Full wwPDB EM Validation Report (i)

Apr 30, 2024 – 12:56 PM EDT

PDB ID	:	8UUA
EMDB ID	:	EMD-42577
Title	:	Cryo-EM structure of the Listeria innocua 50S ribosomal subunit in complex with HflXr (structure III)
Authors	:	Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on	:	2023-10-31
Resolution	:	2.70 Å(reported)
Based on initial model	:	7NHN

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

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

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

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

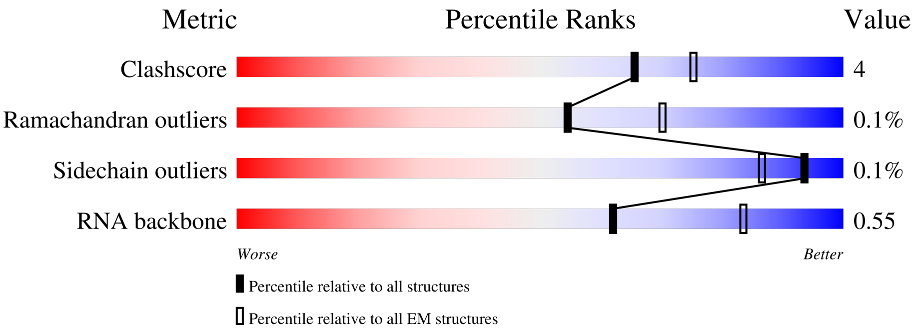
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
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	v	418	8% / 100%
2	A	2932	• / 71% 23% • •
3	B	116	70% 28% • •
4	C	277	87% 12% •
5	D	209	85% 13% •
6	E	207	89% 9% •
7	F	179	• / 76% 21% • •

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Mol	Chain	Length	Quality of chain
8	G	178	78% 21%
9	L	145	90% 8%
10	M	122	84% 16%
11	N	146	91% 8%
12	O	144	82% 10% 8%
13	P	135	85% 10%
14	Q	119	82% 18%
15	R	114	83% 7% 10%
16	S	119	91% 7%
17	T	102	93% 6%
18	U	118	79% 14% 7%
19	V	94	88% 7%
20	W	103	82% 17%
21	Y	96	73% 6% 21%
22	Z	62	81% 15% 5%
23	1	63	81% 13% 6%
24	2	59	90% 5% 5%
25	3	81	9% 70% 27%
26	4	57	88% 5% 7%
27	5	49	88% 8%
28	6	44	82% 16%
29	7	66	89% 6% 5%
30	8	37	84% 14%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 91008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	v	418	3294	2073	566	644	11	0	0

- Molecule 2 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A	2894	62168	27745	11501	20028	2894	0	0

- Molecule 3 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	B	114	2428	1082	428	804	114	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	273	2108	1307	415	379	7	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D	206	1583	995	291	293	4	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	E	203	1539	974	285	280	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	175	Total 1171	C 730	N 207	O 229	S 5	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	177	Total 1355	C 851	N 251	O 252	S 1	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	142	Total 1117	C 709	N 201	O 204	S 3	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	122	Total 925	C 573	N 175	O 172	S 5	0	0

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	N	144	Total 1057	C 654	N 207	O 196	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	133	Total 1045	C 669	N 201	O 170	S 5	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	122	Total 957	C 601	N 187	O 168	S 1	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	Q	118	913	563	176	174	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	R	103	802	508	156	137	1	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	S	116	939	596	185	154	4	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	101	762	493	131	137	1	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	U	110	823	521	155	147	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	V	90	720	457	123	138	2	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	W	102	719	459	135	122	3	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Y	76	571	350	111	109	1	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	Z	59	450	277	95	76	2	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	1	59	483	296	94	92	1	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	2	56	433	272	82	78	1	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	3	59	292	174	59	59	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	4	53	425	259	87	74	5	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	5	47	390	238	78	71	3	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	43	Total 365	C 222	N 88	O 53	S 2	0	0

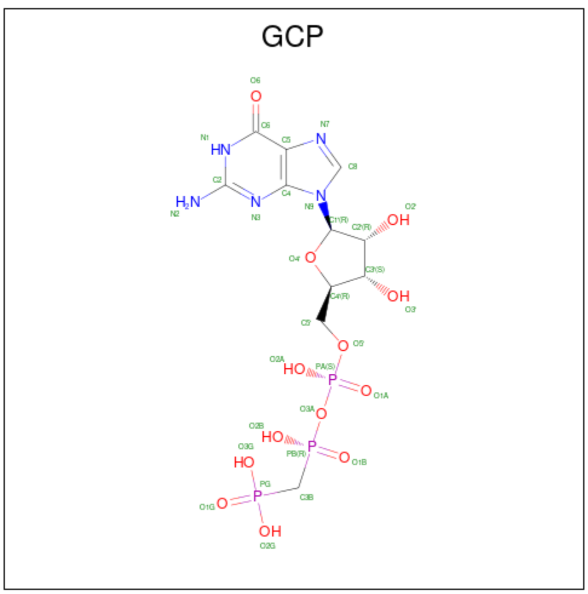
- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	63	Total 512	C 317	N 113	O 78	S 4	0	0

- Molecule 30 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	36	Total 292	C 183	N 59	O 44	S 6	0	0

- Molecule 31 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
31	v	1	Total 32	C 11	N 5	O 13	P 3	0

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	A	192	Total 192	Mg 192	0

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Mol	Chain	Residues	Atoms		AltConf
32	C	2	Total 2	Mg 2	0
32	D	1	Total 1	Mg 1	0
32	M	1	Total 1	Mg 1	0
32	N	1	Total 1	Mg 1	0
32	V	1	Total 1	Mg 1	0
32	Z	1	Total 1	Mg 1	0
32	6	1	Total 1	Mg 1	0

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
33	O	1	Total 1	K 1	0

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

Mol	Chain	Residues	Atoms		AltConf
34	4	1	Total 1	Zn 1	0
34	5	1	Total 1	Zn 1	0
34	8	1	Total 1	Zn 1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	A	130	Total 130	O 130	0
35	N	1	Total 1	O 1	0
35	P	1	Total 1	O 1	0
35	4	1	Total 1	O 1	0

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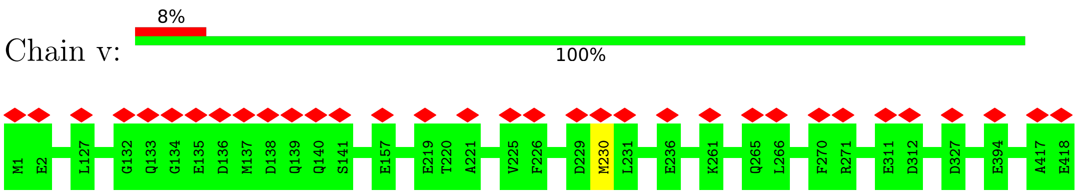
Mol	Chain	Residues	Atoms	AltConf
35	8	1	Total O 1 1	0

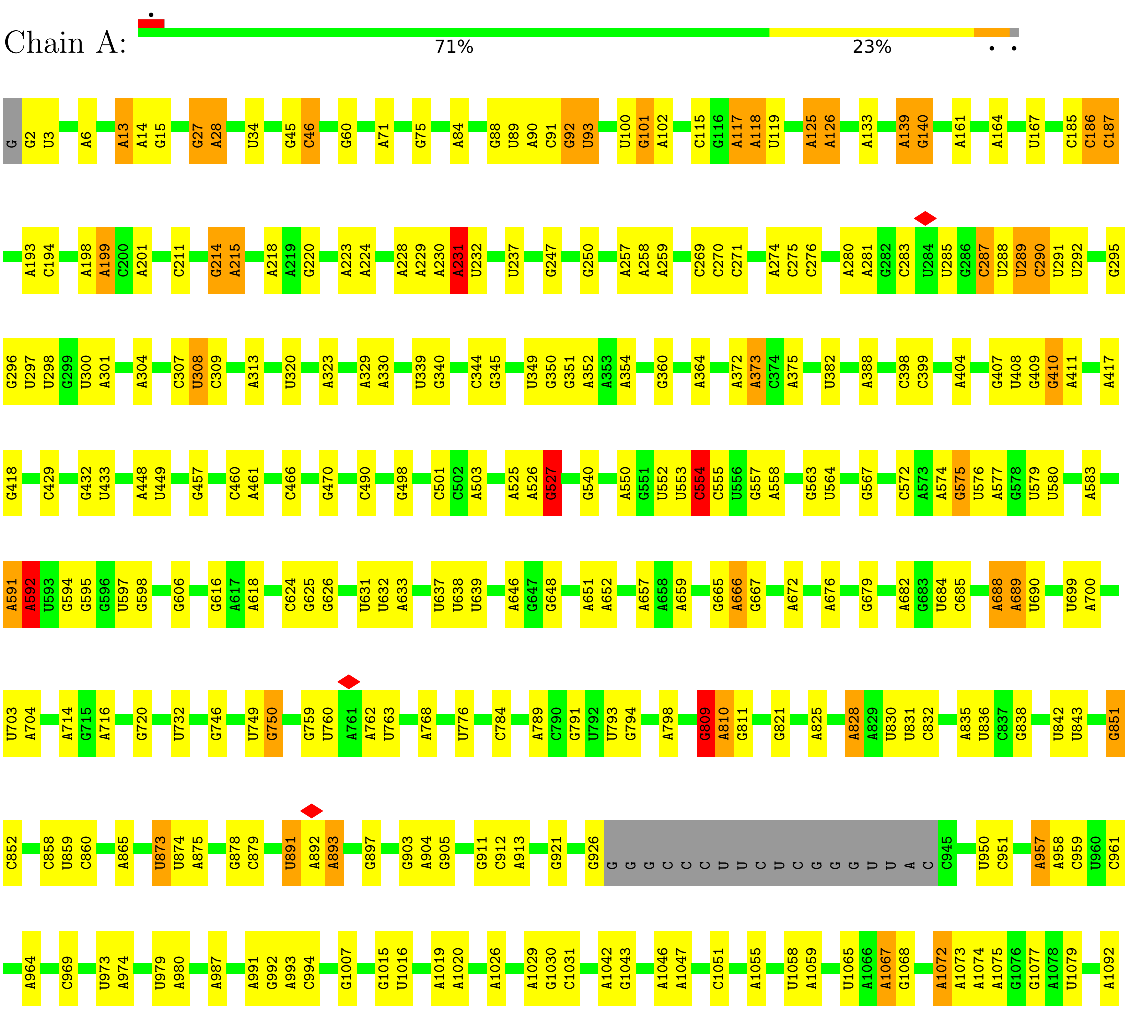
3 Residue-property plots

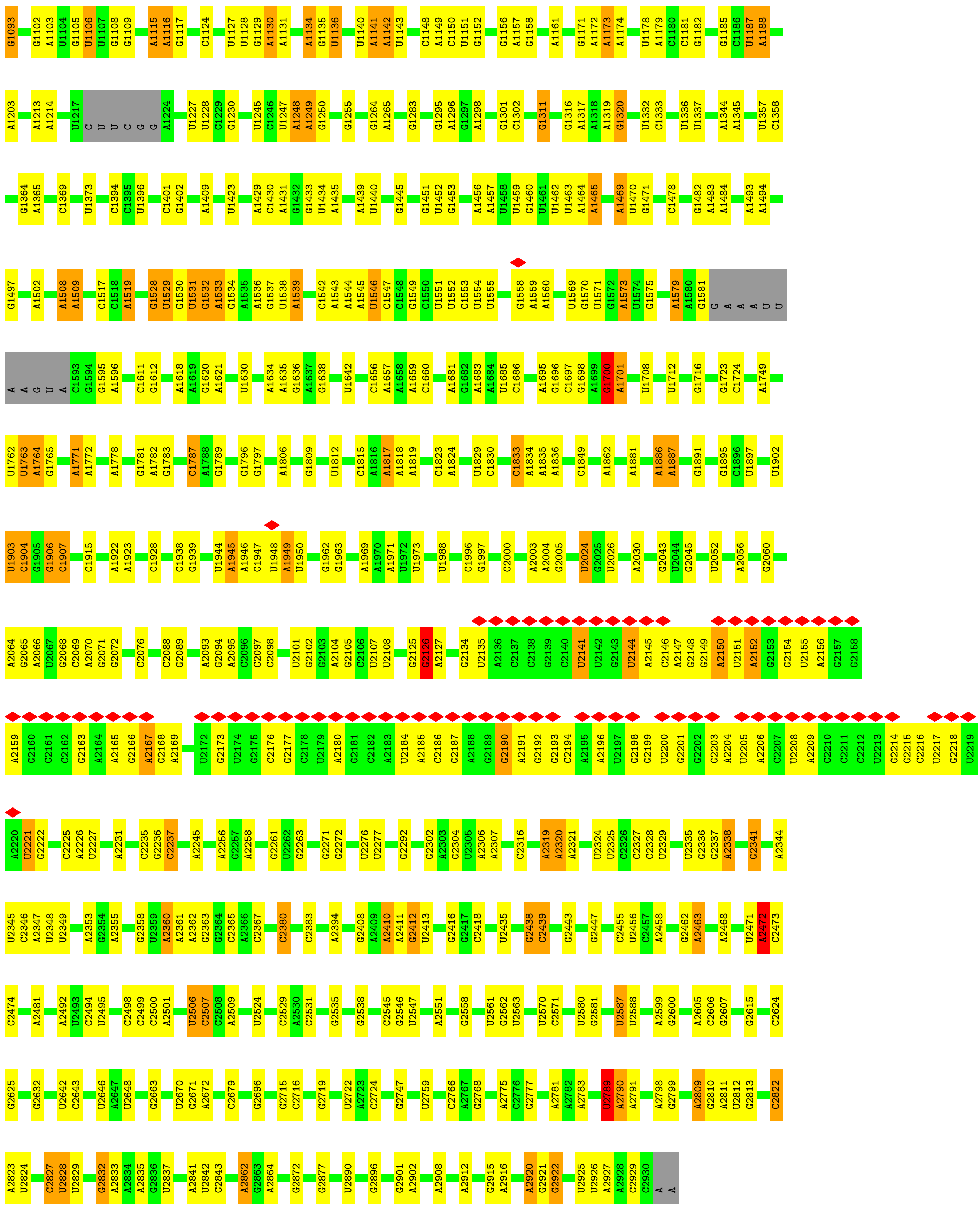
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: GTPase HflX

