Full wwPDB EM Validation Report ⓘ

Apr 20, 2024 – 10:03 pm BST

PDB ID	:	7ZAI
EMDB ID	:	EMD-14581
Title	:	Cryo-EM structure of a Pyrococcus abyssi 30S bound to Met-initiator tRNA, mRNA and aIF1A.
Authors	:	Coureux, P.D.; Bourgeois, G.; Mechulam, Y.; Schmitt, E.; Kazan, R.
Deposited on	:	2022-03-22
Resolution	:	2.60 Å(reported)
Based on initial model	:	7ZHG

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

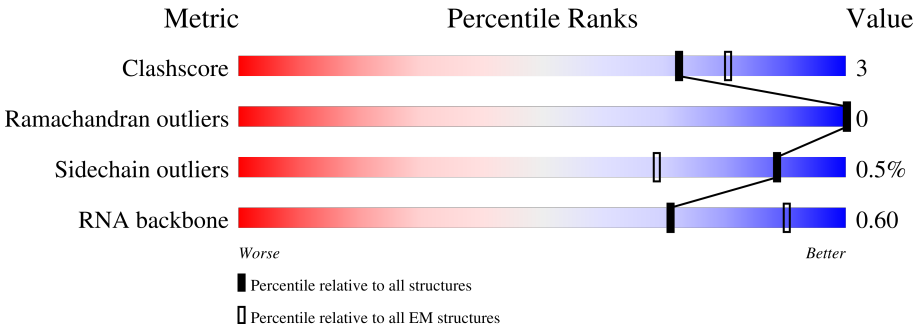
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	2	1497	76% 20% •
2	A	199	92% • 6%
3	B	202	94% • •
4	C	63	84% 6% 10%
5	D	180	91% 5% • •
6	E	243	91% 9%
7	F	236	92% 6% •

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Mol	Chain	Length	Quality of chain
8	G	125	90% 9%
9	H	215	89% 10%
10	I	130	93% 6%
11	J	127	87% 11%
12	K	135	93% 7%
13	L	102	88% 10%
14	M	137	88% 5% 7%
15	N	147	93% 6%
16	O	148	93% 5%
17	P	56	91% 7%
18	Q	158	90% 6%
19	R	113	94% 5%
20	S	67	88% 7%
21	T	132	89% 5% 6%
22	U	150	94%
23	V	99	88% 9%
24	W	65	94% 6%
25	X	71	83% 8% 8%
26	Y	51	49% 47%
27	Z	210	86% 7% 7%
28	0	36	100%
29	3	123	70% 28%
30	5	25	72% 16% 12%
31	4	77	39% 40% 17%
32	6	134	55% 13% 31%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 64649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1497	32312	14418	5959	10438	1497	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	17	4AC	C	modified residue	GB 5457433
2	53	4AC	C	modified residue	GB 5457433
2	286	4AC	C	modified residue	GB 5457433
2	303	4AC	C	modified residue	GB 5457433
2	319	4AC	C	modified residue	GB 5457433
2	379	4AC	C	modified residue	GB 5457433
2	394	4AC	C	modified residue	GB 5457433
2	479	4AC	C	modified residue	GB 5457433
2	511	4AC	C	modified residue	GB 5457433
2	546	4AC	C	modified residue	GB 5457433
2	590	4AC	C	modified residue	GB 5457433
2	626	4AC	C	modified residue	GB 5457433
2	636	4AC	C	modified residue	GB 5457433
2	703	4AC	C	modified residue	GB 5457433
2	718	4AC	C	modified residue	GB 5457433
2	731	4AC	C	modified residue	GB 5457433
2	751	4AC	C	modified residue	GB 5457433
2	828	4AC	C	modified residue	GB 5457433
2	839	4AC	C	modified residue	GB 5457433
2	848	4AC	C	modified residue	GB 5457433
2	851	4AC	C	modified residue	GB 5457433
2	868	4AC	C	modified residue	GB 5457433
2	957	4AC	C	modified residue	GB 5457433
2	1028	4AC	C	modified residue	GB 5457433
2	1147	4AC	C	modified residue	GB 5457433
2	1184	4AC	C	modified residue	GB 5457433
2	1233	4AC	C	modified residue	GB 5457433
2	1239	4AC	C	modified residue	GB 5457433

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Chain	Residue	Modelled	Actual	Comment	Reference
2	1479	4AC	C	modified residue	GB 5457433

- Molecule 2 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	188	Total	C	N	O	S	0	0
			1531	993	268	266	4		

- Molecule 3 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	196	Total	C	N	O	S	0	0
			1571	1017	269	281	4		

- Molecule 4 is a protein called Zn-ribbon RNA-binding protein involved in translation.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	57	Total	C	N	O	S	0	0
			449	285	80	76	8		

- Molecule 5 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	173	Total	C	N	O	S	0	0
			1452	913	280	255	4		

- Molecule 6 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	242	Total	C	N	O	S	0	0
			1983	1281	358	339	5		

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	229	Total	C	N	O	S	0	0
			1808	1147	334	320	7		

- Molecule 8 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	124	Total 977	C 621	N 178	O 176	S 2	0	0

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	214	Total 1725	C 1095	N 323	O 300	S 7	0	0

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	129	Total 1034	C 668	N 184	O 180	S 2	0	0

- Molecule 11 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	J	125	Total 986	C 612	N 205	O 169	0	0

- Molecule 12 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	K	135	Total 1073	C 673	N 207	O 189	S 4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	100	Total 809	C 502	N 157	O 147	S 3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	127	Total 955	C 591	N 190	O 172	S 2	0	0

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	146	Total	C	N	O	S	0	0
			1148	727	224	194	3		

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	141	Total	C	N	O	S	0	0
			1134	712	224	193	5		

- Molecule 17 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	55	Total	C	N	O	S	0	0
			455	288	95	67	5		

- Molecule 18 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	151	Total	C	N	O	S	0	0
			1257	801	239	213	4		

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	107	Total	C	N	O	S	0	0
			884	562	172	147	3		

- Molecule 20 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	64	Total	C	N	O	S	0	0
			541	343	104	93	1		

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	124	Total	C	N	O	S	0	0
			1007	641	191	168	7		

- Molecule 22 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	U	149	Total	C	N	O	0	0
			1223	790	221	212		

- Molecule 23 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	96	Total	C	N	O	S	0	0
			808	528	129	148	3		

- Molecule 24 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	61	Total	C	N	O	S	0	0
			470	294	91	80	5		

- Molecule 25 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	65	Total	C	N	O	0	0
			516	316	103	97		

- Molecule 26 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	49	Total	C	N	O	S	0	0
			400	257	76	62	5		

- Molecule 27 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Z	196	Total	C	N	O	S	0	0
			1541	983	284	270	4		

- Molecule 28 is a protein called 50S ribosomal protein L41e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	0	36	Total	C	N	O	S	0	0
			343	218	84	39	2		

- Molecule 29 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	3	122	Total	C	N	O	S	0	0
			933	594	156	180	3		

- Molecule 30 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	5	22	Total	C	N	O	P	0	0
			474	212	88	152	22		

- Molecule 31 is a RNA chain called tRNA-MET.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	4	77	Total	C	N	O	P	S	0	0
			1644	734	296	536	77	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	A	-	engineered mutation	GB 1334604293
4	72	U	A	engineered mutation	GB 1334604293

- Molecule 32 is a protein called Translation initiation factor 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	6	92	Total	C	N	O	S	0	0
			751	479	142	127	3		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	-20	MET	-	initiating methionine	UNP Q9V138
6	-19	GLY	-	expression tag	UNP Q9V138
6	-18	SER	-	expression tag	UNP Q9V138
6	-17	SER	-	expression tag	UNP Q9V138
6	-16	SER	-	expression tag	UNP Q9V138
6	-15	HIS	-	expression tag	UNP Q9V138
6	-14	HIS	-	expression tag	UNP Q9V138
6	-13	HIS	-	expression tag	UNP Q9V138
6	-12	HIS	-	expression tag	UNP Q9V138
6	-11	HIS	-	expression tag	UNP Q9V138
6	-10	HIS	-	expression tag	UNP Q9V138
6	-9	SER	-	expression tag	UNP Q9V138
6	-8	SER	-	expression tag	UNP Q9V138

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Chain	Residue	Modelled	Actual	Comment	Reference
6	-7	GLY	-	expression tag	UNP Q9V138
6	-6	LEU	-	expression tag	UNP Q9V138
6	-5	VAL	-	expression tag	UNP Q9V138
6	-4	PRO	-	expression tag	UNP Q9V138
6	-3	ARG	-	expression tag	UNP Q9V138
6	-2	GLY	-	expression tag	UNP Q9V138
6	-1	SER	-	expression tag	UNP Q9V138
6	0	HIS	-	expression tag	UNP Q9V138

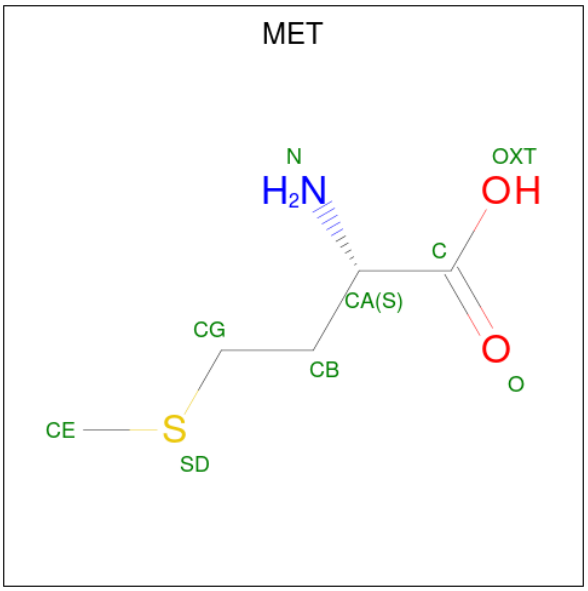
- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	2	59	Total Mg 59 59	0
33	F	1	Total Mg 1 1	0
33	5	1	Total Mg 1 1	0
33	4	1	Total Mg 1 1	0

- Molecule 34 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
34	C	2	Total Zn 2 2	0
34	F	1	Total Zn 1 1	0
34	P	1	Total Zn 1 1	0
34	R	1	Total Zn 1 1	0
34	W	1	Total Zn 1 1	0

- Molecule 35 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



Mol	Chain	Residues	Atoms					AltConf
35	4	1	Total	C	N	O	S	0
			8	5	1	1	1	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	2	342	Total	O	0
			342	342	
36	D	1	Total	O	0
			1	1	
36	F	2	Total	O	0
			2	2	
36	H	2	Total	O	0
			2	2	
36	K	4	Total	O	0
			4	4	
36	L	1	Total	O	0
			1	1	
36	M	7	Total	O	0
			7	7	
36	N	1	Total	O	0
			1	1	
36	Q	3	Total	O	0
			3	3	
36	S	1	Total	O	0
			1	1	
36	U	3	Total	O	0
			3	3	

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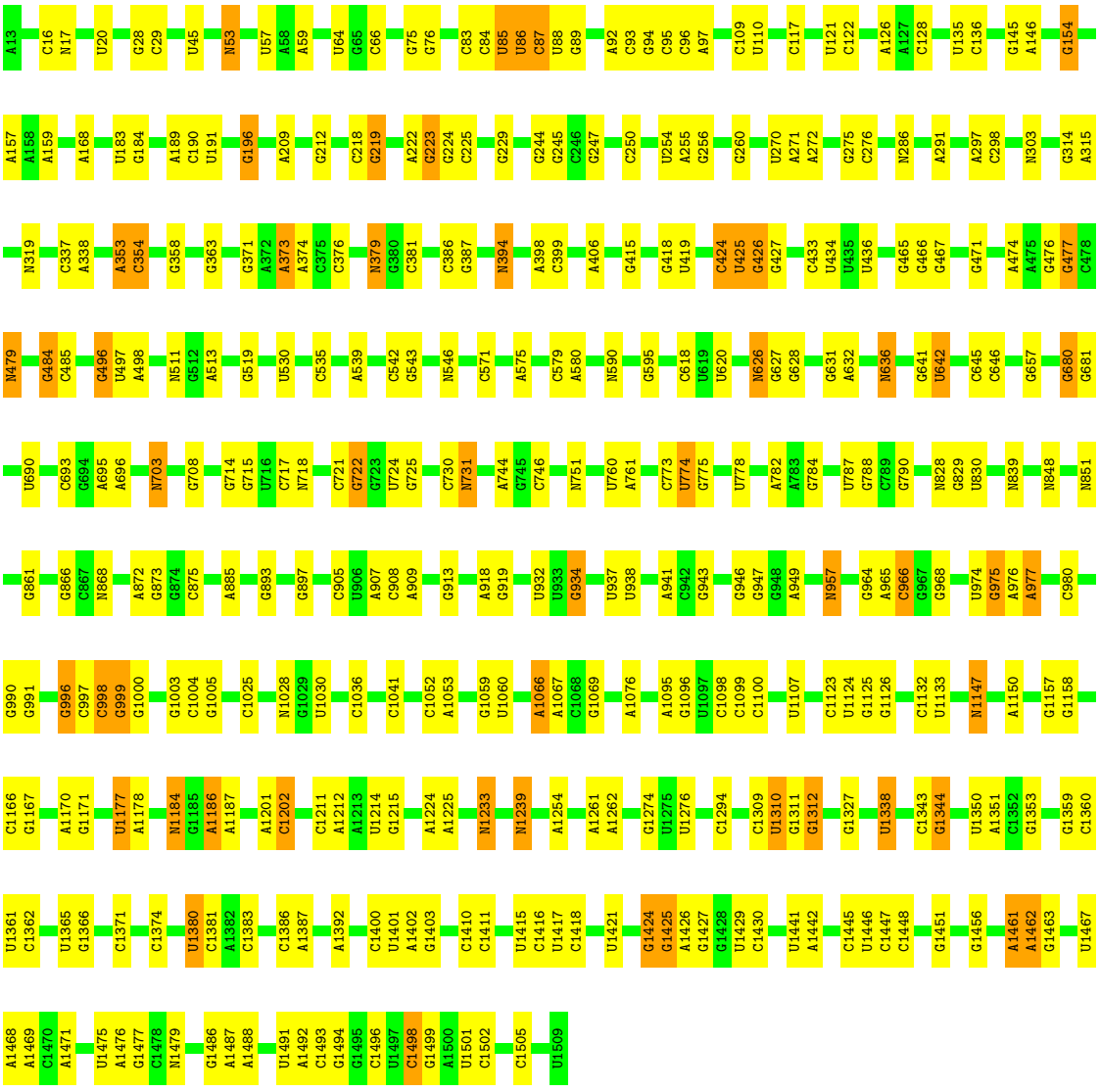
Mol	Chain	Residues	Atoms	AltConf
36	0	3	Total O 3 3	0
36	5	4	Total O 4 4	0
36	4	5	Total O 5 5	0

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.

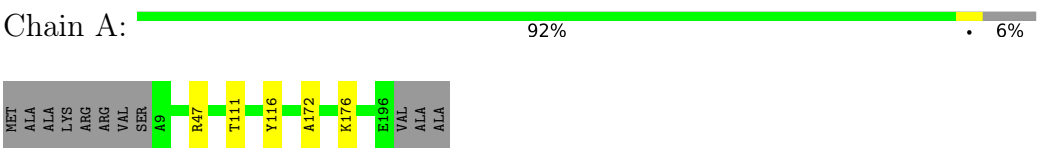
- Molecule 1: 16S rRNA

Chain 2:



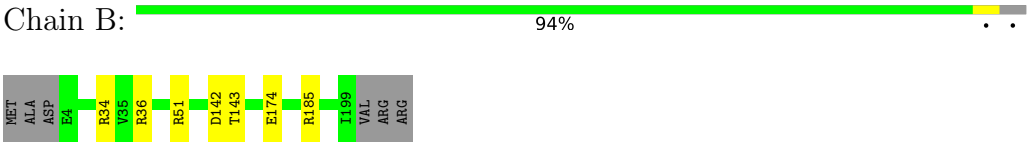
- Molecule 2: 30S ribosomal protein S3Ae

Chain A:



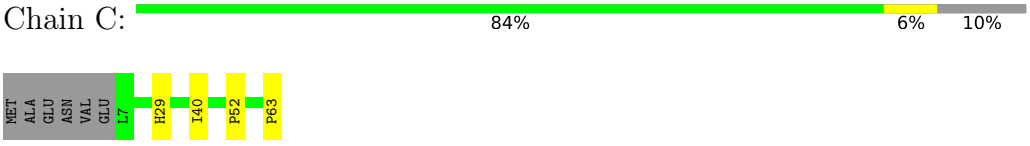
• Molecule 3: 30S ribosomal protein S2

Chain B:



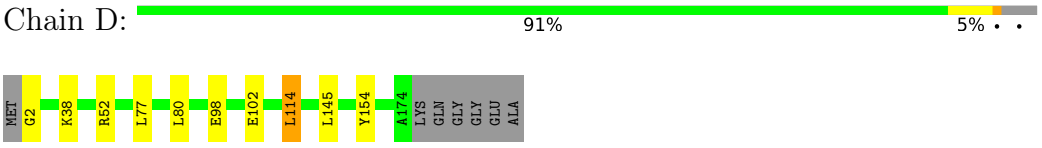
• Molecule 4: Zn-ribbon RNA-binding protein involved in translation

Chain C:



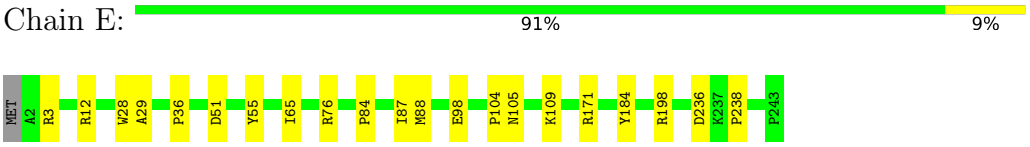
• Molecule 5: 30S ribosomal protein S4

Chain D:



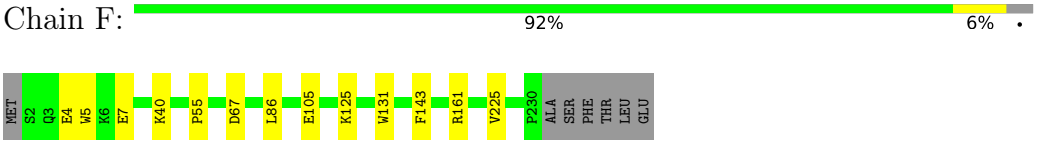
• Molecule 6: 30S ribosomal protein S4e

Chain E:



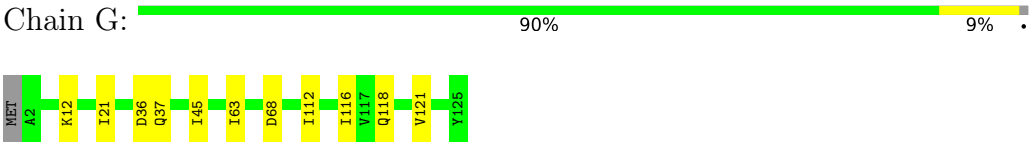
• Molecule 7: 30S ribosomal protein S5

Chain F:



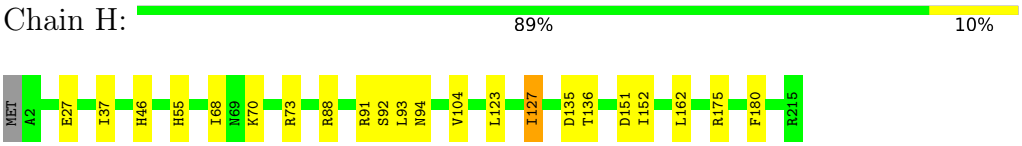
• Molecule 8: 30S ribosomal protein S6e

Chain G:



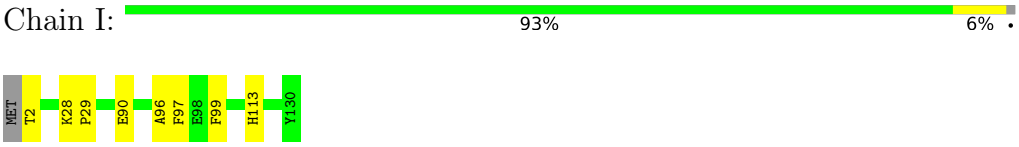
• Molecule 9: 30S ribosomal protein S7

Chain H:



