



## Full wwPDB EM Validation Report ⓘ

Mar 9, 2023 – 10:38 am GMT

PDB ID : 8B6C  
EMDB ID : EMD-15863  
Title : Cryo-EM structure of ribosome-Sec61 in complex with cyclotriazadisulfonamide derivative CK147  
Authors : Pauwels, E.; Shewakramani, N.R.; De Wijngaert, B.; Vermeire, K.; Das, K.  
Deposited on : 2022-09-26  
Resolution : 2.79 Å (reported)  
Based on initial models : 3J7Q, 6MTE

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

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

A user guide is available at

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

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

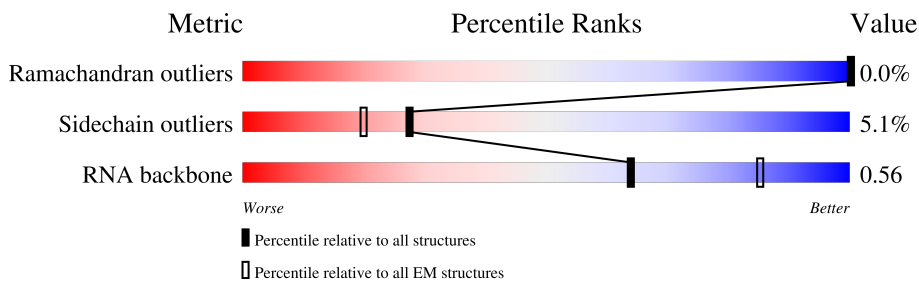
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.1

# 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 2.79 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.





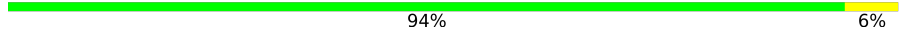

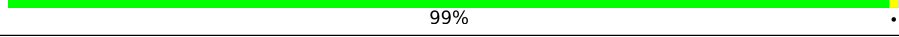


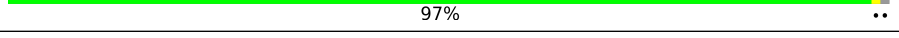
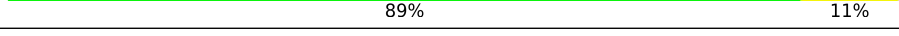
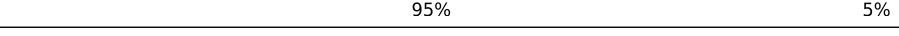
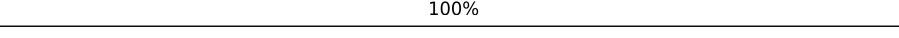
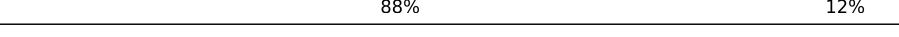
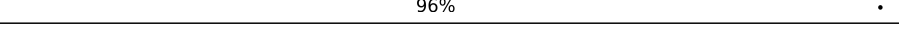
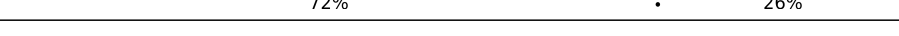
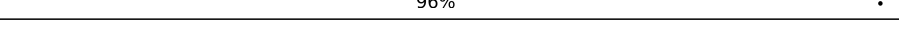

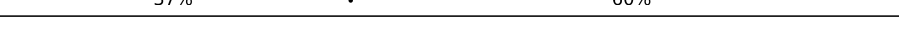
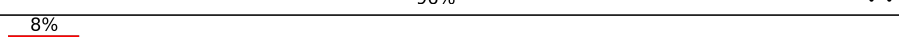
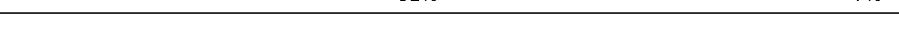






Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	159	
2	5	4808	
3	F	225	
4	D	293	
5	S	176	
6	b	245	
7	B	394	
8	d	107	

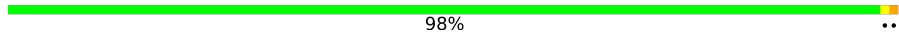
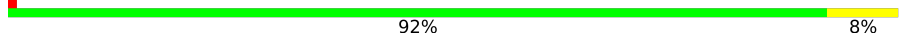

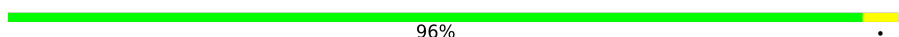
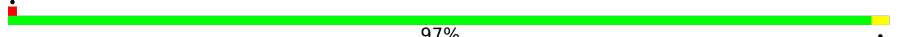

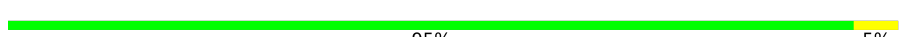



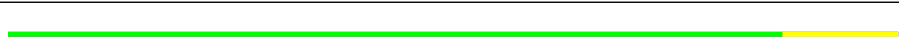


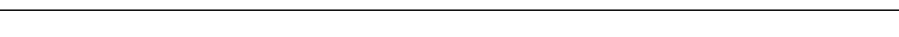
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Mol	Chain	Length	Quality of chain
9	8	156	 80% 17%
10	G	319	 70% 27%
11	J	170	 94% 6%
12	c	98	 90% 10%
13	j	86	 99%
14	A	257	 91% 5%
15	I	214	 90% 6%
16	q	68	 97%
17	p	91	 89% 11%
18	V	131	 95% 5%
19	m	52	 100%
20	l	50	 88% 12%
21	P	153	 96%
22	E	291	 72% 26%
23	Q	188	 96%
24	R	196	 85% 7% 8%
25	W	157	 37% 60%
26	O	203	 96%
27	K	476	 92% 7%
28	C	362	 97%
29	o	103	 95% 5%
30	r	124	 94% 6%
31	f	109	 96%
32	e	128	 98%
33	Z	135	 93% 7%

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Mol	Chain	Length	Quality of chain
34	a	147	 98%
35	g	114	 92% 8%
36	k	70	 90% 9%
37	H	190	 96%
38	L	211	 97%
39	7	120	 90% 10%
40	N	203	 95% 5%
41	i	105	 89% 9%
42	h	122	 94% 6%
43	M	138	 98%
44	Y	134	 87% 13%
45	X	118	 95% 5%
46	U	99	 88% 12%
47	n	25	 76% 24%

## 2 Entry composition [i](#)

There are 50 unique types of molecules in this entry. The entry contains 139959 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 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	T	159	1298	823	252	217	6	0	0

- Molecule 2 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	5	3619	77665	34619	14204	25223	3619	0	0

- Molecule 3 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	225	1875	1205	358	303	9	0	0

- Molecule 4 is a protein called Ribosomal\_L18\_c domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	293	2391	1512	438	427	14	0	0

- Molecule 5 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	S	176	1462	930	285	236	11	0	0

- Molecule 6 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	b	104	848	527	189	129	3	0	0

- Molecule 7 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	B	394	3172	2020	597	542	13	0	0

- Molecule 8 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	d	107	888	560	171	155	2	0	0

- Molecule 9 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	8	151	3208	1432	564	1062	150	0	0

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	233	1879	1199	361	315	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 11 is a protein called 60S ribosomal protein L11.

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

- Molecule 12 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	c	98	761	481	134	140	6	0	0

- Molecule 13 is a protein called Ribosomal protein L37.

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

- Molecule 14 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 15 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 16 is a protein called Protein transport protein Sec61 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	q	67	Total	C	N	O	S	0	0
			535	350	93	88	4		

- Molecule 17 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 18 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 19 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	m	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 20 is a protein called 60S ribosomal protein L39-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 21 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 22 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 23 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	134	ARG	CYS	conflict	UNP F6QKI9

- Molecule 24 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 25 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	63	Total	C	N	O	S	0	0
			528	337	103	85	3		

- Molecule 26 is a protein called 60S ribosomal protein L13a.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 27 is a protein called Protein transport protein Sec61 subunit alpha isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	K	444	Total	C	N	O	S	0	0
			3427	2243	555	607	22		

- Molecule 28 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	C	362	Total	C	N	O	S	0	0
			2884	1813	577	480	14		

- Molecule 29 is a protein called 60S ribosomal protein L36a-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	o	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 31 is a protein called 60S ribosomal protein L35a.

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

- Molecule 32 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 33 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	135	1107	714	208	182	3	0	0

- Molecule 34 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	a	147	1162	734	239	185	4	0	0

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	g	114	906	566	187	147	6	0	0

- Molecule 36 is a protein called 60S ribosomal protein L38.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 37 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	H	190	1516	954	284	272	6	0	0

- Molecule 38 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	L	210	1702	1065	354	279	4	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	74	ARG	HIS	conflict	UNP G1TKB3

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Chain	Residue	Modelled	Actual	Comment	Reference
L	190	ARG	HIS	conflict	UNP G1TKB3

- Molecule 39 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
39	7	120	2558	1141	456	842	119	0	0

- Molecule 40 is a protein called Ribosomal protein L15.

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

- Molecule 41 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	i	102	830	520	176	129	5	0	0

- Molecule 42 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h	122	1013	640	204	168	1	0	0

- Molecule 43 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	M	138	1137	727	221	182	7	0	0

- Molecule 44 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Y	134	1115	700	226	186	3	0	0

- Molecule 45 is a protein called Ribosomal\_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	X	118	967	618	181	167	1	0	0

- Molecule 46 is a protein called 60S ribosomal protein L22 (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	U	99	809	519	141	147	2	0	0

- Molecule 47 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	n	25	239	145	64	27	3	0	0

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
48	5	161	161	161	0
48	8	5	5	5	0
48	A	1	1	1	0
48	I	1	1	1	0
48	V	1	1	1	0
48	P	1	1	1	0
48	a	1	1	1	0
48	7	7	7	7	0

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

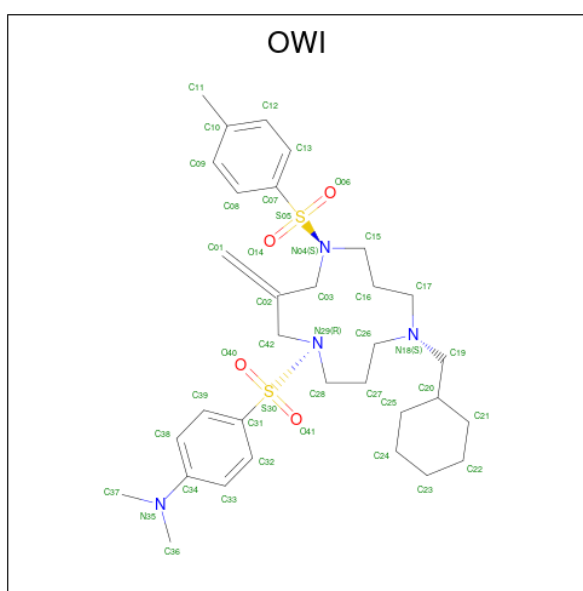
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
49	j	1	1	1	0
49	p	1	1	1	0

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Mol	Chain	Residues	Atoms	AltConf
49	m	1	Total Zn 1 1	0
49	o	1	Total Zn 1 1	0
49	g	1	Total Zn 1 1	0

- Molecule 50 is 4-[[9-(cyclohexylmethyl)-3-methylidene-5-(4-methylphenyl)sulfonyl-1,5,9-triazacyclododec-1-yl]sulfonyl]-{N}, {N}-dimethyl-aniline (three-letter code: OWI) (formula:  $C_{32}H_{48}N_4O_4S_2$ ) (labeled as "Ligand of Interest" by depositor).



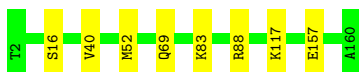
Mol	Chain	Residues	Atoms	AltConf
50	K	1	Total C N O S 42 32 4 4 2	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

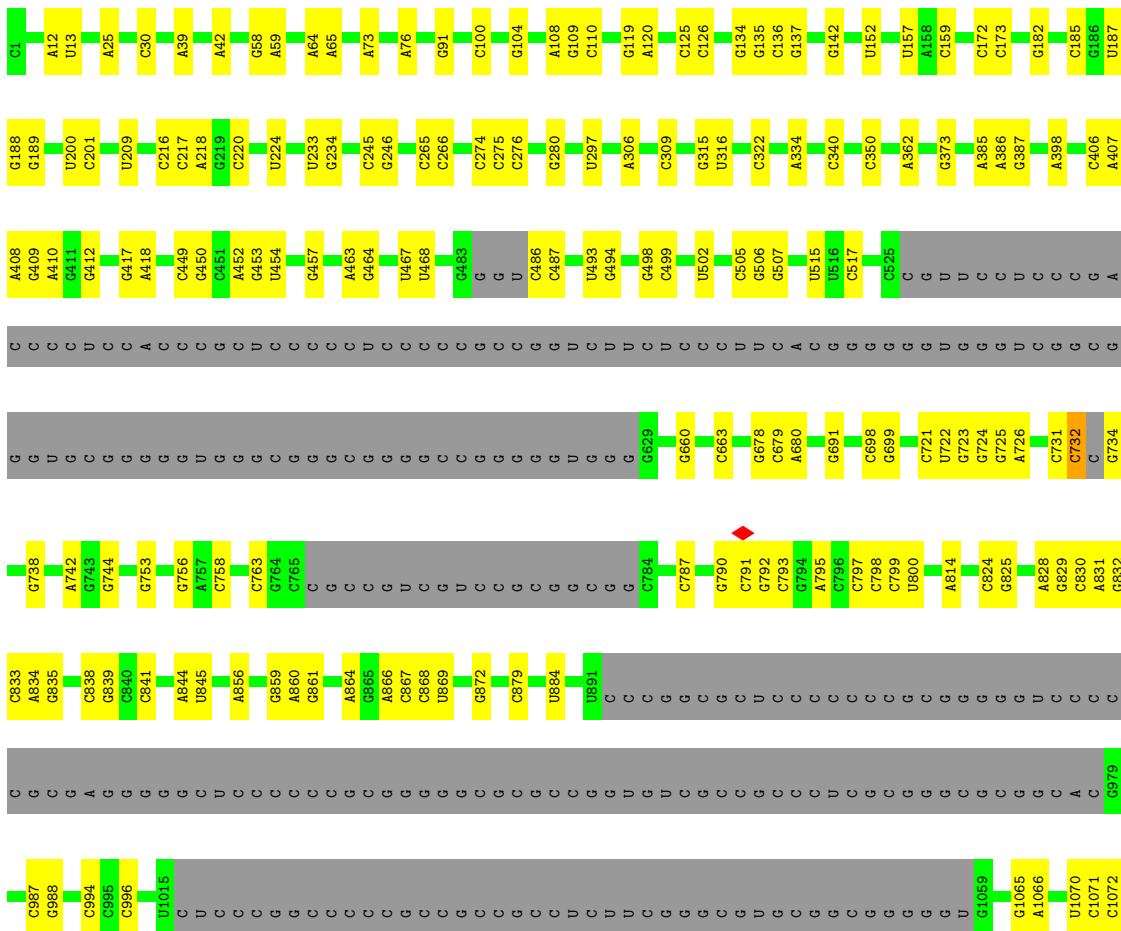
- Molecule 1: 60S ribosomal protein L21

Chain T:  95% 5%

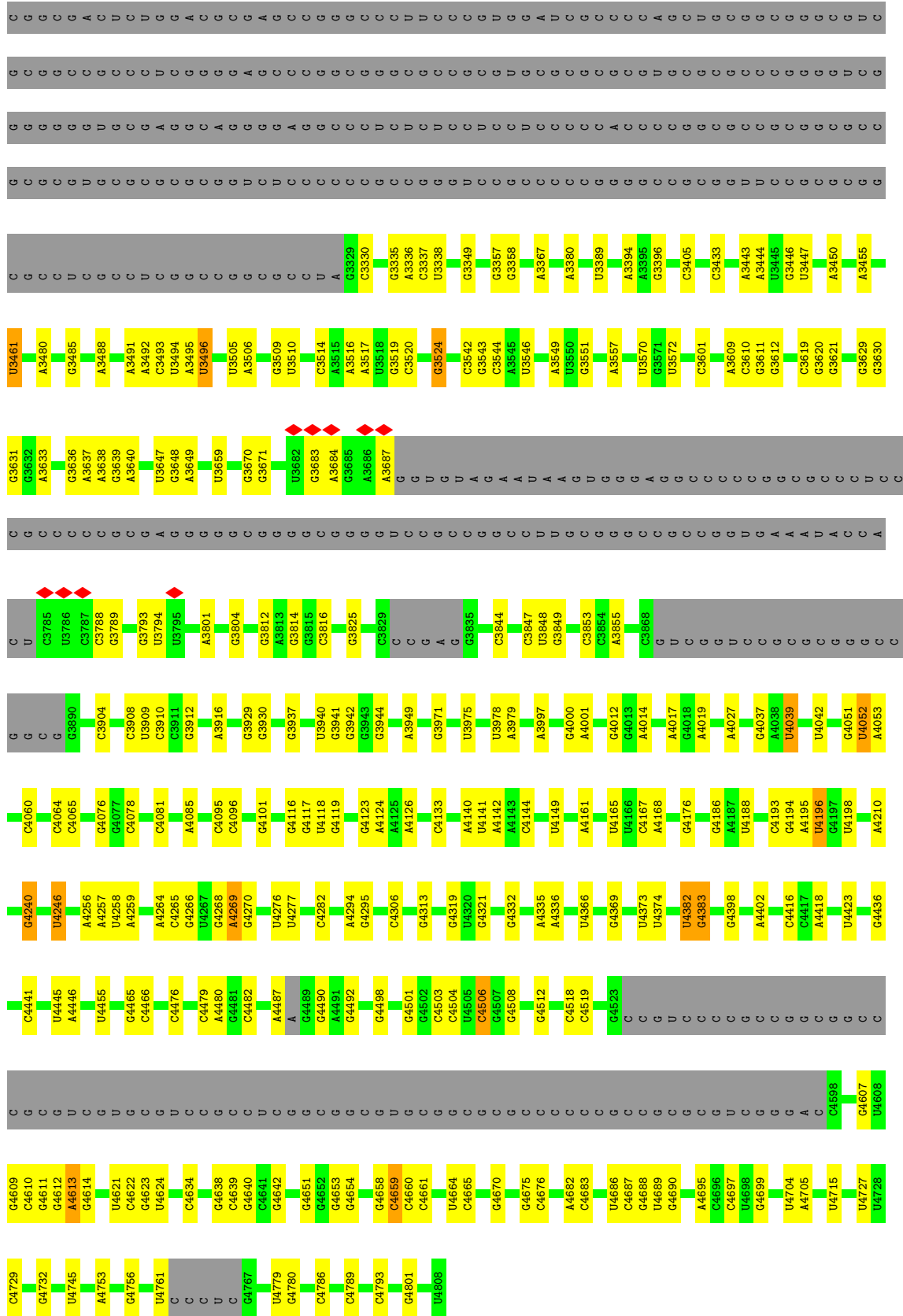


- Molecule 2: 28S rRNA

Chain 5:  59% 16% 25%







• Molecule 3: 60S ribosomal protein L7

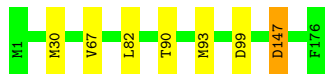




- Molecule 4: Ribosomal\_L18\_c domain-containing protein



- Molecule 5: 60S ribosomal protein L18a



- Molecule 6: 60S ribosomal protein L29



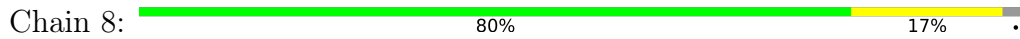
- Molecule 7: Ribosomal protein L3



- Molecule 8: 60S ribosomal protein L31

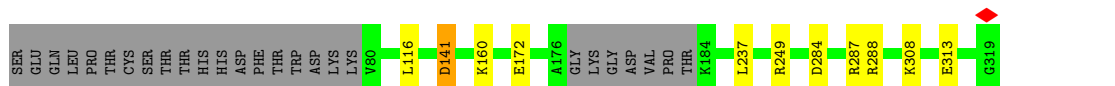
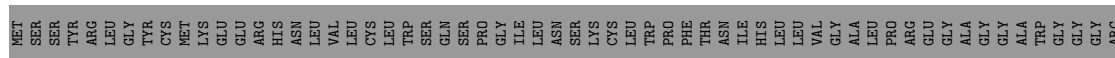


- Molecule 9: 5.8S rRNA





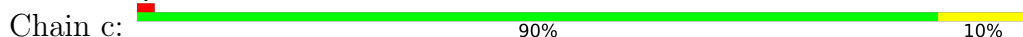
• Molecule 10: 60S ribosomal protein L7a



• Molecule 11: 60S ribosomal protein L11



• Molecule 12: 60S ribosomal protein L30



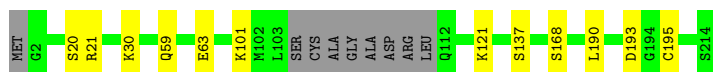
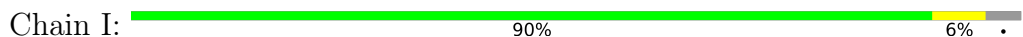
• Molecule 13: Ribosomal protein L37



