Full wwPDB EM Validation Report (i)

Apr 16, 2024 – 04:32 am BST

PDB ID	:	7QGG
EMDB ID	:	EMD-13954
Title	:	Neuronal RNA granules are ribosome complexes stalled at the pre-translocation state
Authors	:	Pulk, A.; Kipper, K.; Mansour, A.
Deposited on	:	2021-12-08
Resolution	:	2.86 Å(reported)
Based on initial model	:	6OLE

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 (i) 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 (i)) were used in the production of this report:

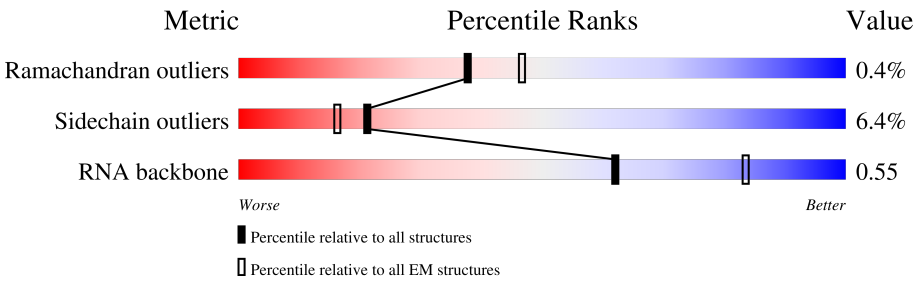
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.86 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)	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 <=5%

Mol	Chain	Length	Quality of chain
1	S2	1872	67% 23% • 8%
2	SA	295	69% • 27%
3	SB	264	78% • 19%
4	SD	243	86% 7% 7%
5	SE	263	92% 6% •
6	SF	204	89% • 7%
7	SH	194	91% 5% •
8	SI	208	91% 7% •
9	SK	165	54% 5% 41%

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Mol	Chain	Length	Quality of chain
10	SL	158	87% 7% 5%
11	SP	145	84% 5% 10%
12	SQ	146	92% 7%
13	SR	135	94% 5%
14	SS	152	88% 7% 5%
15	ST	145	93% 6%
16	SU	119	83% 13%
17	SV	83	87% 11%
18	SX	143	95%
19	Sa	115	84% 5% 10%
20	Sc	69	83% 10% 7%
21	Sd	56	93% 5%
22	Sg	317	89% 9%
23	SC	293	71% 5% 23%
24	SG	249	90% 6% 5%
25	SJ	194	86% 9% 5%
26	SM	132	82% 8% 11%
27	SN	151	96%
28	SO	151	83% 7% 9%
29	SW	130	92% 8%
30	SY	133	92% 7%
31	SZ	125	54% 5% 42%
32	Sb	84	89% 8%
33	Se	59	86% 10%
34	Sf	156	42% 57%

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Mol	Chain	Length	Quality of chain
35	A	257	94%
36	B	403	95%
37	C	421	80% 6% 14%
38	D	157	79% 21%
39	E	121	88% 10%
40	F	297	95%
41	G	298	79% 18%
42	H	260	83% 13%
43	I	266	85% 5% 9%
44	J	192	93% 6%
45	K	214	91% 7%
46	L	178	87% 8%
47	M	211	90% 7%
48	N	214	63% 35%
49	O	204	95% 5%
50	P	203	91% 6%
51	Q	184	82% 14%
52	R	188	95% 5%
53	S	196	89% 7%
54	T	176	96%
55	U	160	90% 8%
56	V	128	66% 11% 23%
57	W	140	91% 5%
58	X	157	37% 61%
59	Y	156	74% 23%

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Mol	Chain	Length	Quality of chain
60	Z	145	86% 7% 8%
61	a	136	90% 8%
62	b	148	98%
63	c	156	57% 39%
64	d	115	81% 7% 12%
65	e	125	81% 15%
66	f	135	91%

2 Entry composition (i)

There are 87 unique types of molecules in this entry. The entry contains 218574 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 RNA (1872-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	S2	1714	36502	16306	6533	11950	1713	0	0

- Molecule 2 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SA	214	1693	1076	297	312	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SB	214	1738	1103	310	311	14	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SD	226	1756	1119	316	314	7	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SE	259	2059	1316	383	352	8	0	0

- Molecule 6 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SF	189	1495	934	284	270	7	0	0

- Molecule 7 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	SH	186	1497	956	274	266	1	0	0

- Molecule 8 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	SI	204	1673	1050	329	289	5	0	0

- Molecule 9 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	SK	98	827	539	148	134	6	0	0

- Molecule 10 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	SL	150	1220	776	228	210	6	0	0

- Molecule 11 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	SP	130	1073	681	205	180	7	0	0

- Molecule 12 is a protein called Rps16 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	SQ	146	1158	736	218	200	4	0	0

- Molecule 13 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	SR	134	1079	676	201	198	4	0	0

- Molecule 14 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	SS	145	1198	751	242	203	2	0	0

- Molecule 15 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	ST	143	1115	698	217	198	2	0	0

- Molecule 16 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	SU	104	822	514	156	148	4	0	0

- Molecule 17 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	SV	82	626	382	118	121	5	0	0

- Molecule 18 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	SX	141	1098	693	219	183	3	0	0

- Molecule 19 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Sa	103	826	515	172	134	5	0	0

- Molecule 20 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Sc	64	506	308	102	94	2	0	0

- Molecule 21 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Sd	55	459	286	94	74	5	0	0

- Molecule 22 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Sg	312	2429	1531	423	463	12	0	0

- Molecule 23 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	SC	225	1755	1134	303	309	9	1	0

- Molecule 24 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	SG	237	1923	1200	387	329	7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	SJ	185	1533	974	309	248	2	1	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	SM	118	912	574	160	171	7	0	0

- Molecule 27 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	SN	150	1208	773	229	205	1	0	0

- Molecule 28 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	SO	137	1024	627	200	191	6	0	0

- Molecule 29 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	SW	129	1034	659	193	176	6	0	0

- Molecule 30 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	SY	131	1073	678	212	178	5	1	0

- Molecule 31 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	SZ	73	579	372	106	100	1	0	0

- Molecule 32 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Sb	82	640	402	118	113	7	0	0

- Molecule 33 is a protein called Ubiquitin-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Se	57	452	281	99	71	1	0	0

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	Sf	67	547	345	102	93	7	0	0

- Molecule 35 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	A	252	1930	1209	395	320	6	0	0

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	B	397	3204	2041	603	546	14	0	0

- Molecule 37 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	C	363	2889	1817	575	481	16	0	0

- Molecule 38 is a RNA chain called RNA (157-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
38	D	157	3337	1489	587	1104	157	0	0

- Molecule 39 is a RNA chain called RNA (121-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	E	119	2541	1132	454	836	119	0	0

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	F	294	2399	1511	442	432	14	0	0

- Molecule 41 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	G	243	1960	1251	375	330	4	0	0

- Molecule 42 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	H	225	1865	1199	357	301	8	0	0

- Molecule 43 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	I	241	1935	1232	372	327	4	0	0

- Molecule 44 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	J	191	1528	961	285	276	6	0	0

- Molecule 45 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	K	208	1692	1074	327	278	13	0	0

- Molecule 46 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	L	170	1362	861	254	241	6	0	0

- Molecule 47 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	M	205	1659	1036	342	276	5	0	0

- Molecule 48 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	N	139	1142	732	221	182	7	0	0

- Molecule 49 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	O	203	1701	1072	359	266	4	0	0

- Molecule 50 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	P	197	1611	1038	316	252	5	0	0

- Molecule 51 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	Q	158	1282	804	248	221	9	0	0

- Molecule 52 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	R	187	1516	949	314	249	4	0	0

- Molecule 53 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	S	188	1572	974	337	252	9	0	0

- Molecule 54 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	T	176	1458	929	284	234	11	0	0

- Molecule 55 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	U	158	1293	821	251	215	6	0	0

- Molecule 56 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	V	99	808	518	141	147	2	0	0

- Molecule 57 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	W	134	993	625	187	176	5	0	0

- Molecule 58 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
58	X	61	511	327	100	82	2	0	0

- Molecule 59 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
59	Y	120	984	630	185	168	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
60	Z	134	1116	700	227	186	3	0	0

- Molecule 61 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	a	134	1103	712	207	181	3	0	0

- Molecule 62 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
62	b	147	1165	736	240	185	4	0	0

- Molecule 63 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
63	c	95	781	487	171	120	3	0	0

- Molecule 64 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
64	d	101	785	498	138	142	7	0	0

- Molecule 65 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
65	e	106	879	555	170	152	2	0	0

- Molecule 66 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
66	f	129	1064	673	220	166	5	0	0

- Molecule 67 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
67	g	109	876	555	174	143	4	0	0

- Molecule 68 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
68	h	116	920	575	190	149	6	0	0

- Molecule 69 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
69	i	122	1015	643	204	167	1	0	0

- Molecule 70 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
70	j	104	849	531	180	133	5	0	0

- Molecule 71 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
71	k	86	705	434	155	111	5	0	0

- Molecule 72 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
72	l	69	569	366	103	99	1	0	0

- Molecule 73 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
73	m	50	444	281	98	64	1	0	0

- Molecule 74 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
74	n	50	411	254	87	64	6	0	0

- Molecule 75 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
75	o	25	240	145	64	28	3	0	0

- Molecule 76 is a protein called Ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
76	p	105	863	542	175	140	6	0	0

- Molecule 77 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
77	q	91	708	444	135	122	7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	87	GLU	LYS	conflict	UNP A0A6J2LF66

- Molecule 78 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
78	r	131	1059	655	224	175	5	0	0

- Molecule 79 is a RNA chain called RNA (4803-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
79	t	3679	78855	35119	14410	25647	3679	0	0

- Molecule 80 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
80	u	76	1613	720	283	535	75	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	34	C	G	conflict	GB 1851728667
u	35	C	A	conflict	GB 1851728667
u	36	G	A	conflict	GB 1851728667
u	37	U	A	conflict	GB 1851728667

- Molecule 81 is a RNA chain called RNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
81	v	76	1618	721	287	534	76	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	?	-	A	deletion	GB 1879656365
v	12	C	U	conflict	GB 1879656365
v	14	C	A	conflict	GB 1879656365
v	16	A	U	conflict	GB 1879656365
v	34	C	G	conflict	GB 1879656365
v	35	C	A	conflict	GB 1879656365
v	36	G	A	conflict	GB 1879656365

- Molecule 82 is a RNA chain called RNA (5'-D(P*()P*()P*()P*())-R(P*UP*UP*AP*CP*GP*GP*CP*GP*GP*UP*()P*()P*()P*()P*()P*())-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
82	w	20	423	189	72	142	20	0	0

- Molecule 83 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
83	Cz	217	1741	1113	312	307	9	0	0

- Molecule 84 is a protein called ALA-ALA-LYS-ALA.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
84	y	4	24	15	5	4	0	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
85	S2	3	3	3	0
85	B	1	1	1	0
85	D	6	6	6	0
85	E	9	9	9	0
85	Z	1	1	1	0
85	t	13	13	13	0

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
86	S2	1	1	1	0
86	Sa	1	1	1	0
86	Sf	1	1	1	0
86	k	1	1	1	0
86	p	1	1	1	0
86	q	1	1	1	0

- Molecule 87 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
87	S2	5	5	5	0
87	SS	1	1	1	0
87	Sf	1	1	1	0
87	u	1	1	1	0

SEQUENCE-PLOTS INFOmissingINFO

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor

4 Model quality (i)

4.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, ZN, UR3, MG, OMU, M7A, 4AC, 6MZ, OMG, B8N, A2M, 5MU, MA6, PSU, OMC, MMX

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	S2	0.24	2/39984 (0.0%)	0.91	101/62292 (0.2%)
2	SA	0.28	0/1730	0.57	0/2350
3	SB	0.31	0/1765	0.61	1/2362 (0.0%)
4	SD	0.41	1/1784 (0.1%)	0.66	2/2402 (0.1%)
5	SE	0.33	1/2101 (0.0%)	0.61	0/2828
6	SF	0.30	0/1516	0.61	0/2037
7	SH	0.32	0/1519	0.59	0/2033
8	SI	0.30	0/1702	0.61	1/2271 (0.0%)
9	SK	0.28	0/851	0.57	0/1147
10	SL	0.32	0/1241	0.62	0/1662
11	SP	0.38	0/1094	0.69	2/1460 (0.1%)
12	SQ	0.38	0/1177	0.70	0/1575
13	SR	0.39	0/1093	0.70	0/1469
14	SS	0.34	0/1216	0.70	1/1628 (0.1%)
15	ST	0.28	0/1134	0.58	1/1519 (0.1%)
16	SU	0.31	0/832	0.62	0/1117
17	SV	0.32	0/632	0.75	2/845 (0.2%)
18	SX	0.31	0/1116	0.66	0/1490
19	Sa	0.28	0/841	0.62	0/1128
20	Sc	0.27	0/508	0.75	1/680 (0.1%)
21	Sd	0.26	0/470	0.58	0/623
22	Sg	0.28	0/2486	0.62	0/3384
23	SC	0.31	0/1795	0.59	1/2424 (0.0%)
24	SG	0.27	0/1946	0.64	1/2590 (0.0%)
25	SJ	0.28	0/1561	0.66	1/2083 (0.0%)
26	SM	0.24	0/922	0.52	0/1237
27	SN	0.24	0/1232	0.53	0/1656
28	SO	0.25	0/1037	0.61	0/1391
29	SW	0.28	0/1051	0.61	0/1406
30	SY	0.27	0/1094	0.59	0/1452
31	SZ	0.33	0/585	0.68	0/785
32	Sb	0.29	0/653	0.59	0/876

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Se	0.29	0/458	0.61	0/604
34	Sf	0.27	0/559	0.54	0/743
35	A	0.28	0/1968	0.57	0/2639
36	B	0.26	0/3272	0.59	3/4380 (0.1%)
37	C	0.31	0/2943	0.60	1/3951 (0.0%)
38	D	0.23	0/3726	0.87	1/5804 (0.0%)
39	E	0.24	0/2839	0.94	7/4425 (0.2%)
40	F	0.26	0/2444	0.53	0/3272
41	G	0.27	0/1998	0.58	0/2676
42	H	0.26	0/1900	0.53	0/2534
43	I	0.26	0/1968	0.58	2/2649 (0.1%)
44	J	0.31	0/1547	0.61	1/2080 (0.0%)
45	K	0.26	0/1730	0.60	2/2311 (0.1%)
46	L	0.29	0/1385	0.63	0/1852
47	M	0.27	0/1690	0.64	1/2261 (0.0%)
48	N	0.29	0/1164	0.64	1/1556 (0.1%)
49	O	0.24	0/1746	0.59	0/2338
50	P	0.29	0/1641	0.59	1/2195 (0.0%)
51	Q	0.24	0/1309	0.54	0/1756
52	R	0.26	0/1540	0.62	0/2054
53	S	0.28	0/1588	0.68	1/2099 (0.0%)
54	T	0.26	0/1498	0.62	1/2010 (0.0%)
55	U	0.28	0/1321	0.59	0/1764
56	V	0.34	0/822	0.69	1/1103 (0.1%)
57	W	0.27	0/1007	0.61	1/1350 (0.1%)
58	X	0.31	0/524	0.60	0/698
59	Y	0.26	0/1001	0.58	0/1345
60	Z	0.29	0/1132	0.63	1/1503 (0.1%)
61	a	0.29	0/1126	0.66	3/1502 (0.2%)
62	b	0.24	0/1194	0.55	0/1594
63	c	0.24	0/794	0.55	0/1045
64	d	0.25	0/796	0.54	0/1068
65	e	0.26	0/894	0.57	0/1204
66	f	0.26	0/1082	0.61	1/1443 (0.1%)
67	g	0.26	0/895	0.60	0/1198
68	h	0.25	0/930	0.59	0/1238
69	i	0.26	0/1023	0.56	0/1350
70	j	0.25	0/860	0.63	0/1137
71	k	0.25	0/720	0.60	0/952
72	l	0.30	0/575	0.60	0/761
73	m	0.24	0/454	0.59	0/599
74	n	0.26	0/417	0.58	0/553
75	o	0.27	0/241	0.79	0/305