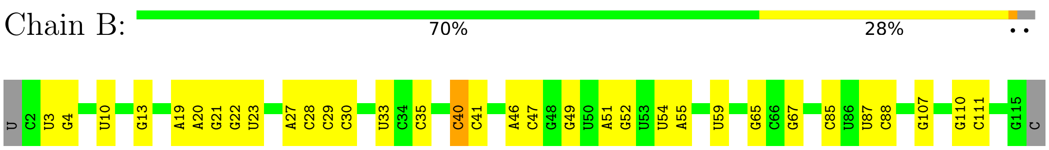


- Molecule 2: 23S Ribosomal RNA

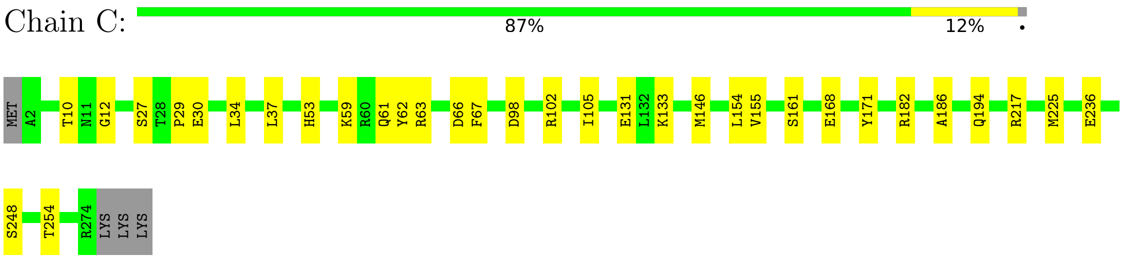




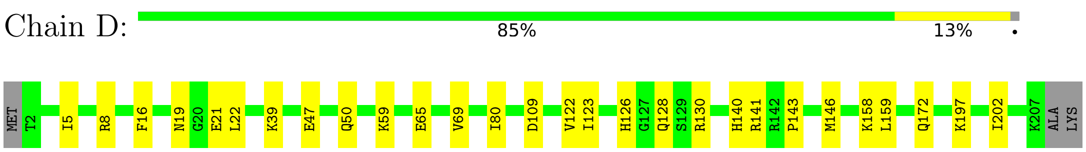
- Molecule 3: 5S Ribosomal RNA



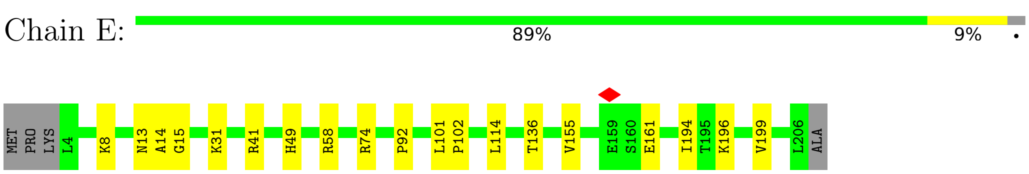
- Molecule 4: Large ribosomal subunit protein uL2



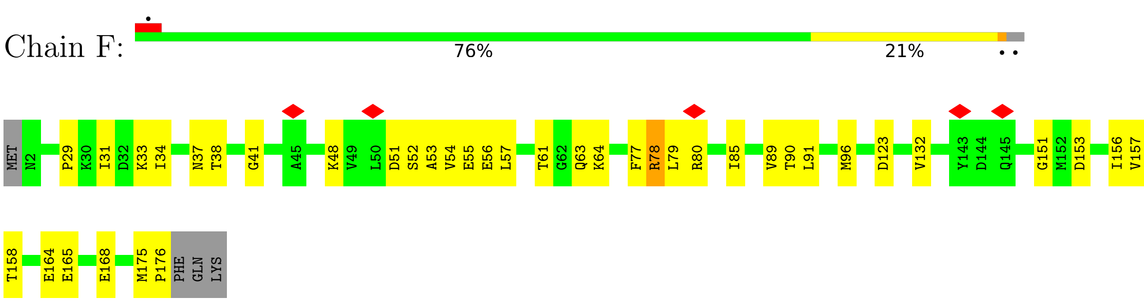
- Molecule 5: Large ribosomal subunit protein uL3



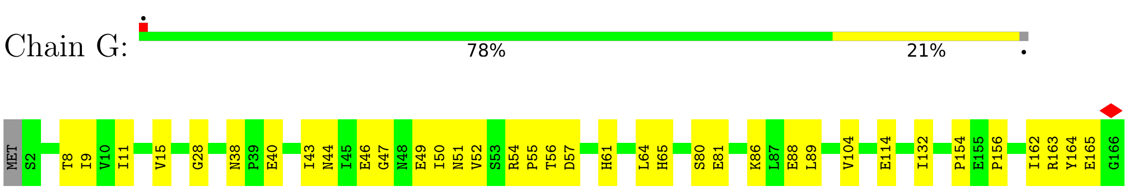
- Molecule 6: Large ribosomal subunit protein uL4

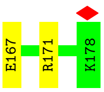


- Molecule 7: Large ribosomal subunit protein uL5



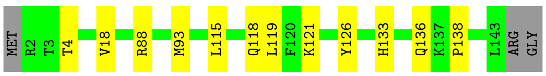
- Molecule 8: Large ribosomal subunit protein uL6





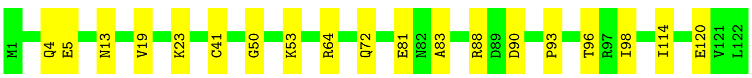
- Molecule 9: Large ribosomal subunit protein uL13

Chain L:



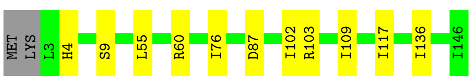
- Molecule 10: Large ribosomal subunit protein uL14

Chain M:



- Molecule 11: Large ribosomal subunit protein uL15

Chain N:

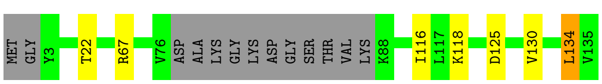


- Molecule 12: Large ribosomal subunit protein uL16

Chain O:

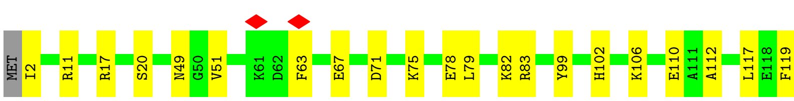
- Molecule 13: Large ribosomal subunit protein bL17

Chain P:



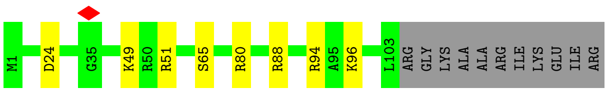
- Molecule 14: Large ribosomal subunit protein uL18

Chain Q:



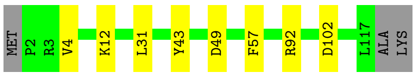
- Molecule 15: Large ribosomal subunit protein bL19

Chain R:



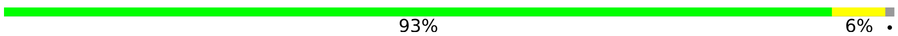
• Molecule 16: Large ribosomal subunit protein bL20

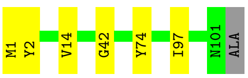
Chain S:



• Molecule 17: Large ribosomal subunit protein bL21

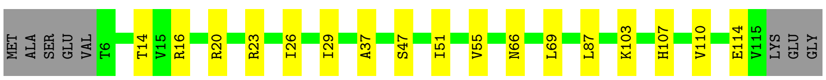
Chain T:





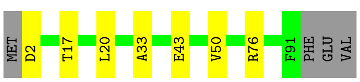
• Molecule 18: Large ribosomal subunit protein uL22

Chain U:



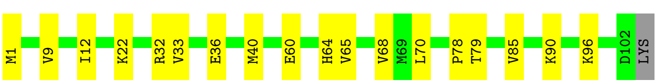
• Molecule 19: Large ribosomal subunit protein uL23

Chain V:



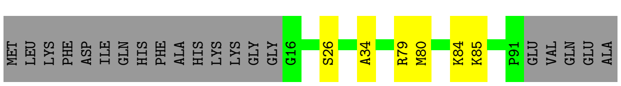
• Molecule 20: Large ribosomal subunit protein uL24

Chain W:



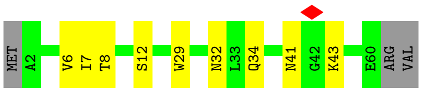
• Molecule 21: Large ribosomal subunit protein bL27

Chain Y:



• Molecule 22: Large ribosomal subunit protein bL28

Chain Z:

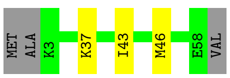


• Molecule 23: Large ribosomal subunit protein uL29

Chain 1:

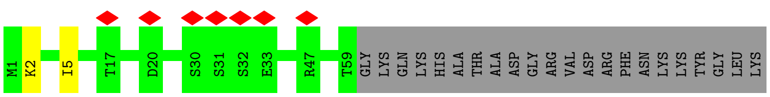
• Molecule 24: Large ribosomal subunit protein uL30

Chain 2:



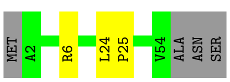
• Molecule 25: Large ribosomal subunit protein bL31B

Chain 3:



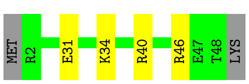
• Molecule 26: Large ribosomal subunit protein bL32

Chain 4:



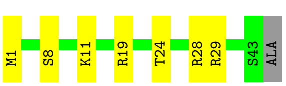
• Molecule 27: Large ribosomal subunit protein bL33

Chain 5:



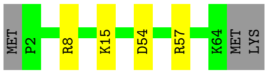
• Molecule 28: Large ribosomal subunit protein bL34

Chain 6:



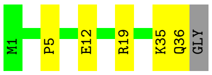
• Molecule 29: Large ribosomal subunit protein bL35

Chain 7:



- Molecule 30: Large ribosomal subunit protein bL36

Chain 8:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	332513	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 $(e^-/\text{Å}^2)$	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.373	Depositor
Minimum map value	-0.712	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, K, MG, ZN

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	v	0.28	0/3336	0.52	0/4499
2	A	0.81	0/69651	0.89	25/108655 (0.0%)
3	B	0.47	0/2711	0.79	0/4224
4	C	0.41	0/2144	0.61	0/2875
5	D	0.42	0/1605	0.59	0/2156
6	E	0.37	0/1559	0.62	1/2104 (0.0%)
7	F	0.30	0/1180	0.57	0/1606
8	G	0.32	0/1377	0.53	0/1857
9	L	0.41	0/1140	0.57	0/1532
10	M	0.41	0/932	0.61	0/1248
11	N	0.36	0/1068	0.57	0/1427
12	O	0.42	0/1067	0.60	0/1428
13	P	0.41	0/968	0.63	1/1297 (0.1%)
14	Q	0.30	0/922	0.55	0/1231
15	R	0.39	0/814	0.61	0/1097
16	S	0.43	0/952	0.60	0/1266
17	T	0.44	0/775	0.54	0/1045
18	U	0.40	0/833	0.61	0/1127
19	V	0.41	0/728	0.53	0/977
20	W	0.36	0/727	0.51	0/976
21	Y	0.42	0/578	0.61	0/770
22	Z	0.39	0/455	0.64	0/604
23	1	0.34	0/484	0.58	0/646
24	2	0.37	0/436	0.58	0/585
25	3	0.24	0/291	0.45	0/404
26	4	0.40	0/433	0.63	0/577
27	5	0.36	0/394	0.60	0/529
28	6	0.41	0/368	0.74	0/479
29	7	0.37	0/519	0.64	0/675
30	8	0.39	0/295	0.55	0/387
All	All	0.71	0/98742	0.82	27/148283 (0.0%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	557	G	O4'-C1'-N9	8.95	115.36	108.20
2	A	1357	U	C2-N1-C1'	7.41	126.60	117.70
2	A	231	A	O4'-C1'-N9	7.22	113.98	108.20
2	A	1067	A	C2-N3-C4	-6.64	107.28	110.60
2	A	1332	U	N3-C2-O2	-6.60	117.58	122.20
2	A	554	C	C2-N1-C1'	6.46	125.91	118.80
2	A	308	U	C2-N1-C1'	6.40	125.38	117.70
2	A	1700	G	O4'-C1'-N9	6.31	113.25	108.20
2	A	1072	A	O4'-C1'-N9	6.05	113.04	108.20
2	A	1358	C	C2-N1-C1'	5.68	125.04	118.80
2	A	2922	G	C4-N9-C1'	5.67	133.87	126.50
2	A	554	C	N1-C2-O2	5.50	122.20	118.90
2	A	2922	G	N7-C8-N9	5.48	115.84	113.10
2	A	1030	G	O4'-C1'-N9	5.44	112.55	108.20
2	A	750	G	O4'-C1'-N9	5.41	112.53	108.20
2	A	592	A	N1-C6-N6	-5.39	115.37	118.60
2	A	2789	U	P-O3'-C3'	5.38	126.16	119.70
2	A	2809	A	P-O3'-C3'	5.25	126.00	119.70
2	A	2472	A	P-O3'-C3'	5.24	125.98	119.70
2	A	2877	G	O4'-C1'-N9	5.21	112.36	108.20
2	A	2126	G	O4'-C1'-N9	5.13	112.31	108.20
13	P	134	LEU	CA-CB-CG	5.12	127.08	115.30
2	A	809	G	C8-N9-C4	-5.09	104.36	106.40
2	A	527	G	O4'-C1'-N9	5.08	112.26	108.20
2	A	2068	G	O4'-C1'-N9	5.05	112.24	108.20
2	A	554	C	C6-N1-C1'	-5.05	114.75	120.80
6	E	114	LEU	CA-CB-CG	5.01	126.82	115.30

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	v	3294	0	3305	0	0
2	A	62168	0	31257	331	0
3	B	2428	0	1229	15	0
4	C	2108	0	2184	23	0
5	D	1583	0	1646	20	0
6	E	1539	0	1624	16	0
7	F	1171	0	1041	31	0
8	G	1355	0	1403	24	0
9	L	1117	0	1145	8	0
10	M	925	0	982	12	0
11	N	1057	0	1073	9	0
12	O	1045	0	1103	8	0
13	P	957	0	993	5	0
14	Q	913	0	939	12	0
15	R	802	0	836	7	0
16	S	939	0	1011	9	0
17	T	762	0	779	4	0
18	U	823	0	861	13	0
19	V	720	0	743	4	0
20	W	719	0	744	11	0
21	Y	571	0	570	5	0
22	Z	450	0	476	6	0
23	1	483	0	500	4	0
24	2	433	0	479	3	0
25	3	292	0	119	2	0
26	4	425	0	423	2	0
27	5	390	0	395	5	0
28	6	365	0	417	5	0
29	7	512	0	562	3	0
30	8	292	0	334	5	0
31	v	32	0	14	0	0
32	6	1	0	0	0	0
32	A	192	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	M	1	0	0	0	0
32	N	1	0	0	0	0
32	V	1	0	0	0	0
32	Z	1	0	0	0	0
33	O	1	0	0	0	0
34	4	1	0	0	0	0
34	5	1	0	0	0	0
34	8	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	4	1	0	0	0	0
35	8	1	0	0	0	0
35	A	130	0	0	0	0
35	N	1	0	0	0	0
35	P	1	0	0	0	0
All	All	91008	0	59187	533	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 4.