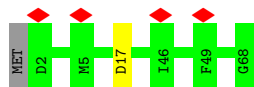
• Molecule 14: Ribosomal protein L8



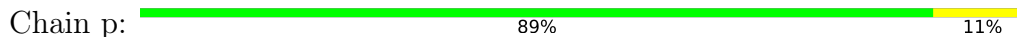
• Molecule 15: Ribosomal protein L10



• Molecule 16: Protein transport protein Sec61 subunit gamma



• Molecule 17: 60S ribosomal protein L37a



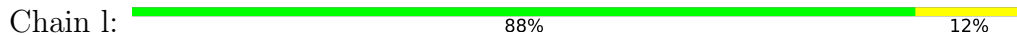
• Molecule 18: 60S ribosomal protein L23



• Molecule 19: 60S ribosomal protein L40



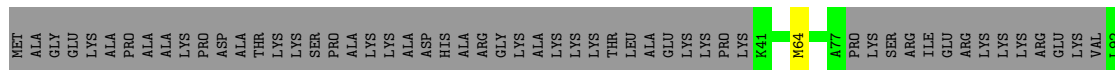
• Molecule 20: 60S ribosomal protein L39-like

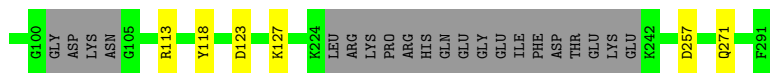


• Molecule 21: 60S ribosomal protein L17



• Molecule 22: 60S ribosomal protein L6

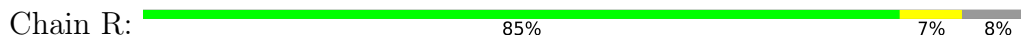




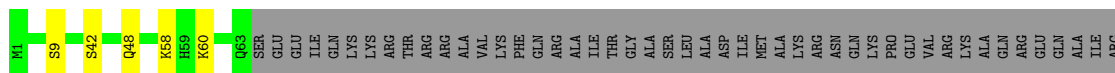
• Molecule 23: eL18



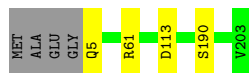
• Molecule 24: 60S ribosomal protein L19



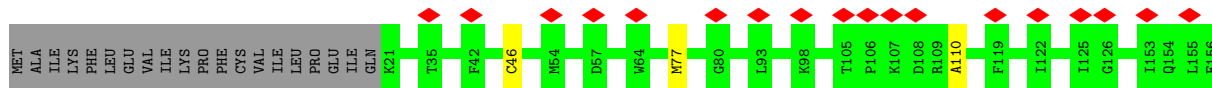
• Molecule 25: Ribosomal protein L24



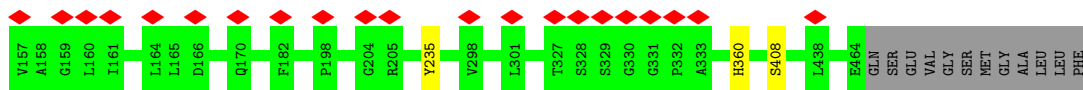
• Molecule 26: 60S ribosomal protein L13a

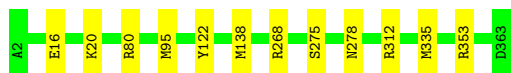


• Molecule 27: Protein transport protein Sec61 subunit alpha isoform 1



• Molecule 28: 60S ribosomal protein L4





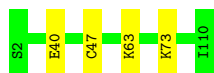
- Molecule 29: 60S ribosomal protein L36a-like



- Molecule 30: 60S ribosomal protein L28



- Molecule 31: 60S ribosomal protein L35a



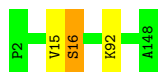
- Molecule 32: Ribosomal protein L32



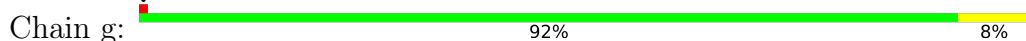
- Molecule 33: 60S ribosomal protein L27



- Molecule 34: 60S ribosomal protein L27a



- Molecule 35: 60S ribosomal protein L34

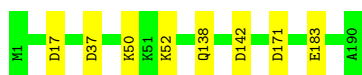




- Molecule 36: 60S ribosomal protein L38



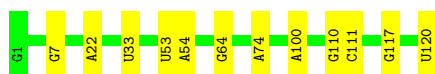
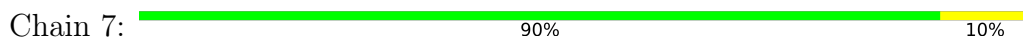
- Molecule 37: 60S ribosomal protein L9



- Molecule 38: 60S ribosomal protein L13



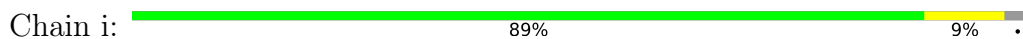
- Molecule 39: 5S rRNA



- Molecule 40: Ribosomal protein L15



- Molecule 41: 60S ribosomal protein L36



- Molecule 42: 60S ribosomal protein L35





- Molecule 43: 60S ribosomal protein L14

Chain M: 98%



- Molecule 44: Ribosomal protein L26

Chain Y: 87%



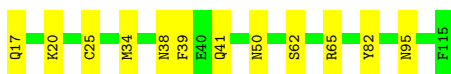
- Molecule 45: Ribosomal\_L23eN domain-containing protein

Chain X: 95%



- Molecule 46: 60S ribosomal protein L22 (Fragment)

Chain U: 88%



- Molecule 47: 60S ribosomal protein L41

Chain n: 76%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132229	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	0.8	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.425	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.01581	Depositor
Map size ( $\text{\AA}$ )	432.96002, 432.96002, 432.96002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.23, 1.23, 1.23	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, P4U, BGH, B8K, OMG, OMC, E7G, OMU, I4U, PSU, B8H, A2M, 1MA, ZN, E6G, MG, UR3, MLZ, OWI, 7MG, P7G

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	T	0.34	0/1326	0.60	0/1770
2	5	0.42	4/85271 (0.0%)	0.79	17/132978 (0.0%)
3	F	0.31	0/1911	0.53	0/2549
4	D	0.33	0/2437	0.56	0/3264
5	S	0.33	0/1501	0.61	2/2012 (0.1%)
6	b	0.31	0/861	0.68	1/1138 (0.1%)
7	B	0.30	0/3240	0.55	0/4339
8	d	0.39	0/903	0.61	0/1216
9	8	0.39	0/3581	0.74	0/5577
10	G	0.33	0/1910	0.61	1/2569 (0.0%)
11	J	0.33	0/1385	0.68	0/1852
12	c	0.31	0/771	0.61	1/1034 (0.1%)
13	j	0.32	0/720	0.60	0/952
14	A	0.37	0/1936	0.61	0/2596
15	I	0.36	0/1702	0.59	1/2272 (0.0%)
16	q	0.30	0/545	0.67	1/728 (0.1%)
17	p	0.34	0/718	0.57	0/953
18	V	0.38	0/993	0.58	0/1332
19	m	0.33	0/425	0.64	0/561
20	l	0.27	0/459	0.59	0/608
21	P	0.33	0/1268	0.62	0/1700
22	E	0.30	0/1762	0.57	0/2362
23	Q	0.31	0/1539	0.63	0/2054
24	R	0.29	0/1524	0.64	0/2013
25	W	0.32	0/541	0.58	0/720
26	O	0.32	0/1662	0.57	0/2222
27	K	0.54	0/3502	0.68	0/4749
28	C	0.35	0/2927	0.58	0/3932
29	o	0.34	0/855	0.61	0/1128
30	r	0.35	0/1010	0.60	0/1354
31	f	0.33	0/895	0.61	0/1198

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	e	0.30	0/1071	0.57	0/1429
33	Z	0.35	0/1130	0.61	2/1507 (0.1%)
34	a	0.30	0/1191	0.77	3/1590 (0.2%)
35	g	0.31	0/916	0.62	0/1220
36	k	0.35	0/575	0.70	0/761
37	H	0.32	0/1535	0.61	2/2063 (0.1%)
38	L	0.33	0/1733	0.62	0/2316
39	7	0.39	0/2858	0.75	0/4455
40	N	0.36	0/1746	0.62	0/2338
41	i	0.29	0/841	0.62	0/1112
42	h	0.28	0/1021	0.58	0/1348
43	M	0.33	0/1158	0.60	0/1547
44	Y	0.32	0/1132	0.63	0/1504
45	X	0.31	0/984	0.68	1/1323 (0.1%)
46	U	0.37	0/823	0.82	1/1104 (0.1%)
47	n	0.26	0/240	0.80	0/305
All	All	0.39	4/149034 (0.0%)	0.73	33/219654 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	732	C	O3'-P	25.73	1.92	1.61
2	5	1390	G	O3'-P	23.27	1.89	1.61
2	5	1392	C	O3'-P	-17.11	1.40	1.61
2	5	731	C	O3'-P	-13.81	1.44	1.61

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	731	C	OP1-P-O3'	-26.75	46.34	105.20
34	a	16	SER	N-CA-CB	17.07	136.11	110.50
2	5	731	C	O3'-P-O5'	14.20	130.97	104.00
34	a	15	VAL	N-CA-C	-10.40	82.92	111.00
2	5	732	C	P-O3'-C3'	-8.94	108.97	119.70
2	5	731	C	OP2-P-O3'	7.37	121.42	105.20
2	5	732	C	O3'-P-O5'	6.54	116.42	104.00
2	5	2253	C	C2-N1-C1'	6.24	125.66	118.80
15	I	193	ASP	CB-CG-OD1	6.17	123.86	118.30
33	Z	103	ASP	CB-CG-OD1	6.14	123.83	118.30
2	5	1594	U	C2-N1-C1'	6.12	125.04	117.70
2	5	732	C	O4'-C4'-C3'	-5.82	98.18	104.00
2	5	100	C	C2-N1-C1'	5.81	125.19	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	732	C	C5'-C4'-O4'	-5.75	102.20	109.10
46	U	41	GLN	CA-CB-CG	5.72	125.99	113.40
5	S	147	ASP	CB-CG-OD1	5.70	123.43	118.30
2	5	1372	C	C2-N1-C1'	5.65	125.02	118.80
2	5	4659	C	N3-C2-O2	-5.64	117.95	121.90
6	b	36	ASP	CB-CG-OD1	5.59	123.34	118.30
12	c	103	ASP	CB-CG-OD1	5.57	123.31	118.30
37	H	142	ASP	CB-CG-OD1	5.45	123.21	118.30
37	H	17	ASP	CB-CG-OD1	5.40	123.16	118.30
2	5	4659	C	N1-C2-O2	5.40	122.14	118.90
34	a	15	VAL	CB-CA-C	-5.38	101.18	111.40
33	Z	92	ASP	CB-CG-OD1	5.30	123.07	118.30
45	X	71	LEU	CA-CB-CG	5.28	127.43	115.30
10	G	141	ASP	CB-CG-OD1	5.18	122.97	118.30
2	5	4613	A	O4'-C1'-N9	5.16	112.33	108.20
16	q	17	ASP	CB-CG-OD1	5.10	122.89	118.30
5	S	82	LEU	CA-CB-CG	5.10	127.03	115.30
2	5	4506	C	N1-C2-O2	5.03	121.92	118.90
2	5	2504	U	P-O3'-C3'	5.02	125.72	119.70
2	5	1594	U	N1-C2-O2	5.01	126.31	122.80

There are no chirality outliers.

There are no planarity outliers.

## 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	T	157/159 (99%)	153 (98%)	4 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
4	D	291/293 (99%)	284 (98%)	7 (2%)	0	100	100
5	S	174/176 (99%)	168 (97%)	6 (3%)	0	100	100
6	b	100/245 (41%)	97 (97%)	3 (3%)	0	100	100
7	B	392/394 (100%)	382 (97%)	10 (3%)	0	100	100
8	d	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
10	G	229/319 (72%)	219 (96%)	10 (4%)	0	100	100
11	J	168/170 (99%)	159 (95%)	9 (5%)	0	100	100
12	c	96/98 (98%)	96 (100%)	0	0	100	100
13	j	84/86 (98%)	84 (100%)	0	0	100	100
14	A	246/257 (96%)	229 (93%)	17 (7%)	0	100	100
15	I	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
16	q	65/68 (96%)	65 (100%)	0	0	100	100
17	p	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
18	V	129/131 (98%)	128 (99%)	1 (1%)	0	100	100
19	m	49/52 (94%)	46 (94%)	3 (6%)	0	100	100
20	l	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
21	P	151/153 (99%)	148 (98%)	3 (2%)	0	100	100
22	E	208/291 (72%)	198 (95%)	9 (4%)	1 (0%)	29	61
23	Q	185/188 (98%)	175 (95%)	10 (5%)	0	100	100
24	R	178/196 (91%)	174 (98%)	4 (2%)	0	100	100
25	W	61/157 (39%)	58 (95%)	3 (5%)	0	100	100
26	O	197/203 (97%)	192 (98%)	5 (2%)	0	100	100
27	K	442/476 (93%)	430 (97%)	11 (2%)	1 (0%)	47	78
28	C	359/362 (99%)	343 (96%)	16 (4%)	0	100	100
29	o	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
30	r	122/124 (98%)	120 (98%)	2 (2%)	0	100	100
31	f	107/109 (98%)	104 (97%)	3 (3%)	0	100	100
32	e	126/128 (98%)	122 (97%)	4 (3%)	0	100	100
33	Z	133/135 (98%)	130 (98%)	3 (2%)	0	100	100
34	a	145/147 (99%)	138 (95%)	6 (4%)	1 (1%)	22	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	g	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	H	188/190 (99%)	184 (98%)	4 (2%)	0	100	100
38	L	208/211 (99%)	201 (97%)	7 (3%)	0	100	100
40	N	201/203 (99%)	193 (96%)	8 (4%)	0	100	100
41	i	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
42	h	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
43	M	136/138 (99%)	131 (96%)	5 (4%)	0	100	100
44	Y	132/134 (98%)	130 (98%)	2 (2%)	0	100	100
45	X	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
46	U	97/99 (98%)	88 (91%)	9 (9%)	0	100	100
47	n	23/25 (92%)	23 (100%)	0	0	100	100
All	All	6861/7436 (92%)	6625 (97%)	233 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
34	a	16	SER
22	E	118	TYR
27	K	110	ALA

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	139/139 (100%)	131 (94%)	8 (6%)	20	50
3	F	196/196 (100%)	192 (98%)	4 (2%)	55	84
4	D	247/247 (100%)	242 (98%)	5 (2%)	55	84
5	S	157/157 (100%)	151 (96%)	6 (4%)	33	67
6	b	84/184 (46%)	78 (93%)	6 (7%)	14	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	B	342/342 (100%)	333 (97%)	9 (3%)	46	79
8	d	98/98 (100%)	92 (94%)	6 (6%)	18	48
10	G	200/272 (74%)	189 (94%)	11 (6%)	21	52
11	J	143/143 (100%)	133 (93%)	10 (7%)	15	40
12	c	84/84 (100%)	75 (89%)	9 (11%)	6	20
13	j	73/73 (100%)	72 (99%)	1 (1%)	67	90
14	A	190/199 (96%)	177 (93%)	13 (7%)	16	42
15	I	175/181 (97%)	164 (94%)	11 (6%)	18	46
16	q	58/59 (98%)	58 (100%)	0	100	100
17	p	74/74 (100%)	64 (86%)	10 (14%)	4	11
18	V	101/101 (100%)	94 (93%)	7 (7%)	15	41
19	m	47/47 (100%)	47 (100%)	0	100	100
20	l	47/47 (100%)	41 (87%)	6 (13%)	4	13
21	P	134/134 (100%)	128 (96%)	6 (4%)	27	60
22	E	190/251 (76%)	184 (97%)	6 (3%)	39	73
23	Q	164/165 (99%)	157 (96%)	7 (4%)	29	62
24	R	159/175 (91%)	146 (92%)	13 (8%)	11	33
25	W	55/126 (44%)	50 (91%)	5 (9%)	9	27
26	O	171/173 (99%)	167 (98%)	4 (2%)	50	82
27	K	370/398 (93%)	365 (99%)	5 (1%)	67	90
28	C	301/301 (100%)	289 (96%)	12 (4%)	31	65
29	o	91/91 (100%)	86 (94%)	5 (6%)	21	52
30	r	108/108 (100%)	100 (93%)	8 (7%)	13	37
31	f	88/88 (100%)	84 (96%)	4 (4%)	27	60
32	e	114/114 (100%)	111 (97%)	3 (3%)	46	79
33	Z	117/117 (100%)	108 (92%)	9 (8%)	13	35
34	a	119/119 (100%)	118 (99%)	1 (1%)	81	94
35	g	98/98 (100%)	89 (91%)	9 (9%)	9	27
36	k	64/65 (98%)	58 (91%)	6 (9%)	8	26
37	H	169/169 (100%)	163 (96%)	6 (4%)	35	69
38	L	175/176 (99%)	170 (97%)	5 (3%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	N	171/171 (100%)	161 (94%)	10 (6%)	20	50
41	i	86/89 (97%)	77 (90%)	9 (10%)	7	20
42	h	109/109 (100%)	102 (94%)	7 (6%)	17	45
43	M	117/117 (100%)	114 (97%)	3 (3%)	46	79
44	Y	124/124 (100%)	106 (86%)	18 (14%)	3	9
45	X	106/106 (100%)	101 (95%)	5 (5%)	26	59
46	U	89/89 (100%)	78 (88%)	11 (12%)	4	14
47	n	24/24 (100%)	18 (75%)	6 (25%)	0	2
All	All	5968/6340 (94%)	5663 (95%)	305 (5%)	27	55

