	51	GLU	2.3
43	DY	64	GLU	2.3
16	AQ	83	ASP	2.3
34	DP	28	GLY	2.3
26	BD	214	TRP	2.3
48	BN	106	MET	2.3
34	BP	128	HIS	2.3
37	DS	57	LYS	2.3
41	BW	106	ILE	2.3
11	AL	11	VAL	2.3
14	CO	34	LEU	2.3
1	CB	128	GLU	2.3
4	AE	128	PRO	2.3
9	CJ	37	PRO	2.3
20	CA	924	C	2.3
44	BZ	100	VAL	2.3
44	DZ	100	VAL	2.3
25	BC	140	ASN	2.3
25	BC	166	ASN	2.3
25	BC	181	PHE	2.3
28	DF	72	ARG	2.3
29	BG	108	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
53	B7	20	ALA	2.3
2	AC	175	LEU	2.3
12	CM	53	VAL	2.3
16	AQ	29	HIS	2.3
36	DR	97	VAL	2.3
46	B1	71	TYR	2.3
11	CL	31	PRO	2.3
26	BD	211	ARG	2.3
32	DK	54	PRO	2.3
36	DR	47	PHE	2.3
37	BS	109	GLY	2.3
28	BF	43	LYS	2.3
29	DG	110	ALA	2.3
38	BT	98	LYS	2.3
39	DU	54	LYS	2.3
16	AQ	53	LEU	2.3
20	CA	883	C	2.3
20	CA	1344	C	2.3
26	DD	259	THR	2.3
59	DB	4	C	2.3
1	CB	100	GLY	2.2
16	AQ	30	PRO	2.2
20	AA	392	G	2.2
23	CY	160	ARG	2.2
26	DD	164	GLN	2.2
38	BT	69	GLY	2.2
43	DY	76	CYS	2.2
16	CQ	40	LYS	2.2
19	CT	74	LYS	2.2
2	CC	181	ASN	2.2
7	AH	111	ILE	2.2
14	CO	85	LEU	2.2
27	BE	192	ASN	2.2
29	DG	92	VAL	2.2
47	D4	14	ILE	2.2
10	AK	57	THR	2.2
3	CD	156	GLU	2.2
26	BD	188	GLU	2.2
27	BE	199	ARG	2.2
29	DG	95	ARG	2.2
7	CH	57	PRO	2.2
16	CQ	17	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
20	AA	106	C	2.2
25	DC	10	ALA	2.2
60	DA	923	C	2.2
32	BK	77	LEU	2.2
34	DP	101	VAL	2.2
20	CA	952	U	2.2
10	CK	45	GLY	2.2
14	CO	8	LYS	2.2
48	BN	2	LYS	2.2
60	DA	1442	G	2.2
60	DA	1661	G	2.2
35	BQ	12	GLN	2.2
19	AT	76	ALA	2.2
25	DC	141	PRO	2.2
29	BG	63	ILE	2.2
34	BP	127	ALA	2.2
7	AH	37	ARG	2.2
36	BR	104	ARG	2.2
60	BA	225	A	2.2
60	BA	804	A	2.2
20	AA	291	C	2.2
25	BC	156	GLU	2.2
29	DG	14	GLU	2.2
60	DA	420	C	2.2
60	DA	589	C	2.2
4	CE	80	ILE	2.2
20	CA	1348	U	2.2
25	DC	42	VAL	2.2
39	DU	113	ALA	2.2
40	DV	96	ILE	2.2
25	BC	224	ARG	2.2
32	DK	76	TYR	2.2
2	AC	35	GLU	2.2
6	CG	109	ASN	2.2
23	AY	346	LYS	2.2
60	BA	1281	G	2.2
27	BE	121	ASN	2.2
1	AB	149	LEU	2.2
28	DF	131	GLY	2.2
29	BG	4	ASP	2.2
37	BS	45	GLY	2.2
25	DC	124	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
34	DP	126	VAL	2.2
42	BX	54	VAL	2.2
46	B1	77	ALA	2.2
60	BA	2360	A	2.2
60	BA	2813	A	2.2
9	AJ	51	ARG	2.2
10	AK	53	SER	2.2
17	CR	54	ARG	2.2
50	B3	35	ARG	2.2
54	D8	48	PHE	2.2
39	BU	51	LYS	2.2
60	BA	971	C	2.2
60	DA	587	C	2.2
19	CT	103	GLY	2.2
1	CB	207	ALA	2.2
2	CC	162	GLN	2.2
7	CH	1	MET	2.2
23	AY	352	VAL	2.2
38	DT	28	VAL	2.2
38	DT	43	GLN	2.2
48	DN	54	VAL	2.2
9	CJ	68	HIS	2.2
16	CQ	25	ARG	2.2
28	BF	90	PHE	2.2
32	BK	67	PHE	2.2
49	B2	69	ARG	2.2
20	CA	68	G	2.2
41	DW	53	SER	2.2
60	BA	1622	G	2.2
15	CP	54	GLU	2.2
28	BF	101	LEU	2.2
53	D7	26	GLY	2.2
60	DA	255	A	2.2
16	AQ	44	ALA	2.2
23	CY	376	ALA	2.2
42	DX	73	ARG	2.2
25	DC	175	PRO	2.2
37	DS	94	TYR	2.2
44	BZ	68	PRO	2.2
27	DE	31	CYS	2.2
1	AB	182	ILE	2.2
1	CB	142	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
12	CM	19	LEU	2.2
44	DZ	120	ILE	2.2
44	DZ	163	LEU	2.2
54	D8	40	GLU	2.2
25	DC	27	ALA	2.2
27	BE	97	LYS	2.2
28	BF	198	ALA	2.2
38	DT	65	LYS	2.2
14	CO	33	THR	2.2
20	CA	926	G	2.2
27	DE	92	THR	2.2
60	DA	1379	A	2.2
60	DA	2813	A	2.2
20	AA	1369	C	2.2
25	BC	223	VAL	2.2
28	BF	91	GLY	2.2
51	D5	59	GLU	2.2
1	AB	161	ALA	2.2
6	CG	62	PHE	2.2
7	AH	21	LYS	2.2
19	CT	76	ALA	2.2
35	BQ	77	LYS	2.2
8	AI	88	TYR	2.2
18	AS	52	TYR	2.2
6	CG	23	VAL	2.2
29	BG	133	LEU	2.2
32	DK	55	VAL	2.2
35	DQ	94	VAL	2.2
43	DY	68	HIS	2.2
19	AT	103	GLY	2.2
23	AY	82	ILE	2.2
26	BD	167	GLY	2.2
26	BD	189	CYS	2.2
29	DG	170	ARG	2.2
33	DO	67	LYS	2.2
36	DR	14	SER	2.2
20	CA	608	A	2.2
23	CY	541	ALA	2.2
42	DX	17	ALA	2.2
60	DA	270(Z)	G	2.2
60	DA	830	G	2.2
60	DA	1699	G	2.2