All (533) 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)
2:A:2141:U:H3	2:A:2214:G:H1	1.10	0.96
20:W:9:VAL:HG13	20:W:68:VAL:HG13	1.50	0.93
2:A:2263:G:H1'	22:Z:32:ASN:HB3	1.50	0.91
2:A:2173:G:H1	2:A:2184:U:H3	0.89	0.88
2:A:2134:G:H1	2:A:2221:U:H3	1.26	0.83
2:A:2125:G:H4'	2:A:2126:G:H5'	1.62	0.82
19:V:33:ALA:O	19:V:76:ARG:NH1	2.14	0.81
14:Q:63:PHE:HB3	14:Q:75:LYS:HD2	1.66	0.78
2:A:2345:U:O2	7:F:37:ASN:ND2	2.17	0.78
2:A:1579:A:N6	2:A:1595:G:O2'	2.17	0.77
2:A:2167:A:H2	2:A:2192:G:H1'	1.50	0.76
2:A:665:G:H4'	2:A:666:A:H5'	1.68	0.76
2:A:1151:U:H2'	2:A:1152:G:H8	1.50	0.75
2:A:84:A:N6	2:A:101:G:O2'	2.20	0.74
2:A:905:G:OP2	21:Y:85:LYS:NZ	2.20	0.74
2:A:211:C:OP1	28:6:29:ARG:NH2	2.22	0.73
2:A:648:G:O6	11:N:103:ARG:NH2	2.21	0.72
2:A:2154:G:OP1	2:A:2203:G:N2	2.23	0.72
2:A:2471:U:O3'	2:A:2472:A:H3'	1.90	0.72
2:A:1886:A:H2'	2:A:1887:A:C8	2.26	0.71
27:5:31:GLU:OE2	27:5:46:ARG:NH1	2.24	0.71
8:G:80:SER:OG	8:G:81:GLU:OE1	2.07	0.71
2:A:2338:A:N6	7:F:38:THR:O	2.24	0.70
2:A:1148:C:H2'	2:A:1149:A:H8	1.57	0.70
22:Z:6:VAL:HG23	22:Z:7:ILE:HD12	1.72	0.69
22:Z:7:ILE:HG22	22:Z:8:THR:HG23	1.73	0.69
2:A:676:A:OP2	29:7:15:LYS:NZ	2.25	0.69
2:A:2545:C:H5"	5:D:128:GLN:OE1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:14:THR:H	18:U:107:HIS:HD2	1.39	0.68
20:W:33:VAL:HG23	20:W:65:VAL:HG22	1.75	0.68
2:A:90:A:H4'	2:A:91:C:H5'	1.75	0.67
2:A:1151:U:H2'	2:A:1152:G:C8	2.30	0.67
8:G:43:ILE:HG13	8:G:52:VAL:HG12	1.77	0.67
23:1:11:THR:HB	23:1:60:ARG:HH11	1.59	0.67
4:C:131:GLU:OE1	4:C:133:LYS:NZ	2.28	0.67
11:N:55:LEU:HD23	11:N:60:ARG:HG2	1.77	0.67
3:B:29:C:H1'	3:B:52:G:H1	1.59	0.67
3:B:3:U:OP1	3:B:59:U:O2'	2.12	0.66
2:A:2361:A:H2'	2:A:2362:A:C8	2.30	0.66
9:L:18:VAL:HG23	9:L:138:PRO:HB2	1.76	0.66
2:A:1833:C:OP2	4:C:182:ARG:NH2	2.29	0.66
2:A:27:G:H1'	2:A:558:A:N6	2.11	0.66
2:A:2337:G:N2	7:F:153:ASP:OD2	2.24	0.66
6:E:49:HIS:HD2	6:E:92:PRO:HB2	1.60	0.66
2:A:1129:G:H21	2:A:1131:A:H8	1.43	0.65
10:M:64:ARG:NH1	10:M:81:GLU:OE2	2.28	0.65
2:A:220:G:H22	2:A:237:U:H4'	1.60	0.65
2:A:2184:U:H2'	2:A:2185:A:H8	1.61	0.65
12:O:64:VAL:HG22	12:O:106:ILE:HG22	1.79	0.65
2:A:2235:C:O2'	2:A:2237:C:OP1	2.14	0.64
2:A:1065:U:HO2'	2:A:1067:A:H2	1.44	0.64
4:C:10:THR:HG22	4:C:12:GLY:H	1.62	0.64
2:A:1530:G:H3'	2:A:1531:U:H5"	1.80	0.64
2:A:1248:A:H2'	2:A:1249:A:C8	2.33	0.64
2:A:2789:U:OP2	30:8:19:ARG:NH1	2.24	0.64
5:D:50:GLN:HE21	5:D:80:ILE:HG21	1.63	0.64
2:A:1131:A:HO2'	2:A:1150:C:HO2'	1.43	0.63
2:A:2173:G:O6	2:A:2184:U:O4	2.15	0.63
2:A:891:U:O2'	2:A:893:A:OP2	2.16	0.63
2:A:2141:U:O2	2:A:2214:G:N2	2.31	0.62
2:A:2341:G:H1	2:A:2344:A:H62	1.45	0.62
2:A:2408:G:H2'	2:A:2410:A:H2	1.65	0.62
2:A:579:U:O2'	16:S:49:ASP:OD2	2.15	0.62
2:A:2410:A:O2'	14:Q:119:PHE:O	2.15	0.62
2:A:1549:G:N2	4:C:98:ASP:O	2.28	0.61
2:A:798:A:H3'	28:6:1:MET:HE1	1.81	0.61
3:B:27:A:H2'	3:B:28:C:C6	2.35	0.61
2:A:1620:G:H4'	4:C:59:LYS:HG3	1.83	0.61
27:5:31:GLU:HG2	27:5:46:ARG:HG3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:498:G:C8	6:E:58:ARG:HD3	2.35	0.61
2:A:1539:A:H2'	4:C:98:ASP:OD2	2.01	0.61
10:M:50:GLY:O	10:M:53:LYS:NZ	2.26	0.61
8:G:40:GLU:HG2	8:G:61:HIS:HE1	1.65	0.60
2:A:1532:G:N2	2:A:1560:A:N1	2.49	0.60
2:A:591:A:H4'	2:A:592:A:H5'	1.83	0.60
6:E:8:LYS:HG3	6:E:14:ALA:HB2	1.83	0.60
11:N:102:ILE:HD13	11:N:109:ILE:HD12	1.84	0.60
2:A:1093:G:N2	2:A:1156:G:O2'	2.34	0.60
2:A:1213:A:H2'	2:A:1214:A:C8	2.37	0.59
2:A:2163:G:O2'	2:A:2191:A:N1	2.35	0.59
2:A:1835:A:H2'	2:A:1836:A:C8	2.37	0.59
7:F:164:GLU:O	7:F:168:GLU:HG3	2.02	0.59
6:E:49:HIS:CD2	6:E:92:PRO:HB2	2.38	0.59
26:4:24:LEU:HD12	26:4:25:PRO:HD2	1.84	0.59
2:A:6:A:O2'	9:L:136:GLN:NE2	2.35	0.59
7:F:61:THR:HG21	7:F:89:VAL:HG11	1.84	0.59
2:A:1141:A:O2'	2:A:1142:A:H8	1.85	0.59
7:F:77:PHE:O	7:F:78:ARG:HD3	2.03	0.59
2:A:2789:U:H5	2:A:2791:A:N7	2.01	0.58
2:A:1135:G:N2	2:A:1136:U:O4	2.32	0.58
20:W:1:MET:SD	20:W:65:VAL:HG21	2.42	0.58
2:A:2716:C:OP1	15:R:51:ARG:NH2	2.29	0.58
2:A:2168:G:H3'	2:A:2169:A:H8	1.69	0.58
29:7:54:ASP:OD1	29:7:57:ARG:NH2	2.37	0.58
2:A:1532:G:HO2'	2:A:1533:A:H8	1.50	0.58
2:A:2208:U:H2'	2:A:2209:A:H8	1.69	0.58
2:A:2125:G:H4'	2:A:2126:G:C5'	2.34	0.58
2:A:2152:A:H2	2:A:2204:A:H5'	1.68	0.58
2:A:1311:G:H5"	18:U:20:ARG:HH22	1.68	0.58
2:A:789:A:O2'	2:A:1708:U:OP1	2.22	0.58
2:A:2438:G:O2'	2:A:2439:C:OP2	2.22	0.58
12:O:54:MET:HB3	12:O:121:ALA:HB2	1.86	0.57
2:A:304:A:H62	2:A:410:G:N2	2.01	0.57
7:F:48:LYS:O	7:F:52:SER:HB3	2.04	0.57
2:A:1532:G:O2'	2:A:1533:A:H8	1.87	0.57
2:A:2319:A:H4'	2:A:2320:A:O4'	2.04	0.57
2:A:1067:A:H62	2:A:1187:U:H3	1.51	0.57
18:U:55:VAL:HG12	18:U:110:VAL:HG12	1.87	0.57
2:A:125:A:H5"	28:6:19:ARG:HG3	1.87	0.56
8:G:46:GLU:OE1	8:G:47:GLY:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1465:A:H8	2:A:1636:G:H21	1.51	0.56
5:D:123:ILE:HD11	5:D:141:ARG:CZ	2.35	0.56
7:F:175:MET:SD	7:F:176:PRO:HD2	2.45	0.56
14:Q:78:GLU:HG2	14:Q:82:LYS:HE2	1.87	0.56
2:A:1456:A:H2'	2:A:1457:A:C8	2.40	0.56
7:F:31:ILE:HA	7:F:158:THR:HG22	1.87	0.56
12:O:32:TYR:OH	12:O:111:GLU:OE2	2.23	0.56
15:R:49:LYS:HB2	15:R:96:LYS:HD3	1.88	0.56
16:S:43:TYR:HB3	17:T:74:TYR:HB3	1.87	0.56
6:E:155:VAL:HB	6:E:194:ILE:HD12	1.87	0.56
8:G:8:THR:HG22	8:G:51:ASN:HD21	1.69	0.56
2:A:304:A:H62	2:A:410:G:H21	1.52	0.56
2:A:1763:U:O2'	2:A:1764:A:H8	1.88	0.56
9:L:4:THR:HG21	16:S:57:PHE:HE1	1.69	0.56
2:A:1140:U:H2'	2:A:1141:A:H2'	1.87	0.56
2:A:2380:C:OP1	27:5:34:LYS:NZ	2.39	0.56
2:A:2822:C:H2'	2:A:2823:A:C8	2.41	0.56
2:A:760:U:O2'	2:A:762:A:N6	2.39	0.55
2:A:1128:U:H2'	2:A:1129:G:O4'	2.06	0.55
7:F:132:VAL:O	7:F:151:GLY:CA	2.53	0.55
2:A:897:G:H21	24:2:46:MET:CE	2.20	0.55
30:8:12:GLU:N	30:8:12:GLU:OE1	2.37	0.55
2:A:27:G:HO2'	2:A:28:A:H8	1.51	0.55
7:F:157:VAL:HB	14:Q:2:ILE:HD11	1.88	0.55
2:A:2155:U:H2'	2:A:2156:A:C8	2.41	0.55
2:A:2177:G:O2'	2:A:2180:A:N6	2.40	0.55
2:A:2201:G:H22	2:A:2204:A:P	2.29	0.55
2:A:1460:G:O2'	2:A:1635:A:N1	2.32	0.54
10:M:13:ASN:ND2	10:M:96:THR:OG1	2.41	0.54
2:A:579:U:H2'	2:A:580:U:C6	2.42	0.54
2:A:92:G:H2'	2:A:93:U:C6	2.42	0.54
4:C:133:LYS:HB3	4:C:186:ALA:HB1	1.89	0.54
5:D:19:ASN:O	15:R:80:ARG:NH2	2.28	0.54
7:F:34:ILE:HG12	7:F:156:ILE:HD13	1.90	0.54
16:S:102:ASP:OD1	17:T:2:TYR:OH	2.24	0.54
2:A:139:A:H2'	2:A:140:G:C8	2.42	0.54
2:A:2438:G:HO2'	2:A:2439:C:P	2.30	0.54
2:A:2832:G:H2'	2:A:2833:A:H8	1.72	0.54
2:A:1245:U:H1'	16:S:4:VAL:HG22	1.89	0.54
20:W:79:THR:HG22	20:W:96:LYS:HD3	1.90	0.54
2:A:288:U:O2'	2:A:289:U:O5'	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1046:A:H2'	2:A:1047:A:C8	2.43	0.54
2:A:2196:A:OP1	2:A:2204:A:O2'	2.26	0.54
2:A:842:U:H2'	2:A:843:U:C6	2.43	0.53
2:A:2184:U:H2'	2:A:2185:A:C8	2.42	0.53
4:C:34:LEU:HD12	4:C:61:GLN:HG2	1.89	0.53
9:L:126:TYR:OH	9:L:133:HIS:NE2	2.39	0.53
4:C:61:GLN:O	4:C:63:ARG:NH1	2.41	0.53
8:G:40:GLU:HG2	8:G:61:HIS:CE1	2.43	0.53
2:A:258:A:H2'	2:A:259:A:C8	2.43	0.53
2:A:859:U:H2'	2:A:860:C:C6	2.43	0.53
2:A:2670:U:H2'	2:A:2671:G:O4'	2.08	0.53
2:A:2199:G:N2	2:A:2204:A:H62	2.05	0.53
7:F:132:VAL:O	7:F:151:GLY:HA2	2.08	0.53
2:A:344:C:H1'	20:W:12:ILE:HD12	1.91	0.53
2:A:2201:G:N2	2:A:2204:A:O5'	2.36	0.53
18:U:16:ARG:HH21	18:U:103:LYS:HD2	1.73	0.53
9:L:88:ARG:HD3	9:L:93:MET:HE2	1.90	0.53
12:O:42:ILE:HD12	12:O:97:VAL:HG21	1.91	0.53
2:A:2148:G:O2'	2:A:2199:G:N2	2.40	0.53
2:A:828:A:C2	4:C:225:MET:HG2	2.44	0.53
4:C:168:GLU:OE2	4:C:171:TYR:HB2	2.10	0.52
5:D:39:LYS:O	5:D:47:GLU:HA	2.09	0.52
2:A:193:A:H2'	2:A:194:C:C6	2.44	0.52
2:A:2199:G:H22	2:A:2204:A:H62	1.56	0.52
2:A:2324:U:H2'	2:A:2325:U:C6	2.45	0.52
2:A:2822:C:H1'	2:A:2920:A:H2	1.73	0.52
17:T:14:VAL:HG23	17:T:97:ILE:HG13	1.92	0.52
2:A:1102:G:H5"	2:A:1103:A:H5'	1.91	0.52
3:B:29:C:O2'	3:B:52:G:N2	2.42	0.52
2:A:1787:C:H5	15:R:94:ARG:NH2	2.08	0.52
2:A:2276:U:H2'	2:A:2277:U:C6	2.45	0.52
5:D:122:VAL:HB	5:D:128:GLN:HG3	1.91	0.52
2:A:2166:G:N2	2:A:2190:G:O2'	2.43	0.52
2:A:2324:U:OP1	2:A:2413:U:O2'	2.24	0.51
6:E:101:LEU:HB2	6:E:102:PRO:HD2	1.91	0.51
8:G:154:PRO:HG3	8:G:163:ARG:HB3	1.92	0.51
2:A:1764:A:H2'	2:A:1765:G:O4'	2.10	0.51
2:A:2346:C:H2'	2:A:2347:A:H8	1.75	0.51
14:Q:106:LYS:NZ	14:Q:110:GLU:OE2	2.30	0.51
15:R:24:ASP:HB2	15:R:88:ARG:O	2.09	0.51
2:A:1127:U:H2'	2:A:1128:U:C6	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:304:A:N6	2:A:410:G:H21	2.08	0.51
2:A:1187:U:H4’	2:A:1188:A:O4’	2.10	0.51
2:A:1922:A:H2’	2:A:1923:A:C8	2.45	0.51
12:O:35:GLN:HE21	12:O:100:GLY:HA2	1.75	0.51
2:A:45:G:H5’	2:A:46:C:OP1	2.10	0.50
2:A:2827:C:H3’	2:A:2828:U:H5”	1.93	0.50
2:A:1248:A:H5’	6:E:41:ARG:HH22	1.77	0.50
2:A:2500:C:H2’	2:A:2501:A:O4’	2.11	0.50
2:A:1172:A:H4’	2:A:1173:A:H5”	1.93	0.50
10:M:4:GLN:HG2	10:M:5:GLU:HG2	1.92	0.50
2:A:624:C:H5’	16:S:31:LEU:HD22	1.93	0.50
7:F:64:LYS:NZ	25:3:5:ILE:O	2.31	0.50
8:G:38:ASN:HD21	8:G:64:LEU:HD13	1.76	0.50
20:W:85:VAL:HA	20:W:90:LYS:HA	1.94	0.50
2:A:27:G:O2’	2:A:28:A:H8	1.93	0.50
2:A:2134:G:H2’	2:A:2135:U:C6	2.47	0.50
2:A:2463:A:H2’	2:A:2463:A:N3	2.26	0.50
2:A:2842:U:H2’	2:A:2843:C:H6	1.76	0.50
2:A:101:G:HO2’	2:A:102:A:H8	1.60	0.50
2:A:2045:G:OP1	18:U:16:ARG:NH2	2.39	0.50
2:A:2043:G:H5”	18:U:47:SER:HB3	1.93	0.50
2:A:684:U:H2’	2:A:685:C:C6	2.47	0.49
2:A:1685:U:H2’	2:A:1686:C:C6	2.47	0.49
2:A:1812:U:H5	2:A:1817:A:N7	2.10	0.49
2:A:2167:A:H2’	2:A:2168:G:H8	1.77	0.49
4:C:37:LEU:HG	4:C:62:TYR:HB2	1.93	0.49
2:A:2546:G:H2’	2:A:2547:U:C6	2.47	0.49
2:A:2789:U:O2’	2:A:2790:A:OP2	2.23	0.49
2:A:746:G:O2’	2:A:1681:A:N3	2.38	0.49
2:A:1065:U:O2’	2:A:1067:A:H2	1.95	0.49
2:A:1483:A:H2’	2:A:1484:A:C8	2.47	0.49
2:A:2:G:H2’	2:A:3:U:C6	2.47	0.49
2:A:290:C:H2’	2:A:291:U:C6	2.48	0.49
2:A:1247:U:O2’	6:E:41:ARG:NH2	2.46	0.49
2:A:1829:U:H2’	2:A:1830:C:C6	2.48	0.49
7:F:63:GLN:HE21	7:F:89:VAL:HG13	1.77	0.49
2:A:2208:U:H2’	2:A:2209:A:C8	2.48	0.49
12:O:17:MET:CE	12:O:41:TRP:HD1	2.26	0.49
17:T:1:MET:HA	17:T:42:GLY:O	2.13	0.49
2:A:2097:C:H2’	2:A:2098:C:C6	2.47	0.48
2:A:2506:U:HO2’	2:A:2507:C:P	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2832:G:H2'	2:A:2833:A:C8	2.48	0.48
2:A:407:G:H2'	2:A:408:U:C6	2.48	0.48
2:A:1519:A:H62	2:A:1573:A:H2	1.61	0.48
5:D:146:MET:HA	5:D:158:LYS:HE3	1.94	0.48
11:N:117:ILE:HD11	11:N:136:ILE:HA	1.95	0.48
7:F:41:GLY:HA2	7:F:85:ILE:HD11	1.96	0.48
2:A:229:A:O4'	2:A:231:A:N6	2.46	0.48
2:A:1700:G:O2'	2:A:1701:A:C8	2.66	0.48
2:A:1700:G:O2'	2:A:1701:A:H8	1.97	0.48
2:A:631:U:H2'	2:A:632:U:C6	2.49	0.48
3:B:46:A:H2'	3:B:47:C:H6	1.78	0.48
19:V:2:ASP:N	19:V:2:ASP:OD1	2.45	0.48
2:A:903:G:H2'	2:A:904:A:C8	2.48	0.48
2:A:2624:C:H2'	2:A:2625:G:C8	2.48	0.48
2:A:2671:G:O2'	2:A:2672:A:H8	1.97	0.48
3:B:30:C:N3	3:B:49:G:N1	2.62	0.48
2:A:373:A:H2	2:A:1255:G:HO2'	1.62	0.48
2:A:2348:U:H2'	2:A:2349:U:C6	2.49	0.48
2:A:1469:A:H2'	2:A:1471:G:N7	2.28	0.48
7:F:29:PRO:HG3	7:F:165:GLU:HB3	1.95	0.48
7:F:53:ALA:HA	7:F:56:GLU:OE2	2.14	0.48
14:Q:49:ASN:HB2	14:Q:51:VAL:HG22	1.96	0.48
2:A:760:U:H1'	2:A:763:U:H5	1.78	0.47
2:A:1897:U:OP1	2:A:2443:G:O2'	2.28	0.47
2:A:632:U:H2'	2:A:633:A:C8	2.49	0.47
2:A:1452:U:H2'	2:A:1453:G:C8	2.49	0.47
2:A:1944:U:H2'	2:A:1945:A:H5'	1.96	0.47
8:G:80:SER:HG	8:G:81:GLU:CD	2.16	0.47
2:A:1546:U:H5"	2:A:1547:C:H5	1.80	0.47
5:D:8:ARG:NH1	5:D:197:LYS:O	2.48	0.47
2:A:897:G:H21	24:2:46:MET:HE2	1.80	0.47
2:A:1105:G:H3'	2:A:1106:U:H2'	1.97	0.47
2:A:2107:U:H2'	2:A:2108:U:C6	2.50	0.47
2:A:2335:U:O2'	7:F:123:ASP:O	2.32	0.47
3:B:35:C:O2	14:Q:102:HIS:HE1	1.96	0.47
2:A:1482:G:H2'	2:A:1483:A:C8	2.50	0.47
2:A:2155:U:H2'	2:A:2156:A:H8	1.78	0.47
2:A:2104:A:H2'	2:A:2105:G:C8	2.50	0.47
2:A:2365:C:OP1	21:Y:84:LYS:NZ	2.48	0.47
9:L:4:THR:HG21	16:S:57:PHE:CE1	2.49	0.47
11:N:55:LEU:O	11:N:60:ARG:NH1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:125:A:O2'	2:A:126:A:C8	2.67	0.47
2:A:809:G:O2'	2:A:810:A:OP1	2.32	0.47
4:C:53:HIS:HA	4:C:217:ARG:HB2	1.95	0.47
4:C:248:SER:HB3	4:C:254:THR:CG2	2.44	0.47
10:M:88:ARG:NH1	10:M:93:PRO:O	2.48	0.47
2:A:287:C:H2'	2:A:288:U:C6	2.50	0.47
2:A:2362:A:H2'	2:A:2363:G:C8	2.50	0.47
18:U:23:ARG:HA	18:U:26:ILE:HG22	1.97	0.47
2:A:2167:A:C2	2:A:2192:G:H1'	2.39	0.47
2:A:2225:C:H2'	2:A:2226:A:H8	1.80	0.47
2:A:2261:G:H22	22:Z:34:GLN:HE22	1.62	0.47
7:F:34:ILE:HD12	7:F:96:MET:HG3	1.96	0.47
8:G:9:ILE:HB	8:G:50:ILE:HB	1.97	0.47
18:U:87:LEU:HB2	18:U:103:LYS:HB2	1.96	0.47
27:5:40:ARG:HG3	27:5:40:ARG:HH11	1.80	0.47
2:A:290:C:H2'	2:A:291:U:H6	1.79	0.46
2:A:1902:U:H2'	2:A:1903:U:H2'	1.96	0.46
2:A:2344:A:N3	7:F:79:LEU:HD11	2.29	0.46
4:C:67:PHE:HE1	4:C:105:ILE:HD11	1.81	0.46
13:P:116:ILE:HG23	13:P:130:VAL:HG21	1.97	0.46
2:A:185:C:H2'	2:A:186:C:H5'	1.96	0.46
2:A:1545:A:H2'	2:A:1547:C:C5	2.50	0.46
2:A:1077:G:H21	30:8:36:GLN:HE22	1.62	0.46
2:A:2925:U:H2'	2:A:2926:U:C6	2.51	0.46
2:A:291:U:H2'	2:A:292:U:C6	2.51	0.46
2:A:993:A:H2'	2:A:994:C:C6	2.50	0.46
2:A:1433:G:H2'	2:A:1434:U:O4'	2.15	0.46
2:A:2304:G:OP1	21:Y:26:SER:HB3	2.16	0.46
2:A:288:U:HO2'	2:A:289:U:H6	1.62	0.46
2:A:651:A:H2'	2:A:652:A:C8	2.50	0.46
2:A:720:G:H1'	6:E:74:ARG:HD3	1.98	0.46
2:A:329:A:H2'	2:A:330:A:C8	2.51	0.46
2:A:1319:A:H4'	2:A:1320:G:OP1	2.14	0.46