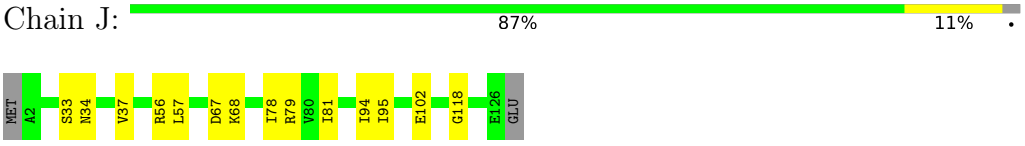
• Molecule 10: 30S ribosomal protein S8

Chain I:



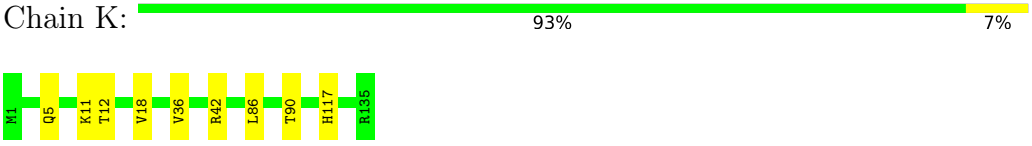
• Molecule 11: 30S ribosomal protein S8e

Chain J:



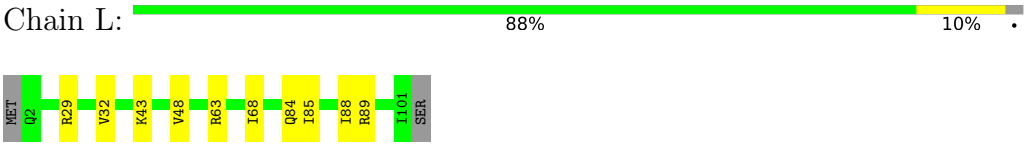
• Molecule 12: 30S ribosomal protein S9

Chain K:



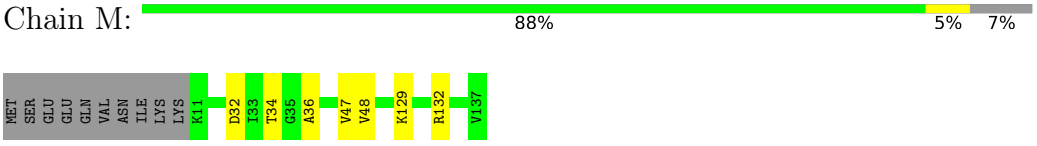
• Molecule 13: 30S ribosomal protein S10

Chain L:



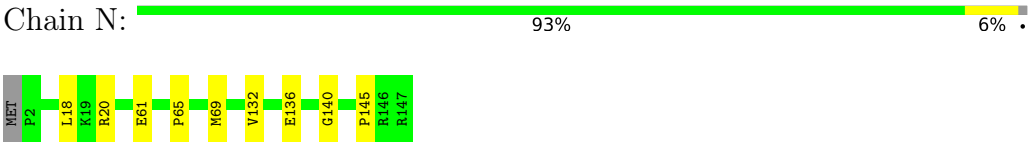
• Molecule 14: 30S ribosomal protein S11

Chain M:



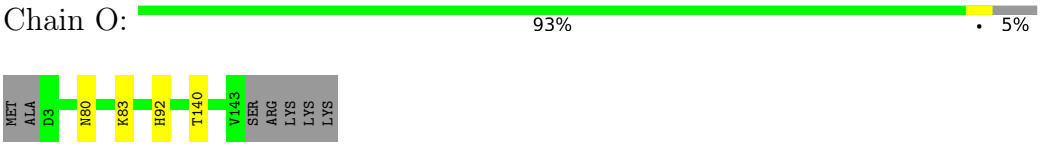
• Molecule 15: 30S ribosomal protein S12

Chain N:



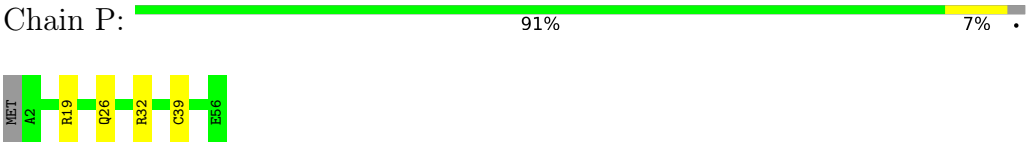
• Molecule 16: 30S ribosomal protein S13

Chain O:



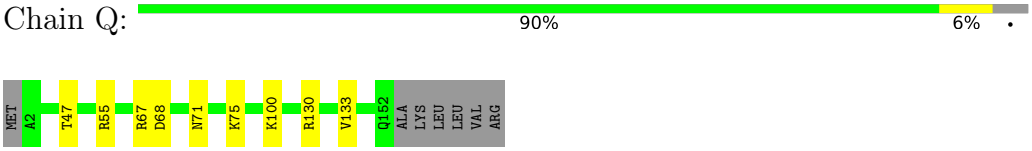
• Molecule 17: 30S ribosomal protein S14 type Z

Chain P:



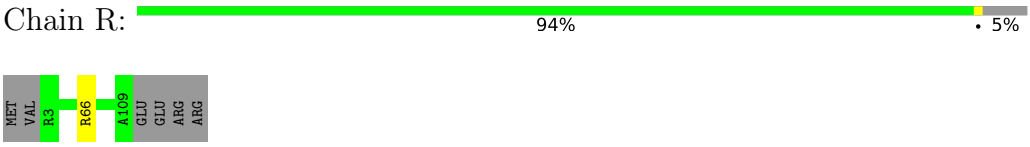
• Molecule 18: 30S ribosomal protein S15

Chain Q:



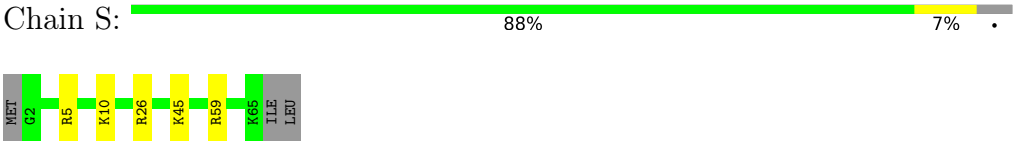
• Molecule 19: 30S ribosomal protein S17

Chain R:



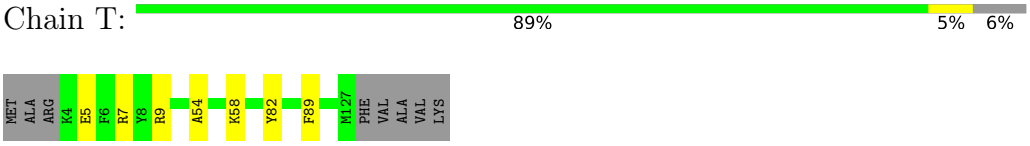
• Molecule 20: 30S ribosomal protein S17e

Chain S:



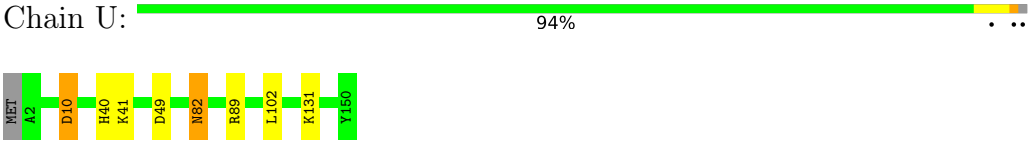
• Molecule 21: 30S ribosomal protein S19

Chain T:



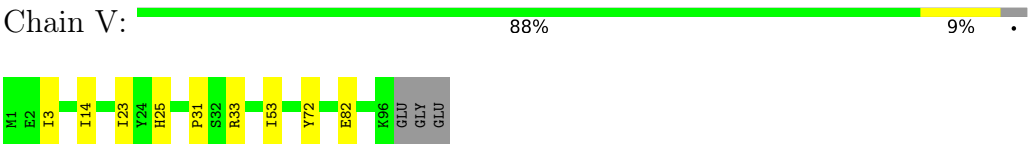
• Molecule 22: 30S ribosomal protein S19e

Chain U:



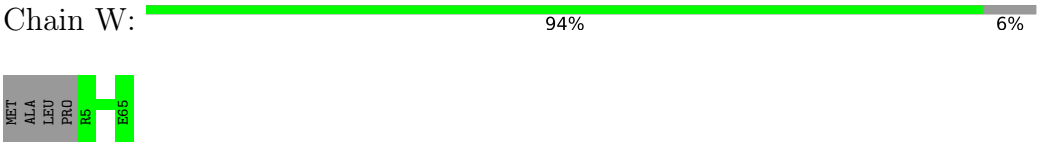
• Molecule 23: 30S ribosomal protein S24e

Chain V:



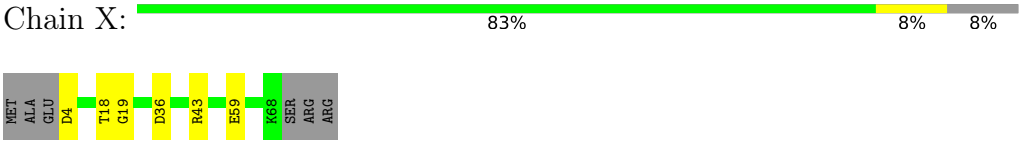
• Molecule 24: 30S ribosomal protein S27e

Chain W:



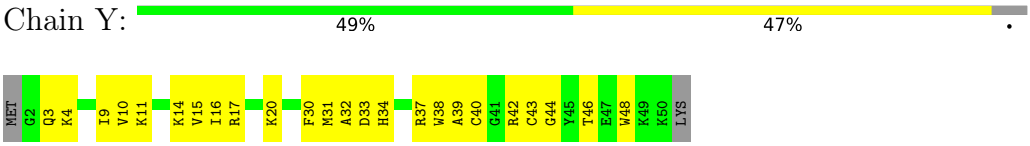
• Molecule 25: 30S ribosomal protein S28e

Chain X:



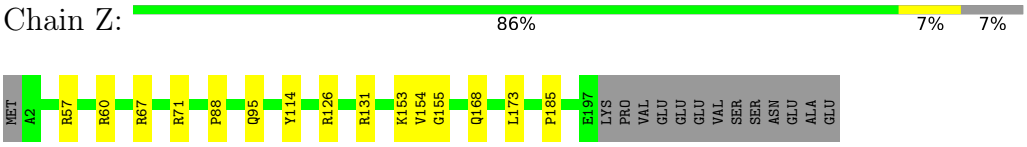
• Molecule 26: 30S ribosomal protein S27ae

Chain Y:



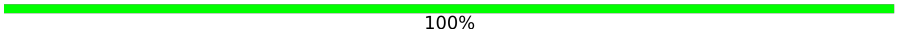
• Molecule 27: 30S ribosomal protein S3

Chain Z:



• Molecule 28: 50S ribosomal protein L41e

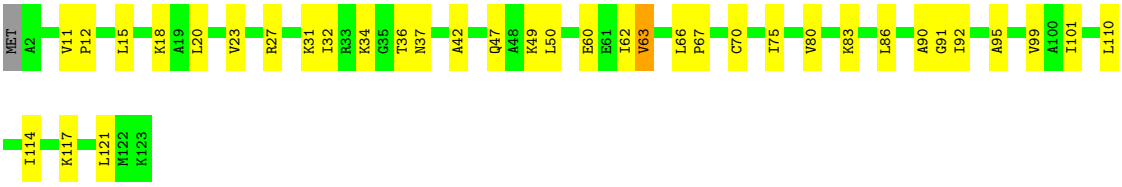
Chain 0:



There are no outlier residues recorded for this chain.

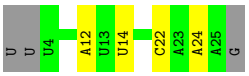
• Molecule 29: 50S ribosomal protein L7Ae

Chain 3:



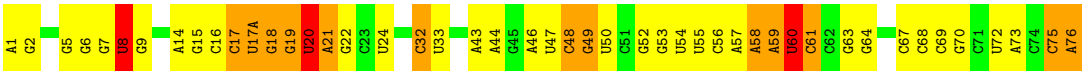
• Molecule 30: mRNA

Chain 5:



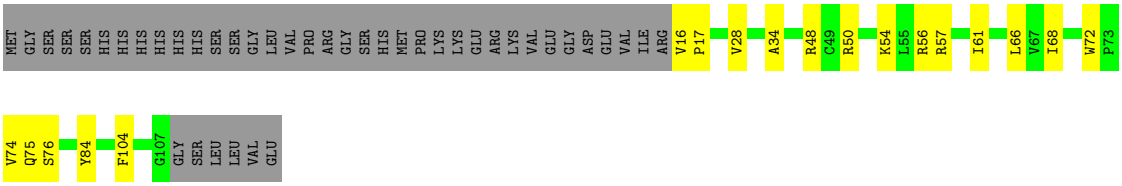
• Molecule 31: tRNA-MET

Chain 4:



• Molecule 32: Translation initiation factor 1A

Chain 6:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	382130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0016	Depositor
Map size (Å)	371.52002, 371.52002, 371.52002	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8600001, 0.8600001, 0.8600001	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHH, PSU, B8H, OMU, ZN, 6MZ, 4SU, MA6, H2U, OMG, 5MC, OMC, UR3, 5MU, 4AC, A2M, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.42	0/34435	0.79	2/53681 (0.0%)
2	A	0.28	0/1557	0.48	0/2087
3	B	0.27	0/1602	0.48	0/2165
4	C	0.28	0/463	0.50	0/628
5	D	0.27	0/1476	0.52	0/1980
6	E	0.28	0/2032	0.53	0/2742
7	F	0.27	0/1838	0.54	0/2478
8	G	0.26	0/993	0.53	0/1329
9	H	0.27	0/1762	0.50	0/2366
10	I	0.29	0/1055	0.54	0/1415
11	J	0.27	0/995	0.58	0/1327
12	K	0.26	0/1089	0.55	0/1459
13	L	0.24	0/817	0.54	0/1097
14	M	0.26	0/973	0.56	0/1311
15	N	0.28	0/1165	0.54	0/1547
16	O	0.26	0/1153	0.54	0/1551
17	P	0.29	0/465	0.58	0/613
18	Q	0.27	0/1285	0.51	0/1727
19	R	0.29	0/907	0.53	0/1225
20	S	0.27	0/548	0.50	0/725
21	T	0.26	0/1026	0.51	0/1371
22	U	0.28	0/1253	0.51	0/1689
23	V	0.29	0/826	0.46	0/1108
24	W	0.26	0/476	0.52	0/641
25	X	0.26	0/518	0.60	0/694
26	Y	0.24	0/412	0.51	0/549
27	Z	0.27	0/1563	0.52	0/2099
28	0	0.28	0/349	0.63	0/451
29	3	0.24	0/945	0.47	0/1274
30	5	0.32	0/531	0.73	0/826
31	4	0.69	8/1724 (0.5%)	1.23	11/2687 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	6	0.23	0/767	0.54	0/1037
All	All	0.37	8/67000 (0.0%)	0.71	13/97879 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	76	A	N3-C4	15.91	1.44	1.34
31	4	76	A	C8-N7	11.15	1.39	1.31
31	4	76	A	C6-N1	9.62	1.42	1.35
31	4	76	A	C5-C4	7.89	1.44	1.38
31	4	76	A	C6-N6	7.10	1.39	1.33
31	4	76	A	N9-C4	6.63	1.41	1.37
31	4	76	A	N1-C2	5.98	1.39	1.34
31	4	76	A	P-OP1	5.07	1.57	1.49