All (305) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	16	SER
1	T	40	VAL
1	T	52	MET
1	T	69	GLN
1	T	83	LYS
1	T	88	ARG
1	T	117	LYS
1	T	157	GLU
3	F	35	LYS
3	F	65	ARG
3	F	182	ASN
3	F	237	ASP
4	D	34	LYS
4	D	45	ASN
4	D	113	PHE
4	D	128	ASP
4	D	293	ARG
5	S	30	MET
5	S	67	VAL
5	S	90	THR
5	S	93	MET
5	S	99	ASP
5	S	147	ASP
6	b	19	ASN
6	b	27	GLN
6	b	50	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	b	57	MET
6	b	63	LYS
6	b	68	ARG
7	B	19	ARG
7	B	134	CYS
7	B	146	LEU
7	B	148	LYS
7	B	194	LEU
7	B	297	LYS
7	B	329	ASP
7	B	362	LYS
7	B	366	LYS
8	d	26	THR
8	d	31	LYS
8	d	61	ASP
8	d	63	ARG
8	d	92	ARG
8	d	101	LYS
10	G	116	LEU
10	G	141	ASP
10	G	160	LYS
10	G	172	GLU
10	G	237	LEU
10	G	249	ARG
10	G	284	ASP
10	G	287	ARG
10	G	288	ARG
10	G	308	LYS
10	G	313	GLU
11	J	12	MET
11	J	14	GLU
11	J	41	GLU
11	J	47	THR
11	J	58	ARG
11	J	59	SER
11	J	72	CYS
11	J	84	GLU
11	J	118	LYS
11	J	119	TYR
12	c	17	ARG
12	c	19	GLN
12	c	24	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	c	52	CYS
12	c	57	LYS
12	c	63	TYR
12	c	66	LEU
12	c	75	SER
12	c	98	ASP
13	j	55	ARG
14	A	14	SER
14	A	28	ARG
14	A	101	VAL
14	A	102	LEU
14	A	115	CYS
14	A	135	THR
14	A	152	SER
14	A	194	ASN
14	A	200	ARG
14	A	208	GLU
14	A	223	SER
14	A	245	ARG
14	A	247	ARG
15	I	20	SER
15	I	21	ARG
15	I	30	LYS
15	I	59	GLN
15	I	63	GLU
15	I	101	LYS
15	I	121	LYS
15	I	137	SER
15	I	168	SER
15	I	190	LEU
15	I	195	CYS
17	p	3	LYS
17	p	21	SER
17	p	24	LYS
17	p	28	LYS
17	p	32	SER
17	p	40	SER
17	p	63	THR
17	p	81	SER
17	p	84	ARG
17	p	90	LYS
18	V	18	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	V	43	LYS
18	V	69	LYS
18	V	87	SER
18	V	111	GLU
18	V	125	CYS
18	V	131	ARG
20	l	2	SER
20	l	20	ASN
20	l	21	ARG
20	l	29	MET
20	l	37	TYR
20	l	46	ARG
21	P	20	SER
21	P	50	ASP
21	P	69	ARG
21	P	100	SER
21	P	111	SER
21	P	137	ASN
22	E	64	MET
22	E	113	ARG
22	E	123	ASP
22	E	127	LYS
22	E	257	ASP
22	E	271	GLN
23	Q	8	ASN
23	Q	53	MET
23	Q	68	ARG
23	Q	79	THR
23	Q	108	ARG
23	Q	134	ARG
23	Q	183	SER
24	R	12	SER
24	R	16	ARG
24	R	52	ARG
24	R	59	SER
24	R	105	LEU
24	R	116	ASP
24	R	119	MET
24	R	122	SER
24	R	136	ARG
24	R	149	LYS
24	R	153	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	R	158	GLN
24	R	175	GLU
25	W	9	SER
25	W	42	SER
25	W	48	GLN
25	W	58	LYS
25	W	60	LYS
26	O	5	GLN
26	O	61	ARG
26	O	113	ASP
26	O	190	SER
27	K	46	CYS
27	K	77	MET
27	K	235	TYR
27	K	360	HIS
27	K	408	SER
28	C	16	GLU
28	C	20	LYS
28	C	80	ARG
28	C	95	MET
28	C	122	TYR
28	C	138	MET
28	C	268	ARG
28	C	275	SER
28	C	278	ASN
28	C	312	ARG
28	C	335	MET
28	C	353	ARG
29	o	27	LYS
29	o	42	ASP
29	o	78	ARG
29	o	99	ARG
29	o	102	GLN
30	r	36	ASN
30	r	58	LYS
30	r	64	MET
30	r	76	SER
30	r	96	MET
30	r	101	LYS
30	r	103	HIS
30	r	125	MET
31	f	40	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
31	f	47	CYS
31	f	63	LYS
31	f	73	LYS
32	e	11	LYS
32	e	25	SER
32	e	70	LEU
33	Z	5	MET
33	Z	53	VAL
33	Z	57	MET
33	Z	59	LYS
33	Z	99	ASP
33	Z	103	ASP
33	Z	106	LEU
33	Z	123	LYS
33	Z	132	GLN
34	a	92	LYS
35	g	31	VAL
35	g	33	LEU
35	g	44	SER
35	g	54	ARG
35	g	67	LEU
35	g	75	SER
35	g	81	SER
35	g	106	VAL
35	g	114	GLN
36	k	6	GLU
36	k	9	LYS
36	k	30	ASP
36	k	40	ARG
36	k	58	GLN
36	k	67	LYS
37	H	37	ASP
37	H	50	LYS
37	H	52	LYS
37	H	138	GLN
37	H	171	ASP
37	H	183	GLU
38	L	106	SER
38	L	124	LEU
38	L	164	GLU
38	L	184	MET
38	L	204	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
40	N	5	LYS
40	N	37	HIS
40	N	80	THR
40	N	90	ASN
40	N	98	LEU
40	N	104	GLU
40	N	126	THR
40	N	140	LYS
40	N	153	LYS
40	N	166	SER
41	i	12	ASN
41	i	19	LYS
41	i	27	SER
41	i	34	THR
41	i	42	ASP
41	i	46	GLU
41	i	56	ARG
41	i	76	ARG
41	i	88	GLU
42	h	5	LYS
42	h	19	LYS
42	h	29	SER
42	h	45	SER
42	h	46	LYS
42	h	88	THR
42	h	105	LYS
43	M	44	ARG
43	M	59	ASP
43	M	62	LEU
44	Y	1	MET
44	Y	20	ASN
44	Y	23	SER
44	Y	30	MET
44	Y	34	LEU
44	Y	37	GLU
44	Y	52	ASP
44	Y	72	GLN
44	Y	74	TYR
44	Y	84	ARG
44	Y	102	SER
44	Y	104	VAL
44	Y	108	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
44	Y	113	LYS
44	Y	120	GLU
44	Y	125	SER
44	Y	127	GLN
44	Y	130	LYS
45	X	50	LYS
45	X	57	GLN
45	X	85	SER
45	X	118	ASP
45	X	151	ASN
46	U	17	GLN
46	U	20	LYS
46	U	25	CYS
46	U	34	MET
46	U	38	ASN
46	U	39	PHE
46	U	50	ASN
46	U	62	SER
46	U	65	ARG
46	U	82	TYR
46	U	95	ASN
47	n	1	MET
47	n	8	LYS
47	n	10	MET
47	n	14	LYS
47	n	17	ARG
47	n	18	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	F	62	GLN
6	b	94	HIS
8	d	121	ASN
10	G	117	GLN
14	A	132	ASN
14	A	162	ASN
14	A	205	ASN
17	p	72	ASN
20	l	20	ASN
21	P	137	ASN
23	Q	57	ASN

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Mol	Chain	Res	Type
27	K	154	GLN
27	K	186	ASN
27	K	360	HIS
29	o	36	GLN
30	r	36	ASN
30	r	83	ASN
45	X	151	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	5	3590/4808 (74%)	695 (19%)	55 (1%)
39	7	119/120 (99%)	12 (10%)	0
9	8	149/156 (95%)	26 (17%)	1 (0%)
All	All	3858/5084 (75%)	733 (18%)	56 (1%)

All (733) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	5	12	A
2	5	13	U
2	5	25	A
2	5	30	C
2	5	39	A
2	5	42	A
2	5	58	G
2	5	59	A
2	5	64	A
2	5	65	A
2	5	73	A
2	5	76	A
2	5	91	G
2	5	104	G
2	5	108	A
2	5	109	G
2	5	110	C
2	5	119	G
2	5	120	A
2	5	126	C
2	5	134	G
2	5	135	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	136	C
2	5	137	G
2	5	142	G
2	5	152	U
2	5	157	U
2	5	159	C
2	5	172	C
2	5	173	C
2	5	182	G
2	5	185	C
2	5	187	U
2	5	188	G
2	5	189	G
2	5	200	U
2	5	201	C
2	5	209	U
2	5	216	C
2	5	217	C
2	5	218	A
2	5	220	C
2	5	224	U
2	5	233	U
2	5	234	G
2	5	246	G
2	5	265	C
2	5	266	C
2	5	274	C
2	5	275	C
2	5	276	C
2	5	280	G
2	5	297	U
2	5	306	A
2	5	309	C
2	5	315	G
2	5	316	U
2	5	322	C
2	5	334	A
2	5	340	C
2	5	350	C
2	5	362	A
2	5	373	G
2	5	386	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	387	G
2	5	406	C
2	5	407	A
2	5	408	A
2	5	409	G
2	5	410	A
2	5	412	G
2	5	418	A
2	5	449	C
2	5	450	G
2	5	452	A
2	5	453	G
2	5	454	U
2	5	457	G
2	5	463	A
2	5	464	G
2	5	467	U
2	5	468	U
2	5	487	C
2	5	493	U
2	5	494	G
2	5	498	G
2	5	499	C
2	5	502	U
2	5	505	C
2	5	506	G
2	5	507	G
2	5	515	U
2	5	517	C
2	5	660	G
2	5	663	C
2	5	678	G
2	5	679	C
2	5	680	A
2	5	691	G
2	5	698	C
2	5	699	G
2	5	721	C
2	5	722	U
2	5	723	G
2	5	724	G
2	5	725	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	726	A
2	5	732	C
2	5	734	G
2	5	738	G
2	5	742	A
2	5	744	G
2	5	753	G
2	5	756	G
2	5	758	C
2	5	763	C
2	5	787	C
2	5	790	G
2	5	791	C
2	5	792	G
2	5	793	C
2	5	795	A
2	5	797	C
2	5	798	C
2	5	799	C
2	5	800	U
2	5	814	A
2	5	824	C
2	5	825	G
2	5	828	A
2	5	830	C
2	5	831	A
2	5	832	G
2	5	833	C
2	5	834	A
2	5	835	G
2	5	838	C
2	5	839	G
2	5	841	C
2	5	844	A
2	5	845	U
2	5	856	A
2	5	859	G
2	5	860	A
2	5	861	G
2	5	864	A
2	5	866	A
2	5	867	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	868	C
2	5	869	U
2	5	872	G
2	5	879	C
2	5	884	U
2	5	987	C
2	5	988	G
2	5	994	C
2	5	996	C
2	5	1066	A
2	5	1070	U
2	5	1071	C
2	5	1072	C
2	5	1073	C
2	5	1074	C
2	5	1084	C
2	5	1086	G
2	5	1101	C
2	5	1102	G
2	5	1103	G
2	5	1105	C
2	5	1106	C
2	5	1107	C
2	5	1121	G
2	5	1122	C
2	5	1123	C
2	5	1124	A
2	5	1126	G
2	5	1127	G
2	5	1129	G
2	5	1131	G
2	5	1132	U
2	5	1133	C
2	5	1135	C
2	5	1136	G
2	5	1206	C
2	5	1208	C
2	5	1209	G
2	5	1210	C
2	5	1214	A
2	5	1215	G
2	5	1216	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	1217	G
2	5	1219	G
2	5	1220	C
2	5	1224	C
2	5	1228	G
2	5	1229	U
2	5	1231	G
2	5	1236	C
2	5	1237	G
2	5	1239	U
2	5	1240	G
2	5	1245	C
2	5	1248	C
2	5	1258	C
2	5	1270	A2M
2	5	1274	A
2	5	1281	A
2	5	1298	A
2	5	1302	G
2	5	1303	G
2	5	1309	C
2	5	1310	G
2	5	1315	A
2	5	1316	A
2	5	1321	G
2	5	1323	C
2	5	1324	G
2	5	1331	A
2	5	1338	G
2	5	1341	A
2	5	1342	A
2	5	1346	C
2	5	1348	G
2	5	1349	C
2	5	1350	G
2	5	1366	C
2	5	1367	G
2	5	1369	C
2	5	1370	G
2	5	1376	G
2	5	1384	C
2	5	1389	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	1393	C
2	5	1394	U
2	5	1395	U
2	5	1400	U
2	5	1401	C
2	5	1402	C
2	5	1412	G
2	5	1437	G
2	5	1438	C
2	5	1439	G
2	5	1452	A
2	5	1453	G
2	5	1456	C
2	5	1457	G
2	5	1469	U
2	5	1472	G
2	5	1478	A
2	5	1479	A2M
2	5	1489	A2M
2	5	1502	A
2	5	1517	G
2	5	1521	C
2	5	1529	G
2	5	1533	U
2	5	1537	PSU
2	5	1546	U
2	5	1551	U
2	5	1557	U
2	5	1567	G
2	5	1568	A
2	5	1579	G
2	5	1580	OMG
2	5	1586	A
2	5	1588	G
2	5	1589	A
2	5	1595	C
2	5	1609	G
2	5	1616	C
2	5	1631	C
2	5	1632	PSU
2	5	1633	C
2	5	1660	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	1670	C
2	5	1673	G
2	5	1680	G
2	5	1681	A
2	5	1685	A
2	5	1689	G
2	5	1692	G
2	5	1694	C
2	5	1695	U
2	5	1696	U
2	5	1699	G
2	5	1700	G
2	5	1703	G
2	5	1707	C
2	5	1711	C
2	5	1712	U
2	5	1714	A
2	5	1715	A
2	5	1720	U
2	5	1726	A
2	5	1743	A
2	5	1744	A
2	5	1746	C
2	5	1751	C
2	5	1754	G
2	5	1758	G
2	5	1760	G
2	5	1767	C
2	5	1774	G
2	5	1775	G
2	5	1776	A
2	5	1781	G
2	5	1794	G
2	5	1808	G
2	5	1821	U
2	5	1828	U
2	5	1829	G
2	5	1836	A
2	5	1838	G
2	5	1857	U
2	5	1859	C
2	5	1860	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	1861	G
2	5	1869	U
2	5	1870	C
2	5	1871	A
2	5	1887	G
2	5	1890	G
2	5	1896	U
2	5	1897	A
2	5	1900	G
2	5	1901	A
2	5	1903	A
2	5	1910	U
2	5	1913	U
2	5	1919	U
2	5	1923	A
2	5	1924	G
2	5	1926	C
2	5	1929	A
2	5	1930	A
2	5	1931	U
2	5	1933	C
2	5	1936	U
2	5	1940	G
2	5	1941	A
2	5	1942	G
2	5	1946	G
2	5	1947	U
2	5	1965	A
2	5	1968	A
2	5	1969	A
2	5	1986	A
2	5	1987	U
2	5	1991	G
2	5	1994	G
2	5	1995	G
2	5	2008	A
2	5	2023	U
2	5	2029	U
2	5	2031	G
2	5	2032	G
2	5	2036	A
2	5	2037	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	2039	G
2	5	2041	G
2	5	2044	A
2	5	2045	G
2	5	2047	G
2	5	2048	A
2	5	2049	G
2	5	2102	G
2	5	2103	C
2	5	2110	U
2	5	2111	A
2	5	2118	G
2	5	2122	A
2	5	2132	C
2	5	2143	A
2	5	2144	G
2	5	2149	G
2	5	2156	A
2	5	2174	G
2	5	2176	G
2	5	2191	G
2	5	2194	C
2	5	2203	A
2	5	2238	A
2	5	2241	U
2	5	2260	A
2	5	2265	OMC
2	5	2267	OMG
2	5	2268	U
2	5	2276	G
2	5	2284	C
2	5	2293	G
2	5	2314	G
2	5	2318	G
2	5	2331	C
2	5	2332	C
2	5	2333	U
2	5	2334	C
2	5	2338	U
2	5	2346	G
2	5	2347	C
2	5	2348	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	2349	G
2	5	2356	A
2	5	2363	C
2	5	2372	A
2	5	2380	A
2	5	2387	G
2	5	2389	G
2	5	2390	G
2	5	2396	A
2	5	2403	C
2	5	2426	C
2	5	2429	G
2	5	2432	C
2	5	2444	A
2	5	2461	G
2	5	2462	G
2	5	2463	G
2	5	2470	C
2	5	2481	G
2	5	2483	G
2	5	2492	G
2	5	2496	C
2	5	2504	U
2	5	2505	G
2	5	2512	C
2	5	2529	G
2	5	2530	U
2	5	2538	A
2	5	2539	A
2	5	2550	U
2	5	2551	U
2	5	2554	G
2	5	2558	G
2	5	2559	C
2	5	2564	G
2	5	2566	U
2	5	2568	A
2	5	2569	G
2	5	2583	U
2	5	2586	A
2	5	2587	A
2	5	2596	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	2597	G
2	5	2598	A
2	5	2602	G
2	5	2606	U
2	5	2607	A
2	5	2612	U
2	5	2630	A
2	5	2631	U
2	5	2633	U
2	5	2657	C
2	5	2669	U
2	5	2670	G
2	5	2685	G
2	5	2688	A
2	5	2698	G
2	5	2741	G
2	5	3330	C
2	5	3336	A
2	5	3337	C
2	5	3338	U
2	5	3349	G
2	5	3357	G
2	5	3358	G
2	5	3367	A
2	5	3380	A
2	5	3389	U
2	5	3394	A
2	5	3396	G
2	5	3405	C
2	5	3443	A
2	5	3444	A
2	5	3446	G
2	5	3461	PSU
2	5	3480	A
2	5	3485	G
2	5	3488	A
2	5	3491	A
2	5	3492	A
2	5	3493	C
2	5	3495	A
2	5	3496	PSU
2	5	3505	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	3506	A
2	5	3509	G
2	5	3510	U
2	5	3516	A
2	5	3517	A
2	5	3519	G
2	5	3520	C
2	5	3524	OMG
2	5	3542	C
2	5	3543	G
2	5	3544	C
2	5	3546	U
2	5	3549	A
2	5	3551	G
2	5	3570	U
2	5	3572	U
2	5	3609	A
2	5	3610	C
2	5	3611	G
2	5	3621	G
2	5	3630	G
2	5	3633	A
2	5	3637	A
2	5	3638	A
2	5	3639	G
2	5	3640	A
2	5	3647	U
2	5	3648	G
2	5	3649	A
2	5	3659	U
2	5	3670	G
2	5	3671	G
2	5	3683	G
2	5	3684	A
2	5	3687	A
2	5	3788	C
2	5	3789	G
2	5	3794	U
2	5	3801	A
2	5	3804	G
2	5	3812	G
2	5	3814	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	3816	C
2	5	3825	G
2	5	3844	C
2	5	3847	C
2	5	3848	U
2	5	3849	G
2	5	3853	C
2	5	3855	A
2	5	3904	C
2	5	3908	C
2	5	3909	U
2	5	3910	C
2	5	3912	G
2	5	3916	A
2	5	3929	G
2	5	3930	G
2	5	3937	G
2	5	3940	U
2	5	3941	G
2	5	3942	G
2	5	3944	G
2	5	3949	A
2	5	3971	G
2	5	3975	U
2	5	3979	A
2	5	3997	A
2	5	4000	G
2	5	4001	A
2	5	4012	G
2	5	4014	A
2	5	4017	A
2	5	4019	A
2	5	4027	A
2	5	4037	G
2	5	4039	PSU
2	5	4051	G
2	5	4052	OMU
2	5	4053	A
2	5	4060	C
2	5	4064	C
2	5	4065	C
2	5	4076	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	4078	C
2	5	4081	C
2	5	4085	A
2	5	4095	C
2	5	4096	C
2	5	4117	G
2	5	4118	U
2	5	4119	G
2	5	4123	G
2	5	4124	A
2	5	4126	A
2	5	4133	C
2	5	4140	A
2	5	4141	U
2	5	4142	A
2	5	4144	C
2	5	4165	U
2	5	4167	C
2	5	4168	A
2	5	4176	G
2	5	4186	G
2	5	4194	G
2	5	4195	A
2	5	4196	PSU
2	5	4198	U
2	5	4210	A
2	5	4240	OMG
2	5	4246	PSU
2	5	4256	A
2	5	4257	A
2	5	4258	U
2	5	4259	A
2	5	4264	A
2	5	4265	C
2	5	4266	G
2	5	4268	G
2	5	4269	A2M
2	5	4270	G
2	5	4294	A
2	5	4295	G
2	5	4306	C
2	5	4313	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	4319	G
2	5	4321	G
2	5	4332	G
2	5	4335	A
2	5	4336	A
2	5	4373	U
2	5	4382	PSU
2	5	4383	OMG
2	5	4398	G
2	5	4402	A
2	5	4416	C
2	5	4418	A
2	5	4423	U
2	5	4441	C
2	5	4446	A
2	5	4455	U
2	5	4465	G
2	5	4466	C
2	5	4476	C
2	5	4479	C
2	5	4480	A
2	5	4482	C
2	5	4487	A
2	5	4490	G
2	5	4492	G
2	5	4498	G
2	5	4501	G
2	5	4503	C
2	5	4504	C
2	5	4506	C
2	5	4508	G
2	5	4512	G
2	5	4518	C
2	5	4519	C
2	5	4607	G
2	5	4609	G
2	5	4610	C
2	5	4611	G
2	5	4612	G
2	5	4613	A
2	5	4614	G
2	5	4621	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	4622	C
2	5	4624	U
2	5	4634	C
2	5	4638	G
2	5	4639	C
2	5	4640	G
2	5	4642	G
2	5	4651	G
2	5	4653	G
2	5	4654	G
2	5	4658	G
2	5	4659	C
2	5	4660	C
2	5	4661	C
2	5	4664	U
2	5	4665	C
2	5	4670	G
2	5	4676	C
2	5	4682	A
2	5	4683	C
2	5	4687	C
2	5	4688	G
2	5	4689	U
2	5	4690	G
2	5	4695	A
2	5	4697	C
2	5	4699	G
2	5	4704	U
2	5	4705	A
2	5	4715	U
2	5	4727	U
2	5	4729	C
2	5	4732	G
2	5	4745	U
2	5	4753	A
2	5	4756	G
2	5	4761	U
2	5	4779	U
2	5	4780	G
2	5	4786	C
2	5	4789	C
2	5	4793	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	5	4801	G
9	8	2	G
9	8	16	G
9	8	34	U
9	8	35	C
9	8	39	G
9	8	59	A
9	8	62	A
9	8	63	U
9	8	86	U
9	8	87	G
9	8	103	A
9	8	105	C
9	8	109	C
9	8	110	U
9	8	111	U
9	8	114	G
9	8	122	G
9	8	124	U
9	8	125	C
9	8	126	C
9	8	127	U
9	8	137	A
9	8	150	C
9	8	151	G
9	8	153	C
9	8	155	C
39	7	7	G
39	7	22	A
39	7	33	U
39	7	53	U
39	7	54	A
39	7	64	G
39	7	74	A
39	7	100	A
39	7	110	G
39	7	111	C
39	7	117	G
39	7	120	U

All (56) RNA pucker outliers are listed below:



Mol	Chain	Res	Type
2	5	12	A
2	5	125	C
2	5	134	G
2	5	217	C
2	5	245	C
2	5	275	C
2	5	385	A
2	5	406	C
2	5	417	G
2	5	486	C
2	5	493	U
2	5	829	G
2	5	987	C
2	5	1065	G
2	5	1102	G
2	5	1123	C
2	5	1125	C
2	5	1207	G
2	5	1235	G
2	5	1273	G
2	5	1314	G
2	5	1400	U
2	5	1588	G
2	5	1743	A
2	5	1757	G
2	5	1918	A
2	5	1929	A
2	5	1985	G
2	5	2028	G
2	5	2109	C
2	5	2345	A
2	5	2482	U
2	5	2504	U
2	5	2538	A
2	5	2597	G
2	5	3335	G
2	5	3357	G
2	5	3620	G
2	5	3636	G
2	5	3793	G
2	5	3847	C
2	5	3940	U
2	5	3978	U