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Mol	Chain	Res	Type	RSRZ
9	AJ	69	ASN	2.2
20	CA	68(Y)	C	2.2
20	CA	314	C	2.2
26	DD	206	LEU	2.2
26	DD	221	VAL	2.2
28	BF	92	PRO	2.2
30	BH	159	GLU	2.2
47	B4	9	LEU	2.2
56	De	74	VAL	2.2
60	DA	32	C	2.2
1	CB	127	ILE	2.2
18	CS	8	GLY	2.2
25	DC	160	GLY	2.2
46	B1	9	GLY	2.2
49	D2	52	ASP	2.2
33	BO	99	PHE	2.2
20	AA	125	U	2.2
2	CC	132	ARG	2.2
25	DC	213	VAL	2.2
3	CD	129	ASN	2.2
11	CL	42	THR	2.2
26	BD	243	GLY	2.2
35	BQ	63	LYS	2.2
35	DQ	23	GLY	2.2
38	DT	73	GLU	2.2
26	DD	10	THR	2.2
28	BF	69	HIS	2.2
60	DA	1637	A	2.2
56	Be	52	ALA	2.2
60	BA	16	G	2.2
60	BA	2454	G	2.2
11	AL	69	TYR	2.2
60	BA	591	C	2.2
60	DA	1694	C	2.2
10	AK	84	VAL	2.2
16	CQ	57	VAL	2.2
35	DQ	15	GLY	2.2
36	DR	110	PRO	2.2
39	BU	88	ILE	2.2
44	BZ	44	PHE	2.2
28	DF	59	TYR	2.2
20	AA	1502	A	2.2