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	75	C	OP1-P-O3'	-27.71	44.24	105.20
31	4	76	A	C2-N3-C4	19.58	120.39	110.60
31	4	75	C	OP2-P-O3'	18.10	145.03	105.20
31	4	76	A	N1-C2-N3	-15.53	121.54	129.30
31	4	76	A	N7-C8-N9	-11.57	108.02	113.80
31	4	76	A	N3-C4-C5	-11.09	119.04	126.80
31	4	76	A	C5-N7-C8	10.36	109.08	103.90
31	4	76	A	N3-C4-N9	9.48	134.99	127.40
31	4	76	A	C8-N9-C4	9.20	109.48	105.80
31	4	76	A	C4-C5-N7	-6.51	107.44	110.70
1	2	1132	C	C2-N1-C1'	5.65	125.02	118.80
1	2	721	C	C2-N1-C1'	5.32	124.65	118.80
31	4	60	U	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32312	0	16354	161	0
2	A	1531	0	1623	3	0
3	B	1571	0	1630	4	0
4	C	449	0	435	2	0
5	D	1452	0	1521	7	0
6	E	1983	0	2060	14	0
7	F	1808	0	1879	8	0
8	G	977	0	1037	9	0
9	H	1725	0	1780	20	0
10	I	1034	0	1069	6	0
11	J	986	0	1070	9	0
12	K	1073	0	1133	5	0
13	L	809	0	859	5	0
14	M	955	0	981	6	0
15	N	1148	0	1248	5	0
16	O	1134	0	1173	2	0
17	P	455	0	476	2	0
18	Q	1257	0	1326	6	0
19	R	884	0	906	1	0
20	S	541	0	573	4	0
21	T	1007	0	1073	4	0
22	U	1223	0	1263	7	0
23	V	808	0	832	6	0
24	W	470	0	496	0	0
25	X	516	0	544	4	0
26	Y	400	0	401	17	0
27	Z	1541	0	1624	10	0
28	0	343	0	407	0	0
29	3	933	0	982	25	0
30	5	474	0	237	0	0
31	4	1644	0	837	50	0
32	6	751	0	773	13	0
33	2	59	0	0	0	0
33	4	1	0	0	0	0
33	5	1	0	0	0	0
33	F	1	0	0	0	0
34	C	2	0	0	0	0
34	F	1	0	0	0	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	W	1	0	0	0	0
35	4	8	0	8	0	0
36	0	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	2	342	0	0	6	0
36	4	5	0	0	0	0
36	5	4	0	0	0	0
36	D	1	0	0	0	0
36	F	2	0	0	0	0
36	H	2	0	0	0	0
36	K	4	0	0	1	0
36	L	1	0	0	0	0
36	M	7	0	0	0	0
36	N	1	0	0	1	0
36	Q	3	0	0	0	0
36	S	1	0	0	1	0
36	U	3	0	0	1	0
All	All	64649	0	48610	377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:16:C:H1'	31:4:61:C:OP1	1.17	1.26
31:4:16:C:C1'	31:4:61:C:OP1	1.90	1.19
31:4:16:C:O2'	31:4:61:C:O5'	1.57	1.18
31:4:16:C:O2'	31:4:61:C:C5'	1.92	1.15
26:Y:34:HIS:CD2	26:Y:39:ALA:HB2	1.86	1.10
31:4:16:C:O2'	31:4:61:C:H5'	1.62	0.96
31:4:16:C:H1'	31:4:60:U:H1'	1.54	0.88
31:4:16:C:C1'	31:4:60:U:H1'	2.03	0.87
9:H:73:ARG:HA	9:H:94:ASN:OD1	1.79	0.82
31:4:17:C:H5'	31:4:17:C:H6	1.44	0.80
1:2:1310:U:O4	9:H:91:ARG:NH2	2.18	0.76
7:F:67:ASP:OD1	7:F:86:LEU:HB3	1.86	0.76
32:6:34:ALA:O	32:6:50:ARG:NH1	2.19	0.75
9:H:88:ARG:HB2	9:H:92:SER:HB3	1.69	0.75
27:Z:57:ARG:O	27:Z:60:ARG:NH2	2.19	0.74
29:3:27:ARG:HD2	29:3:90:ALA:HA	1.69	0.74
12:K:117:HIS:NE2	36:K:201:HOH:O	2.22	0.71
5:D:52:ARG:NH2	7:F:161:ARG:O	2.26	0.69
6:E:12:ARG:HD3	6:E:28:TRP:O	1.93	0.68
26:Y:37:ARG:HG2	26:Y:48:TRP:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:28:LYS:HB3	10:I:29:PRO:HD3	1.76	0.66
31:4:15:G:H21	31:4:59:A:H2	1.43	0.66
1:2:977:A:H62	1:2:999:G:H21	1.41	0.66
26:Y:9:ILE:HG23	26:Y:16:ILE:HG23	1.78	0.65
21:T:82:TYR:HB3	21:T:89:PHE:HB3	1.79	0.64
1:2:866:G:N7	36:2:1738:HOH:O	2.30	0.64
29:3:23:VAL:HG13	29:3:101:ILE:HD13	1.77	0.64
8:G:63:ILE:HA	8:G:121:VAL:HG12	1.80	0.64
1:2:636:4AC:HM73	1:2:703:4AC:HM73	1.80	0.63
31:4:6:G:H2'	31:4:7:G:H8	1.65	0.62
26:Y:34:HIS:NE2	26:Y:39:ALA:HB2	2.14	0.62
31:4:16:C:O2'	31:4:61:C:P	2.57	0.61
31:4:17:C:H5'	31:4:17:C:C6	2.32	0.61
31:4:52:G:H2'	31:4:53:G:H8	1.65	0.61
6:E:198:ARG:NH2	6:E:236:ASP:O	2.32	0.61
26:Y:37:ARG:HD2	26:Y:46:THR:HA	1.82	0.61
1:2:96:C:H2'	1:2:97:A:C8	2.35	0.60
6:E:36:PRO:HD2	6:E:84:PRO:HG2	1.82	0.60
31:4:16:C:C2	31:4:61:C:OP1	2.55	0.60
1:2:485:C:H4'	32:6:54:LYS:HE2	1.83	0.60
12:K:36:VAL:O	12:K:42:ARG:NH1	2.34	0.60
32:6:74:VAL:HG12	32:6:75:GLN:HG2	1.84	0.60
31:4:16:C:H1'	31:4:60:U:C1'	2.29	0.60
1:2:1462:A:OP1	32:6:56:ARG:NH1	2.35	0.59
1:2:1491:U:H2'	1:2:1492:A:H8	1.67	0.59
31:4:48:C:N3	31:4:59:A:N6	2.49	0.59
1:2:790:G:HO2'	10:I:2:THR:N	2.00	0.59
6:E:198:ARG:HH22	6:E:236:ASP:HB2	1.68	0.59
20:S:10:LYS:NZ	36:S:101:HOH:O	2.34	0.59
31:4:8:4SU:O2'	31:4:21:A:N1	2.34	0.59
29:3:11:VAL:HG23	29:3:11:VAL:O	2.04	0.58
31:4:16:C:H1'	31:4:61:C:P	2.37	0.58
31:4:16:C:C2'	31:4:61:C:C5'	2.82	0.58
31:4:16:C:C2'	31:4:61:C:OP1	2.51	0.58
31:4:32:OMC:HM22	31:4:33:U:H5'	1.86	0.57
31:4:21:A:H1'	31:4:59:A:H61	1.70	0.56
26:Y:31:MET:HG2	26:Y:40:CYS:HA	1.87	0.56
27:Z:154:VAL:HG12	27:Z:155:GLY:N	2.20	0.56
29:3:23:VAL:O	29:3:27:ARG:N	2.39	0.56
1:2:83:C:H2'	1:2:84:C:C6	2.41	0.56
1:2:964:G:N2	1:2:1186:A:OP2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:965:A:H5”	1:2:966:C:H5	1.71	0.56
1:2:1076:A:N7	36:2:1755:HOH:O	2.33	0.56
31:4:16:C:O2	31:4:61:C:OP1	2.24	0.55
6:E:12:ARG:HD2	6:E:29:ALA:HB2	1.89	0.55
29:3:70:CYS:HA	29:3:75:ILE:HG21	1.87	0.55
31:4:16:C:C2’	31:4:61:C:H5’	2.37	0.55
1:2:386:C:H2’	1:2:387:G:H8	1.72	0.55
29:3:83:LYS:HD2	29:3:95:ALA:HB1	1.88	0.54
31:4:17:C:H6	31:4:17:C:C5’	2.16	0.54
1:2:575:A:N7	36:2:1756:HOH:O	2.33	0.54
1:2:717:C:H4’	18:Q:47:THR:HG22	1.88	0.54
2:A:47:ARG:HD3	14:M:34:THR:HG21	1.88	0.54
1:2:1214:U:C4	9:H:88:ARG:NE	2.75	0.54
9:H:135:ASP:HB2	9:H:152:ILE:HD11	1.89	0.54
31:4:16:C:N1	31:4:61:C:OP1	2.40	0.54
1:2:1338:U:OP2	22:U:89:ARG:NH1	2.40	0.54
6:E:87:ILE:HD12	6:E:104:PRO:HD3	1.90	0.54
29:3:12:PRO:HB2	29:3:15:LEU:HD13	1.90	0.54
1:2:778:U:O2’	1:2:872:A:N1	2.40	0.54
1:2:1177:OMU:HM22	1:2:1178:A:H5’	1.88	0.54
1:2:386:C:H2’	1:2:387:G:C8	2.43	0.53
1:2:774:OMU:HM22	1:2:775:G:H5’	1.89	0.53
13:L:48:VAL:HG22	13:L:63:ARG:HG2	1.91	0.53
1:2:627:G:H2’	1:2:628:G:C8	2.43	0.53
1:2:484:G:N2	15:N:65:PRO:O	2.40	0.53
29:3:15:LEU:HD12	29:3:114:ILE:HD11	1.90	0.53
1:2:1424:G:O2’	1:2:1425:G:OP1	2.26	0.53
16:O:83:LYS:O	21:T:9:ARG:NH1	2.42	0.52
1:2:247:G:OP1	19:R:66:ARG:NH1	2.42	0.52
1:2:271:A:H2’	1:2:272:A:C8	2.44	0.52
1:2:641:G:H2’	1:2:642:U:C6	2.44	0.52
7:F:125:LYS:HG2	7:F:225:VAL:HG22	1.91	0.52
8:G:68:ASP:HA	8:G:116:ILE:HA	1.90	0.52
11:J:78:ILE:HB	11:J:102:GLU:HG3	1.91	0.52
27:Z:126:ARG:HG3	27:Z:185:PRO:HA	1.91	0.52
1:2:918:A:H2’	1:2:919:G:C8	2.44	0.52
31:4:69:C:H2’	31:4:70:G:H8	1.74	0.52
29:3:36:THR:HG23	29:3:37:ASN:OD1	2.10	0.52
32:6:72:TRP:O	32:6:76:SER:OG	2.24	0.52
31:4:16:C:H2’	31:4:17:C:H5”	1.91	0.52
29:3:50:LEU:HD22	29:3:101:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:157:A:OP1	36:2:1702:HOH:O	2.18	0.51
1:2:1386:C:H2'	1:2:1387:A:C8	2.46	0.51
31:4:68:C:H2'	31:4:69:C:H6	1.74	0.51
29:3:66:LEU:HB2	29:3:67:PRO:HD3	1.92	0.51
1:2:121:U:H2'	1:2:122:C:C6	2.46	0.51
1:2:135:U:H2'	1:2:136:C:C6	2.46	0.51
1:2:908:C:H2'	1:2:909:A:H8	1.76	0.51
22:U:10:ASP:OD1	22:U:10:ASP:N	2.34	0.51
22:U:82:ASN:OD1	36:U:201:HOH:O	2.19	0.51
1:2:1461:A:O2'	1:2:1462:A:H5"	2.11	0.51
26:Y:40:CYS:HB3	26:Y:44:GLY:H	1.76	0.51
1:2:976:A:P	1:2:1000:G:H22	2.34	0.51
27:Z:154:VAL:CG1	27:Z:155:GLY:N	2.73	0.51
1:2:75:G:H2'	1:2:76:G:C8	2.46	0.50
1:2:908:C:C2	1:2:909:A:C8	2.99	0.50
13:L:89:ARG:NH1	13:L:89:ARG:HA	2.26	0.50
10:I:96:ALA:HB3	10:I:99:PHE:HB2	1.92	0.50
11:J:33:SER:HB3	11:J:56:ARG:HD3	1.92	0.50
29:3:18:LYS:HD2	29:3:110:LEU:HB3	1.93	0.50
31:4:6:G:H2'	31:4:7:G:C8	2.45	0.50
1:2:1166:C:OP1	27:Z:153:LYS:NZ	2.39	0.50
31:4:60:U:O2'	31:4:61:C:O5'	2.30	0.50
1:2:154:G:H21	8:G:118:GLN:HE22	1.59	0.50
1:2:145:G:H2'	1:2:146:A:C8	2.47	0.50
1:2:1214:U:N3	9:H:88:ARG:NE	2.60	0.50
9:H:151:ASP:OD1	9:H:152:ILE:N	2.44	0.50
1:2:724:U:H2'	1:2:725:G:O4'	2.10	0.50
1:2:1214:U:C2	9:H:88:ARG:CD	2.94	0.50
1:2:1494:G:OP2	14:M:132:ARG:NH1	2.41	0.50
1:2:85:U:H2'	1:2:86:U:H4'	1.94	0.49
1:2:135:U:H2'	1:2:136:C:H6	1.76	0.49
18:Q:130:ARG:HA	18:Q:133:VAL:HG12	1.94	0.49
4:C:52:PRO:HA	4:C:63:PRO:HD3	1.93	0.49
1:2:1214:U:C2	9:H:88:ARG:HD2	2.47	0.49
1:2:270:U:P	11:J:56:ARG:HH22	2.36	0.49
1:2:1392:A:N6	1:2:1451:G:O2'	2.39	0.49
1:2:1211:C:OP2	9:H:91:ARG:NH1	2.46	0.49
23:V:33:ARG:NH2	23:V:53:ILE:O	2.46	0.49
1:2:1383:C:O3'	32:6:48:ARG:NH1	2.46	0.49
6:E:55:TYR:OH	6:E:98:GLU:OE2	2.30	0.49
20:S:26:ARG:NH2	20:S:59:ARG:HE	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:49:LYS:HG3	29:3:50:LEU:HD12	1.94	0.49
1:2:636:4AC:O7	1:2:636:4AC:H5	2.13	0.48
1:2:996:G:H5"	26:Y:4:LYS:HZ3	1.78	0.48
9:H:37:ILE:HD11	9:H:127:ILE:HD11	1.93	0.48
26:Y:32:ALA:HB3	26:Y:39:ALA:HB3	1.93	0.48
1:2:271:A:H2'	1:2:272:A:H8	1.78	0.48
1:2:695:A:H2'	1:2:696:A:C8	2.49	0.48
1:2:183:U:H2'	1:2:184:G:H8	1.78	0.48
6:E:87:ILE:HG22	6:E:88:MET:HG2	1.95	0.48
12:K:86:LEU:O	12:K:90:THR:HG22	2.13	0.48
11:J:67:ASP:OD1	11:J:68:LYS:N	2.44	0.48
1:2:1461:A:N3	32:6:34:ALA:HB2	2.28	0.48
26:Y:17:ARG:HH11	26:Y:30:PHE:HZ	1.60	0.48
1:2:1417:U:H2'	1:2:1418:C:C6	2.48	0.48
11:J:34:ASN:HB3	11:J:94:ILE:HD12	1.94	0.48
29:3:31:LYS:O	29:3:101:ILE:HA	2.14	0.48
1:2:223:G:H2'	1:2:224:G:H8	1.79	0.47
1:2:965:A:H5"	1:2:966:C:C5	2.49	0.47
14:M:34:THR:HG23	14:M:36:ALA:H	1.78	0.47
32:6:28:VAL:HG21	32:6:61:ILE:HD11	1.95	0.47
1:2:190:C:H2'	1:2:191:U:C6	2.48	0.47
1:2:1167:G:OP2	27:Z:131:ARG:NH2	2.47	0.47
9:H:123:LEU:O	9:H:127:ILE:HG23	2.14	0.47
31:4:1:A:H2'	31:4:2:G:H8	1.77	0.47
1:2:680:OMG:H2'	1:2:681:G:C8	2.49	0.47
1:2:1491:U:H2'	1:2:1492:A:C8	2.47	0.47
6:E:105:ASN:N	6:E:109:LYS:O	2.46	0.47
29:3:80:VAL:HG11	29:3:86:LEU:HD13	1.95	0.47
1:2:109:C:H2'	1:2:110:U:C6	2.49	0.47
23:V:25:HIS:O	23:V:25:HIS:ND1	2.48	0.47
31:4:1:A:H2'	31:4:2:G:C8	2.50	0.47
1:2:426:G:H2'	1:2:427:G:C8	2.50	0.47
11:J:78:ILE:HG22	11:J:79:ARG:HG2	1.96	0.47
1:2:223:G:H2'	1:2:224:G:C8	2.50	0.47
1:2:1066:A:H4'	1:2:1067:A:O5'	2.14	0.47
5:D:80:LEU:HD23	5:D:145:LEU:HD23	1.97	0.47
6:E:65:ILE:HD11	23:V:14:ILE:HD13	1.96	0.47
25:X:36:ASP:OD1	25:X:36:ASP:N	2.40	0.47
1:2:703:4AC:H5	1:2:703:4AC:O7	2.15	0.47
31:4:67:C:H2'	31:4:68:C:C6	2.50	0.47
1:2:433:C:H2'	1:2:434:U:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:98:GLU:O	5:D:102:GLU:HG2	2.16	0.46
1:2:398:A:H3'	1:2:399:C:H6	1.80	0.46
1:2:93:C:H2'	1:2:94:G:C8	2.50	0.46
1:2:579:C:H2'	1:2:580:A:C8	2.50	0.46
25:X:43:ARG:NH2	25:X:59:GLU:O	2.48	0.46
8:G:112:ILE:HA	8:G:116:ILE:HD12	1.97	0.46
15:N:20:ARG:NH2	36:N:201:HOH:O	2.24	0.46
1:2:1461:A:H1'	32:6:34:ALA:HA	1.96	0.46
7:F:5:TRP:HB3	7:F:55:PRO:HB2	1.97	0.46
27:Z:88:PRO:O	27:Z:95:GLN:NE2	2.45	0.46
1:2:1441:U:H2'	1:2:1442:A:H8	1.80	0.46
23:V:23:ILE:HG21	23:V:31:PRO:HG2	1.98	0.46
26:Y:33:ASP:OD1	26:Y:33:ASP:N	2.46	0.46
1:2:1402:A:H2'	1:2:1403:G:C8	2.51	0.46
1:2:1476:A:H2'	1:2:1477:G:C8	2.51	0.46
31:4:43:A:H2'	31:4:44:A:C8	2.51	0.46
31:4:59:A:O2'	31:4:60:U:O5'	2.29	0.46
31:4:67:C:H2'	31:4:68:C:H6	1.80	0.45
7:F:4:GLU:O	7:F:7:GLU:HG3	2.16	0.45
13:L:85:ILE:O	13:L:88:ILE:HG22	2.16	0.45
1:2:168:A:OP2	36:2:1705:HOH:O	2.21	0.45
23:V:72:TYR:OH	23:V:82:GLU:OE2	2.19	0.45
25:X:18:THR:OG1	25:X:19:GLY:N	2.48	0.45
31:4:17(A):U:O2	31:4:17(A):U:O2'	2.28	0.45
31:4:72:U:H2'	31:4:73:A:H8	1.81	0.45
1:2:86:U:H3'	1:2:87:C:H5"	1.98	0.45
1:2:1214:U:H1'	9:H:93:LEU:HG	1.98	0.45
15:N:136:GLU:O	15:N:140:GLY:N	2.45	0.45
12:K:5:GLN:HG2	12:K:18:VAL:HG22	1.99	0.45
18:Q:68:ASP:HB3	18:Q:71:ASN:O	2.17	0.45
11:J:37:VAL:HG22	11:J:95:ILE:HD11	1.99	0.44
1:2:496:G:H22	32:6:57:ARG:HG2	1.81	0.44
2:A:172:ALA:O	2:A:176:LYS:HG3	2.18	0.44
8:G:37:GLN:N	8:G:37:GLN:OE1	2.50	0.44
25:X:4:ASP:N	25:X:4:ASP:OD1	2.50	0.44
31:4:14:A:H61	31:4:21:A:H2	1.64	0.44
1:2:353:A:H5"	1:2:354:C:H5	1.81	0.44
3:B:142:ASP:OD1	3:B:143:THR:N	2.43	0.44
9:H:88:ARG:HB2	9:H:92:SER:CB	2.44	0.44
1:2:714:G:O2'	18:Q:55:ARG:NH1	2.51	0.44
1:2:1493:C:H2'	1:2:1494:G:C8	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:5:G:H2'	31:4:6:G:C8	2.52	0.44
18:Q:100:LYS:HB2	18:Q:100:LYS:HE3	1.77	0.44
32:6:66:LEU:HD13	32:6:104:PHE:HE2	1.83	0.44
1:2:631:G:H22	1:2:708:G:H1	1.66	0.44
1:2:1098:C:H2'	1:2:1099:C:H6	1.82	0.44
5:D:114:LEU:HD12	5:D:154:TYR:CZ	2.53	0.44
21:T:5:GLU:OE2	21:T:7:ARG:NE	2.50	0.44
31:4:58:A:O3'	31:4:59:A:H8	2.00	0.44
29:3:20:LEU:HD11	29:3:80:VAL:HG13	2.00	0.44
1:2:1224:A:H2'	1:2:1225:A:C8	2.53	0.44
15:N:132:VAL:HG21	15:N:145:PRO:HD3	2.00	0.44
1:2:1461:A:HO2'	1:2:1462:A:H8	1.65	0.44
1:2:93:C:H2'	1:2:94:G:H8	1.83	0.43
31:4:20:H2U:N3	31:4:21:A:O2'	2.45	0.43
29:3:42:ALA:O	29:3:47:GLN:N	2.48	0.43
1:2:1095:A:H2'	1:2:1096:G:C8	2.54	0.43
1:2:1361:U:H2'	1:2:1362:C:C6	2.54	0.43
20:S:5:ARG:HB2	20:S:10:LYS:HE3	2.00	0.43
29:3:50:LEU:HD13	29:3:101:ILE:HG13	2.00	0.43
1:2:244:G:H2'	1:2:245:G:H8	1.83	0.43
1:2:1416:C:H2'	1:2:1417:U:C6	2.54	0.43
1:2:1446:U:H2'	1:2:1447:C:C6	2.54	0.43
7:F:40:LYS:HE2	7:F:40:LYS:HB3	1.83	0.43
3:B:51:ARG:HA	3:B:51:ARG:HD3	1.77	0.43
5:D:38:LYS:HA	5:D:38:LYS:HD2	1.89	0.43
7:F:105:GLU:OE2	27:Z:114:TYR:OH	2.35	0.43
9:H:88:ARG:CB	9:H:92:SER:HB3	2.45	0.43
26:Y:42:ARG:NH1	26:Y:43:CYS:SG	2.92	0.43
1:2:645:C:H2'	1:2:646:C:H6	1.84	0.43
6:E:3:ARG:HB3	6:E:3:ARG:NH1	2.33	0.43
6:E:3:ARG:HB3	6:E:3:ARG:HH11	1.83	0.43
7:F:131:TRP:CE2	10:I:97:PHE:HA	2.53	0.43
10:I:90:GLU:OE2	10:I:113:HIS:NE2	2.49	0.43
26:Y:11:LYS:HG2	26:Y:14:LYS:HB2	1.99	0.43
11:J:57:LEU:HB2	11:J:118:GLY:HA2	2.01	0.43
26:Y:34:HIS:NE2	26:Y:39:ALA:CB	2.79	0.43
32:6:16:VAL:HB	32:6:17:PRO:HD3	2.00	0.43
1:2:1125:G:HO2'	1:2:1126:G:H8	1.66	0.43
9:H:68:ILE:HG12	9:H:104:VAL:HG21	1.99	0.43
13:L:43:LYS:HB2	13:L:68:ILE:HB	1.99	0.43
31:4:18:G:C6	31:4:57:A:C6	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:4:69:C:H2'	31:4:70:G:C8	2.52	0.43
1:2:1311:G:H5"	1:2:1312:G:OP1	2.18	0.43
1:2:1380:OMU:HM22	1:2:1381:C:H5'	2.01	0.43
14:M:47:VAL:HG23	14:M:48:VAL:HG13	2.01	0.43
26:Y:20:LYS:HE2	26:Y:38:TRP:CE2	2.54	0.43
31:4:63:G:N1	31:4:64:G:O6	2.52	0.43
1:2:28:G:H2'	1:2:29:C:C6	2.54	0.43
1:2:730:C:H2'	1:2:731:4AC:H6	2.01	0.43
1:2:998:C:N4	1:2:999:G:O6	2.52	0.43
1:2:1447:C:H2'	1:2:1448:C:C6	2.53	0.43
17:P:19:ARG:HD2	17:P:32:ARG:HD3	2.01	0.43
20:S:45:LYS:HB2	20:S:45:LYS:HE2	1.76	0.43
1:2:353:A:H3'	1:2:354:C:H6	1.83	0.42
1:2:975:G:H2'	1:2:1000:G:N2	2.33	0.42
1:2:1365:U:H2'	1:2:1366:G:C8	2.54	0.42
2:A:111:THR:HA	2:A:116:TYR:O	2.19	0.42
1:2:244:G:H2'	1:2:245:G:C8	2.53	0.42
1:2:618:C:OP1	18:Q:75:LYS:HG2	2.20	0.42
13:L:29:ARG:NH2	13:L:84:GLN:OE1	2.52	0.42
31:4:19:G:N2	31:4:57:A:H1'	2.33	0.42
31:4:56:C:H2'	31:4:57:A:O4'	2.18	0.42
32:6:68:ILE:HD12	32:6:84:TYR:HB3	2.02	0.42
1:2:1261:A:H2'	1:2:1262:A:C8	2.55	0.42
1:2:1359:G:H2'	1:2:1360:C:H6	1.84	0.42
6:E:184:TYR:CE1	6:E:238:PRO:HG3	2.54	0.42
11:J:81:ILE:HD11	11:J:102:GLU:HB3	2.02	0.42
26:Y:10:VAL:HG13	26:Y:15:VAL:HG22	2.01	0.42
1:2:1309:C:O2'	9:H:175:ARG:NH1	2.53	0.42
23:V:3:ILE:HG12	23:V:23:ILE:HG12	2.01	0.42
1:2:314:G:HO2'	5:D:2:GLY:N	2.18	0.42
22:U:131:LYS:HE3	22:U:131:LYS:HB2	1.79	0.42
31:4:16:C:O4'	31:4:60:U:H1'	2.17	0.42
1:2:196:G:N3	1:2:196:G:H2'	2.34	0.42
15:N:61:GLU:HG2	15:N:69:MET:SD	2.60	0.42
29:3:36:THR:HG23	29:3:37:ASN:N	2.35	0.42
1:2:218:C:H3'	1:2:219:G:H5"	2.02	0.42
6:E:76:ARG:NH2	6:E:171:ARG:HD2	2.35	0.42
1:2:1076:A:H61	27:Z:155:GLY:HA3	1.84	0.42
1:2:379:4AC:H5	1:2:379:4AC:O7	2.19	0.42
1:2:424:C:H4'	1:2:425:U:C5	2.54	0.42
1:2:479:4AC:H5	1:2:479:4AC:O7	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:H:27:GLU:OE1	9:H:27:GLU:N	2.52	0.42
1:2:85:U:N3	1:2:86:U:H1'	2.35	0.41
1:2:722:G:O2'	10:I:2:THR:HG21	2.20	0.41
1:2:1343:C:H2'	1:2:1344:G:C8	2.55	0.41
1:2:918:A:H2'	1:2:919:G:H8	1.85	0.41
17:P:26:GLN:HB3	17:P:39:CYS:SG	2.60	0.41
1:2:398:A:H3'	1:2:399:C:C6	2.55	0.41
1:2:465:G:H2'	1:2:466:G:C8	2.55	0.41
1:2:476:G:O2'	1:2:477:G:H5'	2.20	0.41
1:2:907:A:H2'	1:2:908:C:H6	1.85	0.41
1:2:975:G:H8	1:2:975:G:OP2	2.02	0.41
1:2:1184:4AC:O7	1:2:1184:4AC:H5	2.19	0.41
1:2:1350:U:H2'	1:2:1351:A:H8	1.84	0.41
1:2:1501:U:H2'	1:2:1502:C:C6	2.54	0.41
9:H:70:LYS:HG3	9:H:162:LEU:HB3	2.01	0.41
16:O:80:ASN:OD1	16:O:92:HIS:ND1	2.53	0.41
1:2:626:4AC:H5	1:2:626:4AC:O7	2.21	0.41
3:B:174:GLU:OE2	3:B:185:ARG:NH1	2.53	0.41
4:C:29:HIS:HA	4:C:40:ILE:O	2.20	0.41
1:2:937:U:OP1	36:2:1708:HOH:O	2.22	0.41
1:2:1402:A:H2'	1:2:1403:G:H8	1.85	0.41
1:2:1410:C:H2'	1:2:1411:C:H6	1.85	0.41
1:2:1415:U:H2'	1:2:1416:C:C6	2.55	0.41
8:G:36:ASP:OD1	8:G:36:ASP:N	2.53	0.41
1:2:636:4AC:HM73	1:2:703:4AC:CM7	2.47	0.41
1:2:1446:U:H2'	1:2:1447:C:H6	1.85	0.41
1:2:1447:C:H2'	1:2:1448:C:H6	1.84	0.41
8:G:21:ILE:HD11	8:G:45:ILE:HD11	2.02	0.41
29:3:34:LYS:HG3	29:3:99:VAL:HG22	2.02	0.41
1:2:1359:G:H2'	1:2:1360:C:C6	2.54	0.41
5:D:77:LEU:HA	5:D:77:LEU:HD23	1.85	0.41
22:U:102:LEU:HD23	22:U:102:LEU:HA	1.93	0.41
29:3:32:ILE:HD12	29:3:91:GLY:HA2	2.03	0.41
1:2:997:C:H2'	1:2:998:C:O4'	2.20	0.41
1:2:1350:U:H2'	1:2:1351:A:C8	2.55	0.41
1:2:1441:U:C2	1:2:1442:A:C8	3.09	0.41
22:U:49:ASP:OD1	22:U:49:ASP:N	2.53	0.41
1:2:645:C:H2'	1:2:646:C:C6	2.56	0.41
1:2:957:4AC:O7	1:2:957:4AC:H5	2.21	0.41
1:2:975:G:N2	1:2:1000:G:O2'	2.36	0.41
1:2:1052:C:H2'	1:2:1053:A:C8	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1099:C:H2'	1:2:1100:C:H6	1.86	0.41
1:2:1233:4AC:O7	1:2:1233:4AC:H5	2.20	0.41
21:T:54:ALA:HA	21:T:58:LYS:O	2.21	0.41
1:2:373:A2M:HM'2	1:2:374:A:C5	2.56	0.41
8:G:12:LYS:HE2	8:G:12:LYS:HB2	1.85	0.41
26:Y:3:GLN:HB3	29:3:62:ILE:HD11	2.03	0.41
29:3:60:GLU:HA	29:3:63:VAL:HG22	2.02	0.41
29:3:117:LYS:HZ2	29:3:121:LEU:HD22	1.86	0.41
1:2:418:G:H2'	1:2:419:U:C6	2.56	0.40
1:2:1123:C:H2'	1:2:1124:U:C6	2.55	0.40
1:2:1147:4AC:O7	1:2:1147:4AC:H5	2.20	0.40
12:K:11:LYS:O	12:K:12:THR:OG1	2.33	0.40
1:2:746:C:H5"	14:M:129:LYS:HG2	2.04	0.40
1:2:1361:U:H2'	1:2:1362:C:H6	1.85	0.40
9:H:135:ASP:OD1	9:H:136:THR:N	2.48	0.40
29:3:92:ILE:HD12	29:3:92:ILE:HA	1.89	0.40
1:2:1239:4AC:O7	1:2:1239:4AC:H5	2.21	0.40
1:2:1429:U:H2'	1:2:1430:C:H6	1.86	0.40
8:G:63:ILE:HD13	8:G:112:ILE:HD11	2.03	0.40
22:U:40:HIS:NE2	22:U:41:LYS:HE3	2.36	0.40
27:Z:67:ARG:HH11	27:Z:71:ARG:HE	1.69	0.40
1:2:353:A:H5"	1:2:354:C:C5	2.56	0.40
1:2:394:4AC:O7	1:2:394:4AC:H5	2.20	0.40
1:2:418:G:H2'	1:2:419:U:H6	1.86	0.40
31:4:7:G:H2'	31:4:49:G:C6	2.56	0.40
1:2:53:4AC:O7	1:2:53:4AC:H5	2.21	0.40
1:2:255:A:C2	1:2:291:A:C5	3.09	0.40
3:B:34:ARG:NH1	3:B:36:ARG:HG2	2.36	0.40
14:M:32:ASP:OD2	14:M:34:THR:HG22	2.21	0.40