16:S:12:LYS:HE3	16:S:12:LYS:HB2	1.70	0.46
20:W:70:LEU:O	20:W:78:PRO:HA	2.16	0.46
2:A:1946:A:N6	2:A:1949:A:N7	2.63	0.46
2:A:2144:U:O4	2:A:2177:G:O2'	2.31	0.46
2:A:2921:G:H8	2:A:2921:G:OP2	1.99	0.46
5:D:123:ILE:HG22	5:D:128:GLN:HB2	1.97	0.46
23:1:10:SER:O	23:1:12:THR:N	2.49	0.46
2:A:1213:A:H2'	2:A:1214:A:H8	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2221:U:H2'	2:A:2222:G:H8	1.81	0.46
2:A:2348:U:H2'	2:A:2349:U:H6	1.81	0.46
8:G:164:TYR:HB2	8:G:167:GLU:HG3	1.97	0.46
18:U:51:ILE:O	18:U:55:VAL:HG23	2.15	0.46
2:A:957:A:H2'	2:A:958:A:C8	2.51	0.46
2:A:2226:A:H2'	2:A:2227:U:C6	2.50	0.46
22:Z:12:SER:HA	22:Z:29:TRP:O	2.16	0.46
2:A:1148:C:H2'	2:A:1149:A:C8	2.46	0.45
2:A:2186:C:H2'	2:A:2187:G:H8	1.81	0.45
2:A:1249:A:N3	11:N:4:HIS:HB3	2.32	0.45
2:A:2200:U:H2'	2:A:2201:G:O4'	2.16	0.45
6:E:13:ASN:OD1	6:E:14:ALA:N	2.49	0.45
8:G:46:GLU:OE2	8:G:49:GLU:N	2.49	0.45
10:M:120:GLU:OE1	15:R:65:SER:OG	2.24	0.45
23:1:13:GLU:O	23:1:17:GLN:HG2	2.16	0.45
24:2:37:LYS:HB3	24:2:43:ILE:HD13	1.98	0.45
5:D:50:GLN:HE21	5:D:80:ILE:CG2	2.29	0.45
5:D:122:VAL:HG21	5:D:143:PRO:HA	1.98	0.45
2:A:1108:G:H2'	2:A:1109:G:H8	1.82	0.45
2:A:1829:U:H2'	2:A:1830:C:H6	1.81	0.45
2:A:2587:U:H2'	2:A:2588:U:C6	2.52	0.45
14:Q:112:ALA:HB1	14:Q:117:LEU:HD12	1.98	0.45
2:A:873:U:O2'	2:A:2101:U:C2	2.70	0.45
2:A:911:G:H2'	2:A:912:C:C6	2.51	0.45
2:A:1551:U:H2'	2:A:1552:U:C6	2.51	0.45
18:U:29:ILE:HG23	18:U:37:ALA:HB1	1.99	0.45
4:C:66:ASP:OD2	4:C:102:ARG:HD3	2.17	0.45
2:A:2148:G:H2'	2:A:2150:A:C8	2.51	0.45
2:A:2921:G:H4'	2:A:2922:G:H8	1.82	0.45
29:7:8:ARG:HD2	29:7:8:ARG:HA	1.83	0.45
2:A:1115:A:H4'	2:A:1116:A:H5"	1.99	0.45
10:M:90:ASP:OD1	10:M:90:ASP:N	2.50	0.45
14:Q:11:ARG:HD2	14:Q:99:TYR:CZ	2.52	0.45
19:V:17:THR:HA	19:V:20:LEU:HD12	1.98	0.45
2:A:1537:G:H2'	2:A:1538:U:C6	2.52	0.45
2:A:2217:U:C2	2:A:2218:G:C8	3.05	0.45
7:F:33:LYS:HA	7:F:96:MET:SD	2.56	0.45
7:F:52:SER:OG	7:F:53:ALA:N	2.49	0.45
8:G:54:ARG:HB2	8:G:65:HIS:ND1	2.31	0.45
8:G:88:GLU:OE2	8:G:165:GLU:HG3	2.17	0.45
2:A:448:A:H2'	2:A:449:U:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1043:G:OP1	16:S:92:ARG:HG2	2.16	0.45
2:A:1544:A:H2'	2:A:1545:A:C8	2.52	0.45
2:A:1903:U:O2'	2:A:1904:C:H5"	2.17	0.45
20:W:40:MET:SD	20:W:60:GLU:HG2	2.56	0.45
2:A:1019:A:OP1	2:A:1019:A:H8	2.00	0.44
2:A:1508:A:H4'	2:A:1509:A:O5'	2.16	0.44
2:A:1716:G:O2'	2:A:2024:U:O4	2.24	0.44
2:A:625:G:H2'	2:A:626:G:C8	2.51	0.44
2:A:2336:G:O6	2:A:2347:A:N6	2.50	0.44
3:B:46:A:H2'	3:B:47:C:C6	2.52	0.44
4:C:29:PRO:HB2	4:C:34:LEU:HD21	1.98	0.44
5:D:21:GLU:OE1	10:M:72:GLN:HG3	2.17	0.44
2:A:349:U:H2'	2:A:350:G:O4'	2.18	0.44
5:D:109:ASP:OD1	5:D:172:GLN:HA	2.18	0.44
2:A:258:A:H2'	2:A:259:A:H8	1.81	0.44
2:A:280:A:H2'	2:A:281:A:C8	2.52	0.44
2:A:2360:A:H2'	2:A:2361:A:C8	2.52	0.44
3:B:21:G:H2'	3:B:22:G:C8	2.52	0.44
2:A:199:A:N6	2:A:2463:A:O2'	2.49	0.44
2:A:351:G:H2'	2:A:352:A:C8	2.52	0.44
2:A:2214:G:H2'	2:A:2215:G:H8	1.83	0.44
2:A:2217:U:H2'	2:A:2218:G:C8	2.53	0.44
2:A:2570:U:H2'	2:A:2571:C:C6	2.51	0.44
5:D:130:ARG:HB2	5:D:140:HIS:O	2.17	0.44
10:M:64:ARG:HG2	10:M:83:ALA:HB3	1.99	0.44
2:A:291:U:H2'	2:A:292:U:H6	1.83	0.44
2:A:749:U:H2'	2:A:750:G:O4'	2.18	0.44
2:A:1497:G:O2'	2:A:1596:A:N3	2.49	0.44
2:A:1698:G:O2'	13:P:125:ASP:OD2	2.21	0.44
2:A:398:C:H2'	2:A:399:C:O4'	2.17	0.44
2:A:904:A:H2'	2:A:905:G:O4'	2.17	0.44
2:A:2146:C:C2	2:A:2147:A:C8	3.05	0.44
2:A:597:U:H2'	2:A:598:G:O4'	2.17	0.44
12:O:34:LEU:HD22	12:O:129:THR:HB	2.00	0.44
9:L:115:LEU:O	9:L:119:LEU:HG	2.17	0.44
20:W:32:ARG:HD3	20:W:64:HIS:HA	1.99	0.44
2:A:703:U:H2'	2:A:704:A:C8	2.52	0.43
2:A:2070:A:H2'	2:A:2071:G:C8	2.53	0.43
2:A:2632:G:C8	4:C:236:GLU:HG2	2.53	0.43
4:C:27:SER:O	4:C:27:SER:OG	2.31	0.43
2:A:831:U:H2'	2:A:832:C:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:950:U:H2'	2:A:951:C:H6	1.82	0.43
2:A:1074:A:H2'	2:A:1075:A:C8	2.52	0.43
2:A:1456:A:H2'	2:A:1457:A:H8	1.81	0.43
2:A:1579:A:H62	2:A:1595:G:HO2'	1.60	0.43
2:A:2915:G:H2'	2:A:2916:A:O4'	2.17	0.43
8:G:55:PRO:HD2	8:G:61:HIS:NE2	2.33	0.43
2:A:339:U:H2'	2:A:340:G:O4'	2.19	0.43
2:A:364:A:H5"	6:E:136:THR:HG23	2.00	0.43
2:A:2922:G:H2'	2:A:2922:G:N3	2.34	0.43
3:B:13:G:OP2	3:B:67:G:N2	2.51	0.43
14:Q:67:GLU:HB2	14:Q:71:ASP:OD2	2.19	0.43
2:A:91:C:H2'	2:A:92:G:O4'	2.18	0.43
2:A:2215:G:H2'	2:A:2216:C:H6	1.82	0.43
3:B:41:C:OP1	25:3:2:LYS:N	2.52	0.43
7:F:51:ASP:O	7:F:55:GLU:OE1	2.37	0.43
8:G:86:LYS:HG2	8:G:132:ILE:HG12	1.99	0.43
2:A:759:G:H2'	2:A:760:U:C6	2.53	0.43
5:D:126:HIS:CD2	5:D:159:LEU:HB3	2.52	0.43
2:A:1130:A:H1'	2:A:1151:U:O2'	2.18	0.43
2:A:1248:A:O4'	6:E:41:ARG:NH2	2.52	0.43
8:G:56:THR:H	8:G:61:HIS:CD2	2.37	0.43
13:P:118:LYS:HA	13:P:130:VAL:HG23	1.99	0.43
2:A:27:G:O2'	2:A:28:A:O5'	2.35	0.43
2:A:271:C:O2	2:A:271:C:H2'	2.18	0.43
2:A:2306:A:H2'	2:A:2307:A:C8	2.54	0.43
3:B:40:C:O2	7:F:90:THR:HG22	2.19	0.43
7:F:52:SER:HA	7:F:55:GLU:OE1	2.18	0.43
2:A:220:G:N2	2:A:237:U:H4'	2.32	0.43
2:A:1401:C:H2'	2:A:1402:G:O4'	2.19	0.43
8:G:44:ASN:OD1	8:G:51:ASN:N	2.48	0.43
2:A:525:A:N3	2:A:527:G:H5"	2.34	0.43
2:A:638:U:H2'	2:A:639:U:C6	2.54	0.43
2:A:1823:C:H2'	2:A:1824:A:C5	2.54	0.43
2:A:2412:G:H2'	2:A:2413:U:C6	2.54	0.43
2:A:2176:C:H2'	2:A:2177:G:O4'	2.19	0.43
3:B:110:G:H2'	3:B:111:C:C6	2.54	0.43
14:Q:79:LEU:O	14:Q:83:ARG:HG3	2.19	0.43
28:6:8:SER:HB3	28:6:11:LYS:HB2	2.00	0.43
18:U:69:LEU:HD22	18:U:114:GLU:OE2	2.19	0.42
28:6:24:THR:O	28:6:28:ARG:HG3	2.18	0.42
2:A:688:A:HO2'	2:A:689:A:P	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1067:A:H3'	2:A:1067:A:C8	2.55	0.42
3:B:30:C:N4	3:B:49:G:O6	2.53	0.42
4:C:248:SER:HB3	4:C:254:THR:HG21	2.01	0.42
5:D:123:ILE:HD11	5:D:141:ARG:NH1	2.35	0.42
9:L:118:GLN:HE22	9:L:121:LYS:NZ	2.17	0.42
13:P:22:THR:HG21	13:P:67:ARG:HB2	2.01	0.42
2:A:409:G:H3'	2:A:410:G:C8	2.55	0.42
2:A:1105:G:H2'	2:A:1106:U:C6	2.55	0.42
8:G:89:LEU:HG	8:G:162:ILE:HG12	2.00	0.42
2:A:297:U:HO2'	2:A:298:U:H5	1.63	0.42
2:A:1015:G:H2'	2:A:1016:U:C6	2.54	0.42
2:A:1336:U:H2'	2:A:1337:U:C6	2.55	0.42
2:A:2494:C:H2'	2:A:2495:U:C6	2.54	0.42
11:N:87:ASP:N	11:N:87:ASP:OD1	2.53	0.42
22:Z:41:ASN:C	22:Z:43:LYS:H	2.23	0.42
2:A:878:G:H2'	2:A:879:C:C6	2.55	0.42
2:A:1906:G:O2'	2:A:1907:C:H6	2.02	0.42
13:P:134:LEU:HD12	13:P:134:LEU:O	2.19	0.42
2:A:117:A:H5'	2:A:118:A:H8	1.85	0.42
7:F:61:THR:HG23	7:F:91:LEU:HD11	2.01	0.42
4:C:146:MET:SD	4:C:154:LEU:HD11	2.60	0.42
2:A:1227:U:H2'	2:A:1228:U:C6	2.54	0.42
2:A:2225:C:H2'	2:A:2226:A:C8	2.55	0.42
2:A:344:C:C5	20:W:78:PRO:HG2	2.55	0.41
2:A:563:G:H2'	2:A:564:U:C6	2.55	0.41
2:A:1074:A:N6	2:A:1171:G:H2'	2.35	0.41
7:F:51:ASP:O	7:F:54:VAL:HB	2.20	0.41
8:G:11:ILE:HD11	8:G:50:ILE:HD11	2.02	0.41
8:G:15:VAL:HG12	8:G:28:GLY:HA3	2.01	0.41
10:M:19:VAL:CG1	10:M:41:CYS:HB2	2.50	0.41
18:U:16:ARG:NH2	18:U:103:LYS:HD2	2.35	0.41
20:W:22:LYS:H	20:W:36:GLU:HG2	1.85	0.41
2:A:540:G:H21	18:U:66:ASN:HD21	1.68	0.41
2:A:2926:U:H2'	2:A:2927:A:C8	2.55	0.41
4:C:30:GLU:O	4:C:34:LEU:HD23	2.20	0.41
2:A:407:G:H2'	2:A:408:U:H6	1.85	0.41
2:A:1430:C:H2'	2:A:1431:A:C8	2.55	0.41
2:A:1528:G:O2'	2:A:1529:U:OP1	2.35	0.41
6:E:196:LYS:O	6:E:199:VAL:HG12	2.20	0.41
2:A:554:C:H6	2:A:554:C:H2'	1.56	0.41
2:A:1763:U:O2'	2:A:1764:A:H5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:V:43:GLU:HG3	19:V:50:VAL:HG23	2.02	0.41
2:A:460:C:H2'	2:A:461:A:C8	2.55	0.41
2:A:2775:A:OP1	30:8:35:LYS:HE3	2.21	0.41
6:E:13:ASN:OD1	6:E:15:GLY:N	2.47	0.41
23:1:14:ILE:HG23	23:1:15:GLN:HG3	2.02	0.41
2:A:115:C:O2'	2:A:125:A:N3	2.48	0.41
2:A:637:U:H2'	2:A:638:U:C6	2.56	0.41
10:M:23:LYS:HE2	10:M:23:LYS:HB2	1.81	0.41
2:A:2347:A:H2'	2:A:2348:U:C6	2.54	0.41
2:A:2561:U:H2'	2:A:2563:U:O5'	2.21	0.41
7:F:53:ALA:HA	7:F:56:GLU:CD	2.41	0.41
8:G:156:PRO:O	8:G:171:ARG:HD3	2.21	0.41
2:A:969:C:O2'	21:Y:34:ALA:HB2	2.21	0.41
2:A:2052:U:OP2	26:4:6:ARG:NH2	2.54	0.41
2:A:214:G:H5"	2:A:215:A:OP2	2.21	0.41
2:A:714:A:H2'	2:A:716:A:H62	1.86	0.41
2:A:1554:U:H2'	2:A:1555:U:O4'	2.21	0.41
2:A:1712:U:O2'	2:A:2719:G:H4'	2.20	0.41
2:A:2410:A:H2'	2:A:2411:A:O4'	2.21	0.41
2:A:2862:A:O2'	5:D:59:LYS:HD2	2.21	0.41
5:D:65:GLU:O	5:D:69:VAL:HG22	2.20	0.41
6:E:161:GLU:HA	6:E:161:GLU:OE1	2.21	0.41
7:F:57:LEU:HD23	7:F:57:LEU:HA	1.95	0.41
27:5:40:ARG:HG3	27:5:40:ARG:NH1	2.36	0.41
2:A:575:G:H2'	2:A:575:G:N3	2.35	0.41
2:A:1465:A:H2	2:A:1634:A:H2	1.69	0.41
2:A:2580:U:H2'	2:A:2581:G:H8	1.85	0.41
11:N:76:ILE:HD13	11:N:76:ILE:HA	1.88	0.41
2:A:13:A:O2'	2:A:15:G:N7	2.48	0.40
2:A:288:U:O2'	2:A:289:U:H6	2.03	0.40
2:A:851:G:N2	2:A:875:A:OP1	2.54	0.40
2:A:1787:C:C5	15:R:94:ARG:NH2	2.89	0.40
2:A:2499:C:OP1	30:8:5:PRO:HD2	2.21	0.40
6:E:31:LYS:HD3	11:N:9:SER:HB2	2.03	0.40
7:F:77:PHE:C	7:F:78:ARG:HD3	2.41	0.40
10:M:98:ILE:HD13	10:M:114:ILE:HG23	2.03	0.40
14:Q:17:ARG:O	14:Q:20:SER:OG	2.24	0.40
21:Y:79:ARG:HD2	21:Y:80:MET:O	2.21	0.40
2:A:1124:C:H1'	2:A:1134:A:H5"	2.03	0.40
2:A:1459:U:H2'	2:A:1460:G:C8	2.56	0.40
2:A:1771:A:H2'	2:A:1772:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:3:U:H2'	3:B:4:G:C8	2.56	0.40
2:A:186:C:O2'	2:A:187:C:H6	2.05	0.40
8:G:56:THR:HG22	8:G:57:ASP:H	1.85	0.40
8:G:104:VAL:HG22	8:G:114:GLU:OE1	2.22	0.40
2:A:2134:G:H2'	2:A:2135:U:H6	1.83	0.40
5:D:16:PHE:CE1	5:D:22:LEU:HD13	2.56	0.40
2:A:1108:G:H2'	2:A:1109:G:C8	2.57	0.40
2:A:2193:G:H2'	2:A:2194:C:H6	1.87	0.40
2:A:2327:C:O2'	2:A:2328:C:H5'	2.21	0.40
2:A:2529:C:OP2	12:O:82:ARG:HD3	2.21	0.40
2:A:2671:G:HO2'	2:A:2672:A:P	2.45	0.40
4:C:161:SER:HB3	4:C:194:GLN:HG3	2.04	0.40
5:D:5:ILE:HG22	5:D:202:ILE:HB	2.04	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	
1	v	416/418 (100%)	393 (94%)	22 (5%)	1 (0%)	47	73
4	C	271/277 (98%)	259 (96%)	11 (4%)	1 (0%)	34	60
5	D	204/209 (98%)	197 (97%)	7 (3%)	0	100	100
6	E	201/207 (97%)	192 (96%)	9 (4%)	0	100	100
7	F	173/179 (97%)	159 (92%)	14 (8%)	0	100	100
8	G	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
9	L	140/145 (97%)	139 (99%)	1 (1%)	0	100	100
10	M	120/122 (98%)	113 (94%)	7 (6%)	0	100	100
11	N	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
12	O	131/144 (91%)	131 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	P	118/135 (87%)	114 (97%)	4 (3%)	0	100	100
14	Q	116/119 (98%)	110 (95%)	6 (5%)	0	100	100
15	R	101/114 (89%)	99 (98%)	2 (2%)	0	100	100
16	S	114/119 (96%)	110 (96%)	4 (4%)	0	100	100
17	T	99/102 (97%)	97 (98%)	2 (2%)	0	100	100
18	U	108/118 (92%)	107 (99%)	1 (1%)	0	100	100
19	V	88/94 (94%)	86 (98%)	2 (2%)	0	100	100
20	W	100/103 (97%)	96 (96%)	4 (4%)	0	100	100
21	Y	74/96 (77%)	68 (92%)	6 (8%)	0	100	100
22	Z	57/62 (92%)	50 (88%)	7 (12%)	0	100	100
23	1	57/63 (90%)	53 (93%)	4 (7%)	0	100	100
24	2	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
25	3	57/81 (70%)	51 (90%)	6 (10%)	0	100	100
26	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
27	5	45/49 (92%)	45 (100%)	0	0	100	100
28	6	41/44 (93%)	41 (100%)	0	0	100	100
29	7	61/66 (92%)	56 (92%)	5 (8%)	0	100	100
30	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	3348/3543 (94%)	3202 (96%)	144 (4%)	2 (0%)	54	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	v	230	MET
4	C	155	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	v	353/365 (97%)	353 (100%)	0	100	100
4	C	221/225 (98%)	221 (100%)	0	100	100
5	D	169/171 (99%)	169 (100%)	0	100	100
6	E	165/174 (95%)	165 (100%)	0	100	100
7	F	97/155 (63%)	95 (98%)	2 (2%)	53	80
8	G	145/147 (99%)	145 (100%)	0	100	100
9	L	119/121 (98%)	119 (100%)	0	100	100
10	M	101/101 (100%)	101 (100%)	0	100	100
11	N	104/115 (90%)	104 (100%)	0	100	100
12	O	103/113 (91%)	103 (100%)	0	100	100
13	P	95/111 (86%)	95 (100%)	0	100	100
14	Q	96/97 (99%)	96 (100%)	0	100	100
15	R	84/99 (85%)	84 (100%)	0	100	100
16	S	95/97 (98%)	95 (100%)	0	100	100
17	T	75/82 (92%)	75 (100%)	0	100	100
18	U	83/97 (86%)	83 (100%)	0	100	100
19	V	78/84 (93%)	78 (100%)	0	100	100
20	W	69/88 (78%)	69 (100%)	0	100	100
21	Y	58/76 (76%)	58 (100%)	0	100	100
22	Z	46/53 (87%)	46 (100%)	0	100	100
23	1	51/55 (93%)	51 (100%)	0	100	100
24	2	50/52 (96%)	50 (100%)	0	100	100
26	4	47/50 (94%)	47 (100%)	0	100	100
27	5	44/48 (92%)	44 (100%)	0	100	100
28	6	39/39 (100%)	39 (100%)	0	100	100
29	7	53/56 (95%)	53 (100%)	0	100	100
30	8	35/35 (100%)	35 (100%)	0	100	100
All	All	2675/2906 (92%)	2673 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	78	ARG
7	F	80	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	v	42	ASN
1	v	67	GLN
1	v	382	ASN
1	v	384	HIS
5	D	33	ASN
5	D	50	GLN
5	D	140	HIS
5	D	152	ASN
6	E	46	GLN
6	E	49	HIS
6	E	75	GLN
6	E	145	ASN
6	E	162	ASN
7	F	63	GLN
8	G	147	ASN
9	L	118	GLN
9	L	136	GLN
10	M	13	ASN
10	M	110	ASN
11	N	35	HIS
12	O	35	GLN
14	Q	15	HIS
16	S	44	GLN
17	T	90	GLN
18	U	66	ASN
18	U	107	HIS
19	V	73	ASN
21	Y	58	ASN
22	Z	34	GLN
26	4	48	GLN
27	5	16	ASN
29	7	26	HIS
29	7	40	GLN
30	8	36	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	A	2890/2932 (98%)	464 (16%)	23 (0%)
3	B	113/116 (97%)	14 (12%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3003/3048 (98%)	478 (15%)	23 (0%)

