



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 10:51 PM EST

PDB ID : 3J9M
EMDB ID : EMD-2876
Title : Structure of the human mitochondrial ribosome (class 1)
Authors : Amunts, A.; Brown, A.; Toots, J.; Scheres, S.H.; Ramakrishnan, V.
Deposited on : 2015-02-08
Resolution : 3.50 Å (reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

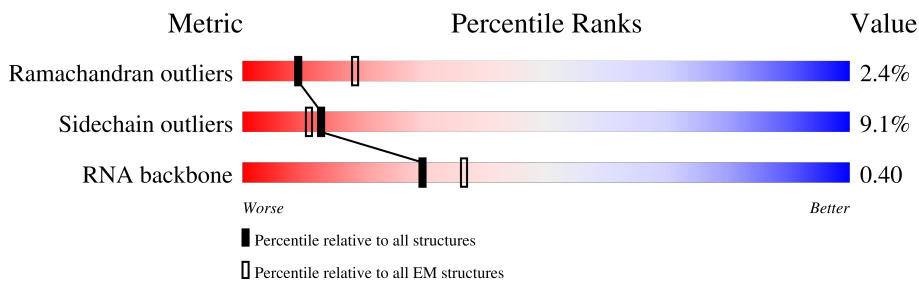
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1559	
2	B	73	
3	D	305	
4	E	348	
5	F	311	
6	H	267	
7	I	261	
8	J	192	
9	K	178	









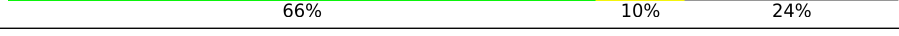

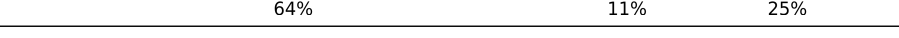
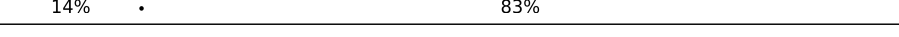

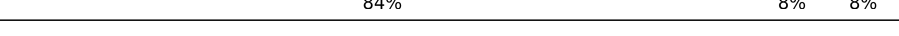


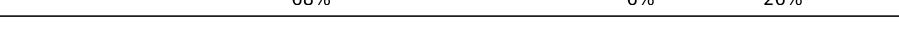

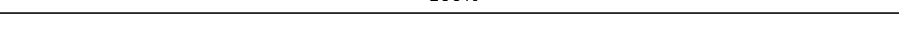






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Mol	Chain	Length	Quality of chain
10	L	145	71% 8% 21%
11	M	296	86% 11%
12	N	251	73% 8% 18%
13	O	175	74% 12% 13%
14	P	179	65% 8% 26%
15	Q	292	67% 7% 25%
16	R	149	83% 10% 6%
17	S	205	70% 6% 24%
18	T	212	75% 22%
19	U	153	63% 9% 27%
20	V	216	80% 7% 12%
21	W	148	69% 6% 25%
22	X	256	85% 9% 5%
23	Y	250	65% 6% 30%
24	Z	161	68% 6% 25%
25	0	188	47% 9% 43%
26	1	65	69% 11% 20%
27	2	92	46% 50%
28	3	188	47% 49%
29	4	103	31% 65%
30	5	423	79% 10% 11%
31	6	380	78% 8% 14%
32	7	338	74% 5% 21%
33	8	206	46% 52%
34	9	137	73% 7% 20%

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Mol	Chain	Length	Quality of chain
35	a	142	
36	b	155	
37	c	332	
38	d	306	
39	e	279	
40	f	194	
41	g	166	
42	h	158	
43	i	128	
44	j	123	
45	k	112	
46	l	138	
47	m	128	
48	o	102	
49	p	206	
50	q	222	
51	r	196	
52	s	439	
53	t	28	
54	u	2	
55	AA	954	
56	AB	296	
57	AC	167	
58	AD	430	
59	AE	125	


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Mol	Chain	Length	Quality of chain
60	AF	242	
61	AG	396	
62	AH	201	
63	AI	194	
64	AJ	138	
65	AK	128	
66	AL	257	
67	AM	137	
68	AN	130	
69	AO	258	
70	AP	142	
71	AQ	87	
72	AR	360	
73	AS	190	
74	AT	173	
75	AU	205	
76	AV	414	
77	AW	187	
78	AX	398	
79	AY	395	
80	AZ	106	
81	A0	218	
82	A1	323	
83	A2	118	
84	A3	199	

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Mol	Chain	Length	Quality of chain
85	A4	579	 A horizontal bar chart representing the quality of the chain. The bar is divided into two segments: a green segment on the left labeled '69%' and a grey segment on the right labeled '28%'. A small yellow dot is located at the boundary between the green and grey segments.

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 158384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1472	31261	14025	5642	10122	1472	0	0

- Molecule 2 is a RNA chain called mt-tRNAVal.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	56	1191	534	214	387	56	0	0

- Molecule 3 is a protein called uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	236	1842	1145	373	315	9	0	0

- Molecule 4 is a protein called uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	300	2365	1523	410	422	10	0	0

- Molecule 5 is a protein called uL4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	250	2013	1294	365	348	6	0	0

- Molecule 6 is a protein called bL9m.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
6	H	95	784	498	152	134	0	0

- Molecule 7 is a protein called uL10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	158	1283	828	235	210	10	0	0

- Molecule 8 is a protein called uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	140	1061	680	192	187	2	0	0

- Molecule 9 is a protein called uL13m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	177	1451	934	259	251	7	0	0

- Molecule 10 is a protein called uL14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	115	889	559	171	154	5	0	0

- Molecule 11 is a protein called uL15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	287	2305	1472	425	402	6	0	0

- Molecule 12 is a protein called uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	N	205	1654	1056	308	280	10	0	0

- Molecule 13 is a protein called bL17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	O	152	1245	784	239	215	7	0	0

- Molecule 14 is a protein called uL18m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	133	Total	C	N	O	S	0	0
			1080	677	209	189	5		

- Molecule 15 is a protein called bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	219	Total	C	N	O	S	0	0
			1822	1168	322	323	9		

- Molecule 16 is a protein called bL20m.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	140	Total	C	N	O	S	0	0
			1153	732	231	186	4		

- Molecule 17 is a protein called bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	156	Total	C	N	O	S	0	0
			1251	806	222	219	4		

- Molecule 18 is a protein called uL22m.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	166	Total	C	N	O	S	0	0
			1368	875	254	232	7		

- Molecule 19 is a protein called uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	111	Total	C	N	O	S	0	0
			922	591	176	153	2		

- Molecule 20 is a protein called uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	189	Total	C	N	O	S	0	0
			1551	987	278	278	8		

- Molecule 21 is a protein called bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	111	Total	C	N	O	S	0	0
			871	558	164	146	3		

- Molecule 22 is a protein called bL28m.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	243	Total	C	N	O	S	0	0
			2027	1310	350	362	5		

- Molecule 23 is a protein called uL29m.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	176	Total	C	N	O	S	0	0
			1517	970	291	252	4		

- Molecule 24 is a protein called uL30m.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	120	Total	C	N	O	S	0	0
			978	626	183	166	3		

- Molecule 25 is a protein called bL32m.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 26 is a protein called bL33m.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 27 is a protein called bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	46	Total	C	N	O	S	0	0
			376	233	83	59	1		

- Molecule 28 is a protein called bL35m.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	36	Total	C	N	O	S	0	0
			322	203	70	46	3		

- Molecule 30 is a protein called mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	376	Total	C	N	O	S	0	0
			3064	1987	529	538	10		

- Molecule 31 is a protein called mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	6	325	Total	C	N	O	S	0	0
			2636	1692	465	470	9		

- Molecule 32 is a protein called mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	7	266	Total	C	N	O	S	0	0
			2158	1383	371	388	16		

- Molecule 33 is a protein called mL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 34 is a protein called mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	9	109	Total	C	N	O	S	0	0
			873	565	152	154	2		

- Molecule 35 is a protein called mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 36 is a protein called mL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	148	Total	C	N	O	S	0	0
			1178	733	229	213	3		

- Molecule 37 is a protein called mL44.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	275	Total	C	N	O	S	0	0
			2217	1415	383	410	9		

- Molecule 38 is a protein called mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	162	Total	C	N	O	S	0	0
			1347	870	234	235	8		

- Molecule 39 is a protein called mL46.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	217	Total	C	N	O	S	0	0
			1762	1124	310	323	5		

- Molecule 40 is a protein called mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	f	131	Total	C	N	O	S	0	0
			1039	663	169	203	4		

- Molecule 41 is a protein called mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	g	129	Total	C	N	O	S	0	0
			1067	690	185	190	2		

- Molecule 42 is a protein called mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	h	100	Total	C	N	O	S	0	0
			827	524	146	155	2		

- Molecule 43 is a protein called mL51.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	i	97	Total	C	N	O	S	0	0
			827	532	165	126	4		

- Molecule 44 is a protein called mL52.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	j	85	Total	C	N	O	S	0	0
			684	423	133	126	2		

- Molecule 45 is a protein called mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	k	84	Total	C	N	O	S	0	0
			655	407	122	121	5		

- Molecule 46 is a protein called mL54.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	l	23	Total	C	N	O	0	0
			221	137	52	32		

- Molecule 47 is a protein called bL31m.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	m	45	Total	C	N	O	S	0	0
			372	232	76	62	2		

- Molecule 48 is a protein called mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	94	Total	C	N	O	S	0	0
			797	501	165	128	3		

- Molecule 49 is a protein called mL62 (ICT1).

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	127	Total	C	N	O	S	0	0
			1058	661	201	192	4		

- Molecule 50 is a protein called mL64 (CRIF1).

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 51 is a protein called mL66 (bS18a).

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	146	Total	C	N	O	S	0	0
			1203	764	232	199	8		

- Molecule 52 is a protein called mL65 (mS30).

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	370	Total	C	N	O	S	0	0
			3036	1946	542	534	14		

- Molecule 53 is a protein called Unknown protein/protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 54 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 55 is a RNA chain called 12S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AA	923	Total	C	N	O	P	0	0
			19606	8790	3535	6358	923		

- Molecule 56 is a protein called uS2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	AB	217	1768	1131	321	306	10	0	0

- Molecule 57 is a protein called uS3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	AC	132	1082	699	195	184	4	0	0

- Molecule 58 is a protein called uS5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	AD	322	2557	1611	476	457	13	0	0

- Molecule 59 is a protein called bS6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	AE	122	972	614	177	177	4	0	0

- Molecule 60 is a protein called uS7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	AF	201	1668	1069	305	283	11	0	0

- Molecule 61 is a protein called uS9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	AG	305	2516	1599	448	455	14	0	0

- Molecule 62 is a protein called uS10m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	AH	122	999	643	168	185	3	0	0

- Molecule 63 is a protein called uS11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AI	136	Total	C	N	O	S	0	0
			1011	637	192	178	4		

- Molecule 64 is a protein called uS12m.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	AJ	108	Total	C	N	O	S	0	0
			838	521	169	142	6		

- Molecule 65 is a protein called uS14m.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AK	101	Total	C	N	O	S	0	0
			861	537	179	140	5		

- Molecule 66 is a protein called uS15m.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	AL	164	Total	C	N	O	S	0	0
			1382	883	257	235	7		

- Molecule 67 is a protein called bS16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AM	116	Total	C	N	O	S	0	0
			920	582	182	150	6		

- Molecule 68 is a protein called uS17m.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	AN	107	Total	C	N	O	S	0	0
			846	549	153	141	3		

- Molecule 69 is a protein called mS40 (bS18b).

Mol	Chain	Residues	Atoms					AltConf	Trace
69	AO	185	Total	C	N	O	S	0	0
			1528	970	285	267	6		

- Molecule 70 is a protein called bS18m (bS18c).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	AP	96	774	498	133	135	8	0	0

- Molecule 71 is a protein called bs21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	AQ	86	740	458	150	124	8	0	0

- Molecule 72 is a protein called mS22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	AR	242	2008	1285	343	372	8	0	0

- Molecule 73 is a protein called mS23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	AS	126	1042	673	183	185	1	0	0

- Molecule 74 is a protein called mS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	AT	162	1330	850	231	238	11	0	0

- Molecule 75 is a protein called mS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	AU	173	1461	900	294	263	4	0	0

- Molecule 76 is a protein called mS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	AV	328	2702	1737	452	502	11	0	0

- Molecule 77 is a protein called bs1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AW	97	Total	C	N	O	S	0	0
			766	486	137	139	4		

- Molecule 78 is a protein called mS29.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	AX	316	Total	C	N	O	S	0	0
			2531	1625	440	455	11		

- Molecule 79 is a protein called mS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	AY	108	Total	C	N	O	S	0	0
			914	593	150	169	2		

- Molecule 80 is a protein called mS33.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	AZ	87	Total	C	N	O	S	0	0
			740	473	133	130	4		

- Molecule 81 is a protein called mS34.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	A0	201	Total	C	N	O	S	0	0
			1684	1065	322	292	5		

- Molecule 82 is a protein called mS35.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	A1	256	Total	C	N	O	S	0	0
			2076	1321	350	395	10		

- Molecule 83 is a protein called mS37.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	A2	116	Total	C	N	O	S	0	0
			925	574	181	162	8		

- Molecule 84 is a protein called mS38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
84	A3	69	610	393	130	86	1	0	0

- Molecule 85 is a protein called mS39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
85	A4	414	2838	1805	490	529	14	0	0

- Molecule 86 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	A	97	Total	Mg	0
			97	97	
86	M	1	Total	Mg	0
			1	1	
86	g	1	Total	Mg	0
			1	1	
86	AA	28	Total	Mg	0
			28	28	

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

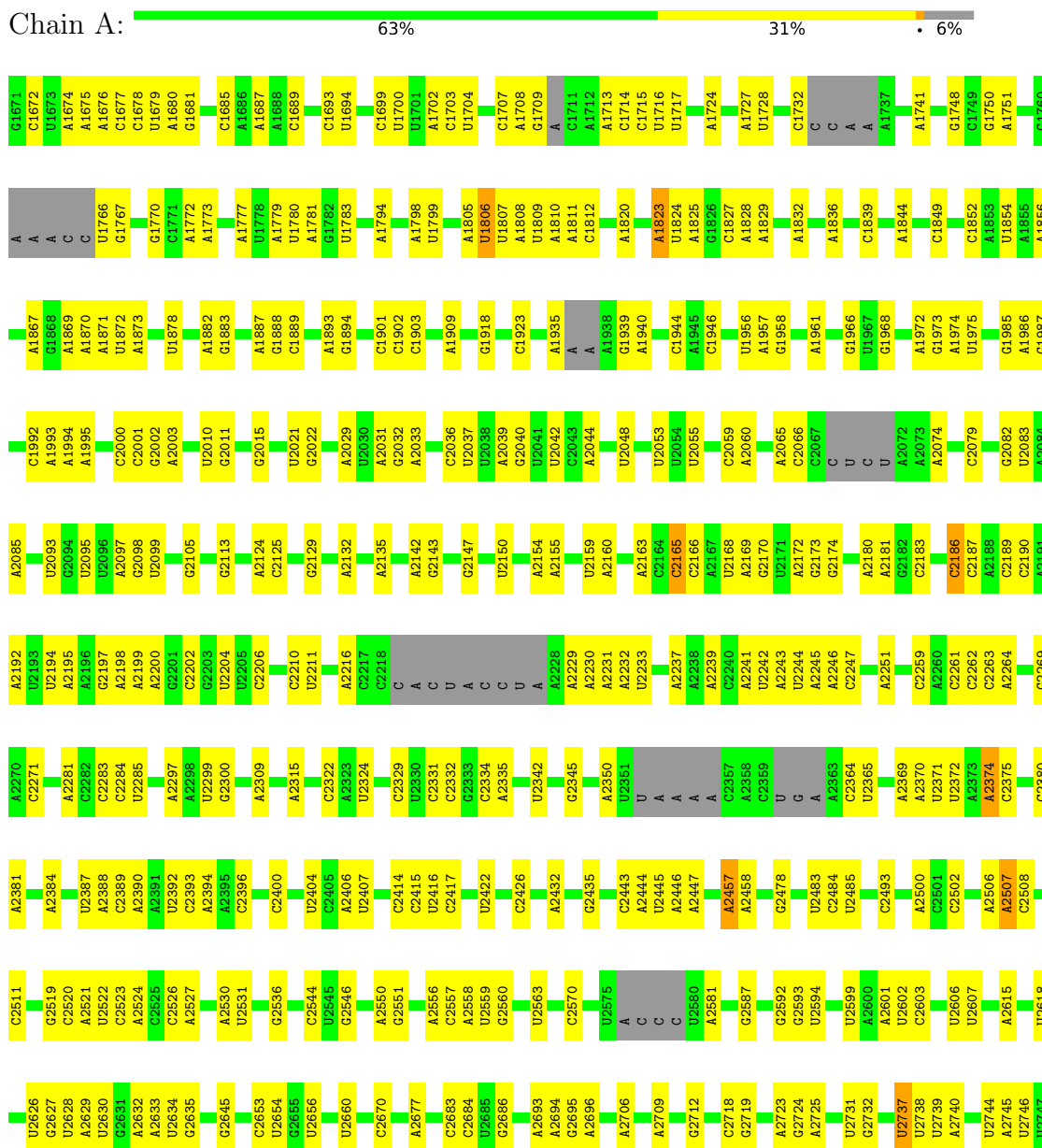
Mol	Chain	Residues	Atoms		AltConf
87	0	1	Total	Zn	0
			1	1	
87	4	1	Total	Zn	0
			1	1	
87	r	1	Total	Zn	0
			1	1	
87	AB	1	Total	Zn	0
			1	1	
87	AO	1	Total	Zn	0
			1	1	
87	AP	1	Total	Zn	0
			1	1	
87	AT	1	Total	Zn	0
			1	1	