There are no symmetry-related clashes.

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	
2	A	186/199 (94%)	183 (98%)	3 (2%)	0	100	100
3	B	194/202 (96%)	190 (98%)	4 (2%)	0	100	100
4	C	55/63 (87%)	55 (100%)	0	0	100	100
5	D	171/180 (95%)	168 (98%)	3 (2%)	0	100	100
6	E	240/243 (99%)	236 (98%)	4 (2%)	0	100	100
7	F	227/236 (96%)	220 (97%)	7 (3%)	0	100	100
8	G	122/125 (98%)	118 (97%)	4 (3%)	0	100	100
9	H	212/215 (99%)	205 (97%)	7 (3%)	0	100	100
10	I	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
11	J	123/127 (97%)	122 (99%)	1 (1%)	0	100	100
12	K	133/135 (98%)	128 (96%)	5 (4%)	0	100	100
13	L	98/102 (96%)	95 (97%)	3 (3%)	0	100	100
14	M	125/137 (91%)	121 (97%)	4 (3%)	0	100	100
15	N	144/147 (98%)	142 (99%)	2 (1%)	0	100	100
16	O	139/148 (94%)	136 (98%)	3 (2%)	0	100	100
17	P	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
18	Q	149/158 (94%)	147 (99%)	2 (1%)	0	100	100
19	R	105/113 (93%)	100 (95%)	5 (5%)	0	100	100
20	S	62/67 (92%)	61 (98%)	1 (2%)	0	100	100
21	T	122/132 (92%)	119 (98%)	3 (2%)	0	100	100
22	U	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
23	V	94/99 (95%)	92 (98%)	2 (2%)	0	100	100
24	W	59/65 (91%)	56 (95%)	3 (5%)	0	100	100
25	X	63/71 (89%)	62 (98%)	1 (2%)	0	100	100
26	Y	47/51 (92%)	41 (87%)	6 (13%)	0	100	100
27	Z	194/210 (92%)	183 (94%)	11 (6%)	0	100	100
28	0	34/36 (94%)	34 (100%)	0	0	100	100
29	3	120/123 (98%)	109 (91%)	11 (9%)	0	100	100
32	6	90/134 (67%)	88 (98%)	2 (2%)	0	100	100
All	All	3635/3854 (94%)	3529 (97%)	106 (3%)	0	100	100

There are no Ramachandran outliers to report.

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
2	A	160/167 (96%)	160 (100%)	0	100 100
3	B	168/173 (97%)	168 (100%)	0	100 100
4	C	50/55 (91%)	50 (100%)	0	100 100
5	D	156/160 (98%)	155 (99%)	1 (1%)	86 95
6	E	213/214 (100%)	212 (100%)	1 (0%)	88 96
7	F	192/198 (97%)	191 (100%)	1 (0%)	88 96
8	G	107/108 (99%)	107 (100%)	0	100 100
9	H	183/184 (100%)	179 (98%)	4 (2%)	52 76
10	I	106/107 (99%)	106 (100%)	0	100 100
11	J	101/103 (98%)	101 (100%)	0	100 100
12	K	111/111 (100%)	111 (100%)	0	100 100
13	L	89/91 (98%)	88 (99%)	1 (1%)	73 88
14	M	94/104 (90%)	94 (100%)	0	100 100
15	N	120/121 (99%)	119 (99%)	1 (1%)	81 92
16	O	117/123 (95%)	116 (99%)	1 (1%)	78 91
17	P	45/46 (98%)	45 (100%)	0	100 100
18	Q	137/143 (96%)	136 (99%)	1 (1%)	84 94
19	R	96/102 (94%)	96 (100%)	0	100 100
20	S	58/61 (95%)	58 (100%)	0	100 100
21	T	108/114 (95%)	108 (100%)	0	100 100
22	U	126/127 (99%)	124 (98%)	2 (2%)	62 82
23	V	88/90 (98%)	88 (100%)	0	100 100
24	W	53/56 (95%)	53 (100%)	0	100 100
25	X	55/60 (92%)	55 (100%)	0	100 100
26	Y	40/42 (95%)	40 (100%)	0	100 100
27	Z	155/168 (92%)	153 (99%)	2 (1%)	69 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
28	0	34/34 (100%)	34 (100%)	0	100 100
29	3	98/99 (99%)	97 (99%)	1 (1%)	76 90
32	6	80/117 (68%)	80 (100%)	0	100 100
All	All	3140/3278 (96%)	3124 (100%)	16 (0%)	89 96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	114	LEU
6	E	51	ASP
7	F	143	PHE
9	H	46	HIS
9	H	55	HIS
9	H	127	ILE
9	H	180	PHE
13	L	32	VAL
15	N	18	LEU
16	O	140	THR
18	Q	67	ARG
22	U	10	ASP
22	U	82	ASN
27	Z	168	GLN
27	Z	173	LEU
29	3	63	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1461/1497 (97%)	147 (10%)	1 (0%)
30	5	21/25 (84%)	4 (19%)	0
31	4	76/77 (98%)	20 (26%)	3 (3%)
All	All	1558/1599 (97%)	171 (10%)	4 (0%)

All (171) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	16	C
1	2	45	U
1	2	57	U
1	2	59	A
1	2	66	C
1	2	85	U
1	2	86	U
1	2	87	C
1	2	88	U
1	2	89	G
1	2	92	A
1	2	95	C
1	2	117	C
1	2	126	A
1	2	128	C
1	2	154	G
1	2	159	A
1	2	189	A
1	2	196	G
1	2	209	A
1	2	212	G
1	2	219	G
1	2	222	A
1	2	223	G
1	2	225	C
1	2	229	G
1	2	254	U
1	2	256	G
1	2	260	G
1	2	275	G
1	2	276	C
1	2	297	A
1	2	298	C
1	2	315	A
1	2	337	C
1	2	338	A
1	2	353	A
1	2	354	C
1	2	358	G
1	2	363	G
1	2	371	G
1	2	376	C
1	2	381	C

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Mol	Chain	Res	Type
1	2	406	A
1	2	415	G
1	2	424	C
1	2	425	U
1	2	426	G
1	2	436	U
1	2	474	A
1	2	477	G
1	2	484	G
1	2	496	G
1	2	497	U
1	2	498	A
1	2	513	A
1	2	530	U
1	2	539	A
1	2	542	C
1	2	543	G
1	2	571	C
1	2	595	G
1	2	620	U
1	2	632	A
1	2	642	U
1	2	690	U
1	2	715	G
1	2	722	G
1	2	744	A
1	2	760	U
1	2	761	A
1	2	782	A
1	2	784	G
1	2	788	G
1	2	829	G
1	2	861	G
1	2	885	A
1	2	893	G
1	2	897	G
1	2	905	C
1	2	932	U
1	2	934	OMG
1	2	941	A
1	2	943	G
1	2	946	G

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Mol	Chain	Res	Type
1	2	947	G
1	2	949	A
1	2	966	C
1	2	968	G
1	2	974	U
1	2	975	G
1	2	977	A
1	2	980	C
1	2	990	G
1	2	991	G
1	2	996	G
1	2	998	C
1	2	999	G
1	2	1003	G
1	2	1004	C
1	2	1005	G
1	2	1030	U
1	2	1059	G
1	2	1060	U
1	2	1066	A
1	2	1107	U
1	2	1133	U
1	2	1150	A
1	2	1157	G
1	2	1158	G
1	2	1170	A
1	2	1171	G
1	2	1186	A
1	2	1187	A
1	2	1201	A
1	2	1202	5MC
1	2	1212	A
1	2	1215	G
1	2	1254	A
1	2	1274	G
1	2	1276	U
1	2	1294	C
1	2	1310	U
1	2	1312	G
1	2	1327	G
1	2	1338	U
1	2	1344	G

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Mol	Chain	Res	Type
1	2	1353	G
1	2	1371	C
1	2	1400	C
1	2	1401	U
1	2	1421	U
1	2	1424	G
1	2	1425	G
1	2	1426	A
1	2	1427	G
1	2	1445	C
1	2	1456	G
1	2	1461	A
1	2	1462	A
1	2	1463	G
1	2	1468	A
1	2	1471	A
1	2	1475	U
1	2	1486	G
1	2	1498	5MC
1	2	1499	G
30	5	12	A
30	5	14	U
30	5	22	C
30	5	24	A
31	4	8	4SU
31	4	9	G
31	4	17	C
31	4	17(A)	U
31	4	18	G
31	4	20	H2U
31	4	21	A
31	4	22	G
31	4	24	U
31	4	46	A
31	4	47	U
31	4	48	C
31	4	49	G
31	4	50	U
31	4	58	A
31	4	59	A
31	4	60	U
31	4	61	C