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Mol	Chain	Res	Type
2	5	4000	G
2	5	4117	G
2	5	4141	U
2	5	4194	G
2	5	4445	U
2	5	4465	G
2	5	4623	G
2	5	4660	C
2	5	4664	U
2	5	4675	G
2	5	4686	U
2	5	4786	C
9	8	124	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMC	5	4282	2	19,22,23	0.95	0	26,31,34	1.03	1 (3%)
2	PSU	5	4277	2	18,21,22	1.93	5 (27%)	22,30,33	1.87	4 (18%)
2	5MC	5	3514	2	18,22,23	1.99	4 (22%)	26,32,35	1.37	3 (11%)
19	MLZ	m	72	19	8,9,10	0.49	0	4,9,11	0.53	0
2	A2M	5	1489	2,48	18,25,26	4.08	5 (27%)	18,36,39	1.22	1 (5%)
2	PSU	5	1537	2	18,21,22	2.02	5 (27%)	22,30,33	1.86	4 (18%)
2	PSU	5	4374	2	18,21,22	2.00	5 (27%)	22,30,33	1.94	4 (18%)
2	I4U	5	1614	2	21,24,25	2.54	7 (33%)	27,34,37	1.07	1 (3%)
2	A2M	5	1270	2	18,25,26	0.96	1 (5%)	18,36,39	1.23	2 (11%)
2	A2M	5	1810	2,48	18,25,26	0.98	0	18,36,39	1.25	2 (11%)
2	OMC	5	2208	2	19,22,23	2.25	5 (26%)	26,31,34	0.94	2 (7%)
2	B8K	5	3629	2	24,28,29	5.87	7 (29%)	30,42,45	2.26	7 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PSU	5	4246	2	18,21,22	1.97	5 (27%)	22,30,33	1.94	5 (22%)
2	5MC	5	4193	2	18,22,23	1.01	2 (11%)	26,32,35	1.37	3 (11%)
2	OMC	5	3619	2	19,22,23	2.25	5 (26%)	26,31,34	0.95	3 (11%)
2	1MA	5	4161	2	16,25,26	2.25	3 (18%)	18,37,40	1.41	3 (16%)
2	OMG	5	1477	2	18,26,27	2.84	5 (27%)	19,38,41	1.25	3 (15%)
2	A2M	5	1479	2	18,25,26	4.05	5 (27%)	18,36,39	1.34	2 (11%)
2	E7G	5	1736	2	24,27,28	5.35	7 (29%)	30,40,43	2.20	10 (33%)
2	B8H	5	4042	2	19,22,23	2.01	7 (36%)	22,32,35	2.04	3 (13%)
2	PSU	5	4188	2	18,21,22	2.01	6 (33%)	22,30,33	1.95	5 (22%)
2	OMC	5	2647	2	19,22,23	2.25	5 (26%)	26,31,34	0.93	2 (7%)
2	A2M	5	3557	2	18,25,26	4.04	5 (27%)	18,36,39	1.22	1 (5%)
2	OMC	5	2265	2,48	19,22,23	2.24	5 (26%)	26,31,34	0.94	2 (7%)
2	P7G	5	3612	2	24,28,29	6.40	6 (25%)	27,41,44	1.38	3 (11%)
2	E6G	5	4101	2	20,27,28	1.99	3 (15%)	22,39,42	2.09	5 (22%)
2	PSU	5	3461	2	18,21,22	2.00	5 (27%)	22,30,33	1.81	4 (18%)
2	B8K	5	4436	2	24,28,29	5.80	7 (29%)	30,42,45	2.30	7 (23%)
2	OMG	5	4240	2	18,26,27	2.83	4 (22%)	19,38,41	1.23	3 (15%)
2	P4U	5	1292	2	21,24,25	2.43	7 (33%)	27,33,36	1.14	2 (7%)
2	OMG	5	1260	2	18,26,27	2.81	4 (22%)	19,38,41	1.22	3 (15%)
2	A2M	5	3450	2	18,25,26	4.09	5 (27%)	18,36,39	1.22	1 (5%)
2	PSU	5	4196	2,48	18,21,22	1.95	5 (27%)	22,30,33	1.90	4 (18%)
2	OMG	5	4383	2	18,26,27	2.84	4 (22%)	19,38,41	1.27	3 (15%)
2	UR3	5	4276	2	19,22,23	1.02	1 (5%)	26,32,35	1.52	2 (7%)
2	OMG	5	4116	2	18,26,27	1.06	1 (5%)	19,38,41	1.22	3 (15%)
2	A2M	5	4269	2,48	18,25,26	4.06	6 (33%)	18,36,39	1.20	1 (5%)
2	OMU	5	4366	2	19,22,23	3.09	7 (36%)	26,31,34	1.84	6 (23%)
28	MLZ	C	333	28	8,9,10	0.46	0	4,9,11	0.64	0
2	A2M	5	398	2	18,25,26	4.08	5 (27%)	18,36,39	1.22	1 (5%)
2	PSU	5	4149	2	18,21,22	1.59	5 (27%)	22,30,33	2.10	5 (22%)
2	PSU	5	1632	2	18,21,22	1.96	5 (27%)	22,30,33	1.95	4 (18%)
2	OMG	5	4369	2	18,26,27	2.83	4 (22%)	19,38,41	1.24	3 (15%)
2	PSU	5	4382	2	18,21,22	1.98	5 (27%)	22,30,33	1.95	5 (22%)
2	PSU	5	4039	2	18,21,22	1.97	5 (27%)	22,30,33	1.91	4 (18%)
2	7MG	5	2365	2	22,26,27	1.45	4 (18%)	29,39,42	2.67	8 (27%)
2	PSU	5	3496	2	18,21,22	1.98	6 (33%)	22,30,33	1.78	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	OMG	5	2267	2	18,26,27	1.05	1 (5%)	19,38,41	1.14	2 (10%)
2	1MA	5	1266	2	16,25,26	2.25	4 (25%)	18,37,40	1.50	3 (16%)
2	OMU	5	4052	2	19,22,23	3.10	7 (36%)	26,31,34	1.81	6 (23%)
2	BGH	5	3631	2	25,29,30	6.34	13 (52%)	31,43,46	2.34	9 (29%)
2	OMG	5	1580	2,48	18,26,27	1.17	1 (5%)	19,38,41	1.15	2 (10%)
2	B8H	5	3494	2	19,22,23	1.98	7 (36%)	22,32,35	1.92	3 (13%)
2	OMC	5	3433	2	19,22,23	2.24	5 (26%)	26,31,34	0.94	2 (7%)
2	OMG	5	2616	2	18,26,27	2.83	4 (22%)	19,38,41	1.25	3 (15%)
2	OMG	5	2207	2	18,26,27	2.84	4 (22%)	19,38,41	1.19	3 (15%)
2	7MG	5	1560	2	22,26,27	5.20	5 (22%)	29,39,42	2.10	8 (27%)
2	OMC	5	2704	2	19,22,23	2.24	5 (26%)	26,31,34	0.95	2 (7%)
2	PSU	5	1638	2	18,21,22	1.99	6 (33%)	22,30,33	1.90	4 (18%)
2	B8H	5	1799	2	19,22,23	2.01	7 (36%)	22,32,35	2.05	3 (13%)
2	A2M	5	3455	2	18,25,26	4.06	5 (27%)	18,36,39	1.23	1 (5%)
2	PSU	5	2351	2	18,21,22	1.98	5 (27%)	22,30,33	1.81	4 (18%)
2	OMG	5	3524	2	18,26,27	2.85	4 (22%)	19,38,41	1.23	3 (15%)
2	P7G	5	1848	2	24,28,29	6.30	6 (25%)	27,41,44	1.34	3 (11%)
2	OMC	5	3601	2	19,22,23	2.25	5 (26%)	26,31,34	0.94	2 (7%)
2	PSU	5	3447	2	18,21,22	1.96	5 (27%)	22,30,33	1.84	4 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OMC	5	4282	2	-	2/9/27/28	0/2/2/2
2	PSU	5	4277	2	-	0/7/25/26	0/2/2/2
2	5MC	5	3514	2	-	0/7/25/26	0/2/2/2
19	MLZ	m	72	19	-	1/7/8/10	-
2	A2M	5	1489	2,48	-	3/5/27/28	0/3/3/3
2	PSU	5	1537	2	-	2/7/25/26	0/2/2/2
2	PSU	5	4374	2	-	0/7/25/26	0/2/2/2
2	I4U	5	1614	2	-	1/9/29/30	0/2/2/2
2	A2M	5	1270	2	-	3/5/27/28	0/3/3/3
2	A2M	5	1810	2,48	-	0/5/27/28	0/3/3/3
2	OMC	5	2208	2	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B8K	5	3629	2	-	3/11/41/42	0/3/3/3
2	PSU	5	4246	2	-	5/7/25/26	0/2/2/2
2	5MC	5	4193	2	-	4/7/25/26	0/2/2/2
2	OMC	5	3619	2	-	1/9/27/28	0/2/2/2
2	1MA	5	4161	2	-	1/3/25/26	0/3/3/3
2	OMG	5	1477	2	-	0/5/27/28	0/3/3/3
2	A2M	5	1479	2	-	2/5/27/28	0/3/3/3
2	E7G	5	1736	2	-	3/9/39/40	0/3/3/3
2	B8H	5	4042	2	-	2/7/25/26	0/2/2/2
2	PSU	5	4188	2	-	0/7/25/26	0/2/2/2
2	OMC	5	2647	2	-	1/9/27/28	0/2/2/2
2	A2M	5	3557	2	-	1/5/27/28	0/3/3/3
2	OMC	5	2265	2,48	-	2/9/27/28	0/2/2/2
2	P7G	5	3612	2	-	3/10/40/41	0/3/3/3
2	E6G	5	4101	2	-	3/6/28/29	0/3/3/3
2	PSU	5	3461	2	-	2/7/25/26	0/2/2/2
2	B8K	5	4436	2	-	0/11/41/42	0/3/3/3
2	OMG	5	4240	2	-	3/5/27/28	0/3/3/3
2	P4U	5	1292	2	-	4/10/29/30	0/2/2/2
2	OMG	5	1260	2	-	1/5/27/28	0/3/3/3
2	A2M	5	3450	2	-	0/5/27/28	0/3/3/3
2	PSU	5	4196	2,48	-	5/7/25/26	0/2/2/2
2	OMG	5	4383	2	-	3/5/27/28	0/3/3/3
2	UR3	5	4276	2	-	0/7/25/26	0/2/2/2
2	OMG	5	4116	2	-	1/5/27/28	0/3/3/3
2	A2M	5	4269	2,48	-	3/5/27/28	0/3/3/3
2	OMU	5	4366	2	-	1/9/27/28	0/2/2/2
28	MLZ	C	333	28	-	0/7/8/10	-
2	A2M	5	398	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4149	2	-	2/7/25/26	0/2/2/2
2	PSU	5	1632	2	-	2/7/25/26	0/2/2/2
2	OMG	5	4369	2	-	1/5/27/28	0/3/3/3
2	PSU	5	4382	2	-	3/7/25/26	0/2/2/2
2	PSU	5	4039	2	-	2/7/25/26	0/2/2/2
2	7MG	5	2365	2	-	0/7/37/38	0/3/3/3
2	PSU	5	3496	2	-	3/7/25/26	0/2/2/2
2	OMG	5	2267	2	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1MA	5	1266	2	-	0/3/25/26	0/3/3/3
2	OMU	5	4052	2	-	3/9/27/28	0/2/2/2
2	BGH	5	3631	2	-	2/13/43/44	0/3/3/3
2	OMG	5	1580	2,48	-	0/5/27/28	0/3/3/3
2	B8H	5	3494	2	-	2/7/25/26	0/2/2/2
2	OMC	5	3433	2	-	4/9/27/28	0/2/2/2
2	OMG	5	2616	2	-	1/5/27/28	0/3/3/3
2	OMG	5	2207	2	-	3/5/27/28	0/3/3/3
2	7MG	5	1560	2	-	0/7/37/38	0/3/3/3
2	OMC	5	2704	2	-	1/9/27/28	0/2/2/2
2	PSU	5	1638	2	-	0/7/25/26	0/2/2/2
2	B8H	5	1799	2	-	0/7/25/26	0/2/2/2
2	A2M	5	3455	2	-	0/5/27/28	0/3/3/3
2	PSU	5	2351	2	-	0/7/25/26	0/2/2/2
2	OMG	5	3524	2	-	2/5/27/28	0/3/3/3
2	P7G	5	1848	2	-	0/10/40/41	0/3/3/3
2	OMC	5	3601	2	-	0/9/27/28	0/2/2/2
2	PSU	5	3447	2	-	0/7/25/26	0/2/2/2