All (478) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	A	13	A
2	A	14	A
2	A	28	A
2	A	34	U
2	A	46	C
2	A	60	G
2	A	71	A
2	A	75	G
2	A	89	U
2	A	93	U
2	A	100	U
2	A	101	G
2	A	117	A
2	A	118	A
2	A	119	U
2	A	125	A
2	A	126	A
2	A	133	A
2	A	140	G
2	A	161	A
2	A	164	A
2	A	167	U
2	A	186	C
2	A	187	C
2	A	198	A
2	A	199	A
2	A	201	A
2	A	214	G
2	A	215	A
2	A	218	A
2	A	223	A
2	A	224	A
2	A	228	A
2	A	230	A
2	A	231	A
2	A	232	U
2	A	247	G

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Mol	Chain	Res	Type
2	A	250	G
2	A	257	A
2	A	269	C
2	A	270	C
2	A	274	A
2	A	275	C
2	A	276	C
2	A	283	C
2	A	285	U
2	A	287	C
2	A	289	U
2	A	290	C
2	A	295	G
2	A	296	G
2	A	300	U
2	A	301	A
2	A	307	C
2	A	308	U
2	A	309	C
2	A	313	A
2	A	320	U
2	A	323	A
2	A	345	G
2	A	354	A
2	A	360	G
2	A	372	A
2	A	373	A
2	A	375	A
2	A	382	U
2	A	388	A
2	A	404	A
2	A	410	G
2	A	411	A
2	A	417	A
2	A	418	G
2	A	429	C
2	A	432	G
2	A	433	U
2	A	457	G
2	A	466	C
2	A	470	G
2	A	490	C

