



Full wwPDB EM Validation Report ⓘ

May 18, 2024 – 11:04 AM EDT

PDB ID : 6WDR
EMDB ID : EMD-21644
Title : Subunit joining exposes nascent pre-40S rRNA for processing and quality control
Authors : Rai, J.; Parker, M.D.; Huang, H.; Choy, S.; Ghalei, H.; Johnson, M.C.; Karbstein, K.; Stroupe, M.E.
Deposited on : 2020-04-01
Resolution : 3.70 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

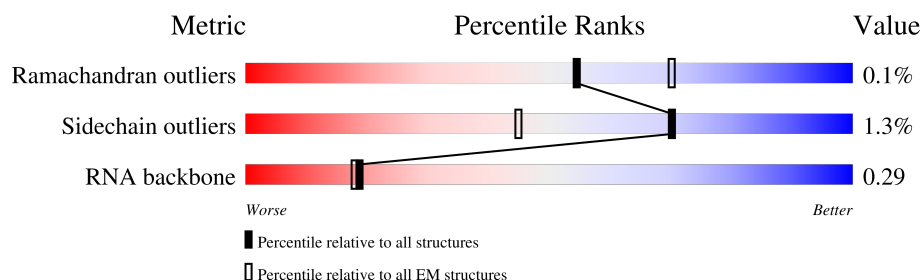
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 Å.

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



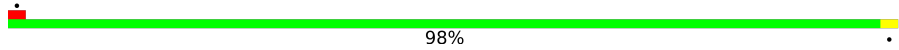
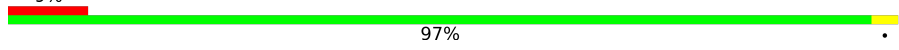
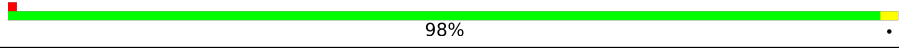
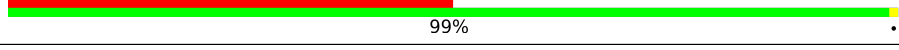
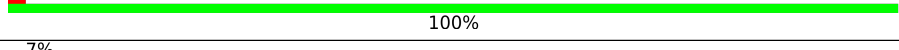
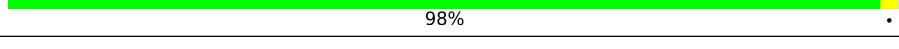
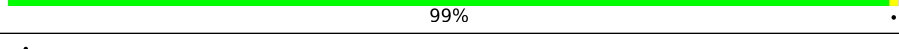
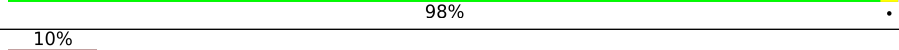
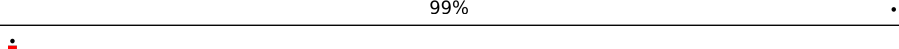
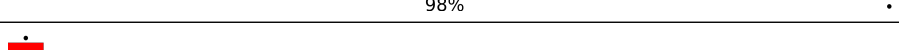
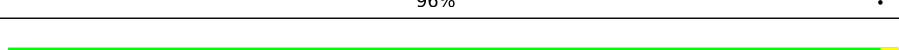
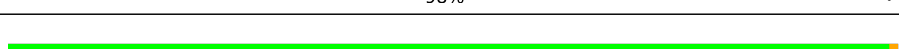


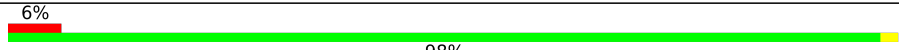
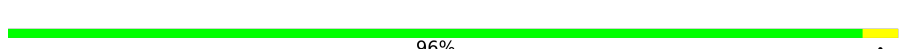

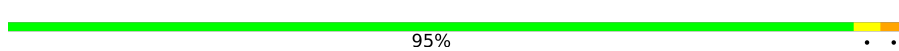

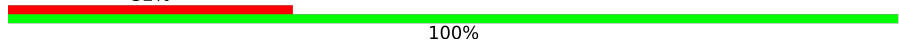
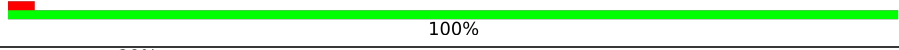



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	
2	C	217	
3	D	223	
4	E	260	
5	F	206	
6	G	232	
7	H	184	
8	I	199	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	J	185	
10	K	96	
11	L	140	
12	M	125	
13	N	150	
14	P	127	
15	Q	127	
16	R	125	
17	S	135	
18	T	143	
19	U	103	
20	V	87	
21	W	129	
22	X	144	
23	Y	134	
24	Z	63	
25	b	81	
26	c	63	
27	d	37	
28	e	63	
29	f	71	
30	g	317	
31	k	788	
32	2	1910	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 74473 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 protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	206	Total	C	N	O	S	0	0
			1611	1036	285	288	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	PHE	ASP	conflict	UNP P32905

- Molecule 2 is a protein called 40S ribosomal protein S2.

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

- Molecule 3 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	260	Total	C	N	O	S	0	0
			2068	1316	389	360	3		

- Molecule 5 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 6 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	232	Total	C	N	O	S	0	0
			1873	1172	366	332	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	184	Total	C	N	O	S	0	0
			1481	951	265	265			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 9 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 10 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 11 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 12 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	125	Total	C	N	O	S	0	0
			941	591	166	182	2		

- Molecule 13 is a protein called 40S ribosomal protein S13.

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

- Molecule 14 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	127	Total	C	N	O	S	0	0
			1001	637	186	171	7		

- Molecule 15 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	127	Total	C	N	O	S	0	0
			993	640	177	176			

- Molecule 16 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	125	Total	C	N	O	S	0	0
			1000	625	188	185	2		

- Molecule 17 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	135	Total	C	N	O	S	0	0
			1110	696	215	197	2		

- Molecule 18 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 19 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	103	Total	C	N	O	S	0	0
			819	519	148	151	1		

- Molecule 20 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 21 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 22 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 23 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 24 is a protein called 40S ribosomal protein S25-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	63	Total	C	N	O	S	0	0
			512	328	94	90			

- Molecule 25 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 26 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 27 is a protein called 40S ribosomal protein S29-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	37	Total	C	N	O	S	0	0
			302	186	62	50	4		

- Molecule 28 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	48	Total	C	N	O	S	0	0
			384	242	81	59	2		

- Molecule 29 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	71	Total	C	N	O	S	0	0
			498	309	93	92	4		

- Molecule 30 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	317	Total	C	N	O	S	0	0
			2431	1538	417	468	8		

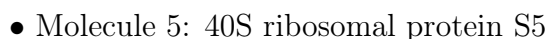
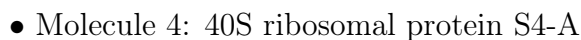
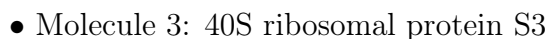
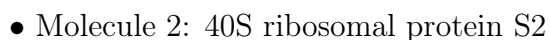
- Molecule 31 is a protein called Ribosome biogenesis protein TSR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	k	638	Total	C	N	O	S	0	0
			5154	3291	896	953	14		

- Molecule 32 is a RNA chain called 20S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	2	1647	Total	C	N	O	P	0	0
			35078	15682	6196	11553	1647		

- Molecule 1: 40S ribosomal protein S0-A



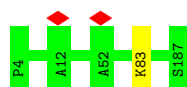
- Molecule 6: 40S ribosomal protein S6-A

Chain G:  98%




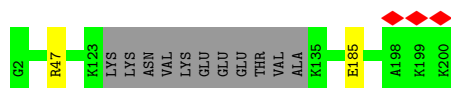
- Molecule 7: 40S ribosomal protein S7-A

Chain H:  99%



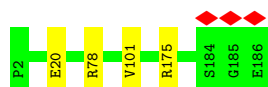
- Molecule 8: 40S ribosomal protein S8-A

Chain I:  93% 6%



- Molecule 9: 40S ribosomal protein S9-A

Chain J:  98%



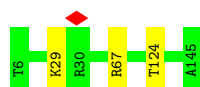
- Molecule 10: 40S ribosomal protein S10-A

Chain K:  9% 97%



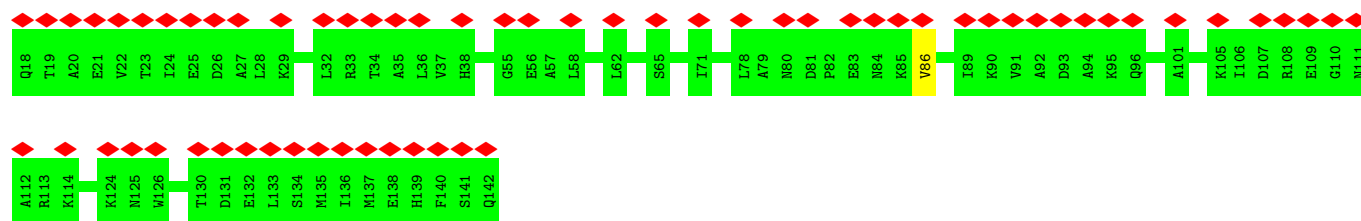
- Molecule 11: 40S ribosomal protein S11-A

Chain L:  98%



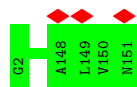
- Molecule 12: 40S ribosomal protein S12

Chain M:  50% 99%



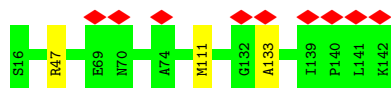
- Molecule 13: 40S ribosomal protein S13

Chain N: 100%



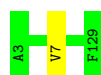
- Molecule 14: 40S ribosomal protein S15

Chain P: 98%



- Molecule 15: 40S ribosomal protein S16-A

Chain Q: 99%



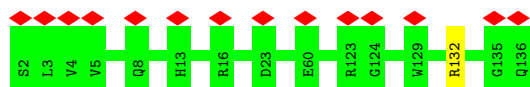
- Molecule 16: 40S ribosomal protein S17-A

Chain R: 98%



- Molecule 17: 40S ribosomal protein S18-A

Chain S: 99%



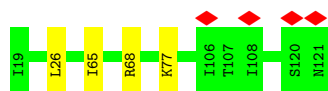
- Molecule 18: 40S ribosomal protein S19-A

Chain T: 98%



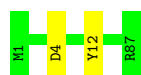
- Molecule 19: 40S ribosomal protein S20

Chain U: 96%



- Molecule 20: 40S ribosomal protein S21-A

Chain V: 98%



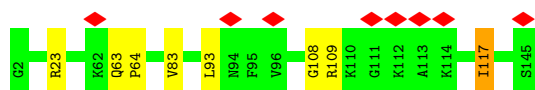
- Molecule 21: 40S ribosomal protein S22-A

Chain W: 99%



- Molecule 22: 40S ribosomal protein S23-A

Chain X: 94% 5%



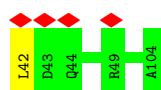
- Molecule 23: 40S ribosomal protein S24-A

Chain Y: 99%



- Molecule 24: 40S ribosomal protein S25-A

Chain Z: 98%



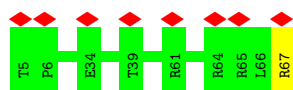
- Molecule 25: 40S ribosomal protein S27-A

Chain b:  96%



- Molecule 26: 40S ribosomal protein S28-A

Chain c:  13% 98%




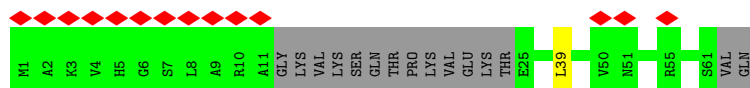
- Molecule 27: 40S ribosomal protein S29-A

Chain d:  95%



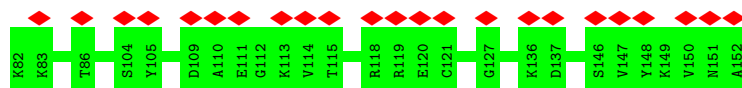
- Molecule 28: 40S ribosomal protein S30-A

Chain e:  22% 75% 24%



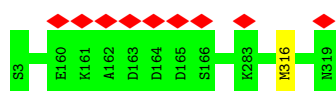
- Molecule 29: Ubiquitin-40S ribosomal protein S31

Chain f:  32% 100%




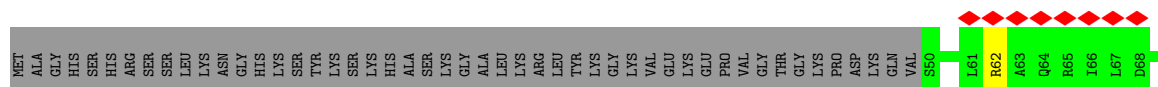
- Molecule 30: Guanine nucleotide-binding protein subunit beta-like protein

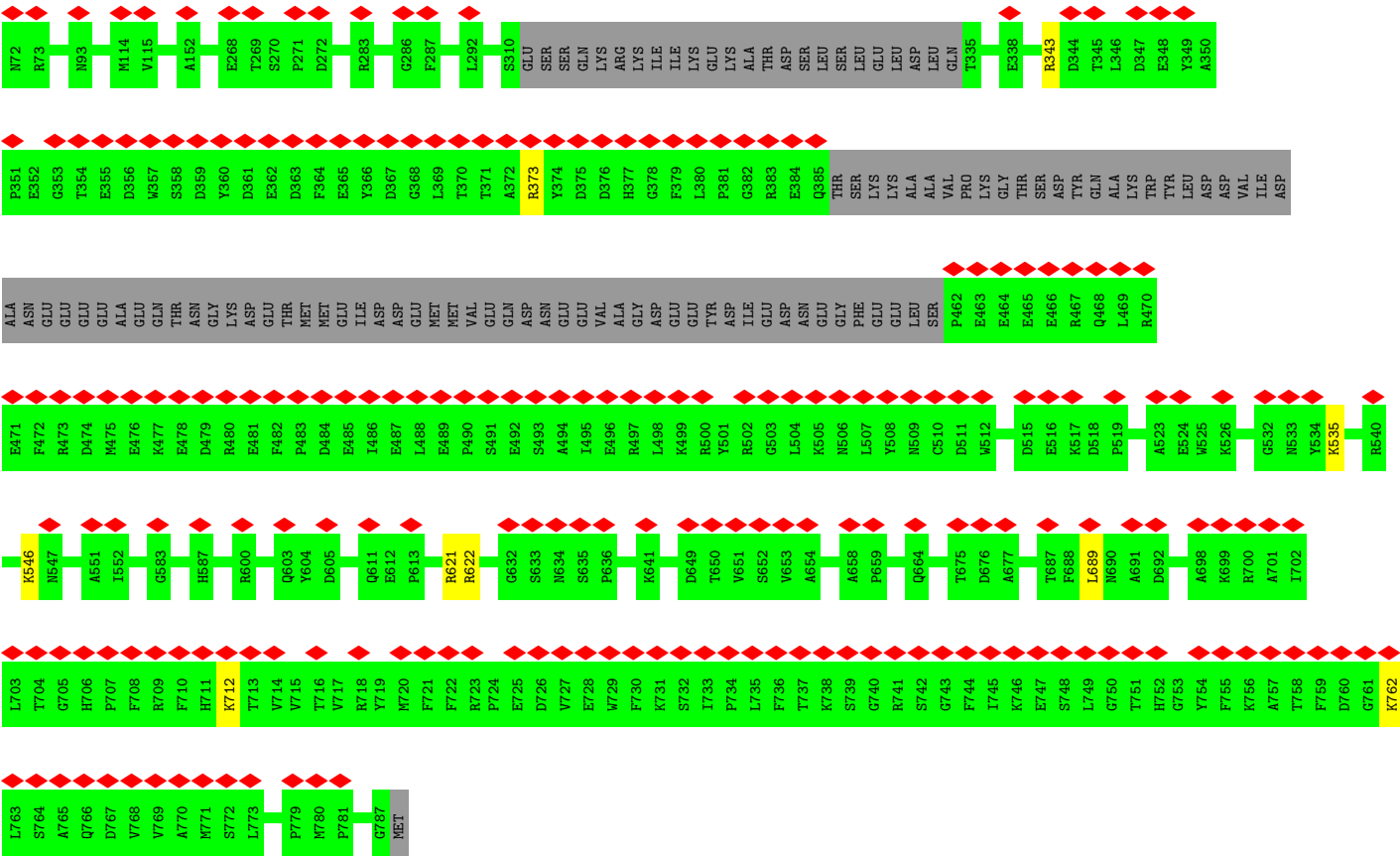
Chain g:  100%



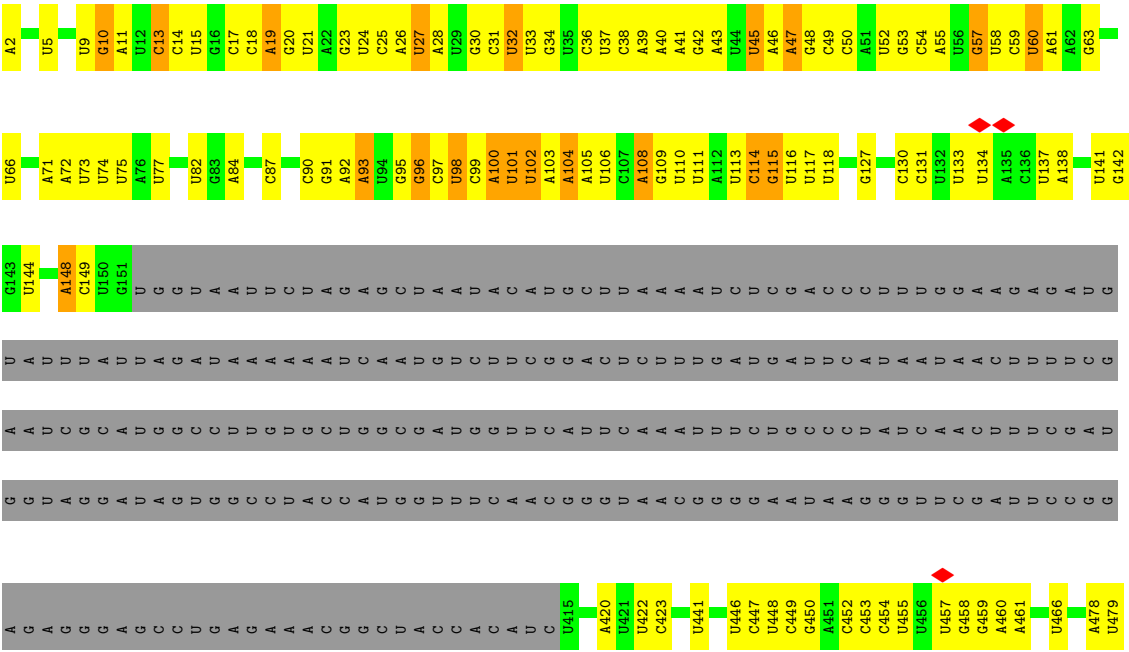
- Molecule 31: Ribosome biogenesis protein TSR1