All (307) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3629	B8K	C8-N9	-26.30	1.31	1.46
2	5	3631	BGH	C8-N9	-26.21	1.31	1.46
2	5	4436	B8K	C8-N9	-25.93	1.31	1.46
2	5	3612	P7G	C8-N9	-25.04	1.32	1.46
2	5	1848	P7G	C8-N9	-24.70	1.32	1.46
2	5	1560	7MG	C8-N9	-21.34	1.34	1.46
2	5	1736	E7G	C8-N9	-19.46	1.35	1.46
2	5	3612	P7G	C8-N7	-14.50	1.32	1.45
2	5	1848	P7G	C8-N7	-14.09	1.32	1.45
2	5	1736	E7G	C8-N7	-13.36	1.33	1.45
2	5	4052	OMU	O4-C4	11.28	1.46	1.24
2	5	4366	OMU	O4-C4	11.21	1.46	1.24
2	5	1489	A2M	O4'-C1'	10.66	1.56	1.41
2	5	3450	A2M	O4'-C1'	10.66	1.55	1.41
2	5	398	A2M	O4'-C1'	10.61	1.55	1.41
2	5	3455	A2M	O4'-C1'	10.58	1.55	1.41
2	5	3557	A2M	O4'-C1'	10.55	1.55	1.41
2	5	4269	A2M	O4'-C1'	10.55	1.55	1.41
2	5	1479	A2M	O4'-C1'	10.46	1.55	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	1479	A2M	C3'-C4'	-10.09	1.27	1.53
2	5	4269	A2M	C3'-C4'	-10.06	1.27	1.53
2	5	1489	A2M	C3'-C4'	-10.06	1.27	1.53
2	5	398	A2M	C3'-C4'	-10.04	1.27	1.53
2	5	3450	A2M	C3'-C4'	-10.03	1.27	1.53
2	5	3557	A2M	C3'-C4'	-9.98	1.27	1.53
2	5	3612	P7G	O6-C6	9.97	1.40	1.23
2	5	1848	P7G	O6-C6	9.94	1.40	1.23
2	5	3455	A2M	C3'-C4'	-9.91	1.27	1.53
2	5	1560	7MG	O6-C6	9.26	1.41	1.23
2	5	3631	BGH	C3'-C4'	-9.17	1.29	1.53
2	5	2616	OMG	O6-C6	8.88	1.41	1.23
2	5	4240	OMG	O6-C6	8.86	1.41	1.23
2	5	3524	OMG	O6-C6	8.86	1.41	1.23
2	5	1614	I4U	O2-C2	8.83	1.40	1.23
2	5	4369	OMG	O6-C6	8.83	1.41	1.23
2	5	2207	OMG	O6-C6	8.82	1.41	1.23
2	5	4383	OMG	O6-C6	8.81	1.41	1.23
2	5	1477	OMG	O6-C6	8.79	1.41	1.23
2	5	1260	OMG	O6-C6	8.72	1.41	1.23
2	5	1736	E7G	O6-C6	8.48	1.39	1.23
2	5	3631	BGH	O6-C6	8.41	1.39	1.23
2	5	1292	P4U	O2-C2	8.39	1.39	1.23
2	5	3629	B8K	O6-C6	8.39	1.39	1.23
2	5	4436	B8K	O6-C6	8.31	1.39	1.23
2	5	4161	1MA	C6-N6	7.64	1.47	1.27
2	5	1266	1MA	C6-N6	7.62	1.47	1.27
2	5	3631	BGH	O4'-C4'	7.50	1.61	1.45
2	5	2208	OMC	C4-N4	6.70	1.49	1.33
2	5	2704	OMC	C4-N4	6.69	1.49	1.33
2	5	3433	OMC	C4-N4	6.68	1.49	1.33
2	5	3619	OMC	C4-N4	6.68	1.49	1.33
2	5	3601	OMC	C4-N4	6.67	1.49	1.33
2	5	2265	OMC	C4-N4	6.67	1.49	1.33
2	5	2647	OMC	C4-N4	6.66	1.49	1.33
2	5	4101	E6G	O6-C6	6.44	1.40	1.35
2	5	2616	OMG	C2-N2	6.28	1.49	1.34
2	5	4383	OMG	C2-N2	6.23	1.49	1.34
2	5	3524	OMG	C2-N2	6.22	1.49	1.34
2	5	2207	OMG	C2-N2	6.20	1.48	1.34
2	5	1477	OMG	C2-N2	6.18	1.48	1.34
2	5	4369	OMG	C2-N2	6.17	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4240	OMG	C2-N2	6.16	1.48	1.34
2	5	1260	OMG	C2-N2	6.05	1.48	1.34
2	5	1479	A2M	C3'-C2'	5.88	1.66	1.52
2	5	3455	A2M	C3'-C2'	5.87	1.66	1.52
2	5	398	A2M	C3'-C2'	5.83	1.65	1.52
2	5	1489	A2M	C3'-C2'	5.81	1.65	1.52
2	5	3450	A2M	C3'-C2'	5.79	1.65	1.52
2	5	3557	A2M	C3'-C2'	5.71	1.65	1.52
2	5	4269	A2M	C3'-C2'	5.69	1.65	1.52
2	5	3455	A2M	O4'-C4'	4.98	1.56	1.45
2	5	3450	A2M	O4'-C4'	4.94	1.56	1.45
2	5	398	A2M	O4'-C4'	4.90	1.55	1.45
2	5	3514	5MC	C4-N4	4.90	1.46	1.34
2	5	1489	A2M	O4'-C4'	4.82	1.55	1.45
2	5	3557	A2M	O4'-C4'	4.77	1.55	1.45
2	5	4269	A2M	O4'-C4'	4.74	1.55	1.45
2	5	3631	BGH	C2-N2	4.69	1.45	1.34
2	5	1736	E7G	C2-N2	4.68	1.45	1.34
2	5	3447	PSU	C6-C5	4.66	1.40	1.35
2	5	4436	B8K	C2-N2	4.65	1.45	1.34
2	5	3496	PSU	C6-C5	4.64	1.40	1.35
2	5	4277	PSU	C6-C5	4.62	1.40	1.35
2	5	3612	P7G	C2-N2	4.62	1.45	1.34
2	5	1848	P7G	C2-N2	4.62	1.45	1.34
2	5	4246	PSU	C6-C5	4.60	1.40	1.35
2	5	1479	A2M	O4'-C4'	4.60	1.55	1.45
2	5	3514	5MC	C2-N1	-4.60	1.30	1.40
2	5	1537	PSU	C6-C5	4.59	1.40	1.35
2	5	3629	B8K	C2-N2	4.59	1.45	1.34
2	5	3631	BGH	O4'-C1'	-4.58	1.31	1.42
2	5	3461	PSU	C6-C5	4.57	1.40	1.35
2	5	4188	PSU	C6-C5	4.50	1.40	1.35
2	5	1632	PSU	C6-C5	4.48	1.40	1.35
2	5	4382	PSU	C6-C5	4.45	1.40	1.35
2	5	4039	PSU	C6-C5	4.44	1.40	1.35
2	5	4052	OMU	C2-N1	-4.43	1.31	1.38
2	5	4374	PSU	C6-C5	4.42	1.40	1.35
2	5	2351	PSU	C6-C5	4.41	1.40	1.35
2	5	1638	PSU	C6-C5	4.31	1.40	1.35
2	5	4366	OMU	C2-N1	-4.31	1.31	1.38
2	5	4196	PSU	C6-C5	4.26	1.40	1.35
2	5	3601	OMC	C2-N1	-4.22	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3433	OMC	C2-N1	-4.18	1.30	1.40
2	5	3619	OMC	C2-N1	-4.17	1.30	1.40
2	5	2208	OMC	C2-N1	-4.16	1.31	1.40
2	5	2647	OMC	C2-N1	-4.10	1.31	1.40
2	5	1560	7MG	C2-N2	4.08	1.43	1.34
2	5	2265	OMC	C2-N1	-4.08	1.31	1.40
2	5	2704	OMC	C2-N1	-4.05	1.31	1.40
2	5	1560	7MG	C4-N9	-4.01	1.33	1.37
2	5	4101	E6G	C2-N2	3.89	1.41	1.33
2	5	2647	OMC	O2-C2	-3.87	1.16	1.23
2	5	3619	OMC	O2-C2	-3.85	1.16	1.23
2	5	2265	OMC	O2-C2	-3.85	1.16	1.23
2	5	3601	OMC	O2-C2	-3.82	1.16	1.23
2	5	4374	PSU	C4-N3	-3.78	1.31	1.38
2	5	1614	I4U	C2-N1	-3.78	1.31	1.40
2	5	2704	OMC	O2-C2	-3.77	1.16	1.23
2	5	1736	E7G	C6-N1	-3.77	1.31	1.38
2	5	2208	OMC	O2-C2	-3.76	1.16	1.23
2	5	2365	7MG	C4-N9	-3.76	1.33	1.37
2	5	3433	OMC	O2-C2	-3.75	1.16	1.23
2	5	3514	5MC	C6-C5	3.70	1.40	1.34
2	5	1560	7MG	C6-N1	-3.69	1.32	1.38
2	5	4382	PSU	C4-N3	-3.69	1.32	1.38
2	5	1632	PSU	C4-N3	-3.68	1.32	1.38
2	5	4196	PSU	C4-N3	-3.65	1.32	1.38
2	5	1537	PSU	C4-N3	-3.64	1.32	1.38
2	5	4039	PSU	C4-N3	-3.63	1.32	1.38
2	5	4188	PSU	C4-N3	-3.63	1.32	1.38
2	5	2351	PSU	C4-N3	-3.63	1.32	1.38
2	5	3631	BGH	C4-N9	-3.61	1.33	1.37
2	5	1638	PSU	C4-N3	-3.58	1.32	1.38
2	5	1799	B8H	C4-N3	-3.58	1.32	1.38
2	5	4246	PSU	C4-N3	-3.57	1.32	1.38
2	5	3447	PSU	C4-N3	-3.56	1.32	1.38
2	5	4042	B8H	C4-N3	-3.54	1.32	1.38
2	5	4277	PSU	C4-N3	-3.54	1.32	1.38
2	5	1799	B8H	C2-N1	-3.51	1.31	1.38
2	5	3461	PSU	C4-N3	-3.50	1.32	1.38
2	5	4366	OMU	C4-N3	-3.47	1.32	1.38
2	5	4042	B8H	C2-N3	-3.46	1.31	1.38
2	5	1292	P4U	O4-C41	-3.46	1.35	1.45
2	5	4042	B8H	C2-N1	-3.45	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3631	BGH	C6-N1	-3.44	1.32	1.38
2	5	3496	PSU	C4-N3	-3.43	1.32	1.38
2	5	1799	B8H	C2-N3	-3.43	1.31	1.38
2	5	4052	OMU	C4-N3	-3.42	1.32	1.38
2	5	3629	B8K	C6-N1	-3.41	1.32	1.38
2	5	3494	B8H	C2-N1	-3.40	1.32	1.38
2	5	4161	1MA	C2-N3	3.37	1.33	1.29
2	5	3629	B8K	C4-N9	-3.36	1.33	1.37
2	5	4436	B8K	C4-N9	-3.36	1.33	1.37
2	5	3494	B8H	C2-N3	-3.33	1.32	1.38
2	5	4436	B8K	C6-N1	-3.33	1.32	1.38
2	5	4149	PSU	C4-N3	-3.33	1.32	1.38
2	5	3494	B8H	C1'-C5	3.32	1.57	1.50
2	5	3494	B8H	C4-N3	-3.32	1.32	1.38
2	5	3631	BGH	C71-N7	3.31	1.47	1.39
2	5	4436	B8K	C71-N7	3.31	1.47	1.39
2	5	3629	B8K	C71-N7	3.27	1.46	1.39
2	5	1638	PSU	C2-N1	-3.25	1.32	1.36
2	5	4039	PSU	C2-N1	-3.22	1.32	1.36
2	5	2351	PSU	C2-N1	-3.20	1.32	1.36
2	5	1580	OMG	C6-N1	-3.19	1.33	1.37
2	5	1477	OMG	C6-N1	-3.19	1.33	1.37
2	5	4188	PSU	C2-N1	-3.19	1.32	1.36
2	5	1848	P7G	C6-N1	-3.19	1.32	1.38
2	5	3461	PSU	C2-N1	-3.16	1.32	1.36
2	5	1614	I4U	C5-C4	-3.15	1.38	1.43
2	5	4383	OMG	C6-N1	-3.15	1.33	1.37
2	5	1537	PSU	C2-N1	-3.15	1.32	1.36
2	5	1614	I4U	O4-C4	3.14	1.41	1.35
2	5	1266	1MA	C2-N3	3.14	1.32	1.29
2	5	3612	P7G	C6-N1	-3.13	1.32	1.38
2	5	2207	OMG	C6-N1	-3.13	1.33	1.37
2	5	4374	PSU	C2-N1	-3.13	1.32	1.36
2	5	398	A2M	C6-N6	3.12	1.45	1.34
2	5	3496	PSU	C2-N1	-3.10	1.32	1.36
2	5	3494	B8H	C6-C5	3.10	1.39	1.34
2	5	4269	A2M	C6-N6	3.10	1.45	1.34
2	5	3455	A2M	C6-N6	3.10	1.45	1.34
2	5	1260	OMG	C6-N1	-3.10	1.33	1.37
2	5	3450	A2M	C6-N6	3.10	1.45	1.34
2	5	1489	A2M	C6-N6	3.10	1.45	1.34
2	5	1292	P4U	O4-C4	3.09	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4369	OMG	C6-N1	-3.08	1.33	1.37
2	5	3557	A2M	C6-N6	3.07	1.45	1.34
2	5	3524	OMG	C6-N1	-3.07	1.33	1.37
2	5	4196	PSU	C2-N1	-3.06	1.32	1.36
2	5	1479	A2M	C6-N6	3.06	1.45	1.34
2	5	3447	PSU	C2-N1	-3.05	1.32	1.36
2	5	4116	OMG	C6-N1	-3.04	1.33	1.37
2	5	4240	OMG	C6-N1	-3.03	1.33	1.37
2	5	3524	OMG	C5-C6	-2.97	1.41	1.47
2	5	4382	PSU	C2-N1	-2.97	1.32	1.36
2	5	1292	P4U	C6-C5	2.97	1.41	1.35
2	5	4246	PSU	C2-N1	-2.96	1.32	1.36
2	5	2616	OMG	C6-N1	-2.94	1.33	1.37
2	5	1260	OMG	C5-C6	-2.94	1.41	1.47
2	5	2365	7MG	C6-N1	-2.93	1.33	1.38
2	5	2207	OMG	C5-C6	-2.89	1.41	1.47
2	5	2267	OMG	C6-N1	-2.89	1.33	1.37
2	5	4369	OMG	C5-C6	-2.87	1.41	1.47
2	5	1799	B8H	C1'-C5	2.86	1.56	1.50
2	5	1632	PSU	C2-N1	-2.86	1.32	1.36
2	5	4277	PSU	C2-N1	-2.86	1.32	1.36
2	5	3631	BGH	O2'-C2'	-2.86	1.35	1.42
2	5	1799	B8H	C6-C5	2.85	1.39	1.34
2	5	3461	PSU	C6-N1	-2.83	1.31	1.36
2	5	4240	OMG	C5-C6	-2.81	1.41	1.47
2	5	1477	OMG	C5-C6	-2.81	1.41	1.47
2	5	4383	OMG	C5-C6	-2.79	1.41	1.47
2	5	4042	B8H	C1'-C5	2.78	1.56	1.50
2	5	4196	PSU	C6-N1	-2.77	1.31	1.36
2	5	4042	B8H	C6-C5	2.77	1.38	1.34
2	5	2365	7MG	C5-N7	-2.75	1.32	1.35
2	5	4366	OMU	C2-N3	-2.75	1.33	1.38
2	5	4193	5MC	C6-N1	-2.75	1.33	1.38
2	5	2616	OMG	C5-C6	-2.72	1.41	1.47
2	5	4382	PSU	C6-N1	-2.71	1.31	1.36
2	5	4188	PSU	C6-N1	-2.69	1.31	1.36
2	5	1638	PSU	C6-N1	-2.68	1.31	1.36
2	5	4052	OMU	C2-N3	-2.67	1.33	1.38
2	5	4039	PSU	C6-N1	-2.64	1.31	1.36
2	5	2351	PSU	C6-N1	-2.64	1.31	1.36
2	5	4246	PSU	C6-N1	-2.62	1.31	1.36
2	5	4374	PSU	C6-N1	-2.62	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	4042	B8H	O4-C4	-2.62	1.18	1.23
2	5	3496	PSU	C6-N1	-2.62	1.31	1.36
2	5	1537	PSU	C6-N1	-2.61	1.31	1.36
2	5	1632	PSU	C6-N1	-2.60	1.31	1.36
2	5	4277	PSU	C6-N1	-2.59	1.31	1.36
2	5	3447	PSU	C6-N1	-2.59	1.31	1.36
2	5	2365	7MG	C5-C4	2.58	1.46	1.38
2	5	1799	B8H	O4-C4	-2.56	1.18	1.23
2	5	1292	P4U	C4-N3	2.55	1.34	1.31
2	5	4193	5MC	C6-C5	2.52	1.38	1.34
2	5	1614	I4U	O4-C41	-2.51	1.41	1.47
2	5	2704	OMC	C6-C5	2.50	1.40	1.35
2	5	2208	OMC	C6-C5	2.49	1.40	1.35
2	5	2265	OMC	C6-C5	2.48	1.40	1.35
2	5	3601	OMC	C6-C5	2.48	1.40	1.35
2	5	4149	PSU	C2'-C1'	-2.47	1.50	1.53
2	5	3433	OMC	C6-C5	2.45	1.40	1.35
2	5	2647	OMC	C6-C5	2.45	1.40	1.35
2	5	1292	P4U	C42-C41	2.44	1.65	1.49
2	5	1614	I4U	C6-N1	-2.44	1.32	1.38
2	5	4042	B8H	O2-C2	-2.43	1.18	1.23
2	5	3619	OMC	C6-C5	2.42	1.40	1.35
2	5	4149	PSU	C2-N3	-2.42	1.33	1.37
2	5	3494	B8H	O4-C4	-2.42	1.19	1.23
2	5	1799	B8H	O2-C2	-2.40	1.18	1.23
2	5	4149	PSU	C6-C5	2.40	1.38	1.35
2	5	2351	PSU	C2-N3	-2.39	1.33	1.37
2	5	3631	BGH	C2-N1	-2.38	1.31	1.37
2	5	4436	B8K	C2-N1	-2.37	1.31	1.37
2	5	3631	BGH	O3'-C3'	2.35	1.48	1.43
2	5	3629	B8K	C2-N1	-2.35	1.31	1.37
2	5	3514	5MC	C6-N1	-2.33	1.34	1.38
2	5	4039	PSU	C2-N3	-2.33	1.33	1.37
2	5	3494	B8H	O2-C2	-2.33	1.18	1.23
2	5	4374	PSU	C2-N3	-2.32	1.33	1.37
2	5	1638	PSU	C2-N3	-2.31	1.33	1.37
2	5	1537	PSU	C2-N3	-2.27	1.33	1.37
2	5	1848	P7G	C2-N3	-2.27	1.32	1.37
2	5	1266	1MA	C5-C4	-2.27	1.37	1.43
2	5	4188	PSU	O4'-C1'	-2.26	1.40	1.43
2	5	1736	E7G	C72-C71	2.25	1.62	1.49
2	5	1292	P4U	C6-N1	-2.24	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	3612	P7G	C2-N3	-2.24	1.32	1.37
2	5	4366	OMU	C6-C5	2.23	1.40	1.35
2	5	3631	BGH	O5'-C5'	-2.22	1.39	1.44
2	5	4101	E6G	C2-N1	-2.22	1.31	1.35
2	5	4196	PSU	C2-N3	-2.22	1.33	1.37
2	5	4382	PSU	C2-N3	-2.21	1.33	1.37
2	5	4149	PSU	C2-N1	-2.20	1.33	1.36
2	5	3496	PSU	C1'-C5	2.19	1.55	1.50
2	5	3461	PSU	C2-N3	-2.19	1.33	1.37
2	5	4188	PSU	C2-N3	-2.17	1.33	1.37
2	5	1632	PSU	C2-N3	-2.17	1.33	1.37
2	5	4161	1MA	C5-C4	-2.16	1.37	1.43
2	5	2647	OMC	C5-C4	-2.15	1.38	1.42
2	5	3496	PSU	C2-N3	-2.13	1.33	1.37
2	5	2704	OMC	C5-C4	-2.13	1.38	1.42
2	5	2208	OMC	C5-C4	-2.13	1.38	1.42
2	5	3601	OMC	C5-C4	-2.13	1.38	1.42
2	5	2265	OMC	C5-C4	-2.12	1.38	1.42
2	5	4366	OMU	C6-N1	-2.12	1.32	1.38
2	5	3447	PSU	C2-N3	-2.12	1.33	1.37
2	5	4246	PSU	C2-N3	-2.12	1.33	1.37
2	5	4052	OMU	C6-C5	2.11	1.39	1.35
2	5	1270	A2M	C5-C4	2.08	1.46	1.40
2	5	4276	UR3	C5-C4	-2.08	1.38	1.43
2	5	4269	A2M	O5'-C5'	-2.06	1.39	1.44
2	5	3619	OMC	C5-C4	-2.06	1.38	1.42
2	5	4052	OMU	C5-C4	-2.05	1.39	1.43
2	5	1614	I4U	C2-N3	-2.05	1.32	1.36
2	5	1266	1MA	C8-N7	-2.05	1.31	1.35
2	5	1638	PSU	O2-C2	-2.04	1.19	1.23
2	5	4366	OMU	C5-C4	-2.03	1.39	1.43
2	5	4052	OMU	C6-N1	-2.03	1.33	1.38
2	5	4277	PSU	C2-N3	-2.03	1.34	1.37
2	5	3433	OMC	C5-C4	-2.02	1.38	1.42
2	5	1477	OMG	C2-N1	-2.02	1.32	1.37
2	5	1736	E7G	C4-N9	-2.01	1.35	1.37