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Mol	Chain	Res	Type
2	A	501	C
2	A	503	A
2	A	526	A
2	A	527	G
2	A	550	A
2	A	552	U
2	A	553	U
2	A	554	C
2	A	555	C
2	A	567	G
2	A	572	C
2	A	574	A
2	A	575	G
2	A	576	U
2	A	577	A
2	A	583	A
2	A	591	A
2	A	592	A
2	A	594	G
2	A	595	G
2	A	606	G
2	A	616	G
2	A	618	A
2	A	646	A
2	A	657	A
2	A	659	A
2	A	666	A
2	A	667	G
2	A	672	A
2	A	679	G
2	A	682	A
2	A	689	A
2	A	690	U
2	A	699	U
2	A	700	A
2	A	732	U
2	A	768	A
2	A	776	U
2	A	784	C
2	A	791	G
2	A	793	U
2	A	794	G

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Mol	Chain	Res	Type
2	A	810	A
2	A	811	G
2	A	821	G
2	A	825	A
2	A	828	A
2	A	830	U
2	A	835	A
2	A	836	U
2	A	838	G
2	A	851	G
2	A	852	C
2	A	858	C
2	A	865	A
2	A	873	U
2	A	874	U
2	A	891	U
2	A	892	A
2	A	893	A
2	A	913	A
2	A	921	G
2	A	926	G
2	A	957	A
2	A	959	C
2	A	961	C
2	A	964	A
2	A	973	U
2	A	974	A
2	A	979	U
2	A	980	A
2	A	987	A
2	A	991	A
2	A	992	G
2	A	1007	G
2	A	1020	A
2	A	1026	A
2	A	1029	A
2	A	1031	C
2	A	1042	A
2	A	1051	C
2	A	1055	A
2	A	1058	U
2	A	1059	A

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Mol	Chain	Res	Type
2	A	1068	G
2	A	1072	A
2	A	1073	A
2	A	1079	U
2	A	1092	A
2	A	1093	G
2	A	1106	U
2	A	1115	A
2	A	1116	A
2	A	1117	G
2	A	1130	A
2	A	1134	A
2	A	1136	U
2	A	1141	A
2	A	1142	A
2	A	1143	U
2	A	1157	A
2	A	1158	G
2	A	1161	A
2	A	1173	A
2	A	1174	A
2	A	1178	U
2	A	1179	A
2	A	1181	C
2	A	1182	G
2	A	1185	G
2	A	1187	U
2	A	1188	A
2	A	1203	A
2	A	1230	G
2	A	1249	A
2	A	1250	G
2	A	1264	G
2	A	1265	A
2	A	1283	G
2	A	1295	G
2	A	1296	A
2	A	1298	A
2	A	1301	G
2	A	1302	C
2	A	1311	G
2	A	1316	G

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Mol	Chain	Res	Type
2	A	1317	A
2	A	1320	G
2	A	1333	C
2	A	1344	A
2	A	1345	A
2	A	1364	G
2	A	1365	A
2	A	1369	C
2	A	1373	U
2	A	1394	C
2	A	1396	U
2	A	1409	A
2	A	1423	U
2	A	1429	A
2	A	1435	A
2	A	1439	A
2	A	1440	U
2	A	1445	G
2	A	1451	G
2	A	1462	U
2	A	1463	U
2	A	1464	A
2	A	1465	A
2	A	1469	A
2	A	1470	U
2	A	1478	C
2	A	1493	A
2	A	1494	A
2	A	1502	A
2	A	1509	A
2	A	1517	C
2	A	1519	A
2	A	1528	G
2	A	1529	U
2	A	1531	U
2	A	1532	G
2	A	1533	A
2	A	1534	G
2	A	1536	A
2	A	1539	A
2	A	1542	C
2	A	1543	A

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Mol	Chain	Res	Type
2	A	1546	U
2	A	1553	C
2	A	1558	G
2	A	1559	A
2	A	1570	G
2	A	1571	U
2	A	1573	A
2	A	1575	G
2	A	1579	A
2	A	1581	G
2	A	1611	C
2	A	1612	G
2	A	1618	A
2	A	1621	A
2	A	1630	U
2	A	1638	G
2	A	1642	U
2	A	1656	C
2	A	1657	A
2	A	1659	A
2	A	1660	C
2	A	1683	A
2	A	1695	A
2	A	1696	G
2	A	1697	C
2	A	1700	G
2	A	1701	A
2	A	1723	G
2	A	1724	C
2	A	1749	A
2	A	1762	U
2	A	1763	U
2	A	1764	A
2	A	1771	A
2	A	1778	A
2	A	1781	G
2	A	1782	A
2	A	1783	G
2	A	1787	C
2	A	1789	G
2	A	1796	G
2	A	1797	G

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Mol	Chain	Res	Type
2	A	1806	A
2	A	1809	G
2	A	1815	C
2	A	1818	A
2	A	1819	A
2	A	1833	C
2	A	1834	A
2	A	1849	C
2	A	1862	A
2	A	1881	A
2	A	1887	A
2	A	1891	G
2	A	1895	G
2	A	1903	U
2	A	1904	C
2	A	1906	G
2	A	1907	C
2	A	1915	C
2	A	1928	C
2	A	1938	C
2	A	1939	G
2	A	1945	A
2	A	1947	C
2	A	1948	U
2	A	1949	A
2	A	1950	U
2	A	1962	G
2	A	1963	G
2	A	1969	A
2	A	1971	A
2	A	1973	U
2	A	1988	U
2	A	1996	C
2	A	1997	G
2	A	2000	C
2	A	2003	A
2	A	2004	A
2	A	2005	G
2	A	2024	U
2	A	2026	U
2	A	2030	A
2	A	2056	A

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Mol	Chain	Res	Type
2	A	2060	G
2	A	2064	A
2	A	2065	G
2	A	2066	A
2	A	2069	C
2	A	2072	G
2	A	2076	C
2	A	2088	C
2	A	2089	G
2	A	2093	A
2	A	2094	G
2	A	2095	A
2	A	2102	G
2	A	2126	G
2	A	2127	A
2	A	2141	U
2	A	2144	U
2	A	2145	A
2	A	2149	G
2	A	2150	A
2	A	2151	U
2	A	2152	A
2	A	2159	A
2	A	2165	A
2	A	2167	A
2	A	2190	G
2	A	2198	G
2	A	2205	U
2	A	2206	A
2	A	2221	U
2	A	2231	A
2	A	2236	G
2	A	2237	C
2	A	2245	A
2	A	2256	A
2	A	2258	A
2	A	2271	G
2	A	2272	G
2	A	2292	G
2	A	2302	G
2	A	2316	C
2	A	2319	A

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Mol	Chain	Res	Type
2	A	2320	A
2	A	2321	A
2	A	2329	U
2	A	2338	A
2	A	2341	G
2	A	2353	A
2	A	2355	A
2	A	2358	G
2	A	2360	A
2	A	2367	C
2	A	2380	C
2	A	2383	C
2	A	2394	A
2	A	2410	A
2	A	2412	G
2	A	2416	G
2	A	2418	C
2	A	2435	U
2	A	2439	C
2	A	2447	G
2	A	2455	C
2	A	2456	U
2	A	2458	A
2	A	2462	G
2	A	2463	A
2	A	2468	A
2	A	2473	C
2	A	2474	C
2	A	2481	A
2	A	2492	A
2	A	2498	C
2	A	2507	C
2	A	2509	A
2	A	2524	U
2	A	2531	C
2	A	2535	G
2	A	2538	G
2	A	2551	A
2	A	2558	G
2	A	2562	G
2	A	2587	U
2	A	2599	A

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Mol	Chain	Res	Type
2	A	2600	G
2	A	2605	A
2	A	2606	C
2	A	2607	G
2	A	2615	G
2	A	2642	U
2	A	2643	C
2	A	2646	U
2	A	2648	U
2	A	2663	G
2	A	2679	C
2	A	2696	G
2	A	2715	G
2	A	2722	U
2	A	2724	C
2	A	2747	G
2	A	2759	U
2	A	2766	C
2	A	2768	G
2	A	2777	G
2	A	2781	A
2	A	2783	A
2	A	2790	A
2	A	2798	A
2	A	2799	G
2	A	2810	G
2	A	2811	A
2	A	2812	U
2	A	2813	G
2	A	2822	C
2	A	2824	U
2	A	2827	C
2	A	2828	U
2	A	2829	U
2	A	2832	G
2	A	2835	A
2	A	2837	U
2	A	2841	A
2	A	2862	A
2	A	2864	A
2	A	2872	G
2	A	2890	U