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	p	0.30	0/877	0.63	0/1156
77	q	0.25	0/718	0.60	1/954 (0.1%)
78	r	0.25	0/1074	0.65	1/1437 (0.1%)
79	t	0.28	15/88201 (0.0%)	0.94	185/137564 (0.1%)
80	u	0.26	0/1800	1.03	7/2804 (0.2%)
81	v	0.26	0/1806	1.00	12/2813 (0.4%)
82	w	0.19	0/471	0.88	1/731 (0.1%)
83	Cz	0.27	0/1769	0.57	0/2371
84	y	0.20	0/23	0.42	0/29
All	All	0.27	19/234128 (0.0%)	0.83	351/343962 (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
12	SQ	0	1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
79	t	479	G	O3'-P	-11.60	1.47	1.61
1	S2	1833	UR3	O3'-P	-10.51	1.48	1.61
4	SD	163	PRO	C-N	9.23	1.55	1.34
79	t	490	G	O3'-P	7.26	1.69	1.61
79	t	1990	G	O5'-C5'	-6.66	1.32	1.42
79	t	480	C	P-OP2	-6.64	1.37	1.49
79	t	478	G	O3'-P	-6.57	1.53	1.61
79	t	4471	C	O3'-P	6.23	1.68	1.61
79	t	1990	G	C5'-C4'	-6.19	1.44	1.51
79	t	3795	U	O3'-P	6.18	1.68	1.61
79	t	489	G	O3'-P	-5.95	1.54	1.61
79	t	480	C	P-OP1	-5.90	1.39	1.49
5	SE	101	LEU	C-N	-5.77	1.20	1.34
79	t	479	G	P-OP1	-5.66	1.39	1.49
79	t	1987	G	O3'-P	-5.63	1.54	1.61
1	S2	1834	A	P-OP1	-5.59	1.39	1.49
79	t	2095	C	C1'-N1	5.51	1.57	1.48
79	t	477	C	O3'-P	-5.47	1.54	1.61
79	t	490	G	C3'-O3'	5.10	1.49	1.42

All (351) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	t	4473	A	O5'-P-OP1	-59.17	39.70	110.70
79	t	3797	G	O5'-P-OP2	-45.67	55.89	110.70
79	t	3797	G	O5'-P-OP1	-34.01	69.89	110.70
79	t	4473	A	O5'-P-OP2	24.62	140.25	110.70
1	S2	115	U	C2-N3-C4	19.48	138.69	127.00
1	S2	1834	A	O5'-P-OP1	-13.84	93.25	105.70
79	t	4473	A	OP1-P-OP2	-12.70	100.55	119.60
79	t	860	C	N1-C2-O2	11.79	125.98	118.90
79	t	860	C	C2-N1-C1'	11.40	131.34	118.80
79	t	853	C	N1-C2-O2	11.36	125.71	118.90
79	t	853	C	C2-N1-C1'	10.88	130.77	118.80
79	t	632	C	N3-C2-O2	-10.75	114.38	121.90
79	t	3380	U	N1-C2-O2	10.54	130.18	122.80
79	t	479	G	C1'-C2'-O2'	-10.43	79.32	110.60
79	t	3380	U	C2-N1-C1'	10.23	129.97	117.70
11	SP	68	PRO	CA-N-CD	-10.12	97.33	111.50
54	T	159	LEU	CA-CB-CG	9.98	138.26	115.30
79	t	4152	U	C2-N1-C1'	9.94	129.63	117.70
1	S2	1317	U	C2-N1-C1'	9.93	129.61	117.70
79	t	1200	C	N3-C2-O2	-9.90	114.97	121.90
79	t	3380	U	N3-C2-O2	-9.85	115.30	122.20
1	S2	1456	C	N1-C2-O2	9.64	124.68	118.90
1	S2	846	C	N3-C2-O2	-9.47	115.27	121.90
79	t	4152	U	N1-C2-O2	9.41	129.39	122.80
1	S2	115	U	N1-C2-N3	9.28	120.47	114.90
1	S2	1456	C	C2-N1-C1'	9.28	129.01	118.80
1	S2	115	U	N3-C4-C5	9.27	120.17	114.60
79	t	1674	C	N3-C2-O2	-9.20	115.46	121.90
79	t	2253	U	C2-N1-C1'	9.15	128.68	117.70
79	t	853	C	N3-C2-O2	-9.11	115.53	121.90
79	t	1990	G	O5'-P-OP2	9.06	121.58	110.70
79	t	860	C	N3-C2-O2	-8.85	115.71	121.90
79	t	863	C	N3-C2-O2	-8.57	115.90	121.90
36	B	360	LEU	CA-CB-CG	8.56	134.99	115.30
79	t	4152	U	N3-C2-O2	-8.53	116.23	122.20
1	S2	1142	C	N1-C2-O2	8.34	123.90	118.90
79	t	222	C	N1-C2-O2	8.34	123.90	118.90
79	t	1135	C	C2-N1-C1'	8.28	127.91	118.80
79	t	1135	C	N1-C2-O2	8.26	123.85	118.90
17	SV	66	ASP	CB-CG-OD1	8.22	125.70	118.30
79	t	4505	C	N3-C2-O2	-8.22	116.15	121.90
79	t	860	C	C6-N1-C1'	-8.17	110.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	t	2253	U	N1-C2-O2	8.17	128.52	122.80
1	S2	1142	C	C2-N1-C1'	8.15	127.76	118.80
79	t	222	C	C2-N1-C1'	8.13	127.75	118.80
1	S2	118	C	C2-N1-C1'	8.09	127.70	118.80
79	t	632	C	C6-N1-C2	-8.04	117.08	120.30
79	t	2253	U	N3-C2-O2	-8.01	116.59	122.20
1	S2	118	C	N1-C2-O2	7.99	123.69	118.90
79	t	2592	C	C2-N1-C1'	7.95	127.55	118.80
79	t	450	G	O4'-C1'-N9	7.93	114.55	108.20
1	S2	1834	A	C5'-C4'-O4'	-7.91	99.61	109.10
36	B	364	ASP	CB-CG-OD1	7.90	125.41	118.30
4	SD	43	PRO	CA-N-CD	-7.90	100.44	111.50
79	t	2312	U	N3-C2-O2	-7.84	116.71	122.20
79	t	2471	C	N1-C2-O2	7.73	123.54	118.90
56	V	35	ASP	CB-CG-OD1	7.63	125.17	118.30
1	S2	976	C	N1-C2-O2	7.57	123.44	118.90
1	S2	1264	C	N1-C2-O2	7.57	123.44	118.90
79	t	1674	C	N1-C2-O2	7.51	123.41	118.90
79	t	853	C	C6-N1-C1'	-7.51	111.79	120.80
8	SI	80	ASP	CB-CG-OD1	7.50	125.05	118.30
1	S2	1456	C	N3-C2-O2	-7.50	116.65	121.90
79	t	3828	C	C6-N1-C2	-7.48	117.31	120.30
23	SC	132	ASP	CB-CG-OD1	7.46	125.01	118.30
79	t	3543	C	N3-C2-O2	-7.45	116.69	121.90
79	t	3828	C	C5-C6-N1	7.41	124.71	121.00
79	t	853	C	C6-N1-C2	-7.41	117.34	120.30
79	t	863	C	N1-C2-O2	7.35	123.31	118.90
1	S2	1719	C	C2-N1-C1'	7.35	126.88	118.80
39	E	29	C	N1-C2-O2	7.33	123.30	118.90
1	S2	1286	C	N1-C2-O2	7.26	123.26	118.90
79	t	2592	C	N1-C2-O2	7.24	123.25	118.90
1	S2	1274	C	N1-C2-O2	7.23	123.24	118.90
61	a	92	ASP	CB-CG-OD1	7.18	124.76	118.30
79	t	2312	U	N1-C2-O2	7.17	127.82	122.80
79	t	480	C	C1'-C2'-O2'	-7.14	89.17	110.60
1	S2	359	C	C2-N1-C1'	7.10	126.61	118.80
79	t	501	G	C4-N9-C1'	7.05	135.67	126.50
1	S2	1523	G	C4-N9-C1'	7.05	135.66	126.50
1	S2	1317	U	C6-N1-C1'	-7.04	111.34	121.20
1	S2	1318	U	N1-C2-O2	7.00	127.70	122.80
79	t	2312	U	C2-N1-C1'	6.96	126.05	117.70
79	t	1985	C	N1-C2-O2	6.93	123.06	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1317	U	N1-C2-O2	6.92	127.65	122.80
79	t	1135	C	N3-C2-O2	-6.92	117.05	121.90
1	S2	306	C	N1-C2-O2	6.92	123.05	118.90
61	a	99	ASP	CB-CG-OD1	6.91	124.52	118.30
79	t	3543	C	N1-C2-O2	6.89	123.04	118.90
1	S2	359	C	N1-C2-O2	6.86	123.02	118.90
79	t	860	C	C6-N1-C2	-6.77	117.59	120.30
79	t	1896	C	N3-C2-O2	-6.76	117.17	121.90
79	t	1350	C	N3-C2-O2	-6.71	117.20	121.90
1	S2	1142	C	N3-C2-O2	-6.70	117.21	121.90
81	v	12	C	N3-C2-O2	-6.69	117.22	121.90
79	t	49	U	N1-C2-O2	6.68	127.48	122.80
80	u	56	C	N1-C2-O2	6.67	122.90	118.90
60	Z	10	ASP	CB-CG-OD1	6.65	124.28	118.30
1	S2	1523	G	N3-C4-N9	6.65	129.99	126.00
79	t	222	C	N3-C2-O2	-6.64	117.25	121.90
79	t	1851	U	C2-N1-C1'	6.63	125.66	117.70
1	S2	1318	U	C2-N1-C1'	6.60	125.62	117.70
79	t	2471	C	C2-N1-C1'	6.60	126.06	118.80
79	t	1388	G	C4-N9-C1'	6.56	135.02	126.50
79	t	137	G	C4-N9-C1'	6.55	135.01	126.50
79	t	4152	U	C6-N1-C1'	-6.55	112.03	121.20
53	S	116	ASP	CB-CG-OD1	6.55	124.19	118.30
79	t	3380	U	C6-N1-C1'	-6.55	112.03	121.20
37	C	59	GLY	N-CA-C	-6.54	96.75	113.10
1	S2	845	C	N1-C2-O2	6.53	122.82	118.90
79	t	632	C	N1-C2-O2	6.53	122.81	118.90
1	S2	1264	C	C2-N1-C1'	6.52	125.98	118.80
81	v	61	C	C2-N1-C1'	6.52	125.97	118.80
4	SD	163	PRO	O-C-N	6.50	133.09	122.70
79	t	851	G	C4-N9-C1'	6.49	134.94	126.50
77	q	89	LEU	CA-CB-CG	6.46	130.16	115.30
79	t	112	C	C2-N1-C1'	6.46	125.90	118.80
11	SP	70	MET	CA-CB-CG	6.45	124.26	113.30
79	t	501	G	N3-C4-N9	6.44	129.86	126.00
78	r	106	LEU	CA-CB-CG	6.40	130.02	115.30
1	S2	1456	C	C6-N1-C1'	-6.38	113.14	120.80
1	S2	118	C	N3-C2-O2	-6.37	117.44	121.90
79	t	477	C	O4'-C4'-C3'	-6.37	97.63	104.00
79	t	2592	C	N3-C2-O2	-6.37	117.44	121.90
79	t	1388	G	N3-C4-N9	6.36	129.81	126.00
1	S2	562	G	P-O3'-C3'	6.36	127.33	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1523	G	N3-C4-C5	-6.34	125.43	128.60
1	S2	1818	A	P-O3'-C3'	6.34	127.30	119.70
1	S2	306	C	C2-N1-C1'	6.32	125.75	118.80
81	v	11	C	N1-C2-O2	6.32	122.69	118.90
1	S2	1318	U	N3-C2-O2	-6.31	117.78	122.20
79	t	860	C	C5-C6-N1	6.31	124.16	121.00
1	S2	1541	C	N1-C2-O2	6.30	122.68	118.90
79	t	137	G	N3-C4-C5	-6.29	125.45	128.60
79	t	2238	G	C4-N9-C1'	6.29	134.67	126.50
79	t	1851	U	N1-C2-O2	6.28	127.20	122.80
79	t	4505	C	N1-C2-O2	6.27	122.66	118.90
81	v	17	A	P-O3'-C3'	6.26	127.21	119.70
1	S2	976	C	C2-N1-C1'	6.24	125.67	118.80
79	t	851	G	N3-C4-C5	-6.22	125.49	128.60
80	u	56	C	C6-N1-C2	-6.22	117.81	120.30
79	t	4441	U	N1-C2-O2	6.21	127.15	122.80
79	t	501	G	N3-C4-C5	-6.21	125.50	128.60
39	E	29	C	N3-C2-O2	-6.21	117.56	121.90
79	t	4037	G	C4-N9-C1'	6.19	134.54	126.50
79	t	2471	C	N3-C2-O2	-6.18	117.57	121.90
25	SJ	50	LEU	CA-CB-CG	6.17	129.50	115.30
79	t	3644	C	N1-C2-O2	6.17	122.60	118.90
79	t	137	G	N3-C4-N9	6.14	129.69	126.00
1	S2	1456	C	C6-N1-C2	-6.13	117.85	120.30
1	S2	1286	C	N3-C2-O2	-6.13	117.61	121.90
1	S2	920	U	C2-N1-C1'	6.12	125.04	117.70
79	t	1486	U	N1-C2-O2	6.11	127.07	122.80
79	t	853	C	C5-C6-N1	6.10	124.05	121.00
79	t	1388	G	N3-C4-C5	-6.10	125.55	128.60
79	t	1851	U	N3-C2-O2	-6.09	117.93	122.20
1	S2	1264	C	N3-C2-O2	-6.07	117.65	121.90
1	S2	875	A	P-O3'-C3'	6.07	126.98	119.70
79	t	2364	C	C2-N1-C1'	6.07	125.47	118.80
79	t	3694	U	P-O3'-C3'	6.03	126.94	119.70
81	v	68	C	C2-N1-C1'	6.03	125.44	118.80
1	S2	1523	G	C8-N9-C1'	-6.03	119.16	127.00
79	t	2253	U	C6-N1-C1'	-6.03	112.76	121.20
1	S2	846	C	N1-C2-O2	6.02	122.51	118.90
81	v	43	C	C2-N1-C1'	6.02	125.42	118.80
79	t	507	G	O4'-C1'-N9	6.02	113.02	108.20
1	S2	1025	U	C2-N1-C1'	6.01	124.92	117.70
36	B	140	ASP	CB-CG-OD1	6.00	123.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
81	v	50	U	P-O3'-C3'	6.00	126.89	119.70
79	t	501	G	C8-N9-C1'	-5.99	119.21	127.00
79	t	1486	U	C2-N1-C1'	5.99	124.88	117.70
1	S2	908	C	N3-C2-O2	-5.98	117.71	121.90
79	t	49	U	C2-N1-C1'	5.98	124.87	117.70
45	K	44	ASP	CB-CG-OD1	5.97	123.68	118.30
79	t	855	C	C2-N1-C1'	5.97	125.36	118.80
1	S2	976	C	N3-C2-O2	-5.95	117.74	121.90
79	t	4130	C	N1-C2-O2	5.95	122.47	118.90
79	t	4693	C	N3-C2-O2	-5.92	117.76	121.90
79	t	851	G	N3-C4-N9	5.92	129.55	126.00
79	t	496	C	N1-C2-O2	5.90	122.44	118.90
39	E	29	C	C2-N1-C1'	5.89	125.28	118.80
79	t	2663	U	N1-C2-O2	5.89	126.92	122.80
81	v	61	C	N1-C2-O2	5.89	122.43	118.90
48	N	81	ASP	CB-CG-OD1	5.88	123.60	118.30
1	S2	1317	U	N3-C2-O2	-5.86	118.10	122.20
79	t	847	U	P-O3'-C3'	5.86	126.74	119.70
79	t	1990	G	O4'-C1'-C2'	-5.85	99.95	105.80
15	ST	110	LEU	CA-CB-CG	5.85	128.75	115.30
57	W	92	ASP	CB-CG-OD1	5.84	123.56	118.30
79	t	4717	U	P-O3'-C3'	5.84	126.71	119.70
79	t	2263	C	C2-N1-C1'	5.83	125.22	118.80
79	t	1985	C	N3-C2-O2	-5.83	117.82	121.90
79	t	2364	C	N1-C2-O2	5.82	122.39	118.90
80	u	62	C	C2-N1-C1'	5.82	125.20	118.80
79	t	480	C	O5'-P-OP1	5.81	117.67	110.70
1	S2	306	C	N3-C2-O2	-5.81	117.83	121.90
79	t	4037	G	N3-C4-C5	-5.80	125.70	128.60
80	u	55	U	C2-N1-C1'	5.79	124.65	117.70
80	u	56	C	C2-N1-C1'	5.79	125.17	118.80
79	t	1146	C	N1-C2-O2	5.79	122.37	118.90
80	u	43	C	C2-N1-C1'	5.78	125.16	118.80
79	t	222	C	C6-N1-C2	-5.78	117.99	120.30
17	SV	11	LEU	CA-CB-CG	5.73	128.47	115.30
79	t	49	U	N3-C2-O2	-5.72	118.19	122.20
44	J	48	LEU	CA-CB-CG	5.72	128.46	115.30
79	t	1135	C	C6-N1-C2	-5.72	118.01	120.30
79	t	1486	U	N3-C2-O2	-5.72	118.20	122.20
1	S2	635	C	C2-N1-C1'	5.71	125.08	118.80
14	SS	23	ARG	CA-CB-CG	5.71	125.95	113.40
1	S2	115	U	N3-C2-O2	-5.70	118.21	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	t	3380	U	C5-C6-N1	5.70	125.55	122.70
79	t	2099	C	C2-N1-C1'	5.68	125.05	118.80
79	t	1896	C	N1-C2-O2	5.68	122.31	118.90
39	E	102	U	N1-C2-O2	5.68	126.78	122.80
80	u	56	C	N3-C2-O2	-5.67	117.93	121.90
1	S2	1142	C	C6-N1-C2	-5.66	118.03	120.30
1	S2	1663	C	C2-N1-C1'	5.66	125.03	118.80
1	S2	1126	C	N1-C2-O2	5.66	122.30	118.90
1	S2	1286	C	C2-N1-C1'	5.65	125.02	118.80
1	S2	1126	C	N3-C2-O2	-5.65	117.94	121.90
79	t	128	C	N1-C2-O2	5.65	122.29	118.90
50	P	141	LEU	CA-CB-CG	5.64	128.28	115.30
79	t	3513	U	N1-C2-O2	5.62	126.74	122.80
1	S2	359	C	N3-C2-O2	-5.62	117.97	121.90
79	t	4441	U	N3-C2-O2	-5.61	118.27	122.20
1	S2	561	G	P-O3'-C3'	5.61	126.43	119.70
79	t	682	C	N1-C2-O2	5.61	122.27	118.90
79	t	1135	C	C6-N1-C1'	-5.61	114.07	120.80
79	t	3947	C	N1-C2-O2	5.60	122.26	118.90
1	S2	118	C	C6-N1-C1'	-5.58	114.10	120.80
79	t	71	C	P-O3'-C3'	5.58	126.39	119.70
79	t	4152	U	C5-C6-N1	5.56	125.48	122.70
79	t	4234	C	N1-C2-O2	5.56	122.24	118.90
1	S2	573	C	N1-C2-O2	5.55	122.23	118.90
79	t	1388	G	C8-N9-C1'	-5.54	119.79	127.00
1	S2	1310	U	C2-N1-C1'	5.54	124.35	117.70
1	S2	1286	C	C6-N1-C2	-5.53	118.09	120.30
1	S2	1142	C	C6-N1-C1'	-5.52	114.18	120.80
66	f	89	LEU	CA-CB-CG	5.52	127.99	115.30
79	t	480	C	N1-C1'-C2'	5.52	121.17	114.00
1	S2	1499	U	C2-N1-C1'	5.51	124.32	117.70
79	t	4643	G	N1-C6-O6	-5.51	116.59	119.90
79	t	2663	U	C2-N1-C1'	5.51	124.31	117.70
79	t	866	C	C2-N1-C1'	5.51	124.86	118.80
24	SG	124	LEU	CA-CB-CG	5.50	127.95	115.30
1	S2	69	C	C2-N1-C1'	5.50	124.85	118.80
79	t	868	C	C2-N1-C1'	5.48	124.83	118.80
47	M	155	MET	CB-CG-SD	5.48	128.84	112.40
1	S2	1274	C	N3-C2-O2	-5.47	118.07	121.90
79	t	222	C	C6-N1-C1'	-5.46	114.25	120.80
1	S2	836	C	N1-C2-O2	5.46	122.17	118.90
79	t	2099	C	N1-C2-O2	5.45	122.17	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	t	1361	G	P-O5'-C5'	-5.45	112.19	120.90
79	t	863	C	C6-N1-C2	-5.44	118.12	120.30
39	E	78	C	C2-N1-C1'	5.44	124.78	118.80
79	t	1923	C	N1-C2-O2	5.43	122.16	118.90
79	t	2592	C	C6-N1-C1'	-5.43	114.28	120.80
79	t	4441	U	C2-N1-C1'	5.43	124.22	117.70
79	t	1990	G	C5'-C4'-O4'	-5.43	102.58	109.10
79	t	2254	C	C2-N1-C1'	5.43	124.77	118.80
1	S2	1264	C	C6-N1-C2	-5.43	118.13	120.30
79	t	3644	C	N3-C2-O2	-5.42	118.11	121.90
3	SB	229	MET	CB-CG-SD	5.42	128.65	112.40
79	t	2121	C	C2-N1-C1'	5.41	124.75	118.80
81	v	68	C	N1-C2-O2	5.41	122.14	118.90
1	S2	1456	C	C5-C6-N1	5.40	123.70	121.00
79	t	137	G	C8-N9-C1'	-5.40	119.98	127.00
79	t	1200	C	N1-C2-O2	5.40	122.14	118.90
1	S2	1473	C	C2-N1-C1'	5.39	124.73	118.80
1	S2	871	G	P-O3'-C3'	5.38	126.16	119.70
79	t	128	C	N3-C2-O2	-5.38	118.14	121.90
79	t	3986	G	N3-C4-C5	-5.38	125.91	128.60
1	S2	118	C	C6-N1-C2	-5.36	118.16	120.30
1	S2	1541	C	C2-N1-C1'	5.36	124.69	118.80
79	t	3513	U	C2-N1-C1'	5.36	124.13	117.70
39	E	29	C	C6-N1-C2	-5.35	118.16	120.30
79	t	1859	U	C2-N1-C1'	5.35	124.12	117.70
79	t	480	C	O4'-C4'-C3'	-5.35	98.65	104.00
79	t	238	C	N3-C2-O2	-5.34	118.16	121.90
43	I	95	LEU	CA-CB-CG	5.34	127.59	115.30
79	t	1923	C	N3-C2-O2	-5.34	118.16	121.90
1	S2	846	C	C6-N1-C2	-5.34	118.17	120.30
79	t	4103	G	P-O3'-C3'	5.33	126.10	119.70
1	S2	836	C	N3-C2-O2	-5.33	118.17	121.90
79	t	4632	C	N3-C2-O2	-5.33	118.17	121.90
1	S2	875	A	OP1-P-O3'	5.33	116.91	105.20
1	S2	1392	C	N1-C2-O2	5.32	122.09	118.90
1	S2	1834	A	C2'-C3'-O3'	-5.32	97.79	109.50
79	t	2592	C	C6-N1-C2	-5.32	118.17	120.30
79	t	4634	G	P-O3'-C3'	5.32	126.08	119.70
79	t	1674	C	C6-N1-C2	-5.32	118.17	120.30
61	a	88	ASP	CB-CG-OD1	5.31	123.08	118.30
79	t	4427	C	N1-C2-O2	5.31	122.09	118.90
79	t	851	G	C8-N9-C1'	-5.30	120.11	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
79	t	2663	U	N3-C2-O2	-5.30	118.49	122.20
1	S2	851	U	N3-C2-O2	-5.29	118.50	122.20
81	v	11	C	N3-C2-O2	-5.29	118.19	121.90
1	S2	860	U	N1-C2-O2	5.29	126.50	122.80
81	v	12	C	C6-N1-C2	-5.28	118.19	120.30
79	t	1909	U	C2-N1-C1'	5.28	124.03	117.70
79	t	1633	C	C2-N1-C1'	5.28	124.60	118.80
82	w	13	C	N1-C2-O2	5.27	122.06	118.90
1	S2	588	C	C2-N1-C1'	5.26	124.59	118.80
1	S2	860	U	C2-N1-C1'	5.26	124.01	117.70
79	t	2312	U	C6-N1-C2	-5.26	117.84	121.00
79	t	866	C	N1-C2-O2	5.25	122.05	118.90
79	t	449	C	C6-N1-C2	-5.25	118.20	120.30
79	t	1575	U	N3-C2-O2	-5.24	118.53	122.20
1	S2	1745	C	C2-N1-C1'	5.24	124.56	118.80
1	S2	976	C	C6-N1-C2	-5.24	118.20	120.30
79	t	520	C	C2-N1-C1'	5.23	124.56	118.80
79	t	1859	U	N1-C2-O2	5.23	126.46	122.80
1	S2	530	C	C2-N1-C1'	5.23	124.55	118.80
1	S2	1834	A	C1'-C2'-O2'	-5.22	94.94	110.60
79	t	4606	C	N1-C2-O2	5.21	122.03	118.90
79	t	3644	C	C2-N1-C1'	5.21	124.53	118.80
79	t	1567	C	C2-N1-C1'	5.20	124.51	118.80
38	D	96	C	N1-C2-O2	5.19	122.02	118.90
1	S2	1719	C	C6-N1-C1'	-5.18	114.58	120.80
1	S2	4	C	C2-N1-C1'	5.18	124.50	118.80
79	t	3497	U	N1-C2-O2	5.18	126.42	122.80
1	S2	430	U	C2-N1-C1'	5.17	123.90	117.70
20	Sc	58	LEU	CA-CB-CG	5.16	127.18	115.30
1	S2	635	C	N1-C2-O2	5.16	122.00	118.90
43	I	136	LEU	CA-CB-CG	5.15	127.16	115.30
79	t	1907	U	N1-C2-O2	5.15	126.41	122.80
1	S2	835	G	N1-C2-N2	-5.15	111.57	116.20
79	t	4632	C	N1-C2-O2	5.13	121.98	118.90
79	t	4037	G	N3-C4-N9	5.13	129.08	126.00
79	t	922	C	N1-C2-O2	5.12	121.97	118.90
1	S2	566	G	P-O3'-C3'	5.11	125.83	119.70
79	t	1197	U	N1-C2-O2	5.10	126.37	122.80
79	t	2664	C	N1-C2-O2	5.10	121.96	118.90
79	t	282	C	N1-C2-O2	5.09	121.95	118.90
1	S2	1022	C	N1-C2-O2	5.08	121.95	118.90
79	t	2238	G	C8-N9-C1'	-5.08	120.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	E	102	U	N3-C2-O2	-5.07	118.65	122.20
1	S2	561	G	OP1-P-O3'	5.06	116.34	105.20
79	t	4472	G	O3'-P-O5'	-5.06	94.39	104.00
79	t	1180	C	N1-C2-O2	5.05	121.93	118.90
79	t	2514	C	C2-N1-C1'	5.05	124.36	118.80
1	S2	804	U	N3-C2-O2	-5.05	118.67	122.20
79	t	1350	C	N1-C2-O2	5.05	121.93	118.90
1	S2	1541	C	N3-C2-O2	-5.04	118.37	121.90
79	t	3380	U	C6-N1-C2	-5.04	117.98	121.00
79	t	4344	C	N1-C2-O2	5.03	121.92	118.90
45	K	83	ASP	CB-CG-OD1	5.02	122.82	118.30
1	S2	908	C	N1-C2-O2	5.02	121.91	118.90
1	S2	1274	C	C2-N1-C1'	5.00	124.30	118.80
79	t	4693	C	N1-C2-O2	5.00	121.90	118.90
81	v	61	C	C6-N1-C1'	-5.00	114.80	120.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	SQ	75	GLY	Peptide