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	2365	7MG	N9-C4-N3	9.34	139.43	125.47
2	5	4149	PSU	N1-C2-N3	6.49	122.49	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1799	B8H	N3-C2-N1	6.08	121.71	115.14
2	5	4042	B8H	N3-C2-N1	6.01	121.64	115.14
2	5	3494	B8H	N3-C2-N1	5.80	121.41	115.14
2	5	4374	PSU	N1-C2-N3	5.69	121.58	115.13
2	5	4276	UR3	C4-N3-C2	-5.66	119.23	124.56
2	5	4188	PSU	N1-C2-N3	5.65	121.53	115.13
2	5	4246	PSU	N1-C2-N3	5.64	121.52	115.13
2	5	2365	7MG	N9-C8-N7	-5.60	95.37	103.38
2	5	3629	B8K	N9-C8-N7	5.54	110.77	103.33
2	5	4039	PSU	N1-C2-N3	5.54	121.41	115.13
2	5	2365	7MG	C5-C4-N3	-5.53	117.59	128.13
2	5	4196	PSU	N1-C2-N3	5.52	121.39	115.13
2	5	4277	PSU	N1-C2-N3	5.51	121.38	115.13
2	5	1537	PSU	N1-C2-N3	5.51	121.38	115.13
2	5	1632	PSU	N1-C2-N3	5.49	121.34	115.13
2	5	1638	PSU	N1-C2-N3	5.47	121.33	115.13
2	5	4382	PSU	N1-C2-N3	5.47	121.32	115.13
2	5	3461	PSU	N1-C2-N3	5.46	121.31	115.13
2	5	1799	B8H	C4-N3-C2	-5.45	120.30	127.35
2	5	3447	PSU	N1-C2-N3	5.42	121.27	115.13
2	5	4042	B8H	C4-N3-C2	-5.41	120.34	127.35
2	5	2351	PSU	N1-C2-N3	5.31	121.15	115.13
2	5	3631	BGH	N9-C8-N7	5.29	110.43	103.33
2	5	4436	B8K	N9-C8-N7	5.27	110.40	103.33
2	5	3496	PSU	N1-C2-N3	5.22	121.04	115.13
2	5	4436	B8K	C5-C6-N1	5.21	120.17	110.99
2	5	4101	E6G	C2-N3-C4	5.20	121.30	115.36
2	5	1560	7MG	N9-C4-N3	5.09	133.08	125.47
2	5	4366	OMU	N3-C2-N1	5.08	121.64	114.89
2	5	3629	B8K	C5-C6-N1	4.99	119.79	110.99
2	5	3494	B8H	C4-N3-C2	-4.96	120.93	127.35
2	5	1736	E7G	N9-C4-N3	4.95	132.88	125.47
2	5	3631	BGH	C5-C6-N1	4.91	119.64	110.99
2	5	4052	OMU	N3-C2-N1	4.89	121.38	114.89
2	5	1736	E7G	C2-N3-C4	4.80	120.84	112.30
2	5	4101	E6G	N3-C2-N1	-4.79	120.84	127.22
2	5	4436	B8K	C2-N3-C4	4.78	120.81	112.30
2	5	4366	OMU	C4-N3-C2	-4.72	120.35	126.58
2	5	4052	OMU	C4-N3-C2	-4.66	120.43	126.58
2	5	1736	E7G	C5-C4-N3	-4.60	119.37	128.13
2	5	3629	B8K	C2-N3-C4	4.55	120.41	112.30
2	5	1736	E7G	N9-C8-N7	4.52	109.84	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1560	7MG	C5-C6-N1	4.51	118.94	110.99
2	5	1736	E7G	C5-C6-N1	4.50	118.92	110.99
2	5	3631	BGH	C2-N3-C4	4.49	120.30	112.30
2	5	1560	7MG	C2-N3-C4	4.48	120.28	112.30
2	5	4101	E6G	C61-O6-C6	-4.41	113.20	117.56
2	5	3631	BGH	C72-C71-N7	4.38	125.45	118.86
2	5	4193	5MC	C5-C6-N1	-4.37	118.84	123.34
2	5	4436	B8K	C72-C71-N7	4.36	125.42	118.86
2	5	1848	P7G	N9-C8-N7	4.31	109.55	103.38
2	5	3612	P7G	N9-C8-N7	4.30	109.52	103.38
2	5	3629	B8K	C72-C71-N7	4.29	125.31	118.86
2	5	1614	I4U	C5-C4-N3	-4.28	118.39	124.91
2	5	3514	5MC	C5-C6-N1	-4.25	118.97	123.34
2	5	1632	PSU	C4-N3-C2	-4.22	120.26	126.34
2	5	3631	BGH	N9-C4-N3	4.21	131.77	125.47
2	5	4382	PSU	C4-N3-C2	-4.21	120.27	126.34
2	5	4149	PSU	C4-N3-C2	-4.17	120.33	126.34
2	5	4246	PSU	C4-N3-C2	-4.16	120.35	126.34
2	5	4196	PSU	C4-N3-C2	-4.14	120.37	126.34
2	5	1638	PSU	C4-N3-C2	-4.13	120.39	126.34
2	5	1560	7MG	C5-C4-N3	-4.11	120.30	128.13
2	5	4039	PSU	C4-N3-C2	-4.09	120.45	126.34
2	5	2365	7MG	C2-N3-C4	4.09	119.58	112.30
2	5	4374	PSU	C4-N3-C2	-4.06	120.49	126.34
2	5	4277	PSU	C4-N3-C2	-4.02	120.55	126.34
2	5	4188	PSU	C4-N3-C2	-4.00	120.58	126.34
2	5	1537	PSU	C4-N3-C2	-3.98	120.60	126.34
2	5	3447	PSU	C4-N3-C2	-3.94	120.67	126.34
2	5	1266	1MA	N1-C2-N3	-3.90	121.48	126.02
2	5	3455	A2M	N3-C2-N1	-3.89	122.60	128.68
2	5	1489	A2M	N3-C2-N1	-3.86	122.64	128.68
2	5	2351	PSU	C4-N3-C2	-3.86	120.78	126.34
2	5	3461	PSU	C4-N3-C2	-3.85	120.80	126.34
2	5	4269	A2M	N3-C2-N1	-3.84	122.67	128.68
2	5	4436	B8K	N9-C4-N3	3.84	131.21	125.47
2	5	398	A2M	N3-C2-N1	-3.83	122.69	128.68
2	5	3631	BGH	C5-C4-N3	-3.81	120.86	128.13
2	5	1479	A2M	N3-C2-N1	-3.78	122.77	128.68
2	5	1560	7MG	N9-C8-N7	3.76	108.75	103.38
2	5	1292	P4U	C5-C4-N3	-3.71	119.27	124.91
2	5	4161	1MA	N1-C2-N3	-3.70	121.71	126.02
2	5	3496	PSU	C4-N3-C2	-3.69	121.02	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3557	A2M	N3-C2-N1	-3.69	122.92	128.68
2	5	3450	A2M	N3-C2-N1	-3.64	122.98	128.68
2	5	4436	B8K	C5-C4-N3	-3.63	121.21	128.13
2	5	3629	B8K	N9-C4-N3	3.60	130.86	125.47
2	5	3629	B8K	C6-C5-C4	-3.58	115.25	122.62
2	5	4436	B8K	C6-C5-C4	-3.58	115.25	122.62
2	5	3629	B8K	C5-C4-N3	-3.48	121.50	128.13
2	5	3514	5MC	C5-C4-N3	-3.43	117.97	121.67
2	5	4149	PSU	C3'-C2'-C1'	3.43	105.63	101.64
2	5	4282	OMC	C2'-C1'-N1	-3.41	107.61	114.22
2	5	4042	B8H	O2-C2-N1	-3.40	119.05	122.87
2	5	1638	PSU	O2-C2-N1	-3.38	119.07	122.79
2	5	4277	PSU	O2-C2-N1	-3.38	119.07	122.79
2	5	1810	A2M	N3-C2-N1	-3.35	123.44	128.68
2	5	1799	B8H	O2-C2-N1	-3.33	119.12	122.87
2	5	3612	P7G	C6-C5-N7	3.33	136.31	130.85
2	5	1266	1MA	C5-C6-N1	3.32	118.86	113.90
2	5	4101	E6G	C2-N1-C6	3.30	121.37	116.08
2	5	4161	1MA	C5-C6-N1	3.29	118.81	113.90
2	5	4374	PSU	O2-C2-N1	-3.29	119.17	122.79
2	5	4246	PSU	O2-C2-N1	-3.27	119.19	122.79
2	5	4039	PSU	O2-C2-N1	-3.26	119.20	122.79
2	5	3461	PSU	O2-C2-N1	-3.25	119.21	122.79
2	5	4188	PSU	O2-C2-N1	-3.25	119.21	122.79
2	5	4149	PSU	O2-C2-N1	-3.24	119.22	122.79
2	5	3631	BGH	C6-C5-C4	-3.21	115.99	122.62
2	5	4382	PSU	C5-C6-N1	-3.21	117.29	122.11
2	5	1537	PSU	O2-C2-N1	-3.19	119.28	122.79
2	5	1848	P7G	C6-C5-N7	3.19	136.07	130.85
2	5	3496	PSU	O2-C2-N1	-3.17	119.30	122.79
2	5	4196	PSU	O2-C2-N1	-3.13	119.35	122.79
2	5	1632	PSU	O2-C2-N1	-3.11	119.37	122.79
2	5	3447	PSU	O2-C2-N1	-3.11	119.37	122.79
2	5	4052	OMU	C5-C4-N3	3.09	119.47	114.84
2	5	4196	PSU	C5-C6-N1	-3.04	117.55	122.11
2	5	4366	OMU	C5-C4-N3	3.04	119.39	114.84
2	5	3494	B8H	O2-C2-N1	-3.03	119.45	122.87
2	5	1632	PSU	C5-C6-N1	-3.03	117.57	122.11
2	5	2616	OMG	C8-N7-C5	2.99	108.69	102.99
2	5	2351	PSU	O2-C2-N1	-2.99	119.50	122.79
2	5	4383	OMG	C8-N7-C5	2.99	108.68	102.99
2	5	4382	PSU	O2-C2-N1	-2.98	119.51	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3631	BGH	C2'-C1'-N9	-2.98	108.08	114.14
2	5	4369	OMG	C8-N7-C5	2.97	108.65	102.99
2	5	1266	1MA	C8-N7-C5	2.95	108.61	102.99
2	5	1477	OMG	C8-N7-C5	2.95	108.61	102.99
2	5	4240	OMG	C8-N7-C5	2.95	108.61	102.99
2	5	3524	OMG	C8-N7-C5	2.92	108.56	102.99
2	5	4277	PSU	C5-C6-N1	-2.91	117.74	122.11
2	5	4161	1MA	C8-N7-C5	2.89	108.50	102.99
2	5	1260	OMG	C8-N7-C5	2.87	108.46	102.99
2	5	1270	A2M	N3-C2-N1	-2.86	124.20	128.68
2	5	4039	PSU	C5-C6-N1	-2.85	117.83	122.11
2	5	4374	PSU	C5-C6-N1	-2.83	117.86	122.11
2	5	1560	7MG	C6-C5-N7	2.83	136.36	131.91
2	5	2207	OMG	C8-N7-C5	2.82	108.37	102.99
2	5	4246	PSU	C5-C6-N1	-2.81	117.90	122.11
2	5	4188	PSU	C5-C6-N1	-2.77	117.96	122.11
2	5	1638	PSU	C5-C6-N1	-2.75	117.98	122.11
2	5	4052	OMU	O4-C4-C5	-2.75	120.33	125.16
2	5	2365	7MG	C5-C6-N1	2.74	115.82	110.99
2	5	1560	7MG	C6-C5-C4	-2.72	117.02	122.62
2	5	3447	PSU	C5-C6-N1	-2.71	118.04	122.11
2	5	2351	PSU	C5-C6-N1	-2.70	118.06	122.11
2	5	4366	OMU	O2-C2-N1	-2.69	119.22	122.79
2	5	4383	OMG	C5-C6-N1	2.68	118.68	113.95
2	5	1537	PSU	C5-C6-N1	-2.67	118.11	122.11
2	5	4052	OMU	O2-C2-N1	-2.65	119.27	122.79
2	5	4116	OMG	C5-C6-N1	2.62	118.58	113.95
2	5	4366	OMU	O4-C4-C5	-2.61	120.57	125.16
2	5	1848	P7G	C5-C4-N3	-2.61	119.40	124.00
2	5	3524	OMG	C5-C6-N1	2.61	118.56	113.95
2	5	2365	7MG	C5-C4-N9	-2.60	102.98	106.35
2	5	1560	7MG	O6-C6-C5	-2.60	121.17	127.54
2	5	4366	OMU	C5-C6-N1	-2.58	117.48	121.81
2	5	1477	OMG	C5-C6-N1	2.57	118.49	113.95
2	5	4369	OMG	C5-C6-N1	2.55	118.45	113.95
2	5	2616	OMG	C5-C6-N1	2.53	118.42	113.95
2	5	3612	P7G	C5-C4-N3	-2.53	119.55	124.00
2	5	4052	OMU	C5-C6-N1	-2.52	117.59	121.81
2	5	1736	E7G	O6-C6-C5	-2.49	121.44	127.54
2	5	1270	A2M	C4-C5-N7	-2.48	106.82	109.40
2	5	4240	OMG	C5-C6-N1	2.47	118.31	113.95
2	5	2207	OMG	C5-C6-N1	2.44	118.27	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	3461	PSU	C5-C6-N1	-2.44	118.44	122.11
2	5	1260	OMG	C5-C6-N1	2.43	118.24	113.95
2	5	4193	5MC	C5-C4-N3	-2.42	119.06	121.67
2	5	1810	A2M	C4-C5-N7	-2.38	106.92	109.40
2	5	2365	7MG	O6-C6-C5	-2.36	121.76	127.54
2	5	2267	OMG	C5-C6-N1	2.34	118.09	113.95
2	5	1736	E7G	C6-C5-N7	2.34	135.67	131.67
2	5	2704	OMC	O2-C2-N3	-2.34	118.53	122.33
2	5	2265	OMC	O2-C2-N3	-2.33	118.54	122.33
2	5	4116	OMG	C8-N7-C5	2.33	107.42	102.99
2	5	1479	A2M	C3'-C2'-C1'	2.32	107.25	102.89
2	5	4383	OMG	C2-N1-C6	-2.32	120.83	125.10
2	5	1580	OMG	C5-C6-N1	2.32	118.05	113.95
2	5	4188	PSU	O4'-C1'-C2'	2.31	108.41	105.14
2	5	3524	OMG	C2-N1-C6	-2.30	120.85	125.10
2	5	1736	E7G	C6-C5-C4	-2.29	117.90	122.62
2	5	3433	OMC	C5-C6-N1	-2.25	118.04	121.81
2	5	2365	7MG	O4'-C1'-N9	2.25	112.36	109.30
2	5	2207	OMG	C2-N1-C6	-2.24	120.97	125.10
2	5	2208	OMC	O2-C2-N3	-2.23	118.70	122.33
2	5	3496	PSU	C5-C6-N1	-2.23	118.77	122.11
2	5	1580	OMG	C8-N7-C5	2.22	107.23	102.99
2	5	1292	P4U	C41-O4-C4	-2.22	112.73	117.24
2	5	4369	OMG	C2-N1-C6	-2.22	121.02	125.10
2	5	4193	5MC	C3'-C2'-C1'	2.22	105.64	101.43
2	5	3514	5MC	O2-C2-N3	-2.21	118.74	122.33
2	5	4149	PSU	C5-C6-N1	-2.21	118.79	122.11
2	5	2647	OMC	O2-C2-N3	-2.20	118.75	122.33
2	5	4276	UR3	C1'-N1-C2	2.20	120.70	116.99
2	5	1477	OMG	C2-N1-C6	-2.20	121.05	125.10
2	5	2267	OMG	C8-N7-C5	2.20	107.17	102.99
2	5	3601	OMC	O2-C2-N3	-2.19	118.76	122.33
2	5	4240	OMG	C2-N1-C6	-2.19	121.06	125.10
2	5	4116	OMG	O6-C6-C5	-2.19	120.09	124.37
2	5	1736	E7G	C8-N7-C71	2.19	125.70	120.50
2	5	2616	OMG	C2-N1-C6	-2.18	121.09	125.10
2	5	2208	OMC	N1-C2-N3	2.17	122.76	118.81
2	5	4101	E6G	C5-C6-N1	-2.17	119.14	123.26
2	5	2704	OMC	N1-C2-N3	2.15	122.73	118.81
2	5	1260	OMG	C2-N1-C6	-2.14	121.15	125.10
2	5	3619	OMC	N1-C2-N3	2.12	122.66	118.81
2	5	2265	OMC	N1-C2-N3	2.12	122.66	118.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	1736	E7G	C2-N1-C6	-2.12	121.24	125.10
2	5	2647	OMC	N1-C2-N3	2.09	122.62	118.81
2	5	3496	PSU	O4'-C1'-C2'	2.09	108.09	105.14
2	5	3601	OMC	N1-C2-N3	2.08	122.60	118.81
2	5	3631	BGH	C2-N1-C6	-2.08	121.31	125.10
2	5	3619	OMC	O2-C2-N3	-2.07	118.97	122.33
2	5	4382	PSU	O4'-C1'-C2'	2.06	108.04	105.14
2	5	3619	OMC	C5-C6-N1	-2.02	118.42	121.81
2	5	3433	OMC	N1-C2-N3	2.02	122.48	118.81
2	5	4246	PSU	O4'-C1'-C2'	2.01	107.98	105.14

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	5	1260	OMG	C1'-C2'-O2'-CM2
2	5	1270	A2M	C1'-C2'-O2'-CM2
2	5	1292	P4U	N3-C4-O4-C41
2	5	1292	P4U	C3'-C4'-C5'-O5'
2	5	1292	P4U	O4'-C4'-C5'-O5'
2	5	1537	PSU	C3'-C4'-C5'-O5'
2	5	1537	PSU	O4'-C4'-C5'-O5'
2	5	1632	PSU	C2'-C1'-C5-C6
2	5	1736	E7G	O4'-C4'-C5'-O5'
2	5	2207	OMG	C1'-C2'-O2'-CM2
2	5	2265	OMC	C1'-C2'-O2'-CM2
2	5	2267	OMG	O4'-C4'-C5'-O5'
2	5	2267	OMG	C3'-C4'-C5'-O5'
2	5	2616	OMG	C1'-C2'-O2'-CM2
2	5	2647	OMC	C1'-C2'-O2'-CM2
2	5	2704	OMC	C1'-C2'-O2'-CM2
2	5	3433	OMC	C2'-C1'-N1-C2
2	5	3433	OMC	C2'-C1'-N1-C6
2	5	3461	PSU	C3'-C4'-C5'-O5'
2	5	3461	PSU	O4'-C4'-C5'-O5'
2	5	3494	B8H	O4'-C4'-C5'-O5'
2	5	3496	PSU	C3'-C4'-C5'-O5'
2	5	3496	PSU	O4'-C4'-C5'-O5'
2	5	3524	OMG	O4'-C4'-C5'-O5'
2	5	3557	A2M	C1'-C2'-O2'-CM2
2	5	3612	P7G	O4'-C4'-C5'-O5'
2	5	3629	B8K	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	5	3631	BGH	C3'-C4'-C5'-O5'
2	5	4052	OMU	C1'-C2'-O2'-CM2
2	5	4052	OMU	C3'-C4'-C5'-O5'
2	5	4101	E6G	C5-C6-O6-C61
2	5	4101	E6G	N1-C6-O6-C61
2	5	4116	OMG	C1'-C2'-O2'-CM2
2	5	4149	PSU	O4'-C1'-C5-C4
2	5	4149	PSU	O4'-C1'-C5-C6
2	5	4193	5MC	C2'-C1'-N1-C6
2	5	4196	PSU	C2'-C1'-C5-C4
2	5	4196	PSU	O4'-C4'-C5'-O5'
2	5	4246	PSU	C3'-C4'-C5'-O5'
2	5	4246	PSU	O4'-C4'-C5'-O5'
2	5	4269	A2M	O4'-C4'-C5'-O5'
2	5	4282	OMC	C1'-C2'-O2'-CM2
2	5	4366	OMU	C1'-C2'-O2'-CM2
2	5	4369	OMG	C1'-C2'-O2'-CM2
2	5	4382	PSU	C3'-C4'-C5'-O5'
2	5	4383	OMG	O4'-C4'-C5'-O5'
2	5	4383	OMG	C1'-C2'-O2'-CM2
19	m	72	MLZ	C-CA-CB-CG
2	5	1736	E7G	C3'-C4'-C5'-O5'
2	5	3524	OMG	C3'-C4'-C5'-O5'
2	5	3612	P7G	C3'-C4'-C5'-O5'
2	5	3629	B8K	C3'-C4'-C5'-O5'
2	5	4039	PSU	C3'-C4'-C5'-O5'
2	5	4196	PSU	C3'-C4'-C5'-O5'
2	5	4269	A2M	C3'-C4'-C5'-O5'
2	5	4382	PSU	O4'-C4'-C5'-O5'
2	5	4383	OMG	C3'-C4'-C5'-O5'
2	5	1292	P4U	O4-C41-C42-C43
2	5	3494	B8H	C3'-C4'-C5'-O5'
2	5	3631	BGH	O4'-C4'-C5'-O5'
2	5	4039	PSU	O4'-C4'-C5'-O5'
2	5	4240	OMG	O4'-C4'-C5'-O5'
2	5	4240	OMG	C3'-C4'-C5'-O5'
2	5	4193	5MC	C2'-C1'-N1-C2
2	5	1736	E7G	C72-C71-N7-C8
2	5	4052	OMU	O4'-C4'-C5'-O5'
2	5	4101	E6G	C62-C61-O6-C6
2	5	4161	1MA	C3'-C4'-C5'-O5'
2	5	2207	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	5	1479	A2M	C3'-C4'-C5'-O5'
2	5	4246	PSU	C4'-C5'-O5'-P
2	5	1489	A2M	C3'-C2'-O2'-CM'
2	5	4240	OMG	C3'-C2'-O2'-CM2
2	5	4193	5MC	O4'-C1'-N1-C6
2	5	4193	5MC	O4'-C1'-N1-C2
2	5	1270	A2M	C4'-C5'-O5'-P
2	5	1489	A2M	C4'-C5'-O5'-P
2	5	3433	OMC	O4'-C1'-N1-C2
2	5	3629	B8K	C4'-C5'-O5'-P
2	5	1270	A2M	C3'-C4'-C5'-O5'
2	5	3433	OMC	O4'-C1'-N1-C6
2	5	3496	PSU	C4'-C5'-O5'-P
2	5	4269	A2M	C3'-C2'-O2'-CM'
2	5	2265	OMC	O4'-C4'-C5'-O5'
2	5	4282	OMC	C3'-C4'-C5'-O5'
2	5	4042	B8H	O4'-C1'-C5-C4
2	5	4196	PSU	O4'-C1'-C5-C4
2	5	4246	PSU	O4'-C1'-C5-C4
2	5	398	A2M	O4'-C4'-C5'-O5'
2	5	1632	PSU	O4'-C1'-C5-C6
2	5	4042	B8H	O4'-C1'-C5-C6
2	5	4196	PSU	O4'-C1'-C5-C6
2	5	4246	PSU	O4'-C1'-C5-C6
2	5	4382	PSU	O4'-C1'-C5-C6
2	5	2207	OMG	C3'-C4'-C5'-O5'
2	5	3612	P7G	C72-C71-N7-C8
2	5	1614	I4U	C42-C41-O4-C4
2	5	1479	A2M	O4'-C4'-C5'-O5'
2	5	1489	A2M	O4'-C4'-C5'-O5'
2	5	3619	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 184 ligands modelled in this entry, 183 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	OWI	K	501	-	45,45,45	2.14	12 (26%)	61,64,64	2.85	13 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	OWI	K	501	-	-	27/52/60/60	0/3/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	K	501	OWI	S05-N04	6.69	1.72	1.63
50	K	501	OWI	S30-N29	6.46	1.72	1.63
50	K	501	OWI	C31-S30	5.39	1.84	1.76
50	K	501	OWI	C07-S05	4.70	1.83	1.76
50	K	501	OWI	C34-N35	3.82	1.46	1.37
50	K	501	OWI	O41-S30	2.98	1.46	1.43
50	K	501	OWI	O06-S05	2.59	1.46	1.43
50	K	501	OWI	O40-S30	2.54	1.46	1.43
50	K	501	OWI	C03-N04	-2.51	1.43	1.47
50	K	501	OWI	O14-S05	2.41	1.46	1.43
50	K	501	OWI	C03-C02	2.15	1.52	1.50
50	K	501	OWI	C42-C02	2.13	1.52	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	K	501	OWI	O41-S30-O40	-11.78	100.43	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	K	501	OWI	O14-S05-O06	-11.49	100.91	119.52
50	K	501	OWI	O41-S30-N29	7.30	113.34	106.69
50	K	501	OWI	O14-S05-N04	6.39	112.52	106.69
50	K	501	OWI	O06-S05-N04	4.78	111.04	106.69
50	K	501	OWI	C31-S30-N29	4.07	112.15	107.30
50	K	501	OWI	C20-C19-N18	-3.69	109.45	114.65
50	K	501	OWI	O40-S30-N29	3.56	109.94	106.69
50	K	501	OWI	O14-S05-C07	3.48	112.45	108.05
50	K	501	OWI	O40-S30-C31	2.46	111.16	108.05
50	K	501	OWI	C07-S05-N04	2.39	110.15	107.30
50	K	501	OWI	C03-C02-C01	-2.24	119.08	122.07
50	K	501	OWI	C26-N18-C19	-2.19	106.74	111.96

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	K	501	OWI	C16-C15-N04-S05
50	K	501	OWI	N18-C19-C20-C21
50	K	501	OWI	N18-C19-C20-C25
50	K	501	OWI	C20-C19-N18-C26
50	K	501	OWI	C02-C42-N29-C28
50	K	501	OWI	C02-C42-N29-S30
50	K	501	OWI	C03-N04-S05-C07
50	K	501	OWI	C32-C31-S30-N29
50	K	501	OWI	C39-C31-S30-N29
50	K	501	OWI	C33-C34-N35-C36
50	K	501	OWI	C38-C34-N35-C37
50	K	501	OWI	C33-C34-N35-C37
50	K	501	OWI	C38-C34-N35-C36
50	K	501	OWI	N18-C26-C27-C28
50	K	501	OWI	C03-N04-S05-O14
50	K	501	OWI	C16-C17-N18-C26
50	K	501	OWI	C15-N04-S05-O14
50	K	501	OWI	C32-C31-S30-O41
50	K	501	OWI	C39-C31-S30-O41
50	K	501	OWI	C02-C03-N04-C15
50	K	501	OWI	C15-N04-S05-O06
50	K	501	OWI	C16-C17-N18-C19
50	K	501	OWI	C15-N04-S05-C07
50	K	501	OWI	C42-N29-S30-O40
50	K	501	OWI	C28-N29-S30-O40

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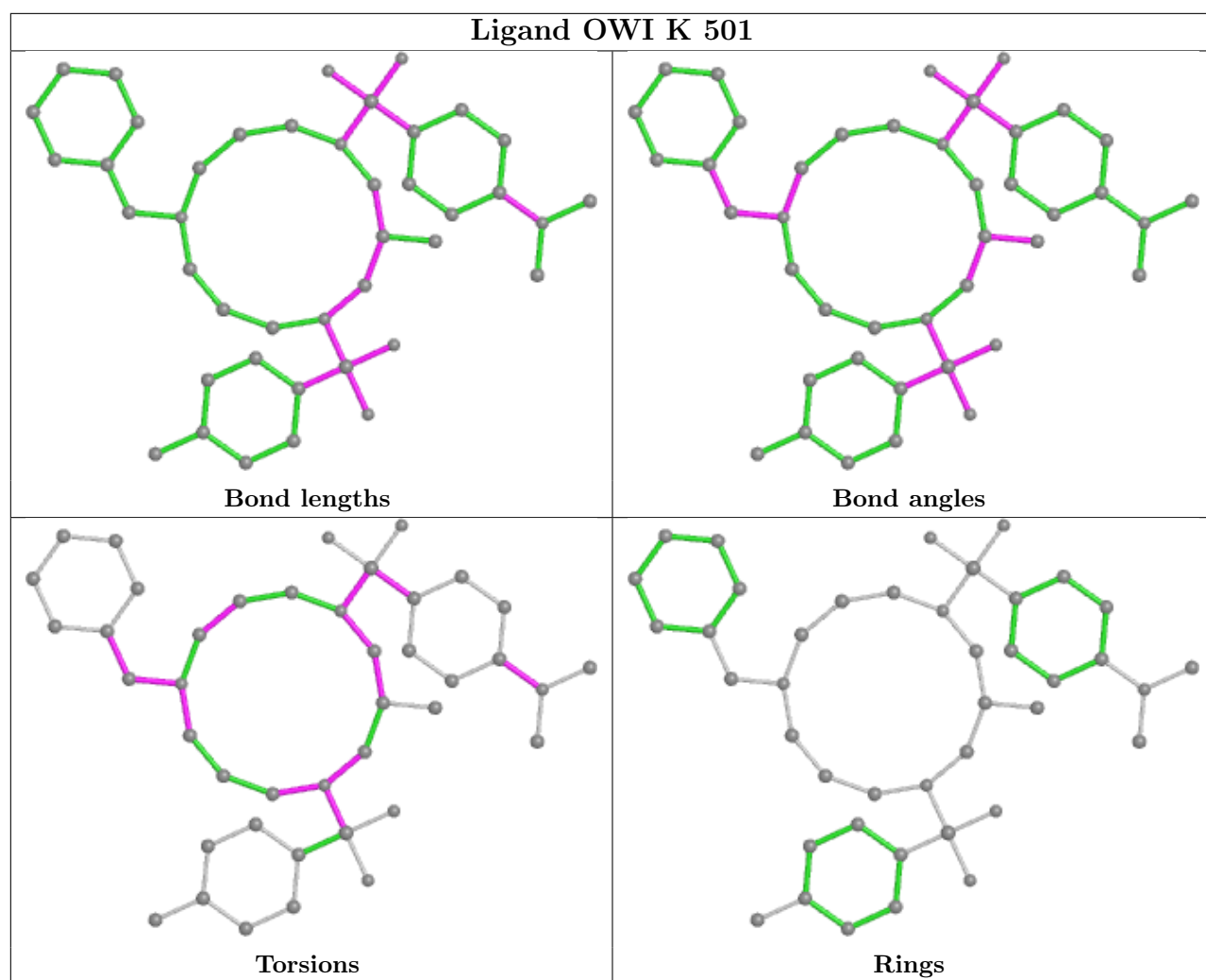
Mol	Chain	Res	Type	Atoms
50	K	501	OWI	C01-C02-C42-N29
50	K	501	OWI	C03-N04-S05-O06

There are no ring outliers.