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Mol	Chain	Res	Type	RSRZ
21	CV	4	A	2.2
25	DC	142	LYS	2.2
40	DV	93	GLU	2.2
43	BY	4	LYS	2.2
49	B2	14	ARG	2.2
20	AA	562	C	2.2
60	BA	174	C	2.2
60	BA	1764	G	2.2
26	BD	172	TYR	2.2
29	DG	19	LEU	2.2
34	DP	77	ARG	2.2
34	DP	107	LYS	2.2
36	BR	26	LYS	2.2
3	AD	81	GLU	2.2
3	AD	204	ILE	2.2
3	CD	90	GLY	2.1
3	CD	183	GLY	2.1
28	DF	127	GLU	2.2
33	DO	41	ALA	2.1
3	AD	174	LEU	2.1
6	AG	12	LEU	2.1
12	AM	34	LEU	2.1
16	CQ	10	VAL	2.1
23	CY	352	VAL	2.1
29	DG	15	VAL	2.1
30	DH	111	HIS	2.1
36	BR	111	LEU	2.1
39	DU	112	ARG	2.1
41	BW	75	TYR	2.1
42	BX	3	THR	2.1
52	B6	14	THR	2.1
27	DE	77	ILE	2.1
38	DT	48	ILE	2.1
26	DD	235	GLY	2.1
45	B0	65	GLY	2.1
60	BA	408	G	2.1
60	BA	2215	G	2.1
1	AB	130	ARG	2.1
1	AB	164	VAL	2.1
3	AD	22	LYS	2.1
4	AE	105	VAL	2.1
12	AM	31	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
17	AR	44	LEU	2.1
45	D0	32	ARG	2.1
60	BA	270(N)	U	2.1
60	DA	12	U	2.1
60	DA	1680	U	2.1
60	DA	1911	U	2.1
3	AD	154	ASN	2.1
4	CE	75	THR	2.1
9	CJ	4	ILE	2.1
25	BC	225	ILE	2.1
29	DG	18	GLU	2.1
2	AC	26	LYS	2.1
11	CL	17	LYS	2.1
12	CM	34	LEU	2.1
32	DK	38	VAL	2.1
36	DR	117	VAL	2.1
39	BU	90	VAL	2.1
39	BU	109	LEU	2.1
42	BX	70	LEU	2.1
3	AD	185	PHE	2.1
20	CA	569	C	2.1
60	DA	1909	C	2.1
12	CM	20	THR	2.1
16	CQ	13	ASP	2.1
25	BC	70	GLY	2.1
35	DQ	19	GLY	2.1
41	BW	40	ASN	2.1
46	B1	5	CYS	2.1
60	DA	411	G	2.1
60	DA	1816	G	2.1
60	DA	2714	G	2.1
60	DA	2807	G	2.1
7	AH	95	VAL	2.1
10	CK	84	VAL	2.1
23	CY	276	VAL	2.1
25	DC	158	LYS	2.1
28	BF	93	LYS	2.1
36	BR	56	LYS	2.1
29	DG	135	LEU	2.1
43	BY	50	ARG	2.1
51	B5	31	VAL	2.1
53	D7	25	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
6	AG	27	ILE	2.1
3	AD	95	GLY	2.1
20	CA	101	A	2.1
46	B1	29	GLY	2.1
52	B6	24	GLU	2.1
52	B6	35	GLU	2.1
60	BA	1780	A	2.1
25	DC	47	LYS	2.1
41	BW	34	ASN	2.1
8	CI	51	ARG	2.1
11	AL	101	VAL	2.1
12	CM	45	VAL	2.1
23	CY	575	VAL	2.1
40	DV	57	VAL	2.1
46	B1	68	PRO	2.1
60	DA	18	C	2.1
30	DH	164	TYR	2.1
60	BA	448	U	2.1
18	CS	72	GLY	2.1
25	BC	99	GLU	2.1
52	B6	15	GLU	2.1
60	DA	89	G	2.1
60	DA	1763	G	2.1
8	AI	44	VAL	2.1
9	AJ	8	LEU	2.1
30	DH	115	VAL	2.1
30	DH	163	TYR	2.1
34	DP	97	PRO	2.1
9	AJ	4	ILE	2.1
60	BA	2361	A	2.1
60	BA	2734	A	2.1
12	CM	26	GLY	2.1
20	AA	1049	U	2.1
25	DC	147	GLY	2.1
33	BO	18	LYS	2.1
34	BP	7	ARG	2.1
59	BB	8	U	2.1
6	CG	100	ALA	2.1
10	CK	24	SER	2.1
25	BC	169	THR	2.1
42	DX	13	LEU	2.1
4	AE	84	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
14	AO	36	ILE	2.1
35	BQ	126	PRO	2.1
20	CA	157	G	2.1
20	CA	1058	G	2.1
60	BA	88	G	2.1
60	BA	1299	G	2.1
60	DA	1171	G	2.1
28	DF	138	GLU	2.1
7	CH	30	ARG	2.1
19	CT	57	ARG	2.1
23	CY	74	TRP	2.1
35	BQ	22	LYS	2.1
42	DX	62	LYS	2.1
53	B7	40	TRP	2.1
7	CH	110	ALA	2.1
20	CA	152	A	2.1
20	CA	611	A	2.1
60	DA	632	A	2.1
23	AY	340	TYR	2.1
60	DA	2743	C	2.1
4	AE	86	ALA	2.1
11	AL	83	VAL	2.1
25	BC	60	ARG	2.1
36	DR	7	GLY	2.1
28	BF	26	ALA	2.1
29	BG	56	ALA	2.1
37	DS	46	VAL	2.1
23	CY	212	TYR	2.1
60	BA	1699	G	2.1
60	DA	940	G	2.1
60	DA	2358	G	2.1
30	BH	52	VAL	2.1
43	DY	23	ARG	2.1
60	DA	2590	A	2.1
18	AS	20	LEU	2.1
60	BA	2613	U	2.1
60	DA	441	U	2.1
2	CC	134	ILE	2.1
20	CA	322	C	2.1
36	BR	27	SER	2.1
36	BR	59	ASP	2.1
2	CC	138	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
4	AE	103	GLY	2.1
28	DF	37	VAL	2.1
32	DK	87	GLY	2.1
27	DE	11	MET	2.1
43	BY	5	MET	2.1
2	CC	170	GLN	2.1
20	AA	156	G	2.1
20	CA	855	G	2.1
48	BN	78	TYR	2.1
60	DA	270(K)	G	2.1
60	DA	2468	G	2.1
2	CC	15	THR	2.1
12	CM	94	ARG	2.1
60	BA	265	A	2.1
60	BA	819	A	2.1
60	BA	2336	A	2.1
12	CM	86	CYS	2.1
14	CO	39	LEU	2.1
26	DD	232	PRO	2.1
27	DE	148	GLY	2.1
20	AA	962	C	2.1
20	AA	1404	C	2.1
20	CA	352	C	2.1
23	AY	313	ALA	2.1
60	BA	672	C	2.1
32	DK	52	ILE	2.1
1	AB	82	ARG	2.1
3	AD	17	VAL	2.1
3	AD	203	VAL	2.1
3	CD	113	SER	2.1
12	AM	91	ARG	2.1
27	DE	190	GLY	2.1
36	DR	13	HIS	2.1
37	BS	24	LEU	2.1
40	DV	18	LEU	2.1
3	AD	79	PHE	2.1
20	AA	1184	G	2.1
20	CA	871	U	2.1
30	DH	160	LYS	2.1
35	DQ	36	ALA	2.1
7	AH	86	ILE	2.1
44	BZ	57	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
60	BA	407	G	2.1
60	DA	882	G	2.1
60	DA	1647	G	2.1
6	CG	13	GLN	2.1
3	CD	19	LEU	2.1
20	AA	972	C	2.1
27	DE	72	VAL	2.1
28	BF	148	LEU	2.1
40	BV	101	GLY	2.1
40	DV	39	LEU	2.1
60	BA	1754	C	2.1
60	BA	2742	C	2.1
60	DA	270(L)	C	2.1
14	AO	16	ALA	2.1
23	CY	275	ALA	2.1
30	BH	106	THR	2.1
26	BD	104	TYR	2.1
28	BF	164	ARG	2.1
1	AB	81	VAL	2.1
4	CE	139	LEU	2.1
20	AA	1506	U	2.1
44	DZ	33	LEU	2.1
60	DA	421	U	2.1
9	AJ	97	GLU	2.1
19	AT	101	GLY	2.1
23	AY	350	GLU	2.1
39	BU	89	GLU	2.1
15	AP	43	LYS	2.0
60	DA	2589	A	2.0
6	CG	39	ALA	2.0
20	AA	886	G	2.0
20	AA	1343	G	2.0
23	AY	209	ALA	2.0
42	DX	22	ALA	2.0
7	CH	54	ASP	2.0
23	AY	212	TYR	2.0
28	BF	149	ASP	2.0
44	BZ	124	ILE	2.0
20	AA	454	C	2.0
23	AY	377	VAL	2.0
59	DB	88	C	2.0
60	DA	163(B)	C	2.0