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 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
2	SA	212/295 (72%)	196 (92%)	16 (8%)	0	100 100
3	SB	212/264 (80%)	201 (95%)	9 (4%)	2 (1%)	17 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	SD	224/243 (92%)	197 (88%)	23 (10%)	4 (2%)	8	25
5	SE	257/263 (98%)	238 (93%)	16 (6%)	3 (1%)	13	35
6	SF	187/204 (92%)	172 (92%)	15 (8%)	0	100	100
7	SH	182/194 (94%)	169 (93%)	12 (7%)	1 (0%)	29	57
8	SI	202/208 (97%)	183 (91%)	17 (8%)	2 (1%)	15	40
9	SK	96/165 (58%)	87 (91%)	9 (9%)	0	100	100
10	SL	148/158 (94%)	140 (95%)	6 (4%)	2 (1%)	11	31
11	SP	128/145 (88%)	121 (94%)	7 (6%)	0	100	100
12	SQ	144/146 (99%)	133 (92%)	9 (6%)	2 (1%)	11	31
13	SR	132/135 (98%)	115 (87%)	16 (12%)	1 (1%)	19	46
14	SS	143/152 (94%)	127 (89%)	15 (10%)	1 (1%)	22	50
15	ST	141/145 (97%)	134 (95%)	7 (5%)	0	100	100
16	SU	102/119 (86%)	95 (93%)	6 (6%)	1 (1%)	15	40
17	SV	80/83 (96%)	75 (94%)	5 (6%)	0	100	100
18	SX	139/143 (97%)	123 (88%)	16 (12%)	0	100	100
19	Sa	101/115 (88%)	95 (94%)	6 (6%)	0	100	100
20	Sc	62/69 (90%)	51 (82%)	11 (18%)	0	100	100
21	Sd	53/56 (95%)	50 (94%)	3 (6%)	0	100	100
22	Sg	310/317 (98%)	273 (88%)	37 (12%)	0	100	100
23	SC	224/293 (76%)	208 (93%)	16 (7%)	0	100	100
24	SG	235/249 (94%)	217 (92%)	18 (8%)	0	100	100
25	SJ	184/194 (95%)	169 (92%)	14 (8%)	1 (0%)	29	57
26	SM	116/132 (88%)	101 (87%)	15 (13%)	0	100	100
27	SN	148/151 (98%)	145 (98%)	3 (2%)	0	100	100
28	SO	135/151 (89%)	120 (89%)	15 (11%)	0	100	100
29	SW	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
30	SY	130/133 (98%)	118 (91%)	12 (9%)	0	100	100
31	SZ	71/125 (57%)	62 (87%)	9 (13%)	0	100	100
32	Sb	80/84 (95%)	75 (94%)	5 (6%)	0	100	100
33	Se	55/59 (93%)	48 (87%)	7 (13%)	0	100	100
34	Sf	65/156 (42%)	51 (78%)	14 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	A	250/257 (97%)	231 (92%)	19 (8%)	0	100	100
36	B	395/403 (98%)	367 (93%)	28 (7%)	0	100	100
37	C	361/421 (86%)	333 (92%)	21 (6%)	7 (2%)	8	24
40	F	292/297 (98%)	275 (94%)	15 (5%)	2 (1%)	22	50
41	G	239/298 (80%)	209 (87%)	28 (12%)	2 (1%)	19	46
42	H	223/260 (86%)	210 (94%)	13 (6%)	0	100	100
43	I	239/266 (90%)	222 (93%)	17 (7%)	0	100	100
44	J	189/192 (98%)	176 (93%)	12 (6%)	1 (0%)	29	57
45	K	204/214 (95%)	193 (95%)	11 (5%)	0	100	100
46	L	168/178 (94%)	159 (95%)	8 (5%)	1 (1%)	25	53
47	M	203/211 (96%)	175 (86%)	25 (12%)	3 (2%)	10	30
48	N	137/214 (64%)	132 (96%)	5 (4%)	0	100	100
49	O	201/204 (98%)	191 (95%)	9 (4%)	1 (0%)	29	57
50	P	195/203 (96%)	189 (97%)	5 (3%)	1 (0%)	29	57
51	Q	156/184 (85%)	151 (97%)	5 (3%)	0	100	100
52	R	185/188 (98%)	172 (93%)	13 (7%)	0	100	100
53	S	186/196 (95%)	180 (97%)	6 (3%)	0	100	100
54	T	174/176 (99%)	160 (92%)	14 (8%)	0	100	100
55	U	156/160 (98%)	149 (96%)	6 (4%)	1 (1%)	25	53
56	V	97/128 (76%)	94 (97%)	3 (3%)	0	100	100
57	W	132/140 (94%)	126 (96%)	6 (4%)	0	100	100
58	X	59/157 (38%)	56 (95%)	3 (5%)	0	100	100
59	Y	118/156 (76%)	114 (97%)	4 (3%)	0	100	100
60	Z	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
61	a	132/136 (97%)	122 (92%)	10 (8%)	0	100	100
62	b	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
63	c	91/156 (58%)	86 (94%)	5 (6%)	0	100	100
64	d	99/115 (86%)	93 (94%)	6 (6%)	0	100	100
65	e	104/125 (83%)	99 (95%)	5 (5%)	0	100	100
66	f	127/135 (94%)	118 (93%)	8 (6%)	1 (1%)	19	46
67	g	107/110 (97%)	102 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	h	114/117 (97%)	106 (93%)	8 (7%)	0	100	100
69	i	120/123 (98%)	113 (94%)	7 (6%)	0	100	100
70	j	102/105 (97%)	95 (93%)	7 (7%)	0	100	100
71	k	84/97 (87%)	79 (94%)	3 (4%)	2 (2%)	6	19
72	l	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
73	m	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
74	n	48/128 (38%)	46 (96%)	2 (4%)	0	100	100
75	o	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
76	p	103/106 (97%)	93 (90%)	9 (9%)	1 (1%)	15	40
77	q	89/92 (97%)	83 (93%)	6 (7%)	0	100	100
78	r	129/137 (94%)	114 (88%)	15 (12%)	0	100	100
83	Cz	215/217 (99%)	183 (85%)	31 (14%)	1 (0%)	29	57
84	y	2/4 (50%)	2 (100%)	0	0	100	100
All	All	11465/12921 (89%)	10600 (92%)	821 (7%)	44 (0%)	38	62