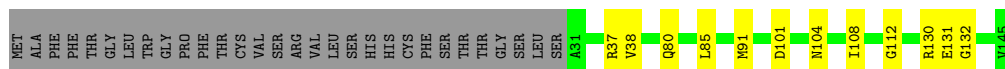
- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

3 Residue-property plots [i](#)

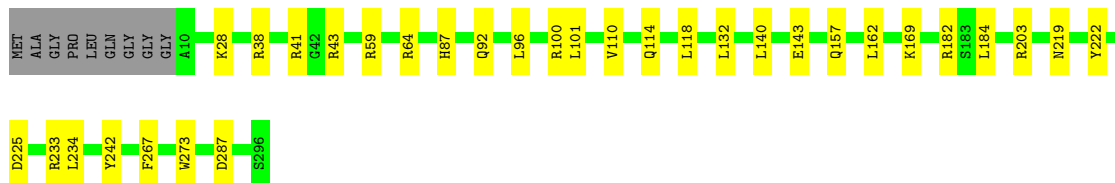
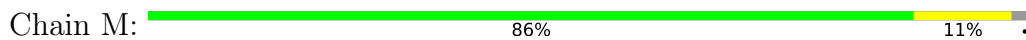
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: 16S rRNA

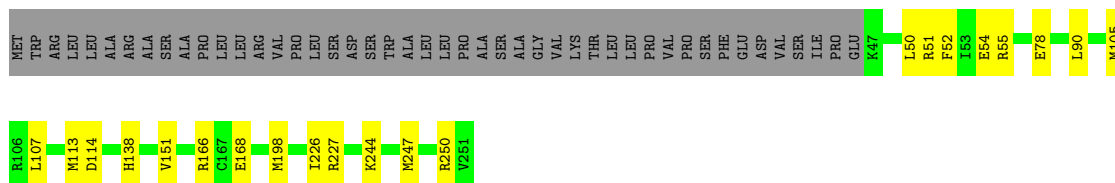




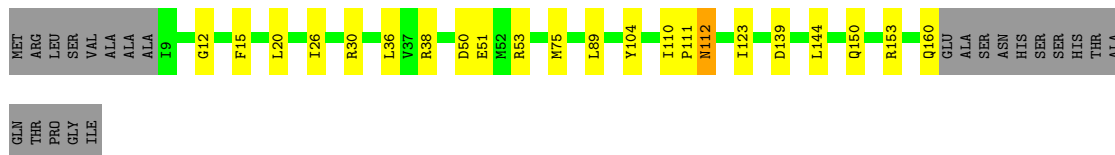
• Molecule 11: uL15m



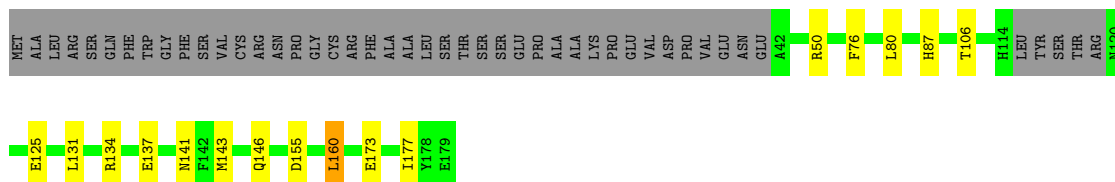
• Molecule 12: uL16m



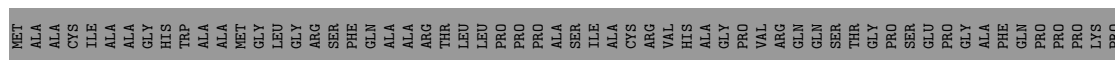
• Molecule 13: bL17m



• Molecule 14: uL18m

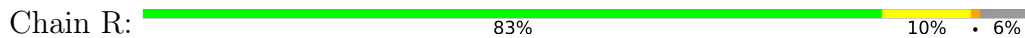


• Molecule 15: bL19m

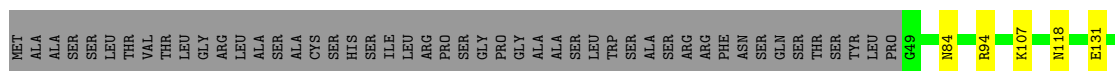




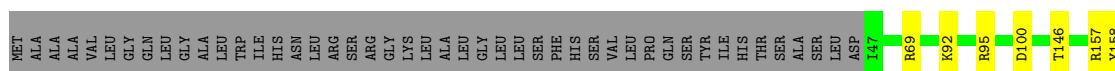
• Molecule 16: bL20m



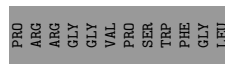
• Molecule 17: bL21m



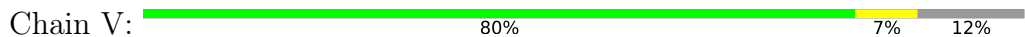
• Molecule 18: uL22m



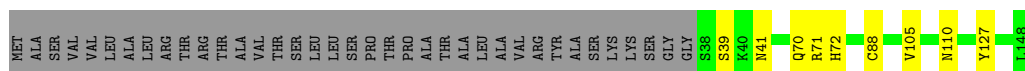
• Molecule 19: uL23m



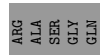
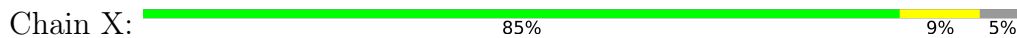
• Molecule 20: uL24m



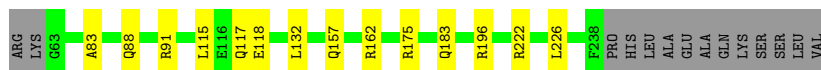
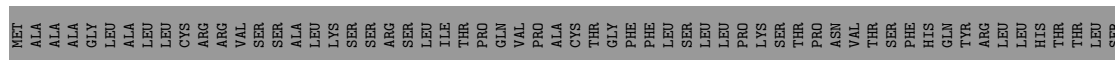
• Molecule 21: bL27m



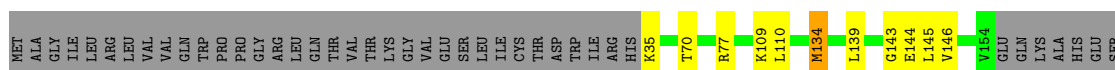
• Molecule 22: bL28m



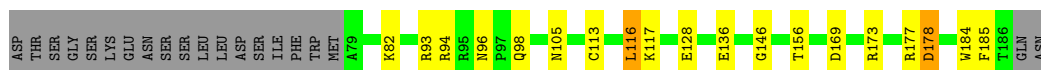
• Molecule 23: uL29m



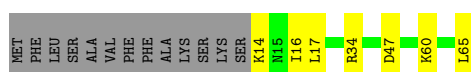
• Molecule 24: uL30m



• Molecule 25: bL32m

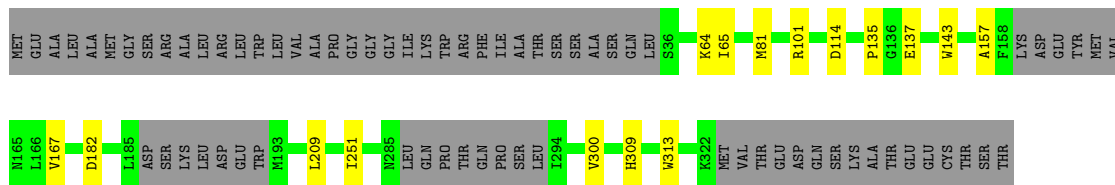


• Molecule 26: bL33m

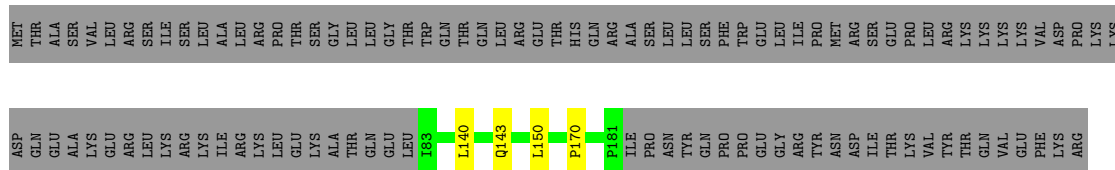


• Molecule 27: bL34m





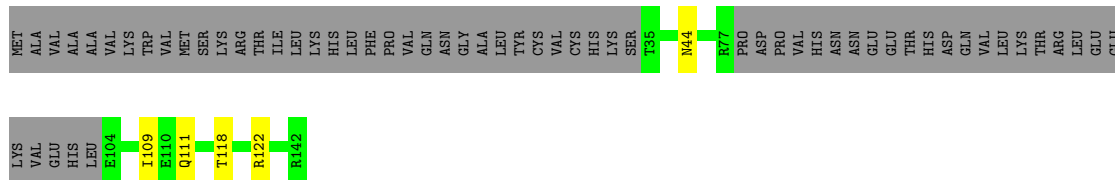
• Molecule 33: mL40



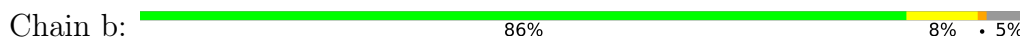
• Molecule 34: mL41



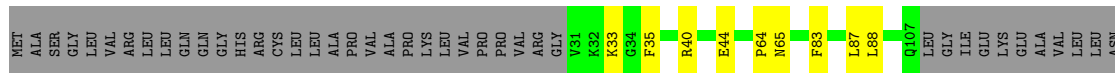
• Molecule 35: mL42



• Molecule 36: mL43

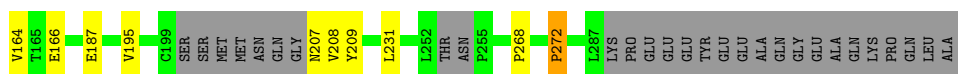
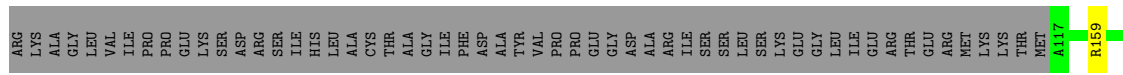
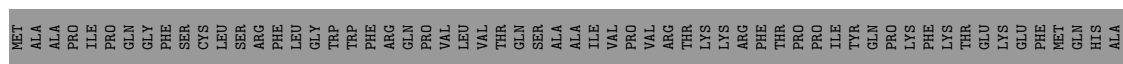


• Molecule 37: mL44

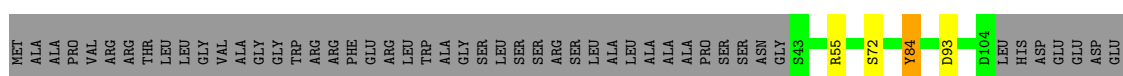




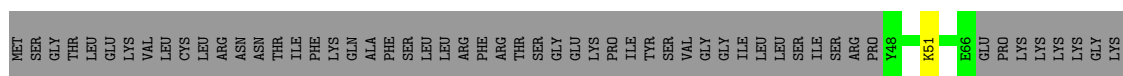
• Molecule 38: mL45



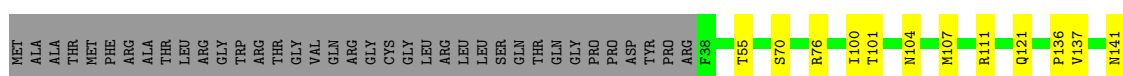
• Molecule 39: mL46



• Molecule 40: mL48




• Molecule 41: mL49



• Molecule 42: mL50

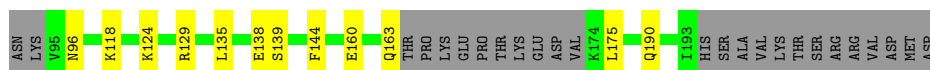
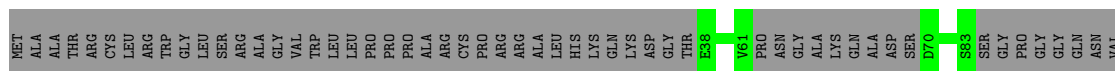


Chain o:  84% 8% 8%



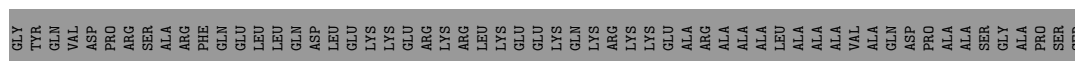
• Molecule 49: mL62 (ICT1)

Chain p:  56% 6% 38%



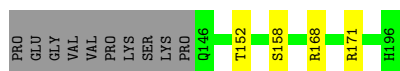
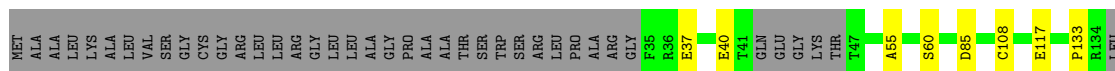
• Molecule 50: mL64 (CRIF1)

Chain q:  53% 5% 42%




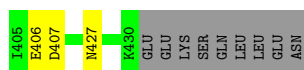
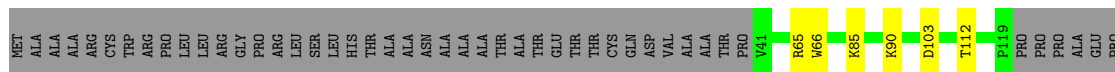
• Molecule 51: mL66 (bS18a)

Chain r:  68% 6% 26%



• Molecule 52: mL65 (mS30)