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Mol	Chain	Res	Type	RSRZ
7	CH	116	LYS	2.0
26	DD	15	PHE	2.0
54	D8	35	GLN	2.0
42	BX	40	LYS	2.0
46	D1	29	GLY	2.0
53	B7	17	GLY	2.0
3	CD	141	ARG	2.0
4	AE	19	MET	2.0
19	AT	37	SER	2.0
27	BE	95	ILE	2.0
28	BF	22	ALA	2.0
28	BF	199	TRP	2.0
60	DA	1033	U	2.0
29	BG	166	ASP	2.0
60	DA	529	A	2.0
20	AA	310	G	2.0
20	CA	710	G	2.0
60	DA	1191	G	2.0
60	DA	2553	G	2.0
1	AB	68	ILE	2.0
1	CB	92	TYR	2.0
13	AN	12	ARG	2.0
20	AA	1321	C	2.0
26	DD	62	TYR	2.0
36	DR	16	HIS	2.0
49	B2	26	ARG	2.0
60	BA	270(L)	C	2.0
23	CY	273	LEU	2.0
28	BF	140	LEU	2.0
30	BH	115	VAL	2.0
38	DT	61	PHE	2.0
40	DV	2	PHE	2.0
50	B3	17	LYS	2.0
32	BK	24	GLY	2.0
14	CO	36	ILE	2.0
29	BG	110	ALA	2.0
6	AG	44	TYR	2.0
11	CL	104	VAL	2.0
20	CA	1268	A	2.0
23	CY	342	TYR	2.0
60	BA	781	A	2.0
60	DA	1307	A	2.0