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	SB	191	ASP
5	SE	165	GLU
10	SL	82	MET
37	C	55	SER
37	C	58	ALA
83	Cz	60	ARG
37	C	54	VAL
37	C	56	GLU
37	C	318	PRO
47	M	46	ILE
55	U	4	THR
71	k	86	PRO
76	p	76	ASN
4	SD	213	PRO
12	SQ	127	CYS
37	C	57	LEU
4	SD	202	LYS
8	SI	98	LYS
16	SU	107	GLU

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Mol	Chain	Res	Type
25	SJ	67	ASP
37	C	319	LEU
41	G	117	VAL
49	O	145	ASN
3	SB	130	THR
4	SD	192	TRP
10	SL	23	VAL
40	F	6	VAL
46	L	111	GLU
47	M	157	ILE
4	SD	162	ASP
5	SE	98	ASN
7	SH	99	ARG
13	SR	129	LYS
14	SS	49	ASP
40	F	253	TYR
44	J	2	LYS
47	M	164	GLU
66	f	19	LYS
8	SI	97	VAL
71	k	85	LYS
5	SE	30	ARG
12	SQ	100	VAL
41	G	116	VAL
50	P	146	GLY

4.3.2 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	
2	SA	179/242 (74%)	170 (95%)	9 (5%)	24	53
3	SB	195/231 (84%)	189 (97%)	6 (3%)	40	71
4	SD	189/202 (94%)	179 (95%)	10 (5%)	22	50
5	SE	222/225 (99%)	210 (95%)	12 (5%)	22	49
6	SF	159/171 (93%)	152 (96%)	7 (4%)	28	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	SH	166/174 (95%)	157 (95%)	9 (5%)	22	49
8	SI	177/180 (98%)	165 (93%)	12 (7%)	16	38
9	SK	89/136 (65%)	80 (90%)	9 (10%)	7	20
10	SL	134/142 (94%)	123 (92%)	11 (8%)	11	29
11	SP	116/130 (89%)	109 (94%)	7 (6%)	19	45
12	SQ	121/121 (100%)	112 (93%)	9 (7%)	13	35
13	SR	120/121 (99%)	114 (95%)	6 (5%)	24	53
14	SS	126/132 (96%)	115 (91%)	11 (9%)	10	27
15	ST	113/115 (98%)	106 (94%)	7 (6%)	18	43
16	SU	94/107 (88%)	90 (96%)	4 (4%)	29	59
17	SV	66/67 (98%)	57 (86%)	9 (14%)	3	9
18	SX	113/115 (98%)	108 (96%)	5 (4%)	28	58
19	Sa	89/98 (91%)	83 (93%)	6 (7%)	16	39
20	Sc	57/62 (92%)	51 (90%)	6 (10%)	7	18
21	Sd	48/49 (98%)	45 (94%)	3 (6%)	18	42
22	Sg	271/275 (98%)	241 (89%)	30 (11%)	6	16
23	SC	191/224 (85%)	176 (92%)	15 (8%)	12	31
24	SG	207/218 (95%)	194 (94%)	13 (6%)	18	42
25	SJ	162/168 (96%)	144 (89%)	18 (11%)	6	16
26	SM	98/108 (91%)	88 (90%)	10 (10%)	7	20
27	SN	130/131 (99%)	125 (96%)	5 (4%)	33	64
28	SO	107/119 (90%)	96 (90%)	11 (10%)	7	19
29	SW	112/113 (99%)	102 (91%)	10 (9%)	9	26
30	SY	114/115 (99%)	105 (92%)	9 (8%)	12	31
31	SZ	64/103 (62%)	58 (91%)	6 (9%)	8	23
32	Sb	74/76 (97%)	67 (90%)	7 (10%)	8	23
33	Se	46/48 (96%)	40 (87%)	6 (13%)	4	11
34	Sf	60/140 (43%)	59 (98%)	1 (2%)	60	83
35	A	194/199 (98%)	183 (94%)	11 (6%)	20	47
36	B	345/349 (99%)	332 (96%)	13 (4%)	33	64
37	C	304/349 (87%)	286 (94%)	18 (6%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	F	248/250 (99%)	238 (96%)	10 (4%)	31	62
41	G	216/256 (84%)	210 (97%)	6 (3%)	43	73
42	H	195/224 (87%)	187 (96%)	8 (4%)	30	61
43	I	205/223 (92%)	191 (93%)	14 (7%)	16	38
44	J	171/172 (99%)	159 (93%)	12 (7%)	15	37
45	K	178/181 (98%)	166 (93%)	12 (7%)	16	39
46	L	143/149 (96%)	129 (90%)	14 (10%)	8	21
47	M	171/177 (97%)	158 (92%)	13 (8%)	13	33
48	N	118/157 (75%)	114 (97%)	4 (3%)	37	67
49	O	171/172 (99%)	162 (95%)	9 (5%)	22	50
50	P	169/173 (98%)	159 (94%)	10 (6%)	19	45
51	Q	139/163 (85%)	131 (94%)	8 (6%)	20	46
52	R	164/165 (99%)	155 (94%)	9 (6%)	21	49
53	S	167/175 (95%)	154 (92%)	13 (8%)	12	32
54	T	156/156 (100%)	150 (96%)	6 (4%)	33	64
55	U	139/140 (99%)	125 (90%)	14 (10%)	7	20
56	V	89/114 (78%)	76 (85%)	13 (15%)	3	8
57	W	102/107 (95%)	96 (94%)	6 (6%)	19	45
58	X	53/126 (42%)	50 (94%)	3 (6%)	20	47
59	Y	108/133 (81%)	103 (95%)	5 (5%)	27	56
60	Z	124/135 (92%)	115 (93%)	9 (7%)	14	35
61	a	117/118 (99%)	109 (93%)	8 (7%)	16	38
62	b	120/121 (99%)	118 (98%)	2 (2%)	60	83
63	c	80/124 (64%)	74 (92%)	6 (8%)	13	34
64	d	86/97 (89%)	78 (91%)	8 (9%)	9	24
65	e	97/110 (88%)	92 (95%)	5 (5%)	23	51
66	f	115/121 (95%)	111 (96%)	4 (4%)	36	67
67	g	88/89 (99%)	84 (96%)	4 (4%)	27	57
68	h	99/100 (99%)	96 (97%)	3 (3%)	41	72
69	i	109/110 (99%)	102 (94%)	7 (6%)	17	41
70	j	88/89 (99%)	86 (98%)	2 (2%)	50	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
71	k	73/80 (91%)	70 (96%)	3 (4%)	30	61
72	l	64/65 (98%)	60 (94%)	4 (6%)	18	42
73	m	47/48 (98%)	44 (94%)	3 (6%)	17	41
74	n	46/116 (40%)	45 (98%)	1 (2%)	52	79
75	o	24/24 (100%)	23 (96%)	1 (4%)	30	60
76	p	93/94 (99%)	89 (96%)	4 (4%)	29	59
77	q	74/75 (99%)	66 (89%)	8 (11%)	6	17
78	r	115/121 (95%)	110 (96%)	5 (4%)	29	59
83	Cz	195/196 (100%)	170 (87%)	25 (13%)	4	11
84	y	1/1 (100%)	1 (100%)	0	100	100
All	All	10009/11002 (91%)	9367 (94%)	642 (6%)	21	41

All (642) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	SA	9	GLN
2	SA	36	GLN
2	SA	42	LYS
2	SA	75	SER
2	SA	76	VAL
2	SA	88	LEU
2	SA	131	HIS
2	SA	193	HIS
2	SA	205	ARG
3	SB	32	ASP
3	SB	38	MET
3	SB	85	LYS
3	SB	167	LYS
3	SB	203	SER
3	SB	227	LYS
4	SD	28	GLU
4	SD	34	TYR
4	SD	76	ARG
4	SD	84	VAL
4	SD	119	CYS
4	SD	169	ASP
4	SD	176	LEU
4	SD	178	ARG

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Mol	Chain	Res	Type
4	SD	204	LEU
4	SD	207	HIS
5	SE	48	LEU
5	SE	50	ASN
5	SE	53	LYS
5	SE	66	MET
5	SE	79	ASP
5	SE	87	MET
5	SE	103	TYR
5	SE	109	PHE
5	SE	120	LYS
5	SE	125	LYS
5	SE	183	VAL
5	SE	233	LYS
6	SF	23	TRP
6	SF	37	ASP
6	SF	97	PHE
6	SF	125	SER
6	SF	163	PHE
6	SF	194	ASP
6	SF	198	ARG
7	SH	39	GLN
7	SH	52	GLU
7	SH	72	PHE
7	SH	111	LYS
7	SH	130	LEU
7	SH	164	ASN
7	SH	165	ASN
7	SH	179	LYS
7	SH	192	PHE
8	SI	23	LYS
8	SI	37	LYS
8	SI	56	ARG
8	SI	96	LEU
8	SI	111	GLN
8	SI	113	TYR
8	SI	115	SER
8	SI	123	ARG
8	SI	128	LYS
8	SI	148	LYS
8	SI	166	PHE
8	SI	167	GLN

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Mol	Chain	Res	Type
9	SK	2	LEU
9	SK	3	MET
9	SK	12	TYR
9	SK	26	ASP
9	SK	29	MET
9	SK	31	LYS
9	SK	43	LEU
9	SK	62	PHE
9	SK	74	GLU
10	SL	17	PHE
10	SL	23	VAL
10	SL	32	LYS
10	SL	48	LYS
10	SL	52	GLU
10	SL	65	ASN
10	SL	69	ARG
10	SL	84	ARG
10	SL	103	GLU
10	SL	104	LYS
10	SL	110	SER
11	SP	9	LYS
11	SP	21	ASP
11	SP	27	ASP
11	SP	50	ARG
11	SP	70	MET
11	SP	89	MET
11	SP	96	VAL
12	SQ	22	VAL
12	SQ	29	ASN
12	SQ	31	LEU
12	SQ	51	LEU
12	SQ	97	GLN
12	SQ	105	LYS
12	SQ	114	GLN
12	SQ	127	CYS
12	SQ	129	SER
13	SR	11	LYS
13	SR	47	ARG
13	SR	70	SER
13	SR	76	GLU
13	SR	78	ARG
13	SR	104	GLU

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Mol	Chain	Res	Type
14	SS	8	LYS
14	SS	10	GLN
14	SS	11	HIS
14	SS	14	ARG
14	SS	23	ARG
14	SS	34	LYS
14	SS	61	GLU
14	SS	73	ASN
14	SS	110	ASP
14	SS	116	LYS
14	SS	144	ARG
15	ST	24	LYS
15	ST	27	LYS
15	ST	35	ASP
15	ST	75	MET
15	ST	79	TYR
15	ST	88	ARG
15	ST	143	LYS
16	SU	49	LYS
16	SU	67	LYS
16	SU	79	ARG
16	SU	92	HIS
17	SV	1	MET
17	SV	10	ASP
17	SV	41	ARG
17	SV	45	ARG
17	SV	50	PHE
17	SV	51	LYS
17	SV	62	MET
17	SV	66	ASP
17	SV	81	LYS
18	SX	8	ARG
18	SX	92	ASN
18	SX	98	ASP
18	SX	105	PHE
18	SX	139	GLU
19	Sa	2	THR
19	Sa	25	ASN
19	Sa	42	ARG
19	Sa	45	VAL
19	Sa	55	GLU
19	Sa	63	VAL

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Mol	Chain	Res	Type
20	Sc	17	VAL
20	Sc	29	GLN
20	Sc	33	GLU
20	Sc	56	LEU
20	Sc	57	THR
20	Sc	64	GLU
21	Sd	19	ARG
21	Sd	39	CYS
21	Sd	41	GLN
22	Sg	3	GLU
22	Sg	14	HIS
22	Sg	30	MET
22	Sg	36	ARG
22	Sg	38	LYS
22	Sg	42	MET
22	Sg	63	SER
22	Sg	64	HIS
22	Sg	71	ILE
22	Sg	87	LEU
22	Sg	96	THR
22	Sg	105	THR
22	Sg	113	PHE
22	Sg	116	ASP
22	Sg	118	ARG
22	Sg	131	LEU
22	Sg	140	TYR
22	Sg	156	PHE
22	Sg	179	LEU
22	Sg	195	LEU
22	Sg	215	GLN
22	Sg	228	TYR
22	Sg	231	ASP
22	Sg	246	TYR
22	Sg	259	TRP
22	Sg	264	LYS
22	Sg	268	ASP
22	Sg	302	TYR
22	Sg	306	LEU
22	Sg	314	ILE
23	SC	66	LEU
23	SC	68	ARG
23	SC	72	ASP

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Mol	Chain	Res	Type
23	SC	74	LYS
23	SC	97	PHE
23	SC	103	LYS
23	SC	121	ARG
23	SC	145	LYS
23	SC	163	VAL
23	SC	167	ARG
23	SC	172	ASN
23	SC	214	LEU
23	SC	236	PHE
23	SC	263	LYS
23	SC	271	ASP
24	SG	1	MET
24	SG	7	PHE
24	SG	12	CYS
24	SG	14	LYS
24	SG	25	ARG
24	SG	31	ARG
24	SG	41	LEU
24	SG	89	THR
24	SG	119	LYS
24	SG	126	ASP
24	SG	201	LYS
24	SG	211	LYS
24	SG	225	GLN
25	SJ	5	ARG
25	SJ	13	TYR
25	SJ	22	LYS
25	SJ	27	GLN
25	SJ	34	GLU
25	SJ	52	LYS
25	SJ	55	LYS
25	SJ	63	LEU
25	SJ	66	LYS
25	SJ	67	ASP
25	SJ	69	ARG
25	SJ	79	ARG
25	SJ	86	VAL
25	SJ	88	ASP
25	SJ	101	LYS
25	SJ	103	GLU
25	SJ	107	GLU

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Mol	Chain	Res	Type
25	SJ	158	ASP
26	SM	33	ARG
26	SM	42	LEU
26	SM	45	ARG
26	SM	46	GLN
26	SM	51	VAL
26	SM	76	LEU
26	SM	93	LYS
26	SM	103	VAL
26	SM	112	LYS
26	SM	116	LYS
27	SN	32	ASP
27	SN	87	ASP
27	SN	89	TYR
27	SN	112	LYS
27	SN	133	ARG
28	SO	27	VAL
28	SO	40	THR
28	SO	60	MET
28	SO	61	LYS
28	SO	75	MET
28	SO	80	ASP
28	SO	104	ARG
28	SO	119	LEU
28	SO	124	MET
28	SO	128	ARG
28	SO	151	LEU
29	SW	13	SER
29	SW	22	LYS
29	SW	23	ARG
29	SW	36	ARG
29	SW	54	ASP
29	SW	68	ARG
29	SW	80	ASP
29	SW	82	GLN
29	SW	118	ARG
29	SW	120	HIS
30	SY	13	MET
30	SY	21	LYS
30	SY	23	MET
30	SY	42	GLU
30	SY	47	MET

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Mol	Chain	Res	Type
30	SY	48	TYR
30	SY	51	THR
30	SY	118	ARG
30	SY	120	THR
31	SZ	44	LEU
31	SZ	46	ASN
31	SZ	50	PHE
31	SZ	78	LYS
31	SZ	111	ARG
31	SZ	113	THR
32	Sb	6	ASP
32	Sb	9	HIS
32	Sb	15	GLU
32	Sb	16	LYS
32	Sb	60	SER
32	Sb	79	PHE
32	Sb	80	ARG
33	Se	8	ARG
33	Se	15	GLN
33	Se	22	GLN
33	Se	24	LYS
33	Se	35	ARG
33	Se	46	VAL
34	Sf	125	GLU
35	A	32	VAL
35	A	80	GLU
35	A	102	LEU
35	A	135	THR
35	A	154	SER
35	A	159	SER
35	A	160	SER
35	A	194	ASN
35	A	198	ARG
35	A	207	VAL
35	A	243	THR
36	B	85	VAL
36	B	90	VAL
36	B	94	GLU
36	B	147	GLU
36	B	181	MET
36	B	344	VAL
36	B	350	SER