No monomer is involved in short contacts.

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





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

There are no such residues in this entry.

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

There are no chain breaks in this entry.

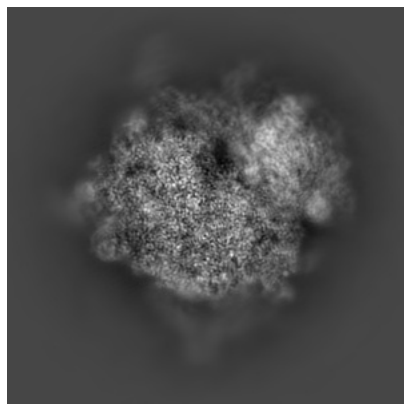
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15863. These allow visual inspection of the internal detail of the map and identification of artifacts.

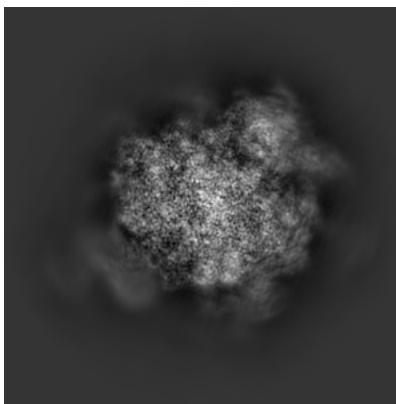
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

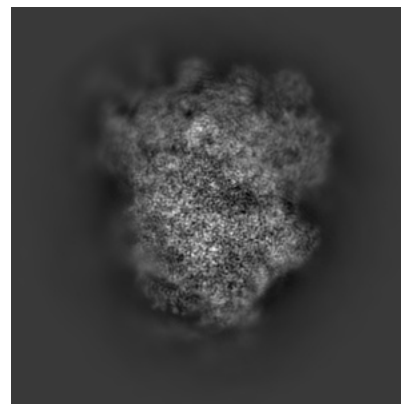
#### 6.1.1 Primary map



X

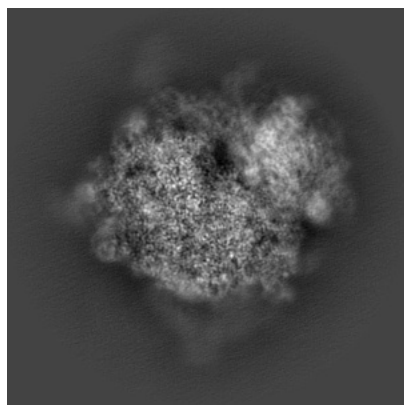


Y

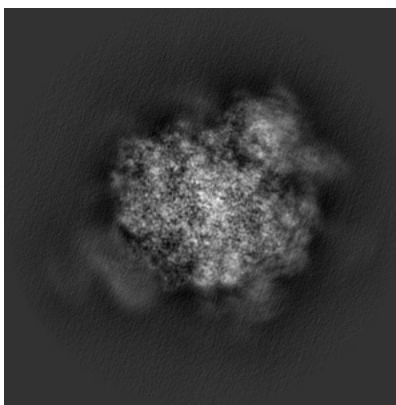


Z

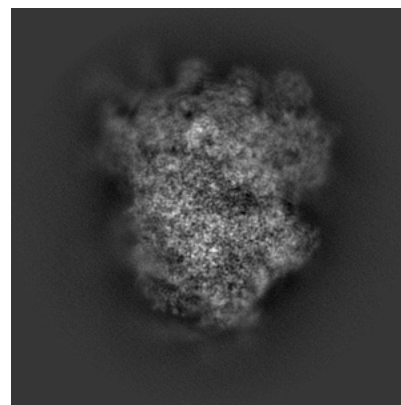
#### 6.1.2 Raw map



X



Y

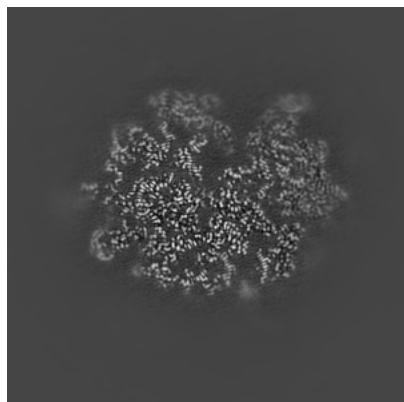


Z

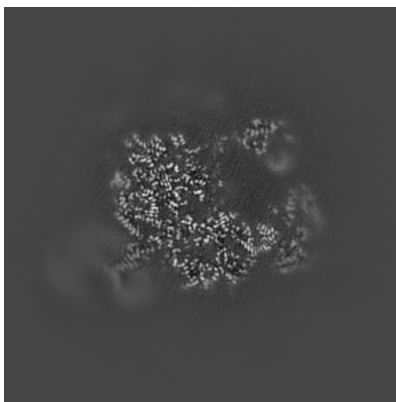
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

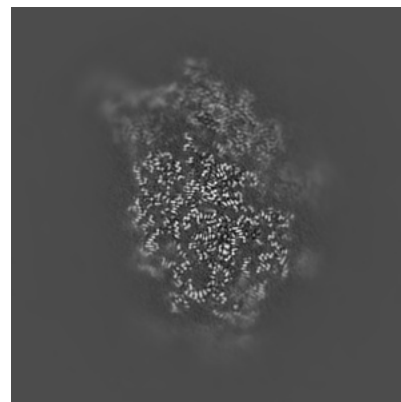
### 6.2.1 Primary map



X Index: 176

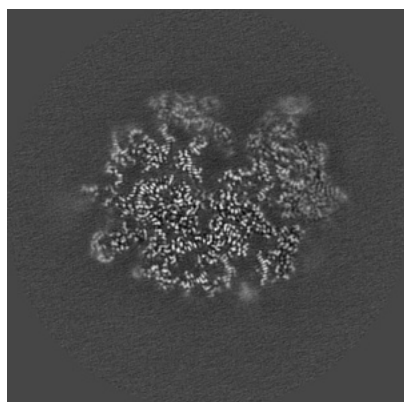


Y Index: 176

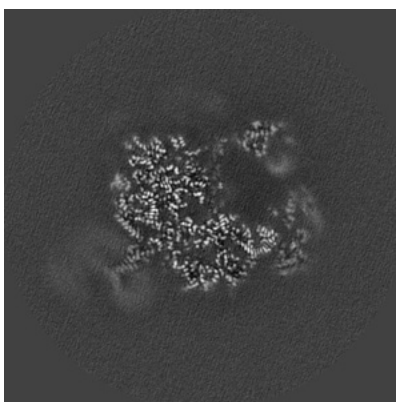


Z Index: 176

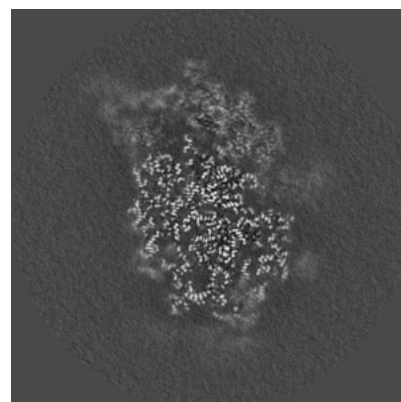
### 6.2.2 Raw map



X Index: 176



Y Index: 176

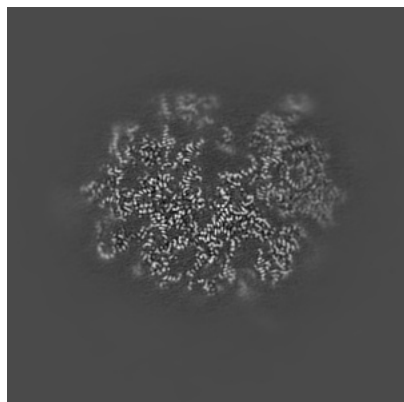


Z Index: 176

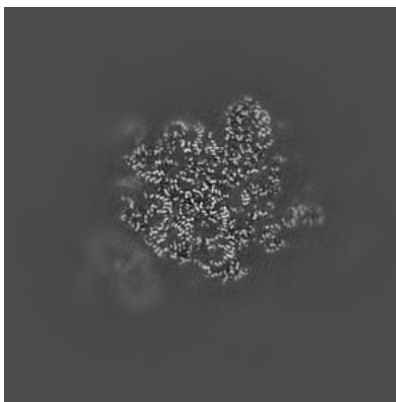
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

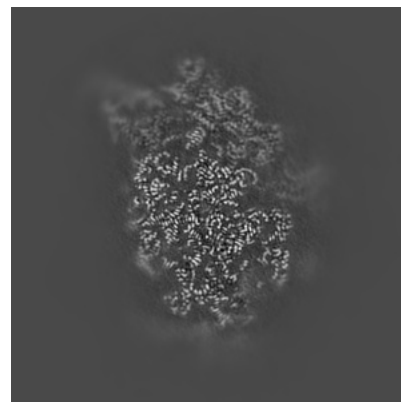
### 6.3.1 Primary map



X Index: 179

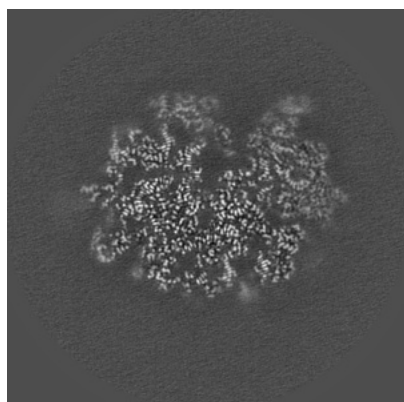


Y Index: 147

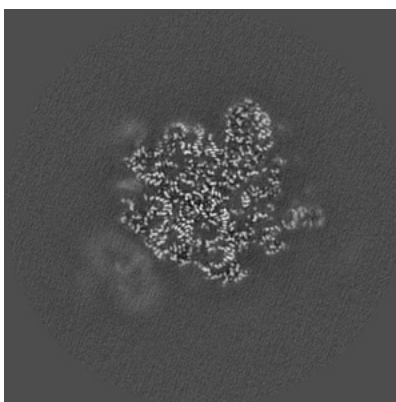


Z Index: 180

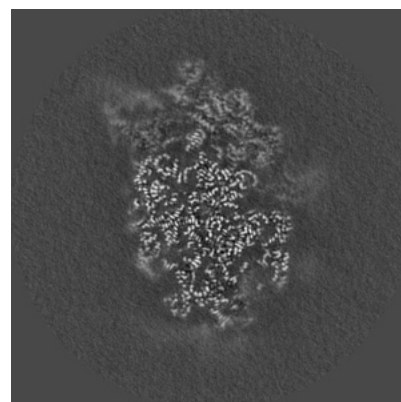
### 6.3.2 Raw map



X Index: 177



Y Index: 147



Z Index: 180

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

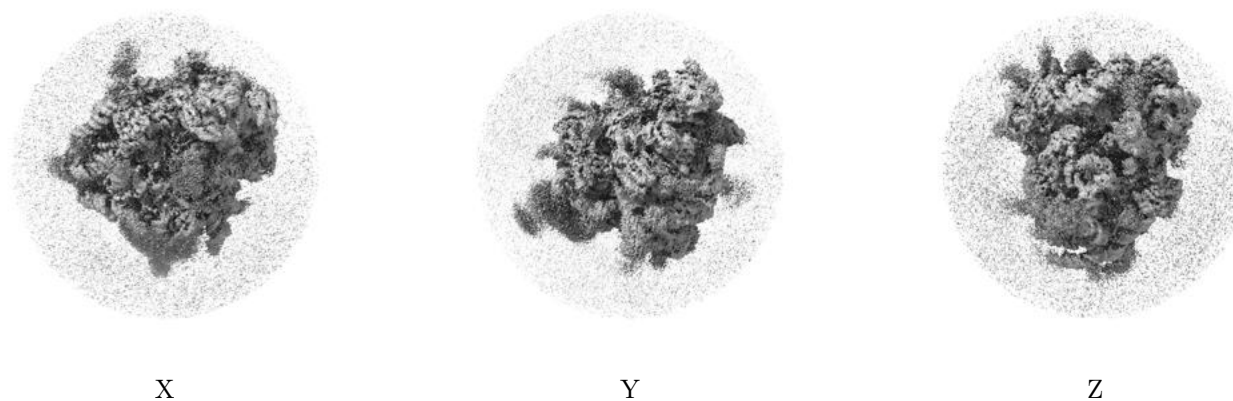
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01581. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

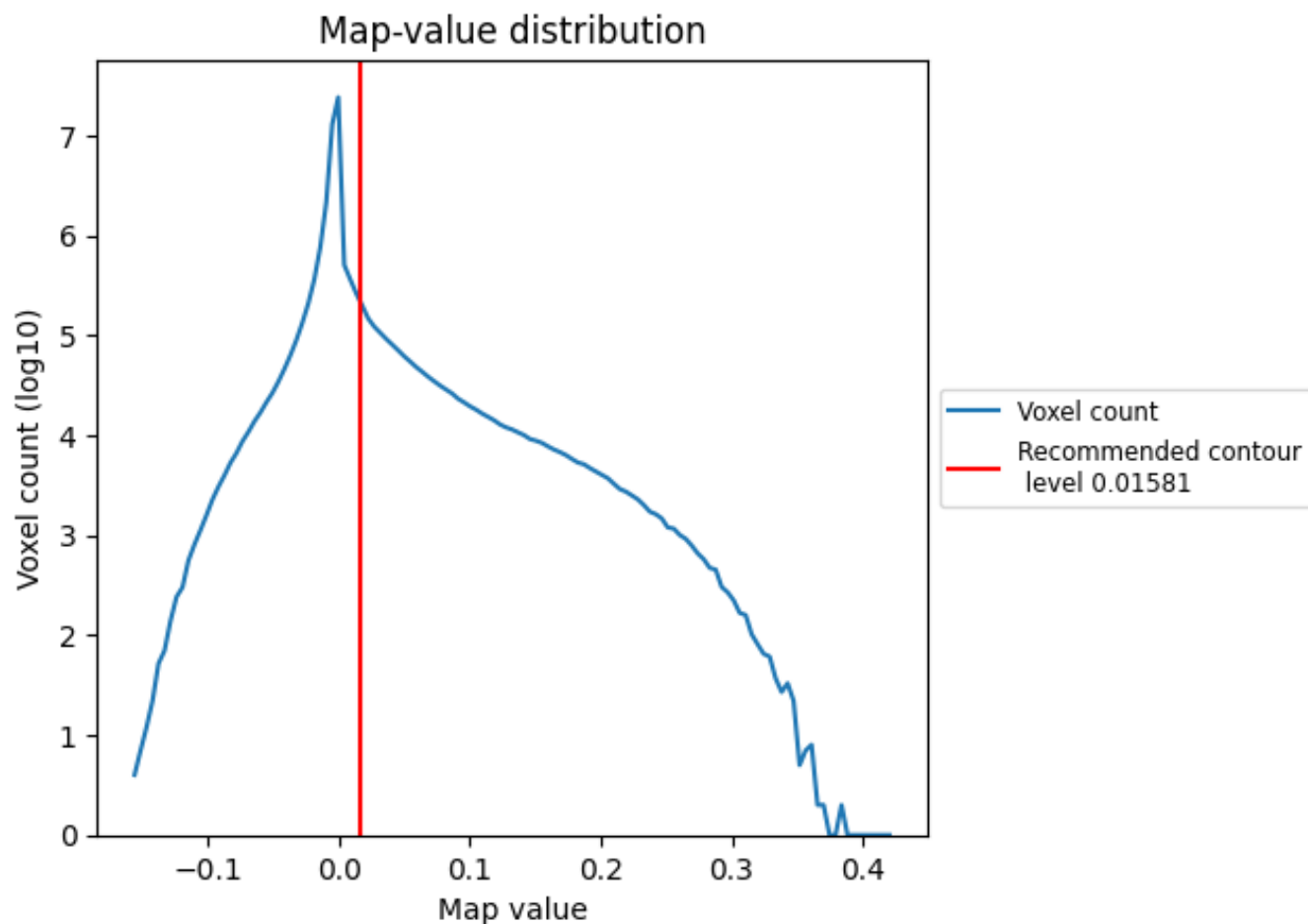
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

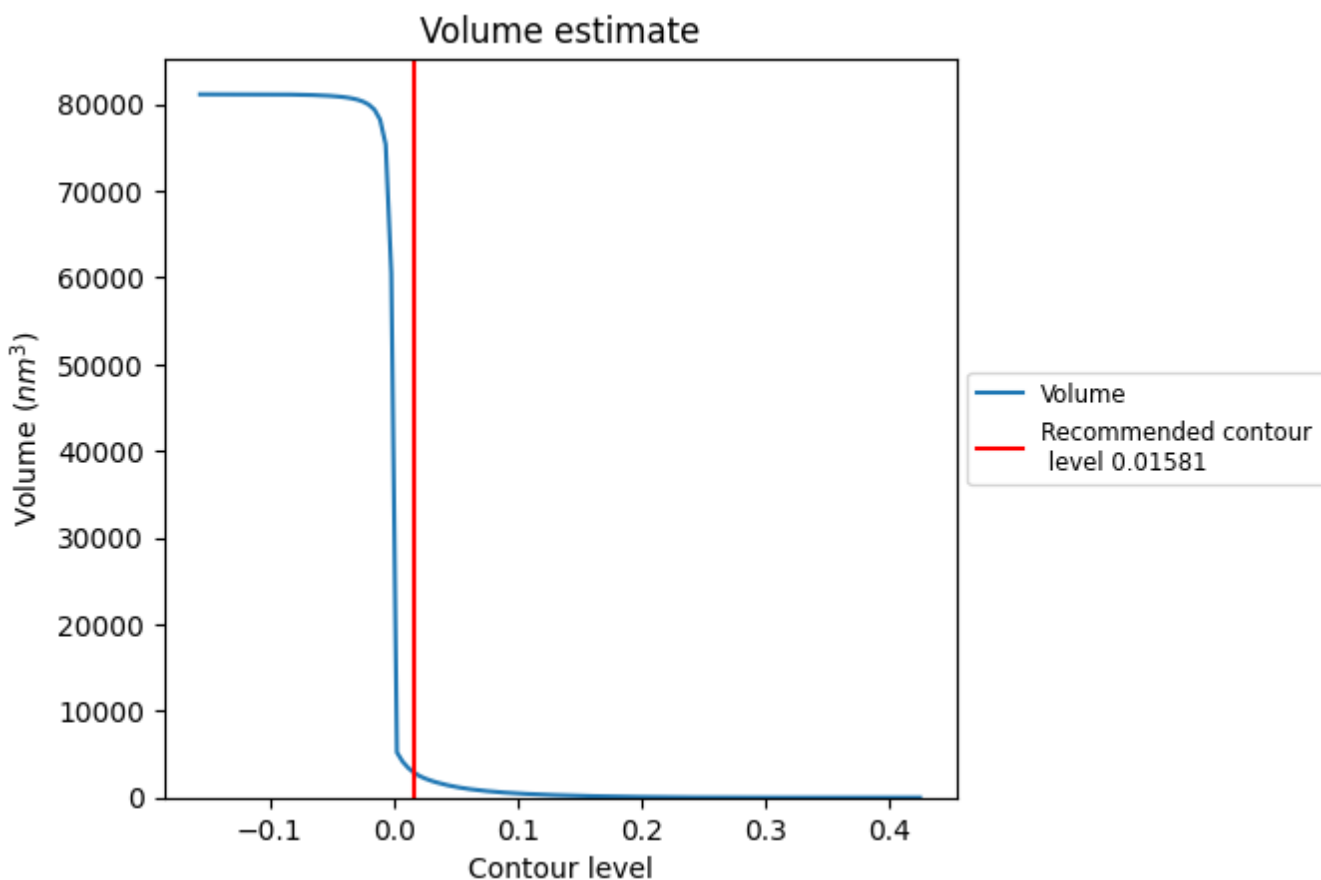
This section contains the results of statistical analysis of the map.