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Mol	Chain	Res	Type	RSRZ
30	DH	68	THR	2.0
35	BQ	98	LYS	2.0
14	AO	21	ASP	2.0
2	CC	24	ALA	2.0
6	AG	50	ILE	2.0
11	CL	15	ARG	2.0
22	CW	75	C	2.0
60	BA	1505	C	2.0
60	BA	2179	C	2.0
60	DA	898	C	2.0
60	DA	1280	G	2.0
33	BO	82	ASN	2.0
36	DR	25	ALA	2.0
60	DA	1350	C	2.0
10	CK	73	MET	2.0
2	CC	173	VAL	2.0
20	AA	1240	U	2.0
20	CA	1196	U	2.0
44	DZ	75	ASN	2.0
1	CB	67	THR	2.0
8	AI	58	ARG	2.0
10	CK	32	ILE	2.0
20	AA	919	A	2.0
44	BZ	172	ALA	2.0
53	B7	33	ARG	2.0
1	CB	149	LEU	2.0
36	DR	65	LEU	2.0
49	B2	65	ASN	2.0
52	B6	45	LYS	2.0
20	CA	450	G	2.0
20	CA	1187	G	2.0
25	DC	156	GLU	2.0
60	BA	264	C	2.0
60	DA	1506	C	2.0
44	DZ	81	ARG	2.0
1	CB	205	ASP	2.0
2	CC	37	GLN	2.0
26	DD	205	VAL	2.0
2	CC	154	SER	2.0
11	AL	109	GLY	2.0
23	CY	350	GLU	2.0
34	DP	44	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
44	DZ	153	SER	2.0
48	BN	100	GLU	2.0
60	DA	394	A	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
24	UAL	AU	5	9/10	0.89	0.18	65,65,65,65	0
24	DPP	CU	2	6/7	0.92	0.10	65,65,65,65	0
24	KBE	CU	1	9/10	0.92	0.30	65,65,65,65	0
24	KBE	AU	1	9/10	0.93	1.01	65,65,65,65	0
24	UAL	CU	5	9/10	0.94	0.10	65,65,65,65	0
24	DPP	AU	2	6/7	0.96	0.12	65,65,65,65	0
24	5OH	AU	6	12/13	0.96	0.25	99,101,102,102	0
24	5OH	CU	6	12/13	0.97	0.09	99,101,102,102	0

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, 95th 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.