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Mol	Chain	Res	Type
36	B	357	ARG
36	B	358	ARG
36	B	360	LEU
36	B	378	ARG
36	B	395	ASP
36	B	396	ARG
37	C	14	LYS
37	C	52	TYR
37	C	69	THR
37	C	94	ASN
37	C	95	MET
37	C	122	TYR
37	C	150	LEU
37	C	188	ARG
37	C	266	THR
37	C	267	TRP
37	C	290	SER
37	C	291	ARG
37	C	313	VAL
37	C	336	ARG
37	C	345	ARG
37	C	350	ARG
37	C	352	LYS
37	C	353	LYS
40	F	68	ARG
40	F	115	MET
40	F	118	ILE
40	F	134	SER
40	F	136	ASP
40	F	155	THR
40	F	172	SER
40	F	239	MET
40	F	262	LYS
40	F	291	GLN
41	G	50	LYS
41	G	53	CYS
41	G	65	ARG
41	G	117	VAL
41	G	220	LYS
41	G	233	ARG
42	H	72	GLU
42	H	75	GLN

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Mol	Chain	Res	Type
42	H	116	LYS
42	H	141	SER
42	H	189	ARG
42	H	201	ASP
42	H	205	GLU
42	H	260	ASN
43	I	22	GLN
43	I	29	ASN
43	I	38	ASN
43	I	71	TYR
43	I	90	GLN
43	I	128	VAL
43	I	136	LEU
43	I	167	VAL
43	I	192	ARG
43	I	215	LEU
43	I	217	LYS
43	I	223	ARG
43	I	230	TYR
43	I	260	GLU
44	J	6	SER
44	J	24	THR
44	J	36	ARG
44	J	48	LEU
44	J	50	LYS
44	J	54	ARG
44	J	66	GLU
44	J	84	VAL
44	J	141	LYS
44	J	163	GLN
44	J	169	ASN
44	J	189	GLN
45	K	21	ARG
45	K	26	VAL
45	K	32	ARG
45	K	52	MET
45	K	102	MET
45	K	109	ASP
45	K	115	MET
45	K	121	LYS
45	K	141	LYS
45	K	146	GLU

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Mol	Chain	Res	Type
45	K	188	LYS
45	K	197	VAL
46	L	28	GLU
46	L	42	GLN
46	L	47	THR
46	L	54	ARG
46	L	63	ARG
46	L	64	ARG
46	L	70	VAL
46	L	84	GLU
46	L	96	LYS
46	L	110	GLN
46	L	118	LYS
46	L	150	CYS
46	L	164	ARG
46	L	168	GLN
47	M	8	MET
47	M	22	VAL
47	M	37	LYS
47	M	59	VAL
47	M	69	LYS
47	M	105	LYS
47	M	121	ARG
47	M	128	PRO
47	M	129	ARG
47	M	144	LEU
47	M	158	ARG
47	M	164	GLU
47	M	200	LYS
48	N	35	ARG
48	N	44	ARG
48	N	113	MET
48	N	121	ARG
49	O	5	LYS
49	O	20	ARG
49	O	24	ARG
49	O	44	ARG
49	O	47	LYS
49	O	75	VAL
49	O	125	SER
49	O	144	ARG
49	O	189	ARG

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Mol	Chain	Res	Type
50	P	31	ARG
50	P	65	ASN
50	P	103	LYS
50	P	117	ARG
50	P	135	PHE
50	P	173	GLN
50	P	183	LYS
50	P	184	ASN
50	P	185	VAL
50	P	187	LYS
51	Q	6	LEU
51	Q	10	ASN
51	Q	20	SER
51	Q	24	VAL
51	Q	28	ASN
51	Q	87	SER
51	Q	110	ASP
51	Q	111	SER
52	R	9	LYS
52	R	14	ARG
52	R	17	GLU
52	R	20	SER
52	R	40	ASN
52	R	98	LEU
52	R	103	LEU
52	R	115	LYS
52	R	183	SER
53	S	12	SER
53	S	23	TRP
53	S	30	ASN
53	S	37	SER
53	S	63	CYS
53	S	96	MET
53	S	108	ARG
53	S	122	SER
53	S	133	LYS
53	S	152	LYS
53	S	153	LYS
53	S	155	LEU
53	S	158	GLN
54	T	16	CYS
54	T	21	LYS

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Mol	Chain	Res	Type
54	T	31	ARG
54	T	82	LEU
54	T	85	ASP
54	T	98	ARG
55	U	4	THR
55	U	14	MET
55	U	38	ASP
55	U	41	ASP
55	U	45	MET
55	U	48	VAL
55	U	80	VAL
55	U	107	LYS
55	U	113	ASP
55	U	117	LYS
55	U	125	TRP
55	U	126	VAL
55	U	129	LYS
55	U	159	MET
56	V	25	CYS
56	V	34	MET
56	V	38	ASN
56	V	43	LEU
56	V	50	ASN
56	V	62	THR
56	V	65	ARG
56	V	67	LYS
56	V	78	PHE
56	V	79	SER
56	V	97	ARG
56	V	98	ASP
56	V	115	PHE
57	W	13	LYS
57	W	28	CYS
57	W	112	MET
57	W	118	THR
57	W	123	LYS
57	W	128	LEU
58	X	12	LYS
58	X	27	LYS
58	X	38	SER
59	Y	43	SER
59	Y	47	ARG

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Mol	Chain	Res	Type
59	Y	67	ARG
59	Y	85	SER
59	Y	88	LYS
60	Z	13	LYS
60	Z	32	SER
60	Z	40	GLN
60	Z	55	VAL
60	Z	74	TYR
60	Z	95	VAL
60	Z	100	ARG
60	Z	108	ARG
60	Z	114	ASP
61	a	13	VAL
61	a	30	ASP
61	a	57	MET
61	a	67	LYS
61	a	75	TYR
61	a	84	ARG
61	a	112	ARG
61	a	120	GLU
62	b	9	ARG
62	b	140	VAL
63	c	14	ARG
63	c	54	LEU
63	c	55	LYS
63	c	91	ARG
63	c	95	ARG
63	c	114	LYS
64	d	23	LYS
64	d	26	LYS
64	d	51	ASN
64	d	68	LYS
64	d	78	ASN
64	d	90	ARG
64	d	98	ASP
64	d	108	MET
65	e	57	MET
65	e	91	LYS
65	e	93	ASN
65	e	98	SER
65	e	122	VAL
66	f	9	LYS

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Mol	Chain	Res	Type
66	f	76	LYS
66	f	109	LYS
66	f	130	ARG
67	g	46	ARG
67	g	95	LYS
67	g	99	HIS
67	g	100	ARG
68	h	5	LEU
68	h	23	SER
68	h	28	ASN
69	i	12	LYS
69	i	15	GLU
69	i	20	GLN
69	i	25	LYS
69	i	30	GLN
69	i	71	LYS
69	i	82	ASP
70	j	29	ARG
70	j	56	ARG
71	k	25	LYS
71	k	79	ARG
71	k	83	THR
72	l	7	GLU
72	l	9	LYS
72	l	18	LYS
72	l	29	LYS
73	m	21	ARG
73	m	29	MET
73	m	36	ARG
74	n	111	ARG
75	o	15	ARG
76	p	27	LYS
76	p	77	CYS
76	p	79	SER
76	p	96	ASP
77	q	7	LYS
77	q	8	VAL
77	q	36	LYS
77	q	48	LYS
77	q	60	CYS
77	q	75	SER
77	q	90	LYS

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Mol	Chain	Res	Type
77	q	91	ASP
78	r	27	THR
78	r	58	LYS
78	r	61	VAL
78	r	80	THR
78	r	119	ARG
83	Cz	1	MET
83	Cz	7	ARG
83	Cz	15	ARG
83	Cz	16	GLU
83	Cz	19	HIS
83	Cz	27	LYS
83	Cz	34	LEU
83	Cz	40	ASN
83	Cz	45	LYS
83	Cz	47	LYS
83	Cz	56	LYS
83	Cz	60	ARG
83	Cz	62	LYS
83	Cz	78	LYS
83	Cz	85	MET
83	Cz	86	ASP
83	Cz	97	LYS
83	Cz	105	LYS
83	Cz	118	LYS
83	Cz	144	MET
83	Cz	162	VAL
83	Cz	174	MET
83	Cz	176	ASP
83	Cz	189	PHE
83	Cz	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
2	SA	141	ASN
5	SE	188	ASN
9	SK	50	GLN
10	SL	65	ASN
12	SQ	80	GLN
12	SQ	86	GLN
13	SR	118	GLN

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Mol	Chain	Res	Type
14	SS	19	ASN
14	SS	72	GLN
14	SS	101	ASN
16	SU	92	HIS
17	SV	33	GLN
18	SX	20	GLN
19	Sa	25	ASN
20	Sc	29	GLN
21	Sd	16	GLN
21	Sd	45	GLN
22	Sg	15	ASN
23	SC	134	ASN
24	SG	56	ASN
26	SM	119	GLN
27	SN	62	GLN
28	SO	103	ASN
29	SW	91	ASN
30	SY	112	ASN
31	SZ	46	ASN
31	SZ	64	ASN
33	Se	44	ASN
35	A	194	ASN
36	B	208	ASN
36	B	258	HIS
40	F	138	GLN
41	G	138	HIS
42	H	138	ASN
42	H	175	ASN
42	H	260	ASN
44	J	63	ASN
45	K	144	ASN
46	L	65	ASN
46	L	71	HIS
46	L	97	ASN
47	M	111	GLN
47	M	115	GLN
47	M	149	GLN
49	O	99	GLN
49	O	196	ASN
50	P	65	ASN
50	P	173	GLN
51	Q	28	ASN

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Mol	Chain	Res	Type
51	Q	116	HIS
52	R	44	ASN
52	R	45	GLN
53	S	40	GLN
54	T	108	GLN
57	W	31	ASN
57	W	135	ASN
59	Y	73	HIS
59	Y	93	ASN
60	Z	56	GLN
61	a	132	GLN
63	c	27	GLN
63	c	58	GLN
64	d	33	GLN
64	d	40	GLN
64	d	51	ASN
66	f	107	ASN
67	g	20	ASN
70	j	80	HIS
74	n	87	GLN
76	p	36	GLN
76	p	102	GLN
78	r	23	GLN
78	r	83	ASN
78	r	100	ASN
83	Cz	19	HIS
83	Cz	158	GLN

4.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	S2	1690/1872 (90%)	391 (23%)	19 (1%)
38	D	156/157 (99%)	32 (20%)	1 (0%)
39	E	118/121 (97%)	11 (9%)	0
79	t	3659/4803 (76%)	687 (18%)	0
80	u	75/76 (98%)	20 (26%)	0
81	v	75/76 (98%)	26 (34%)	0
82	w	19/20 (95%)	8 (42%)	0
All	All	5792/7125 (81%)	1175 (20%)	20 (0%)

All (1175) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	S2	2	A
1	S2	9	U
1	S2	25	A
1	S2	33	G
1	S2	41	G
1	S2	42	A
1	S2	43	U
1	S2	44	U
1	S2	46	A
1	S2	55	U
1	S2	56	G
1	S2	60	A
1	S2	61	A
1	S2	64	A
1	S2	66	G
1	S2	67	C
1	S2	68	A
1	S2	70	G
1	S2	73	C
1	S2	74	G
1	S2	76	U
1	S2	80	G
1	S2	113	G
1	S2	114	G
1	S2	115	U
1	S2	116	OMU
1	S2	125	C
1	S2	126	G
1	S2	139	C
1	S2	142	C
1	S2	143	U
1	S2	155	G
1	S2	159	A2M
1	S2	160	U
1	S2	161	U
1	S2	168	C
1	S2	173	A
1	S2	176	U
1	S2	189	U
1	S2	190	G
1	S2	191	A
1	S2	193	C
1	S2	194	C

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Mol	Chain	Res	Type
1	S2	195	C
1	S2	196	C
1	S2	197	C
1	S2	198	U
1	S2	206	G
1	S2	207	G
1	S2	209	G
1	S2	211	G
1	S2	212	A
1	S2	213	U
1	S2	218	G
1	S2	297	U
1	S2	298	C
1	S2	308	U
1	S2	311	G
1	S2	315	G
1	S2	316	A
1	S2	321	A
1	S2	322	C
1	S2	326	C
1	S2	327	U
1	S2	328	C
1	S2	329	C
1	S2	330	G
1	S2	331	U
1	S2	332	G
1	S2	335	G
1	S2	338	G
1	S2	343	C
1	S2	350	G
1	S2	363	A
1	S2	367	A
1	S2	371	U
1	S2	372	C
1	S2	388	G
1	S2	389	C
1	S2	390	C
1	S2	411	A
1	S2	412	C
1	S2	419	U
1	S2	420	C
1	S2	432	C

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Mol	Chain	Res	Type
1	S2	439	G
1	S2	449	G
1	S2	451	A
1	S2	452	A
1	S2	453	C
1	S2	455	G
1	S2	467	A
1	S2	473	G
1	S2	475	C
1	S2	476	A
1	S2	488	A
1	S2	490	U
1	S2	491	U
1	S2	505	C
1	S2	506	C
1	S2	520	OMC
1	S2	528	A
1	S2	534	A
1	S2	537	G
1	S2	550	G
1	S2	552	C
1	S2	556	U
1	S2	557	A
1	S2	558	A
1	S2	559	U
1	S2	561	G
1	S2	562	G
1	S2	563	A
1	S2	564	A
1	S2	567	A
1	S2	573	C
1	S2	579	A
1	S2	581	C
1	S2	582	C
1	S2	586	A
1	S2	591	G
1	S2	592	G
1	S2	593	A
1	S2	594	U
1	S2	603	G
1	S2	607	A
1	S2	610	U

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Mol	Chain	Res	Type
1	S2	611	C
1	S2	617	C
1	S2	620	G
1	S2	629	G
1	S2	630	U
1	S2	631	A
1	S2	632	A
1	S2	646	A
1	S2	658	A
1	S2	663	C
1	S2	666	C
1	S2	671	A2M
1	S2	672	A
1	S2	674	A
1	S2	675	A
1	S2	676	G
1	S2	686	OMG
1	S2	693	G
1	S2	694	G
1	S2	695	G
1	S2	696	A
1	S2	697	G
1	S2	698	C
1	S2	700	G
1	S2	734	G
1	S2	736	C
1	S2	737	C
1	S2	738	C
1	S2	740	G
1	S2	741	C
1	S2	742	C
1	S2	751	C
1	S2	754	G
1	S2	755	G
1	S2	756	C
1	S2	792	G
1	S2	793	C
1	S2	794	C
1	S2	795	C
1	S2	800	C
1	S2	801	G
1	S2	802	U

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Mol	Chain	Res	Type
1	S2	804	U
1	S2	818	U
1	S2	820	G
1	S2	824	G
1	S2	825	PSU
1	S2	833	A
1	S2	834	G
1	S2	838	C
1	S2	839	G
1	S2	840	A
1	S2	841	G
1	S2	842	C
1	S2	844	G
1	S2	845	C
1	S2	850	A
1	S2	861	A
1	S2	862	G
1	S2	872	A
1	S2	873	A
1	S2	875	A
1	S2	876	G
1	S2	890	U
1	S2	891	U
1	S2	893	U
1	S2	894	G
1	S2	897	G
1	S2	898	G
1	S2	900	U
1	S2	906	A
1	S2	908	C
1	S2	910	G
1	S2	916	A
1	S2	917	U
1	S2	920	U
1	S2	923	A
1	S2	936	G
1	S2	958	A
1	S2	972	U
1	S2	973	G
1	S2	974	G
1	S2	976	C
1	S2	993	A

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Mol	Chain	Res	Type
1	S2	995	A
1	S2	1002	G
1	S2	1004	A
1	S2	1005	U
1	S2	1019	U
1	S2	1020	U
1	S2	1024	U
1	S2	1026	A
1	S2	1048	U
1	S2	1052	A
1	S2	1064	U
1	S2	1065	A
1	S2	1086	A
1	S2	1087	A
1	S2	1088	C
1	S2	1091	U
1	S2	1112	C
1	S2	1117	U
1	S2	1118	U
1	S2	1119	C
1	S2	1120	C
1	S2	1122	A
1	S2	1124	G
1	S2	1136	A
1	S2	1141	C
1	S2	1152	A
1	S2	1153	A
1	S2	1157	U
1	S2	1173	A
1	S2	1198	A
1	S2	1210	G
1	S2	1211	A
1	S2	1218	C
1	S2	1220	A
1	S2	1222	C
1	S2	1223	A
1	S2	1227	G
1	S2	1236	G
1	S2	1245	U
1	S2	1246	PSU
1	S2	1254	A
1	S2	1256	A