Chain s:  77% 7% 16%



• Molecule 53: Unknown protein/protein extension

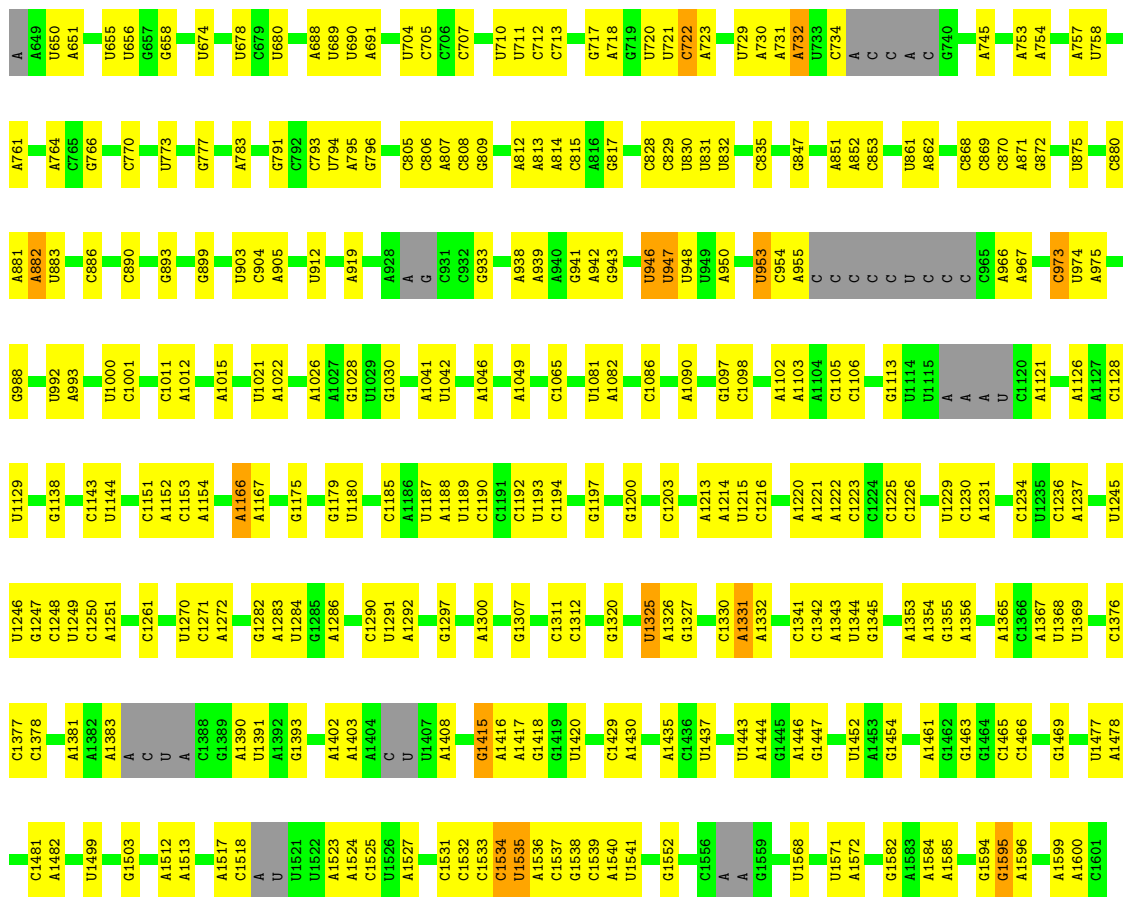


There are no outlier residues recorded for this chain.

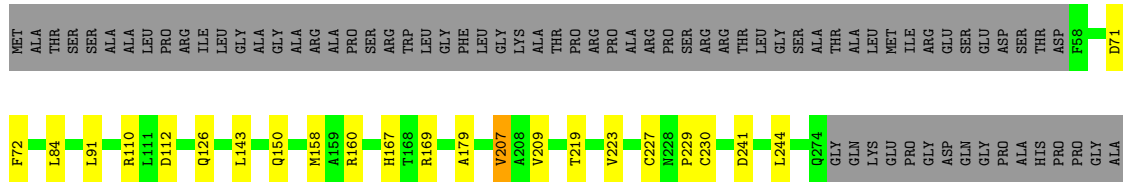
• Molecule 54: E-site tRNA



• Molecule 55: 12S rRNA

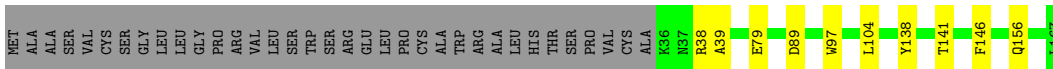


• Molecule 56: uS2m

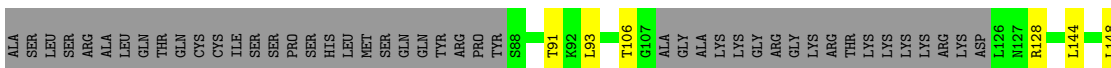
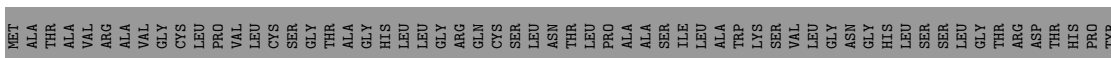


ASP
MET
SER
HIS
SER
LEU

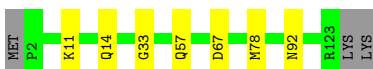
• Molecule 57: uS3m



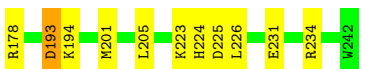
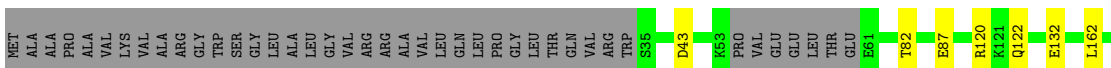
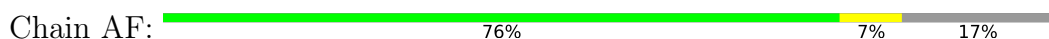
• Molecule 58: uS5m



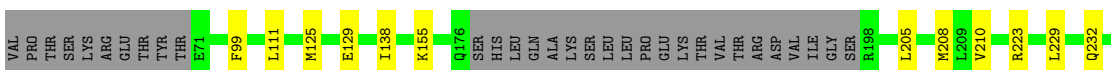
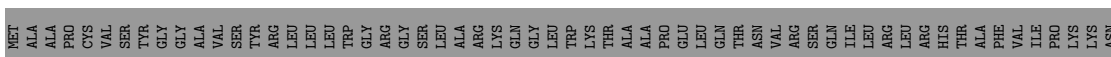
• Molecule 59: bS6m



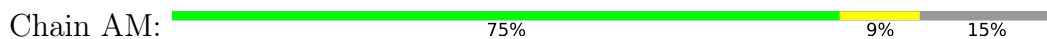
• Molecule 60: uS7m



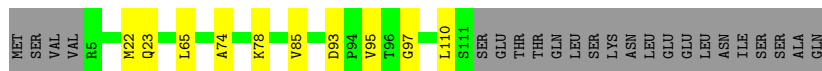
• Molecule 61: uS9m



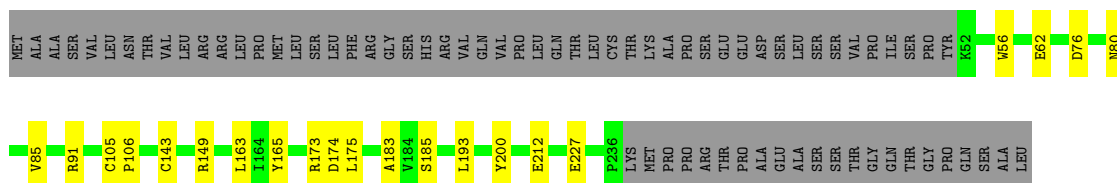
• Molecule 67: bS16m



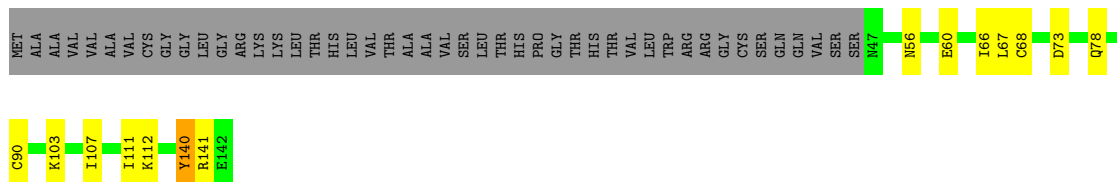
• Molecule 68: uS17m



• Molecule 69: mS40 (bS18b)



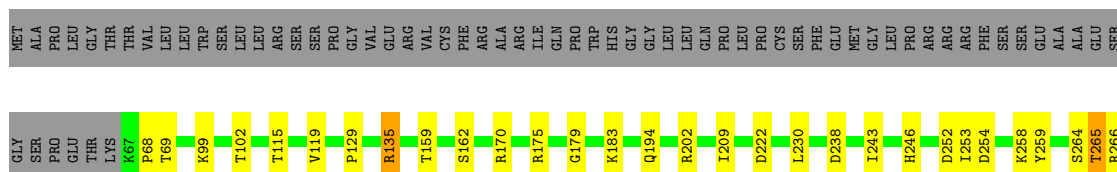
• Molecule 70: bS18m (bS18c)



• Molecule 71: bS21m

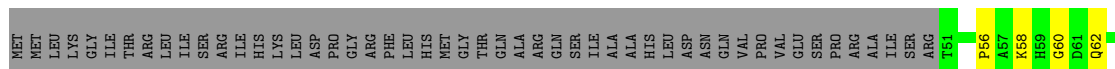


• Molecule 72: mS22

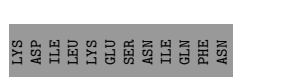
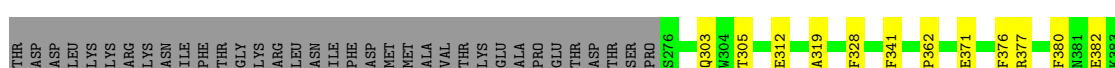
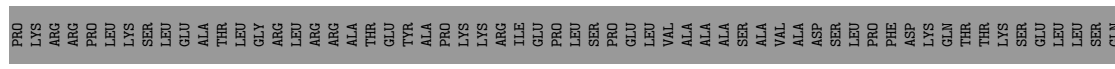
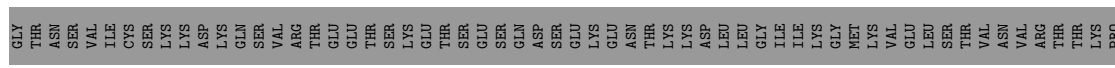
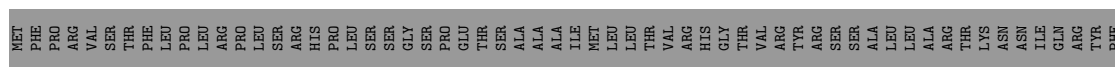




• Molecule 78: mS29



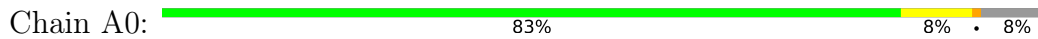
• Molecule 79: mS31



• Molecule 80: mS33



• Molecule 81: mS34



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	884122	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS, FEI TITAN KRIOS	Depositor
Voltage (kV)	300, 300, 300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1500, 1500, 1500, 1500	Depositor
Maximum defocus (nm)	3500, 3500, 3500, 3500	Depositor
Magnification	104478, 104478, 104478, 104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

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: ZN, GDP, MG

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	A	0.27	0/34967	0.75	14/54407 (0.0%)
2	B	0.22	0/1328	0.67	1/2056 (0.0%)
3	D	0.39	1/1879 (0.1%)	0.73	0/2527
4	E	0.37	0/2433	0.69	0/3299
5	F	0.39	0/2071	0.73	0/2817
6	H	0.41	0/798	0.72	0/1073
7	I	0.42	0/1308	0.79	0/1761
8	J	0.42	0/1077	0.73	0/1452
9	K	0.45	0/1495	0.78	1/2029 (0.0%)
10	L	0.35	0/904	0.70	0/1218
11	M	0.44	0/2359	0.78	0/3185
12	N	0.38	0/1697	0.72	0/2281
13	O	0.42	0/1269	0.84	0/1708
14	P	0.42	0/1103	0.77	1/1491 (0.1%)
15	Q	0.43	0/1863	0.73	1/2509 (0.0%)
16	R	0.43	0/1174	0.86	0/1572
17	S	0.37	0/1276	0.71	0/1729
18	T	0.37	0/1402	0.73	0/1886
19	U	0.39	0/946	0.77	0/1283
20	V	0.39	0/1590	0.67	0/2151
21	W	0.35	0/893	0.70	0/1204
22	X	0.42	0/2081	0.73	0/2812
23	Y	0.43	0/1552	0.80	0/2079
24	Z	0.36	0/1003	0.68	0/1354
25	0	0.44	0/895	0.80	0/1201
26	1	0.37	0/438	0.70	0/583
27	2	0.40	0/382	0.97	1/507 (0.2%)
28	3	0.39	0/852	0.74	1/1136 (0.1%)
29	4	0.36	0/329	0.71	0/435
30	5	0.41	0/3154	0.75	1/4295 (0.0%)
31	6	0.41	0/2722	0.71	0/3709
32	7	0.39	0/2207	0.69	0/2978

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	8	0.42	0/855	0.73	0/1152
34	9	0.40	0/896	0.73	0/1205
35	a	0.40	0/709	0.61	0/963
36	b	0.39	0/1202	0.74	0/1626
37	c	0.42	0/2264	0.76	0/3059
38	d	0.40	0/1385	0.65	0/1877
39	e	0.40	0/1797	0.66	1/2422 (0.0%)
40	f	0.38	0/1055	0.61	0/1427
41	g	0.39	0/1102	0.69	0/1503
42	h	0.43	0/847	0.74	0/1150
43	i	0.42	0/849	0.86	0/1135
44	j	0.43	0/698	0.79	0/940
45	k	0.46	0/665	0.73	0/897
46	l	0.45	0/226	0.87	0/299
47	m	0.38	0/379	0.70	0/510
48	o	0.44	0/818	0.88	0/1097
49	p	0.38	0/1071	0.68	0/1433
50	q	0.46	0/1107	0.76	0/1498
51	r	0.39	0/1238	0.67	0/1676
52	s	0.40	0/3114	0.73	0/4225
54	u	0.29	0/46	1.12	0/69
55	AA	0.25	0/21926	0.76	17/34121 (0.0%)
56	AB	0.42	0/1811	0.79	0/2451
57	AC	0.41	0/1112	0.67	0/1505
58	AD	0.46	2/2607 (0.1%)	0.73	0/3498
59	AE	0.38	0/989	0.78	0/1335
60	AF	0.42	0/1708	0.80	0/2291
61	AG	0.41	0/2570	0.75	0/3443
62	AH	0.39	0/1019	0.73	0/1379
63	AI	0.36	0/1031	0.69	0/1390
64	AJ	0.36	0/854	0.67	0/1148
65	AK	0.40	0/879	0.85	1/1182 (0.1%)
66	AL	0.43	0/1406	0.79	0/1878
67	AM	0.41	0/941	0.82	0/1265
68	AN	0.35	0/864	0.66	0/1169
69	AO	0.41	0/1580	0.73	0/2150
70	AP	0.42	0/791	0.71	0/1062
71	AQ	0.42	0/752	0.91	0/1001
72	AR	0.44	0/2050	0.82	4/2770 (0.1%)
73	AS	0.43	0/1069	0.75	0/1441
74	AT	0.40	0/1361	0.73	0/1829
75	AU	0.43	0/1482	0.84	0/1987
76	AV	0.45	0/2758	0.83	2/3724 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
77	AW	0.41	0/778	0.74	0/1048
78	AX	0.44	0/2596	0.76	3/3519 (0.1%)
79	AY	0.57	2/943 (0.2%)	0.71	0/1274
80	AZ	0.45	0/757	0.82	0/1011
81	A0	0.40	0/1727	0.78	1/2338 (0.0%)
82	A1	0.41	0/2121	0.70	1/2873 (0.0%)
83	A2	0.42	0/939	0.79	0/1256
84	A3	0.43	0/621	0.92	0/820
85	A4	0.42	0/2137	0.75	0/2872
All	All	0.37	5/165949 (0.0%)	0.75	51/235920 (0.0%)

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
8	J	0	1
15	Q	0	1
58	AD	0	1
72	AR	0	1
74	AT	0	1
78	AX	0	2
80	AZ	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	AY	371	GLU	CD-OE1	8.47	1.34	1.25
79	AY	371	GLU	CD-OE2	7.81	1.34	1.25
58	AD	283	GLU	CD-OE2	7.25	1.33	1.25
58	AD	283	GLU	CD-OE1	6.94	1.33	1.25
3	D	115	GLU	CD-OE1	5.13	1.31	1.25