Chain k:  29% 80% 19%

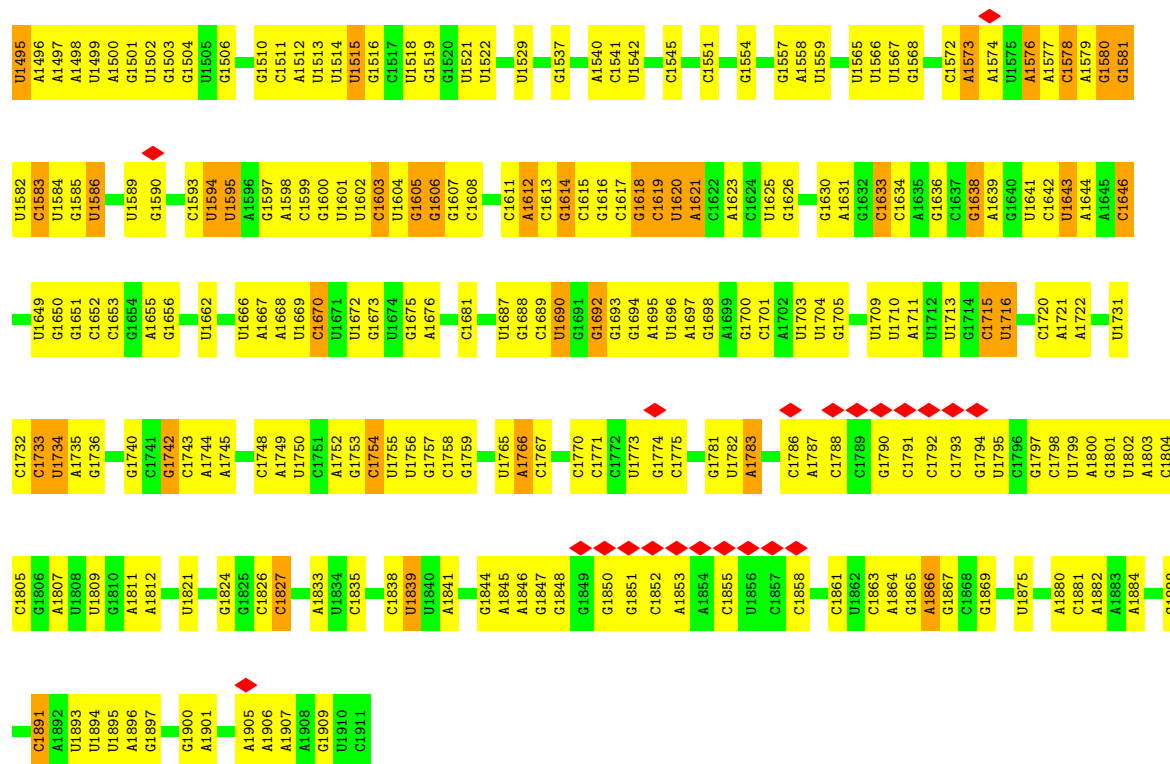




● Molecule 32: 20S ribosomal RNA







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, POINT	Depositor
Number of particles used	90692, 90692	Depositor
Resolution determination method	FSC 0.143 CUT-OFF, FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION, PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25.00	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	DIRECT ELECTRON DE-64 (8k x 8k)	Depositor
Maximum map value	0.172	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (\AA)	476.16, 476.16, 476.16	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.24, 1.24, 1.24	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.73	0/1653	0.65	0/2261
2	C	0.78	1/1665 (0.1%)	0.70	0/2263
3	D	0.46	0/1758	0.77	3/2365 (0.1%)
4	E	0.81	0/2109	0.69	1/2839 (0.0%)
5	F	0.36	0/1628	0.59	0/2199
6	G	0.57	0/1897	0.59	0/2532
7	H	0.55	0/1506	0.60	0/2028
8	I	0.72	0/1514	0.63	0/2021
9	J	0.79	0/1519	0.67	0/2035
10	K	0.40	0/836	0.63	0/1128
11	L	0.97	0/1155	0.71	0/1557
12	M	0.27	0/949	0.64	0/1284
13	N	0.66	0/1215	0.61	0/1638
14	P	0.34	0/1019	0.62	0/1363
15	Q	0.45	0/1011	0.61	0/1362
16	R	0.49	0/1010	0.64	1/1355 (0.1%)
17	S	0.31	0/1128	0.62	0/1518
18	T	0.38	0/1130	0.53	0/1517
19	U	0.44	0/829	0.62	1/1121 (0.1%)
20	V	0.73	0/693	0.66	0/935
21	W	1.03	0/1038	0.82	1/1395 (0.1%)
22	X	0.79	0/1139	0.79	1/1518 (0.1%)
23	Y	0.68	0/1087	0.66	0/1449
24	Z	0.30	0/519	0.59	1/696 (0.1%)
25	b	0.62	0/620	0.68	2/838 (0.2%)
26	c	0.35	0/499	0.62	0/670
27	d	0.54	0/306	0.73	0/404
28	e	0.56	0/390	0.68	0/517
29	f	0.31	0/502	0.65	0/673
30	g	0.36	0/2484	0.60	0/3382
31	k	0.35	0/5273	0.59	1/7129 (0.0%)
32	2	1.56	433/39196 (1.1%)	1.49	733/60993 (1.2%)
All	All	1.18	434/79277 (0.5%)	1.17	745/114985 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	C	0	1
3	D	0	1
8	I	0	1
9	J	0	1
10	K	0	1
14	P	0	2
16	R	0	1
18	T	0	1
19	U	0	1
22	X	0	4
27	d	0	1
All	All	0	16

All (434) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	627	G	C6-N1	-8.99	1.33	1.39
32	2	649	G	N7-C5	-8.66	1.34	1.39
32	2	1185	C	N3-C4	-8.38	1.28	1.33
32	2	893	A	N9-C8	-8.20	1.31	1.37
32	2	646	G	C5-C4	-8.16	1.32	1.38
32	2	97	C	C4-C5	-8.05	1.36	1.43
32	2	1168	U	P-O5'	8.00	1.67	1.59
32	2	628	G	N9-C8	-7.88	1.32	1.37
32	2	875	U	C2-N3	-7.84	1.32	1.37
32	2	724	G	C5-C4	-7.83	1.32	1.38
32	2	646	G	N1-C2	-7.76	1.31	1.37
32	2	649	G	C5-C4	-7.60	1.33	1.38
32	2	1185	C	C2-O2	-7.60	1.17	1.24
32	2	1255	U	C2-N3	-7.54	1.32	1.37
32	2	1289	A	N7-C5	-7.50	1.34	1.39
32	2	564	A	N7-C5	-7.50	1.34	1.39
32	2	647	G	C6-N1	-7.49	1.34	1.39
32	2	627	G	C5-C4	-7.47	1.33	1.38
32	2	876	G	C5-C4	-7.47	1.33	1.38
32	2	891	G	C6-N1	-7.46	1.34	1.39
32	2	568	C	N3-C4	-7.43	1.28	1.33
32	2	594	A	N9-C4	-7.43	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	630	A	N9-C4	-7.35	1.33	1.37
32	2	835	C	N1-C6	-7.34	1.32	1.37
32	2	650	A	N7-C5	-7.31	1.34	1.39
32	2	10	G	N9-C4	-7.31	1.32	1.38
32	2	600	G	C5-C4	-7.25	1.33	1.38
32	2	562	A	N7-C5	-7.20	1.34	1.39
32	2	659	G	N1-C2	-7.16	1.32	1.37
32	2	712	C	N1-C6	-7.14	1.32	1.37
32	2	659	G	C5-C4	-7.08	1.33	1.38
32	2	627	G	N1-C2	-7.04	1.32	1.37
32	2	891	G	N1-C2	-7.04	1.32	1.37
32	2	724	G	C6-N1	-7.02	1.34	1.39
32	2	725	G	C5-C4	-7.00	1.33	1.38
32	2	571	C	N3-C4	-6.98	1.29	1.33
32	2	894	G	C6-N1	-6.97	1.34	1.39
32	2	1452	A	N9-C4	-6.92	1.33	1.37
32	2	628	G	C5-C4	-6.89	1.33	1.38
32	2	564	A	N9-C4	-6.89	1.33	1.37
32	2	873	G	C8-N7	-6.89	1.26	1.30
32	2	90	C	N3-C4	-6.87	1.29	1.33
32	2	893	A	N7-C5	-6.86	1.35	1.39
32	2	99	C	N3-C4	-6.84	1.29	1.33
32	2	10	G	N7-C5	-6.84	1.35	1.39
32	2	629	A	N9-C4	-6.83	1.33	1.37
32	2	109	G	N1-C2	-6.83	1.32	1.37
32	2	1452	A	N3-C4	-6.82	1.30	1.34
32	2	1452	A	C5-C4	-6.79	1.33	1.38
32	2	733	A	C5-C4	-6.79	1.33	1.38
32	2	109	G	C6-N1	-6.78	1.34	1.39
32	2	624	C	C4-C5	-6.75	1.37	1.43
32	2	39	A	N9-C4	-6.74	1.33	1.37
32	2	1056	G	N9-C4	-6.74	1.32	1.38
32	2	98	U	N3-C4	-6.73	1.32	1.38
32	2	108	A	N7-C5	-6.71	1.35	1.39
32	2	640	G	C5-C4	-6.69	1.33	1.38
32	2	100	A	C5-C4	-6.69	1.34	1.38
32	2	894	G	C5-C4	-6.68	1.33	1.38
32	2	894	G	N7-C5	-6.68	1.35	1.39
32	2	1260	G	C5-C4	-6.66	1.33	1.38
32	2	635	G	C5-C4	-6.64	1.33	1.38
32	2	876	G	N7-C5	-6.63	1.35	1.39
32	2	621	U	C2-N3	-6.62	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	57	G	N9-C8	-6.62	1.33	1.37
32	2	655	G	C5-C4	-6.60	1.33	1.38
32	2	730	G	N7-C5	-6.57	1.35	1.39
32	2	893	A	N9-C4	-6.55	1.33	1.37
32	2	561	C	C4-C5	-6.54	1.37	1.43
32	2	570	G	C5-C4	-6.54	1.33	1.38
32	2	1880	A	N9-C4	-6.53	1.33	1.37
32	2	877	C	C4-C5	-6.52	1.37	1.43
32	2	628	G	N7-C5	-6.52	1.35	1.39
32	2	650	A	N9-C4	-6.51	1.33	1.37
32	2	578	A	N7-C5	-6.51	1.35	1.39
32	2	1168	U	C4-C5	-6.50	1.37	1.43
32	2	1448	A	N9-C4	-6.48	1.33	1.37
32	2	100	A	N9-C8	-6.48	1.32	1.37
32	2	714	A	N9-C4	-6.47	1.33	1.37
32	2	1256	U	C2-N3	-6.47	1.33	1.37
32	2	1573	A	C5-C6	-6.47	1.35	1.41
32	2	873	G	N7-C5	-6.46	1.35	1.39
2	C	60	SER	C-N	-6.41	1.19	1.34
32	2	1443	G	N7-C5	-6.41	1.35	1.39
32	2	115	G	C5-C4	-6.40	1.33	1.38
32	2	1006	A	N9-C4	-6.39	1.34	1.37
32	2	870	G	N7-C5	-6.38	1.35	1.39
32	2	655	G	C6-N1	-6.37	1.35	1.39
32	2	1184	G	N7-C5	-6.36	1.35	1.39
32	2	647	G	N1-C2	-6.36	1.32	1.37
32	2	1295	A	N9-C4	-6.34	1.34	1.37
32	2	714	A	N3-C4	-6.34	1.31	1.34
32	2	894	G	C8-N7	-6.33	1.27	1.30
32	2	624	C	N3-C4	-6.32	1.29	1.33
32	2	657	C	C4-C5	-6.32	1.37	1.43
32	2	108	A	C5-C4	-6.31	1.34	1.38
32	2	109	G	C5-C4	-6.31	1.33	1.38
32	2	30	G	N9-C4	-6.31	1.32	1.38
32	2	873	G	N1-C2	-6.31	1.32	1.37
32	2	1456	G	C5-C4	-6.30	1.33	1.38
32	2	102	U	C4-C5	-6.30	1.37	1.43
32	2	615	A	N9-C4	-6.29	1.34	1.37
32	2	1185	C	C2-N3	-6.29	1.30	1.35
32	2	1191	A	N7-C5	-6.29	1.35	1.39
32	2	1827	C	N1-C6	-6.28	1.33	1.37
32	2	712	C	N3-C4	-6.27	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	647	G	C5-C4	-6.27	1.33	1.38
32	2	568	C	C4-C5	-6.26	1.38	1.43
32	2	659	G	N7-C5	-6.26	1.35	1.39
32	2	724	G	N1-C2	-6.24	1.32	1.37
32	2	1052	A	C5-C4	-6.23	1.34	1.38
32	2	109	G	N7-C5	-6.22	1.35	1.39
32	2	711	C	N3-C4	-6.22	1.29	1.33
32	2	646	G	N7-C5	-6.21	1.35	1.39
32	2	1184	G	C8-N7	-6.20	1.27	1.30
32	2	659	G	C6-N1	-6.19	1.35	1.39
32	2	2	A	N7-C5	-6.19	1.35	1.39
32	2	894	G	C5-C6	-6.18	1.36	1.42
32	2	1443	G	C5-C6	-6.18	1.36	1.42
32	2	656	C	N3-C4	-6.17	1.29	1.33
32	2	1254	G	C5-C4	-6.17	1.34	1.38
32	2	24	U	C2-N3	-6.16	1.33	1.37
32	2	599	G	C5-C4	-6.16	1.34	1.38
32	2	834	G	C5-C4	-6.16	1.34	1.38
32	2	570	G	N1-C2	-6.16	1.32	1.37
32	2	1019	C	N1-C6	-6.15	1.33	1.37
32	2	873	G	C6-N1	-6.15	1.35	1.39
32	2	1184	G	C5-C6	-6.15	1.36	1.42
32	2	99	C	N1-C6	-6.14	1.33	1.37
32	2	23	G	C5-C4	-6.13	1.34	1.38
32	2	108	A	N3-C4	-6.11	1.31	1.34
32	2	644	C	C4-C5	-6.11	1.38	1.43
32	2	875	U	N1-C2	-6.10	1.33	1.38
32	2	720	G	C5-C4	-6.10	1.34	1.38
32	2	1042	A	N7-C5	-6.10	1.35	1.39
32	2	1182	A	C5-C6	-6.09	1.35	1.41
32	2	1618	G	N9-C4	-6.09	1.33	1.38
32	2	1043	G	C5-C4	-6.08	1.34	1.38
32	2	664	A	C5-C4	-6.04	1.34	1.38
32	2	630	A	N7-C5	-6.03	1.35	1.39
32	2	111	U	N3-C4	-6.03	1.33	1.38
32	2	648	A	C5-C4	-6.02	1.34	1.38
32	2	1655	A	N9-C4	6.02	1.41	1.37
32	2	95	G	C5-C4	-6.01	1.34	1.38
32	2	1258	U	C2-N3	-6.00	1.33	1.37
32	2	599	G	N3-C4	-5.99	1.31	1.35
32	2	568	C	N1-C6	-5.99	1.33	1.37
32	2	91	G	N7-C5	-5.98	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	1236	A	C5-C4	-5.97	1.34	1.38
32	2	565	U	C2-N3	-5.97	1.33	1.37
32	2	659	G	C8-N7	-5.96	1.27	1.30
32	2	640	G	N1-C2	-5.96	1.32	1.37
32	2	649	G	N1-C2	-5.96	1.32	1.37
32	2	667	G	C6-N1	-5.96	1.35	1.39
32	2	650	A	N9-C8	-5.95	1.32	1.37
32	2	707	C	C4-C5	-5.95	1.38	1.43
32	2	688	A	N7-C5	-5.93	1.35	1.39
32	2	623	A	N7-C5	-5.92	1.35	1.39
32	2	1053	A	N7-C5	-5.92	1.35	1.39
32	2	615	A	C5-C4	-5.91	1.34	1.38
32	2	722	G	N9-C8	-5.91	1.33	1.37
32	2	735	U	C2-N3	-5.89	1.33	1.37
32	2	870	G	N3-C4	-5.89	1.31	1.35
32	2	621	U	N3-C4	-5.89	1.33	1.38
32	2	597	G	C5-C4	-5.87	1.34	1.38
32	2	1253	G	N7-C5	-5.87	1.35	1.39
32	2	573	C	N1-C6	-5.86	1.33	1.37
32	2	636	G	N9-C4	-5.86	1.33	1.38
32	2	1140	A	N9-C4	-5.85	1.34	1.37
32	2	1163	A	N7-C5	-5.84	1.35	1.39
32	2	790	A	N9-C4	-5.83	1.34	1.37
32	2	873	G	N9-C8	-5.83	1.33	1.37
32	2	580	C	N3-C4	-5.83	1.29	1.33
32	2	47	A	N7-C5	-5.82	1.35	1.39
32	2	653	G	N9-C8	-5.82	1.33	1.37
32	2	866	U	N1-C2	-5.80	1.33	1.38
32	2	685	G	C6-N1	-5.80	1.35	1.39
32	2	1444	G	C5-C4	-5.78	1.34	1.38
32	2	97	C	N3-C4	-5.78	1.29	1.33
32	2	1881	C	N3-C4	-5.77	1.29	1.33
32	2	893	A	N3-C4	-5.76	1.31	1.34
32	2	878	A	N7-C5	-5.76	1.35	1.39
32	2	725	G	N1-C2	-5.76	1.33	1.37
32	2	655	G	N1-C2	-5.76	1.33	1.37
32	2	1016	A	N7-C5	-5.76	1.35	1.39
32	2	95	G	N7-C5	-5.75	1.35	1.39
32	2	1003	A	N9-C4	-5.75	1.34	1.37
32	2	697	G	C5-C4	-5.74	1.34	1.38
32	2	1003	A	C5-C4	-5.74	1.34	1.38
32	2	569	U	C2-N3	-5.74	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	620	G	N7-C5	-5.74	1.35	1.39
32	2	563	A	N9-C4	-5.71	1.34	1.37
32	2	636	G	N7-C5	-5.71	1.35	1.39
32	2	896	U	C2-N3	-5.71	1.33	1.37
32	2	1053	A	N9-C4	-5.70	1.34	1.37
32	2	1258	U	N3-C4	-5.70	1.33	1.38
32	2	564	A	N3-C4	-5.70	1.31	1.34
32	2	706	C	C4-C5	-5.69	1.38	1.43
32	2	20	G	N7-C5	-5.68	1.35	1.39
32	2	657	C	N1-C6	-5.68	1.33	1.37
32	2	885	A	N9-C4	-5.68	1.34	1.37
32	2	1260	G	N7-C5	-5.66	1.35	1.39
32	2	999	A	C6-N1	-5.66	1.31	1.35
32	2	625	G	C6-N1	-5.66	1.35	1.39
32	2	24	U	N1-C2	-5.65	1.33	1.38
32	2	1042	A	C5-C6	-5.65	1.35	1.41
32	2	96	G	C6-N1	-5.65	1.35	1.39
32	2	655	G	N7-C5	-5.64	1.35	1.39
32	2	660	A	C5-C4	-5.64	1.34	1.38
32	2	19	A	N3-C4	-5.64	1.31	1.34
32	2	895	U	C2-N3	-5.64	1.33	1.37
32	2	1050	A	N7-C5	-5.64	1.35	1.39
32	2	698	C	N1-C6	-5.63	1.33	1.37
32	2	20	G	N9-C8	-5.62	1.33	1.37
32	2	1253	G	C5-C4	-5.62	1.34	1.38
32	2	1485	C	N3-C4	-5.61	1.30	1.33
32	2	1824	G	C6-N1	-5.61	1.35	1.39
32	2	581	U	C2-N3	-5.61	1.33	1.37
32	2	664	A	N7-C5	-5.60	1.35	1.39
32	2	1260	G	C6-N1	-5.59	1.35	1.39
32	2	898	A	N9-C4	-5.59	1.34	1.37
32	2	614	C	N1-C6	-5.58	1.33	1.37
32	2	1007	G	C6-N1	-5.58	1.35	1.39
32	2	655	G	N9-C8	-5.58	1.33	1.37
32	2	1255	U	N3-C4	-5.57	1.33	1.38
32	2	1168	U	C3'-O3'	5.56	1.50	1.42
32	2	1449	G	C5-C4	-5.56	1.34	1.38
32	2	1488	A	N9-C4	-5.56	1.34	1.37
32	2	649	G	C8-N7	-5.56	1.27	1.30
32	2	713	U	N1-C2	-5.56	1.33	1.38
32	2	669	U	C2-N3	-5.55	1.33	1.37
32	2	1043	G	N1-C2	-5.55	1.33	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	866	U	C2-N3	-5.55	1.33	1.37
32	2	90	C	N1-C6	-5.54	1.33	1.37
32	2	651	G	C8-N7	-5.54	1.27	1.30
32	2	660	A	N7-C5	-5.54	1.35	1.39
32	2	617	C	C4-C5	-5.53	1.38	1.43
32	2	38	C	N3-C4	-5.52	1.30	1.33
32	2	898	A	N7-C5	-5.52	1.35	1.39
32	2	624	C	N1-C2	-5.51	1.34	1.40
32	2	627	G	N3-C4	-5.51	1.31	1.35
32	2	725	G	C6-N1	-5.51	1.35	1.39
32	2	732	C	N1-C6	-5.51	1.33	1.37
32	2	615	A	N7-C5	-5.50	1.35	1.39
32	2	1568	G	N7-C5	-5.50	1.35	1.39
32	2	637	U	C4-C5	-5.48	1.38	1.43
32	2	668	C	N3-C4	-5.47	1.30	1.33
32	2	631	U	C2-N3	-5.47	1.33	1.37
32	2	646	G	N9-C8	-5.47	1.34	1.37
32	2	885	A	C5-C6	-5.47	1.36	1.41
32	2	115	G	N9-C8	-5.47	1.34	1.37
32	2	1251	U	C2-N3	-5.47	1.33	1.37
32	2	1257	C	C4-C5	-5.46	1.38	1.43
32	2	854	A	N9-C4	-5.46	1.34	1.37
32	2	897	G	N1-C2	-5.45	1.33	1.37
32	2	1037	A	N7-C5	-5.44	1.35	1.39
32	2	1168	U	O3'-P	5.43	1.67	1.61
32	2	99	C	C2-N3	-5.43	1.31	1.35
32	2	700	A	C6-N1	-5.43	1.31	1.35
32	2	1280	A	N9-C4	-5.43	1.34	1.37
32	2	862	A	N7-C5	-5.42	1.35	1.39
32	2	699	A	N7-C5	-5.42	1.35	1.39
32	2	656	C	N1-C6	-5.42	1.33	1.37
32	2	720	G	N1-C2	-5.42	1.33	1.37
32	2	997	G	C2-N3	-5.42	1.28	1.32
32	2	108	A	C6-N1	-5.42	1.31	1.35
32	2	92	A	N7-C5	-5.41	1.36	1.39
32	2	1042	A	C5-C4	-5.41	1.34	1.38
32	2	613	U	C2-N3	-5.40	1.33	1.37
32	2	644	C	C2-N3	-5.40	1.31	1.35
32	2	721	G	N1-C2	-5.40	1.33	1.37
32	2	662	A	N9-C8	-5.40	1.33	1.37
32	2	63	G	C6-N1	-5.40	1.35	1.39
32	2	560	U	C4-C5	-5.40	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	602	C	N3-C4	-5.40	1.30	1.33
32	2	57	G	N7-C5	-5.40	1.36	1.39
32	2	43	A	N9-C4	-5.39	1.34	1.37
32	2	111	U	C2-N3	-5.39	1.33	1.37
32	2	588	G	N9-C8	-5.39	1.34	1.37
32	2	630	A	C5-C4	-5.39	1.34	1.38
32	2	721	G	C6-N1	-5.38	1.35	1.39
32	2	662	A	N7-C5	-5.38	1.36	1.39
32	2	890	C	N3-C4	-5.38	1.30	1.33
32	2	1572	C	N1-C6	-5.38	1.33	1.37
32	2	876	G	C8-N7	-5.38	1.27	1.30
32	2	41	A	C5-C4	-5.37	1.34	1.38
32	2	789	A	N9-C4	-5.37	1.34	1.37
32	2	835	C	C4-C5	-5.36	1.38	1.43
32	2	662	A	C5-C4	-5.36	1.34	1.38
32	2	650	A	C8-N7	-5.36	1.27	1.31
32	2	667	G	N1-C2	-5.36	1.33	1.37
32	2	1260	G	N9-C8	-5.36	1.34	1.37
32	2	894	G	C6-O6	-5.35	1.19	1.24
32	2	640	G	C6-N1	-5.35	1.35	1.39
32	2	627	G	N9-C8	-5.34	1.34	1.37
32	2	36	C	N1-C6	-5.34	1.33	1.37
32	2	113	U	N1-C2	-5.34	1.33	1.38
32	2	570	G	C6-N1	-5.34	1.35	1.39
32	2	885	A	N3-C4	-5.34	1.31	1.34
32	2	1258	U	C4-C5	-5.34	1.38	1.43
32	2	636	G	C5-C4	-5.33	1.34	1.38
32	2	894	G	N1-C2	-5.33	1.33	1.37
32	2	1247	U	N1-C2	-5.33	1.33	1.38
32	2	633	A	N7-C5	-5.32	1.36	1.39
32	2	93	A	N7-C5	-5.32	1.36	1.39
32	2	618	G	N7-C5	-5.31	1.36	1.39
32	2	654	A	C5-C4	-5.30	1.35	1.38
32	2	23	G	N9-C8	-5.30	1.34	1.37
32	2	556	U	C2-N3	-5.30	1.34	1.37
32	2	1008	A	N9-C4	-5.30	1.34	1.37
32	2	1009	G	C5-C4	-5.29	1.34	1.38
32	2	653	G	N7-C5	-5.29	1.36	1.39
32	2	580	C	N1-C6	-5.28	1.33	1.37
32	2	838	C	C2-N3	-5.28	1.31	1.35
32	2	867	A	C5-C4	-5.27	1.35	1.38
32	2	688	A	C6-N6	-5.27	1.29	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	647	G	N3-C4	-5.27	1.31	1.35
32	2	715	A	N7-C5	-5.27	1.36	1.39
32	2	571	C	C2-N3	-5.26	1.31	1.35
32	2	599	G	N9-C8	-5.26	1.34	1.37
32	2	601	C	N3-C4	-5.26	1.30	1.33
32	2	624	C	C2-N3	-5.26	1.31	1.35
32	2	1005	U	C2-N3	-5.26	1.34	1.37
32	2	629	A	C5-C4	-5.25	1.35	1.38
32	2	1182	A	C5-C4	-5.25	1.35	1.38
32	2	854	A	N3-C4	-5.25	1.31	1.34
32	2	665	C	N1-C6	-5.25	1.34	1.37
32	2	867	A	N9-C8	-5.24	1.33	1.37
32	2	601	C	N1-C6	-5.23	1.34	1.37
32	2	1043	G	C6-N1	-5.23	1.35	1.39
32	2	1455	U	C2-N3	-5.23	1.34	1.37
32	2	725	G	C8-N7	-5.23	1.27	1.30
32	2	28	A	N9-C4	-5.22	1.34	1.37
32	2	585	G	N7-C5	-5.22	1.36	1.39
32	2	654	A	N9-C8	-5.21	1.33	1.37
32	2	1045	A	C5-C4	-5.21	1.35	1.38
32	2	1244	A	N7-C5	-5.21	1.36	1.39
32	2	95	G	C6-N1	-5.21	1.35	1.39
32	2	1112	G	C6-N1	-5.21	1.35	1.39
32	2	1427	A	N9-C4	5.21	1.41	1.37
32	2	720	G	N9-C8	-5.21	1.34	1.37
32	2	27	U	C2-N3	-5.20	1.34	1.37
32	2	722	G	C6-N1	-5.20	1.35	1.39
32	2	1015	A	N9-C4	-5.20	1.34	1.37
32	2	628	G	C8-N7	-5.20	1.27	1.30
32	2	649	G	N9-C8	-5.20	1.34	1.37
32	2	1448	A	C5-C4	-5.20	1.35	1.38
32	2	61	A	N7-C5	-5.19	1.36	1.39
32	2	423	C	C4-C5	-5.19	1.38	1.43
32	2	871	U	C2-N3	-5.19	1.34	1.37
32	2	644	C	N1-C2	-5.18	1.34	1.40
32	2	574	U	N1-C2	-5.18	1.33	1.38
32	2	889	U	C4-C5	-5.18	1.38	1.43
32	2	103	A	C6-N1	-5.18	1.31	1.35
32	2	103	A	N7-C5	-5.17	1.36	1.39
32	2	597	G	N3-C4	-5.17	1.31	1.35
32	2	645	C	N1-C2	-5.17	1.34	1.40
32	2	21	U	C2-N3	-5.17	1.34	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	53	G	C5-C4	-5.17	1.34	1.38
32	2	724	G	N9-C8	-5.17	1.34	1.37
32	2	868	A	C5-C4	-5.17	1.35	1.38
32	2	1053	A	C5-C6	-5.16	1.36	1.41
32	2	20	G	C8-N7	-5.16	1.27	1.30
32	2	115	G	N1-C2	-5.16	1.33	1.37
32	2	898	A	N3-C4	-5.16	1.31	1.34
32	2	651	G	C2-N3	-5.16	1.28	1.32
32	2	1450	U	C2-N3	-5.16	1.34	1.37
32	2	710	U	N1-C2	-5.16	1.33	1.38
32	2	993	C	N3-C4	-5.15	1.30	1.33
32	2	1006	A	N7-C5	-5.15	1.36	1.39
32	2	1044	C	N1-C6	-5.15	1.34	1.37
32	2	1295	A	C5-C4	-5.15	1.35	1.38
32	2	609	G	N7-C5	-5.14	1.36	1.39
32	2	1260	G	N1-C2	-5.14	1.33	1.37
32	2	90	C	C2-N3	-5.14	1.31	1.35
32	2	664	A	N9-C4	-5.14	1.34	1.37
32	2	638	U	C2-N3	-5.14	1.34	1.37
32	2	1155	A	N9-C4	-5.14	1.34	1.37
32	2	95	G	N1-C2	-5.13	1.33	1.37
32	2	567	U	C2-N3	-5.13	1.34	1.37
32	2	110	U	C2-N3	-5.13	1.34	1.37
32	2	1189	C	N3-C4	-5.13	1.30	1.33
32	2	573	C	C4-C5	-5.12	1.38	1.43
32	2	697	G	N3-C4	-5.12	1.31	1.35
32	2	876	G	N9-C8	-5.12	1.34	1.37
32	2	41	A	N7-C5	-5.11	1.36	1.39
32	2	571	C	N1-C6	-5.11	1.34	1.37
32	2	593	G	C6-N1	-5.11	1.35	1.39
32	2	1294	A	C5-C4	-5.11	1.35	1.38
32	2	878	A	C6-N1	-5.11	1.31	1.35
32	2	1259	G	N7-C5	-5.11	1.36	1.39
32	2	721	G	C5-C4	-5.11	1.34	1.38
32	2	1165	U	C4-C5	-5.11	1.39	1.43
32	2	1003	A	C5-C6	-5.10	1.36	1.41
32	2	1448	A	N3-C4	-5.09	1.31	1.34
32	2	106	U	C4-C5	-5.09	1.39	1.43
32	2	597	G	N7-C5	-5.09	1.36	1.39
32	2	1243	A	N9-C4	-5.09	1.34	1.37
32	2	629	A	C6-N1	-5.08	1.31	1.35
32	2	710	U	C4-C5	-5.08	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	645	C	C4-C5	-5.07	1.38	1.43
32	2	1020	A	N9-C4	-5.07	1.34	1.37
32	2	891	G	N9-C8	-5.07	1.34	1.37
32	2	1294	A	N9-C4	-5.07	1.34	1.37
32	2	1433	G	N9-C4	-5.07	1.33	1.38
32	2	667	G	N7-C5	-5.07	1.36	1.39
32	2	569	U	N1-C2	-5.06	1.33	1.38
32	2	110	U	C4-C5	-5.06	1.39	1.43
32	2	562	A	C5-C6	-5.06	1.36	1.41
32	2	870	G	C6-N1	-5.06	1.36	1.39
32	2	714	A	C5-C4	-5.05	1.35	1.38
32	2	1586	U	C4-O4	-5.05	1.19	1.23
32	2	651	G	C5-C4	-5.05	1.34	1.38
32	2	96	G	C2-N3	-5.05	1.28	1.32
32	2	707	C	N3-C4	-5.05	1.30	1.33
32	2	858	G	N9-C8	-5.05	1.34	1.37
32	2	567	U	C4-C5	-5.05	1.39	1.43
32	2	1294	A	N7-C5	-5.05	1.36	1.39
32	2	1048	G	C6-N1	-5.04	1.36	1.39
32	2	700	A	N9-C4	-5.04	1.34	1.37
32	2	646	G	C5-C6	-5.03	1.37	1.42
32	2	510	A	C5-C4	-5.03	1.35	1.38
32	2	1137	C	N1-C6	-5.03	1.34	1.37
32	2	573	C	N1-C2	-5.03	1.35	1.40
32	2	627	G	C8-N7	-5.03	1.27	1.30
32	2	1042	A	C6-N1	-5.02	1.32	1.35
32	2	558	A	C5-C4	-5.02	1.35	1.38
32	2	723	A	N9-C8	-5.02	1.33	1.37
32	2	725	G	N9-C8	-5.01	1.34	1.37
32	2	724	G	C8-N7	-5.01	1.27	1.30
32	2	1483	A	N3-C4	-5.01	1.31	1.34
32	2	601	C	N1-C2	-5.01	1.35	1.40
32	2	109	G	C8-N7	-5.01	1.27	1.30
32	2	18	C	N1-C6	-5.00	1.34	1.37