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Mol	Chain	Res	Type
1	S2	1259	G
1	S2	1260	G
1	S2	1262	A
1	S2	1263	A
1	S2	1268	A
1	S2	1277	G
1	S2	1278	G
1	S2	1286	C
1	S2	1287	A
1	S2	1288	G
1	S2	1289	G
1	S2	1290	A
1	S2	1292	U
1	S2	1298	A
1	S2	1299	U
1	S2	1303	U
1	S2	1304	A
1	S2	1305	G
1	S2	1306	C
1	S2	1312	C
1	S2	1315	G
1	S2	1316	A
1	S2	1325	G
1	S2	1330	G
1	S2	1333	G
1	S2	1336	U
1	S2	1344	C
1	S2	1345	U
1	S2	1374	U
1	S2	1379	A
1	S2	1381	A
1	S2	1400	U
1	S2	1401	G
1	S2	1406	C
1	S2	1407	U
1	S2	1421	C
1	S2	1423	G
1	S2	1424	A
1	S2	1436	C
1	S2	1437	C
1	S2	1439	C
1	S2	1440	C

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Mol	Chain	Res	Type
1	S2	1441	A
1	S2	1442	A
1	S2	1445	U
1	S2	1449	A
1	S2	1450	G
1	S2	1457	A
1	S2	1461	G
1	S2	1465	U
1	S2	1466	U
1	S2	1469	G
1	S2	1473	C
1	S2	1480	U
1	S2	1492	A
1	S2	1493	G
1	S2	1497	U
1	S2	1498	G
1	S2	1500	G
1	S2	1501	A
1	S2	1510	G
1	S2	1511	A
1	S2	1522	U
1	S2	1523	G
1	S2	1524	C
1	S2	1536	A
1	S2	1537	C
1	S2	1539	G
1	S2	1540	A
1	S2	1547	C
1	S2	1548	A
1	S2	1555	G
1	S2	1559	A
1	S2	1560	C
1	S2	1561	C
1	S2	1563	U
1	S2	1571	C
1	S2	1573	G
1	S2	1576	G
1	S2	1583	A
1	S2	1584	C
1	S2	1588	U
1	S2	1589	U
1	S2	1591	A

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Mol	Chain	Res	Type
1	S2	1601	G
1	S2	1602	U
1	S2	1603	G
1	S2	1609	G
1	S2	1624	U
1	S2	1626	A
1	S2	1650	A
1	S2	1651	G
1	S2	1657	G
1	S2	1665	U
1	S2	1668	G
1	S2	1674	G
1	S2	1678	A
1	S2	1679	U
1	S2	1680	U
1	S2	1685	C
1	S2	1689	G
1	S2	1698	A
1	S2	1702	A
1	S2	1725	G
1	S2	1731	U
1	S2	1732	U
1	S2	1752	G
1	S2	1754	C
1	S2	1783	G
1	S2	1784	A
1	S2	1785	G
1	S2	1786	C
1	S2	1787	G
1	S2	1788	C
1	S2	1789	U
1	S2	1794	A
1	S2	1806	U
1	S2	1808	G
1	S2	1817	G
1	S2	1818	A
1	S2	1819	G
1	S2	1827	A
1	S2	1828	A
1	S2	1829	G
1	S2	1832	G
1	S2	1834	A

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Mol	Chain	Res	Type
1	S2	1836	C
1	S2	1838	A
1	S2	1839	G
1	S2	1841	U
1	S2	1843	U
1	S2	1852	G
1	S2	1855	C
1	S2	1864	G
1	S2	1865	G
1	S2	1866	A
1	S2	1868	C
1	S2	1872	A
38	D	16	G
38	D	23	C
38	D	34	U
38	D	35	C
38	D	38	U
38	D	39	G
38	D	59	A
38	D	63	U
38	D	71	A
38	D	72	A
38	D	77	A
38	D	78	G
38	D	79	G
38	D	81	C
38	D	83	C
38	D	84	A
38	D	85	U
38	D	86	U
38	D	87	G
38	D	94	G
38	D	103	A
38	D	105	C
38	D	109	C
38	D	110	U
38	D	111	U
38	D	122	G
38	D	124	U
38	D	125	C
38	D	126	C
38	D	128	C

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Mol	Chain	Res	Type
38	D	129	C
38	D	148	A
39	E	7	G
39	E	22	A
39	E	33	U
39	E	50	A
39	E	51	G
39	E	53	U
39	E	54	A
39	E	63	C
39	E	64	G
39	E	102	U
39	E	110	G
79	t	9	C
79	t	25	A
79	t	32	G
79	t	39	A
79	t	40	G
79	t	42	A
79	t	48	G
79	t	49	U
79	t	59	A
79	t	64	A
79	t	65	A
79	t	66	A
79	t	71	C
79	t	72	C
79	t	76	A
79	t	91	G
79	t	108	A
79	t	110	C
79	t	119	G
79	t	129	C
79	t	130	G
79	t	131	C
79	t	132	G
79	t	137	G
79	t	138	C
79	t	139	G
79	t	142	G
79	t	152	U
79	t	160	G

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Mol	Chain	Res	Type
79	t	166	C
79	t	176	G
79	t	179	G
79	t	182	G
79	t	183	C
79	t	184	U
79	t	185	C
79	t	186	G
79	t	187	U
79	t	199	G
79	t	208	A
79	t	215	C
79	t	216	C
79	t	217	C
79	t	218	A
79	t	232	G
79	t	233	U
79	t	236	G
79	t	247	G
79	t	255	C
79	t	256	G
79	t	257	C
79	t	258	G
79	t	264	C
79	t	266	C
79	t	295	A
79	t	297	U
79	t	306	A
79	t	310	G
79	t	315	G
79	t	316	U
79	t	317	A
79	t	340	C
79	t	349	A
79	t	373	G
79	t	376	A
79	t	381	U
79	t	387	G
79	t	410	A
79	t	411	G
79	t	412	G
79	t	431	G

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Mol	Chain	Res	Type
79	t	440	U
79	t	451	C
79	t	452	A
79	t	453	G
79	t	454	U
79	t	455	C
79	t	464	G
79	t	469	C
79	t	480	C
79	t	482	C
79	t	483	G
79	t	484	C
79	t	485	G
79	t	487	C
79	t	488	C
79	t	489	G
79	t	497	C
79	t	500	U
79	t	501	G
79	t	502	G
79	t	507	G
79	t	508	G
79	t	513	U
79	t	516	U
79	t	517	U
79	t	518	C
79	t	520	C
79	t	524	C
79	t	616	U
79	t	617	C
79	t	626	A
79	t	632	C
79	t	644	G
79	t	646	C
79	t	657	C
79	t	661	C
79	t	662	G
79	t	677	C
79	t	680	U
79	t	682	C
79	t	685	C
79	t	706	U

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Mol	Chain	Res	Type
79	t	707	G
79	t	708	G
79	t	713	G
79	t	714	C
79	t	715	C
79	t	717	G
79	t	724	A
79	t	725	A
79	t	726	G
79	t	727	G
79	t	728	U
79	t	730	G
79	t	838	C
79	t	845	G
79	t	848	A
79	t	850	A
79	t	851	G
79	t	853	C
79	t	859	G
79	t	860	C
79	t	862	G
79	t	864	A
79	t	867	G
79	t	869	U
79	t	877	U
79	t	878	C
79	t	879	C
79	t	889	G
79	t	890	G
79	t	891	G
79	t	892	A
79	t	893	G
79	t	895	C
79	t	898	A
79	t	899	U
79	t	902	C
79	t	904	G
79	t	982	C
79	t	987	C
79	t	988	G
79	t	990	C
79	t	992	C

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Mol	Chain	Res	Type
79	t	1010	U
79	t	1013	C
79	t	1014	C
79	t	1065	G
79	t	1066	C
79	t	1067	G
79	t	1068	G
79	t	1072	G
79	t	1078	U
79	t	1079	C
79	t	1080	C
79	t	1090	C
79	t	1096	C
79	t	1097	G
79	t	1098	U
79	t	1099	C
79	t	1100	G
79	t	1102	C
79	t	1109	U
79	t	1110	C
79	t	1113	G
79	t	1114	C
79	t	1118	G
79	t	1137	C
79	t	1138	U
79	t	1139	C
79	t	1140	U
79	t	1141	C
79	t	1142	C
79	t	1143	C
79	t	1144	U
79	t	1146	C
79	t	1147	C
79	t	1150	U
79	t	1154	G
79	t	1155	G
79	t	1156	G
79	t	1158	U
79	t	1167	G
79	t	1169	G
79	t	1176	A
79	t	1178	C

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Mol	Chain	Res	Type
79	t	1183	G
79	t	1187	U
79	t	1188	C
79	t	1190	G
79	t	1196	A
79	t	1197	U
79	t	1198	G
79	t	1204	U
79	t	1205	A
79	t	1206	C
79	t	1228	A
79	t	1256	A
79	t	1260	A
79	t	1261	G
79	t	1267	C
79	t	1268	G
79	t	1269	U
79	t	1279	G
79	t	1289	A
79	t	1299	A
79	t	1300	A
79	t	1310	U
79	t	1311	C
79	t	1312	C
79	t	1313	C
79	t	1324	A
79	t	1341	C
79	t	1343	C
79	t	1345	C
79	t	1346	C
79	t	1347	A
79	t	1348	G
79	t	1379	G
79	t	1385	C
79	t	1386	G
79	t	1387	C
79	t	1388	G
79	t	1390	C
79	t	1401	A
79	t	1402	G
79	t	1406	G
79	t	1427	A

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Mol	Chain	Res	Type
79	t	1429	A
79	t	1438	A
79	t	1451	A
79	t	1467	A
79	t	1470	C
79	t	1478	G
79	t	1482	U
79	t	1495	U
79	t	1500	U
79	t	1505	A
79	t	1511	C
79	t	1516	G
79	t	1517	A
79	t	1528	G
79	t	1529	G
79	t	1535	A
79	t	1537	G
79	t	1538	A
79	t	1542	A
79	t	1545	G
79	t	1558	G
79	t	1565	C
79	t	1574	G
79	t	1595	G
79	t	1598	C
79	t	1603	A
79	t	1606	G
79	t	1607	C
79	t	1608	G
79	t	1609	G
79	t	1633	C
79	t	1643	G
79	t	1666	G
79	t	1667	A
79	t	1668	A
79	t	1674	C
79	t	1675	U
79	t	1683	U
79	t	1689	A
79	t	1696	A
79	t	1705	G
79	t	1706	A

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Mol	Chain	Res	Type
79	t	1723	G
79	t	1735	G
79	t	1736	U
79	t	1737	G
79	t	1738	G
79	t	1739	A
79	t	1744	G
79	t	1757	G
79	t	1771	G
79	t	1791	U
79	t	1793	A
79	t	1794	A
79	t	1800	C
79	t	1817	C
79	t	1820	U
79	t	1823	C
79	t	1824	G
79	t	1833	C
79	t	1842	G
79	t	1849	U
79	t	1850	G
79	t	1859	U
79	t	1860	A
79	t	1862	A
79	t	1863	G
79	t	1864	A
79	t	1878	G
79	t	1881	A
79	t	1882	U
79	t	1884	G
79	t	1885	A
79	t	1887	G
79	t	1889	C
79	t	1895	C
79	t	1900	A
79	t	1904	G
79	t	1905	U
79	t	1909	U
79	t	1914	A
79	t	1927	A
79	t	1932	C
79	t	1935	G

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Mol	Chain	Res	Type
79	t	1947	G
79	t	1949	U
79	t	1956	G
79	t	1957	G
79	t	1970	A
79	t	1971	U
79	t	1985	C
79	t	1992	C
79	t	1993	G
79	t	1994	G
79	t	1995	A
79	t	1996	A
79	t	1997	C
79	t	1998	G
79	t	1999	G
79	t	2002	C
79	t	2003	G
79	t	2005	G
79	t	2008	C
79	t	2009	G
79	t	2011	C
79	t	2012	C
79	t	2013	G
79	t	2096	G
79	t	2098	G
79	t	2099	C
79	t	2100	C
79	t	2102	C
79	t	2106	G
79	t	2112	A
79	t	2133	C
79	t	2143	G
79	t	2144	A
79	t	2145	G
79	t	2150	G
79	t	2157	A
79	t	2173	U
79	t	2175	G
79	t	2176	A
79	t	2192	G
79	t	2194	U
79	t	2195	C

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Mol	Chain	Res	Type
79	t	2204	A
79	t	2205	G
79	t	2239	A
79	t	2240	A
79	t	2246	G
79	t	2254	C
79	t	2261	A
79	t	2262	A
79	t	2265	G
79	t	2266	C
79	t	2269	U
79	t	2291	U
79	t	2294	G
79	t	2307	G
79	t	2314	C
79	t	2315	G
79	t	2323	G
79	t	2332	C
79	t	2333	C
79	t	2334	U
79	t	2337	G
79	t	2338	U
79	t	2347	G
79	t	2348	C
79	t	2349	C
79	t	2350	G
79	t	2357	A
79	t	2388	G
79	t	2389	U
79	t	2390	G
79	t	2391	G
79	t	2397	A
79	t	2398	U
79	t	2410	G
79	t	2425	A
79	t	2430	G
79	t	2431	A
79	t	2433	C
79	t	2435	A
79	t	2445	A
79	t	2450	G
79	t	2462	G

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Mol	Chain	Res	Type
79	t	2471	C
79	t	2482	G
79	t	2484	G
79	t	2504	A
79	t	2513	C
79	t	2517	G
79	t	2531	U
79	t	2538	G
79	t	2539	A
79	t	2540	A
79	t	2552	U
79	t	2554	C
79	t	2555	G
79	t	2556	G
79	t	2565	G
79	t	2570	G
79	t	2584	U
79	t	2587	A
79	t	2591	U
79	t	2603	G
79	t	2604	G
79	t	2605	U
79	t	2606	G
79	t	2608	A
79	t	2610	A
79	t	2613	U
79	t	2631	A
79	t	2632	U
79	t	2634	U
79	t	2640	G
79	t	2641	C
79	t	2643	G
79	t	2650	A
79	t	2658	C
79	t	2670	U
79	t	2671	G
79	t	2687	U
79	t	2699	G
79	t	2725	A
79	t	2741	G
79	t	2746	G
79	t	3334	A

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Mol	Chain	Res	Type
79	t	3336	C
79	t	3340	C
79	t	3341	U
79	t	3353	C
79	t	3360	G
79	t	3361	G
79	t	3370	A
79	t	3376	U
79	t	3397	A
79	t	3399	G
79	t	3407	G
79	t	3408	C
79	t	3433	G
79	t	3445	G
79	t	3446	A
79	t	3447	A
79	t	3464	U
79	t	3471	A
79	t	3483	A
79	t	3492	G
79	t	3494	A
79	t	3495	A
79	t	3508	U
79	t	3509	A
79	t	3511	G
79	t	3512	G
79	t	3513	U
79	t	3515	G
79	t	3519	A
79	t	3545	C
79	t	3546	G
79	t	3547	C
79	t	3549	U
79	t	3552	A
79	t	3553	U
79	t	3554	G
79	t	3559	A
79	t	3564	G
79	t	3573	U
79	t	3574	G
79	t	3575	U
79	t	3612	A

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Mol	Chain	Res	Type
79	t	3614	G
79	t	3627	U
79	t	3632	G
79	t	3636	A
79	t	3641	A
79	t	3642	G
79	t	3644	C
79	t	3650	U
79	t	3658	A
79	t	3674	G
79	t	3685	U
79	t	3690	G
79	t	3695	A
79	t	3696	G
79	t	3697	A
79	t	3698	A
79	t	3699	U
79	t	3701	A
79	t	3708	G
79	t	3769	C
79	t	3773	C
79	t	3775	G
79	t	3779	A
79	t	3780	A
79	t	3781	U
79	t	3794	A
79	t	3796	C
79	t	3797	G
79	t	3808	G
79	t	3825	G
79	t	3826	G
79	t	3827	G
79	t	3828	C
79	t	3829	G
79	t	3833	C
79	t	3834	C
79	t	3835	C
79	t	3836	G
79	t	3837	A
79	t	3842	C
79	t	3844	C
79	t	3846	C