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	947	U	N1-C1'-C2'	-12.05	98.33	114.00
55	AA	946	U	N1-C1'-C2'	-9.06	102.04	112.00
55	AA	1596	A	N9-C1'-C2'	-8.73	102.40	112.00
72	AR	135	ARG	NE-CZ-NH2	7.44	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2507	A	C2'-C3'-O3'	7.32	125.61	109.50
55	AA	953	U	C2'-C3'-O3'	7.05	125.02	109.50
55	AA	1595	G	N9-C1'-C2'	-6.80	104.52	112.00
1	A	2807	U	C5'-C4'-O4'	6.74	117.19	109.10
55	AA	973	C	N1-C1'-C2'	-6.60	104.74	112.00
55	AA	1415	G	C2'-C3'-O3'	6.57	124.21	113.70
81	A0	118	LEU	CA-CB-CG	6.54	130.33	115.30
55	AA	1325	U	N1-C1'-C2'	-6.35	105.02	112.00
55	AA	722	C	C2'-C3'-O3'	6.26	123.71	113.70
82	A1	229	LEU	CA-CB-CG	6.25	129.69	115.30
55	AA	882	A	C2'-C3'-O3'	6.19	123.61	113.70
1	A	2457	A	C2'-C3'-O3'	6.08	123.42	113.70
55	AA	1535	U	C2'-C3'-O3'	6.04	123.37	113.70
76	AV	107	TRP	CA-CB-CG	6.03	125.15	113.70
1	A	2737	U	O4'-C1'-N1	6.00	113.00	108.20
28	3	169	ARG	NE-CZ-NH1	5.97	123.28	120.30
55	AA	1166	A	C2'-C3'-O3'	5.94	123.20	113.70
9	K	145	LEU	CA-CB-CG	5.90	128.88	115.30
1	A	2165	C	C2'-C3'-O3'	5.73	122.87	113.70
1	A	3092	U	C2'-C3'-O3'	5.66	122.75	113.70
15	Q	215	VAL	C-N-CD	5.54	140.04	128.40
65	AK	63	LEU	CA-CB-CG	5.53	128.02	115.30
1	A	1806	U	C2'-C3'-O3'	5.51	122.51	113.70
1	A	2374	A	C2'-C3'-O3'	5.49	122.49	113.70
1	A	2737	U	C5'-C4'-O4'	5.48	115.68	109.10
55	AA	947	U	P-O3'-C3'	5.48	126.27	119.70
1	A	2186	C	C2'-C3'-O3'	5.45	122.41	113.70
1	A	2737	U	C1'-O4'-C4'	-5.44	105.55	109.90
72	AR	265	THR	CA-C-N	5.42	129.13	117.20
78	AX	222	LEU	CA-CB-CG	5.27	127.42	115.30
72	AR	265	THR	C-N-CA	5.22	134.76	121.70
55	AA	1331	A	C2'-C3'-O3'	5.17	121.97	113.70
1	A	2807	U	O4'-C4'-C3'	-5.15	98.85	104.00
55	AA	1534	C	C2'-C3'-O3'	5.14	121.92	113.70
39	e	258	ASP	CB-CG-OD2	5.11	122.90	118.30
78	AX	397	TYR	CB-CA-C	-5.08	100.23	110.40
14	P	160	LEU	CA-CB-CG	5.08	126.98	115.30
30	5	257	TYR	C-N-CD	5.08	139.06	128.40
76	AV	75	LEU	CA-CB-CG	5.08	126.98	115.30
27	2	60	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	1823	A	C2'-C3'-O3'	5.06	121.80	113.70
2	B	1607	U	C2'-C3'-O3'	5.06	121.79	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	AA	1596	A	C4'-C3'-O3'	5.03	123.07	113.00
78	AX	397	TYR	CA-CB-CG	5.03	122.95	113.40
72	AR	265	THR	CB-CA-C	5.02	125.14	111.60
1	A	3041	U	C2'-C3'-O3'	5.01	121.72	113.70
55	AA	732	A	N9-C1'-C2'	-5.01	106.49	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
58	AD	287	ASP	Peptide
72	AR	265	THR	Peptide
74	AT	147	VAL	Peptide
78	AX	94	PHE	Peptide
78	AX	95	SER	Peptide
80	AZ	89	ARG	Peptide
8	J	30	MET	Peptide
15	Q	215	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
3	D	234/305 (77%)	214 (92%)	18 (8%)	2 (1%)	17	56
4	E	296/348 (85%)	266 (90%)	20 (7%)	10 (3%)	3	28
5	F	248/311 (80%)	228 (92%)	13 (5%)	7 (3%)	5	32
6	H	93/267 (35%)	84 (90%)	8 (9%)	1 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	I	154/261 (59%)	139 (90%)	11 (7%)	4 (3%)	5	33
8	J	138/192 (72%)	126 (91%)	11 (8%)	1 (1%)	22	61
9	K	175/178 (98%)	156 (89%)	11 (6%)	8 (5%)	2	21
10	L	113/145 (78%)	100 (88%)	11 (10%)	2 (2%)	8	41
11	M	285/296 (96%)	247 (87%)	34 (12%)	4 (1%)	11	46
12	N	203/251 (81%)	186 (92%)	16 (8%)	1 (0%)	29	68
13	O	150/175 (86%)	130 (87%)	16 (11%)	4 (3%)	5	33
14	P	129/179 (72%)	117 (91%)	9 (7%)	3 (2%)	6	36
15	Q	217/292 (74%)	186 (86%)	22 (10%)	9 (4%)	3	23
16	R	138/149 (93%)	126 (91%)	9 (6%)	3 (2%)	6	37
17	S	154/205 (75%)	141 (92%)	11 (7%)	2 (1%)	12	48
18	T	164/212 (77%)	154 (94%)	7 (4%)	3 (2%)	8	41
19	U	109/153 (71%)	95 (87%)	10 (9%)	4 (4%)	3	26
20	V	183/216 (85%)	159 (87%)	20 (11%)	4 (2%)	6	37
21	W	109/148 (74%)	100 (92%)	6 (6%)	3 (3%)	5	32
22	X	241/256 (94%)	211 (88%)	22 (9%)	8 (3%)	4	28
23	Y	174/250 (70%)	162 (93%)	9 (5%)	3 (2%)	9	42
24	Z	118/161 (73%)	110 (93%)	5 (4%)	3 (2%)	5	34
25	0	106/188 (56%)	93 (88%)	8 (8%)	5 (5%)	2	20
26	1	50/65 (77%)	44 (88%)	5 (10%)	1 (2%)	7	39
27	2	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	88 (95%)	4 (4%)	1 (1%)	14	52
29	4	34/103 (33%)	34 (100%)	0	0	100	100
30	5	368/423 (87%)	326 (89%)	32 (9%)	10 (3%)	5	33
31	6	313/380 (82%)	281 (90%)	25 (8%)	7 (2%)	6	37
32	7	258/338 (76%)	226 (88%)	28 (11%)	4 (2%)	9	43
33	8	97/206 (47%)	90 (93%)	6 (6%)	1 (1%)	15	54
34	9	105/137 (77%)	92 (88%)	10 (10%)	3 (3%)	4	31
35	a	78/142 (55%)	74 (95%)	3 (4%)	1 (1%)	12	48
36	b	146/155 (94%)	127 (87%)	16 (11%)	3 (2%)	7	38
37	c	271/332 (82%)	236 (87%)	28 (10%)	7 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	d	156/306 (51%)	137 (88%)	12 (8%)	7 (4%)	2	21
39	e	211/279 (76%)	193 (92%)	14 (7%)	4 (2%)	8	40
40	f	125/194 (64%)	115 (92%)	6 (5%)	4 (3%)	4	29
41	g	127/166 (76%)	114 (90%)	8 (6%)	5 (4%)	3	25
42	h	96/158 (61%)	82 (85%)	9 (9%)	5 (5%)	2	18
43	i	95/128 (74%)	76 (80%)	16 (17%)	3 (3%)	4	29
44	j	83/123 (68%)	77 (93%)	4 (5%)	2 (2%)	6	35
45	k	82/112 (73%)	64 (78%)	12 (15%)	6 (7%)	1	11
46	l	21/138 (15%)	20 (95%)	1 (5%)	0	100	100
47	m	43/128 (34%)	39 (91%)	4 (9%)	0	100	100
48	o	92/102 (90%)	77 (84%)	12 (13%)	3 (3%)	4	28
49	p	119/206 (58%)	113 (95%)	4 (3%)	2 (2%)	9	42
50	q	126/222 (57%)	118 (94%)	8 (6%)	0	100	100
51	r	140/196 (71%)	124 (89%)	13 (9%)	3 (2%)	7	38
52	s	366/439 (83%)	332 (91%)	28 (8%)	6 (2%)	9	43
56	AB	215/296 (73%)	193 (90%)	18 (8%)	4 (2%)	8	40
57	AC	130/167 (78%)	117 (90%)	12 (9%)	1 (1%)	19	58
58	AD	316/430 (74%)	284 (90%)	28 (9%)	4 (1%)	12	48
59	AE	120/125 (96%)	114 (95%)	5 (4%)	1 (1%)	19	58
60	AF	197/242 (81%)	183 (93%)	12 (6%)	2 (1%)	15	54
61	AG	301/396 (76%)	265 (88%)	30 (10%)	6 (2%)	7	39
62	AH	120/201 (60%)	105 (88%)	11 (9%)	4 (3%)	4	28
63	AI	134/194 (69%)	116 (87%)	11 (8%)	7 (5%)	2	18
64	AJ	106/138 (77%)	91 (86%)	14 (13%)	1 (1%)	17	56
65	AK	99/128 (77%)	96 (97%)	2 (2%)	1 (1%)	15	54
66	AL	162/257 (63%)	148 (91%)	13 (8%)	1 (1%)	25	64
67	AM	114/137 (83%)	105 (92%)	9 (8%)	0	100	100
68	AN	105/130 (81%)	94 (90%)	8 (8%)	3 (3%)	4	31
69	AO	183/258 (71%)	157 (86%)	21 (12%)	5 (3%)	5	33
70	AP	94/142 (66%)	85 (90%)	6 (6%)	3 (3%)	4	29
71	AQ	84/87 (97%)	75 (89%)	6 (7%)	3 (4%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
72	AR	240/360 (67%)	202 (84%)	28 (12%)	10 (4%)	3	23
73	AS	124/190 (65%)	110 (89%)	14 (11%)	0	100	100
74	AT	160/173 (92%)	144 (90%)	8 (5%)	8 (5%)	2	19
75	AU	171/205 (83%)	163 (95%)	8 (5%)	0	100	100
76	AV	320/414 (77%)	283 (88%)	29 (9%)	8 (2%)	5	34
77	AW	95/187 (51%)	82 (86%)	9 (10%)	4 (4%)	3	23
78	AX	310/398 (78%)	263 (85%)	30 (10%)	17 (6%)	2	17
79	AY	106/395 (27%)	95 (90%)	8 (8%)	3 (3%)	5	32
80	AZ	85/106 (80%)	72 (85%)	8 (9%)	5 (6%)	1	15
81	A0	197/218 (90%)	175 (89%)	19 (10%)	3 (2%)	10	45
82	A1	252/323 (78%)	212 (84%)	34 (14%)	6 (2%)	6	35
83	A2	114/118 (97%)	97 (85%)	13 (11%)	4 (4%)	3	27
84	A3	67/199 (34%)	62 (92%)	4 (6%)	1 (2%)	10	45
85	A4	237/579 (41%)	230 (97%)	5 (2%)	2 (1%)	19	58
All	All	12628/17789 (71%)	11290 (89%)	1039 (8%)	299 (2%)	9	35

All (299) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	170	LEU
4	E	245	THR
5	F	223	HIS
7	I	102	VAL
8	J	70	ILE
9	K	15	ALA
9	K	115	ASN
11	M	242	TYR
13	O	112	ASN
17	S	94	ARG
19	U	79	ARG
22	X	69	ILE
22	X	127	VAL
24	Z	134	MET
25	0	178	ASP
30	5	190	SER
30	5	263	ILE
30	5	420	HIS

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Mol	Chain	Res	Type
32	7	251	ILE
33	8	170	PRO
34	9	131	TYR
36	b	69	PRO
36	b	116	ARG
37	c	64	PRO
37	c	123	GLN
37	c	314	TRP
38	d	164	VAL
38	d	231	LEU
38	d	272	PRO
39	e	174	PRO
40	f	164	ALA
40	f	190	THR
42	h	65	ASP
42	h	147	ASN
43	i	99	GLY
45	k	61	GLU
45	k	62	PRO
52	s	285	GLY
56	AB	179	ALA
56	AB	230	CYS
60	AF	193	ASP
61	AG	210	VAL
61	AG	315	PHE
61	AG	392	THR
63	AI	116	GLY
64	AJ	104	GLU
69	AO	183	ALA
70	AP	66	ILE
70	AP	141	ARG
71	AQ	81	ALA
71	AQ	85	GLN
72	AR	179	GLY
74	AT	131	PRO
74	AT	137	ARG
76	AV	156	ASN
76	AV	251	TRP
77	AW	109	GLU
78	AX	97	ALA
78	AX	149	ASP
78	AX	251	SER

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Mol	Chain	Res	Type
78	AX	364	ASN
79	AY	328	PHE
80	AZ	21	GLU
80	AZ	54	ASN
83	A2	60	GLU
85	A4	68	VAL
3	D	67	LYS
4	E	292	HIS
5	F	117	ARG
9	K	3	SER
9	K	143	GLU
11	M	287	ASP
12	N	78	GLU
15	Q	214	LYS
16	R	12	ASN
16	R	143	SER
17	S	140	ASN
18	T	158	TYR
19	U	46	MET
20	V	155	PRO
20	V	171	ILE
22	X	139	TYR
22	X	221	LYS
25	0	146	GLY
25	0	184	TRP
31	6	307	HIS
32	7	157	ALA
32	7	309	HIS
37	c	264	THR
38	d	187	GLU
39	e	151	ARG
40	f	90	VAL
41	g	145	GLY
42	h	146	SER
43	i	59	ASN
43	i	65	ASN
44	j	34	ALA
45	k	18	VAL
48	o	14	GLY
48	o	15	ARG
49	p	139	SER
49	p	190	GLN

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Mol	Chain	Res	Type
52	s	364	GLY
57	AC	39	ALA
58	AD	196	ASN
60	AF	194	LYS
61	AG	261	GLN
62	AH	62	VAL
62	AH	75	ARG
62	AH	126	ILE
63	AI	94	ASN
63	AI	184	ASN
69	AO	56	TRP
72	AR	69	THR
72	AR	202	ARG
72	AR	279	LYS
72	AR	292	ASP
76	AV	198	TRP
78	AX	95	SER
78	AX	152	ILE
78	AX	164	ASN
78	AX	250	GLN
78	AX	343	ILE
79	AY	319	ALA
80	AZ	89	ARG
81	A0	108	ASN
81	A0	112	GLY
82	A1	149	ILE
4	E	326	GLU
5	F	59	ARG
7	I	172	PRO
9	K	47	TYR
15	Q	76	LEU
15	Q	212	ASN
18	T	95	ARG
20	V	118	ARG
21	W	39	SER
21	W	72	HIS
22	X	177	HIS
25	0	177	ARG
30	5	35	VAL
30	5	383	TYR
31	6	73	THR
34	9	46	SER

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Mol	Chain	Res	Type
37	c	35	PHE
41	g	70	SER
44	j	40	TYR
51	r	158	SER
52	s	85	LYS
61	AG	321	ASP
63	AI	156	PRO
66	AL	80	PRO
68	AN	22	MET
68	AN	74	ALA
69	AO	185	SER
70	AP	140	TYR
72	AR	68	PRO
72	AR	264	SER
74	AT	132	ARG
76	AV	155	GLU
76	AV	197	SER
77	AW	149	LEU
78	AX	120	PRO
80	AZ	22	VAL
82	A1	63	ASP
82	A1	71	PRO
83	A2	16	PRO
85	A4	132	ILE
4	E	126	ASP
4	E	127	CYS
5	F	92	ARG
6	H	61	LYS
9	K	151	ILE
14	P	173	GLU
15	Q	216	PRO
16	R	137	GLU
18	T	69	ARG
19	U	12	LEU
21	W	127	TYR
22	X	81	GLY
26	1	60	LYS
30	5	296	LYS
31	6	130	VAL
31	6	350	TYR
31	6	351	HIS
35	a	44	ASN