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Mol	Chain	Res	Type
31	4	75	C
31	4	76	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1424	G
31	4	19	G
31	4	60	U
31	4	75	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	OMG	2	913	1	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)
1	OMC	2	773	1	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
1	OMC	2	1036	1	19,22,23	0.82	0	26,31,34	0.83	1 (3%)
1	4AC	2	17	1	21,24,25	1.01	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	718	1	21,24,25	1.00	2 (9%)	29,34,37	1.29	4 (13%)
1	6MZ	2	1469	33,1	18,25,26	0.83	1 (5%)	16,36,39	2.14	3 (18%)
1	4AC	2	636	1	21,24,25	1.02	2 (9%)	29,34,37	1.53	4 (13%)
1	4AC	2	868	1	21,24,25	1.03	2 (9%)	29,34,37	1.31	5 (17%)
1	OMC	2	1376	1	19,22,23	0.82	0	26,31,34	0.81	0
1	5MC	2	1498	1	18,22,23	0.92	2 (11%)	26,32,35	1.24	4 (15%)
1	OMU	2	774	1	19,22,23	1.24	3 (15%)	26,31,34	1.74	4 (15%)
1	5MC	2	1505	1,30	18,22,23	0.94	2 (11%)	26,32,35	1.12	3 (11%)
1	4AC	2	479	1	21,24,25	1.01	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	751	1	21,24,25	1.02	2 (9%)	29,34,37	1.31	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	4AC	2	1239	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	319	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	2	590	1	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	546	1	21,24,25	1.00	2 (9%)	29,34,37	1.34	4 (13%)
1	LHH	2	1041	1	22,25,26	2.52	8 (36%)	29,35,38	1.24	5 (17%)
1	4AC	2	1147	1	21,24,25	1.02	2 (9%)	29,34,37	1.36	4 (13%)
1	UR3	2	1467	1	19,22,23	0.92	0	26,32,35	1.42	1 (3%)
1	4AC	2	1028	1	21,24,25	0.99	2 (9%)	29,34,37	1.32	4 (13%)
1	OMG	2	873	1	18,26,27	0.93	1 (5%)	19,38,41	1.10	2 (10%)
1	OMG	2	1069	1	18,26,27	0.95	1 (5%)	19,38,41	1.08	2 (10%)
1	OMU	2	1380	1	19,22,23	1.25	3 (15%)	26,31,34	1.76	5 (19%)
1	A2M	2	373	1	18,25,26	0.96	1 (5%)	18,36,39	1.25	2 (11%)
1	OMC	2	1040	1	19,22,23	0.82	0	26,31,34	0.77	0
31	OMC	4	32	31	19,22,23	0.85	0	26,31,34	1.05	2 (7%)
1	4AC	2	839	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	2	1202	1	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
1	4AC	2	1233	1	21,24,25	1.01	2 (9%)	29,34,37	1.39	4 (13%)
1	4AC	2	957	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	B8H	2	938	1	19,22,23	0.78	0	22,32,35	1.37	3 (13%)
1	5MC	2	1496	1	18,22,23	0.92	2 (11%)	26,32,35	1.11	2 (7%)
1	4AC	2	379	1	21,24,25	1.00	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	1479	1	21,24,25	1.00	2 (9%)	29,34,37	1.33	4 (13%)
1	OMU	2	64	1	19,22,23	1.24	3 (15%)	26,31,34	1.72	4 (15%)
1	OMG	2	680	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	5MC	2	1374	1	18,22,23	0.94	2 (11%)	26,32,35	1.09	2 (7%)
1	MA6	2	1487	1	18,26,27	0.89	1 (5%)	19,38,41	1.26	2 (10%)
1	OMU	2	830	1	19,22,23	1.26	3 (15%)	26,31,34	1.73	4 (15%)
31	H2U	4	20	31	18,21,22	1.01	2 (11%)	21,30,33	1.98	1 (4%)
1	4AC	2	626	1	21,24,25	1.01	2 (9%)	29,34,37	1.37	4 (13%)
1	4AC	2	848	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	286	1	21,24,25	1.02	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	394	1	21,24,25	1.00	2 (9%)	29,34,37	1.35	4 (13%)
1	OMU	2	1177	1	19,22,23	1.23	3 (15%)	26,31,34	1.74	5 (19%)
1	4AC	2	511	1	21,24,25	1.03	2 (9%)	29,34,37	1.38	4 (13%)
1	4AC	2	1184	1	21,24,25	1.02	2 (9%)	29,34,37	1.33	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OMG	2	467	1	18,26,27	0.95	1 (5%)	19,38,41	1.11	2 (10%)
1	5MC	2	1025	1	18,22,23	0.94	2 (11%)	26,32,35	1.10	3 (11%)
1	OMC	2	129	1	19,22,23	0.82	0	26,31,34	0.83	0
1	4AC	2	731	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	5MC	2	535	1	18,22,23	0.95	2 (11%)	26,32,35	1.08	2 (7%)
31	5MU	4	54	31	19,22,23	1.42	6 (31%)	28,32,35	1.86	5 (17%)
31	4SU	4	8	31	18,21,22	1.72	4 (22%)	26,30,33	2.22	5 (19%)
1	4AC	2	703	1	21,24,25	1.02	2 (9%)	29,34,37	1.49	4 (13%)
1	5MC	2	875	1	18,22,23	0.95	2 (11%)	26,32,35	1.11	3 (11%)
1	OMU	2	20	1	19,22,23	1.25	3 (15%)	26,31,34	1.81	5 (19%)
1	OMG	2	657	1	18,26,27	0.94	1 (5%)	19,38,41	1.06	2 (10%)
1	OMC	2	846	1	19,22,23	0.81	0	26,31,34	0.82	0
1	4AC	2	828	1	21,24,25	1.01	2 (9%)	29,34,37	1.33	4 (13%)
1	MA6	2	1488	1	18,26,27	0.90	1 (5%)	19,38,41	1.28	2 (10%)
1	4AC	2	53	1	21,24,25	1.00	2 (9%)	29,34,37	1.32	4 (13%)
1	4AC	2	303	1	21,24,25	1.02	2 (9%)	29,34,37	1.34	4 (13%)
1	4AC	2	851	1	21,24,25	1.04	2 (9%)	29,34,37	1.33	5 (17%)
1	OMU	2	787	1	19,22,23	1.26	3 (15%)	26,31,34	1.80	5 (19%)
1	OMG	2	934	1	18,26,27	0.95	1 (5%)	19,38,41	1.15	2 (10%)
31	PSU	4	55	31	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
1	LHH	2	250	1	22,25,26	2.53	8 (36%)	29,35,38	1.26	6 (20%)
1	OMG	2	471	1	18,26,27	0.96	1 (5%)	19,38,41	1.06	2 (10%)
1	5MC	2	693	1	18,22,23	0.93	2 (11%)	26,32,35	1.09	3 (11%)
1	OMG	2	519	1	18,26,27	0.95	1 (5%)	19,38,41	1.12	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	2	913	1	-	1/5/27/28	0/3/3/3
1	OMC	2	773	1	-	0/9/27/28	0/2/2/2
1	OMC	2	1036	1	-	0/9/27/28	0/2/2/2
1	4AC	2	17	1	-	0/11/29/30	0/2/2/2
1	4AC	2	718	1	-	0/11/29/30	0/2/2/2
1	6MZ	2	1469	33,1	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	636	1	-	0/11/29/30	0/2/2/2
1	4AC	2	868	1	-	0/11/29/30	0/2/2/2
1	OMC	2	1376	1	-	2/9/27/28	0/2/2/2
1	5MC	2	1498	1	-	4/7/25/26	0/2/2/2
1	OMU	2	774	1	-	1/9/27/28	0/2/2/2
1	5MC	2	1505	1,30	-	0/7/25/26	0/2/2/2
1	4AC	2	479	1	-	0/11/29/30	0/2/2/2
1	4AC	2	751	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1239	1	-	0/11/29/30	0/2/2/2
1	4AC	2	319	1	-	0/11/29/30	0/2/2/2
1	4AC	2	590	1	-	0/11/29/30	0/2/2/2
1	4AC	2	546	1	-	0/11/29/30	0/2/2/2
1	LHH	2	1041	1	-	0/13/31/32	0/2/2/2
1	4AC	2	1147	1	-	0/11/29/30	0/2/2/2
1	UR3	2	1467	1	-	0/7/25/26	0/2/2/2
1	4AC	2	1028	1	-	0/11/29/30	0/2/2/2
1	OMG	2	873	1	-	1/5/27/28	0/3/3/3
1	OMG	2	1069	1	-	0/5/27/28	0/3/3/3
1	OMU	2	1380	1	-	0/9/27/28	0/2/2/2
1	A2M	2	373	1	-	0/5/27/28	0/3/3/3
1	OMC	2	1040	1	-	0/9/27/28	0/2/2/2
31	OMC	4	32	31	-	2/9/27/28	0/2/2/2
1	4AC	2	839	1	-	0/11/29/30	0/2/2/2
1	5MC	2	1202	1	-	2/7/25/26	0/2/2/2
1	4AC	2	1233	1	-	0/11/29/30	0/2/2/2
1	4AC	2	957	1	-	0/11/29/30	0/2/2/2
1	B8H	2	938	1	-	0/7/25/26	0/2/2/2
1	5MC	2	1496	1	-	0/7/25/26	0/2/2/2
1	4AC	2	379	1	-	0/11/29/30	0/2/2/2
1	4AC	2	1479	1	-	0/11/29/30	0/2/2/2
1	OMU	2	64	1	-	2/9/27/28	0/2/2/2
1	OMG	2	680	1	-	0/5/27/28	0/3/3/3
1	5MC	2	1374	1	-	0/7/25/26	0/2/2/2
1	MA6	2	1487	1	-	0/7/29/30	0/3/3/3
1	OMU	2	830	1	-	0/9/27/28	0/2/2/2
31	H2U	4	20	31	-	7/7/38/39	0/2/2/2
1	4AC	2	626	1	-	0/11/29/30	0/2/2/2
1	4AC	2	848	1	-	0/11/29/30	0/2/2/2
1	4AC	2	286	1	-	0/11/29/30	0/2/2/2
1	4AC	2	394	1	-	0/11/29/30	0/2/2/2
1	OMU	2	1177	1	-	2/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4AC	2	511	1	-	1/11/29/30	0/2/2/2
1	4AC	2	1184	1	-	0/11/29/30	0/2/2/2
1	OMG	2	467	1	-	1/5/27/28	0/3/3/3
1	5MC	2	1025	1	-	1/7/25/26	0/2/2/2
1	OMC	2	129	1	-	0/9/27/28	0/2/2/2
1	4AC	2	731	1	-	0/11/29/30	0/2/2/2
1	5MC	2	535	1	-	0/7/25/26	0/2/2/2
31	5MU	4	54	31	-	0/7/25/26	0/2/2/2
31	4SU	4	8	31	-	0/7/25/26	0/2/2/2
1	4AC	2	703	1	-	0/11/29/30	0/2/2/2
1	5MC	2	875	1	-	0/7/25/26	0/2/2/2
1	OMU	2	20	1	-	5/9/27/28	0/2/2/2
1	OMG	2	657	1	-	0/5/27/28	0/3/3/3
1	OMC	2	846	1	-	0/9/27/28	0/2/2/2
1	4AC	2	828	1	-	0/11/29/30	0/2/2/2
1	MA6	2	1488	1	-	1/7/29/30	0/3/3/3
1	4AC	2	53	1	-	0/11/29/30	0/2/2/2
1	4AC	2	303	1	-	0/11/29/30	0/2/2/2
1	4AC	2	851	1	-	0/11/29/30	0/2/2/2
1	OMU	2	787	1	-	2/9/27/28	0/2/2/2
1	OMG	2	934	1	-	2/5/27/28	0/3/3/3
31	PSU	4	55	31	-	0/7/25/26	0/2/2/2
1	LHH	2	250	1	-	0/13/31/32	0/2/2/2
1	OMG	2	471	1	-	0/5/27/28	0/3/3/3
1	5MC	2	693	1	-	0/7/25/26	0/2/2/2
1	OMG	2	519	1	-	0/5/27/28	0/3/3/3

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	250	LHH	C4-N4	6.99	1.49	1.39
1	2	1041	LHH	C4-N4	6.96	1.49	1.39
1	2	250	LHH	C7-N4	6.36	1.49	1.37
1	2	1041	LHH	C7-N4	6.27	1.48	1.37
31	4	8	4SU	C4-S4	-4.49	1.59	1.68
1	2	250	LHH	O2-C2	-4.13	1.16	1.23
1	2	1041	LHH	O2-C2	-4.10	1.16	1.23
31	4	8	4SU	C4-N3	-3.32	1.34	1.37
31	4	55	PSU	C6-C5	3.20	1.39	1.35
1	2	957	4AC	C5-C4	2.90	1.47	1.40
1	2	868	4AC	C5-C4	2.89	1.47	1.40
1	2	511	4AC	C5-C4	2.89	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1147	4AC	C5-C4	2.89	1.47	1.40
1	2	1239	4AC	C5-C4	2.89	1.47	1.40
1	2	20	OMU	C4-N3	-2.88	1.33	1.38
1	2	1184	4AC	C5-C4	2.88	1.47	1.40
1	2	839	4AC	C5-C4	2.87	1.47	1.40
1	2	751	4AC	C5-C4	2.86	1.46	1.40
31	4	54	5MU	C6-C5	2.85	1.39	1.34
1	2	286	4AC	C5-C4	2.85	1.46	1.40
1	2	471	OMG	C6-N1	-2.84	1.33	1.37
1	2	787	OMU	C4-N3	-2.83	1.33	1.38
1	2	590	4AC	C5-C4	2.83	1.46	1.40
1	2	851	4AC	C5-C4	2.83	1.46	1.40
1	2	479	4AC	C5-C4	2.82	1.46	1.40
1	2	848	4AC	C5-C4	2.82	1.46	1.40
1	2	53	4AC	C5-C4	2.81	1.46	1.40
1	2	303	4AC	C5-C4	2.80	1.46	1.40
1	2	319	4AC	C5-C4	2.80	1.46	1.40
1	2	828	4AC	C5-C4	2.79	1.46	1.40
1	2	830	OMU	C4-N3	-2.79	1.33	1.38
1	2	718	4AC	C5-C4	2.78	1.46	1.40
1	2	519	OMG	C6-N1	-2.78	1.33	1.37
1	2	657	OMG	C6-N1	-2.78	1.33	1.37
1	2	17	4AC	C5-C4	2.77	1.46	1.40
1	2	379	4AC	C5-C4	2.77	1.46	1.40
1	2	1233	4AC	C5-C4	2.77	1.46	1.40
1	2	1028	4AC	C5-C4	2.77	1.46	1.40
1	2	394	4AC	C5-C4	2.76	1.46	1.40
1	2	546	4AC	C5-C4	2.76	1.46	1.40
1	2	731	4AC	C5-C4	2.75	1.46	1.40
1	2	1380	OMU	C4-N3	-2.75	1.33	1.38
1	2	626	4AC	C5-C4	2.75	1.46	1.40
1	2	467	OMG	C6-N1	-2.75	1.33	1.37
1	2	1479	4AC	C5-C4	2.74	1.46	1.40
1	2	1177	OMU	C4-N3	-2.74	1.33	1.38
1	2	680	OMG	C6-N1	-2.74	1.33	1.37
1	2	774	OMU	C4-N3	-2.73	1.33	1.38
1	2	913	OMG	C6-N1	-2.73	1.33	1.37
31	4	54	5MU	C4-N3	-2.73	1.33	1.38
1	2	636	4AC	C5-C4	2.71	1.46	1.40
1	2	1069	OMG	C6-N1	-2.71	1.33	1.37
1	2	1041	LHH	C2-N1	-2.70	1.34	1.40
1	2	703	4AC	C5-C4	2.70	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	64	OMU	C4-N3	-2.70	1.33	1.38
1	2	873	OMG	C6-N1	-2.69	1.33	1.37
1	2	934	OMG	C6-N1	-2.66	1.33	1.37
1	2	250	LHH	C2-N1	-2.66	1.34	1.40
31	4	20	H2U	C2-N3	-2.65	1.33	1.38
31	4	55	PSU	C4-N3	-2.65	1.33	1.38
1	2	1202	5MC	C6-C5	2.62	1.38	1.34
1	2	851	4AC	C4-N3	-2.61	1.28	1.32
1	2	1505	5MC	C6-C5	2.60	1.38	1.34
1	2	1374	5MC	C6-C5	2.60	1.38	1.34
1	2	1041	LHH	C6-C5	2.58	1.41	1.35
1	2	535	5MC	C6-C5	2.56	1.38	1.34
1	2	787	OMU	C2-N3	-2.56	1.33	1.38
1	2	250	LHH	C6-C5	2.55	1.41	1.35
1	2	535	5MC	C6-N1	-2.55	1.33	1.38
1	2	875	5MC	C6-N1	-2.54	1.33	1.38
1	2	875	5MC	C6-C5	2.54	1.38	1.34
1	2	1025	5MC	C6-C5	2.52	1.38	1.34
1	2	1025	5MC	C6-N1	-2.51	1.33	1.38
1	2	693	5MC	C6-C5	2.51	1.38	1.34
1	2	1374	5MC	C6-N1	-2.51	1.33	1.38
1	2	1498	5MC	C6-C5	2.50	1.38	1.34
1	2	20	OMU	C2-N3	-2.49	1.33	1.38
1	2	693	5MC	C6-N1	-2.49	1.33	1.38
1	2	1496	5MC	C6-N1	-2.48	1.33	1.38
1	2	868	4AC	C4-N3	-2.47	1.28	1.32
1	2	731	4AC	C4-N3	-2.45	1.28	1.32
1	2	1496	5MC	C6-C5	2.44	1.38	1.34
1	2	1202	5MC	C6-N1	-2.44	1.33	1.38
1	2	848	4AC	C4-N3	-2.43	1.28	1.32
1	2	1041	LHH	C6-N1	-2.43	1.32	1.38
1	2	17	4AC	C4-N3	-2.42	1.28	1.32
1	2	1469	6MZ	C5-C4	2.42	1.47	1.40
1	2	1498	5MC	C6-N1	-2.42	1.33	1.38
1	2	250	LHH	C6-N1	-2.41	1.32	1.38
1	2	830	OMU	C2-N3	-2.41	1.33	1.38
1	2	718	4AC	C4-N3	-2.41	1.28	1.32
1	2	774	OMU	C2-N3	-2.41	1.33	1.38
1	2	319	4AC	C4-N3	-2.40	1.28	1.32
1	2	1479	4AC	C4-N3	-2.40	1.28	1.32
1	2	1380	OMU	C2-N3	-2.40	1.33	1.38
1	2	511	4AC	C4-N3	-2.40	1.28	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	8	4SU	C5-C4	-2.39	1.39	1.42
1	2	839	4AC	C4-N3	-2.39	1.28	1.32
1	2	751	4AC	C4-N3	-2.38	1.28	1.32
1	2	1505	5MC	C6-N1	-2.38	1.34	1.38
1	2	286	4AC	C4-N3	-2.37	1.28	1.32
1	2	1487	MA6	C5-C4	2.37	1.47	1.40
1	2	303	4AC	C4-N3	-2.37	1.28	1.32
1	2	828	4AC	C4-N3	-2.37	1.28	1.32
1	2	590	4AC	C4-N3	-2.37	1.28	1.32
31	4	20	H2U	C4-N3	-2.35	1.33	1.37
1	2	1239	4AC	C4-N3	-2.35	1.28	1.32
1	2	957	4AC	C4-N3	-2.33	1.28	1.32
1	2	64	OMU	C2-N3	-2.33	1.33	1.38
1	2	626	4AC	C4-N3	-2.33	1.28	1.32
1	2	1177	OMU	C2-N3	-2.33	1.33	1.38
1	2	1488	MA6	C5-C4	2.33	1.47	1.40
1	2	379	4AC	C4-N3	-2.32	1.28	1.32
1	2	53	4AC	C4-N3	-2.32	1.28	1.32
1	2	703	4AC	C4-N3	-2.31	1.28	1.32
1	2	546	4AC	C4-N3	-2.30	1.28	1.32
1	2	1028	4AC	C4-N3	-2.29	1.28	1.32
1	2	373	A2M	C5-C4	2.28	1.47	1.40
1	2	1147	4AC	C4-N3	-2.28	1.28	1.32
1	2	1184	4AC	C4-N3	-2.27	1.28	1.32
1	2	636	4AC	C4-N3	-2.26	1.28	1.32
1	2	394	4AC	C4-N3	-2.26	1.28	1.32
1	2	1233	4AC	C4-N3	-2.21	1.29	1.32
1	2	479	4AC	C4-N3	-2.18	1.29	1.32
31	4	54	5MU	C4-C5	2.17	1.48	1.44
1	2	1041	LHH	C2-N3	-2.16	1.32	1.36
1	2	1177	OMU	C5-C4	-2.15	1.38	1.43
1	2	774	OMU	C5-C4	-2.15	1.38	1.43
1	2	64	OMU	C5-C4	-2.12	1.38	1.43
1	2	830	OMU	C5-C4	-2.11	1.39	1.43
1	2	250	LHH	C2-N3	-2.11	1.32	1.36
31	4	54	5MU	C2-N1	2.11	1.41	1.38
1	2	20	OMU	C5-C4	-2.10	1.39	1.43
1	2	1380	OMU	C5-C4	-2.09	1.39	1.43
1	2	250	LHH	CM7-C7	2.09	1.54	1.50
1	2	1041	LHH	CM7-C7	2.08	1.54	1.50
31	4	8	4SU	C2-N3	-2.08	1.34	1.38
31	4	54	5MU	C6-N1	-2.07	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	787	OMU	C5-C4	-2.07	1.39	1.43
31	4	54	5MU	C2-N3	-2.06	1.34	1.38