All (745) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1168	U	C5-C6-N1	15.46	130.43	122.70
32	2	892	U	C6-N1-C2	-14.21	112.48	121.00
32	2	1168	U	OP1-P-OP2	-13.91	98.73	119.60
32	2	97	C	C6-N1-C2	-13.89	114.75	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1731	U	C2-N1-C1'	13.25	133.60	117.70
32	2	1168	U	O5'-P-OP2	12.82	126.09	110.70
32	2	1733	C	C6-N1-C2	-12.75	115.20	120.30
32	2	1437	U	C2-N1-C1'	12.72	132.96	117.70
32	2	423	C	C6-N1-C2	-12.66	115.24	120.30
32	2	716	U	C2-N1-C1'	12.45	132.64	117.70
32	2	1159	U	N3-C2-O2	-12.39	113.53	122.20
32	2	144	U	N3-C2-O2	-12.22	113.64	122.20
32	2	1731	U	N1-C2-O2	12.18	131.32	122.80
32	2	1437	U	N1-C2-O2	12.16	131.32	122.80
32	2	832	C	N1-C2-O2	12.15	126.19	118.90
32	2	716	U	N1-C2-O2	12.03	131.22	122.80
32	2	836	C	O5'-P-OP1	-11.66	95.21	105.70
32	2	716	U	N3-C2-O2	-11.49	114.16	122.20
32	2	1168	U	C6-N1-C2	-11.35	114.19	121.00
32	2	1437	U	N3-C2-O2	-11.29	114.30	122.20
32	2	1204	U	N1-C2-O2	11.29	130.70	122.80
32	2	1583	C	N1-C2-O2	11.22	125.63	118.90
32	2	1427	A	C2-N3-C4	11.14	116.17	110.60
32	2	1159	U	N1-C2-O2	11.05	130.53	122.80
32	2	1184	G	N1-C6-O6	11.02	126.51	119.90
32	2	693	G	N3-C4-C5	-10.98	123.11	128.60
32	2	832	C	C2-N1-C1'	10.89	130.77	118.80
32	2	1731	U	N3-C2-O2	-10.72	114.69	122.20
32	2	693	G	C2-N3-C4	10.72	117.26	111.90
32	2	1040	U	N3-C2-O2	-10.69	114.72	122.20
32	2	1443	G	C4-C5-N7	10.58	115.03	110.80
32	2	1204	U	C2-N1-C1'	10.54	130.35	117.70
32	2	1168	U	C2-N1-C1'	10.50	130.30	117.70
32	2	836	C	C6-N1-C2	-10.41	116.14	120.30
32	2	890	C	N1-C2-O2	10.32	125.09	118.90
32	2	873	G	C4-N9-C1'	10.25	139.82	126.50
32	2	1184	G	C5-C6-O6	-10.12	122.53	128.60
32	2	1443	G	C6-C5-N7	-9.99	124.41	130.40
32	2	1165	U	C5-C6-N1	9.96	127.68	122.70
32	2	890	C	N3-C2-O2	-9.96	114.93	121.90
32	2	1426	C	C6-N1-C2	-9.95	116.32	120.30
32	2	144	U	N1-C2-O2	9.91	129.74	122.80
32	2	1783	A	C5-C6-N6	-9.81	115.85	123.70
32	2	873	G	C8-N9-C1'	-9.57	114.56	127.00
32	2	890	C	C6-N1-C2	-9.57	116.47	120.30
32	2	1578	C	C5-C6-N1	9.56	125.78	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1618	G	N3-C4-C5	9.56	133.38	128.60
32	2	1204	U	N3-C2-O2	-9.49	115.55	122.20
32	2	892	U	N1-C2-N3	9.46	120.58	114.90
32	2	97	C	C5-C6-N1	9.41	125.71	121.00
32	2	1056	G	N3-C4-C5	9.38	133.29	128.60
32	2	423	C	C5-C6-N1	9.37	125.69	121.00
32	2	1615	C	C2-N1-C1'	9.36	129.09	118.80
32	2	101	U	N3-C2-O2	-9.34	115.66	122.20
32	2	892	U	N3-C4-C5	-9.34	108.99	114.60
32	2	1426	C	N1-C2-O2	9.32	124.49	118.90
32	2	1110	U	N3-C2-O2	-9.30	115.69	122.20
32	2	1166	A	O4'-C1'-N9	9.30	115.64	108.20
32	2	835	C	C5-C6-N1	9.28	125.64	121.00
32	2	1731	U	C6-N1-C1'	-9.25	108.25	121.20
32	2	846	C	N1-C2-O2	9.24	124.45	118.90
32	2	539	C	N1-C2-O2	9.23	124.44	118.90
32	2	1426	C	N3-C2-O2	-9.18	115.47	121.90
32	2	716	U	C6-N1-C1'	-9.15	108.39	121.20
32	2	1603	C	N1-C2-O2	9.10	124.36	118.90
32	2	1618	G	C4-N9-C1'	-9.05	114.74	126.50
32	2	1576	A	C2-N3-C4	8.98	115.09	110.60
32	2	671	C	C6-N1-C2	-8.96	116.72	120.30
32	2	1159	U	C2-N1-C1'	8.95	128.43	117.70
32	2	1184	G	C6-C5-N7	-8.93	125.04	130.40
32	2	1583	C	N3-C2-O2	-8.93	115.65	121.90
32	2	858	G	N3-C4-N9	8.90	131.34	126.00
32	2	641	A	C8-N9-C4	-8.89	102.24	105.80
32	2	1030	C	N1-C2-O2	8.87	124.22	118.90
32	2	1110	U	C2-N1-C1'	8.85	128.32	117.70
22	X	93	LEU	CA-CB-CG	8.84	135.63	115.30
32	2	892	U	O4'-C1'-N1	8.79	115.23	108.20
32	2	693	G	N3-C4-N9	8.78	131.27	126.00
32	2	846	C	C6-N1-C2	-8.74	116.80	120.30
32	2	838	C	N3-C4-C5	8.70	125.38	121.90
32	2	17	C	C6-N1-C2	-8.65	116.84	120.30
32	2	832	C	N3-C2-O2	-8.65	115.84	121.90
32	2	1169	C	O5'-P-OP2	-8.64	97.92	105.70
32	2	1184	G	C4-C5-N7	8.62	114.25	110.80
32	2	1185	C	C6-N1-C2	-8.61	116.86	120.30
32	2	1615	C	N1-C2-O2	8.59	124.06	118.90
32	2	846	C	C2-N1-C1'	8.58	128.24	118.80
32	2	641	A	C2-N3-C4	8.48	114.84	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	890	C	C2-N1-C1'	8.47	128.12	118.80
32	2	1783	A	N1-C6-N6	8.45	123.67	118.60
32	2	832	C	C6-N1-C1'	-8.45	110.66	120.80
32	2	1180	C	C2-N1-C1'	8.45	128.09	118.80
32	2	1185	C	N3-C2-O2	-8.44	115.99	121.90
32	2	572	C	C6-N1-C2	-8.41	116.94	120.30
32	2	100	A	C2-N3-C4	8.41	114.80	110.60
32	2	144	U	C2-N1-C1'	8.40	127.78	117.70
32	2	835	C	C6-N1-C2	-8.39	116.94	120.30
32	2	780	U	N3-C2-O2	-8.37	116.34	122.20
32	2	671	C	C5-C6-N1	8.36	125.18	121.00
32	2	1289	A	N7-C8-N9	8.32	117.96	113.80
32	2	1309	A	C8-N9-C4	-8.31	102.47	105.80
32	2	1182	A	N9-C4-C5	-8.31	102.48	105.80
32	2	627	G	N1-C6-O6	-8.29	114.92	119.90
32	2	1040	U	N1-C2-O2	8.29	128.60	122.80
32	2	1443	G	C5-N7-C8	-8.29	100.16	104.30
32	2	858	G	N3-C4-C5	-8.25	124.47	128.60
32	2	1312	A	C8-N9-C4	-8.25	102.50	105.80
32	2	1616	G	C4-N9-C1'	8.23	137.20	126.50
32	2	1168	U	P-O3'-C3'	8.21	129.56	119.70
32	2	1573	A	O4'-C1'-N9	8.18	114.75	108.20
32	2	1437	U	C6-N1-C1'	-8.18	109.75	121.20
32	2	836	C	C5-C6-N1	8.16	125.08	121.00
32	2	1604	U	N1-C2-O2	8.14	128.50	122.80
32	2	1409	U	N3-C2-O2	-8.13	116.51	122.20
32	2	846	C	C5-C6-N1	8.06	125.03	121.00
32	2	117	U	C5-C6-N1	8.04	126.72	122.70
32	2	1013	U	C2-N1-C1'	8.01	127.32	117.70
32	2	693	G	C5-C6-N1	8.01	115.50	111.50
32	2	1595	U	C2-N1-C1'	8.00	127.31	117.70
32	2	639	C	N1-C2-O2	7.99	123.70	118.90
32	2	857	A	C5-C6-N1	7.99	121.69	117.70
32	2	1641	U	N3-C2-O2	-7.97	116.62	122.20
32	2	873	G	N3-C4-N9	7.97	130.78	126.00
32	2	857	A	C2-N3-C4	7.92	114.56	110.60
32	2	1578	C	C4-C5-C6	-7.91	113.44	117.40
32	2	1040	U	C2-N1-C1'	7.90	127.19	117.70
32	2	1606	G	N7-C8-N9	7.86	117.03	113.10
32	2	693	G	C4-N9-C1'	7.86	136.72	126.50
32	2	780	U	N1-C2-O2	7.86	128.30	122.80
32	2	17	C	C5-C6-N1	7.84	124.92	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1618	G	C8-N9-C1'	7.82	137.16	127.00
32	2	1040	U	C6-N1-C2	-7.81	116.31	121.00
32	2	1541	C	N1-C2-O2	7.80	123.58	118.90
32	2	1110	U	N1-C2-O2	7.79	128.25	122.80
32	2	14	C	C6-N1-C2	-7.76	117.20	120.30
32	2	1731	U	C5-C6-N1	7.72	126.56	122.70
32	2	1185	C	N1-C2-N3	7.71	124.60	119.20
32	2	1257	C	C5-C6-N1	7.70	124.85	121.00
32	2	892	U	C6-N1-C1'	7.69	131.97	121.20
32	2	1302	G	N3-C4-N9	7.69	130.61	126.00
32	2	877	C	C5-C6-N1	7.67	124.83	121.00
32	2	54	C	N3-C2-O2	-7.66	116.54	121.90
32	2	1581	G	C6-C5-N7	-7.64	125.81	130.40
32	2	1589	U	O4'-C1'-N1	7.62	114.30	108.20
32	2	641	A	C5-C6-N1	7.61	121.51	117.70
32	2	841	U	C5-C6-N1	7.61	126.50	122.70
32	2	14	C	C5-C6-N1	7.60	124.80	121.00
32	2	1742	G	N3-C4-C5	-7.58	124.81	128.60
32	2	824	G	N3-C4-C5	-7.57	124.81	128.60
32	2	1606	G	C8-N9-C4	-7.57	103.37	106.40
32	2	943	C	O4'-C1'-N1	7.55	114.24	108.20
32	2	1476	G	C4-C5-N7	7.54	113.82	110.80
32	2	1692	G	C4-N9-C1'	7.52	136.27	126.50
32	2	824	G	C4-N9-C1'	7.51	136.26	126.50
32	2	1409	U	C2-N1-C1'	7.50	126.70	117.70
3	D	96	LEU	CA-CB-CG	7.50	132.54	115.30
32	2	1692	G	N3-C4-N9	7.48	130.49	126.00
32	2	1655	A	C2-N3-C4	7.48	114.34	110.60
32	2	1692	G	N3-C4-C5	-7.47	124.86	128.60
32	2	846	C	N3-C2-O2	-7.46	116.68	121.90
32	2	724	G	N1-C6-O6	-7.45	115.43	119.90
32	2	61	A	C5-N7-C8	-7.43	100.19	103.90
32	2	1204	U	C6-N1-C1'	-7.41	110.82	121.20
32	2	100	A	C5-C6-N1	7.41	121.41	117.70
32	2	539	C	N3-C2-O2	-7.41	116.71	121.90
32	2	1605	G	O4'-C1'-N9	7.41	114.12	108.20
32	2	1773	U	C5-C6-N1	7.40	126.40	122.70
32	2	1351	G	C4-N9-C1'	7.39	136.11	126.50
32	2	1742	G	N3-C4-N9	7.36	130.42	126.00
32	2	892	U	C5-C6-N1	7.35	126.38	122.70
3	D	113	LEU	CA-CB-CG	7.35	132.21	115.30
32	2	101	U	N1-C2-O2	7.33	127.93	122.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1583	C	C2-N1-C1'	7.33	126.86	118.80
32	2	1639	A	O4'-C1'-N9	7.33	114.06	108.20
32	2	672	C	C6-N1-C2	-7.32	117.37	120.30
32	2	1218	C	N3-C2-O2	-7.29	116.80	121.90
32	2	873	G	C6-C5-N7	-7.29	126.03	130.40
32	2	1734	U	C6-N1-C2	7.27	125.36	121.00
32	2	1615	C	C6-N1-C2	-7.25	117.40	120.30
32	2	857	A	N1-C2-N3	-7.25	125.68	129.30
32	2	1581	G	C5-C6-O6	-7.24	124.25	128.60
32	2	1438	U	C2-N1-C1'	7.22	126.37	117.70
32	2	1257	C	C6-N1-C2	-7.20	117.42	120.30
32	2	1289	A	O4'-C1'-N9	7.19	113.95	108.20
32	2	1595	U	N1-C2-O2	7.19	127.83	122.80
32	2	940	U	N3-C2-O2	-7.18	117.17	122.20
32	2	1638	G	C4-N9-C1'	7.17	135.83	126.50
32	2	101	U	C2-N1-C1'	7.14	126.27	117.70
32	2	1289	A	C8-N9-C4	-7.13	102.95	105.80
32	2	1185	C	O5'-P-OP1	-7.12	99.29	105.70
32	2	54	C	N1-C2-O2	7.11	123.17	118.90
32	2	1181	U	P-O3'-C3'	7.11	128.23	119.70
32	2	880	U	C5-C6-N1	7.09	126.25	122.70
32	2	568	C	C6-N1-C2	-7.07	117.47	120.30
32	2	1185	C	C5-C4-N4	7.04	125.13	120.20
32	2	110	U	C5-C6-N1	7.03	126.22	122.70
32	2	1541	C	C2-N1-C1'	7.03	126.53	118.80
32	2	1615	C	C5-C6-N1	7.03	124.52	121.00
32	2	1643	U	P-O3'-C3'	7.03	128.14	119.70
32	2	1616	G	N3-C4-C5	-7.02	125.09	128.60
32	2	1427	A	C5-C6-N1	7.02	121.21	117.70
32	2	1289	A	C5-N7-C8	-7.00	100.40	103.90
32	2	1437	U	C5-C6-N1	7.00	126.20	122.70
32	2	49	C	N1-C2-O2	6.99	123.10	118.90
32	2	1000	A	O5'-P-OP2	-6.99	99.41	105.70
32	2	641	A	N7-C8-N9	6.98	117.29	113.80
32	2	31	C	C6-N1-C2	-6.98	117.51	120.30
32	2	894	G	C5-N7-C8	-6.97	100.81	104.30
32	2	1603	C	C2-N1-C1'	6.96	126.46	118.80
32	2	1027	U	N3-C2-O2	-6.96	117.33	122.20
32	2	1039	A	O4'-C1'-N9	6.93	113.74	108.20
32	2	1545	C	N1-C2-O2	6.92	123.05	118.90
32	2	1604	U	C2-N1-C1'	6.92	126.00	117.70
32	2	1438	U	O4'-C1'-N1	6.90	113.72	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1289	A	C6-C5-N7	-6.89	127.47	132.30
32	2	1742	G	C2-N3-C4	6.89	115.34	111.90
32	2	891	G	N1-C2-N2	-6.89	110.00	116.20
32	2	1618	G	N3-C4-N9	-6.89	121.87	126.00
32	2	1783	A	N9-C4-C5	-6.88	103.05	105.80
32	2	712	C	C6-N1-C2	-6.87	117.55	120.30
32	2	1218	C	N1-C2-O2	6.87	123.02	118.90
32	2	1541	C	N3-C2-O2	-6.86	117.09	121.90
32	2	730	G	C8-N9-C4	-6.86	103.66	106.40
32	2	110	U	C6-N1-C2	-6.84	116.90	121.00
32	2	1641	U	C2-N1-C1'	6.83	125.89	117.70
32	2	867	A	N1-C6-N6	-6.82	114.51	118.60
32	2	1441	U	C5-C6-N1	6.81	126.11	122.70
32	2	631	U	N3-C2-O2	-6.81	117.44	122.20
32	2	1360	A	C4-N9-C1'	6.81	138.55	126.30
32	2	1734	U	N1-C2-O2	6.80	127.56	122.80
32	2	1485	C	N1-C2-O2	6.80	122.98	118.90
32	2	1580	G	C4-N9-C1'	6.80	135.34	126.50
32	2	891	G	C4-N9-C1'	6.80	135.33	126.50
32	2	1185	C	N3-C4-N4	-6.79	113.25	118.00
32	2	1027	U	C5-C6-N1	6.78	126.09	122.70
32	2	1758	C	C5-C6-N1	6.78	124.39	121.00
32	2	1758	C	C6-N1-C2	-6.78	117.59	120.30
32	2	858	G	C5-C6-N1	6.78	114.89	111.50
32	2	1566	U	N3-C2-O2	-6.78	117.45	122.20
32	2	1604	U	N3-C2-O2	-6.77	117.46	122.20
32	2	1427	A	N1-C6-N6	-6.76	114.55	118.60
32	2	1243	A	C5-N7-C8	-6.75	100.52	103.90
32	2	1409	U	N1-C2-O2	6.74	127.52	122.80
32	2	1463	U	N3-C2-O2	-6.73	117.49	122.20
32	2	855	A	N1-C6-N6	-6.72	114.57	118.60
32	2	1615	C	N3-C2-O2	-6.72	117.20	121.90
32	2	1182	A	N1-C6-N6	6.71	122.63	118.60
32	2	1030	C	N3-C2-O2	-6.70	117.21	121.90
32	2	1576	A	C5-C6-N1	6.69	121.05	117.70
32	2	1056	G	N3-C4-N9	-6.67	122.00	126.00
32	2	1476	G	C6-C5-N7	-6.67	126.40	130.40
32	2	1453	U	N1-C2-O2	6.67	127.47	122.80
32	2	693	G	C8-N9-C4	-6.65	103.74	106.40
32	2	1482	G	C8-N9-C4	-6.64	103.74	106.40
32	2	1641	U	N1-C2-O2	6.64	127.45	122.80
32	2	1182	A	N1-C2-N3	-6.64	125.98	129.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1302	G	N3-C4-C5	-6.63	125.28	128.60
32	2	1581	G	C4-C5-N7	6.62	113.45	110.80
32	2	18	C	C5-C6-N1	6.62	124.31	121.00
32	2	1027	U	N1-C2-O2	6.62	127.43	122.80
32	2	1182	A	C4-C5-N7	6.61	114.01	110.70
32	2	1580	G	N7-C8-N9	6.59	116.39	113.10
32	2	1180	C	N1-C2-O2	6.59	122.85	118.90
32	2	1184	G	N9-C4-C5	-6.58	102.77	105.40
32	2	839	G	C8-N9-C4	-6.58	103.77	106.40
32	2	1891	C	N3-C2-O2	-6.58	117.30	121.90
32	2	824	G	N3-C4-N9	6.57	129.94	126.00
32	2	1056	G	C4-N9-C1'	-6.56	117.97	126.50
32	2	1302	G	C4-N9-C1'	6.56	135.03	126.50
32	2	144	U	C6-N1-C2	-6.53	117.08	121.00
32	2	87	C	N1-C2-O2	6.53	122.82	118.90
32	2	639	C	N3-C2-O2	-6.52	117.33	121.90
32	2	1110	U	C6-N1-C1'	-6.52	112.07	121.20
32	2	1013	U	C6-N1-C1'	-6.51	112.08	121.20
32	2	688	A	C5-C6-N1	6.51	120.95	117.70
32	2	873	G	C4-C5-N7	6.50	113.40	110.80
32	2	1690	U	N1-C2-O2	6.50	127.35	122.80
32	2	102	U	C5-C6-N1	6.50	125.95	122.70
32	2	1445	U	N3-C2-O2	-6.49	117.65	122.20
32	2	670	A	C5-C6-N1	6.49	120.94	117.70
32	2	894	G	C4-C5-N7	6.49	113.39	110.80
32	2	835	C	OP2-P-O3'	6.48	119.46	105.20
32	2	1748	C	N1-C2-O2	6.48	122.79	118.90
32	2	1595	U	C5-C6-N1	6.47	125.94	122.70
32	2	1835	C	N3-C2-O2	-6.47	117.37	121.90
32	2	1168	U	P-O5'-C5'	6.47	131.25	120.90
32	2	1485	C	N3-C2-O2	-6.46	117.38	121.90
32	2	43	A	C4-C5-C6	-6.46	113.77	117.00
32	2	835	C	P-O3'-C3'	-6.45	111.95	119.70
32	2	105	A	N1-C6-N6	-6.45	114.73	118.60
32	2	48	G	C6-C5-N7	-6.44	126.53	130.40
32	2	561	C	C5-C6-N1	6.44	124.22	121.00
32	2	552	U	N1-C2-O2	6.44	127.31	122.80
32	2	552	U	N3-C2-O2	-6.44	117.69	122.20
32	2	601	C	C6-N1-C2	-6.43	117.73	120.30
32	2	1023	C	N3-C2-O2	-6.43	117.40	121.90
32	2	1168	U	N3-C4-O4	6.43	123.90	119.40
32	2	1385	G	O4'-C1'-N9	6.43	113.34	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1638	G	C8-N9-C1'	-6.43	118.65	127.00
32	2	1182	A	C5-C6-N6	-6.42	118.56	123.70
32	2	894	G	N7-C8-N9	6.42	116.31	113.10
32	2	61	A	C4-C5-N7	6.42	113.91	110.70
32	2	1476	G	C5-N7-C8	-6.41	101.09	104.30
32	2	881	U	O5'-P-OP1	-6.41	99.94	105.70
25	b	36	LYS	C-N-CA	6.40	137.71	121.70
32	2	892	U	C5-C4-O4	6.40	129.74	125.90
32	2	1357	C	N3-C2-O2	-6.39	117.43	121.90
32	2	18	C	C6-N1-C2	-6.38	117.75	120.30
32	2	1401	U	C5-C6-N1	6.37	125.89	122.70
32	2	1605	G	C4-N9-C1'	6.36	134.77	126.50
32	2	1289	A	C4-C5-N7	6.35	113.88	110.70
32	2	1426	C	C5-C6-N1	6.35	124.17	121.00
32	2	423	C	C6-N1-C1'	6.35	128.42	120.80
32	2	1013	U	N1-C2-O2	6.34	127.24	122.80
32	2	1573	A	N1-C6-N6	6.34	122.40	118.60
32	2	836	C	OP1-P-OP2	6.34	129.10	119.60
32	2	1595	U	N3-C2-O2	-6.33	117.77	122.20
32	2	1783	A	N3-C4-N9	6.33	132.46	127.40
32	2	565	U	N3-C2-O2	-6.32	117.77	122.20
32	2	858	G	C2-N3-C4	6.32	115.06	111.90
32	2	1620	U	N3-C2-O2	-6.32	117.78	122.20
32	2	872	U	O5'-P-OP2	-6.31	100.02	105.70
32	2	901	U	N1-C2-O2	6.30	127.21	122.80
32	2	649	G	C8-N9-C4	-6.29	103.88	106.40
32	2	1891	C	N1-C2-O2	6.29	122.68	118.90
32	2	1137	C	N3-C2-O2	-6.29	117.50	121.90
32	2	1616	G	C8-N9-C1'	-6.29	118.83	127.00
32	2	1437	U	C6-N1-C2	-6.28	117.23	121.00
32	2	1443	G	N7-C8-N9	6.28	116.24	113.10
32	2	1754	C	C5-C6-N1	6.28	124.14	121.00
32	2	1439	A	C5-C6-N1	6.28	120.84	117.70
32	2	87	C	N3-C2-O2	-6.27	117.51	121.90
32	2	1692	G	C8-N9-C1'	-6.26	118.86	127.00
32	2	102	U	C6-N1-C2	-6.26	117.25	121.00
32	2	1495	U	P-O3'-C3'	6.25	127.20	119.70
32	2	1633	C	C6-N1-C2	-6.24	117.81	120.30
32	2	1362	C	C6-N1-C2	-6.23	117.81	120.30
32	2	452	C	N1-C2-O2	6.22	122.64	118.90
32	2	573	C	C6-N1-C2	-6.21	117.82	120.30
32	2	1165	U	C4-C5-C6	-6.20	115.98	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	561	C	C6-N1-C2	-6.20	117.82	120.30
32	2	1482	G	N7-C8-N9	6.20	116.20	113.10
32	2	845	U	N1-C2-O2	6.19	127.14	122.80
25	b	41	LEU	CA-CB-CG	6.19	129.54	115.30
32	2	1875	U	N3-C2-O2	-6.18	117.88	122.20
32	2	668	C	C6-N1-C2	-6.17	117.83	120.30
32	2	1443	G	N9-C4-C5	-6.17	102.93	105.40
32	2	648	A	N1-C2-N3	-6.17	126.22	129.30
32	2	1302	G	C8-N9-C1'	-6.16	118.99	127.00
32	2	1615	C	C6-N1-C1'	-6.16	113.41	120.80
32	2	1443	G	N1-C6-O6	6.16	123.59	119.90
32	2	1583	C	C6-N1-C1'	-6.15	113.42	120.80
32	2	1690	U	N3-C2-O2	-6.15	117.90	122.20
32	2	1620	U	N1-C2-O2	6.14	127.10	122.80
32	2	1754	C	C6-N1-C2	-6.14	117.84	120.30
32	2	570	G	O5'-P-OP2	-6.14	100.17	105.70
32	2	627	G	C5-C6-N1	6.14	114.57	111.50
32	2	891	G	N3-C4-C5	-6.14	125.53	128.60
32	2	1742	G	C4-N9-C1'	6.14	134.48	126.50
32	2	606	C	C5-C6-N1	6.13	124.07	121.00
32	2	1453	U	N3-C2-O2	-6.13	117.91	122.20
32	2	1441	U	N1-C2-O2	6.13	127.09	122.80
32	2	61	A	N7-C8-N9	6.13	116.86	113.80
32	2	1182	A	C8-N9-C4	6.12	108.25	105.80
32	2	539	C	C2-N1-C1'	6.11	125.52	118.80
32	2	1165	U	C5-C4-O4	-6.11	122.23	125.90
32	2	1383	U	C5-C6-N1	6.11	125.75	122.70
32	2	564	A	C8-N9-C4	-6.11	103.36	105.80
32	2	1616	G	C8-N9-C4	-6.10	103.96	106.40
32	2	804	A	C8-N9-C4	6.10	108.24	105.80
32	2	891	G	C8-N9-C1'	-6.09	119.09	127.00