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Mol	Chain	Res	Type
2	A	2896	G
2	A	2901	G
2	A	2902	A
2	A	2908	A
2	A	2912	A
2	A	2920	A
2	A	2929	C
3	B	10	U
3	B	19	A
3	B	20	A
3	B	23	U
3	B	33	U
3	B	40	C
3	B	51	A
3	B	54	U
3	B	55	A
3	B	65	G
3	B	85	C
3	B	87	U
3	B	88	C
3	B	107	G

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A	27	G
2	A	88	G
2	A	92	G
2	A	139	A
2	A	553	U
2	A	688	A
2	A	809	G
2	A	979	U
2	A	1248	A
2	A	1249	A
2	A	1508	A
2	A	1528	G
2	A	1532	G
2	A	1533	A
2	A	1569	U
2	A	1817	A
2	A	1886	A

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Mol	Chain	Res	Type
2	A	2438	G
2	A	2463	A
2	A	2472	A
2	A	2506	U
2	A	2789	U
2	A	2809	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 205 ligands modelled in this entry, 204 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	$\#\|Z\| > 2$
31	GCP	v	501	-	27,34,34	1.43	5 (18%)	34,54,54	1.92	8 (23%)

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
31	GCP	v	501	-	-	5/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	v	501	GCP	C5-C6	4.00	1.48	1.41
31	v	501	GCP	PG-O3G	2.73	1.61	1.54
31	v	501	GCP	PG-O2G	2.59	1.60	1.54
31	v	501	GCP	C5-C4	2.36	1.47	1.40
31	v	501	GCP	PB-O2B	2.12	1.61	1.56

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	v	501	GCP	C2-N3-C4	4.76	120.79	115.36
31	v	501	GCP	C2-N1-C6	3.98	122.26	115.93
31	v	501	GCP	C5-C6-N1	-3.97	118.00	123.43
31	v	501	GCP	C4-C5-C6	-3.54	117.42	120.80
31	v	501	GCP	PB-O3A-PA	-3.50	121.47	132.56
31	v	501	GCP	C3'-C2'-C1'	3.35	106.02	100.98
31	v	501	GCP	N3-C2-N1	-3.18	122.98	127.22
31	v	501	GCP	C4-C5-N7	-2.49	106.81	109.40

There are no chirality outliers.

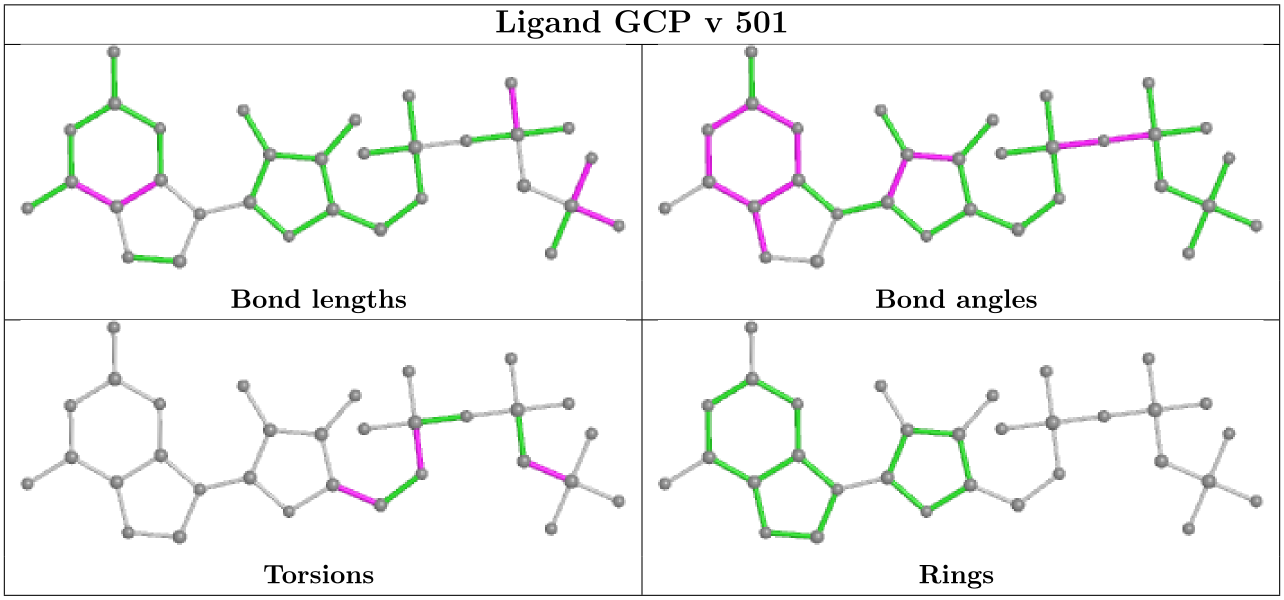
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	v	501	GCP	C5'-O5'-PA-O1A
31	v	501	GCP	C5'-O5'-PA-O3A
31	v	501	GCP	O4'-C4'-C5'-O5'
31	v	501	GCP	PB-C3B-PG-O1G
31	v	501	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

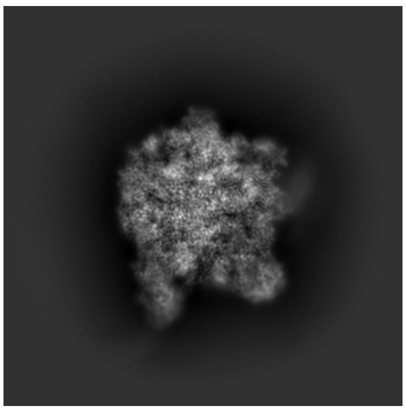
6 Map visualisation (i)

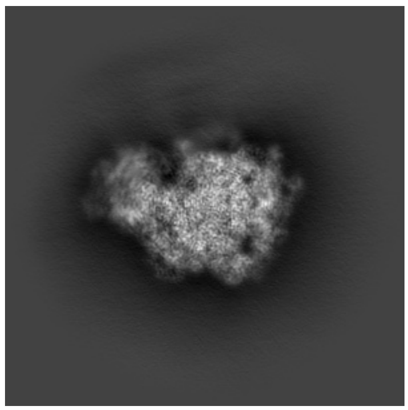
This section contains visualisations of the EMDB entry EMD-42577. These allow visual inspection of the internal detail of the map and identification of artifacts.

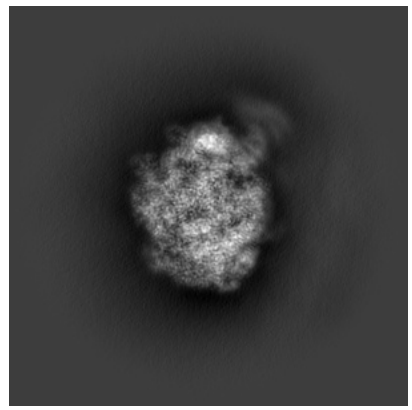
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

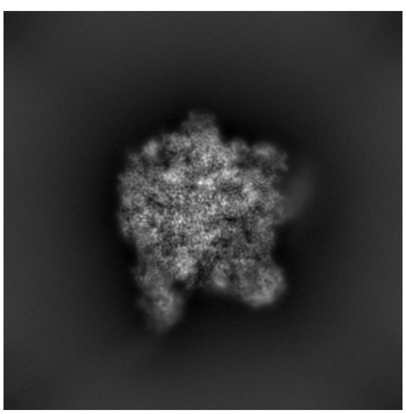
6.1.1 Primary map

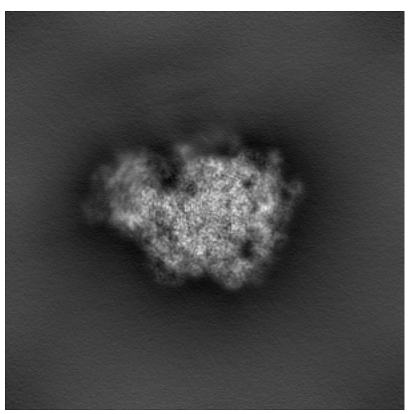

X

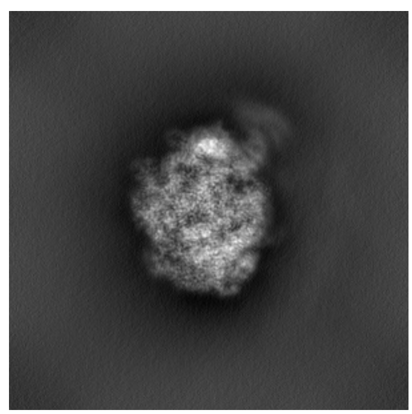

Y


Z

6.1.2 Raw map


X

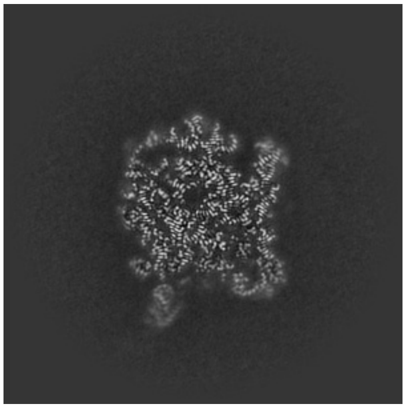

Y

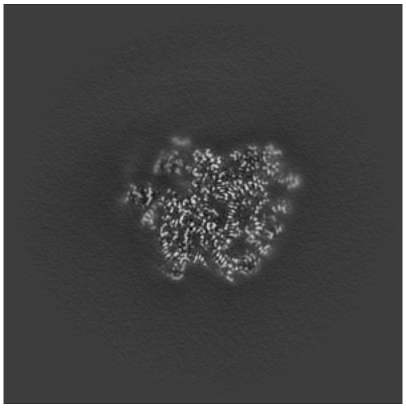

Z

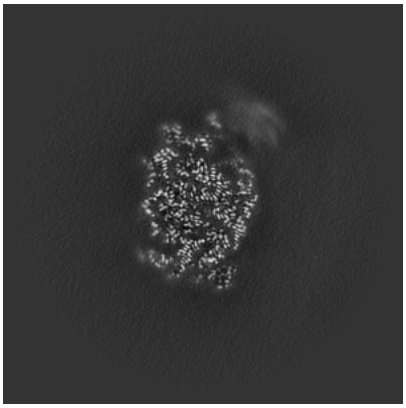
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

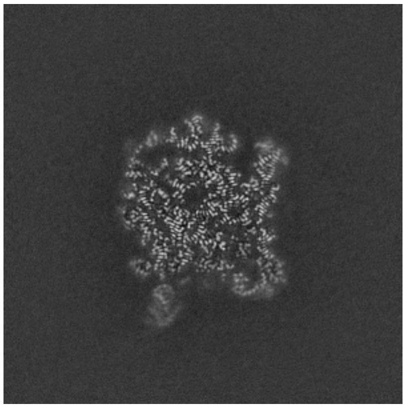
6.2.1 Primary map

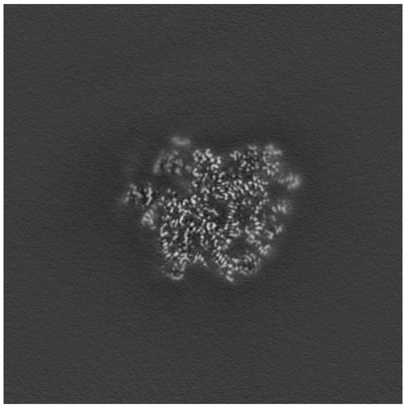

X Index: 256

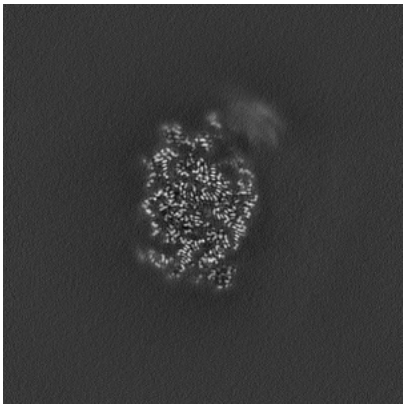

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

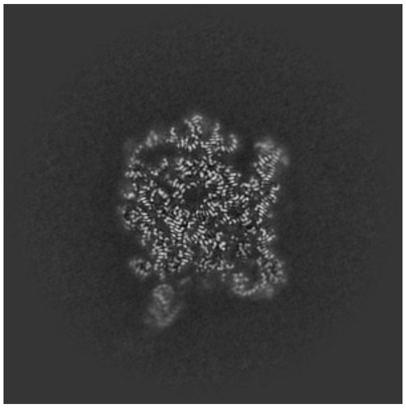

Y Index: 256

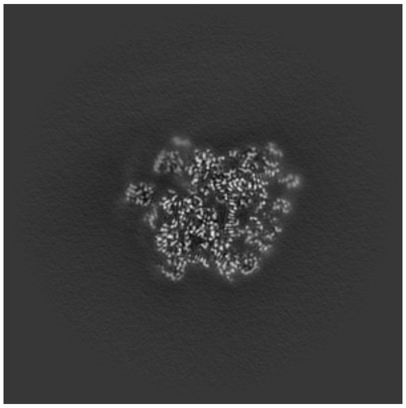

Z Index: 256

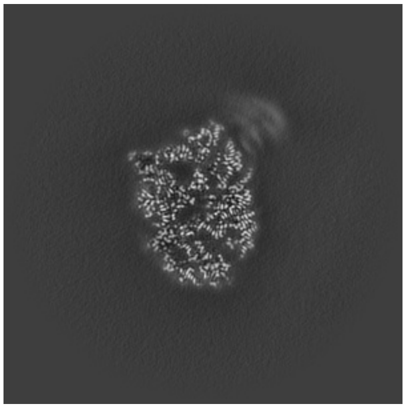
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