All (235) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	4	20	H2U	C4-N3-C2	-8.41	118.82	125.79
31	4	8	4SU	C4-N3-C2	-7.00	120.54	127.34
1	2	1469	6MZ	C2-N1-C6	6.71	122.34	116.59
31	4	8	4SU	C5-C4-N3	5.97	120.23	114.69
31	4	55	PSU	N1-C2-N3	5.91	121.83	115.13
1	2	1467	UR3	C4-N3-C2	-5.77	119.13	124.56
1	2	703	4AC	O7-C7-N4	4.94	129.82	121.82
1	2	636	4AC	O7-C7-N4	4.86	129.69	121.82
1	2	938	B8H	C4-N3-C2	-4.83	121.10	127.35
1	2	787	OMU	C4-N3-C2	-4.81	120.23	126.58
1	2	20	OMU	C4-N3-C2	-4.78	120.27	126.58
1	2	1380	OMU	C4-N3-C2	-4.67	120.42	126.58
1	2	1233	4AC	O7-C7-N4	4.56	129.20	121.82
1	2	1177	OMU	C4-N3-C2	-4.56	120.57	126.58
1	2	830	OMU	C4-N3-C2	-4.55	120.58	126.58
1	2	626	4AC	O7-C7-N4	4.54	129.17	121.82
1	2	774	OMU	C4-N3-C2	-4.54	120.60	126.58
1	2	20	OMU	N3-C2-N1	4.53	120.90	114.89
31	4	54	5MU	C4-N3-C2	-4.51	121.51	127.35
1	2	379	4AC	O7-C7-N4	4.50	129.10	121.82
1	2	479	4AC	O7-C7-N4	4.49	129.08	121.82
1	2	303	4AC	O7-C7-N4	4.46	129.04	121.82
1	2	839	4AC	O7-C7-N4	4.46	129.04	121.82
1	2	546	4AC	O7-C7-N4	4.46	129.04	121.82
31	4	54	5MU	N3-C2-N1	4.45	120.80	114.89
1	2	787	OMU	N3-C2-N1	4.45	120.80	114.89
1	2	1028	4AC	O7-C7-N4	4.45	129.02	121.82
1	2	319	4AC	O7-C7-N4	4.45	129.01	121.82
1	2	1147	4AC	O7-C7-N4	4.44	129.00	121.82
1	2	590	4AC	O7-C7-N4	4.43	128.98	121.82
1	2	511	4AC	O7-C7-N4	4.42	128.97	121.82
1	2	828	4AC	O7-C7-N4	4.41	128.96	121.82
1	2	64	OMU	C4-N3-C2	-4.40	120.78	126.58
1	2	1380	OMU	N3-C2-N1	4.40	120.72	114.89
1	2	394	4AC	O7-C7-N4	4.39	128.93	121.82
1	2	53	4AC	O7-C7-N4	4.39	128.92	121.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	848	4AC	O7-C7-N4	4.39	128.92	121.82
1	2	17	4AC	O7-C7-N4	4.38	128.91	121.82
1	2	731	4AC	O7-C7-N4	4.38	128.91	121.82
1	2	1184	4AC	O7-C7-N4	4.38	128.90	121.82
1	2	957	4AC	O7-C7-N4	4.34	128.85	121.82
1	2	286	4AC	O7-C7-N4	4.34	128.85	121.82
1	2	830	OMU	N3-C2-N1	4.34	120.65	114.89
1	2	1479	4AC	O7-C7-N4	4.33	128.82	121.82
1	2	851	4AC	O7-C7-N4	4.31	128.79	121.82
1	2	751	4AC	O7-C7-N4	4.30	128.78	121.82
1	2	1177	OMU	N3-C2-N1	4.30	120.59	114.89
1	2	718	4AC	O7-C7-N4	4.27	128.73	121.82
1	2	868	4AC	O7-C7-N4	4.25	128.70	121.82
1	2	1239	4AC	O7-C7-N4	4.25	128.70	121.82
1	2	774	OMU	N3-C2-N1	4.19	120.46	114.89
31	4	8	4SU	N3-C2-N1	4.18	120.44	114.89
1	2	64	OMU	N3-C2-N1	4.14	120.39	114.89
31	4	54	5MU	C5-C4-N3	4.05	118.77	115.31
31	4	55	PSU	C4-N3-C2	-3.94	120.66	126.34
1	2	787	OMU	C5-C4-N3	3.69	120.36	114.84
31	4	54	5MU	C5-C6-N1	-3.68	119.56	123.34
31	4	54	5MU	O4-C4-C5	-3.67	120.64	124.90
1	2	20	OMU	C5-C4-N3	3.66	120.31	114.84
1	2	774	OMU	C5-C4-N3	3.65	120.31	114.84
1	2	1380	OMU	C5-C4-N3	3.65	120.30	114.84
1	2	1469	6MZ	C4-C5-N7	-3.63	105.62	109.40
1	2	830	OMU	C5-C4-N3	3.59	120.22	114.84
1	2	64	OMU	C5-C4-N3	3.59	120.21	114.84
1	2	1177	OMU	C5-C4-N3	3.55	120.15	114.84
1	2	636	4AC	C5-C4-N4	-3.54	116.78	122.92
1	2	636	4AC	N4-C4-N3	3.53	119.78	113.85
31	4	8	4SU	C5-C4-S4	-3.46	120.01	124.47
1	2	1487	MA6	C4-C5-N7	-3.44	105.81	109.40
1	2	1488	MA6	N3-C2-N1	-3.44	123.30	128.68
1	2	1488	MA6	C4-C5-N7	-3.43	105.82	109.40
1	2	1505	5MC	C5-C6-N1	-3.37	119.87	123.34
1	2	1025	5MC	C5-C6-N1	-3.36	119.88	123.34
31	4	55	PSU	O2-C2-N1	-3.34	119.11	122.79
1	2	703	4AC	C5-C4-N4	-3.33	117.14	122.92
1	2	1469	6MZ	N3-C2-N1	-3.29	123.54	128.68
1	2	1487	MA6	N3-C2-N1	-3.26	123.58	128.68
1	2	535	5MC	C5-C6-N1	-3.25	120.00	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1374	5MC	C5-C6-N1	-3.24	120.00	123.34
1	2	1202	5MC	C5-C6-N1	-3.23	120.01	123.34
1	2	373	A2M	N3-C2-N1	-3.20	123.68	128.68
1	2	703	4AC	CM7-C7-N4	-3.19	109.78	115.29
1	2	693	5MC	C5-C6-N1	-3.18	120.07	123.34
1	2	875	5MC	C5-C6-N1	-3.14	120.11	123.34
1	2	1233	4AC	N4-C4-N3	3.09	119.04	113.85
1	2	703	4AC	N4-C4-N3	3.07	119.01	113.85
1	2	379	4AC	N4-C4-N3	3.05	118.97	113.85
1	2	64	OMU	O4-C4-C5	-3.04	119.81	125.16
1	2	774	OMU	O4-C4-C5	-3.02	119.85	125.16
1	2	394	4AC	N4-C4-N3	3.02	118.92	113.85
1	2	1233	4AC	C5-C4-N4	-3.01	117.69	122.92
1	2	479	4AC	N4-C4-N3	2.99	118.86	113.85
1	2	1380	OMU	O4-C4-C5	-2.98	119.91	125.16
1	2	379	4AC	C5-C4-N4	-2.98	117.75	122.92
1	2	546	4AC	N4-C4-N3	2.97	118.83	113.85
1	2	1177	OMU	O4-C4-C5	-2.96	119.95	125.16
1	2	1496	5MC	C5-C6-N1	-2.96	120.29	123.34
1	2	839	4AC	CM7-C7-N4	-2.93	110.22	115.29
1	2	828	4AC	CM7-C7-N4	-2.93	110.23	115.29
1	2	479	4AC	C5-C4-N4	-2.92	117.84	122.92
1	2	590	4AC	CM7-C7-N4	-2.91	110.25	115.29
1	2	1147	4AC	N4-C4-N3	2.91	118.74	113.85
1	2	319	4AC	N4-C4-N3	2.91	118.74	113.85
1	2	17	4AC	CM7-C7-N4	-2.91	110.26	115.29
1	2	731	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	2	303	4AC	CM7-C7-N4	-2.89	110.29	115.29
1	2	511	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	2	1184	4AC	C5-C4-N4	-2.89	117.90	122.92
1	2	626	4AC	CM7-C7-N4	-2.89	110.30	115.29
1	2	626	4AC	N4-C4-N3	2.88	118.69	113.85
1	2	1479	4AC	N4-C4-N3	2.86	118.66	113.85
1	2	787	OMU	O4-C4-C5	-2.86	120.13	125.16
1	2	626	4AC	C5-C4-N4	-2.86	117.95	122.92
1	2	1028	4AC	N4-C4-N3	2.85	118.64	113.85
1	2	20	OMU	O4-C4-C5	-2.85	120.15	125.16
1	2	830	OMU	O4-C4-C5	-2.84	120.16	125.16
1	2	1147	4AC	C5-C4-N4	-2.84	117.98	122.92
1	2	53	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	2	479	4AC	CM7-C7-N4	-2.84	110.38	115.29
1	2	394	4AC	C5-C4-N4	-2.84	117.99	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	1233	4AC	CM7-C7-N4	-2.83	110.39	115.29
31	4	32	OMC	O2-C2-N3	-2.83	117.73	122.33
1	2	546	4AC	C5-C4-N4	-2.83	118.00	122.92
1	2	1184	4AC	N4-C4-N3	2.83	118.60	113.85
1	2	286	4AC	CM7-C7-N4	-2.83	110.41	115.29
1	2	1147	4AC	CM7-C7-N4	-2.82	110.42	115.29
1	2	851	4AC	CM7-C7-N4	-2.81	110.42	115.29
1	2	319	4AC	CM7-C7-N4	-2.81	110.43	115.29
1	2	319	4AC	C5-C4-N4	-2.81	118.04	122.92
1	2	848	4AC	CM7-C7-N4	-2.80	110.46	115.29
1	2	379	4AC	CM7-C7-N4	-2.79	110.46	115.29
1	2	957	4AC	N4-C4-N3	2.79	118.53	113.85
1	2	868	4AC	CM7-C7-N4	-2.78	110.49	115.29
1	2	1239	4AC	N4-C4-N3	2.77	118.50	113.85
1	2	53	4AC	N4-C4-N3	2.76	118.49	113.85
1	2	1028	4AC	CM7-C7-N4	-2.76	110.52	115.29
1	2	511	4AC	N4-C4-N3	2.75	118.47	113.85
1	2	394	4AC	CM7-C7-N4	-2.75	110.53	115.29
1	2	751	4AC	N4-C4-N3	2.75	118.46	113.85
1	2	1028	4AC	C5-C4-N4	-2.74	118.16	122.92
1	2	957	4AC	C5-C4-N4	-2.73	118.18	122.92
1	2	546	4AC	CM7-C7-N4	-2.73	110.58	115.29
1	2	731	4AC	N4-C4-N3	2.71	118.39	113.85
1	2	848	4AC	N4-C4-N3	2.70	118.39	113.85
1	2	751	4AC	CM7-C7-N4	-2.70	110.62	115.29
1	2	373	A2M	C4-C5-N7	-2.69	106.60	109.40
1	2	53	4AC	C5-C4-N4	-2.69	118.25	122.92
1	2	1498	5MC	C5-C6-N1	-2.69	120.57	123.34
1	2	1479	4AC	C5-C4-N4	-2.69	118.25	122.92
1	2	511	4AC	C5-C4-N4	-2.68	118.26	122.92
1	2	718	4AC	CM7-C7-N4	-2.68	110.66	115.29
1	2	1239	4AC	C5-C4-N4	-2.67	118.27	122.92
1	2	303	4AC	N4-C4-N3	2.66	118.33	113.85
1	2	1498	5MC	C5-C4-N3	-2.66	118.80	121.67
1	2	839	4AC	N4-C4-N3	2.66	118.32	113.85
1	2	848	4AC	C5-C4-N4	-2.66	118.29	122.92
1	2	751	4AC	C5-C4-N4	-2.66	118.30	122.92
1	2	636	4AC	CM7-C7-N4	-2.65	110.70	115.29
1	2	957	4AC	CM7-C7-N4	-2.64	110.72	115.29
1	2	1479	4AC	CM7-C7-N4	-2.64	110.73	115.29
1	2	731	4AC	C5-C4-N4	-2.64	118.34	122.92
1	2	303	4AC	C5-C4-N4	-2.64	118.34	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	718	4AC	N4-C4-N3	2.61	118.24	113.85
1	2	1496	5MC	C5-C4-N3	-2.61	118.86	121.67
1	2	17	4AC	N4-C4-N3	2.60	118.22	113.85
1	2	875	5MC	C5-C4-N3	-2.60	118.87	121.67
1	2	828	4AC	N4-C4-N3	2.59	118.20	113.85
1	2	828	4AC	C5-C4-N4	-2.58	118.43	122.92
1	2	17	4AC	C5-C4-N4	-2.58	118.44	122.92
1	2	839	4AC	C5-C4-N4	-2.57	118.45	122.92
1	2	590	4AC	N4-C4-N3	2.57	118.17	113.85
1	2	1498	5MC	O2-C2-N3	-2.57	118.15	122.33
1	2	1202	5MC	C5-C4-N3	-2.56	118.92	121.67
1	2	1184	4AC	CM7-C7-N4	-2.55	110.88	115.29
1	2	250	LHH	N4-C4-N3	2.54	118.11	113.85
1	2	286	4AC	N4-C4-N3	2.52	118.08	113.85
1	2	1239	4AC	CM7-C7-N4	-2.52	110.94	115.29
1	2	693	5MC	C5-C4-N3	-2.51	118.97	121.67
1	2	535	5MC	C5-C4-N3	-2.49	118.98	121.67
1	2	718	4AC	C5-C4-N4	-2.49	118.59	122.92
1	2	1505	5MC	C5-C4-N3	-2.48	119.00	121.67
1	2	250	LHH	C5-C4-N3	-2.48	118.60	122.59
1	2	787	OMU	O2-C2-N1	-2.48	119.49	122.79
1	2	286	4AC	C5-C4-N4	-2.48	118.62	122.92
1	2	20	OMU	O2-C2-N1	-2.46	119.52	122.79
1	2	1025	5MC	C5-C4-N3	-2.45	119.03	121.67
1	2	1374	5MC	C5-C4-N3	-2.45	119.03	121.67
1	2	1041	LHH	C5-C4-N3	-2.44	118.67	122.59
1	2	590	4AC	C5-C4-N4	-2.43	118.69	122.92
1	2	250	LHH	C5-C6-N1	-2.43	117.73	121.81
1	2	1041	LHH	C5-C6-N1	-2.42	117.75	121.81
1	2	519	OMG	C5-C6-N1	2.42	118.22	113.95
1	2	934	OMG	C8-N7-C5	2.41	107.59	102.99
1	2	934	OMG	C5-C6-N1	2.40	118.19	113.95
1	2	467	OMG	C5-C6-N1	2.40	118.18	113.95
1	2	467	OMG	C8-N7-C5	2.39	107.54	102.99
1	2	519	OMG	C8-N7-C5	2.39	107.54	102.99
1	2	471	OMG	C5-C6-N1	2.38	118.15	113.95
1	2	913	OMG	C5-C6-N1	2.38	118.15	113.95
1	2	1069	OMG	C5-C6-N1	2.36	118.12	113.95
1	2	913	OMG	C8-N7-C5	2.36	107.49	102.99
1	2	657	OMG	C5-C6-N1	2.35	118.11	113.95
1	2	1041	LHH	N4-C4-N3	2.35	117.80	113.85
1	2	873	OMG	C5-C6-N1	2.35	118.10	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	868	4AC	N4-C4-N3	2.35	117.80	113.85
1	2	680	OMG	C5-C6-N1	2.35	118.10	113.95
1	2	873	OMG	C8-N7-C5	2.34	107.45	102.99
1	2	1069	OMG	C8-N7-C5	2.32	107.42	102.99
1	2	471	OMG	C8-N7-C5	2.29	107.36	102.99
1	2	773	OMC	O2-C2-N3	-2.28	118.62	122.33
1	2	680	OMG	C8-N7-C5	2.28	107.33	102.99
1	2	938	B8H	N3-C2-N1	2.28	117.60	115.14
1	2	868	4AC	C5-C4-N4	-2.27	118.97	122.92
1	2	657	OMG	C8-N7-C5	2.22	107.22	102.99
1	2	851	4AC	C5-C4-N4	-2.21	119.08	122.92
1	2	851	4AC	N4-C4-N3	2.21	117.56	113.85
1	2	1041	LHH	CM7-C7-N4	2.21	119.11	115.29
1	2	1498	5MC	C1'-N1-C6	-2.19	117.47	121.12
31	4	8	4SU	O2-C2-N1	-2.19	119.88	122.79
31	4	32	OMC	C1'-N1-C2	2.17	123.27	118.42
1	2	851	4AC	O2-C2-N3	-2.17	118.81	122.33
1	2	875	5MC	O2-C2-N3	-2.13	118.86	122.33
1	2	1036	OMC	O2-C2-N3	-2.10	118.91	122.33
1	2	250	LHH	CM7-C7-N4	2.10	118.92	115.29
1	2	1505	5MC	O2-C2-N3	-2.08	118.95	122.33
1	2	938	B8H	O4'-C1'-C2'	2.07	108.07	105.14
1	2	1202	5MC	O2-C2-N3	-2.07	118.97	122.33
1	2	250	LHH	O2-C2-N3	-2.07	118.97	122.33
1	2	1177	OMU	O2-C2-N1	-2.05	120.07	122.79
1	2	1380	OMU	O2-C2-N1	-2.04	120.08	122.79
1	2	250	LHH	C6-C5-C4	2.03	119.45	116.96
1	2	868	4AC	O2-C2-N3	-2.03	119.04	122.33
1	2	1041	LHH	O2-C2-N3	-2.02	119.05	122.33
1	2	1025	5MC	O2-C2-N3	-2.01	119.07	122.33
1	2	693	5MC	O2-C2-N3	-2.01	119.07	122.33

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	934	OMG	O4'-C4'-C5'-O5'
31	4	20	H2U	C3'-C4'-C5'-O5'
31	4	20	H2U	O4'-C1'-N1-C6
1	2	934	OMG	C3'-C4'-C5'-O5'
1	2	1202	5MC	O4'-C4'-C5'-O5'
1	2	1202	5MC	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	4	20	H2U	O4'-C4'-C5'-O5'
1	2	20	OMU	C2'-C1'-N1-C6
1	2	1376	OMC	O4'-C4'-C5'-O5'
1	2	20	OMU	O4'-C1'-N1-C6
1	2	1498	5MC	O4'-C1'-N1-C6
1	2	913	OMG	C3'-C2'-O2'-CM2
1	2	1498	5MC	O4'-C1'-N1-C2
1	2	511	4AC	O4'-C4'-C5'-O5'
31	4	32	OMC	C2'-C1'-N1-C6
31	4	20	H2U	C2'-C1'-N1-C6
1	2	20	OMU	O4'-C4'-C5'-O5'
1	2	20	OMU	O4'-C1'-N1-C2
1	2	1177	OMU	C3'-C2'-O2'-CM2
1	2	787	OMU	O4'-C1'-N1-C6
1	2	787	OMU	C2'-C1'-N1-C6
1	2	20	OMU	C2'-C1'-N1-C2
1	2	1025	5MC	O4'-C4'-C5'-O5'
1	2	1376	OMC	C3'-C4'-C5'-O5'
1	2	64	OMU	C1'-C2'-O2'-CM2
1	2	1177	OMU	C1'-C2'-O2'-CM2
31	4	20	H2U	C2'-C1'-N1-C2
31	4	32	OMC	C2'-C1'-N1-C2
31	4	20	H2U	O4'-C1'-N1-C2
31	4	20	H2U	C4'-C5'-O5'-P
1	2	64	OMU	C3'-C2'-O2'-CM2
1	2	774	OMU	C3'-C2'-O2'-CM2
1	2	467	OMG	O4'-C4'-C5'-O5'
1	2	1498	5MC	O4'-C4'-C5'-O5'
1	2	1498	5MC	C2'-C1'-N1-C2
1	2	873	OMG	C4'-C5'-O5'-P
1	2	1488	MA6	C4'-C5'-O5'-P

There are no ring outliers.

21 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	636	4AC	3	0
1	2	774	OMU	1	0
1	2	479	4AC	1	0
1	2	1239	4AC	1	0
1	2	1147	4AC	1	0
1	2	1380	OMU	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	2	373	A2M	1	0
31	4	32	OMC	1	0
1	2	1233	4AC	1	0
1	2	957	4AC	1	0
1	2	379	4AC	1	0
1	2	680	OMG	1	0
31	4	20	H2U	1	0
1	2	626	4AC	1	0
1	2	394	4AC	1	0
1	2	1177	OMU	1	0
1	2	1184	4AC	1	0
1	2	731	4AC	1	0
31	4	8	4SU	1	0
1	2	703	4AC	3	0
1	2	53	4AC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 69 ligands modelled in this entry, 68 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	$\#\|Z\| > 2$
35	MET	4	101	31	6,7,8	1.23	1 (16%)	2,7,9	1.97	1 (50%)

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
35	MET	4	101	31	-	1/5/6/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	101	MET	CB-CA	-2.78	1.49	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	4	101	MET	CE-SD-CG	2.68	109.60	100.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	4	101	MET	CA-CB-CG-SD

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

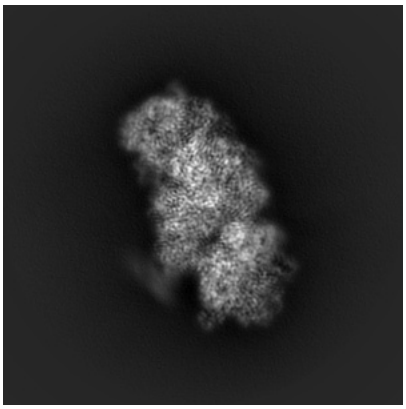
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14581. These allow visual inspection of the internal detail of the map and identification of artifacts.