32	2	855	A	C2-N3-C4	6.08	113.64	110.60
32	2	61	A	N1-C6-N6	6.08	122.25	118.60
32	2	1327	U	N3-C2-O2	-6.08	117.94	122.20
32	2	95	G	N1-C6-O6	-6.07	116.26	119.90
32	2	627	G	C6-N1-C2	-6.07	121.46	125.10
32	2	1168	U	C5'-C4'-O4'	-6.07	101.81	109.10
32	2	1670	C	C6-N1-C2	-6.07	117.87	120.30
32	2	43	A	C6-C5-N7	6.07	136.55	132.30
32	2	1349	C	C6-N1-C2	6.05	122.72	120.30
32	2	1614	G	N3-C4-N9	6.05	129.63	126.00
32	2	530	U	N3-C2-O2	-6.04	117.97	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	877	C	C4-C5-C6	-6.04	114.38	117.40
32	2	672	C	C5-C6-N1	6.04	124.02	121.00
32	2	1351	G	N3-C4-N9	6.03	129.62	126.00
32	2	1427	A	N1-C2-N3	-6.03	126.28	129.30
32	2	1351	G	C8-N9-C1'	-6.03	119.16	127.00
32	2	1484	C	N1-C2-O2	6.03	122.52	118.90
32	2	1312	A	N7-C8-N9	6.03	116.81	113.80
32	2	566	U	C6-N1-C2	-6.02	117.39	121.00
32	2	13	C	C5-C6-N1	6.02	124.01	121.00
32	2	1289	A	C4-N9-C1'	6.02	137.13	126.30
32	2	1168	U	C5-C4-O4	-6.01	122.29	125.90
32	2	1351	G	N3-C4-C5	-6.01	125.59	128.60
32	2	1165	U	N1-C2-O2	6.00	127.00	122.80
32	2	853	C	C6-N1-C1'	6.00	128.00	120.80
32	2	30	G	N3-C4-N9	-5.99	122.41	126.00
32	2	1116	C	N1-C2-O2	5.99	122.49	118.90
32	2	1603	C	C6-N1-C1'	-5.99	113.61	120.80
32	2	641	A	N3-C4-C5	-5.98	122.62	126.80
32	2	1638	G	N3-C4-N9	5.98	129.59	126.00
32	2	982	C	N3-C2-O2	-5.97	117.72	121.90
32	2	861	U	N3-C2-O2	-5.97	118.02	122.20
32	2	1024	G	O4'-C1'-N9	5.96	112.97	108.20
32	2	1580	G	N3-C4-N9	5.96	129.58	126.00
32	2	1023	C	N1-C2-O2	5.96	122.48	118.90
32	2	32	U	C5-C6-N1	5.96	125.68	122.70
32	2	1051	U	C5-C6-N1	5.96	125.68	122.70
32	2	1580	G	C8-N9-C4	-5.96	104.02	106.40
32	2	1438	U	N3-C4-C5	-5.95	111.03	114.60
32	2	1839	U	N1-C2-O2	5.95	126.97	122.80
32	2	1027	U	C6-N1-C2	-5.95	117.43	121.00
32	2	1156	C	C6-N1-C2	-5.95	117.92	120.30
32	2	1692	G	C2-N3-C4	5.95	114.88	111.90
32	2	657	C	C5-C6-N1	5.94	123.97	121.00
32	2	793	C	N1-C2-O2	5.93	122.46	118.90
32	2	1487	U	N3-C2-O2	-5.93	118.05	122.20
32	2	662	A	O5'-P-OP2	-5.93	100.36	105.70
32	2	857	A	C4-C5-C6	-5.93	114.03	117.00
32	2	1107	U	N3-C2-O2	-5.92	118.06	122.20
32	2	1292	G	N7-C8-N9	5.92	116.06	113.10
32	2	530	U	N1-C2-O2	5.91	126.94	122.80
32	2	580	C	N1-C2-O2	5.91	122.45	118.90
32	2	1617	C	N1-C2-O2	5.91	122.45	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	655	G	N1-C6-O6	-5.89	116.36	119.90
32	2	1204	U	C5-C6-N1	5.89	125.64	122.70
32	2	1168	U	N1-C2-O2	5.88	126.92	122.80
32	2	1439	A	C2-N3-C4	5.88	113.54	110.60
32	2	11	A	C4-C5-N7	5.88	113.64	110.70
32	2	624	C	C4-C5-C6	-5.88	114.46	117.40
32	2	598	U	C2-N1-C1'	5.87	124.74	117.70
32	2	1748	C	N3-C2-O2	-5.86	117.80	121.90
32	2	1417	G	N3-C4-N9	5.85	129.51	126.00
32	2	1330	G	N3-C2-N2	-5.84	115.81	119.90
32	2	853	C	C6-N1-C2	-5.83	117.97	120.30
32	2	891	G	N3-C4-N9	5.83	129.50	126.00
32	2	900	C	O5'-P-OP1	-5.83	100.45	105.70
32	2	1748	C	C2-N1-C1'	5.83	125.21	118.80
32	2	108	A	C8-N9-C4	-5.82	103.47	105.80
4	E	9	LEU	CB-CG-CD2	-5.81	101.12	111.00
32	2	1258	U	N1-C2-O2	5.81	126.87	122.80
32	2	771	U	N1-C2-O2	5.81	126.87	122.80
32	2	31	C	C6-N1-C1'	5.80	127.76	120.80
31	k	689	LEU	CA-CB-CG	5.79	128.62	115.30
32	2	1180	C	C6-N1-C1'	-5.79	113.85	120.80
32	2	1168	U	OP1-P-O3'	5.79	117.93	105.20
32	2	1618	G	O4'-C1'-N9	5.78	112.83	108.20
32	2	54	C	C6-N1-C2	-5.78	117.99	120.30
32	2	33	U	C5-C6-N1	5.78	125.59	122.70
32	2	693	G	C8-N9-C1'	-5.77	119.50	127.00
32	2	1766	A	O4'-C1'-N9	5.77	112.81	108.20
32	2	1881	C	N3-C2-O2	-5.77	117.86	121.90
32	2	1029	G	N3-C4-N9	5.75	129.45	126.00
32	2	893	A	N7-C8-N9	5.75	116.68	113.80
32	2	1655	A	N3-C4-N9	5.75	132.00	127.40
32	2	572	C	C5-C6-N1	5.75	123.87	121.00
32	2	824	G	C8-N9-C1'	-5.74	119.53	127.00
32	2	1040	U	C5-C4-O4	5.73	129.34	125.90
32	2	1337	U	N1-C2-O2	5.73	126.81	122.80
32	2	15	U	C5-C6-N1	5.73	125.57	122.70
32	2	1135	U	N1-C2-O2	5.73	126.81	122.80
32	2	1576	A	N3-C4-C5	-5.72	122.80	126.80
32	2	39	A	C8-N9-C4	5.71	108.09	105.80
32	2	1457	U	N3-C2-O2	-5.71	118.20	122.20
32	2	37	U	N3-C2-O2	-5.71	118.21	122.20
32	2	530	U	C5-C6-N1	5.71	125.55	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	687	C	C6-N1-C2	-5.70	118.02	120.30
32	2	1048	G	N1-C6-O6	-5.70	116.48	119.90
32	2	1580	G	N3-C4-C5	-5.69	125.75	128.60
32	2	991	U	N3-C2-O2	-5.69	118.22	122.20
32	2	1409	U	C6-N1-C2	-5.69	117.58	121.00
32	2	1341	A	C8-N9-C4	5.69	108.08	105.80
32	2	48	G	C4-C5-N7	5.69	113.08	110.80
32	2	1742	G	C8-N9-C1'	-5.69	119.61	127.00
32	2	856	U	P-O3'-C3'	5.68	126.52	119.70
32	2	993	C	C6-N1-C2	-5.68	118.03	120.30
32	2	48	G	N3-C4-N9	5.67	129.40	126.00
32	2	1417	G	C4-N9-C1'	5.67	133.88	126.50
32	2	1027	U	C2-N1-C1'	5.67	124.50	117.70
32	2	1734	U	N1-C2-N3	-5.67	111.50	114.90
32	2	873	G	N7-C8-N9	5.66	115.93	113.10
32	2	1310	C	N1-C2-O2	5.66	122.30	118.90
32	2	894	G	C5-C6-N1	5.66	114.33	111.50
32	2	1835	C	N1-C2-O2	5.65	122.29	118.90
32	2	1484	C	C6-N1-C2	-5.65	118.04	120.30
32	2	118	U	C6-N1-C2	-5.64	117.61	121.00
32	2	669	U	C5-C4-O4	5.64	129.29	125.90
32	2	1484	C	N3-C2-O2	-5.64	117.95	121.90
32	2	1357	C	N1-C2-O2	5.64	122.28	118.90
32	2	674	C	N3-C2-O2	-5.64	117.95	121.90
32	2	1417	G	N3-C4-C5	-5.64	125.78	128.60
32	2	61	A	O4'-C1'-N9	5.63	112.71	108.20
32	2	1655	A	N3-C4-C5	-5.63	122.86	126.80
32	2	873	G	N3-C4-C5	-5.63	125.79	128.60
32	2	896	U	C4-C5-C6	-5.63	116.32	119.70
32	2	1180	C	C6-N1-C2	-5.62	118.05	120.30
32	2	52	U	C5-C6-N1	5.62	125.51	122.70
32	2	1433	G	C5-C6-O6	-5.62	125.23	128.60
32	2	670	A	C2-N3-C4	5.61	113.41	110.60
32	2	1566	U	N1-C2-O2	5.61	126.73	122.80
19	U	26	LEU	CA-CB-CG	5.60	128.19	115.30
32	2	580	C	N3-C2-O2	-5.60	117.98	121.90
32	2	1573	A	C3'-C2'-C1'	-5.60	97.02	101.50
32	2	659	G	N1-C2-N2	-5.59	111.17	116.20
32	2	539	C	C6-N1-C2	-5.59	118.06	120.30
32	2	624	C	C5-C6-N1	5.59	123.80	121.00
32	2	1833	A	O4'-C1'-N9	5.59	112.67	108.20
32	2	771	U	N3-C2-O2	-5.59	118.29	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1427	A	N3-C4-N9	5.59	131.87	127.40
32	2	1839	U	N3-C2-O2	-5.59	118.29	122.20
32	2	824	G	C8-N9-C4	-5.58	104.17	106.40
32	2	1056	G	C2-N3-C4	-5.58	109.11	111.90
32	2	148	A	C8-N9-C4	5.58	108.03	105.80
32	2	833	A	N1-C6-N6	-5.58	115.25	118.60
32	2	1426	C	C2-N1-C1'	5.57	124.93	118.80
32	2	571	C	N3-C4-N4	-5.57	114.10	118.00
32	2	1427	A	N3-C4-C5	-5.57	122.90	126.80
32	2	1458	C	C6-N1-C2	-5.57	118.07	120.30
32	2	103	A	C8-N9-C4	-5.56	103.58	105.80
32	2	669	U	N1-C2-N3	5.56	118.24	114.90
32	2	1783	A	C5-C6-N1	5.56	120.48	117.70
32	2	1180	C	C5-C6-N1	5.56	123.78	121.00
32	2	631	U	N1-C2-O2	5.55	126.69	122.80
32	2	1360	A	C8-N9-C1'	-5.55	117.70	127.70
32	2	1441	U	N3-C2-O2	-5.55	118.31	122.20
32	2	1433	G	N1-C6-O6	5.55	123.23	119.90
32	2	1300	C	C5-C6-N1	-5.55	118.22	121.00
3	D	210	GLU	C-N-CD	-5.55	108.40	120.60
32	2	1029	G	C8-N9-C1'	-5.54	119.79	127.00
32	2	1312	A	N3-C4-C5	-5.54	122.92	126.80
32	2	1783	A	C4-C5-N7	5.54	113.47	110.70
32	2	835	C	OP1-P-O3'	-5.54	93.02	105.20
32	2	1443	G	C2-N3-C4	-5.54	109.13	111.90
32	2	1168	U	C2-N3-C4	5.54	130.32	127.00
32	2	1646	C	N3-C2-O2	-5.54	118.03	121.90
32	2	109	G	C5-C6-N1	5.53	114.27	111.50
32	2	11	A	O4'-C1'-N9	5.53	112.63	108.20
32	2	60	U	C5-C6-N1	5.53	125.46	122.70
32	2	541	U	P-O3'-C3'	5.53	126.33	119.70
32	2	530	U	C2-N1-C1'	5.52	124.33	117.70
32	2	1617	C	N3-C2-O2	-5.52	118.03	121.90
32	2	639	C	C5-C6-N1	5.52	123.76	121.00
32	2	1116	C	N3-C2-O2	-5.52	118.04	121.90
32	2	1734	U	N3-C4-O4	-5.52	115.54	119.40
32	2	838	C	C5-C4-N4	-5.51	116.34	120.20
32	2	624	C	N1-C2-O2	5.51	122.21	118.90
32	2	43	A	C4-N9-C1'	-5.51	116.39	126.30
32	2	1044	C	C6-N1-C2	-5.51	118.10	120.30
32	2	892	U	C4-C5-C6	5.50	123.00	119.70
32	2	513	C	N1-C2-O2	5.50	122.20	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1457	U	N1-C2-O2	5.50	126.65	122.80
32	2	893	A	C5-N7-C8	-5.49	101.16	103.90
32	2	1231	U	N3-C2-O2	-5.49	118.36	122.20
32	2	1322	G	N3-C4-N9	5.48	129.29	126.00
32	2	894	G	C8-N9-C4	-5.48	104.21	106.40
32	2	1495	U	OP1-P-O3'	5.47	117.25	105.20
32	2	1484	C	C2-N1-C1'	5.47	124.82	118.80
32	2	569	U	C6-N1-C2	-5.47	117.72	121.00
32	2	31	C	C5-C6-N1	5.46	123.73	121.00
32	2	855	A	C5-C6-N1	5.45	120.43	117.70
32	2	1716	U	N3-C2-O2	-5.45	118.38	122.20
16	R	26	LEU	CA-CB-CG	5.45	127.83	115.30
32	2	890	C	C5-C6-N1	5.45	123.72	121.00
32	2	1292	G	C4-N9-C1'	5.44	133.58	126.50
32	2	117	U	C6-N1-C2	-5.44	117.73	121.00
32	2	447	C	N3-C2-O2	-5.44	118.09	121.90
32	2	1594	U	C2-N1-C1'	5.43	124.22	117.70
32	2	730	G	C4-N9-C1'	5.43	133.55	126.50
32	2	897	G	N3-C4-N9	5.42	129.25	126.00
32	2	733	A	C2-N3-C4	5.41	113.31	110.60
32	2	1482	G	C6-C5-N7	-5.41	127.16	130.40
32	2	45	U	O4'-C1'-N1	5.41	112.52	108.20
32	2	698	C	N1-C2-O2	5.40	122.14	118.90
32	2	891	G	N1-C2-N3	5.40	127.14	123.90
32	2	1581	G	N3-C4-N9	5.39	129.24	126.00
32	2	1243	A	N7-C8-N9	5.39	116.49	113.80
32	2	1135	U	N3-C2-O2	-5.38	118.43	122.20
32	2	15	U	C6-N1-C2	-5.38	117.77	121.00
32	2	1034	A	C8-N9-C4	5.38	107.95	105.80
32	2	1159	U	C6-N1-C2	-5.38	117.78	121.00
32	2	104	A	C5-C6-N1	5.37	120.39	117.70
32	2	1655	A	C4-N9-C1'	5.37	135.97	126.30
32	2	894	G	C6-C5-N7	-5.37	127.18	130.40
32	2	1242	C	C6-N1-C2	-5.37	118.15	120.30
32	2	1327	U	N1-C2-O2	5.37	126.56	122.80
32	2	569	U	N3-C2-O2	-5.35	118.45	122.20
32	2	1005	U	O5'-P-OP2	-5.35	100.88	105.70
32	2	826	U	P-O3'-C3'	5.35	126.12	119.70
32	2	1332	C	O5'-P-OP1	5.35	117.12	110.70
32	2	1073	C	C6-N1-C2	-5.35	118.16	120.30
32	2	617	C	C6-N1-C2	-5.34	118.16	120.30
32	2	873	G	O5'-P-OP2	-5.34	100.90	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	43	A	C8-N9-C1'	5.33	137.30	127.70
32	2	999	A	N1-C6-N6	-5.33	115.40	118.60
32	2	1247	U	C5-C6-N1	5.33	125.37	122.70
32	2	1866	A	P-O3'-C3'	5.33	126.09	119.70
32	2	1292	G	C8-N9-C4	-5.32	104.27	106.40
32	2	606	C	C4-C5-C6	-5.32	114.74	117.40
32	2	827	G	O4'-C1'-N9	-5.32	103.95	108.20
32	2	1254	G	O5'-P-OP1	-5.32	100.92	105.70
32	2	711	C	O5'-P-OP2	-5.31	100.92	105.70
32	2	1443	G	C4-N9-C1'	5.31	133.40	126.50
32	2	1603	C	N3-C2-O2	-5.31	118.18	121.90
32	2	109	G	N1-C6-O6	-5.31	116.72	119.90
32	2	878	A	C8-N9-C4	-5.31	103.68	105.80
32	2	908	C	C5-C6-N1	5.30	123.65	121.00
32	2	1358	U	N3-C2-O2	-5.30	118.49	122.20
32	2	1456	G	N1-C6-O6	-5.30	116.72	119.90
32	2	1159	U	C6-N1-C1'	-5.30	113.78	121.20
32	2	1581	G	N1-C6-O6	5.30	123.08	119.90
32	2	1616	G	N3-C4-N9	5.30	129.18	126.00
32	2	645	C	C5-C6-N1	5.29	123.65	121.00
32	2	674	C	N1-C2-O2	5.29	122.08	118.90
32	2	1051	U	C6-N1-C2	-5.29	117.82	121.00
32	2	98	U	N3-C2-O2	-5.29	118.50	122.20
32	2	571	C	N1-C2-N3	5.28	122.90	119.20
32	2	142	G	C4-C5-N7	5.28	112.91	110.80
32	2	835	C	O3'-P-O5'	5.28	114.02	104.00
32	2	845	U	N3-C2-O2	-5.27	118.51	122.20
32	2	1612	A	P-O3'-C3'	5.27	126.02	119.70
32	2	1352	G	C4-N9-C1'	5.27	133.35	126.50
32	2	1541	C	C6-N1-C1'	-5.27	114.48	120.80
32	2	707	C	C5-C6-N1	5.27	123.63	121.00
32	2	1733	C	N3-C4-C5	-5.26	119.80	121.90
32	2	867	A	C2-N3-C4	5.26	113.23	110.60
32	2	452	C	N3-C2-O2	-5.26	118.22	121.90
21	W	103	ILE	CG1-CB-CG2	-5.25	99.84	111.40
32	2	21	U	N3-C2-O2	-5.25	118.52	122.20
32	2	805	A	O4'-C1'-N9	5.25	112.40	108.20
32	2	1346	A	P-O3'-C3'	5.25	126.00	119.70
32	2	21	U	N1-C2-O2	5.24	126.47	122.80
32	2	1024	G	C4-N9-C1'	5.24	133.31	126.50
32	2	831	G	N1-C6-O6	5.23	123.04	119.90
32	2	1360	A	C8-N9-C4	-5.23	103.71	105.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	645	C	C4-C5-C6	-5.23	114.79	117.40
32	2	877	C	C6-N1-C2	-5.23	118.21	120.30
32	2	1431	C	P-O3'-C3'	5.22	125.97	119.70
32	2	1384	U	C5-C6-N1	5.22	125.31	122.70
32	2	1515	U	N1-C2-O2	5.22	126.45	122.80
32	2	659	G	N3-C4-N9	5.22	129.13	126.00
32	2	11	A	N9-C4-C5	-5.22	103.71	105.80
32	2	106	U	O5'-P-OP1	-5.22	101.00	105.70
32	2	1619	C	C6-N1-C2	-5.22	118.21	120.30
32	2	1167	A	N9-C1'-C2'	-5.22	106.26	112.00
32	2	1328	G	N9-C4-C5	-5.21	103.31	105.40
32	2	1465	A	C5-N7-C8	-5.21	101.29	103.90
32	2	570	G	N1-C6-O6	-5.21	116.77	119.90
32	2	1716	U	N1-C2-O2	5.21	126.45	122.80
32	2	114	C	N3-C4-C5	5.21	123.98	121.90
32	2	1715	C	N1-C2-O2	5.21	122.03	118.90
32	2	1052	A	O5'-P-OP2	-5.21	101.01	105.70
32	2	688	A	N7-C8-N9	5.20	116.40	113.80
32	2	1566	U	C2-N1-C1'	5.20	123.94	117.70
32	2	104	A	O5'-P-OP1	-5.20	101.02	105.70
32	2	827	G	C8-N9-C1'	5.20	133.76	127.00
32	2	724	G	C5-C6-N1	5.20	114.10	111.50
32	2	571	C	N3-C2-O2	-5.19	118.27	121.90
32	2	1255	U	N3-C2-O2	-5.19	118.57	122.20
32	2	1875	U	N1-C2-O2	5.19	126.43	122.80
32	2	977	C	N1-C2-O2	5.19	122.01	118.90
32	2	1039	A	N1-C6-N6	-5.19	115.49	118.60
32	2	826	U	OP2-P-O3'	5.19	116.61	105.20
32	2	838	C	C4-C5-C6	-5.18	114.81	117.40
32	2	1409	U	O4'-C1'-N1	5.18	112.34	108.20
32	2	1168	U	O3'-P-O5'	5.18	113.83	104.00
32	2	1073	C	C5-C6-N1	5.17	123.59	121.00
32	2	1286	C	N1-C2-O2	5.17	122.00	118.90
32	2	549	C	N3-C2-O2	-5.17	118.28	121.90
32	2	596	A	C5-N7-C8	-5.17	101.32	103.90
32	2	11	A	N3-C4-N9	5.16	131.53	127.40
32	2	61	A	C6-C5-N7	-5.16	128.69	132.30
32	2	11	A	C4-N9-C1'	5.16	135.58	126.30
32	2	688	A	C5-N7-C8	-5.16	101.32	103.90
32	2	1433	G	N3-C2-N2	-5.15	116.29	119.90
32	2	1439	A	N1-C6-N6	-5.15	115.51	118.60
32	2	1441	U	C6-N1-C2	-5.15	117.91	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	1184	G	C2-N3-C4	-5.15	109.33	111.90
32	2	549	C	N1-C2-O2	5.15	121.99	118.90
32	2	1433	G	N1-C2-N2	5.15	120.83	116.20
32	2	447	C	N1-C2-O2	5.14	121.99	118.90
32	2	627	G	N3-C4-C5	-5.14	126.03	128.60
32	2	1163	A	C8-N9-C4	-5.14	103.74	105.80
32	2	1260	G	N3-C4-C5	-5.14	126.03	128.60
32	2	1424	U	O4'-C1'-N1	5.14	112.31	108.20
32	2	20	G	C6-C5-N7	-5.14	127.32	130.40
32	2	546	U	N1-C2-O2	5.14	126.39	122.80
32	2	643	U	OP2-P-O3'	5.13	116.50	105.20
32	2	661	G	N9-C4-C5	5.13	107.45	105.40
32	2	501	U	C2-N1-C1'	5.12	123.84	117.70
32	2	892	U	N3-C2-O2	-5.12	118.62	122.20
32	2	1311	C	OP1-P-O3'	5.12	116.46	105.20
32	2	567	U	C5-C6-N1	5.12	125.26	122.70
24	Z	42	LEU	CA-CB-CG	5.11	127.06	115.30
32	2	1312	A	C4-N9-C1'	5.11	135.50	126.30
32	2	560	U	C5-C6-N1	5.11	125.25	122.70
32	2	857	A	O4'-C1'-N9	-5.11	104.12	108.20
32	2	1004	U	C5-C6-N1	5.11	125.25	122.70
32	2	1360	A	N7-C8-N9	5.11	116.35	113.80
32	2	1330	G	C5-C6-O6	-5.10	125.54	128.60
32	2	558	A	C8-N9-C4	5.10	107.84	105.80
32	2	1212	U	C2-N1-C1'	5.09	123.81	117.70
32	2	1056	G	C8-N9-C4	5.09	108.44	106.40
32	2	663	A	OP2-P-O3'	5.09	116.39	105.20
32	2	880	U	OP1-P-OP2	5.08	127.23	119.60
32	2	43	A	O4'-C1'-N9	5.08	112.27	108.20
32	2	693	G	C6-N1-C2	-5.08	122.05	125.10
32	2	901	U	N3-C2-O2	-5.08	118.64	122.20
32	2	1186	C	N3-C2-O2	-5.08	118.34	121.90
32	2	57	G	C4-N9-C1'	5.08	133.10	126.50
32	2	730	G	N3-C4-C5	-5.08	126.06	128.60
32	2	1616	G	C4-C5-C6	5.07	121.84	118.80
32	2	1621	A	N9-C4-C5	-5.07	103.77	105.80
32	2	982	C	N1-C2-O2	5.07	121.94	118.90
32	2	873	G	N9-C4-C5	-5.07	103.37	105.40
32	2	1030	C	C5-C6-N1	5.07	123.53	121.00
32	2	1167	A	C4-C5-N7	5.07	113.23	110.70
32	2	1487	U	N1-C2-O2	5.06	126.34	122.80
32	2	659	G	N3-C2-N2	5.06	123.44	119.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	845	U	C2-N1-C1'	5.05	123.77	117.70
32	2	1417	G	C8-N9-C1'	-5.05	120.43	127.00
32	2	817	C	O5'-P-OP1	-5.04	101.16	105.70
32	2	832	C	C5-C6-N1	5.04	123.52	121.00
32	2	11	A	C8-N9-C1'	-5.04	118.62	127.70
32	2	571	C	C5-C6-N1	-5.04	118.48	121.00
32	2	640	G	C5-C6-N1	5.04	114.02	111.50
32	2	1438	U	C6-N1-C2	-5.04	117.98	121.00
32	2	149	C	C6-N1-C2	-5.04	118.29	120.30
32	2	1001	A	C8-N9-C4	-5.04	103.79	105.80
32	2	877	C	N1-C2-O2	5.03	121.92	118.90
32	2	605	C	N1-C2-O2	5.03	121.92	118.90
32	2	1247	U	C4-C5-C6	-5.03	116.68	119.70
32	2	1013	U	N3-C2-O2	-5.03	118.68	122.20
32	2	1604	U	C5-C6-N1	5.03	125.21	122.70
32	2	1292	G	C5-N7-C8	-5.03	101.79	104.30
32	2	1833	A	N7-C8-N9	5.02	116.31	113.80
32	2	1257	C	C4-C5-C6	-5.02	114.89	117.40
32	2	873	G	C5-N7-C8	-5.02	101.79	104.30
32	2	885	A	N3-C4-C5	5.02	130.31	126.80
32	2	1440	G	O5'-P-OP1	-5.01	101.19	105.70
32	2	1605	G	C8-N9-C1'	-5.01	120.48	127.00
32	2	733	A	C5-C6-N1	5.01	120.21	117.70
32	2	71	A	N7-C8-N9	5.01	116.31	113.80
32	2	662	A	C5-C6-N1	5.01	120.20	117.70
32	2	872	U	N3-C4-C5	5.00	117.60	114.60
32	2	1360	A	C4-C5-C6	5.00	119.50	117.00