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Mol	Chain	Res	Type
36	b	117	LYS
38	d	268	PRO
39	e	84	TYR
39	e	245	GLN
41	g	101	THR
41	g	104	ASN
42	h	66	LEU
48	o	50	SER
51	r	133	PRO
52	s	250	PHE
58	AD	299	LYS
62	AH	147	HIS
63	AI	60	PHE
74	AT	149	CYS
74	AT	152	LEU
78	AX	301	TRP
79	AY	362	PRO
80	AZ	20	GLY
83	A2	11	ALA
83	A2	61	PHE
4	E	141	LYS
4	E	322	ASP
5	F	128	TRP
5	F	142	ARG
7	I	61	HIS
11	M	143	GLU
14	P	87	HIS
14	P	177	ILE
15	Q	147	ALA
15	Q	171	VAL
15	Q	211	PRO
15	Q	242	GLY
19	U	34	ALA
20	V	178	SER
22	X	52	ILE
23	Y	162	ARG
23	Y	183	GLN
24	Z	146	VAL
25	0	116	LEU
30	5	272	ASP
30	5	297	ALA
31	6	165	ALA

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Mol	Chain	Res	Type
38	d	195	VAL
38	d	208	VAL
40	f	83	GLY
42	h	138	SER
52	s	264	ILE
56	AB	229	PRO
63	AI	157	GLY
65	AK	81	ASP
68	AN	97	GLY
71	AQ	86	GLY
72	AR	162	SER
74	AT	126	PRO
77	AW	144	LEU
77	AW	166	ASN
78	AX	94	PHE
78	AX	325	PRO
82	A1	53	LEU
84	A3	185	ALA
3	D	281	TRP
4	E	241	GLY
4	E	317	PRO
5	F	222	THR
10	L	112	GLY
11	M	110	VAL
13	O	15	PHE
23	Y	83	ALA
24	Z	143	GLY
28	3	95	THR
34	9	121	PRO
41	g	137	VAL
45	k	37	VAL
45	k	73	ARG
51	r	55	ALA
52	s	272	PRO
58	AD	148	LEU
58	AD	423	SER
61	AG	138	ILE
74	AT	148	PRO
76	AV	44	GLU
76	AV	132	LYS
78	AX	156	PRO
82	A1	240	GLU

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Mol	Chain	Res	Type
13	O	111	PRO
30	5	270	ILE
32	7	135	PRO
37	c	313	PRO
56	AB	207	VAL
81	A0	69	GLY
82	A1	195	GLY
7	I	178	GLY
13	O	12	GLY
45	k	78	GLY
74	AT	72	PRO
78	AX	56	PRO
78	AX	342	PRO
9	K	23	GLY
10	L	132	GLY
15	Q	108	ILE
22	X	174	PRO
59	AE	33	GLY
9	K	148	PRO
31	6	68	PRO
37	c	250	VAL
63	AI	145	ILE
69	AO	200	TYR
76	AV	212	GLY
30	5	305	GLN
69	AO	106	PRO
72	AR	270	GLY
78	AX	60	GLY
72	AR	129	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 PDB entries followed by that with respect to all EM entries.

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
3	D	190/245 (78%)	173 (91%)	17 (9%)	9 37
4	E	255/290 (88%)	233 (91%)	22 (9%)	10 38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	217/262 (83%)	198 (91%)	19 (9%)	10	38
6	H	86/228 (38%)	83 (96%)	3 (4%)	36	67
7	I	145/232 (62%)	133 (92%)	12 (8%)	11	40
8	J	113/150 (75%)	103 (91%)	10 (9%)	10	38
9	K	155/156 (99%)	145 (94%)	10 (6%)	17	50
10	L	98/124 (79%)	88 (90%)	10 (10%)	7	32
11	M	245/249 (98%)	217 (89%)	28 (11%)	5	26
12	N	172/211 (82%)	152 (88%)	20 (12%)	5	26
13	O	133/150 (89%)	114 (86%)	19 (14%)	3	19
14	P	115/154 (75%)	102 (89%)	13 (11%)	6	27
15	Q	201/256 (78%)	187 (93%)	14 (7%)	15	46
16	R	118/126 (94%)	104 (88%)	14 (12%)	5	25
17	S	141/180 (78%)	130 (92%)	11 (8%)	12	42
18	T	146/182 (80%)	141 (97%)	5 (3%)	37	68
19	U	99/135 (73%)	89 (90%)	10 (10%)	7	32
20	V	169/191 (88%)	157 (93%)	12 (7%)	14	46
21	W	91/119 (76%)	85 (93%)	6 (7%)	16	49
22	X	217/227 (96%)	199 (92%)	18 (8%)	11	40
23	Y	159/223 (71%)	148 (93%)	11 (7%)	15	47
24	Z	111/147 (76%)	102 (92%)	9 (8%)	11	41
25	0	97/164 (59%)	81 (84%)	16 (16%)	2	13
26	1	49/60 (82%)	43 (88%)	6 (12%)	5	23
27	2	40/72 (56%)	37 (92%)	3 (8%)	13	43
28	3	88/166 (53%)	83 (94%)	5 (6%)	20	53
29	4	35/89 (39%)	31 (89%)	4 (11%)	5	26
30	5	337/368 (92%)	305 (90%)	32 (10%)	8	34
31	6	266/332 (80%)	242 (91%)	24 (9%)	9	37
32	7	242/303 (80%)	230 (95%)	12 (5%)	24	58
33	8	91/190 (48%)	88 (97%)	3 (3%)	38	68
34	9	91/112 (81%)	85 (93%)	6 (7%)	16	49
35	a	78/133 (59%)	74 (95%)	4 (5%)	24	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	b	130/135 (96%)	118 (91%)	12 (9%)	9	36
37	c	241/288 (84%)	220 (91%)	21 (9%)	10	38
38	d	151/274 (55%)	146 (97%)	5 (3%)	38	68
39	e	188/236 (80%)	178 (95%)	10 (5%)	22	55
40	f	117/173 (68%)	113 (97%)	4 (3%)	37	68
41	g	119/148 (80%)	109 (92%)	10 (8%)	11	40
42	h	95/148 (64%)	84 (88%)	11 (12%)	5	26
43	i	86/110 (78%)	76 (88%)	10 (12%)	5	26
44	j	68/97 (70%)	61 (90%)	7 (10%)	7	32
45	k	74/90 (82%)	68 (92%)	6 (8%)	11	41
46	l	23/116 (20%)	20 (87%)	3 (13%)	4	21
47	m	40/113 (35%)	39 (98%)	1 (2%)	47	75
48	o	80/87 (92%)	75 (94%)	5 (6%)	18	51
49	p	117/181 (65%)	107 (92%)	10 (8%)	10	39
50	q	110/178 (62%)	99 (90%)	11 (10%)	7	32
51	r	133/169 (79%)	124 (93%)	9 (7%)	16	48
52	s	326/381 (86%)	299 (92%)	27 (8%)	11	40
56	AB	191/249 (77%)	171 (90%)	20 (10%)	7	31
57	AC	115/143 (80%)	106 (92%)	9 (8%)	12	42
58	AD	269/357 (75%)	239 (89%)	30 (11%)	6	27
59	AE	104/107 (97%)	98 (94%)	6 (6%)	20	53
60	AF	178/209 (85%)	161 (90%)	17 (10%)	8	34
61	AG	265/342 (78%)	243 (92%)	22 (8%)	11	40
62	AH	112/180 (62%)	93 (83%)	19 (17%)	2	12
63	AI	104/147 (71%)	89 (86%)	15 (14%)	3	18
64	AJ	93/118 (79%)	86 (92%)	7 (8%)	13	43
65	AK	91/113 (80%)	82 (90%)	9 (10%)	8	33
66	AL	152/226 (67%)	131 (86%)	21 (14%)	3	20
67	AM	95/113 (84%)	82 (86%)	13 (14%)	3	20
68	AN	93/115 (81%)	86 (92%)	7 (8%)	13	43
69	AO	166/230 (72%)	150 (90%)	16 (10%)	8	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
70	AP	87/123 (71%)	75 (86%)	12 (14%)	3	20
71	AQ	78/79 (99%)	73 (94%)	5 (6%)	17	50
72	AR	224/318 (70%)	198 (88%)	26 (12%)	5	26
73	AS	109/164 (66%)	103 (94%)	6 (6%)	21	54
74	AT	150/157 (96%)	128 (85%)	22 (15%)	3	18
75	AU	149/174 (86%)	137 (92%)	12 (8%)	11	41
76	AV	295/364 (81%)	266 (90%)	29 (10%)	8	33
77	AW	84/158 (53%)	76 (90%)	8 (10%)	8	34
78	AX	275/351 (78%)	231 (84%)	44 (16%)	2	14
79	AY	99/357 (28%)	91 (92%)	8 (8%)	11	41
80	AZ	80/95 (84%)	72 (90%)	8 (10%)	7	32
81	A0	176/190 (93%)	158 (90%)	18 (10%)	7	32
82	A1	237/291 (81%)	218 (92%)	19 (8%)	12	41
83	A2	99/101 (98%)	84 (85%)	15 (15%)	3	17
84	A3	63/166 (38%)	58 (92%)	5 (8%)	12	41
85	A4	226/379 (60%)	211 (93%)	15 (7%)	16	49
All	All	11347/15266 (74%)	10314 (91%)	1033 (9%)	13	36

All (1033) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	65	SER
3	D	71	LYS
3	D	73	THR
3	D	113	ARG
3	D	117	THR
3	D	142	VAL
3	D	147	ARG
3	D	152	ILE
3	D	187	LEU
3	D	202	ARG
3	D	205	GLN
3	D	232	ARG
3	D	236	VAL
3	D	243	THR
3	D	262	ARG

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Mol	Chain	Res	Type
3	D	263	ASN
3	D	274	ARG
4	E	51	GLU
4	E	60	PHE
4	E	82	ASP
4	E	97	VAL
4	E	106	MET
4	E	154	ARG
4	E	168	LEU
4	E	187	ILE
4	E	207	THR
4	E	218	VAL
4	E	227	GLN
4	E	231	HIS
4	E	271	LEU
4	E	276	ILE
4	E	294	ASN
4	E	300	LYS
4	E	304	LEU
4	E	310	LEU
4	E	318	THR
4	E	324	ASP
4	E	330	GLU
4	E	331	ASP
5	F	59	ARG
5	F	76	ARG
5	F	86	VAL
5	F	101	MET
5	F	108	ARG
5	F	121	ARG
5	F	125	ARG
5	F	141	ILE
5	F	147	ARG
5	F	174	LEU
5	F	184	GLN
5	F	185	ASP
5	F	203	LEU
5	F	221	LEU
5	F	226	MET
5	F	228	GLN
5	F	243	ILE
5	F	255	LYS

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Mol	Chain	Res	Type
5	F	259	LEU
6	H	56	VAL
6	H	75	ARG
6	H	87	LYS
7	I	44	ARG
7	I	45	GLN
7	I	47	LEU
7	I	79	ILE
7	I	85	GLU
7	I	90	PHE
7	I	93	ASN
7	I	136	GLU
7	I	160	LYS
7	I	170	THR
7	I	191	PHE
7	I	192	ILE
8	J	50	CYS
8	J	56	ARG
8	J	71	LEU
8	J	84	GLN
8	J	86	THR
8	J	116	HIS
8	J	120	ILE
8	J	123	ILE
8	J	141	VAL
8	J	142	ARG
9	K	9	GLN
9	K	13	THR
9	K	21	LEU
9	K	38	ARG
9	K	73	GLU
9	K	95	LEU
9	K	125	LEU
9	K	145	LEU
9	K	154	ARG
9	K	158	TYR
10	L	37	ARG
10	L	38	VAL
10	L	80	GLN
10	L	85	LEU
10	L	91	MET
10	L	101	ASP

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Mol	Chain	Res	Type
10	L	104	ASN
10	L	108	ILE
10	L	130	ARG
10	L	131	GLU
11	M	28	LYS
11	M	38	ARG
11	M	41	ARG
11	M	43	ARG
11	M	59	ARG
11	M	64	ARG
11	M	87	HIS
11	M	92	GLN
11	M	96	LEU
11	M	100	ARG
11	M	101	LEU
11	M	114	GLN
11	M	118	LEU
11	M	132	LEU
11	M	140	LEU
11	M	157	GLN
11	M	162	LEU
11	M	169	LYS
11	M	182	ARG
11	M	184	LEU
11	M	203	ARG
11	M	219	ASN
11	M	222	TYR
11	M	225	ASP
11	M	233	ARG
11	M	234	LEU
11	M	267	PHE
11	M	273	TRP
12	N	50	LEU
12	N	51	ARG
12	N	52	PHE
12	N	54	GLU
12	N	55	ARG
12	N	90	LEU
12	N	105	MET
12	N	107	LEU
12	N	113	MET
12	N	114	ASP

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Mol	Chain	Res	Type
12	N	138	HIS
12	N	151	VAL
12	N	166	ARG
12	N	168	GLU
12	N	198	MET
12	N	226	ILE
12	N	227	ARG
12	N	244	LYS
12	N	247	MET
12	N	250	ARG
13	O	20	LEU
13	O	26	ILE
13	O	30	ARG
13	O	36	LEU
13	O	38	ARG
13	O	50	ASP
13	O	51	GLU
13	O	53	ARG
13	O	75	MET
13	O	89	LEU
13	O	104	TYR
13	O	110	ILE
13	O	112	ASN
13	O	123	ILE
13	O	139	ASP
13	O	144	LEU
13	O	150	GLN
13	O	153	ARG
13	O	160	GLN
14	P	50	ARG
14	P	76	PHE
14	P	80	LEU
14	P	106	THR
14	P	125	GLU
14	P	131	LEU
14	P	134	ARG
14	P	137	GLU
14	P	141	ASN
14	P	143	MET
14	P	146	GLN
14	P	155	ASP
14	P	160	LEU

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Mol	Chain	Res	Type
15	Q	87	THR
15	Q	98	ASP
15	Q	102	ARG
15	Q	129	LYS
15	Q	136	ILE
15	Q	194	LEU
15	Q	212	ASN
15	Q	232	ARG
15	Q	235	ARG
15	Q	237	ASN
15	Q	248	CYS
15	Q	261	ASN
15	Q	271	ARG
15	Q	275	THR
16	R	10	LEU
16	R	11	ARG
16	R	12	ASN
16	R	17	ARG
16	R	22	GLN
16	R	34	ARG
16	R	36	ASN
16	R	67	LEU
16	R	93	CYS
16	R	98	ASN
16	R	119	LEU
16	R	122	ARG
16	R	123	ARG
16	R	124	ARG
17	S	84	ASN
17	S	107	LYS
17	S	118	ASN
17	S	131	GLU
17	S	134	LEU
17	S	135	LEU
17	S	144	LEU
17	S	153	LEU
17	S	172	MET
17	S	173	ARG
17	S	178	LYS
18	T	92	LYS
18	T	100	ASP
18	T	146	THR

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Mol	Chain	Res	Type
18	T	157	ARG
18	T	207	THR
19	U	3	ARG
19	U	17	LEU
19	U	25	PHE
19	U	28	LEU
19	U	38	ASP
19	U	50	ARG
19	U	53	LEU
19	U	71	ARG
19	U	91	ASP
19	U	99	LEU
20	V	20	ARG
20	V	40	ARG
20	V	101	THR
20	V	104	TYR
20	V	108	MET
20	V	117	HIS
20	V	126	MET
20	V	145	ARG
20	V	149	ARG
20	V	152	ARG
20	V	185	ARG
20	V	196	GLU
21	W	41	ASN
21	W	70	GLN
21	W	71	ARG
21	W	88	CYS
21	W	105	VAL
21	W	110	ASN
22	X	20	ILE
22	X	62	VAL
22	X	63	GLU
22	X	69	ILE
22	X	77	ARG
22	X	79	LEU
22	X	96	LYS
22	X	99	LYS
22	X	130	ARG
22	X	142	ASP
22	X	153	LEU
22	X	160	ASP