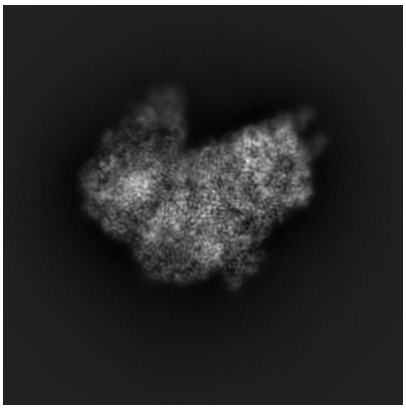
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

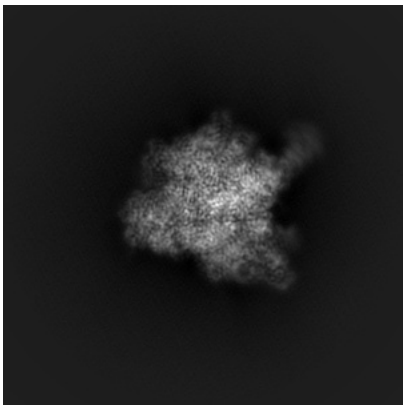
6.1.1 Primary map



X

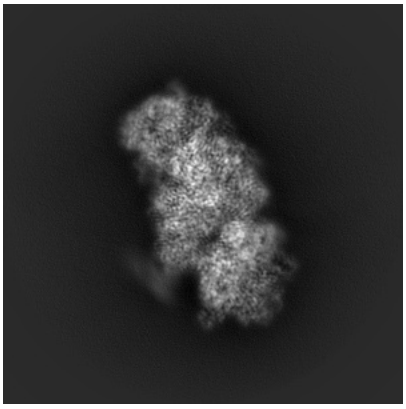


Y

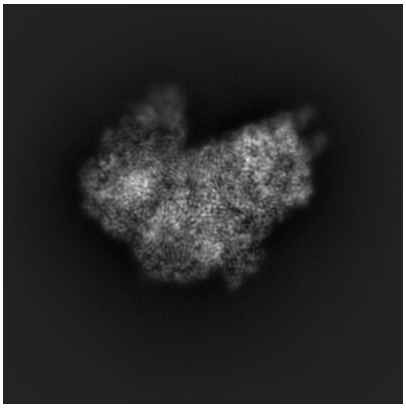


Z

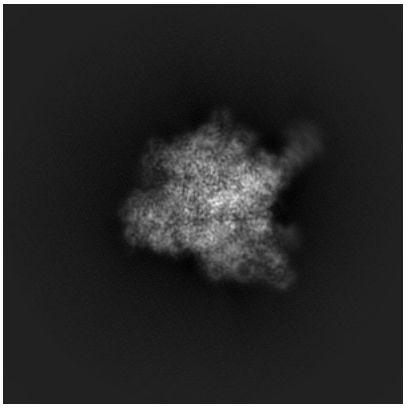
6.1.2 Raw map



X



Y

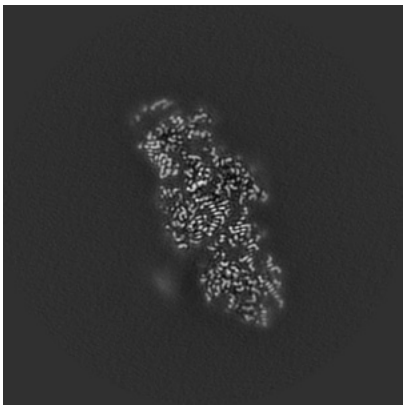


Z

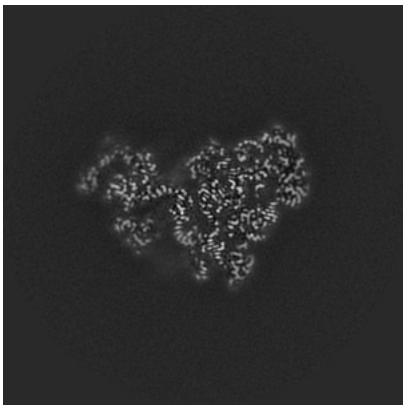
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

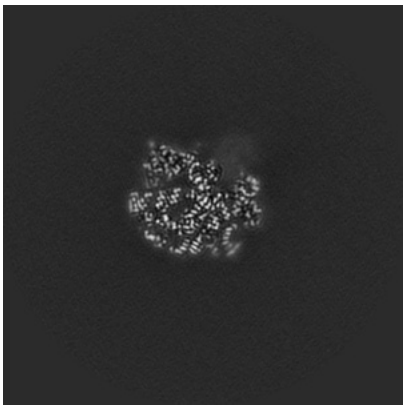
6.2.1 Primary map



X Index: 216

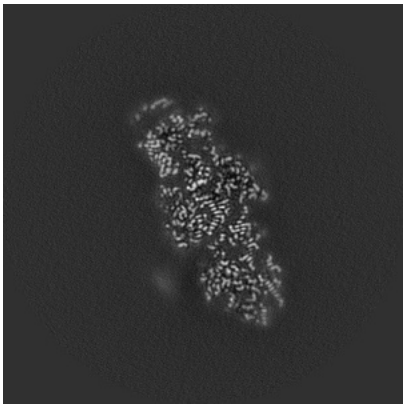


Y Index: 216

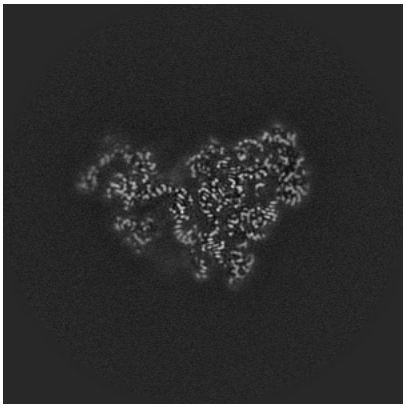


Z Index: 216

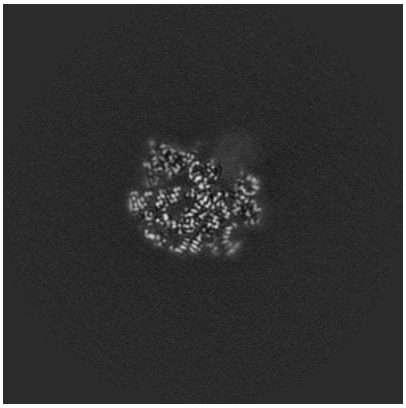
6.2.2 Raw map



X Index: 216



Y Index: 216

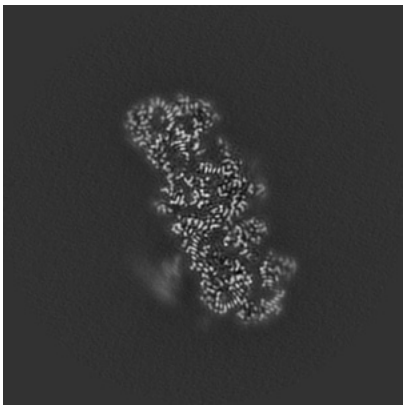


Z Index: 216

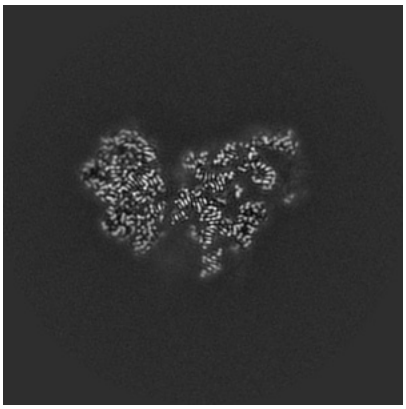
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

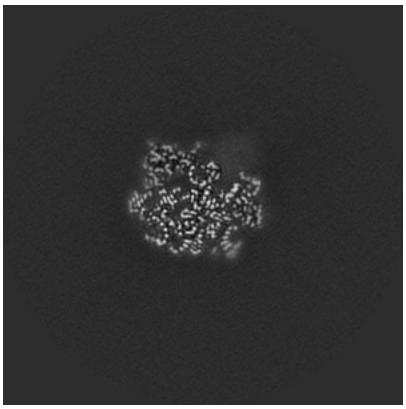
6.3.1 Primary map



X Index: 226

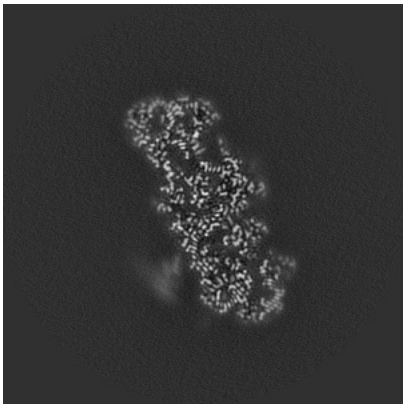


Y Index: 228

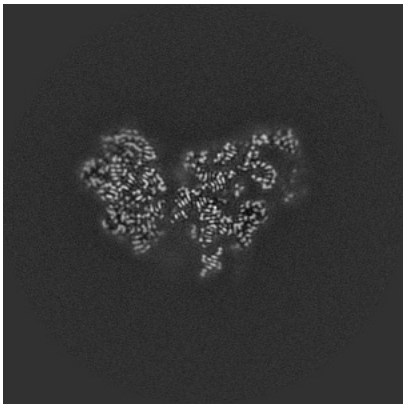


Z Index: 218

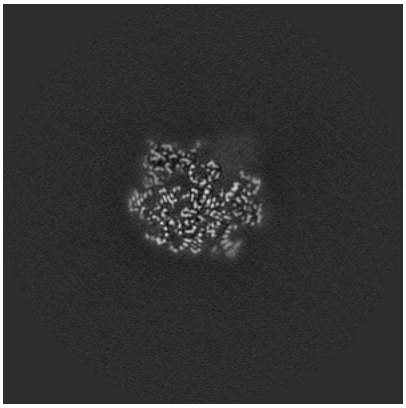
6.3.2 Raw map



X Index: 225



Y Index: 227

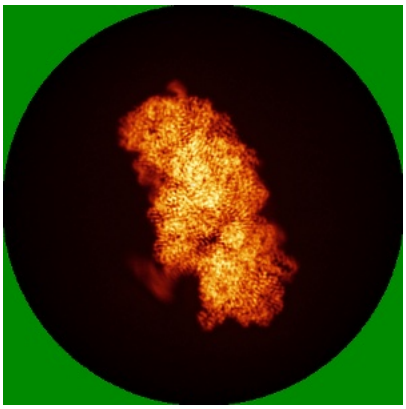


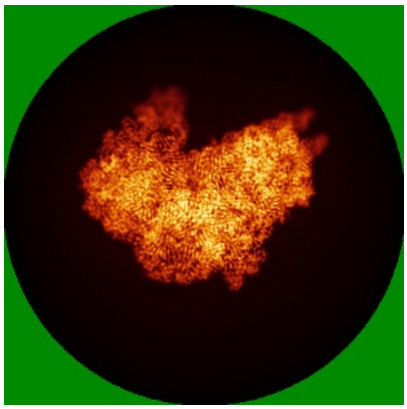
Z Index: 218

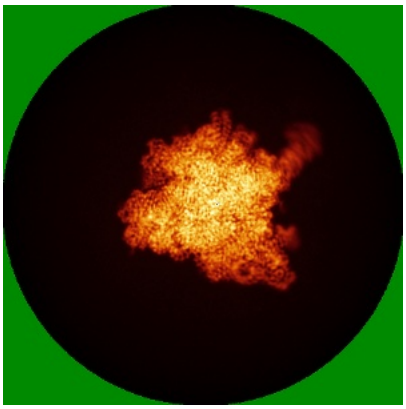
The images above show the largest variance slices of the map in three orthogonal directions.

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

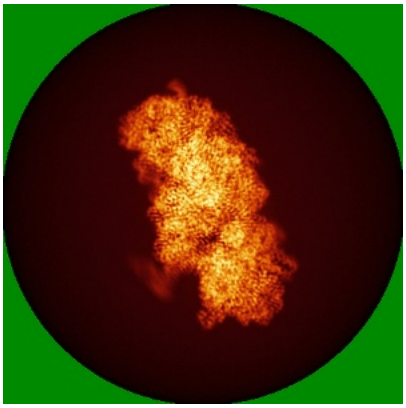
6.4.1 Primary map

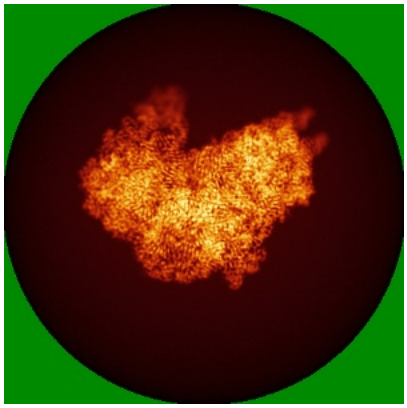

X

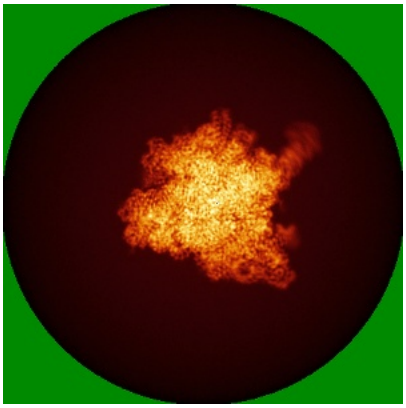

Y


Z

6.4.2 Raw map


X

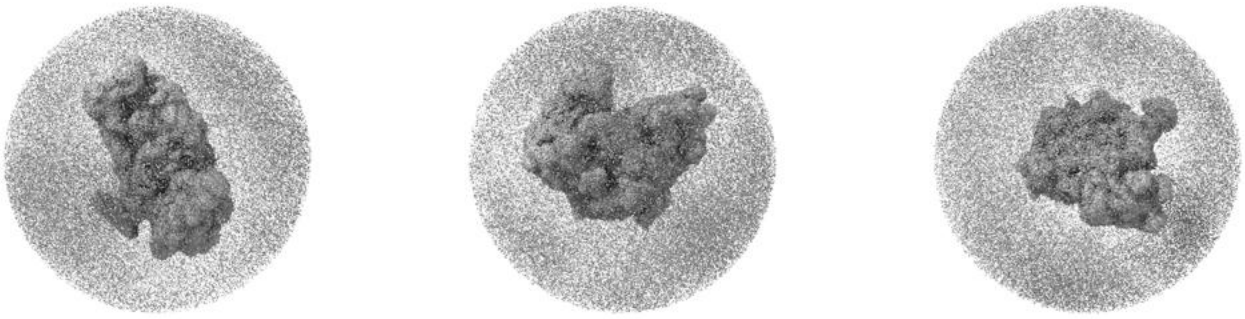

Y


Z

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

6.5 Orthogonal surface views (i)

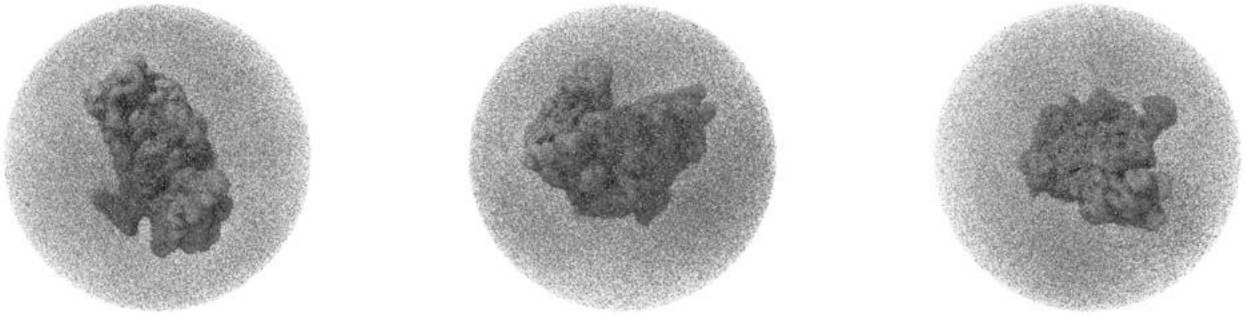
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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.

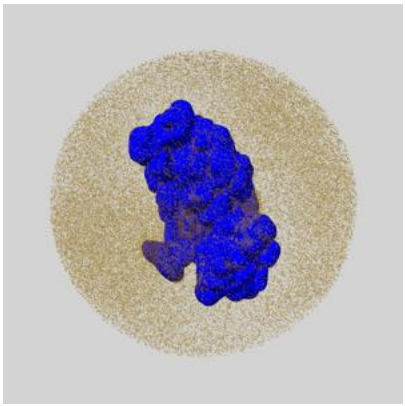
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

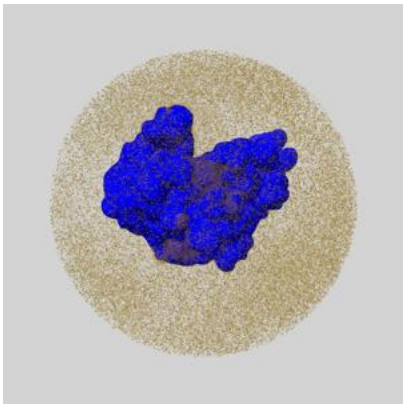
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

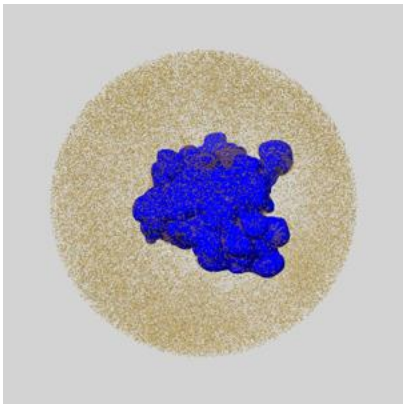
6.6.1 emd_14581_msk_1.map (i)