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	VAL	Peptide
2	C	106	ASP	Peptide
3	D	210	GLU	Peptide
8	I	185	GLU	Peptide
9	J	20	GLU	Peptide
10	K	87	VAL	Peptide
14	P	111	MET	Peptide
14	P	133	ALA	Peptide
16	R	83	GLN	Peptide
18	T	79	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
19	U	77	LYS	Peptide
22	X	108	GLY	Peptide
22	X	109	ARG	Peptide
22	X	117	ILE	Peptide
22	X	63	GLN	Peptide
27	d	23	VAL	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/206 (99%)	181 (89%)	23 (11%)	0	100	100
2	C	215/217 (99%)	199 (93%)	16 (7%)	0	100	100
3	D	220/223 (99%)	177 (80%)	41 (19%)	2 (1%)	17	54
4	E	258/260 (99%)	231 (90%)	27 (10%)	0	100	100
5	F	203/206 (98%)	181 (89%)	22 (11%)	0	100	100
6	G	230/232 (99%)	214 (93%)	16 (7%)	0	100	100
7	H	182/184 (99%)	170 (93%)	12 (7%)	0	100	100
8	I	184/199 (92%)	165 (90%)	19 (10%)	0	100	100
9	J	183/185 (99%)	163 (89%)	20 (11%)	0	100	100
10	K	92/96 (96%)	72 (78%)	19 (21%)	1 (1%)	14	50
11	L	138/140 (99%)	123 (89%)	15 (11%)	0	100	100
12	M	123/125 (98%)	99 (80%)	24 (20%)	0	100	100
13	N	148/150 (99%)	134 (90%)	14 (10%)	0	100	100
14	P	119/127 (94%)	89 (75%)	30 (25%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Q	125/127 (98%)	115 (92%)	10 (8%)	0	100	100
16	R	123/125 (98%)	112 (91%)	11 (9%)	0	100	100
17	S	133/135 (98%)	108 (81%)	25 (19%)	0	100	100
18	T	141/143 (99%)	129 (92%)	12 (8%)	0	100	100
19	U	101/103 (98%)	91 (90%)	10 (10%)	0	100	100
20	V	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
21	W	127/129 (98%)	112 (88%)	15 (12%)	0	100	100
22	X	142/144 (99%)	116 (82%)	24 (17%)	2 (1%)	11	45
23	Y	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
24	Z	61/63 (97%)	52 (85%)	9 (15%)	0	100	100
25	b	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
26	c	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
27	d	35/37 (95%)	29 (83%)	6 (17%)	0	100	100
28	e	44/63 (70%)	37 (84%)	7 (16%)	0	100	100
29	f	64/71 (90%)	47 (73%)	17 (27%)	0	100	100
30	g	315/317 (99%)	279 (89%)	36 (11%)	0	100	100
31	k	630/788 (80%)	572 (91%)	58 (9%)	0	100	100
All	All	4897/5160 (95%)	4318 (88%)	574 (12%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	X	117	ILE
3	D	211	PRO
10	K	54	TYR
3	D	216	PRO
22	X	64	PRO