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Mol	Chain	Res	Type
22	X	180	ASP
22	X	183	ARG
22	X	208	LEU
22	X	213	GLU
22	X	215	GLN
22	X	234	LEU
23	Y	88	GLN
23	Y	91	ARG
23	Y	115	LEU
23	Y	117	GLN
23	Y	118	GLU
23	Y	132	LEU
23	Y	157	GLN
23	Y	175	ARG
23	Y	196	ARG
23	Y	222	ARG
23	Y	226	LEU
24	Z	35	LYS
24	Z	70	THR
24	Z	77	ARG
24	Z	109	LYS
24	Z	110	LEU
24	Z	134	MET
24	Z	139	LEU
24	Z	144	GLU
24	Z	145	LEU
25	0	82	LYS
25	0	93	ARG
25	0	94	ARG
25	0	96	ASN
25	0	98	GLN
25	0	105	ASN
25	0	113	CYS
25	0	116	LEU
25	0	117	LYS
25	0	128	GLU
25	0	136	GLU
25	0	156	THR
25	0	169	ASP
25	0	173	ARG
25	0	178	ASP
25	0	185	PHE

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Mol	Chain	Res	Type
26	1	14	LYS
26	1	16	ILE
26	1	17	LEU
26	1	34	ARG
26	1	47	ASP
26	1	65	LEU
27	2	49	ARG
27	2	51	ASN
27	2	69	ARG
28	3	94	LEU
28	3	143	ARG
28	3	167	LYS
28	3	168	ARG
28	3	169	ARG
29	4	68	ASN
29	4	85	ARG
29	4	87	ARG
29	4	98	HIS
30	5	31	TYR
30	5	55	LEU
30	5	67	VAL
30	5	70	LEU
30	5	82	TYR
30	5	98	LEU
30	5	102	GLN
30	5	106	ILE
30	5	108	HIS
30	5	110	ARG
30	5	113	LEU
30	5	115	GLU
30	5	170	ILE
30	5	218	LEU
30	5	223	ARG
30	5	230	LEU
30	5	251	HIS
30	5	256	PHE
30	5	262	ILE
30	5	264	ASP
30	5	275	ASN
30	5	294	LEU
30	5	295	ASP
30	5	300	ARG

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Mol	Chain	Res	Type
30	5	305	GLN
30	5	312	LYS
30	5	337	GLU
30	5	365	ASP
30	5	371	LYS
30	5	381	LEU
30	5	382	LEU
30	5	415	LEU
31	6	40	ILE
31	6	52	ARG
31	6	60	ARG
31	6	72	ARG
31	6	73	THR
31	6	136	ARG
31	6	146	TYR
31	6	173	LEU
31	6	185	MET
31	6	189	CYS
31	6	233	LEU
31	6	234	HIS
31	6	235	TRP
31	6	236	LEU
31	6	272	LEU
31	6	277	GLN
31	6	298	PHE
31	6	324	ASP
31	6	328	THR
31	6	334	LEU
31	6	356	ARG
31	6	361	GLN
31	6	370	ARG
31	6	371	ASP
32	7	64	LYS
32	7	65	ILE
32	7	81	MET
32	7	101	ARG
32	7	114	ASP
32	7	137	GLU
32	7	143	TRP
32	7	167	VAL
32	7	182	ASP
32	7	209	LEU

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Mol	Chain	Res	Type
32	7	300	VAL
32	7	313	TRP
33	8	140	LEU
33	8	143	GLN
33	8	150	LEU
34	9	17	ARG
34	9	23	SER
34	9	25	ARG
34	9	41	ILE
34	9	96	VAL
34	9	123	GLN
35	a	109	ILE
35	a	111	GLN
35	a	118	THR
35	a	122	ARG
36	b	9	ARG
36	b	11	LEU
36	b	15	LEU
36	b	26	LEU
36	b	49	ARG
36	b	68	ARG
36	b	71	CYS
36	b	85	ARG
36	b	96	GLU
36	b	103	LYS
36	b	116	ARG
36	b	135	ASN
37	c	33	LYS
37	c	40	ARG
37	c	44	GLU
37	c	65	ASN
37	c	83	PHE
37	c	87	LEU
37	c	88	LEU
37	c	123	GLN
37	c	147	ASP
37	c	183	GLU
37	c	191	LEU
37	c	211	THR
37	c	241	LEU
37	c	260	GLN
37	c	268	PRO

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Mol	Chain	Res	Type
37	c	269	LEU
37	c	271	PHE
37	c	280	LEU
37	c	283	GLU
37	c	310	ASN
37	c	311	ARG
38	d	159	ARG
38	d	166	GLU
38	d	207	ASN
38	d	209	TYR
38	d	272	PRO
39	e	55	ARG
39	e	72	SER
39	e	84	TYR
39	e	93	ASP
39	e	126	GLN
39	e	139	GLU
39	e	145	ASP
39	e	157	LEU
39	e	242	ASP
39	e	243	PHE
40	f	51	LYS
40	f	166	PHE
40	f	185	SER
40	f	188	GLU
41	g	55	THR
41	g	76	ARG
41	g	100	ILE
41	g	107	MET
41	g	111	ARG
41	g	121	GLN
41	g	136	PRO
41	g	141	ASN
41	g	147	LEU
41	g	155	GLN
42	h	70	LEU
42	h	73	TYR
42	h	92	GLU
42	h	100	LEU
42	h	117	LEU
42	h	120	MET
42	h	125	ASP

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Mol	Chain	Res	Type
42	h	131	ASN
42	h	137	ARG
42	h	147	ASN
42	h	156	TRP
43	i	35	ARG
43	i	51	ARG
43	i	63	LEU
43	i	74	ILE
43	i	88	LEU
43	i	95	ARG
43	i	105	ASP
43	i	107	LEU
43	i	113	ARG
43	i	128	ARG
44	j	30	GLN
44	j	40	TYR
44	j	43	LEU
44	j	63	GLN
44	j	66	ARG
44	j	80	LEU
44	j	88	LEU
45	k	21	CYS
45	k	25	LYS
45	k	42	VAL
45	k	56	ARG
45	k	87	LEU
45	k	93	HIS
46	l	120	ARG
46	l	121	LEU
46	l	131	ARG
47	m	72	ARG
48	o	22	ARG
48	o	42	GLU
48	o	59	GLU
48	o	62	HIS
48	o	90	ASP
49	p	96	ASN
49	p	118	LYS
49	p	124	LYS
49	p	129	ARG
49	p	135	LEU
49	p	138	GLU

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Mol	Chain	Res	Type
49	p	144	PHE
49	p	160	GLU
49	p	163	GLN
49	p	175	LEU
50	q	43	GLU
50	q	44	ASP
50	q	46	LEU
50	q	60	GLN
50	q	70	VAL
50	q	89	GLU
50	q	104	ARG
50	q	108	LEU
50	q	112	GLN
50	q	114	ARG
50	q	143	TRP
51	r	37	GLU
51	r	40	GLU
51	r	60	SER
51	r	85	ASP
51	r	108	CYS
51	r	117	GLU
51	r	152	THR
51	r	168	ARG
51	r	171	ARG
52	s	65	ARG
52	s	66	TRP
52	s	90	LYS
52	s	103	ASP
52	s	112	THR
52	s	148	ASP
52	s	177	LEU
52	s	201	ASP
52	s	204	CYS
52	s	229	LEU
52	s	238	ASN
52	s	243	ILE
52	s	264	ILE
52	s	270	LYS
52	s	276	ARG
52	s	280	ASN
52	s	301	LEU
52	s	321	GLU

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Mol	Chain	Res	Type
52	s	336	THR
52	s	353	ARG
52	s	363	ASP
52	s	368	SER
52	s	373	GLN
52	s	404	THR
52	s	406	GLU
52	s	407	ASP
52	s	427	ASN
56	AB	71	ASP
56	AB	72	PHE
56	AB	84	LEU
56	AB	91	LEU
56	AB	110	ARG
56	AB	112	ASP
56	AB	126	GLN
56	AB	143	LEU
56	AB	150	GLN
56	AB	158	MET
56	AB	160	ARG
56	AB	167	HIS
56	AB	169	ARG
56	AB	207	VAL
56	AB	209	VAL
56	AB	219	THR
56	AB	223	VAL
56	AB	227	CYS
56	AB	241	ASP
56	AB	244	LEU
57	AC	38	ARG
57	AC	79	GLU
57	AC	89	ASP
57	AC	97	TRP
57	AC	104	LEU
57	AC	138	TYR
57	AC	141	THR
57	AC	146	PHE
57	AC	156	GLN
58	AD	91	THR
58	AD	93	LEU
58	AD	106	THR
58	AD	128	ARG

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Mol	Chain	Res	Type
58	AD	144	LEU
58	AD	167	LYS
58	AD	179	TRP
58	AD	186	LYS
58	AD	230	THR
58	AD	234	LYS
58	AD	239	LYS
58	AD	244	LEU
58	AD	260	LYS
58	AD	264	ARG
58	AD	269	ARG
58	AD	276	VAL
58	AD	283	GLU
58	AD	286	GLU
58	AD	289	THR
58	AD	316	CYS
58	AD	318	ARG
58	AD	332	MET
58	AD	341	ASN
58	AD	343	LEU
58	AD	355	ARG
58	AD	356	GLN
58	AD	380	LEU
58	AD	407	ASP
58	AD	419	ARG
58	AD	425	LEU
59	AE	11	LYS
59	AE	14	GLN
59	AE	57	GLN
59	AE	67	ASP
59	AE	78	MET
59	AE	92	ASN
60	AF	43	ASP
60	AF	82	THR
60	AF	87	GLU
60	AF	120	ARG
60	AF	122	GLN
60	AF	132	GLU
60	AF	162	LEU
60	AF	178	ARG
60	AF	193	ASP
60	AF	201	MET

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Mol	Chain	Res	Type
60	AF	205	LEU
60	AF	223	LYS
60	AF	224	HIS
60	AF	225	ASP
60	AF	226	LEU
60	AF	231	GLU
60	AF	234	ARG
61	AG	99	PHE
61	AG	111	LEU
61	AG	125	MET
61	AG	129	GLU
61	AG	155	LYS
61	AG	205	LEU
61	AG	208	MET
61	AG	223	ARG
61	AG	229	LEU
61	AG	232	GLN
61	AG	263	ASP
61	AG	310	ARG
61	AG	312	GLN
61	AG	313	LEU
61	AG	323	LEU
61	AG	327	ASP
61	AG	331	THR
61	AG	363	TRP
61	AG	373	ASP
61	AG	385	GLU
61	AG	389	ARG
61	AG	393	TRP
62	AH	72	LEU
62	AH	76	LEU
62	AH	84	ASP
62	AH	90	SER
62	AH	92	GLU
62	AH	97	LEU
62	AH	110	GLU
62	AH	119	THR
62	AH	120	LEU
62	AH	126	ILE
62	AH	131	ARG
62	AH	132	VAL
62	AH	136	MET

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Mol	Chain	Res	Type
62	AH	139	LEU
62	AH	142	CYS
62	AH	148	LEU
62	AH	160	ILE
62	AH	164	LEU
62	AH	166	GLU
63	AI	62	ILE
63	AI	74	ARG
63	AI	81	GLU
63	AI	93	ASN
63	AI	95	THR
63	AI	98	GLN
63	AI	115	GLU
63	AI	159	LEU
63	AI	163	HIS
63	AI	171	GLU
63	AI	173	ILE
63	AI	175	ILE
63	AI	176	THR
63	AI	178	ASN
63	AI	187	ARG
64	AJ	43	LYS
64	AJ	49	LEU
64	AJ	74	ASN
64	AJ	79	LYS
64	AJ	89	ARG
64	AJ	104	GLU
64	AJ	109	LEU
65	AK	49	ASP
65	AK	63	LEU
65	AK	72	ASP
65	AK	75	ILE
65	AK	81	ASP
65	AK	103	ARG
65	AK	106	LEU
65	AK	112	ARG
65	AK	128	TRP
66	AL	75	ASP
66	AL	96	GLU
66	AL	97	MET
66	AL	99	ASN
66	AL	102	GLU

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Mol	Chain	Res	Type
66	AL	104	LEU
66	AL	109	GLU
66	AL	125	LEU
66	AL	137	ARG
66	AL	145	LYS
66	AL	148	LYS
66	AL	156	LEU
66	AL	161	ASP
66	AL	170	LEU
66	AL	181	ILE
66	AL	187	ILE
66	AL	198	ARG
66	AL	205	THR
66	AL	213	VAL
66	AL	216	GLU
66	AL	223	ARG
67	AM	17	LEU
67	AM	29	ARG
67	AM	33	ARG
67	AM	34	ILE
67	AM	43	ARG
67	AM	50	GLN
67	AM	53	SER
67	AM	59	ASN
67	AM	65	LEU
67	AM	69	ASN
67	AM	71	ASP
67	AM	74	ARG
67	AM	110	LEU
68	AN	23	GLN
68	AN	65	LEU
68	AN	78	LYS
68	AN	85	VAL
68	AN	93	ASP
68	AN	95	VAL
68	AN	110	LEU
69	AO	62	GLU
69	AO	76	ASP
69	AO	80	ASN
69	AO	85	VAL
69	AO	91	ARG
69	AO	105	CYS

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Mol	Chain	Res	Type
69	AO	143	CYS
69	AO	149	ARG
69	AO	163	LEU
69	AO	165	TYR
69	AO	173	ARG
69	AO	174	ASP
69	AO	175	LEU
69	AO	193	LEU
69	AO	212	GLU
69	AO	227	GLU
70	AP	56	ASN
70	AP	60	GLU
70	AP	67	LEU
70	AP	68	CYS
70	AP	73	ASP
70	AP	78	GLN
70	AP	90	CYS
70	AP	103	LYS
70	AP	107	ILE
70	AP	111	ILE
70	AP	112	LYS
70	AP	140	TYR
71	AQ	10	ARG
71	AQ	28	ARG
71	AQ	50	ARG
71	AQ	54	ARG
71	AQ	55	GLU
72	AR	99	LYS
72	AR	102	THR
72	AR	115	THR
72	AR	119	VAL
72	AR	135	ARG
72	AR	159	THR
72	AR	170	ARG
72	AR	175	ARG
72	AR	183	LYS
72	AR	194	GLN
72	AR	209	ILE
72	AR	222	ASP
72	AR	230	LEU
72	AR	238	ASP
72	AR	243	ILE

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Mol	Chain	Res	Type
72	AR	246	HIS
72	AR	252	ASP
72	AR	253	ILE
72	AR	254	ASP
72	AR	258	LYS
72	AR	259	TYR
72	AR	266	ARG
72	AR	267	TYR
72	AR	284	LEU
72	AR	292	ASP
72	AR	307	LEU
73	AS	61	GLN
73	AS	89	ASN
73	AS	97	GLN
73	AS	108	LYS
73	AS	111	GLU
73	AS	121	THR
74	AT	6	ARG
74	AT	9	ILE
74	AT	10	ARG
74	AT	11	ARG
74	AT	25	ASP
74	AT	28	LYS
74	AT	33	ASN
74	AT	35	ASN
74	AT	39	GLU
74	AT	42	GLU
74	AT	45	ARG
74	AT	59	ASN
74	AT	66	MET
74	AT	70	MET
74	AT	77	ARG
74	AT	96	LYS
74	AT	98	ILE
74	AT	99	MET
74	AT	102	ILE
74	AT	114	ARG
74	AT	133	LYS
74	AT	158	GLU
75	AU	27	ARG
75	AU	30	ARG
75	AU	32	ASP