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Mol	Chain	Res	Type
79	t	3847	G
79	t	3851	C
79	t	3869	C
79	t	3894	C
79	t	3895	U
79	t	3896	C
79	t	3902	A
79	t	3915	G
79	t	3916	G
79	t	3923	G
79	t	3928	G
79	t	3935	A
79	t	3944	A
79	t	3946	A
79	t	3957	G
79	t	3961	U
79	t	3965	A
79	t	3966	A
79	t	3981	G
79	t	3983	A
79	t	3986	G
79	t	3987	A
79	t	3998	G
79	t	4000	A
79	t	4004	G
79	t	4006	A
79	t	4013	A
79	t	4036	A
79	t	4037	G
79	t	4038	U
79	t	4046	C
79	t	4062	G
79	t	4064	C
79	t	4081	C
79	t	4086	U
79	t	4100	G
79	t	4103	G
79	t	4104	U
79	t	4108	A
79	t	4109	G
79	t	4110	A
79	t	4111	A

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Mol	Chain	Res	Type
79	t	4119	C
79	t	4125	G
79	t	4126	A
79	t	4128	A
79	t	4137	G
79	t	4153	C
79	t	4154	A
79	t	4169	U
79	t	4176	C
79	t	4185	C
79	t	4196	A
79	t	4198	C
79	t	4207	G
79	t	4225	U
79	t	4226	G
79	t	4244	U
79	t	4245	A
79	t	4250	A
79	t	4251	C
79	t	4256	G
79	t	4280	A
79	t	4287	U
79	t	4289	U
79	t	4292	C
79	t	4299	G
79	t	4321	A
79	t	4322	A
79	t	4349	G
79	t	4356	A
79	t	4368	U
79	t	4369	G
79	t	4371	G
79	t	4388	A
79	t	4402	C
79	t	4410	G
79	t	4427	C
79	t	4432	A
79	t	4441	U
79	t	4452	C
79	t	4462	C
79	t	4463	G
79	t	4464	G

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Mol	Chain	Res	Type
79	t	4466	A
79	t	4467	G
79	t	4472	G
79	t	4473	A
79	t	4474	A
79	t	4475	G
79	t	4483	G
79	t	4486	U
79	t	4489	C
79	t	4491	C
79	t	4493	G
79	t	4497	A
79	t	4502	G
79	t	4507	C
79	t	4591	U
79	t	4593	C
79	t	4596	U
79	t	4597	G
79	t	4600	G
79	t	4601	A
79	t	4602	G
79	t	4603	A
79	t	4609	U
79	t	4610	C
79	t	4623	G
79	t	4624	G
79	t	4627	U
79	t	4628	G
79	t	4633	C
79	t	4634	G
79	t	4635	G
79	t	4637	A
79	t	4639	G
79	t	4640	G
79	t	4641	G
79	t	4647	C
79	t	4652	U
79	t	4655	C
79	t	4664	C
79	t	4665	U
79	t	4666	U
79	t	4667	A

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Mol	Chain	Res	Type
79	t	4669	C
79	t	4672	A
79	t	4673	C
79	t	4680	G
79	t	4688	U
79	t	4692	G
79	t	4693	C
79	t	4695	A
79	t	4705	U
79	t	4714	U
79	t	4717	U
79	t	4718	U
79	t	4719	C
79	t	4720	U
79	t	4721	G
79	t	4735	U
79	t	4742	C
79	t	4746	G
79	t	4753	C
79	t	4755	U
79	t	4756	C
79	t	4770	G
79	t	4778	G
79	t	4779	C
79	t	4783	C
79	t	4784	G
79	t	4787	A
79	t	4790	A
80	u	4	C
80	u	6	G
80	u	7	A
80	u	8	U
80	u	14	A
80	u	16	U
80	u	17	C
80	u	18	G
80	u	19	G
80	u	20	U
80	u	21	A
80	u	23	A
80	u	46	G
80	u	47	U

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Mol	Chain	Res	Type
80	u	52	G
80	u	56	C
80	u	57	G
80	u	59	U
80	u	74	C
80	u	76	A
81	v	8	U
81	v	9	A
81	v	11	C
81	v	12	C
81	v	13	C
81	v	14	C
81	v	16	A
81	v	18	G
81	v	19	G
81	v	20	U
81	v	21	A
81	v	22	G
81	v	23	A
81	v	47	U
81	v	48	C
81	v	49	C
81	v	51	U
81	v	55	U
81	v	56	C
81	v	57	G
81	v	61	C
81	v	62	C
81	v	67	C
81	v	69	G
81	v	73	A
81	v	76	A
82	w	10	C
82	w	11	A
82	w	12	U
82	w	21	G
82	w	24	G
82	w	25	A
82	w	27	C
82	w	28	U

All (20) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	S2	42	A
1	S2	60	A
1	S2	196	C
1	S2	307	C
1	S2	320	C
1	S2	448	A
1	S2	561	G
1	S2	562	G
1	S2	566	G
1	S2	673	A
1	S2	871	G
1	S2	875	A
1	S2	1399	A
1	S2	1570	G
1	S2	1575	C
1	S2	1684	U
1	S2	1805	C
1	S2	1818	A
1	S2	1827	A
38	D	86	U

4.4 Non-standard residues in protein, DNA, RNA chains (i)

33 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	$\#\|Z\| > 2$
1	OMC	S2	1706	1	19,22,23	0.50	0	26,31,34	0.66	0
1	4AC	S2	1845	1	21,24,25	3.56	10 (47%)	29,34,37	1.13	3 (10%)
1	5MU	S2	817	1	19,22,23	0.40	0	28,32,35	0.91	2 (7%)
1	PSU	S2	1084	1	18,21,22	1.06	1 (5%)	22,30,33	1.71	4 (18%)
1	PSU	S2	1246	1	18,21,22	1.08	1 (5%)	22,30,33	1.72	4 (18%)
1	PSU	S2	825	1	18,21,22	1.10	1 (5%)	22,30,33	1.70	4 (18%)
1	OMU	S2	121	1	19,22,23	1.39	3 (15%)	26,31,34	1.96	7 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	UR3	S2	1833	1	19,22,23	3.00	7 (36%)	26,32,35	1.65	4 (15%)
1	OMC	S2	520	1	19,22,23	0.52	0	26,31,34	0.77	0
1	4AC	S2	1340	1	21,24,25	3.56	10 (47%)	29,34,37	1.12	3 (10%)
1	OMG	S2	686	1	18,26,27	1.10	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	S2	1681	1	18,25,26	3.56	8 (44%)	18,36,39	3.34	4 (22%)
1	MMX	S2	571	1	19,23,24	4.00	4 (21%)	22,33,36	2.83	6 (27%)
1	OMU	S2	116	1	19,22,23	3.10	8 (42%)	26,31,34	1.69	5 (19%)
1	M7A	S2	1809	1	20,25,26	2.07	3 (15%)	28,37,40	4.10	8 (28%)
1	B8N	S2	1251	1	24,29,30	3.06	5 (20%)	29,42,45	1.74	5 (17%)
1	6MZ	S2	1835	1	18,25,26	5.58	13 (72%)	16,36,39	5.12	11 (68%)
1	A2M	S2	671	1	18,25,26	3.61	8 (44%)	18,36,39	3.47	6 (33%)
1	A2M	S2	166	1	18,25,26	3.58	8 (44%)	18,36,39	3.36	3 (16%)
1	OMG	S2	512	1	18,26,27	1.11	2 (11%)	19,38,41	0.85	1 (5%)
1	A2M	S2	27	1	18,25,26	3.59	8 (44%)	18,36,39	3.32	4 (22%)
1	A2M	S2	487	1	18,25,26	3.63	8 (44%)	18,36,39	3.41	3 (16%)
1	A2M	S2	159	1	18,25,26	3.61	8 (44%)	18,36,39	3.44	5 (27%)
1	OMC	S2	1713	1	19,22,23	0.51	0	26,31,34	0.67	0
1	MA6	S2	1853	1	18,26,27	1.04	2 (11%)	19,38,41	3.32	2 (10%)
1	A2M	S2	1034	1	18,25,26	3.58	8 (44%)	18,36,39	3.36	4 (22%)
1	PSU	S2	119	1	18,21,22	1.10	1 (5%)	22,30,33	1.71	4 (18%)
1	PSU	S2	615	1	18,21,22	1.02	1 (5%)	22,30,33	1.66	4 (18%)
1	OMG	S2	647	1	18,26,27	1.11	2 (11%)	19,38,41	0.85	1 (5%)
1	PSU	S2	826	1	18,21,22	1.08	1 (5%)	22,30,33	1.66	5 (22%)
1	5MC	S2	1377	1	18,22,23	0.53	0	26,32,35	0.75	0
1	MA6	S2	1854	1	18,26,27	1.03	2 (11%)	19,38,41	3.36	2 (10%)
1	OMC	S2	174	1	19,22,23	0.51	0	26,31,34	0.67	0

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
1	OMC	S2	1706	1	-	0/9/27/28	0/2/2/2
1	4AC	S2	1845	1	-	0/11/29/30	0/2/2/2
1	5MU	S2	817	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	1084	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	S2	1246	1	-	2/7/25/26	0/2/2/2
1	PSU	S2	825	1	-	0/7/25/26	0/2/2/2
1	OMU	S2	121	1	-	1/9/27/28	0/2/2/2
1	UR3	S2	1833	1	-	2/7/25/26	0/2/2/2
1	OMC	S2	520	1	-	2/9/27/28	0/2/2/2
1	4AC	S2	1340	1	-	0/11/29/30	0/2/2/2
1	OMG	S2	686	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	1681	1	-	2/5/27/28	0/3/3/3
1	MMX	S2	571	1	-	4/9/44/45	0/2/2/2
1	OMU	S2	116	1	-	2/9/27/28	0/2/2/2
1	M7A	S2	1809	1	-	1/7/37/38	0/3/3/3
1	B8N	S2	1251	1	-	2/16/34/35	0/2/2/2
1	6MZ	S2	1835	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	671	1	-	1/5/27/28	0/3/3/3
1	A2M	S2	166	1	-	0/5/27/28	0/3/3/3
1	OMG	S2	512	1	-	0/5/27/28	0/3/3/3
1	A2M	S2	27	1	-	2/5/27/28	0/3/3/3
1	A2M	S2	487	1	-	0/5/27/28	0/3/3/3
1	A2M	S2	159	1	-	1/5/27/28	0/3/3/3
1	OMC	S2	1713	1	-	0/9/27/28	0/2/2/2
1	MA6	S2	1853	1	-	5/7/29/30	0/3/3/3
1	A2M	S2	1034	1	-	0/5/27/28	0/3/3/3
1	PSU	S2	119	1	-	0/7/25/26	0/2/2/2
1	PSU	S2	615	1	-	0/7/25/26	0/2/2/2
1	OMG	S2	647	1	-	2/5/27/28	0/3/3/3
1	PSU	S2	826	1	-	2/7/25/26	0/2/2/2
1	5MC	S2	1377	1	-	0/7/25/26	0/2/2/2
1	MA6	S2	1854	1	-	6/7/29/30	0/3/3/3
1	OMC	S2	174	1	-	0/9/27/28	0/2/2/2

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1835	6MZ	O3'-C3'	11.94	1.71	1.43
1	S2	1835	6MZ	O4'-C1'	-11.56	1.24	1.41
1	S2	571	MMX	C2-N1	10.18	1.50	1.37
1	S2	571	MMX	C4-N3	9.93	1.53	1.45
1	S2	1835	6MZ	C3'-C4'	-8.85	1.30	1.53
1	S2	166	A2M	C3'-C4'	-8.82	1.30	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	27	A2M	C3'-C4'	-8.76	1.30	1.53
1	S2	1034	A2M	C3'-C4'	-8.74	1.30	1.53
1	S2	1681	A2M	C3'-C4'	-8.73	1.30	1.53
1	S2	487	A2M	C3'-C4'	-8.69	1.30	1.53
1	S2	159	A2M	C3'-C4'	-8.62	1.31	1.53
1	S2	571	MMX	C2-N3	8.56	1.48	1.37
1	S2	671	A2M	C3'-C4'	-8.56	1.31	1.53
1	S2	1251	B8N	C6-N1	7.91	1.56	1.36
1	S2	159	A2M	O4'-C4'	7.72	1.62	1.45
1	S2	27	A2M	O4'-C4'	7.69	1.62	1.45
1	S2	1034	A2M	O4'-C4'	7.66	1.62	1.45
1	S2	671	A2M	O4'-C4'	7.65	1.62	1.45
1	S2	487	A2M	O4'-C4'	7.64	1.62	1.45
1	S2	166	A2M	O4'-C4'	7.62	1.62	1.45
1	S2	1833	UR3	C2-N1	7.61	1.49	1.38
1	S2	1845	4AC	C4-N3	7.48	1.45	1.32
1	S2	1340	4AC	C4-N3	7.46	1.45	1.32
1	S2	487	A2M	O4'-C1'	-7.45	1.30	1.41
1	S2	1681	A2M	O4'-C4'	7.45	1.61	1.45
1	S2	671	A2M	O4'-C1'	-7.42	1.30	1.41
1	S2	1251	B8N	C4-N3	-7.39	1.26	1.40
1	S2	116	OMU	C2-N1	7.36	1.50	1.38
1	S2	159	A2M	O4'-C1'	-7.34	1.30	1.41
1	S2	1681	A2M	O4'-C1'	-7.03	1.31	1.41
1	S2	116	OMU	C2-N3	6.99	1.50	1.38
1	S2	27	A2M	O4'-C1'	-6.96	1.31	1.41
1	S2	1034	A2M	O4'-C1'	-6.94	1.31	1.41
1	S2	166	A2M	O4'-C1'	-6.90	1.31	1.41
1	S2	1340	4AC	C6-C5	6.83	1.50	1.35
1	S2	1833	UR3	C6-C5	6.82	1.50	1.35
1	S2	1845	4AC	C6-C5	6.77	1.50	1.35
1	S2	1809	M7A	C4-N9	6.12	1.49	1.38
1	S2	1251	B8N	C2-N1	5.90	1.56	1.39
1	S2	1833	UR3	C2-N3	5.89	1.50	1.39
1	S2	1835	6MZ	O4'-C4'	5.82	1.58	1.45
1	S2	116	OMU	C6-C5	5.69	1.48	1.35
1	S2	1845	4AC	C7-N4	5.65	1.47	1.37
1	S2	1340	4AC	C7-N4	5.65	1.47	1.37
1	S2	1835	6MZ	C5-C4	-5.55	1.26	1.40
1	S2	1251	B8N	C6-C5	5.54	1.42	1.34
1	S2	1340	4AC	C4-N4	5.29	1.47	1.39
1	S2	1845	4AC	C2-N3	5.29	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1845	4AC	C2-N1	5.28	1.51	1.40
1	S2	1340	4AC	C2-N1	5.27	1.51	1.40
1	S2	1845	4AC	C4-N4	5.24	1.47	1.39
1	S2	1340	4AC	C2-N3	5.23	1.47	1.36
1	S2	1835	6MZ	O2'-C2'	-5.17	1.30	1.43
1	S2	1835	6MZ	C6-N1	-4.91	1.27	1.34
1	S2	1835	6MZ	C8-N7	-4.76	1.26	1.34
1	S2	1835	6MZ	C4-N3	-4.74	1.29	1.35
1	S2	1809	M7A	C6-N6	4.41	1.45	1.34
1	S2	116	OMU	C4-N3	4.36	1.46	1.38
1	S2	571	MMX	C5-C4	-4.22	1.48	1.52
1	S2	1845	4AC	C5-C4	4.18	1.49	1.40
1	S2	1340	4AC	C5-C4	4.12	1.49	1.40
1	S2	1340	4AC	CM7-C7	4.11	1.59	1.50
1	S2	1845	4AC	CM7-C7	4.09	1.59	1.50
1	S2	1809	M7A	C5-N7	4.03	1.49	1.39
1	S2	1251	B8N	C1'-C5	3.97	1.59	1.50
1	S2	119	PSU	C6-C5	3.69	1.39	1.35
1	S2	825	PSU	C6-C5	3.65	1.39	1.35
1	S2	1246	PSU	C6-C5	3.62	1.39	1.35
1	S2	826	PSU	C6-C5	3.58	1.39	1.35
1	S2	1833	UR3	C6-N1	3.49	1.46	1.38
1	S2	1084	PSU	C6-C5	3.44	1.39	1.35
1	S2	615	PSU	C6-C5	3.39	1.39	1.35
1	S2	121	OMU	C4-N3	-3.32	1.32	1.38
1	S2	1835	6MZ	C2'-C1'	-3.26	1.48	1.53
1	S2	166	A2M	C6-N6	3.18	1.45	1.34
1	S2	159	A2M	C6-N6	3.18	1.45	1.34
1	S2	1681	A2M	C6-N6	3.18	1.45	1.34
1	S2	487	A2M	C6-N6	3.18	1.45	1.34
1	S2	671	A2M	C6-N6	3.17	1.45	1.34
1	S2	27	A2M	C6-N6	3.16	1.45	1.34
1	S2	1835	6MZ	C5-N7	-3.15	1.28	1.39
1	S2	1034	A2M	C6-N6	3.14	1.45	1.34
1	S2	121	OMU	C2-N3	-3.07	1.32	1.38
1	S2	671	A2M	O3'-C3'	3.06	1.50	1.43
1	S2	1835	6MZ	C2-N1	-2.96	1.28	1.33
1	S2	1034	A2M	O3'-C3'	2.92	1.49	1.43
1	S2	159	A2M	O3'-C3'	2.91	1.49	1.43
1	S2	27	A2M	O3'-C3'	2.90	1.49	1.43
1	S2	487	A2M	O3'-C3'	2.89	1.49	1.43
1	S2	116	OMU	O4-C4	-2.88	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	116	OMU	C6-N1	2.86	1.44	1.38
1	S2	1681	A2M	O3'-C3'	2.84	1.49	1.43
1	S2	166	A2M	O3'-C3'	2.84	1.49	1.43
1	S2	686	OMG	C8-N7	-2.77	1.30	1.35
1	S2	647	OMG	C8-N7	-2.77	1.30	1.35
1	S2	512	OMG	C8-N7	-2.76	1.30	1.35
1	S2	1853	MA6	C2-N3	2.66	1.36	1.32
1	S2	166	A2M	C5-C4	-2.65	1.33	1.40
1	S2	1835	6MZ	C6-N6	2.62	1.39	1.35
1	S2	159	A2M	C5-C4	-2.61	1.34	1.40
1	S2	27	A2M	C5-C4	-2.60	1.34	1.40
1	S2	487	A2M	C5-C4	-2.60	1.34	1.40
1	S2	1034	A2M	C5-C4	-2.60	1.34	1.40
1	S2	671	A2M	C5-C4	-2.59	1.34	1.40
1	S2	1340	4AC	C6-N1	2.58	1.44	1.38
1	S2	1681	A2M	C5-C4	-2.57	1.34	1.40
1	S2	166	A2M	O2'-C2'	-2.57	1.36	1.42
1	S2	27	A2M	O2'-C2'	-2.56	1.36	1.42
1	S2	1854	MA6	C2-N3	2.56	1.36	1.32
1	S2	1034	A2M	O2'-C2'	-2.56	1.36	1.42
1	S2	1854	MA6	C5-C4	-2.56	1.34	1.40
1	S2	121	OMU	C5-C4	-2.56	1.38	1.43
1	S2	1845	4AC	C6-N1	2.55	1.44	1.38
1	S2	1853	MA6	C5-C4	-2.54	1.34	1.40
1	S2	671	A2M	O2'-C2'	-2.52	1.36	1.42
1	S2	1681	A2M	O2'-C2'	-2.52	1.36	1.42
1	S2	487	A2M	O2'-C2'	-2.50	1.36	1.42
1	S2	159	A2M	O2'-C2'	-2.50	1.36	1.42
1	S2	116	OMU	C5-C4	2.35	1.48	1.43
1	S2	27	A2M	C2-N3	2.32	1.35	1.32
1	S2	512	OMG	C5-C6	-2.31	1.42	1.47
1	S2	1833	UR3	C4-N3	2.29	1.45	1.40
1	S2	1034	A2M	C2-N3	2.28	1.35	1.32
1	S2	647	OMG	C5-C6	-2.28	1.42	1.47
1	S2	1681	A2M	C2-N3	2.28	1.35	1.32
1	S2	487	A2M	C2-N3	2.25	1.35	1.32
1	S2	116	OMU	O2-C2	-2.25	1.18	1.23
1	S2	686	OMG	C5-C6	-2.23	1.42	1.47
1	S2	166	A2M	C2-N3	2.23	1.35	1.32
1	S2	159	A2M	C2-N3	2.23	1.35	1.32
1	S2	1845	4AC	O7-C7	-2.21	1.18	1.23
1	S2	1340	4AC	O7-C7	-2.20	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S2	1833	UR3	C5-C4	2.19	1.49	1.43
1	S2	671	A2M	C2-N3	2.15	1.35	1.32
1	S2	1833	UR3	O2-C2	-2.14	1.18	1.22