5.3.2 Protein sidechains ⓘ

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	
1	A	171/173 (99%)	171 (100%)	0	100	100
2	C	176/176 (100%)	172 (98%)	4 (2%)	50	71
3	D	182/182 (100%)	178 (98%)	4 (2%)	52	72
4	E	221/221 (100%)	220 (100%)	1 (0%)	88	94
5	F	173/173 (100%)	172 (99%)	1 (1%)	86	93
6	G	198/198 (100%)	193 (98%)	5 (2%)	47	70
7	H	165/165 (100%)	164 (99%)	1 (1%)	86	93
8	I	150/160 (94%)	149 (99%)	1 (1%)	84	91
9	J	158/158 (100%)	155 (98%)	3 (2%)	57	76
10	K	89/89 (100%)	88 (99%)	1 (1%)	73	85
11	L	125/125 (100%)	122 (98%)	3 (2%)	49	71
12	M	101/101 (100%)	100 (99%)	1 (1%)	76	86
13	N	127/127 (100%)	127 (100%)	0	100	100
14	P	105/105 (100%)	104 (99%)	1 (1%)	76	86
15	Q	107/107 (100%)	106 (99%)	1 (1%)	78	88
16	R	113/113 (100%)	113 (100%)	0	100	100
17	S	120/120 (100%)	119 (99%)	1 (1%)	81	89
18	T	115/115 (100%)	113 (98%)	2 (2%)	60	79
19	U	96/96 (100%)	94 (98%)	2 (2%)	53	74
20	V	74/74 (100%)	72 (97%)	2 (3%)	44	68
21	W	110/110 (100%)	109 (99%)	1 (1%)	78	88
22	X	119/119 (100%)	117 (98%)	2 (2%)	60	79
23	Y	112/112 (100%)	110 (98%)	2 (2%)	59	77
24	Z	56/56 (100%)	56 (100%)	0	100	100
25	b	70/70 (100%)	69 (99%)	1 (1%)	67	82
26	c	56/56 (100%)	55 (98%)	1 (2%)	59	77
27	d	33/33 (100%)	31 (94%)	2 (6%)	18	50
28	e	40/54 (74%)	39 (98%)	1 (2%)	47	70
29	f	43/62 (69%)	43 (100%)	0	100	100
30	g	259/261 (99%)	258 (100%)	1 (0%)	91	95
31	k	553/703 (79%)	544 (98%)	9 (2%)	62	80
All	All	4217/4414 (96%)	4163 (99%)	54 (1%)	70	83

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	89	GLN
2	C	111	VAL
2	C	113	LEU
2	C	179	VAL
3	D	76	ARG
3	D	154	ASP
3	D	190	ARG
3	D	212	LYS
4	E	106	LYS
5	F	166	ARG
6	G	25	ARG
6	G	98	ARG
6	G	129	VAL
6	G	151	ASP
6	G	214	LYS
7	H	83	LYS
8	I	47	ARG
9	J	78	ARG
9	J	101	VAL
9	J	175	ARG
10	K	55	VAL
11	L	29	LYS
11	L	67	ARG
11	L	124	THR
12	M	86	VAL
14	P	47	ARG
15	Q	7	VAL
17	S	132	ARG
18	T	63	ARG
18	T	105	LEU
19	U	65	ILE
19	U	68	ARG
20	V	4	ASP
20	V	12	TYR
21	W	103	ILE
22	X	23	ARG
22	X	83	VAL
23	Y	112	LYS
23	Y	115	ASP
25	b	65	THR
26	c	67	ARG
27	d	23	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	d	28	THR
28	e	39	LEU
30	g	316	MET
31	k	62	ARG
31	k	343	ARG
31	k	373	ARG
31	k	535	LYS
31	k	546	LYS
31	k	621	ARG
31	k	622	ARG
31	k	712	LYS
31	k	762	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
2	C	59	HIS
2	C	209	ASN
3	D	101	GLN
3	D	165	ASN
3	D	174	HIS
4	E	57	ASN
4	E	98	ASN
4	E	209	HIS
5	F	122	ASN
5	F	169	ASN
7	H	74	GLN
7	H	108	GLN
7	H	147	ASN
8	I	111	GLN
9	J	48	GLN
9	J	112	GLN
10	K	17	GLN
13	N	21	ASN
13	N	69	ASN
13	N	105	ASN
13	N	123	HIS
14	P	98	ASN
14	P	103	ASN
15	Q	83	GLN
15	Q	100	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	Q	103	ASN
16	R	48	ASN
16	R	105	GLN
17	S	12	GLN
17	S	63	GLN
17	S	71	GLN
17	S	122	HIS
17	S	127	HIS
18	T	77	ASN
19	U	40	ASN
19	U	48	HIS
20	V	33	GLN
20	V	35	ASN
21	W	80	ASN
21	W	92	ASN
23	Y	77	ASN
23	Y	110	GLN
25	b	51	GLN
27	d	20	GLN
29	f	123	ASN
30	g	187	GLN
30	g	237	GLN
31	k	56	ASN
31	k	255	ASN
31	k	302	GLN
31	k	377	HIS
31	k	506	ASN
31	k	513	GLN
31	k	547	ASN
31	k	638	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	2	1613/1910 (84%)	714 (44%)	22 (1%)