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Mol	Chain	Res	Type
75	AU	34	LEU
75	AU	39	ILE
75	AU	43	ASN
75	AU	49	ASP
75	AU	96	LEU
75	AU	110	GLN
75	AU	149	TRP
75	AU	152	ARG
75	AU	176	ARG
76	AV	36	ASP
76	AV	52	ASP
76	AV	62	GLU
76	AV	72	ILE
76	AV	82	ARG
76	AV	86	ASP
76	AV	90	TYR
76	AV	93	TYR
76	AV	100	ASN
76	AV	102	TRP
76	AV	106	ASN
76	AV	107	TRP
76	AV	119	TYR
76	AV	146	LEU
76	AV	161	LEU
76	AV	168	MET
76	AV	183	LEU
76	AV	184	TYR
76	AV	192	LYS
76	AV	209	LEU
76	AV	215	GLN
76	AV	217	ASN
76	AV	240	LEU
76	AV	241	ARG
76	AV	266	VAL
76	AV	366	THR
76	AV	375	TYR
76	AV	380	GLN
76	AV	393	GLU
77	AW	103	ARG
77	AW	104	ILE
77	AW	119	LYS
77	AW	133	LYS

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Mol	Chain	Res	Type
77	AW	142	LEU
77	AW	146	ASP
77	AW	154	LEU
77	AW	163	LEU
78	AX	58	LYS
78	AX	62	GLN
78	AX	68	TYR
78	AX	70	ILE
78	AX	75	LEU
78	AX	76	GLU
78	AX	79	PHE
78	AX	81	HIS
78	AX	93	THR
78	AX	94	PHE
78	AX	123	ARG
78	AX	138	LEU
78	AX	155	ILE
78	AX	164	ASN
78	AX	179	ASP
78	AX	180	GLN
78	AX	182	LEU
78	AX	188	LEU
78	AX	189	LYS
78	AX	195	ASN
78	AX	222	LEU
78	AX	225	VAL
78	AX	228	GLN
78	AX	240	VAL
78	AX	242	ILE
78	AX	243	VAL
78	AX	246	GLU
78	AX	248	LYS
78	AX	256	PHE
78	AX	257	HIS
78	AX	263	ASP
78	AX	266	ASN
78	AX	272	THR
78	AX	278	ASP
78	AX	290	VAL
78	AX	293	LEU
78	AX	295	LYS
78	AX	338	ASP

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Mol	Chain	Res	Type
78	AX	341	ILE
78	AX	365	TRP
78	AX	381	LEU
78	AX	383	LEU
78	AX	391	LEU
78	AX	392	GLU
79	AY	303	GLN
79	AY	305	THR
79	AY	312	GLU
79	AY	341	PHE
79	AY	376	PHE
79	AY	377	ARG
79	AY	380	PHE
79	AY	382	GLU
80	AZ	14	LEU
80	AZ	32	LYS
80	AZ	48	THR
80	AZ	54	ASN
80	AZ	55	HIS
80	AZ	62	MET
80	AZ	76	GLN
80	AZ	81	GLU
81	A0	27	ARG
81	A0	33	LEU
81	A0	65	LEU
81	A0	66	GLN
81	A0	76	LEU
81	A0	82	ARG
81	A0	103	ASP
81	A0	107	GLN
81	A0	108	ASN
81	A0	118	LEU
81	A0	119	THR
81	A0	132	GLU
81	A0	171	ARG
81	A0	177	GLU
81	A0	190	MET
81	A0	192	ASN
81	A0	199	GLU
81	A0	202	ASP
82	A1	92	LYS
82	A1	112	LEU

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Mol	Chain	Res	Type
82	A1	113	HIS
82	A1	133	TRP
82	A1	145	LYS
82	A1	173	LEU
82	A1	177	LEU
82	A1	187	LYS
82	A1	205	LEU
82	A1	211	ARG
82	A1	212	CYS
82	A1	216	ARG
82	A1	219	TYR
82	A1	226	LEU
82	A1	232	GLU
82	A1	247	ASP
82	A1	249	GLU
82	A1	254	GLU
82	A1	259	GLU
83	A2	12	ARG
83	A2	24	ASN
83	A2	29	LEU
83	A2	37	ARG
83	A2	38	ARG
83	A2	53	MET
83	A2	60	GLU
83	A2	61	PHE
83	A2	71	GLN
83	A2	82	GLU
83	A2	85	LYS
83	A2	86	MET
83	A2	87	ARG
83	A2	99	LEU
83	A2	107	LEU
84	A3	146	LEU
84	A3	153	LEU
84	A3	165	LYS
84	A3	179	LYS
84	A3	182	LEU
85	A4	61	LYS
85	A4	92	ASP
85	A4	105	SER
85	A4	141	MET
85	A4	379	PHE

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Mol	Chain	Res	Type
85	A4	417	GLN
85	A4	420	MET
85	A4	441	THR
85	A4	454	ARG
85	A4	457	TYR
85	A4	458	TYR
85	A4	477	TRP
85	A4	478	TYR
85	A4	544	LEU
85	A4	583	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	195	ASN
3	D	235	GLN
3	D	276	HIS
4	E	57	ASN
4	E	231	HIS
4	E	233	GLN
5	F	74	GLN
5	F	228	GLN
5	F	249	ASN
8	J	116	HIS
9	K	48	HIS
9	K	80	HIS
9	K	140	ASN
10	L	104	ASN
11	M	130	GLN
12	N	237	HIS
13	O	150	GLN
14	P	120	ASN
15	Q	212	ASN
15	Q	213	GLN
15	Q	258	GLN
15	Q	261	ASN
17	S	91	GLN
18	T	210	HIS
19	U	41	GLN
19	U	82	HIS
21	W	110	ASN
22	X	175	GLN

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Mol	Chain	Res	Type
22	X	241	GLN
23	Y	183	GLN
25	0	170	GLN
26	1	15	ASN
27	2	57	ASN
30	5	102	GLN
30	5	186	GLN
30	5	205	GLN
30	5	289	HIS
30	5	305	GLN
30	5	353	HIS
31	6	292	GLN
31	6	354	GLN
32	7	55	GLN
32	7	247	ASN
32	7	285	ASN
32	7	298	GLN
33	8	126	GLN
35	a	44	ASN
35	a	62	HIS
36	b	27	GLN
36	b	129	GLN
37	c	94	ASN
37	c	123	GLN
37	c	128	GLN
37	c	172	ASN
37	c	192	GLN
38	d	207	ASN
39	e	156	ASN
39	e	198	ASN
39	e	245	GLN
41	g	104	ASN
42	h	99	ASN
42	h	147	ASN
43	i	89	GLN
43	i	120	HIS
45	k	19	GLN
45	k	26	ASN
48	o	46	HIS
48	o	85	HIS
48	o	91	GLN
49	p	176	HIS

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Mol	Chain	Res	Type
50	q	137	GLN
51	r	65	ASN
51	r	112	HIS
52	s	315	ASN
52	s	358	GLN
52	s	385	GLN
52	s	414	ASN
52	s	420	GLN
57	AC	156	GLN
58	AD	155	GLN
59	AE	57	GLN
59	AE	81	HIS
60	AF	103	ASN
60	AF	207	HIS
61	AG	312	GLN
64	AJ	37	HIS
64	AJ	74	ASN
66	AL	162	GLN
67	AM	59	ASN
70	AP	78	GLN
70	AP	115	GLN
71	AQ	15	GLN
73	AS	89	ASN
73	AS	97	GLN
74	AT	54	GLN
74	AT	125	HIS
76	AV	245	HIS
78	AX	66	GLN
78	AX	164	ASN
78	AX	266	ASN
78	AX	363	ASN
80	AZ	27	ASN
81	A0	145	HIS
84	A3	141	HIS
84	A3	158	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1459/1559 (93%)	470 (32%)	99 (6%)
2	B	51/73 (69%)	19 (37%)	3 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	u	1/2 (50%)	1 (100%)	0
55	AA	914/954 (95%)	273 (29%)	57 (6%)
All	All	2425/2588 (93%)	763 (31%)	159 (6%)

All (763) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1672	C
1	A	1674	A
1	A	1675	A
1	A	1676	A
1	A	1678	C
1	A	1679	U
1	A	1680	A
1	A	1681	G
1	A	1685	C
1	A	1687	A
1	A	1689	C
1	A	1693	C
1	A	1694	U
1	A	1699	C
1	A	1700	U
1	A	1702	A
1	A	1703	C
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1709	G
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1716	U
1	A	1717	U
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1732	C
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1767	G

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Mol	Chain	Res	Type
1	A	1770	G
1	A	1772	A
1	A	1773	A
1	A	1777	A
1	A	1779	A
1	A	1780	U
1	A	1781	A
1	A	1783	U
1	A	1794	A
1	A	1798	A
1	A	1799	U
1	A	1805	A
1	A	1806	U
1	A	1807	U
1	A	1808	A
1	A	1809	U
1	A	1810	A
1	A	1811	A
1	A	1812	C
1	A	1820	A
1	A	1823	A
1	A	1824	U
1	A	1825	A
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1839	C
1	A	1844	A
1	A	1849	C
1	A	1852	C
1	A	1854	U
1	A	1856	A
1	A	1867	A
1	A	1869	A
1	A	1870	A
1	A	1871	A
1	A	1872	U
1	A	1873	A
1	A	1878	U
1	A	1882	A

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Mol	Chain	Res	Type
1	A	1883	G
1	A	1887	A
1	A	1888	G
1	A	1889	C
1	A	1893	A
1	A	1894	G
1	A	1901	C
1	A	1902	C
1	A	1903	C
1	A	1909	A
1	A	1918	G
1	A	1923	C
1	A	1935	A
1	A	1939	G
1	A	1940	A
1	A	1944	C
1	A	1946	C
1	A	1956	U
1	A	1957	A
1	A	1958	G
1	A	1961	A
1	A	1966	G
1	A	1968	G
1	A	1973	G
1	A	1974	A
1	A	1975	U
1	A	1985	G
1	A	1986	A
1	A	1987	G
1	A	1992	C
1	A	1993	A
1	A	1994	A
1	A	1995	A
1	A	2000	C
1	A	2001	C
1	A	2002	G
1	A	2003	A
1	A	2011	G
1	A	2015	G
1	A	2021	U
1	A	2022	G
1	A	2029	A

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Mol	Chain	Res	Type
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2040	G
1	A	2042	U
1	A	2044	A
1	A	2048	U
1	A	2053	U
1	A	2055	U
1	A	2059	C
1	A	2060	A
1	A	2065	A
1	A	2066	C
1	A	2074	A
1	A	2079	C
1	A	2082	G
1	A	2083	U
1	A	2085	A
1	A	2093	U
1	A	2095	U
1	A	2097	A
1	A	2098	G
1	A	2099	U
1	A	2105	G
1	A	2113	G
1	A	2124	A
1	A	2125	C
1	A	2129	G
1	A	2132	A
1	A	2135	A
1	A	2142	A
1	A	2143	G
1	A	2147	G
1	A	2150	U
1	A	2154	A
1	A	2155	A
1	A	2159	U
1	A	2160	A
1	A	2163	A

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Mol	Chain	Res	Type
1	A	2165	C
1	A	2166	C
1	A	2168	U
1	A	2169	A
1	A	2170	G
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2180	A
1	A	2181	A
1	A	2183	C
1	A	2187	C
1	A	2190	C
1	A	2192	A
1	A	2194	U
1	A	2195	A
1	A	2197	G
1	A	2198	A
1	A	2199	A
1	A	2200	A
1	A	2202	C
1	A	2204	U
1	A	2206	C
1	A	2210	C
1	A	2211	U
1	A	2216	A
1	A	2229	A
1	A	2230	A
1	A	2231	A
1	A	2232	A
1	A	2233	U
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2242	U
1	A	2243	A
1	A	2244	U
1	A	2245	A
1	A	2246	A
1	A	2247	C
1	A	2259	C
1	A	2262	C

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Mol	Chain	Res	Type
1	A	2263	C
1	A	2264	A
1	A	2269	G
1	A	2271	C
1	A	2281	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2309	A
1	A	2315	A
1	A	2322	C
1	A	2324	U
1	A	2329	C
1	A	2331	C
1	A	2332	C
1	A	2334	C
1	A	2335	A
1	A	2342	U
1	A	2345	G
1	A	2350	A
1	A	2364	C
1	A	2365	U
1	A	2369	A
1	A	2370	A
1	A	2371	U
1	A	2372	U
1	A	2374	A
1	A	2375	C
1	A	2381	A
1	A	2384	A
1	A	2387	U
1	A	2388	A
1	A	2390	A
1	A	2392	U
1	A	2393	C
1	A	2394	A
1	A	2396	C
1	A	2406	A
1	A	2407	U

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Mol	Chain	Res	Type
1	A	2414	C
1	A	2415	C
1	A	2416	U
1	A	2426	C
1	A	2432	A
1	A	2435	G
1	A	2443	C
1	A	2444	A
1	A	2445	U
1	A	2446	A
1	A	2447	A
1	A	2458	A
1	A	2478	G
1	A	2483	U
1	A	2484	C
1	A	2485	U
1	A	2493	C
1	A	2500	A
1	A	2502	C
1	A	2507	A
1	A	2508	C
1	A	2511	C
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2527	A
1	A	2530	A
1	A	2531	U
1	A	2536	G
1	A	2544	C
1	A	2546	G
1	A	2550	A
1	A	2551	G
1	A	2556	A
1	A	2557	C
1	A	2558	A
1	A	2559	U
1	A	2560	G
1	A	2563	U
1	A	2570	C

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Mol	Chain	Res	Type
1	A	2581	A
1	A	2587	G
1	A	2592	G
1	A	2593	G
1	A	2594	U
1	A	2599	U
1	A	2601	A
1	A	2602	U
1	A	2603	C
1	A	2607	U
1	A	2615	A
1	A	2618	U
1	A	2626	U
1	A	2627	G
1	A	2628	U
1	A	2629	A
1	A	2630	U
1	A	2632	A
1	A	2633	A
1	A	2634	U
1	A	2635	G
1	A	2645	G
1	A	2654	U
1	A	2656	U
1	A	2660	U
1	A	2670	C
1	A	2677	A
1	A	2683	C
1	A	2686	G
1	A	2693	A
1	A	2694	A
1	A	2695	G
1	A	2696	A
1	A	2706	A
1	A	2709	A
1	A	2712	G
1	A	2718	C
1	A	2719	G
1	A	2723	A
1	A	2724	G
1	A	2725	A
1	A	2731	U

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Mol	Chain	Res	Type
1	A	2732	G
1	A	2737	U
1	A	2738	U
1	A	2739	U
1	A	2740	A
1	A	2744	U
1	A	2745	A
1	A	2746	U
1	A	2748	A
1	A	2749	A
1	A	2750	U
1	A	2755	A
1	A	2756	C
1	A	2757	A
1	A	2758	G
1	A	2804	A
1	A	2807	U
1	A	2808	U
1	A	2810	G
1	A	2813	U
1	A	2814	G
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2842	C
1	A	2844	G
1	A	2846	G
1	A	2847	C
1	A	2851	A
1	A	2854	U
1	A	2859	A
1	A	2864	U
1	A	2865	C
1	A	2870	G
1	A	2871	U
1	A	2880	A
1	A	2893	A
1	A	2895	U
1	A	2901	A
1	A	2906	C
1	A	2910	A
1	A	2911	C

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Mol	Chain	Res	Type
1	A	2912	C
1	A	2913	A
1	A	2916	G
1	A	2917	G
1	A	2919	A
1	A	2922	A
1	A	2923	G
1	A	2926	A
1	A	2927	C
1	A	2928	C
1	A	2935	A
1	A	2936	U
1	A	2955	U
1	A	2956	A
1	A	2960	U
1	A	2961	C
1	A	2962	C
1	A	2963	A
1	A	2964	U
1	A	2971	A
1	A	2979	U
1	A	2981	A
1	A	2986	C
1	A	2989	G
1	A	2990	A
1	A	2992	G
1	A	2994	U
1	A	3004	C
1	A	3005	A
1	A	3007	C
1	A	3016	G
1	A	3022	G
1	A	3029	A
1	A	3040	G
1	A	3041	U
1	A	3042	U
1	A	3049	U
1	A	3053	A
1	A	3054	G
1	A	3056	C
1	A	3060	C
1	A	3063	G