X



Y

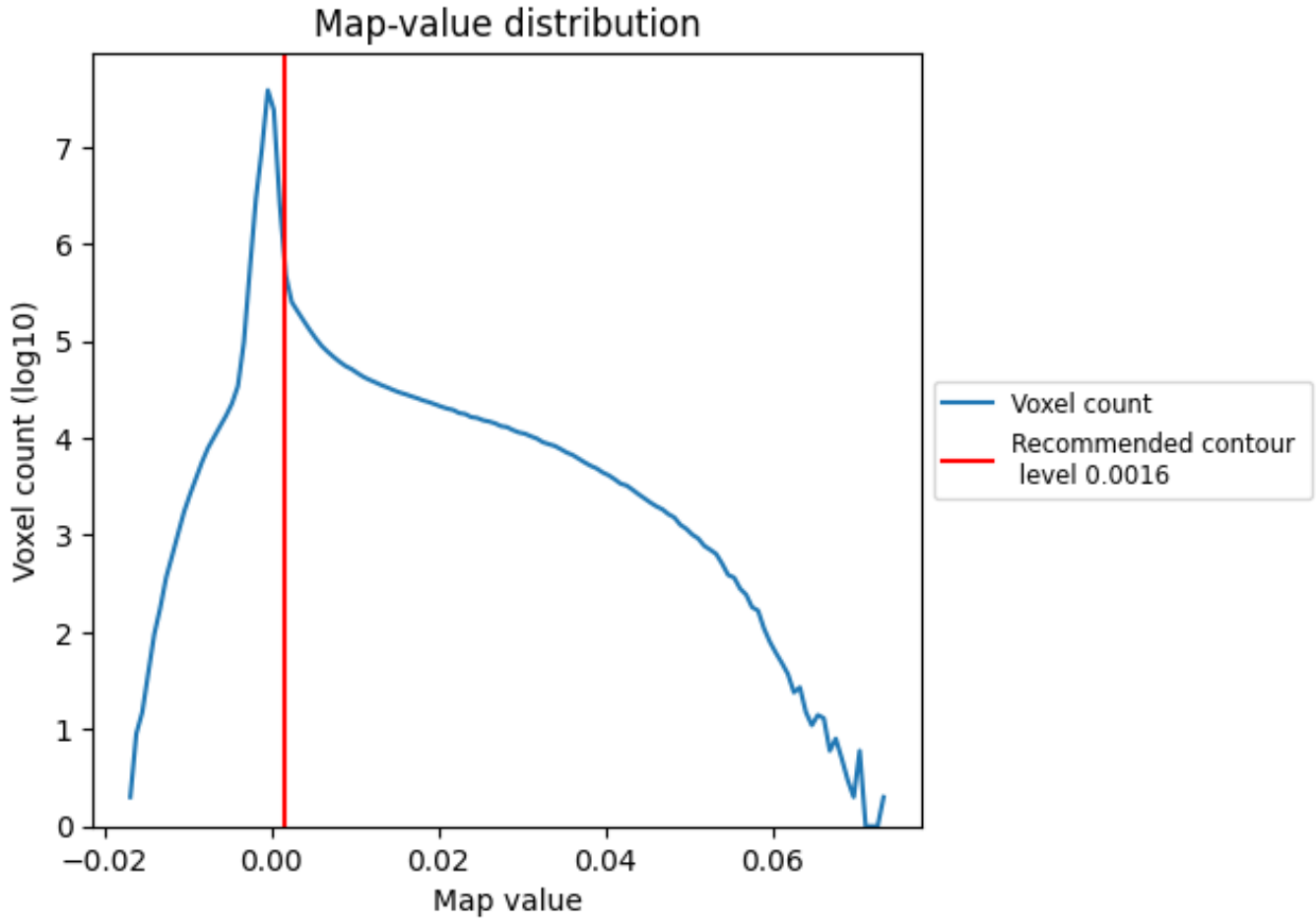


Z

7 Map analysis

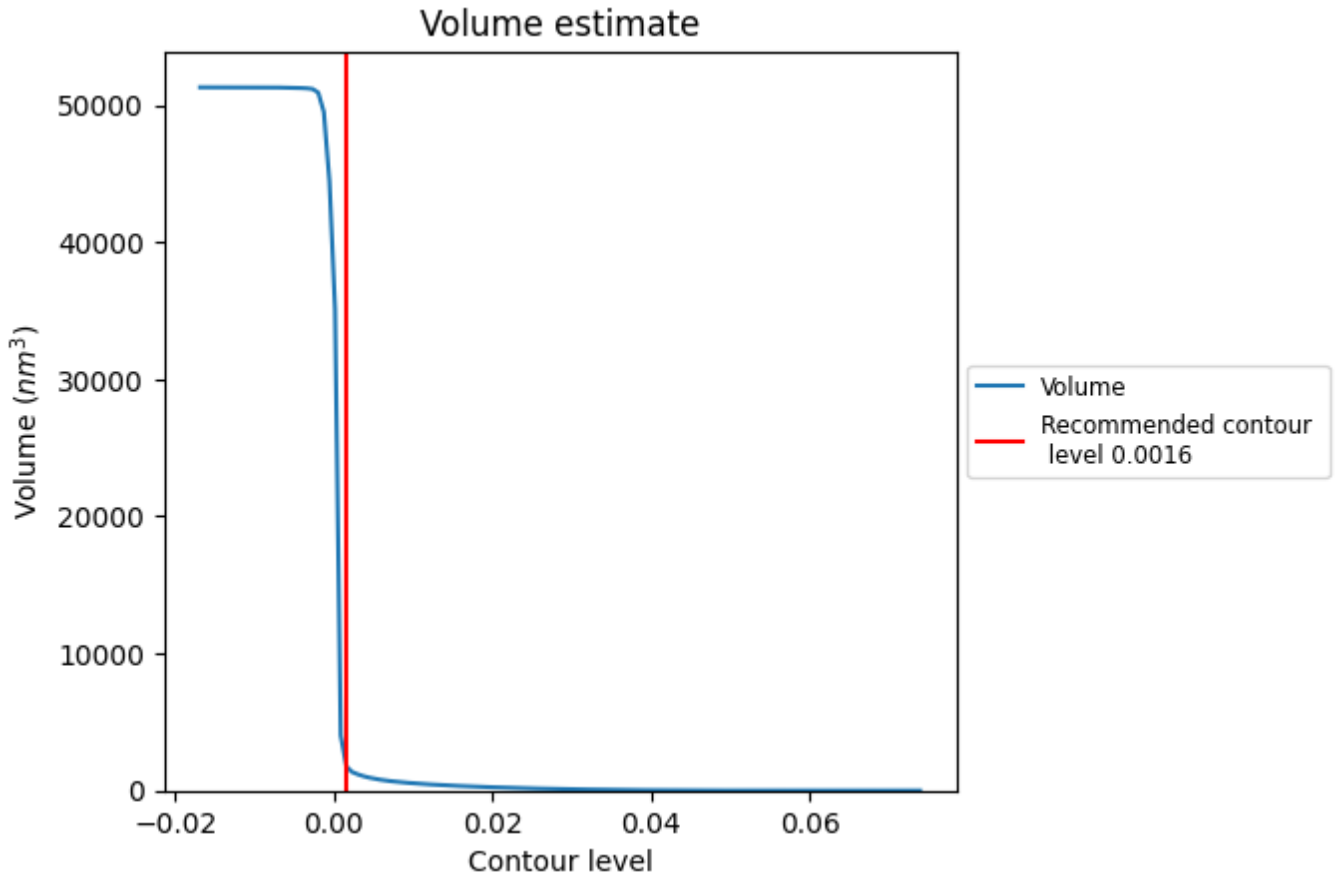
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

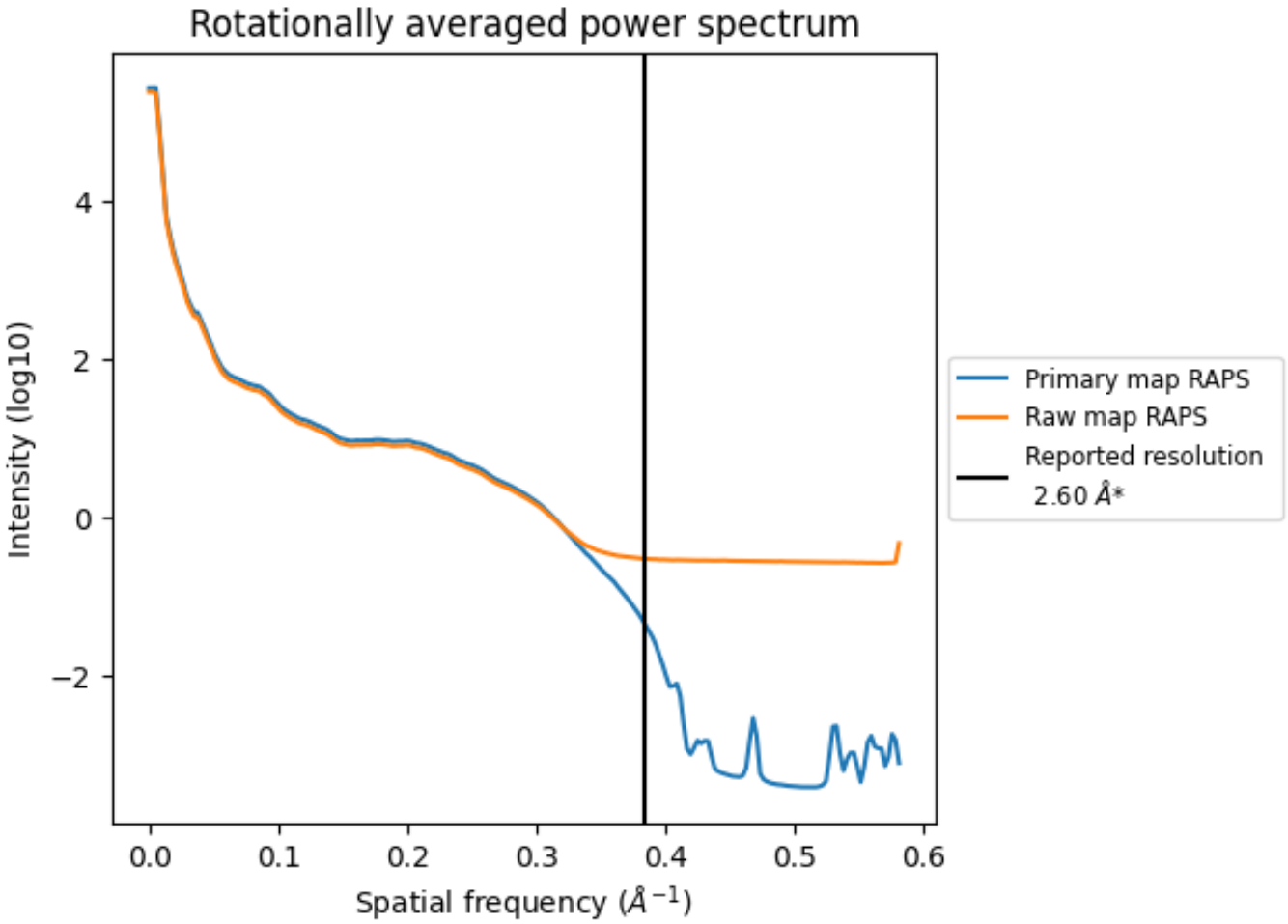
7.2 Volume estimate



The volume at the recommended contour level is 1745 nm^3; this corresponds to an approximate mass of 1576 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)

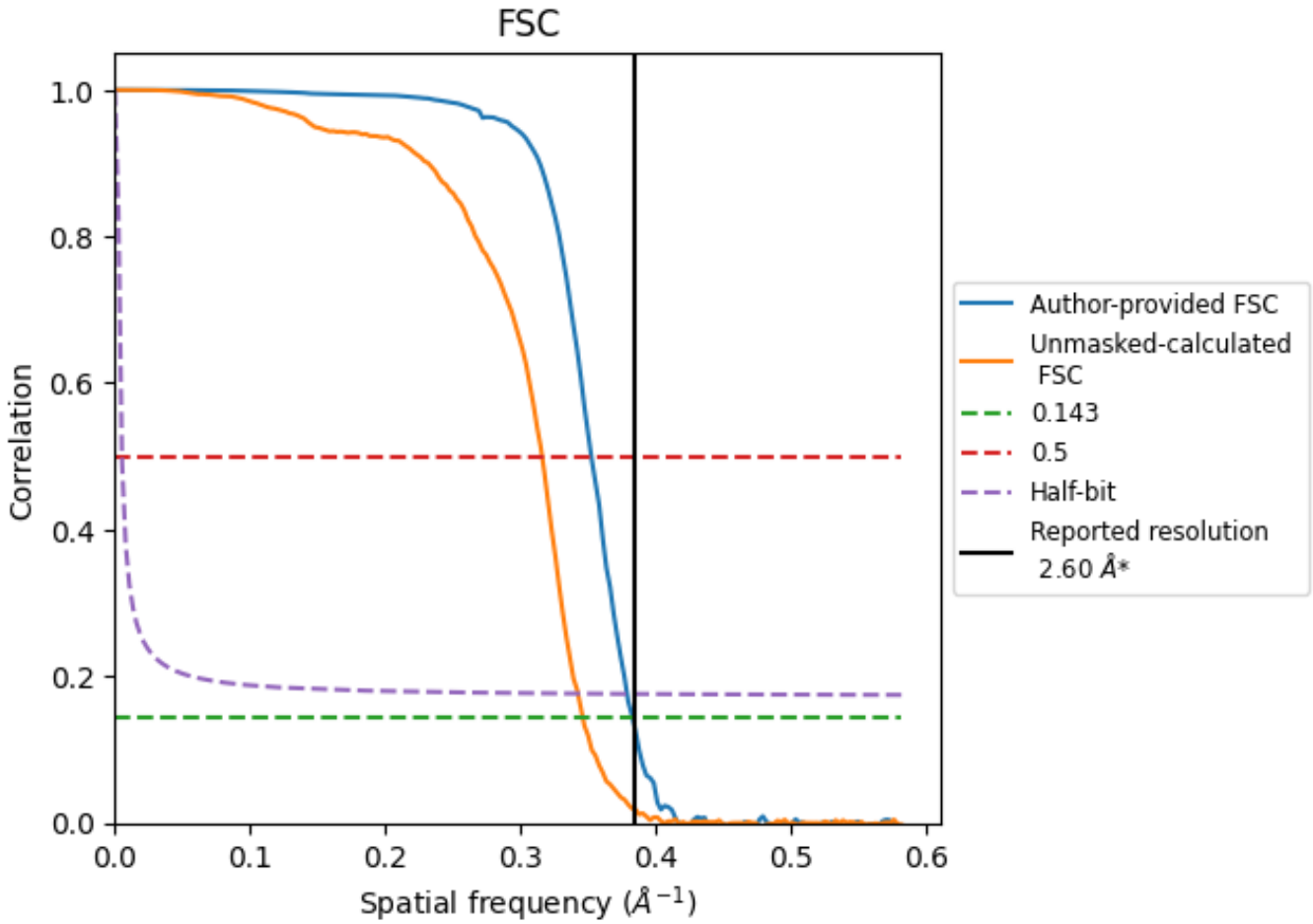


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

8.2 Resolution estimates (i)

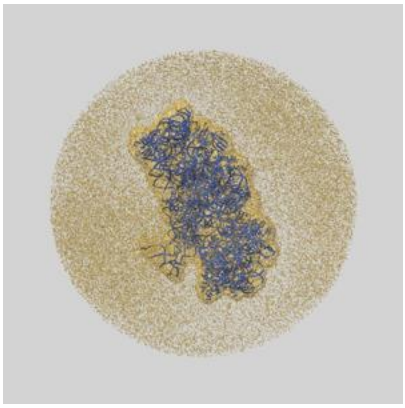
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	2.61	2.84	2.64
Unmasked-calculated*	2.89	3.17	2.92

*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 2.89 differs from the reported value 2.6 by more than 10 %

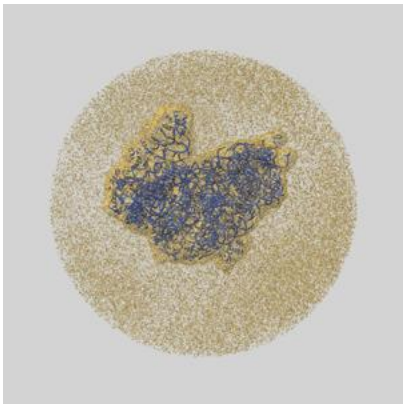
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14581 and PDB model 7ZAI. Per-residue inclusion information can be found in section 3 on page 13.

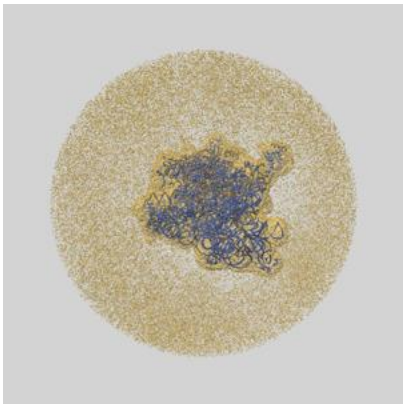
9.1 Map-model overlay



X



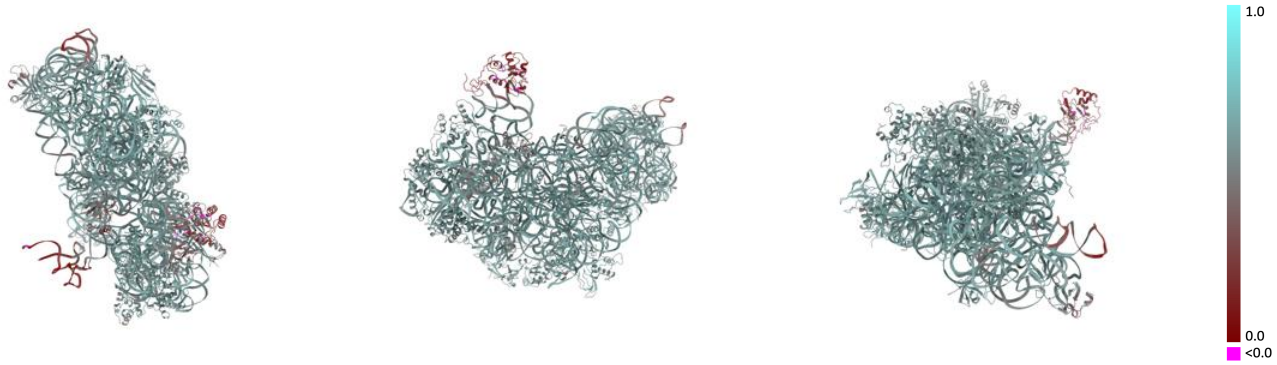
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0016 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.

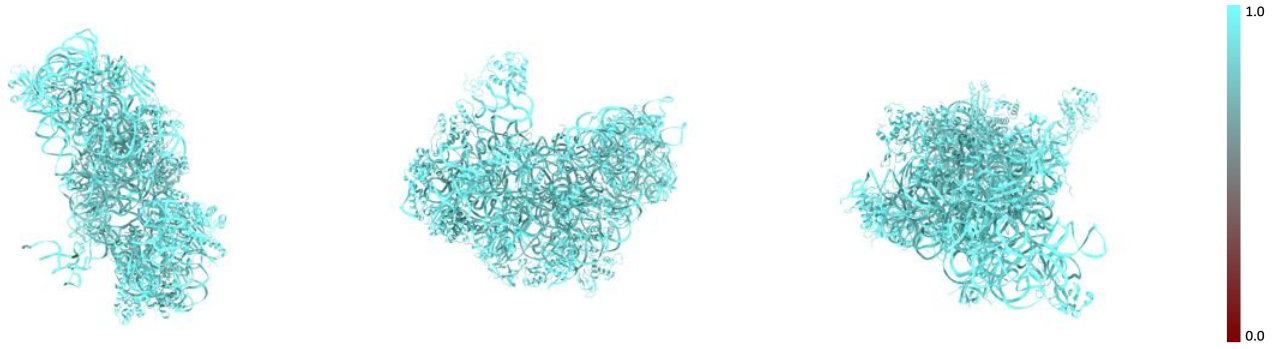
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

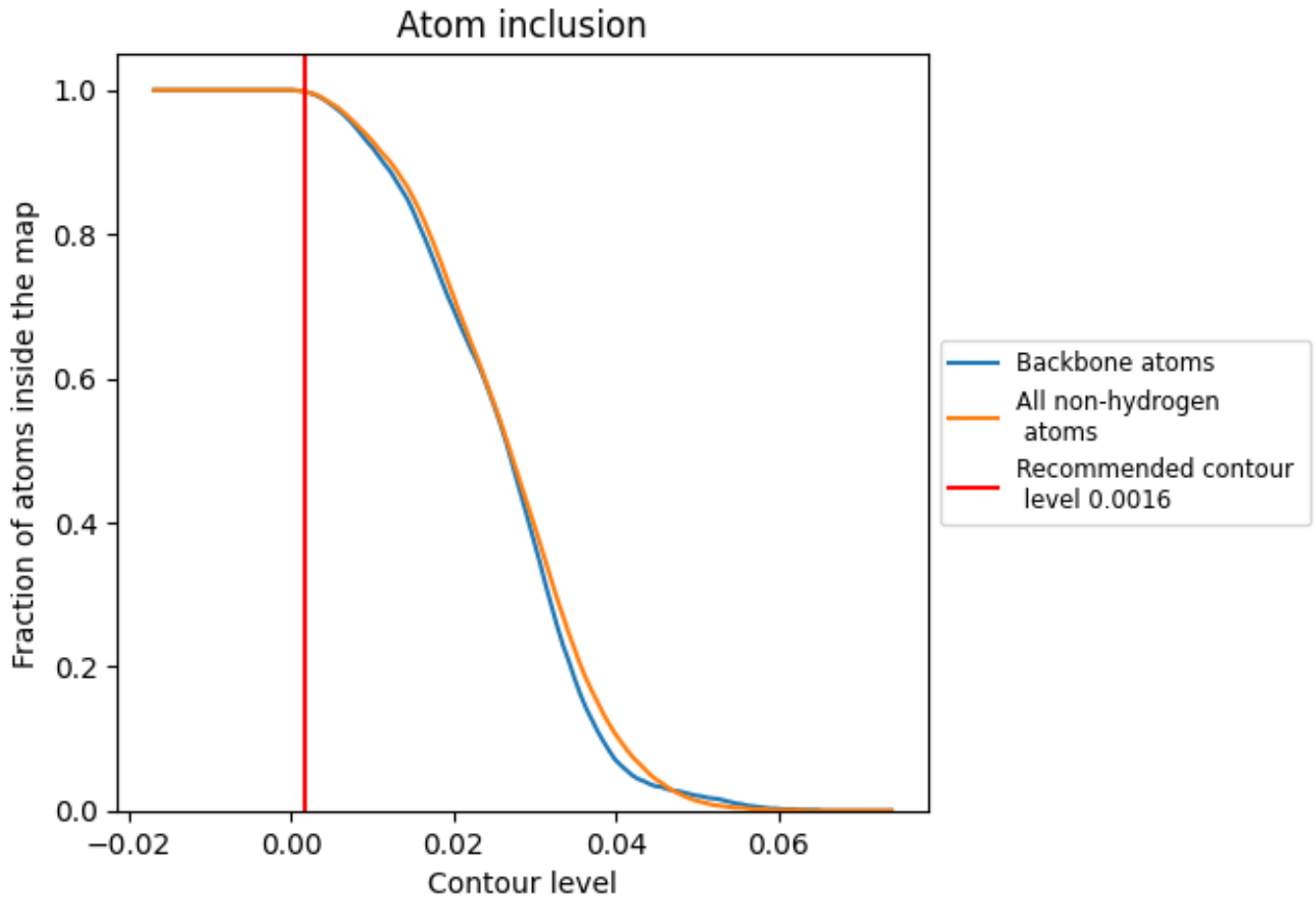
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0016).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9980	0.5870
0	1.0000	0.6320
2	1.0000	0.6130
3	0.9950	0.2100
4	0.9860	0.3190
5	1.0000	0.5630
6	0.9130	0.4080
A	1.0000	0.5920
B	0.9990	0.5920
C	1.0000	0.6110
D	1.0000	0.6190
E	1.0000	0.6070
F	0.9990	0.6170
G	1.0000	0.5310
H	0.9980	0.5960
I	0.9990	0.6270
J	1.0000	0.5980
K	1.0000	0.6030
L	1.0000	0.5620
M	0.9990	0.6110
N	0.9980	0.6130
O	0.9990	0.5760
P	0.9980	0.6010
Q	1.0000	0.6020
R	1.0000	0.6260
S	1.0000	0.5480
T	1.0000	0.5750
U	1.0000	0.5950
V	0.9990	0.5890
W	1.0000	0.5890
X	1.0000	0.5940
Y	0.9970	0.1770
Z	0.9990	0.5670