All (714) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
32	2	5	U
32	2	9	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	10	G
32	2	13	C
32	2	19	A
32	2	25	C
32	2	26	A
32	2	27	U
32	2	32	U
32	2	34	G
32	2	40	A
32	2	42	G
32	2	45	U
32	2	46	A
32	2	47	A
32	2	50	C
32	2	55	A
32	2	57	G
32	2	58	U
32	2	59	C
32	2	60	U
32	2	66	U
32	2	72	A
32	2	73	U
32	2	74	U
32	2	75	U
32	2	77	U
32	2	82	U
32	2	84	A
32	2	93	A
32	2	96	G
32	2	98	U
32	2	100	A
32	2	101	U
32	2	102	U
32	2	104	A
32	2	108	A
32	2	114	C
32	2	115	G
32	2	116	U
32	2	127	G
32	2	130	C
32	2	131	C
32	2	133	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	134	U
32	2	137	U
32	2	138	A
32	2	141	U
32	2	148	A
32	2	420	A
32	2	422	U
32	2	441	U
32	2	446	U
32	2	448	U
32	2	449	C
32	2	450	G
32	2	453	C
32	2	454	C
32	2	455	U
32	2	457	U
32	2	458	G
32	2	459	G
32	2	460	A
32	2	461	A
32	2	466	U
32	2	478	A
32	2	479	U
32	2	480	A
32	2	481	A
32	2	482	A
32	2	488	A
32	2	490	U
32	2	491	G
32	2	492	U
32	2	493	C
32	2	494	U
32	2	496	C
32	2	498	G
32	2	499	A
32	2	500	C
32	2	503	U
32	2	504	U
32	2	505	U
32	2	513	C
32	2	514	A
32	2	519	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	520	A
32	2	524	U
32	2	525	U
32	2	526	C
32	2	529	A
32	2	530	U
32	2	534	A
32	2	535	U
32	2	537	G
32	2	539	C
32	2	540	U
32	2	542	G
32	2	543	U
32	2	544	G
32	2	551	A
32	2	558	A
32	2	562	A
32	2	568	C
32	2	571	C
32	2	573	C
32	2	577	C
32	2	579	A
32	2	584	C
32	2	585	G
32	2	587	U
32	2	592	G
32	2	599	G
32	2	600	G
32	2	601	C
32	2	604	A
32	2	605	C
32	2	606	C
32	2	615	A
32	2	622	A
32	2	623	A
32	2	624	C
32	2	626	G
32	2	631	U
32	2	635	G
32	2	644	C
32	2	647	G
32	2	656	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	659	G
32	2	663	A
32	2	664	A
32	2	665	C
32	2	667	G
32	2	674	C
32	2	675	A
32	2	679	A
32	2	680	A
32	2	682	G
32	2	686	G
32	2	687	C
32	2	688	A
32	2	689	G
32	2	693	G
32	2	694	C
32	2	695	G
32	2	698	C
32	2	700	A
32	2	701	A
32	2	702	U
32	2	707	C
32	2	708	A
32	2	711	C
32	2	717	U
32	2	718	C
32	2	720	G
32	2	722	G
32	2	730	G
32	2	731	A
32	2	732	C
32	2	738	A
32	2	740	A
32	2	743	G
32	2	744	A
32	2	745	U
32	2	748	A
32	2	749	G
32	2	753	C
32	2	754	C
32	2	755	A
32	2	756	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	758	C
32	2	759	G
32	2	760	G
32	2	763	C
32	2	765	U
32	2	766	G
32	2	767	U
32	2	769	A
32	2	770	U
32	2	771	U
32	2	773	G
32	2	774	A
32	2	782	C
32	2	783	A
32	2	786	G
32	2	790	A
32	2	797	A
32	2	803	G
32	2	804	A
32	2	805	A
32	2	806	C
32	2	808	A
32	2	814	G
32	2	820	G
32	2	822	C
32	2	823	U
32	2	824	G
32	2	825	G
32	2	826	U
32	2	827	G
32	2	828	C
32	2	829	C
32	2	830	A
32	2	831	G
32	2	833	A
32	2	835	C
32	2	836	C
32	2	837	G
32	2	839	G
32	2	840	G
32	2	841	U
32	2	842	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	843	A
32	2	844	U
32	2	845	U
32	2	848	A
32	2	855	A
32	2	856	U
32	2	857	A
32	2	858	G
32	2	859	C
32	2	869	A
32	2	876	G
32	2	879	G
32	2	880	U
32	2	883	A
32	2	885	A
32	2	886	A
32	2	887	G
32	2	889	U
32	2	890	C
32	2	891	G
32	2	892	U
32	2	893	A
32	2	902	U
32	2	903	U
32	2	904	G
32	2	915	G
32	2	916	C
32	2	918	G
32	2	919	G
32	2	921	C
32	2	923	G
32	2	926	U
32	2	927	U
32	2	928	C
32	2	929	C
32	2	930	A
32	2	931	A
32	2	933	G
32	2	937	C
32	2	942	C
32	2	943	C
32	2	944	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	949	G
32	2	951	U
32	2	952	A
32	2	954	C
32	2	959	A
32	2	960	G
32	2	962	C
32	2	963	C
32	2	964	U
32	2	968	G
32	2	969	G
32	2	972	C
32	2	974	U
32	2	977	C
32	2	980	A
32	2	984	G
32	2	985	G
32	2	986	A
32	2	987	C
32	2	989	U
32	2	997	G
32	2	998	A
32	2	999	A
32	2	1000	A
32	2	1007	G
32	2	1011	G
32	2	1012	U
32	2	1014	C
32	2	1020	A
32	2	1021	G
32	2	1025	U
32	2	1027	U
32	2	1028	U
32	2	1029	G
32	2	1030	C
32	2	1035	A
32	2	1036	U
32	2	1039	A
32	2	1040	U
32	2	1049	A
32	2	1053	A
32	2	1056	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1057	A
32	2	1058	A
32	2	1060	A
32	2	1061	G
32	2	1062	G
32	2	1065	G
32	2	1066	U
32	2	1067	U
32	2	1069	G
32	2	1070	G
32	2	1072	U
32	2	1073	C
32	2	1076	U
32	2	1077	U
32	2	1079	U
32	2	1087	U
32	2	1090	A
32	2	1095	C
32	2	1096	A
32	2	1097	U
32	2	1098	C
32	2	1099	G
32	2	1102	A
32	2	1106	U
32	2	1108	A
32	2	1109	A
32	2	1115	A
32	2	1118	G
32	2	1122	G
32	2	1131	C
32	2	1132	U
32	2	1133	A
32	2	1134	C
32	2	1135	U
32	2	1142	G
32	2	1144	A
32	2	1149	C
32	2	1151	A
32	2	1159	U
32	2	1160	U
32	2	1162	C
32	2	1167	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1168	U
32	2	1169	C
32	2	1173	C
32	2	1176	U
32	2	1179	A
32	2	1182	A
32	2	1186	C
32	2	1202	G
32	2	1203	G
32	2	1204	U
32	2	1205	G
32	2	1209	U
32	2	1210	U
32	2	1213	A
32	2	1214	A
32	2	1215	U
32	2	1217	A
32	2	1218	C
32	2	1225	G
32	2	1228	A
32	2	1232	U
32	2	1234	C
32	2	1235	G
32	2	1244	A
32	2	1248	C
32	2	1252	G
32	2	1254	G
32	2	1255	U
32	2	1257	C
32	2	1263	G
32	2	1264	G
32	2	1265	A
32	2	1276	A
32	2	1284	A
32	2	1286	C
32	2	1290	A
32	2	1295	A
32	2	1297	U
32	2	1299	A
32	2	1300	C
32	2	1301	G
32	2	1302	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1303	A
32	2	1304	A
32	2	1307	G
32	2	1308	C
32	2	1309	A
32	2	1310	C
32	2	1311	C
32	2	1312	A
32	2	1313	C
32	2	1315	A
32	2	1318	A
32	2	1319	G
32	2	1321	G
32	2	1322	G
32	2	1327	U
32	2	1328	G
32	2	1331	G
32	2	1332	C
32	2	1333	U
32	2	1336	A
32	2	1337	U
32	2	1339	U
32	2	1340	G
32	2	1341	A
32	2	1342	C
32	2	1343	U
32	2	1346	A
32	2	1347	C
32	2	1349	C
32	2	1350	G
32	2	1351	G
32	2	1353	G
32	2	1354	A
32	2	1355	A
32	2	1356	A
32	2	1357	C
32	2	1358	U
32	2	1359	C
32	2	1361	C
32	2	1362	C
32	2	1363	A
32	2	1364	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1366	U
32	2	1367	C
32	2	1369	A
32	2	1370	G
32	2	1371	A
32	2	1372	C
32	2	1374	C
32	2	1375	A
32	2	1376	A
32	2	1378	A
32	2	1379	A
32	2	1380	G
32	2	1381	G
32	2	1382	A
32	2	1383	U
32	2	1384	U
32	2	1385	G
32	2	1386	A
32	2	1387	C
32	2	1388	A
32	2	1391	U
32	2	1392	U
32	2	1393	G
32	2	1394	A
32	2	1396	A
32	2	1397	G
32	2	1398	C
32	2	1399	U
32	2	1400	C
32	2	1403	U
32	2	1404	C
32	2	1405	U
32	2	1406	U
32	2	1408	A
32	2	1409	U
32	2	1410	U
32	2	1411	U
32	2	1412	U
32	2	1413	G
32	2	1414	U
32	2	1415	G
32	2	1417	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1418	U
32	2	1419	G
32	2	1420	G
32	2	1421	U
32	2	1422	G
32	2	1423	G
32	2	1425	G
32	2	1426	C
32	2	1427	A
32	2	1429	G
32	2	1431	C
32	2	1432	C
32	2	1437	U
32	2	1438	U
32	2	1439	A
32	2	1440	G
32	2	1445	U
32	2	1446	G
32	2	1450	U
32	2	1454	U
32	2	1455	U
32	2	1458	C
32	2	1459	U
32	2	1466	U
32	2	1467	U
32	2	1468	G
32	2	1471	A
32	2	1473	A
32	2	1474	A
32	2	1475	C
32	2	1476	G
32	2	1477	A
32	2	1478	A
32	2	1482	G
32	2	1491	C
32	2	1492	U
32	2	1493	A
32	2	1494	C
32	2	1495	U
32	2	1496	A
32	2	1497	A
32	2	1498	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1499	U
32	2	1500	A
32	2	1501	G
32	2	1502	U
32	2	1503	G
32	2	1504	G
32	2	1506	G
32	2	1510	G
32	2	1511	C
32	2	1512	A
32	2	1513	U
32	2	1514	U
32	2	1515	U
32	2	1516	G
32	2	1518	U
32	2	1519	G
32	2	1521	U
32	2	1522	U
32	2	1529	U
32	2	1537	G
32	2	1540	A
32	2	1542	U
32	2	1551	C
32	2	1554	G
32	2	1557	G
32	2	1558	A
32	2	1559	U
32	2	1565	U
32	2	1567	U
32	2	1573	A
32	2	1574	A
32	2	1576	A
32	2	1577	A
32	2	1578	C
32	2	1579	A
32	2	1580	G
32	2	1581	G
32	2	1582	U
32	2	1583	C
32	2	1584	U
32	2	1585	G
32	2	1586	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1590	G
32	2	1593	C
32	2	1594	U
32	2	1595	U
32	2	1597	G
32	2	1598	A
32	2	1599	C
32	2	1600	G
32	2	1601	U
32	2	1602	U
32	2	1603	C
32	2	1605	G
32	2	1606	G
32	2	1607	G
32	2	1608	C
32	2	1611	C
32	2	1612	A
32	2	1613	C
32	2	1614	G
32	2	1618	G
32	2	1619	C
32	2	1620	U
32	2	1621	A
32	2	1623	A
32	2	1625	U
32	2	1626	G
32	2	1630	G
32	2	1631	A
32	2	1634	C
32	2	1636	G
32	2	1638	G
32	2	1642	C
32	2	1643	U
32	2	1644	A
32	2	1646	C
32	2	1649	U
32	2	1650	G
32	2	1651	G
32	2	1652	C
32	2	1653	C
32	2	1656	G
32	2	1662	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1666	U
32	2	1667	A
32	2	1668	A
32	2	1669	U
32	2	1670	C
32	2	1672	U
32	2	1673	G
32	2	1675	G
32	2	1676	A
32	2	1681	C
32	2	1687	U
32	2	1688	G
32	2	1689	C
32	2	1690	U
32	2	1692	G
32	2	1693	G
32	2	1694	G
32	2	1695	A
32	2	1696	U
32	2	1697	A
32	2	1698	G
32	2	1700	G
32	2	1701	C
32	2	1703	U
32	2	1704	U
32	2	1705	G
32	2	1709	U
32	2	1710	U
32	2	1711	A
32	2	1713	U
32	2	1715	C
32	2	1716	U
32	2	1720	C
32	2	1721	A
32	2	1722	A
32	2	1732	C
32	2	1733	C
32	2	1734	U
32	2	1735	A
32	2	1736	G
32	2	1740	G
32	2	1742	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1743	C
32	2	1744	A
32	2	1745	A
32	2	1749	A
32	2	1750	U
32	2	1752	A
32	2	1753	G
32	2	1754	C
32	2	1755	U
32	2	1756	U
32	2	1757	G
32	2	1759	G
32	2	1765	U
32	2	1766	A
32	2	1767	C
32	2	1770	C
32	2	1771	C
32	2	1774	G
32	2	1775	C
32	2	1781	G
32	2	1782	U
32	2	1783	A
32	2	1786	C
32	2	1787	A
32	2	1788	C
32	2	1790	G
32	2	1791	C
32	2	1792	C
32	2	1793	C
32	2	1794	G
32	2	1795	U
32	2	1797	G
32	2	1798	C
32	2	1799	U
32	2	1800	A
32	2	1801	G
32	2	1802	U
32	2	1803	A
32	2	1804	C
32	2	1805	C
32	2	1807	A
32	2	1809	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	2	1811	A
32	2	1812	A
32	2	1821	U
32	2	1826	C
32	2	1827	C
32	2	1838	C
32	2	1839	U
32	2	1841	A
32	2	1844	G
32	2	1845	A
32	2	1846	A
32	2	1847	G
32	2	1848	G
32	2	1850	G
32	2	1851	G
32	2	1852	C
32	2	1853	A
32	2	1855	C
32	2	1858	C
32	2	1861	C
32	2	1863	C
32	2	1864	A
32	2	1865	G
32	2	1867	G
32	2	1869	G
32	2	1882	A
32	2	1884	A
32	2	1888	G
32	2	1891	C
32	2	1893	U
32	2	1894	U
32	2	1895	U
32	2	1896	A
32	2	1897	G
32	2	1900	G
32	2	1901	A
32	2	1905	A
32	2	1906	A
32	2	1907	A
32	2	1909	G

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	2	541	U
32	2	826	U
32	2	856	U
32	2	1056	G
32	2	1108	A
32	2	1168	U
32	2	1181	U
32	2	1346	A
32	2	1358	U
32	2	1383	U
32	2	1430	G
32	2	1431	C
32	2	1495	U
32	2	1502	U
32	2	1578	C
32	2	1605	G
32	2	1633	C
32	2	1643	U
32	2	1667	A
32	2	1734	U
32	2	1753	G
32	2	1866	A

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
32	2	34
29	f	3
14	P	3
10	K	1
5	F	1
3	D	1
31	k	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1169:C	O3'	1170:U	P	30.51
1	2	921:C	O3'	922:G	P	23.31
1	2	1128:U	O3'	1129:A	P	22.80
1	2	1588:A	O3'	1589:U	P	17.38
1	2	1616:G	O3'	1617:C	P	13.69
1	f	137:ASP	C	138:ARG	N	12.35
1	2	1179:A	O3'	1180:C	P	11.43
1	2	1859:A	O3'	1860:U	P	11.20
1	2	1164:U	O3'	1165:U	P	10.82
1	2	1165:U	O3'	1166:A	P	10.56
1	2	1784:C	O3'	1785:A	P	10.46
1	2	1182:A	O3'	1183:U	P	10.22
1	2	1184:G	O3'	1185:C	P	9.57
1	2	1590:G	O3'	1591:C	P	7.83
1	2	1609:C	O3'	1610:G	P	7.76
1	f	136:LYS	C	137:ASP	N	6.90
1	2	1586:U	O3'	1587:G	P	6.33
1	2	1180:C	O3'	1181:U	P	6.32
1	2	1183:U	O3'	1184:G	P	6.23
1	2	1858:C	O3'	1859:A	P	6.11
1	2	1591:C	O3'	1592:C	P	5.49
1	2	1297:U	O3'	1298:G	P	5.36
1	2	1163:A	O3'	1164:U	P	4.79
1	K	26:ASP	C	27:PHE	N	4.75
1	2	1783:A	O3'	1784:C	P	4.69
1	2	1595:U	O3'	1596:A	P	4.65
1	f	129:GLY	C	130:VAL	N	4.44
1	2	1176:U	O3'	1177:A	P	4.40

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	224:ASN	C	225:ARG	N	4.34
1	2	1522:U	O3'	1523:A	P	4.21
1	2	1177:A	O3'	1178:A	P	3.95
1	P	79:HIS	C	80:MET	N	3.90
1	2	1205:G	O3'	1206:U	P	3.58
1	2	1280:A	O3'	1281:U	P	3.32
1	2	1529:U	O3'	1530:U	P	3.32
1	D	224:ASP	C	225:TYR	N	3.22
1	2	1647:C	O3'	1648:U	P	3.20
1	2	1193:G	O3'	1194:G	P	3.18
1	2	1351:G	O3'	1352:G	P	3.18
1	P	70:ASN	C	71:GLU	N	3.17
1	2	1223:U	O3'	1224:C	P	3.17
1	k	60:GLN	C	61:LEU	N	3.16
1	P	108:ARG	C	109:PRO	N	3.14
1	2	1587:G	O3'	1588:A	P	3.11
1	C	60:SER	C	61:LEU	N	1.19

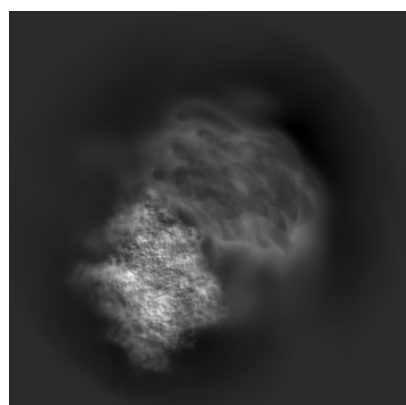
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21644. These allow visual inspection of the internal detail of the map and identification of artifacts.

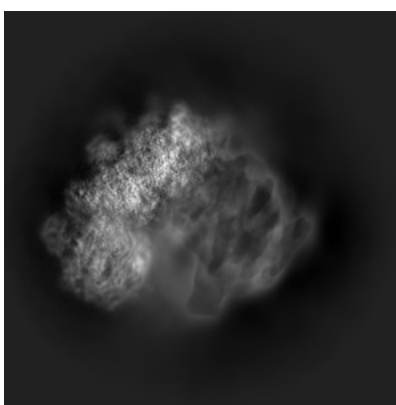
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

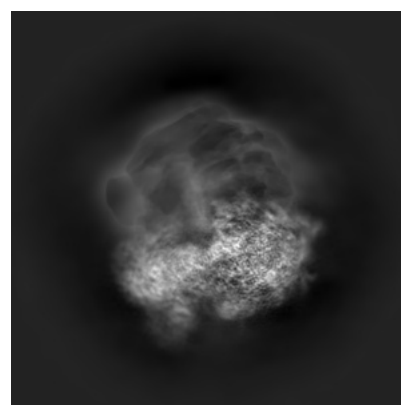
6.1.1 Primary map



X



Y

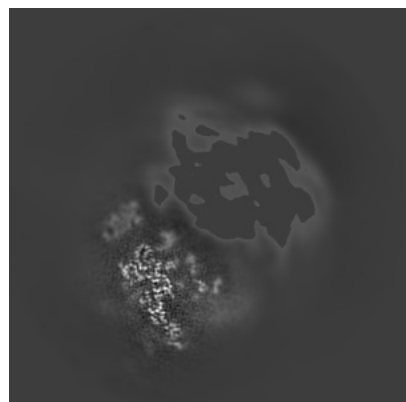


Z

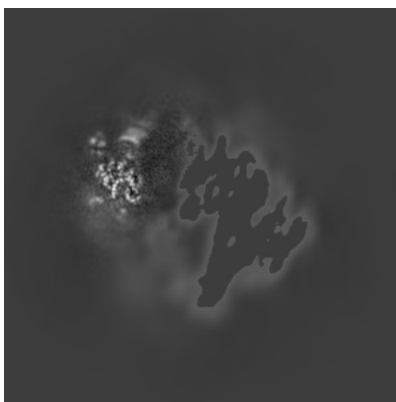
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192

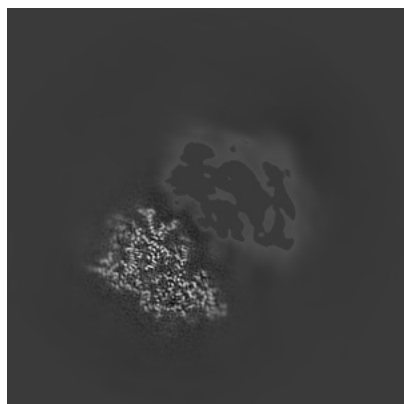


Z Index: 192

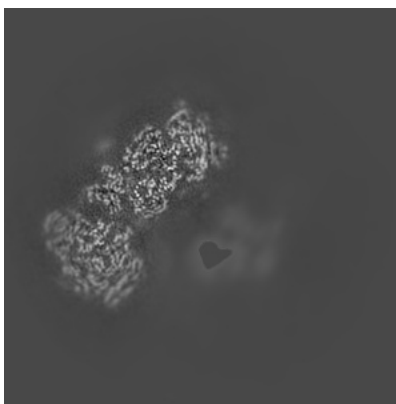
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

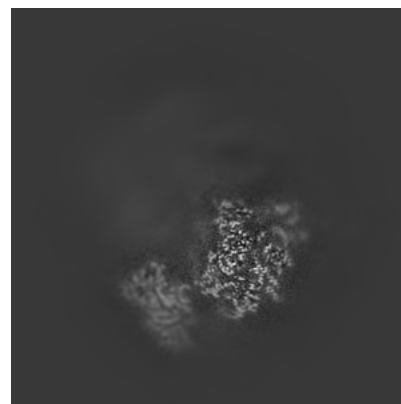
6.3.1 Primary map



X Index: 224



Y Index: 131

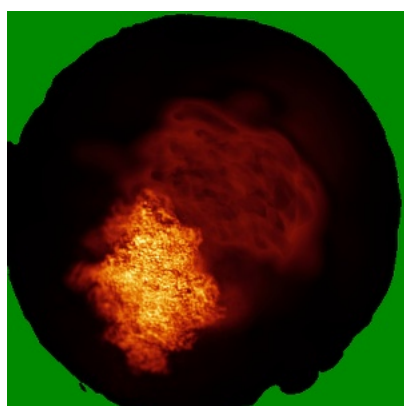


Z Index: 127

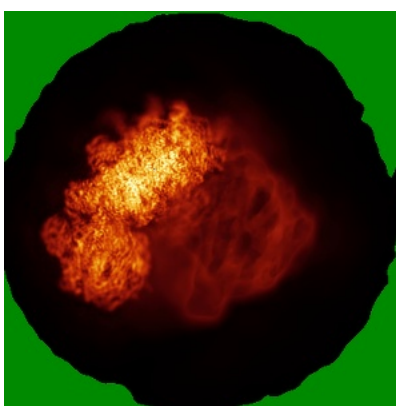
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

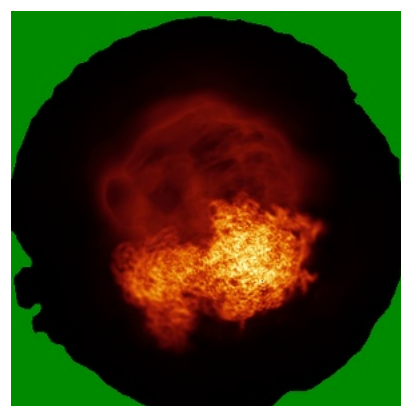
6.4.1 Primary map



X



Y

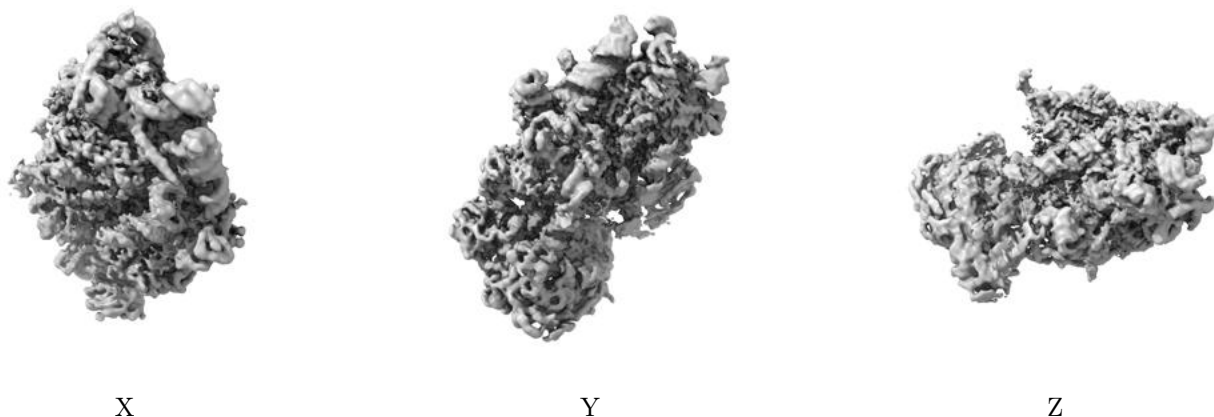


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

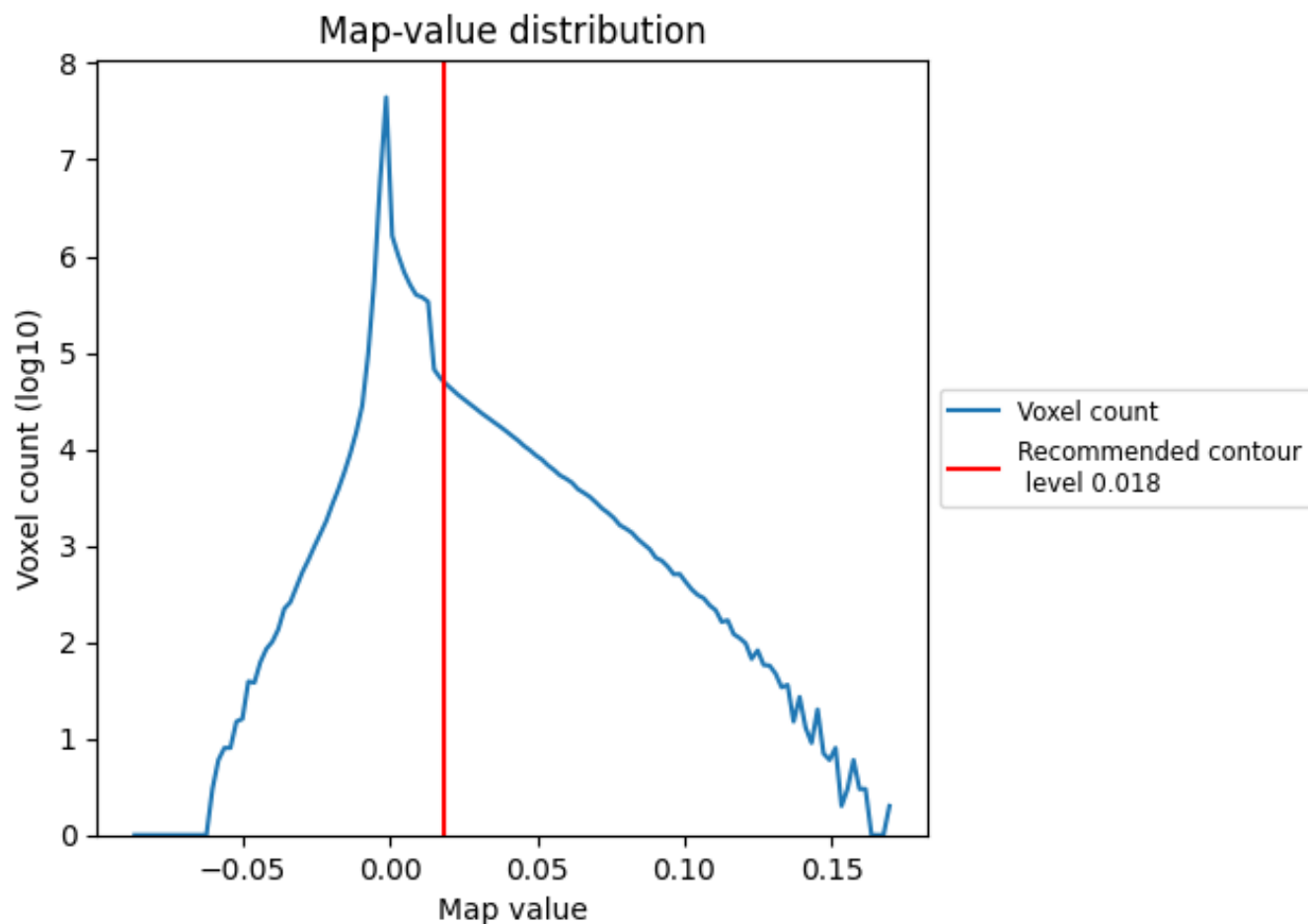
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