### 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.

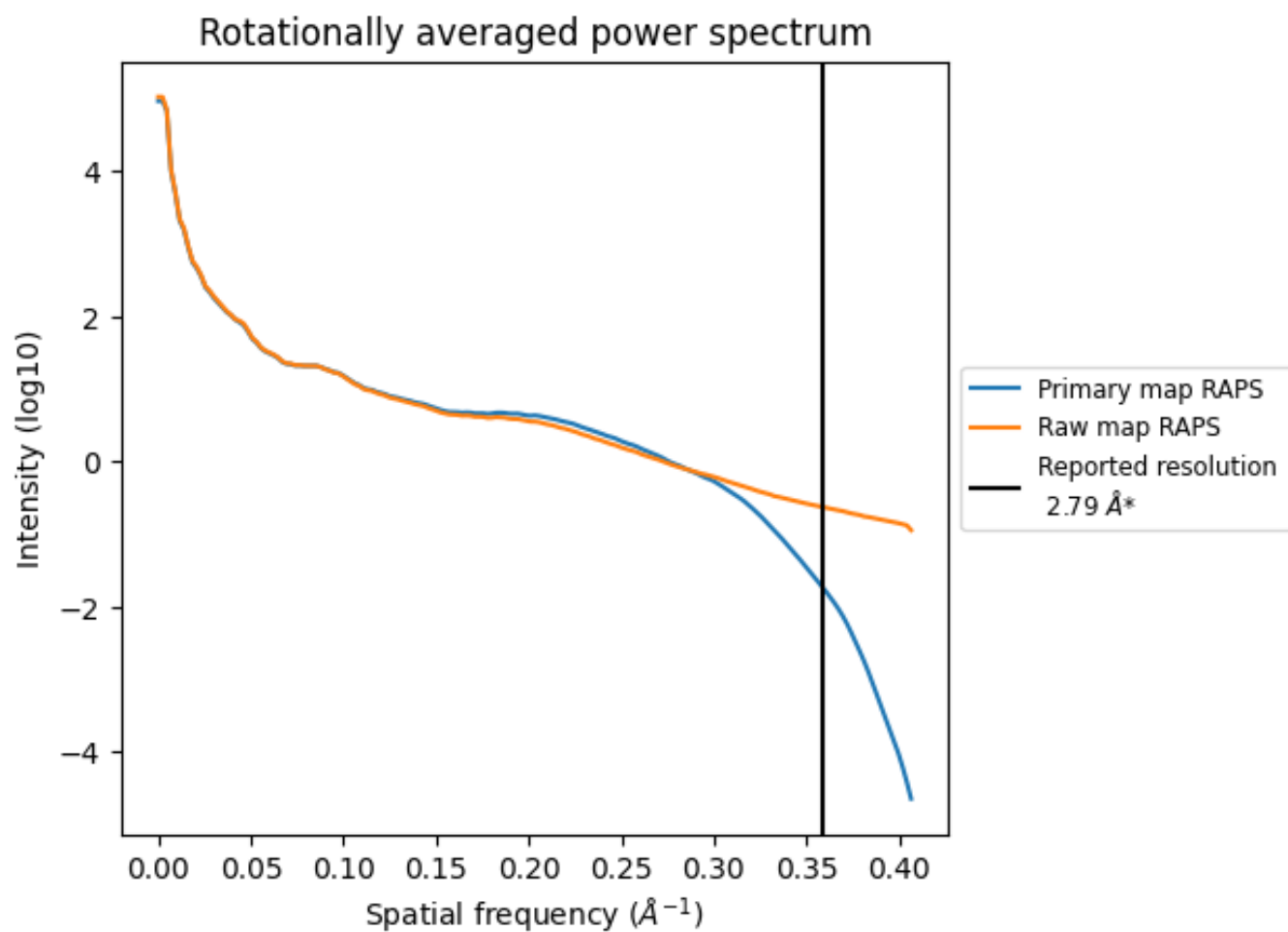
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2951 nm<sup>3</sup>; this corresponds to an approximate mass of 2665 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 i



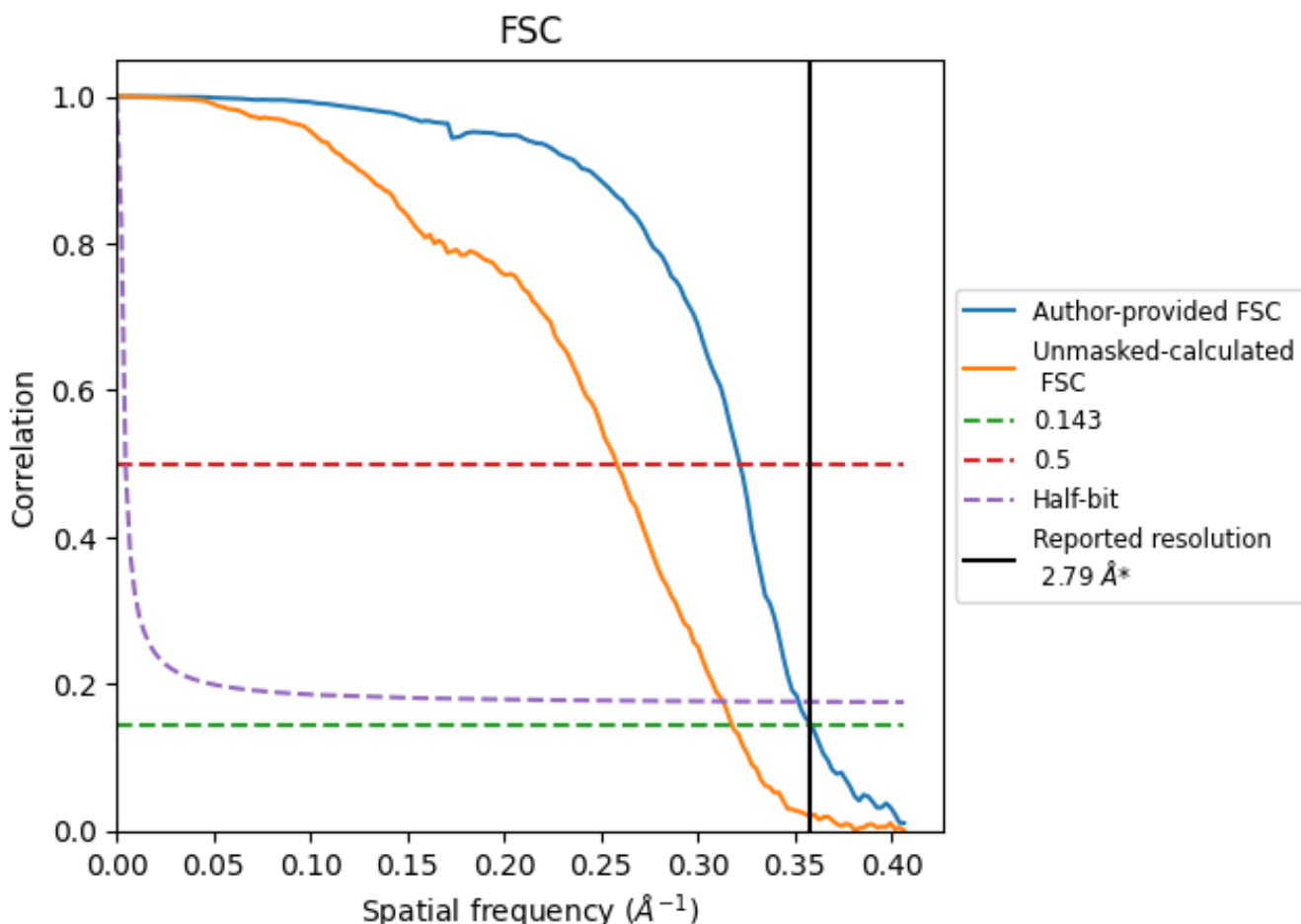
\*Reported resolution corresponds to spatial frequency of  $0.358 \text{ \AA}^{-1}$



## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.358 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

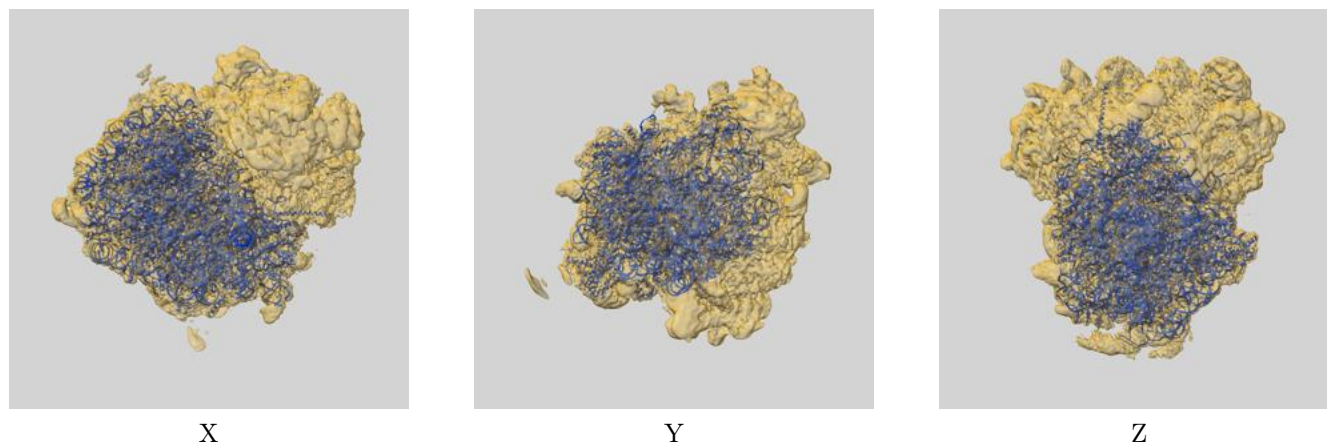
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.11	2.84
Unmasked-calculated*	3.15	3.87	3.19

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.15 differs from the reported value 2.79 by more than 10 %

## 9 Map-model fit [i](#)

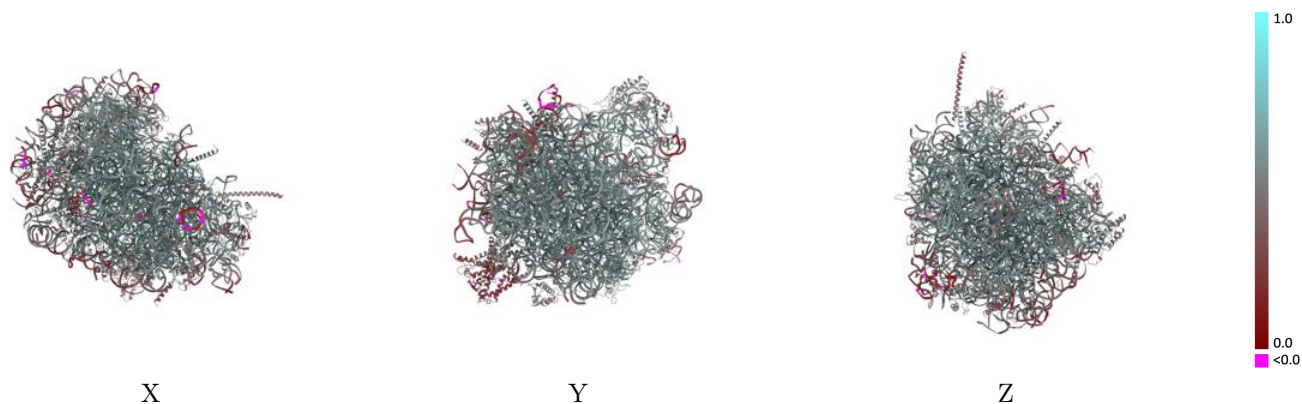
This section contains information regarding the fit between EMDB map EMD-15863 and PDB model 8B6C. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



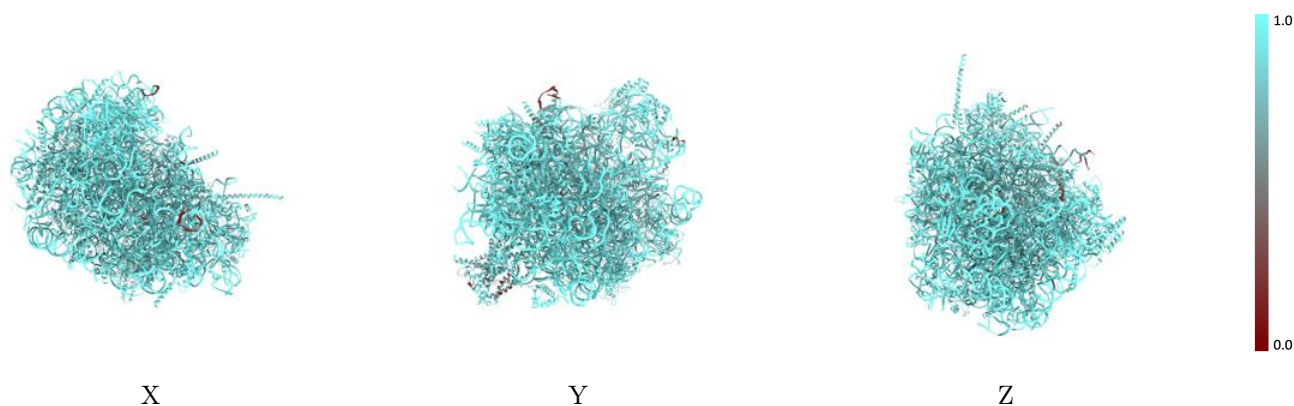
The images above show the 3D surface view of the map at the recommended contour level 0.01581 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



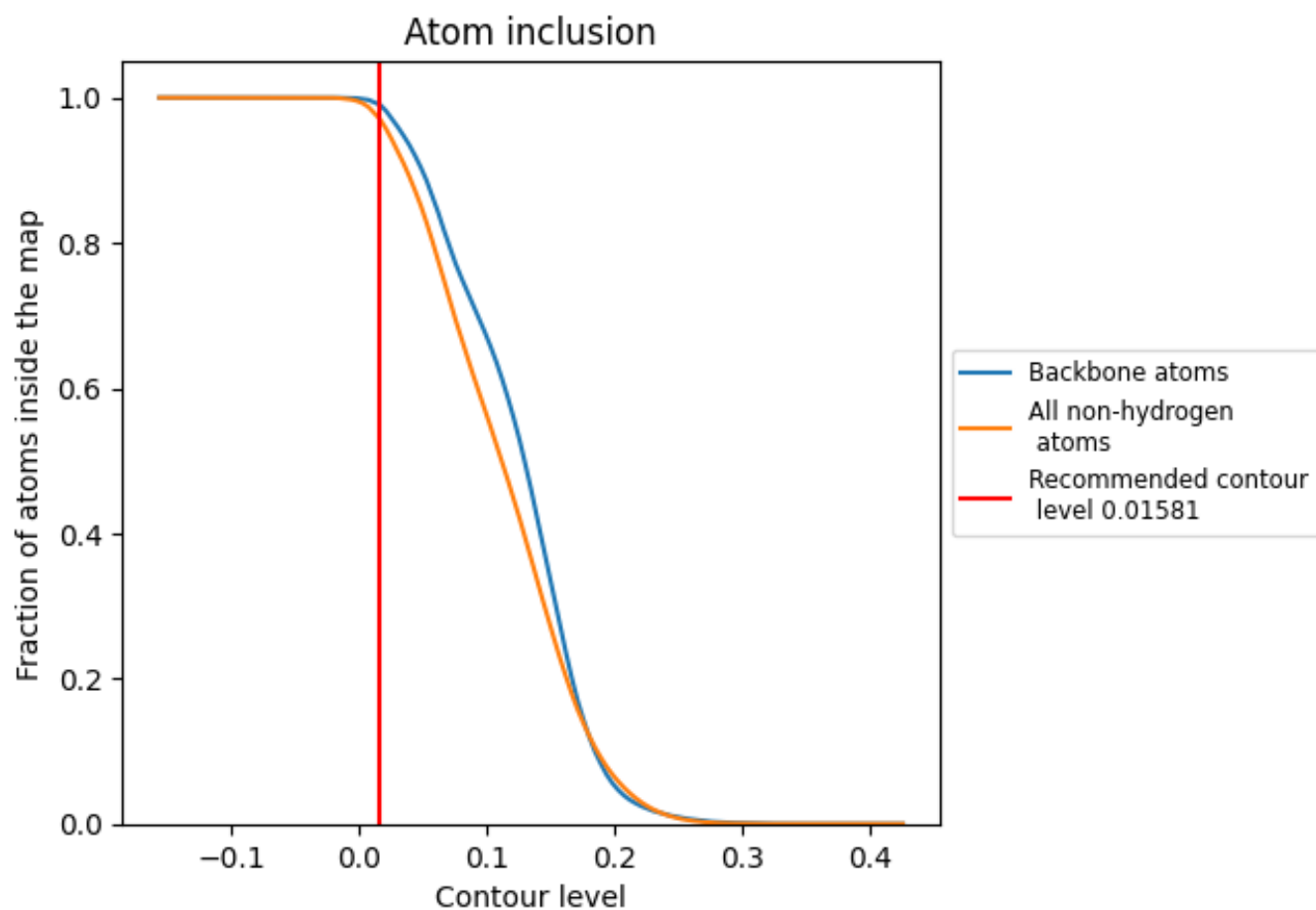
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01581).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% 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 (0.01581) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9712	 0.5160
5	 0.9873	 0.5160
7	 0.9977	 0.5520
8	 0.9953	 0.5410
A	 0.9695	 0.5720
B	 0.9690	 0.5500
C	 0.9655	 0.5490
D	 0.9720	 0.5050
E	 0.9708	 0.5230
F	 0.9587	 0.5510
G	 0.9556	 0.4800
H	 0.9547	 0.5320
I	 0.9585	 0.5400
J	 0.9500	 0.4670
K	 0.7718	 0.2550
L	 0.9370	 0.5110
M	 0.9718	 0.5320
N	 0.9722	 0.5760
O	 0.9753	 0.5530
P	 0.9619	 0.5550
Q	 0.9579	 0.5600
R	 0.9403	 0.4920
S	 0.9716	 0.5580
T	 0.9596	 0.5390
U	 0.9444	 0.4390
V	 0.9562	 0.5610
W	 0.9568	 0.5450
X	 0.9309	 0.5240
Y	 0.9453	 0.5250
Z	 0.9702	 0.5140
a	 0.9752	 0.5680
b	 0.9325	 0.4730
c	 0.9395	 0.4970
d	 0.9510	 0.5230
e	 0.9656	 0.5670



*Continued on next page...*

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Chain	Atom inclusion	Q-score
f	 0.9667	 0.5760
g	 0.9448	 0.5440
h	 0.9367	 0.5150
i	 0.9472	 0.4970
j	 0.9777	 0.5790
k	 0.9174	 0.4660
l	 0.9555	 0.5470
m	 0.9520	 0.5540
n	 0.8853	 0.4620
o	 0.9621	 0.5470
p	 0.9419	 0.5400
q	 0.8046	 0.2950
r	 0.9770	 0.5530