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Mol	Chain	Res	Type
1	A	3065	U
1	A	3068	G
1	A	3069	A
1	A	3070	G
1	A	3072	U
1	A	3073	C
1	A	3074	A
1	A	3085	A
1	A	3086	U
1	A	3093	C
1	A	3096	U
1	A	3097	U
1	A	3098	U
1	A	3100	U
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3114	U
1	A	3120	C
1	A	3123	G
1	A	3127	G
1	A	3128	A
1	A	3129	A
1	A	3131	G
1	A	3135	A
1	A	3141	A
1	A	3149	C
1	A	3150	U
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3169	C
1	A	3170	C
1	A	3172	C
1	A	3173	G
1	A	3176	A
1	A	3180	A
1	A	3183	U
1	A	3184	C

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Mol	Chain	Res	Type
1	A	3185	A
1	A	3187	C
1	A	3188	U
1	A	3189	C
1	A	3190	A
1	A	3192	C
1	A	3196	G
1	A	3202	U
1	A	3204	C
1	A	3207	A
1	A	3213	A
1	A	3217	A
1	A	3218	A
1	A	3223	A
1	A	3228	U
2	B	1604	G
2	B	1608	G
2	B	1609	U
2	B	1610	A
2	B	1611	G
2	B	1613	U
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1632	U
2	B	1634	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1649	C
2	B	1650	A
2	B	1659	U
2	B	1665	C
2	B	1669	G
54	u	2	A
55	AA	650	U
55	AA	651	A
55	AA	655	U
55	AA	656	U
55	AA	658	G
55	AA	674	U
55	AA	678	U

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Mol	Chain	Res	Type
55	AA	680	U
55	AA	688	A
55	AA	689	U
55	AA	690	U
55	AA	691	A
55	AA	704	U
55	AA	705	C
55	AA	707	C
55	AA	710	U
55	AA	711	U
55	AA	712	C
55	AA	713	C
55	AA	718	A
55	AA	720	U
55	AA	721	U
55	AA	723	A
55	AA	729	U
55	AA	730	A
55	AA	731	A
55	AA	732	A
55	AA	734	C
55	AA	745	A
55	AA	753	A
55	AA	754	A
55	AA	757	A
55	AA	758	U
55	AA	761	A
55	AA	764	A
55	AA	766	G
55	AA	770	C
55	AA	773	U
55	AA	777	G
55	AA	783	A
55	AA	791	G
55	AA	793	C
55	AA	794	U
55	AA	795	A
55	AA	796	G
55	AA	805	C
55	AA	806	C
55	AA	807	A
55	AA	808	C

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Mol	Chain	Res	Type
55	AA	809	G
55	AA	812	A
55	AA	813	A
55	AA	814	A
55	AA	815	C
55	AA	817	G
55	AA	829	C
55	AA	830	U
55	AA	831	U
55	AA	832	U
55	AA	835	C
55	AA	847	G
55	AA	851	A
55	AA	852	A
55	AA	853	C
55	AA	861	U
55	AA	862	A
55	AA	868	C
55	AA	869	C
55	AA	870	C
55	AA	871	A
55	AA	872	G
55	AA	875	U
55	AA	880	C
55	AA	881	A
55	AA	883	U
55	AA	886	C
55	AA	890	C
55	AA	893	G
55	AA	899	G
55	AA	904	C
55	AA	905	A
55	AA	912	U
55	AA	919	A
55	AA	933	G
55	AA	938	A
55	AA	939	A
55	AA	941	G
55	AA	942	A
55	AA	943	G
55	AA	946	U
55	AA	947	U

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Mol	Chain	Res	Type
55	AA	948	U
55	AA	950	A
55	AA	954	C
55	AA	955	A
55	AA	966	A
55	AA	967	A
55	AA	973	C
55	AA	974	U
55	AA	975	A
55	AA	988	G
55	AA	992	U
55	AA	993	A
55	AA	1000	U
55	AA	1001	C
55	AA	1011	C
55	AA	1012	A
55	AA	1015	A
55	AA	1021	U
55	AA	1022	A
55	AA	1026	A
55	AA	1028	G
55	AA	1030	G
55	AA	1041	A
55	AA	1042	U
55	AA	1046	A
55	AA	1049	A
55	AA	1065	C
55	AA	1082	A
55	AA	1086	C
55	AA	1090	A
55	AA	1097	G
55	AA	1098	C
55	AA	1102	A
55	AA	1103	A
55	AA	1105	C
55	AA	1106	C
55	AA	1113	G
55	AA	1121	A
55	AA	1126	A
55	AA	1128	C
55	AA	1129	U
55	AA	1138	G

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Mol	Chain	Res	Type
55	AA	1143	C
55	AA	1144	U
55	AA	1151	C
55	AA	1153	C
55	AA	1154	A
55	AA	1166	A
55	AA	1167	A
55	AA	1175	G
55	AA	1179	G
55	AA	1180	U
55	AA	1185	C
55	AA	1187	U
55	AA	1188	A
55	AA	1189	U
55	AA	1190	C
55	AA	1192	C
55	AA	1193	U
55	AA	1194	C
55	AA	1197	G
55	AA	1200	G
55	AA	1203	C
55	AA	1214	A
55	AA	1215	U
55	AA	1216	C
55	AA	1220	A
55	AA	1221	A
55	AA	1222	A
55	AA	1223	C
55	AA	1225	C
55	AA	1226	C
55	AA	1229	U
55	AA	1230	C
55	AA	1231	A
55	AA	1234	C
55	AA	1236	C
55	AA	1237	A
55	AA	1245	U
55	AA	1246	U
55	AA	1247	G
55	AA	1248	C
55	AA	1249	U
55	AA	1250	C

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Mol	Chain	Res	Type
55	AA	1251	A
55	AA	1261	C
55	AA	1270	U
55	AA	1271	C
55	AA	1272	A
55	AA	1282	G
55	AA	1283	A
55	AA	1284	U
55	AA	1286	A
55	AA	1290	C
55	AA	1292	A
55	AA	1297	G
55	AA	1300	A
55	AA	1307	G
55	AA	1311	C
55	AA	1312	C
55	AA	1320	G
55	AA	1325	U
55	AA	1326	A
55	AA	1327	G
55	AA	1330	C
55	AA	1332	A
55	AA	1341	C
55	AA	1342	C
55	AA	1343	A
55	AA	1344	U
55	AA	1345	G
55	AA	1353	A
55	AA	1354	A
55	AA	1355	G
55	AA	1356	A
55	AA	1365	A
55	AA	1367	A
55	AA	1368	U
55	AA	1369	U
55	AA	1376	C
55	AA	1377	C
55	AA	1378	C
55	AA	1381	A
55	AA	1383	A
55	AA	1390	A
55	AA	1391	U

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Mol	Chain	Res	Type
55	AA	1393	G
55	AA	1402	A
55	AA	1403	A
55	AA	1408	A
55	AA	1416	A
55	AA	1417	A
55	AA	1418	G
55	AA	1420	U
55	AA	1430	A
55	AA	1435	A
55	AA	1437	U
55	AA	1443	U
55	AA	1444	A
55	AA	1447	G
55	AA	1452	U
55	AA	1454	G
55	AA	1461	A
55	AA	1463	G
55	AA	1465	C
55	AA	1466	C
55	AA	1469	G
55	AA	1477	U
55	AA	1478	A
55	AA	1481	C
55	AA	1482	A
55	AA	1499	U
55	AA	1503	G
55	AA	1512	A
55	AA	1513	A
55	AA	1517	A
55	AA	1518	C
55	AA	1523	A
55	AA	1524	A
55	AA	1525	C
55	AA	1527	A
55	AA	1532	C
55	AA	1533	C
55	AA	1534	C
55	AA	1535	U
55	AA	1536	A
55	AA	1537	C
55	AA	1538	G

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Mol	Chain	Res	Type
55	AA	1539	C
55	AA	1540	A
55	AA	1541	U
55	AA	1552	G
55	AA	1568	U
55	AA	1571	U
55	AA	1572	A
55	AA	1582	G
55	AA	1584	A
55	AA	1585	A
55	AA	1594	G
55	AA	1595	G
55	AA	1599	A
55	AA	1600	A

All (159) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1677	C
1	A	1700	U
1	A	1703	C
1	A	1707	C
1	A	1713	A
1	A	1715	C
1	A	1724	A
1	A	1727	A
1	A	1766	U
1	A	1772	A
1	A	1780	U
1	A	1798	A
1	A	1805	A
1	A	1806	U
1	A	1807	U
1	A	1809	U
1	A	1823	A
1	A	1824	U
1	A	1828	A
1	A	1852	C
1	A	1870	A
1	A	1871	A
1	A	1888	G
1	A	1901	C

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Mol	Chain	Res	Type
1	A	1956	U
1	A	1972	A
1	A	1974	A
1	A	1995	A
1	A	2001	C
1	A	2010	U
1	A	2036	C
1	A	2125	C
1	A	2135	A
1	A	2154	A
1	A	2160	A
1	A	2165	C
1	A	2172	A
1	A	2173	G
1	A	2186	C
1	A	2189	C
1	A	2197	G
1	A	2229	A
1	A	2231	A
1	A	2239	A
1	A	2243	A
1	A	2245	A
1	A	2251	A
1	A	2261	C
1	A	2342	U
1	A	2370	A
1	A	2374	A
1	A	2380	C
1	A	2389	C
1	A	2400	C
1	A	2404	U
1	A	2417	C
1	A	2422	U
1	A	2444	A
1	A	2457	A
1	A	2493	C
1	A	2506	A
1	A	2507	A
1	A	2519	G
1	A	2523	C
1	A	2526	C
1	A	2530	A

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Mol	Chain	Res	Type
1	A	2558	A
1	A	2559	U
1	A	2601	A
1	A	2602	U
1	A	2606	U
1	A	2618	U
1	A	2628	U
1	A	2653	C
1	A	2684	C
1	A	2693	A
1	A	2737	U
1	A	2740	A
1	A	2744	U
1	A	2807	U
1	A	2846	G
1	A	2853	A
1	A	2865	C
1	A	2905	A
1	A	2918	A
1	A	2922	A
1	A	2945	A
1	A	2955	U
1	A	2960	U
1	A	2989	G
1	A	3004	C
1	A	3029	A
1	A	3041	U
1	A	3068	G
1	A	3092	U
1	A	3149	C
1	A	3168	C
1	A	3188	U
1	A	3201	A
2	B	1607	U
2	B	1608	G
2	B	1611	G
55	AA	655	U
55	AA	689	U
55	AA	717	G
55	AA	722	C
55	AA	729	U
55	AA	730	A

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Mol	Chain	Res	Type
55	AA	757	A
55	AA	783	A
55	AA	793	C
55	AA	806	C
55	AA	828	C
55	AA	868	C
55	AA	871	A
55	AA	882	A
55	AA	903	U
55	AA	946	U
55	AA	947	U
55	AA	953	U
55	AA	974	U
55	AA	992	U
55	AA	1021	U
55	AA	1030	G
55	AA	1041	A
55	AA	1081	U
55	AA	1106	C
55	AA	1113	G
55	AA	1152	A
55	AA	1166	A
55	AA	1189	U
55	AA	1213	A
55	AA	1229	U
55	AA	1236	C
55	AA	1245	U
55	AA	1246	U
55	AA	1249	U
55	AA	1271	C
55	AA	1291	U
55	AA	1326	A
55	AA	1331	A
55	AA	1342	C
55	AA	1343	A
55	AA	1353	A
55	AA	1368	U
55	AA	1402	A
55	AA	1415	G
55	AA	1429	C
55	AA	1430	A
55	AA	1446	A

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Mol	Chain	Res	Type
55	AA	1465	C
55	AA	1512	A
55	AA	1531	C
55	AA	1532	C
55	AA	1534	C
55	AA	1535	U
55	AA	1537	C
55	AA	1539	C
55	AA	1568	U

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 135 ligands modelled in this entry, 134 are monoatomic - leaving 1 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
88	GDP	AX	500	-	24,30,30	0.95	1 (4%)	30,47,47	1.35	4 (13%)

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
88	GDP	AX	500	-	-	4/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
88	AX	500	GDP	C6-N1	-2.03	1.34	1.37

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	AX	500	GDP	C3'-C2'-C1'	3.83	106.74	100.98
88	AX	500	GDP	PA-O3A-PB	-2.91	122.85	132.83
88	AX	500	GDP	C5-C6-N1	2.47	118.31	113.95
88	AX	500	GDP	C8-N7-C5	2.36	107.49	102.99

There are no chirality outliers.

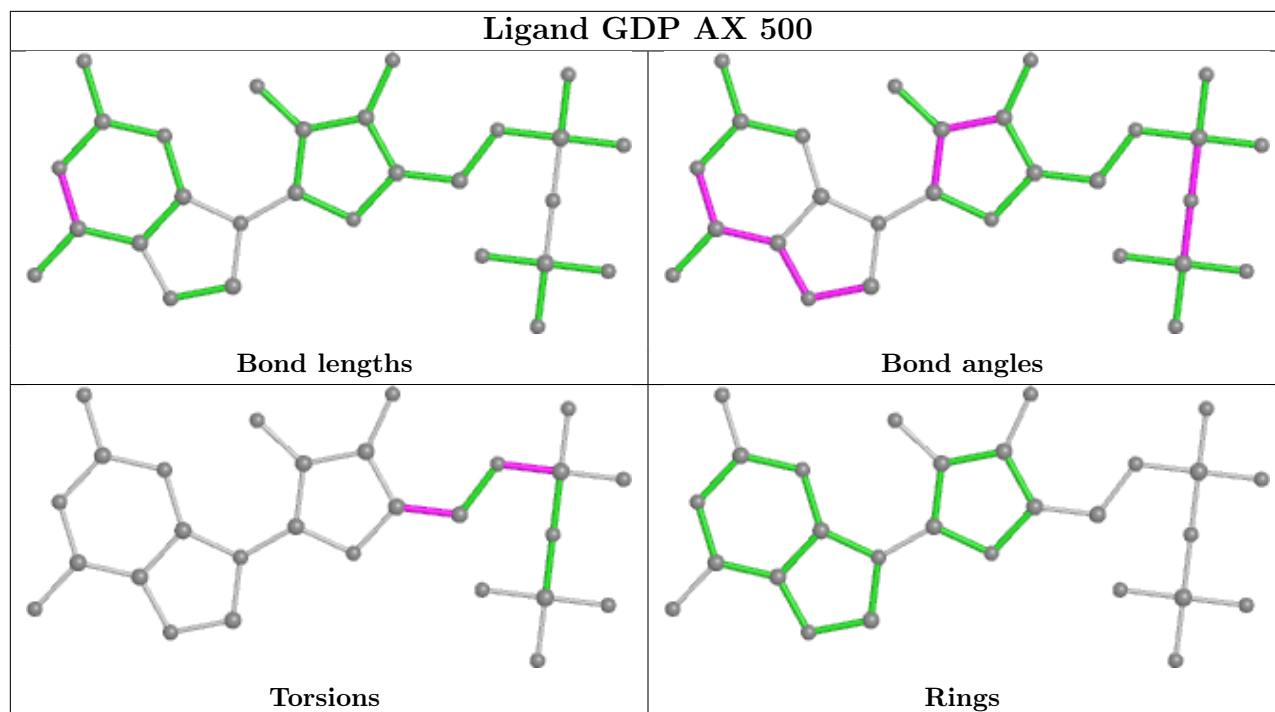
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	AX	500	GDP	C5'-O5'-PA-O3A
88	AX	500	GDP	C3'-C4'-C5'-O5'
88	AX	500	GDP	O4'-C4'-C5'-O5'
88	AX	500	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
85	A4	13

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A4	380:ASP	C	386:UNK	N	26.68
1	A4	143:GLU	C	145:UNK	N	21.71
1	A4	399:UNK	C	414:LYS	N	20.81
1	A4	173:UNK	C	220:UNK	N	13.65
1	A4	300:UNK	C	311:UNK	N	13.15
1	A4	285:UNK	C	290:UNK	N	12.01
1	A4	362:UNK	C	368:SER	N	11.59
1	A4	326:UNK	C	331:UNK	N	10.66
1	A4	232:UNK	C	237:UNK	N	10.09
1	A4	345:UNK	C	353:UNK	N	9.25
1	A4	250:UNK	C	255:UNK	N	7.95

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A4	156:UNK	C	161:UNK	N	6.10
1	A4	269:UNK	C	272:UNK	N	5.11

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2876. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.