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1809	M7A	C5-C6-N6	13.86	147.41	123.74
1	S2	1854	MA6	N1-C6-N6	-13.27	103.09	117.06
1	S2	1853	MA6	N1-C6-N6	-13.16	103.21	117.06
1	S2	1809	M7A	N6-C6-N1	-11.78	92.55	118.35
1	S2	671	A2M	C5-C6-N6	10.59	136.44	120.35
1	S2	1034	A2M	C5-C6-N6	10.57	136.41	120.35
1	S2	159	A2M	C5-C6-N6	10.51	136.33	120.35
1	S2	166	A2M	C5-C6-N6	10.49	136.29	120.35
1	S2	487	A2M	C5-C6-N6	10.48	136.28	120.35
1	S2	27	A2M	C5-C6-N6	10.35	136.08	120.35
1	S2	1681	A2M	C5-C6-N6	10.28	135.97	120.35
1	S2	1835	6MZ	C3'-C2'-C1'	9.29	114.97	100.98
1	S2	1835	6MZ	O4'-C1'-C2'	-8.69	94.23	106.93
1	S2	571	MMX	N3-C2-N1	8.58	122.47	116.83
1	S2	1835	6MZ	O2'-C2'-C1'	-8.50	79.48	110.85
1	S2	1835	6MZ	C1'-N9-C4	-8.43	111.83	126.64
1	S2	671	A2M	N6-C6-N1	-7.23	103.56	118.57
1	S2	1034	A2M	N6-C6-N1	-7.22	103.59	118.57
1	S2	487	A2M	N6-C6-N1	-7.17	103.70	118.57
1	S2	166	A2M	N6-C6-N1	-7.16	103.72	118.57
1	S2	159	A2M	N6-C6-N1	-7.14	103.76	118.57
1	S2	1681	A2M	N6-C6-N1	-7.01	104.01	118.57
1	S2	27	A2M	N6-C6-N1	-7.01	104.03	118.57
1	S2	1809	M7A	C4-N9-C1'	-6.55	111.05	126.60
1	S2	1835	6MZ	O3'-C3'-C4'	6.01	128.43	111.05
1	S2	166	A2M	N3-C2-N1	-5.85	119.54	128.68
1	S2	1681	A2M	N3-C2-N1	-5.67	119.81	128.68
1	S2	1034	A2M	N3-C2-N1	-5.58	119.95	128.68
1	S2	487	A2M	N3-C2-N1	-5.58	119.95	128.68
1	S2	1854	MA6	N3-C2-N1	-5.58	119.96	128.68
1	S2	1809	M7A	N3-C2-N1	-5.57	119.89	128.60
1	S2	27	A2M	N3-C2-N1	-5.56	119.99	128.68
1	S2	671	A2M	N3-C2-N1	-5.54	120.02	128.68
1	S2	159	A2M	N3-C2-N1	-5.52	120.05	128.68
1	S2	571	MMX	C4-N3-C2	-5.49	116.49	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	571	MMX	O2-C2-N3	-5.47	115.14	122.07
1	S2	1853	MA6	N3-C2-N1	-5.46	120.14	128.68
1	S2	121	OMU	C2'-C1'-N1	-5.24	104.05	114.22
1	S2	1251	B8N	C5-C4-N3	5.15	125.71	116.17
1	S2	116	OMU	C4-N3-C2	-5.03	119.95	126.58
1	S2	1835	6MZ	O4'-C4'-C5'	-4.88	93.31	109.37
1	S2	1809	M7A	N3-C4-N9	4.63	132.72	126.87
1	S2	1084	PSU	C4-N3-C2	-4.48	119.88	126.34
1	S2	1251	B8N	C4-N3-C2	-4.45	119.83	125.46
1	S2	1246	PSU	N1-C2-N3	4.44	120.16	115.13
1	S2	119	PSU	C4-N3-C2	-4.44	119.95	126.34
1	S2	825	PSU	C4-N3-C2	-4.41	119.99	126.34
1	S2	571	MMX	C5-C6-N1	4.40	117.94	110.71
1	S2	119	PSU	N1-C2-N3	4.38	120.09	115.13
1	S2	825	PSU	N1-C2-N3	4.36	120.08	115.13
1	S2	1246	PSU	C4-N3-C2	-4.33	120.10	126.34
1	S2	1833	UR3	C1'-N1-C2	4.33	124.30	116.99
1	S2	826	PSU	C4-N3-C2	-4.31	120.13	126.34
1	S2	615	PSU	N1-C2-N3	4.30	120.00	115.13
1	S2	1084	PSU	N1-C2-N3	4.30	120.00	115.13
1	S2	826	PSU	N1-C2-N3	4.21	119.91	115.13
1	S2	1833	UR3	C4-N3-C2	-4.20	120.61	124.56
1	S2	615	PSU	C4-N3-C2	-4.18	120.31	126.34
1	S2	1835	6MZ	N3-C2-N1	-4.10	122.27	128.68
1	S2	121	OMU	N3-C2-N1	4.02	120.22	114.89
1	S2	1809	M7A	C71-N7-C5	-3.87	109.15	124.01
1	S2	1833	UR3	C6-N1-C2	-3.68	118.50	121.79
1	S2	116	OMU	N3-C2-N1	3.62	119.70	114.89
1	S2	121	OMU	C4-N3-C2	-3.61	121.82	126.58
1	S2	1809	M7A	C2-N3-C4	3.52	120.06	111.75
1	S2	121	OMU	C5-C4-N3	3.34	119.84	114.84
1	S2	116	OMU	C5-C4-N3	3.24	119.69	114.84
1	S2	116	OMU	O4-C4-C5	-3.05	119.79	125.16
1	S2	571	MMX	C6-C5-C4	2.99	117.32	110.92
1	S2	1681	A2M	C1'-N9-C4	2.98	131.88	126.64
1	S2	1835	6MZ	C2'-C3'-C4'	-2.98	96.84	102.64
1	S2	1251	B8N	N3-C2-N1	2.95	120.92	116.76
1	S2	571	MMX	C31-N3-C2	2.93	121.21	117.44
1	S2	1835	6MZ	O3'-C3'-C2'	2.93	121.29	111.82
1	S2	1845	4AC	C6-C5-C4	2.82	120.42	116.96
1	S2	1833	UR3	O2-C2-N3	-2.80	117.39	121.34
1	S2	1835	6MZ	C2-N1-C6	-2.76	114.22	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S2	1340	4AC	C6-C5-C4	2.75	120.33	116.96
1	S2	1809	M7A	C5-C4-N3	-2.73	120.21	126.62
1	S2	1246	PSU	O2-C2-N1	-2.64	119.89	122.79
1	S2	119	PSU	O2-C2-N1	-2.62	119.91	122.79
1	S2	817	5MU	C1'-N1-C2	2.61	122.29	117.57
1	S2	121	OMU	O4-C4-C5	-2.58	120.62	125.16
1	S2	615	PSU	O2-C2-N1	-2.57	119.96	122.79
1	S2	825	PSU	O2-C2-N1	-2.57	119.96	122.79
1	S2	121	OMU	O2'-C2'-C1'	2.54	114.03	109.08
1	S2	1845	4AC	C5-C4-N3	-2.53	118.53	122.59
1	S2	1340	4AC	C5-C4-N3	-2.52	118.53	122.59
1	S2	1084	PSU	O2-C2-N1	-2.50	120.04	122.79
1	S2	826	PSU	O2-C2-N1	-2.46	120.08	122.79
1	S2	1251	B8N	O4-C4-N3	-2.46	115.81	119.98
1	S2	27	A2M	C1'-N9-C4	2.43	130.91	126.64
1	S2	1246	PSU	C6-N1-C2	-2.39	120.24	122.68
1	S2	512	OMG	O6-C6-C5	2.36	128.98	124.37
1	S2	647	OMG	O6-C6-C5	2.33	128.93	124.37
1	S2	615	PSU	C6-N1-C2	-2.33	120.30	122.68
1	S2	1835	6MZ	O5'-C5'-C4'	2.30	116.83	108.99
1	S2	1251	B8N	O4'-C1'-C2'	2.29	108.38	105.14
1	S2	159	A2M	C2'-C3'-C4'	2.29	106.96	101.99
1	S2	686	OMG	O6-C6-C5	2.28	128.83	124.37
1	S2	119	PSU	C6-N1-C2	-2.26	120.37	122.68
1	S2	825	PSU	C6-N1-C2	-2.19	120.44	122.68
1	S2	159	A2M	C1'-N9-C4	2.19	130.49	126.64
1	S2	826	PSU	C6-N1-C2	-2.18	120.46	122.68
1	S2	671	A2M	C3'-C2'-C1'	2.17	106.96	102.89
1	S2	817	5MU	C1'-N1-C6	-2.15	117.54	121.12
1	S2	116	OMU	C1'-N1-C2	2.14	121.45	117.57
1	S2	671	A2M	C2'-C3'-C4'	2.12	106.59	101.99
1	S2	671	A2M	O4'-C4'-C3'	2.11	109.29	105.11
1	S2	1340	4AC	N4-C4-N3	2.09	117.36	113.85
1	S2	1084	PSU	C6-N1-C2	-2.08	120.56	122.68
1	S2	1845	4AC	N4-C4-N3	2.06	117.31	113.85
1	S2	826	PSU	O4'-C1'-C2'	2.05	108.04	105.14
1	S2	1034	A2M	C1'-N9-C4	2.04	130.22	126.64
1	S2	121	OMU	O4'-C1'-N1	2.01	112.95	108.36

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	S2	27	A2M	C3'-C4'-C5'-O5'
1	S2	116	OMU	C3'-C4'-C5'-O5'
1	S2	116	OMU	O4'-C4'-C5'-O5'
1	S2	121	OMU	C1'-C2'-O2'-CM2
1	S2	520	OMC	O4'-C4'-C5'-O5'
1	S2	571	MMX	O4'-C1'-N1-C2
1	S2	571	MMX	O4'-C1'-N1-C6
1	S2	686	OMG	C3'-C4'-C5'-O5'
1	S2	826	PSU	O4'-C1'-C5-C4
1	S2	826	PSU	O4'-C1'-C5-C6
1	S2	1251	B8N	N3-C31-C32-C33
1	S2	1833	UR3	O4'-C1'-N1-C6
1	S2	1833	UR3	O4'-C1'-N1-C2
1	S2	1853	MA6	O4'-C4'-C5'-O5'
1	S2	1853	MA6	C3'-C4'-C5'-O5'
1	S2	1853	MA6	C5-C6-N6-C9
1	S2	1853	MA6	C5-C6-N6-C10
1	S2	1854	MA6	C5-C6-N6-C10
1	S2	27	A2M	O4'-C4'-C5'-O5'
1	S2	520	OMC	C3'-C4'-C5'-O5'
1	S2	571	MMX	C3'-C4'-C5'-O5'
1	S2	571	MMX	O4'-C4'-C5'-O5'
1	S2	1246	PSU	C3'-C4'-C5'-O5'
1	S2	1854	MA6	O4'-C4'-C5'-O5'
1	S2	1246	PSU	O4'-C4'-C5'-O5'
1	S2	1854	MA6	C3'-C4'-C5'-O5'
1	S2	1853	MA6	N1-C6-N6-C9
1	S2	1854	MA6	N1-C6-N6-C10
1	S2	1835	6MZ	O4'-C4'-C5'-O5'
1	S2	686	OMG	O4'-C4'-C5'-O5'
1	S2	1681	A2M	O4'-C4'-C5'-O5'
1	S2	1854	MA6	C5-C6-N6-C9
1	S2	1809	M7A	C2'-C1'-N9-C8
1	S2	159	A2M	C4'-C5'-O5'-P
1	S2	671	A2M	C4'-C5'-O5'-P
1	S2	1251	B8N	N34-C33-C34-O35
1	S2	1854	MA6	C4'-C5'-O5'-P
1	S2	1681	A2M	C3'-C4'-C5'-O5'
1	S2	647	OMG	C3'-C4'-C5'-O5'
1	S2	647	OMG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 39 ligands modelled in this entry, 39 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-13954. 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.

5.1 Orthogonal projections (i)

This section was not generated.

5.2 Central slices (i)

This section was not generated.

5.3 Largest variance slices (i)

This section was not generated.

5.4 Orthogonal standard-deviation projections (False-color) (i)

This section was not generated.

5.5 Orthogonal surface views (i)

This section was not generated.

5.6 Mask visualisation (i)

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

6 Map analysis (i)

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

6.1 Map-value distribution (i)

This section was not generated.

6.2 Volume estimate versus contour level (i)

This section was not generated.

6.3 Rotationally averaged power spectrum (i)

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

7 Fourier-Shell correlation (i)

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

8 Map-model fit (i)

This section was not generated.