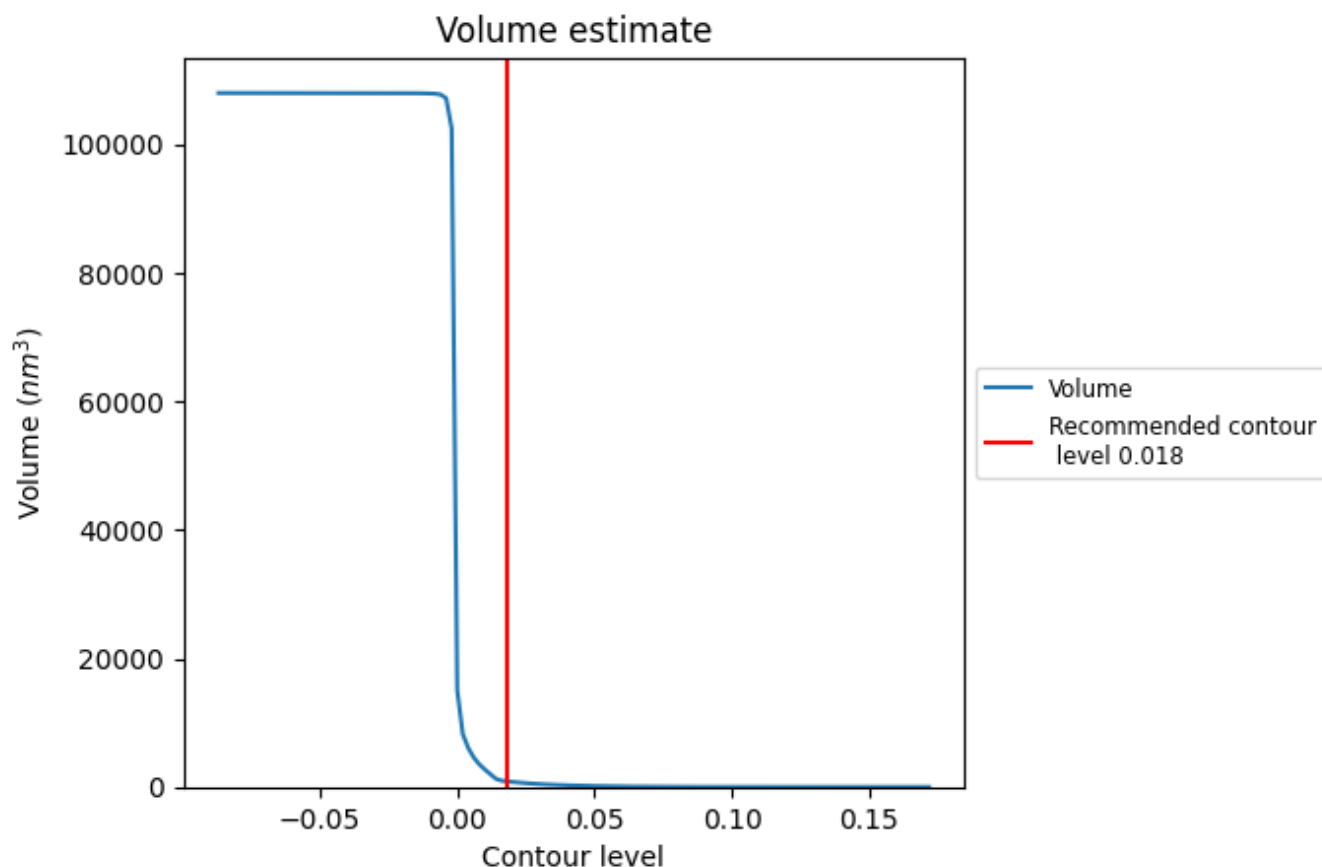
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

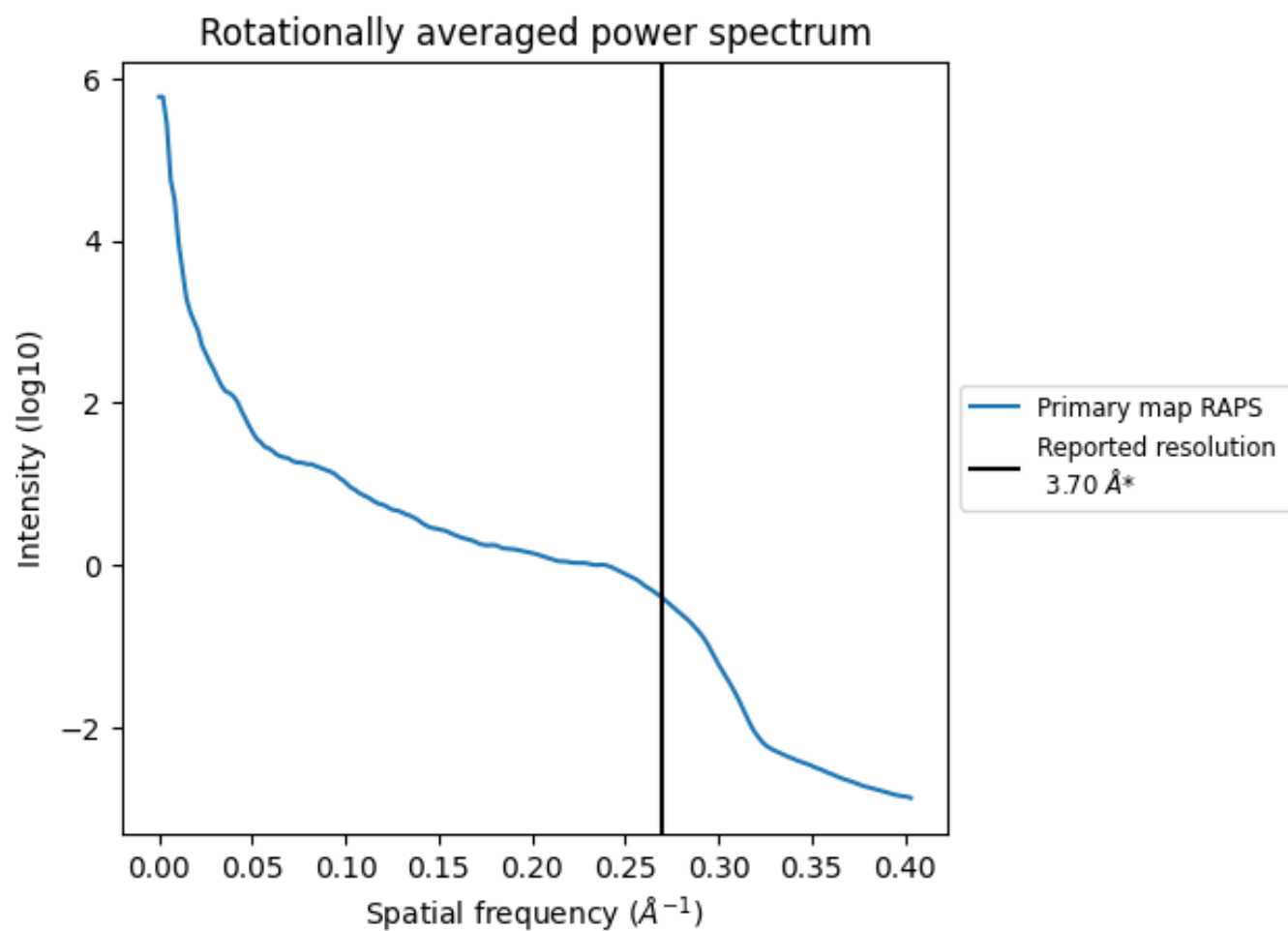
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 881 nm^3 ; this corresponds to an approximate mass of 796 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

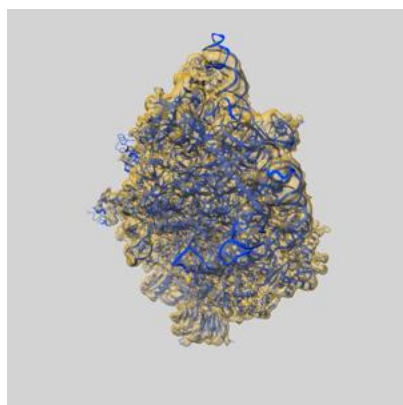
8 Fourier-Shell correlation

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

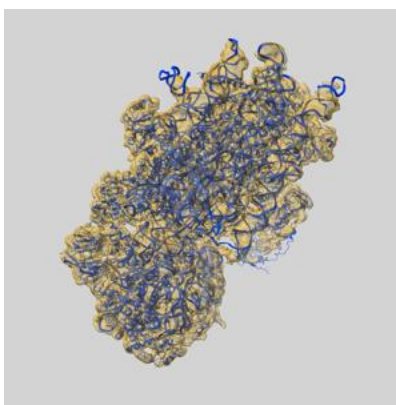
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21644 and PDB model 6WDR. Per-residue inclusion information can be found in section [3](#) on page [9](#).

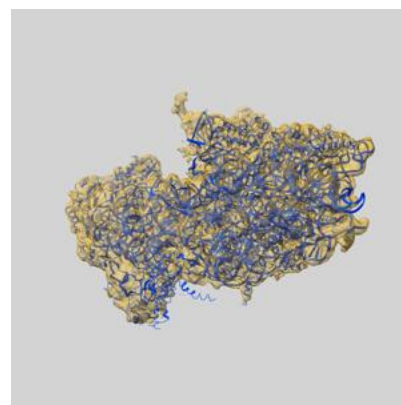
9.1 Map-model overlay [i](#)



X



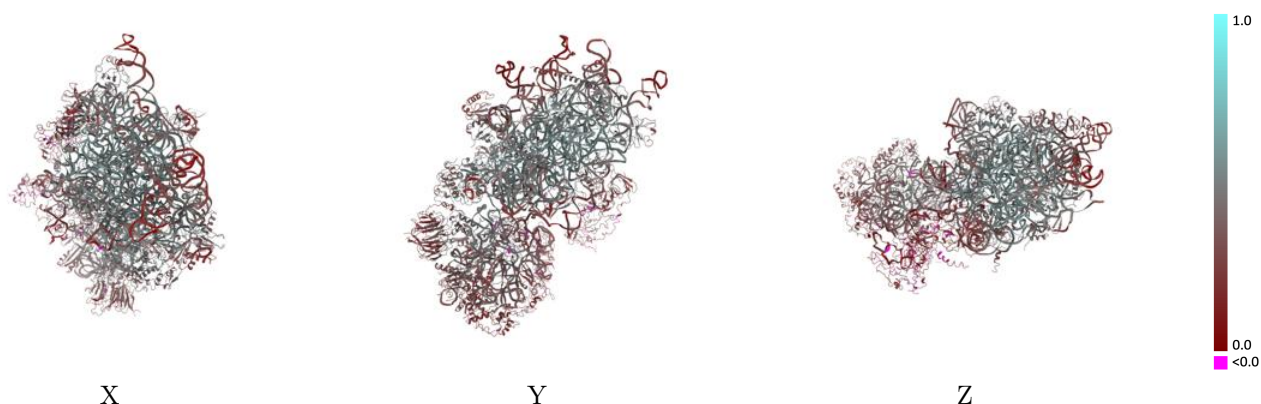
Y



Z

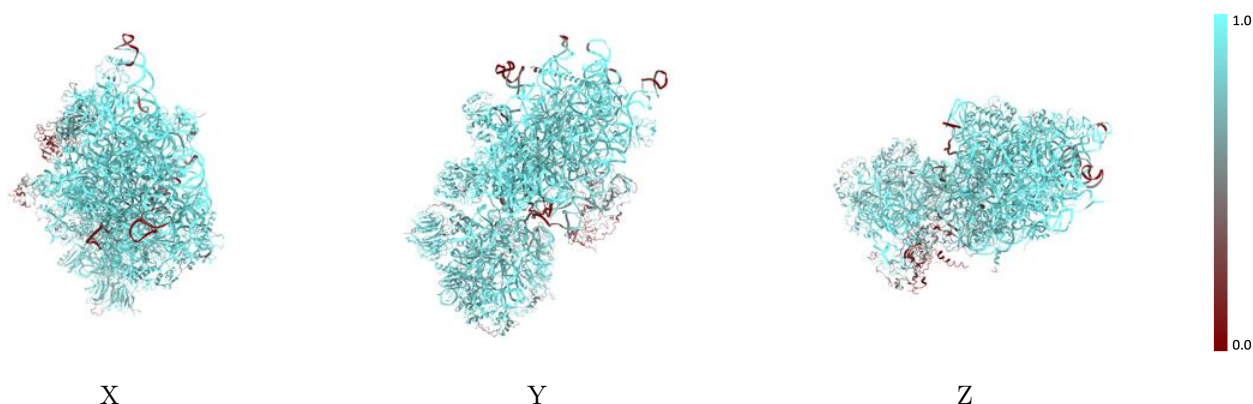
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



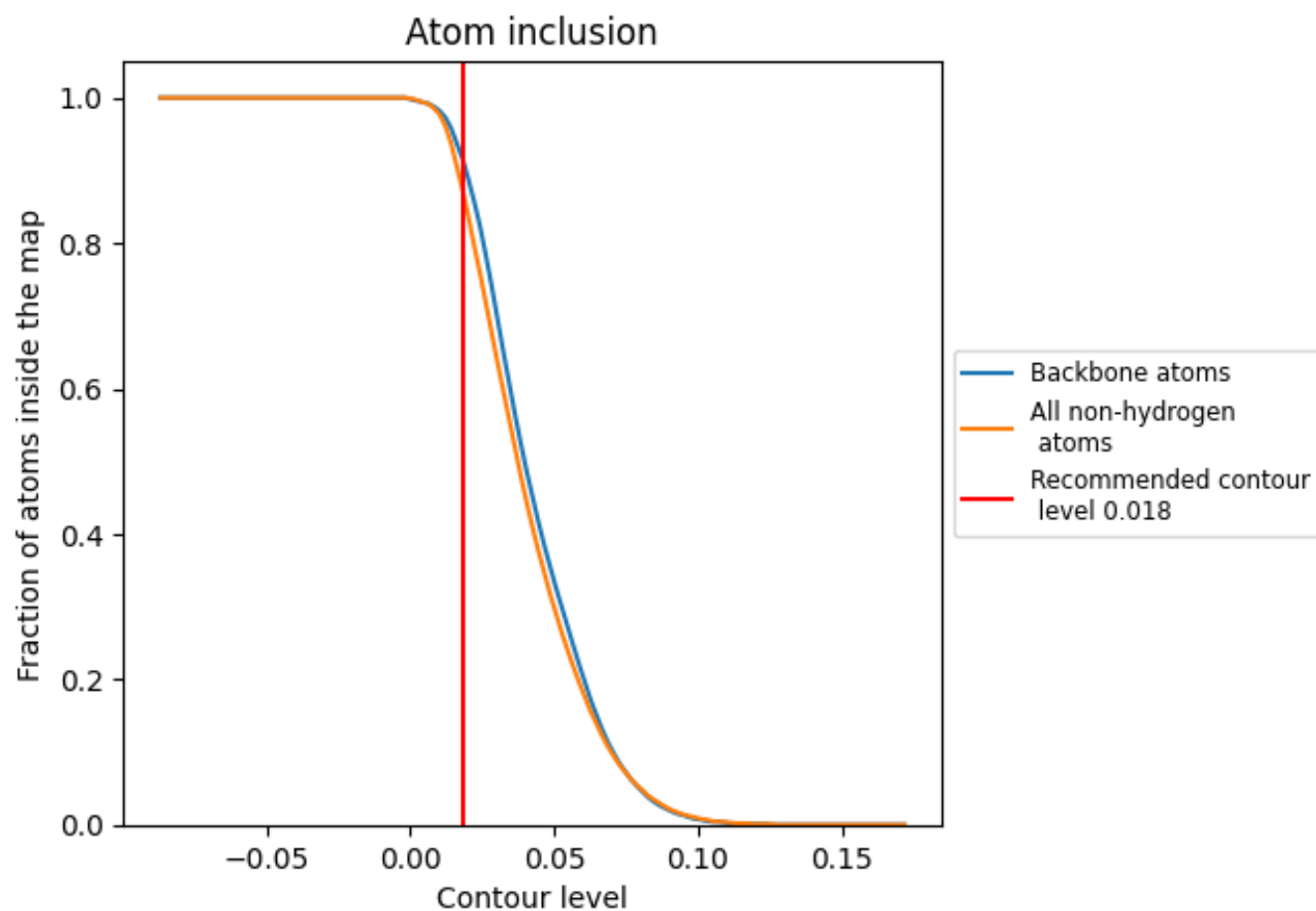
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).



































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.3970
2	 0.9390	 0.4170
A	 0.9480	 0.4780
C	 0.9450	 0.5100
D	 0.7440	 0.2880
E	 0.9580	 0.5260
F	 0.7810	 0.3070
G	 0.9140	 0.4250
H	 0.8810	 0.3970
I	 0.9190	 0.4800
J	 0.9490	 0.4960
K	 0.8360	 0.2430
L	 0.9550	 0.5420
M	 0.4310	 0.1370
N	 0.9010	 0.4590
P	 0.8070	 0.2300
Q	 0.8950	 0.3780
R	 0.8460	 0.3910
S	 0.7420	 0.2260
T	 0.8940	 0.3060
U	 0.8350	 0.3810
V	 0.9350	 0.5080
W	 0.9790	 0.5620
X	 0.9040	 0.4970
Y	 0.9440	 0.4850
Z	 0.7460	 0.2200
b	 0.9500	 0.4720
c	 0.6980	 0.3250
d	 0.9280	 0.4310
e	 0.6850	 0.4080
f	 0.6110	 0.1540
g	 0.8470	 0.3050
k	 0.5170	 0.2580