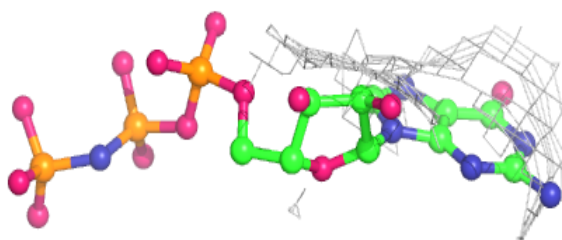
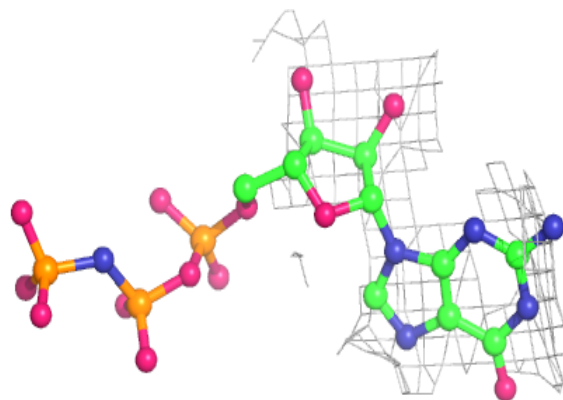
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
61	GNP	CY	702	32/32	0.94	0.13	58,71,81,83	0
61	GNP	AY	701	32/32	0.95	0.20	58,71,81,83	0
62	MG	AY	702	1/1	0.96	0.20	124,124,124,124	0
62	MG	CY	701	1/1	0.97	0.11	104,104,104,104	0

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.

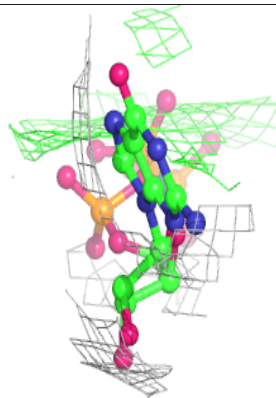
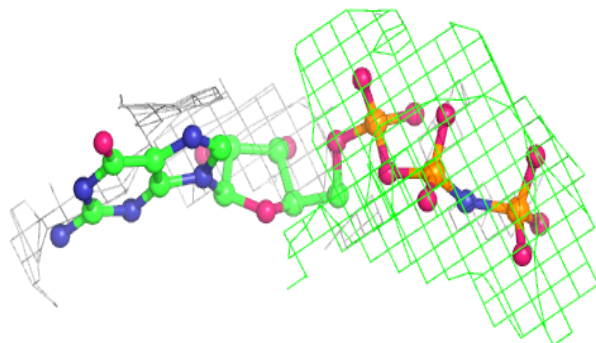
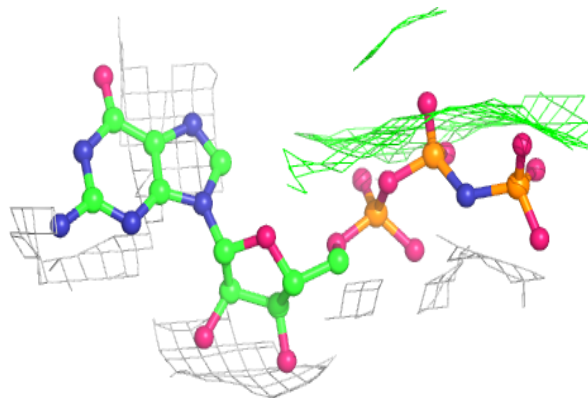
Electron density around GNP CY 702:

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



Electron density around GNP AY 701:

$2mF_o-DF_c$ (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.