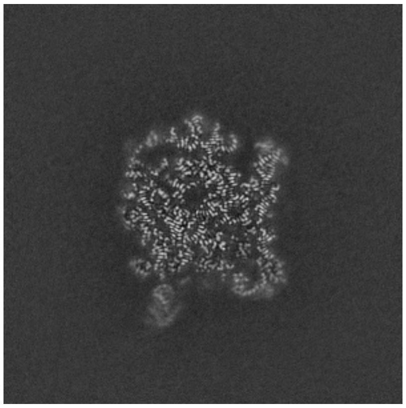
6.3.1 Primary map

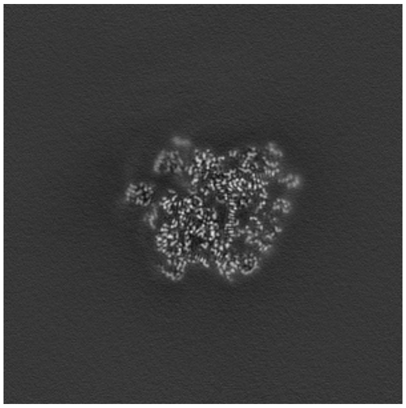

X Index: 256

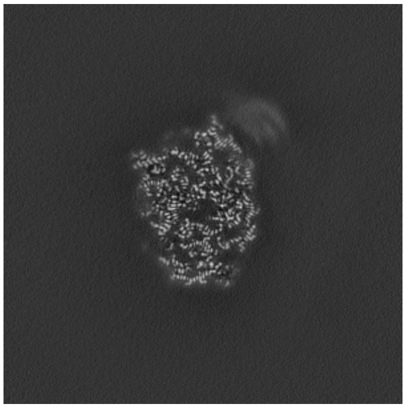

Y Index: 254


Z Index: 274

6.3.2 Raw map


X Index: 256

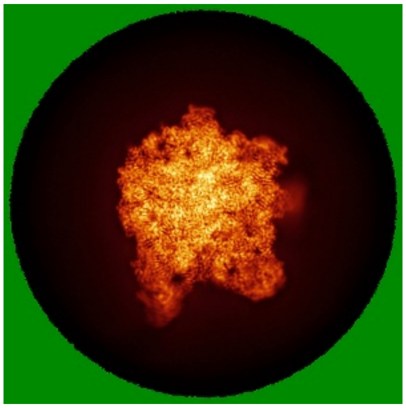

Y Index: 254


Z Index: 267

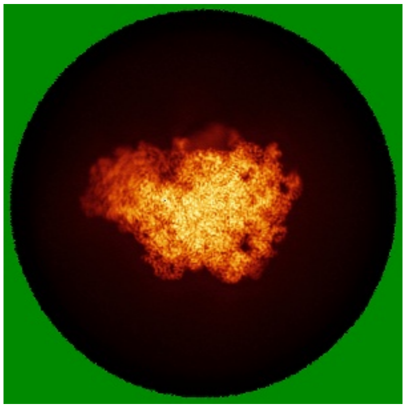
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

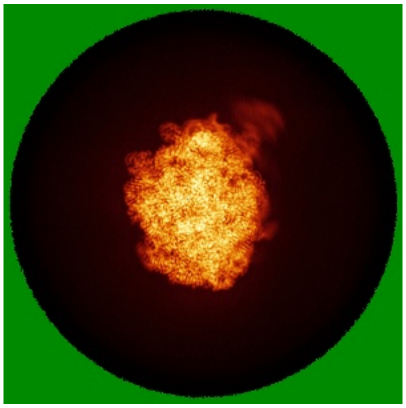
6.4.1 Primary map



X

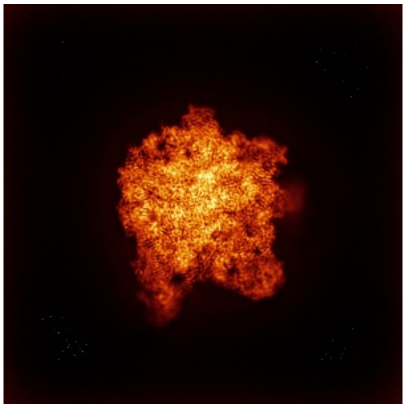


Y

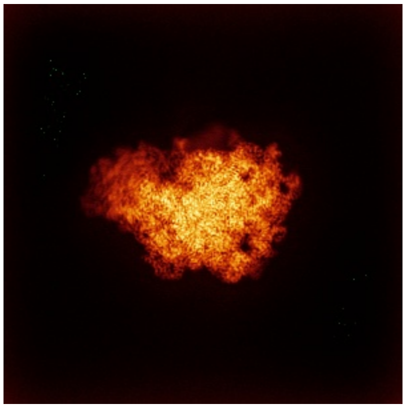


Z

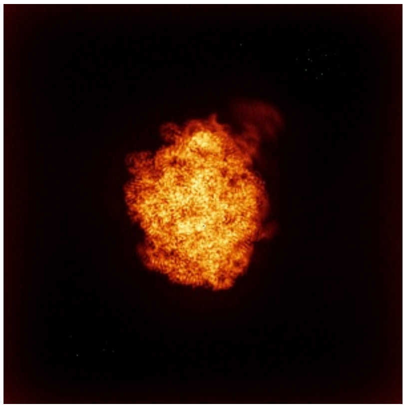
6.4.2 Raw map



X



Y

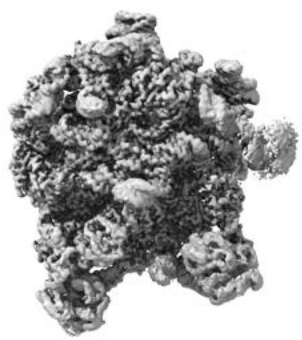


Z

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



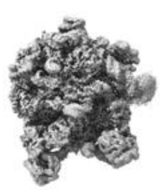
X

Y

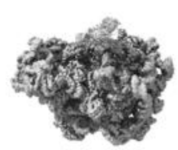
Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. 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.

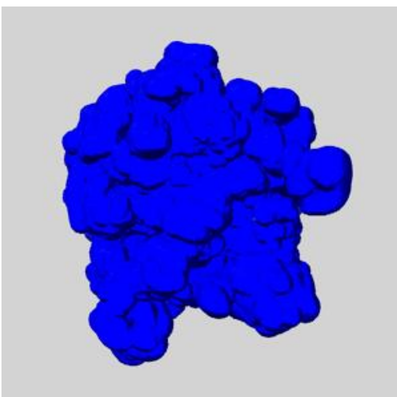
6.6 Mask visualisation (i)

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

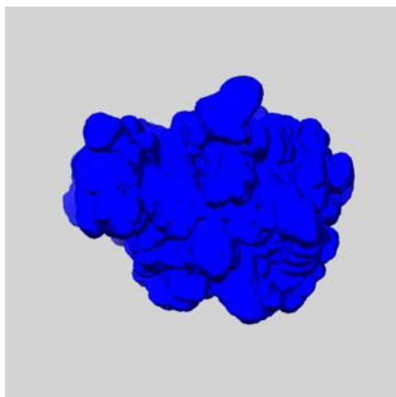
A mask typically either:

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

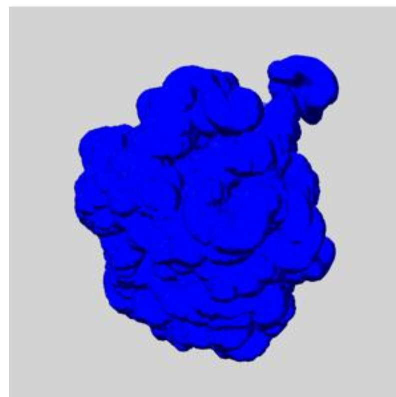
6.6.1 emd_42577_msk_1.map (i)



X



Y

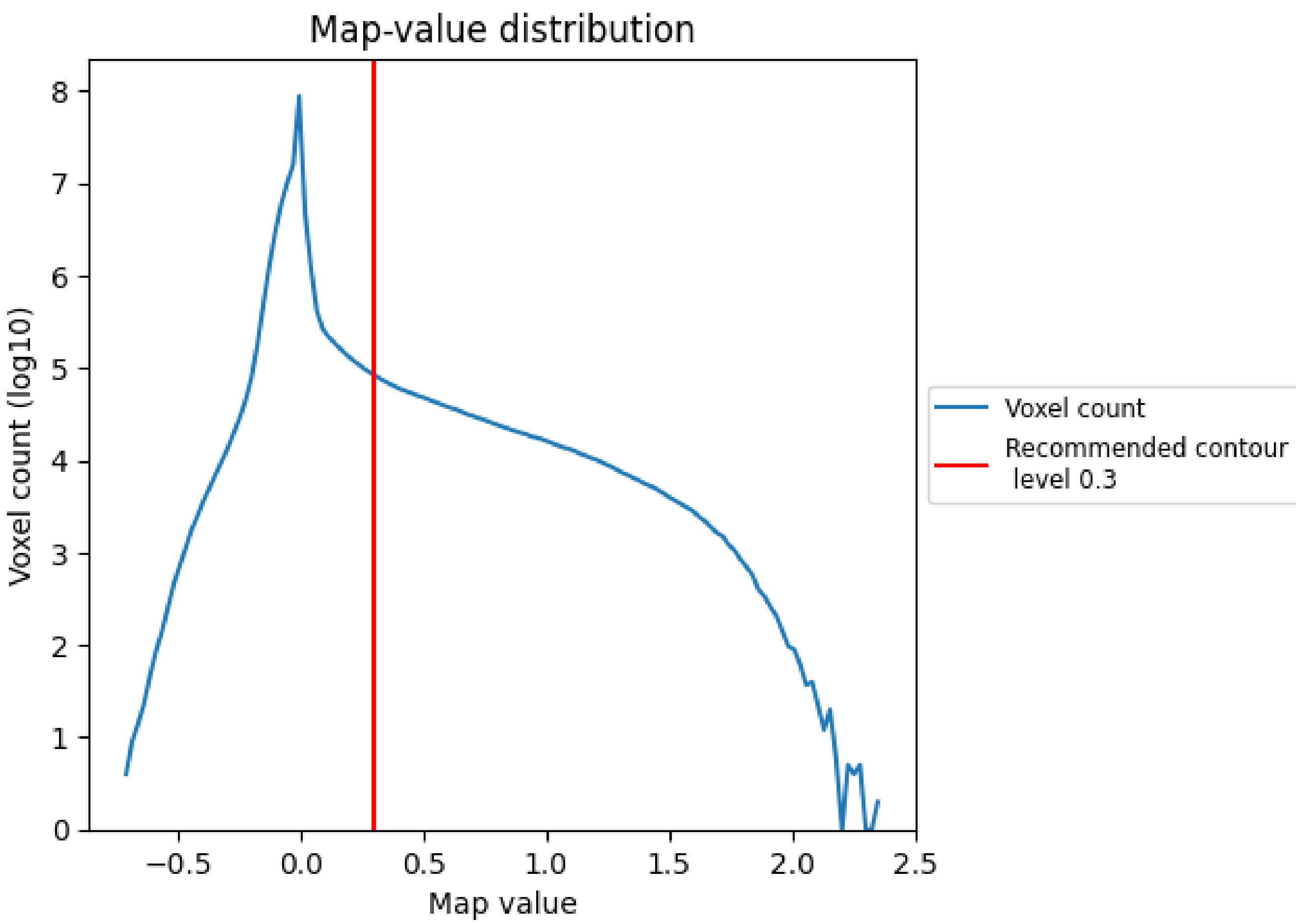


Z

7 Map analysis ⓘ

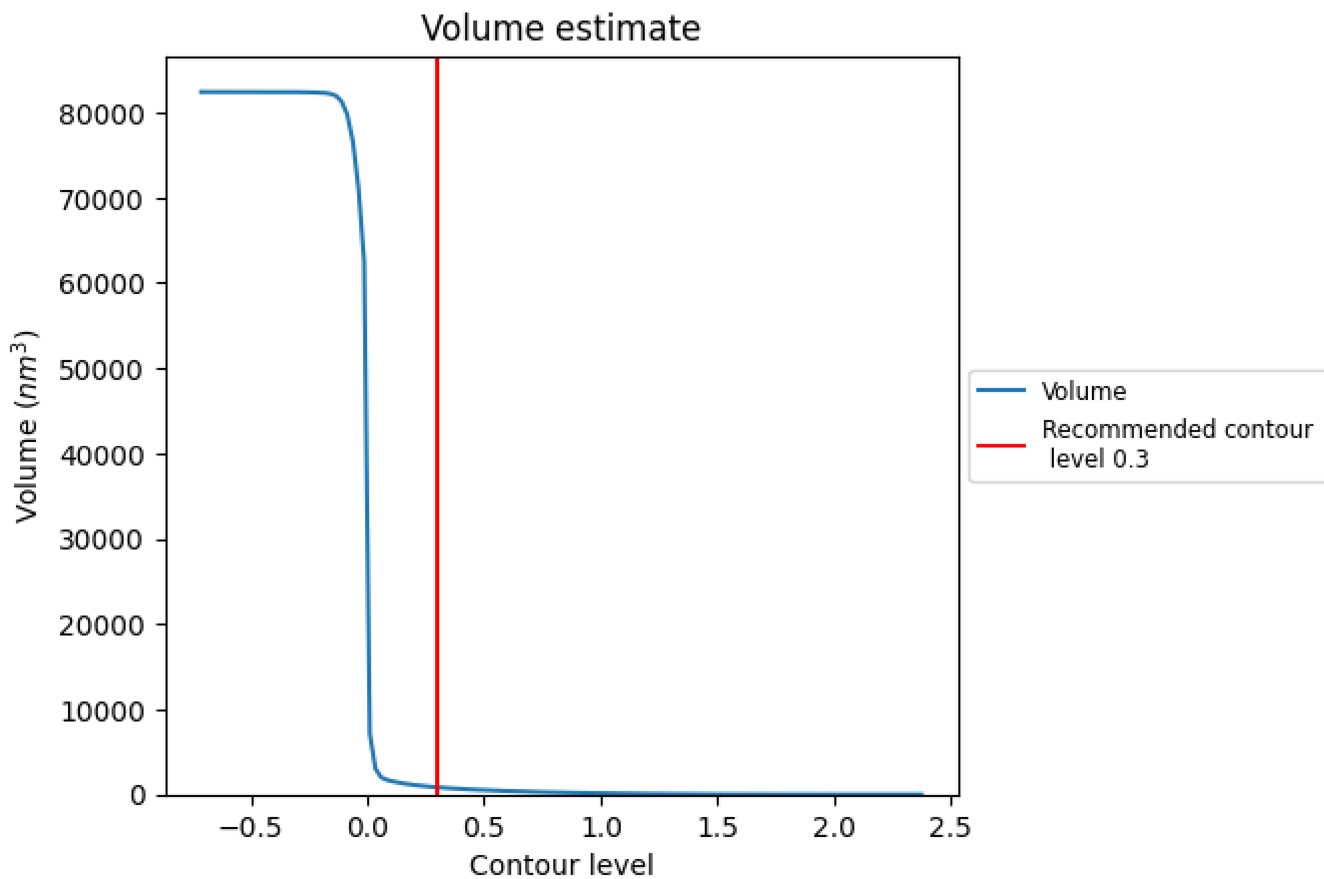
This section contains the results of statistical analysis of the map.

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.

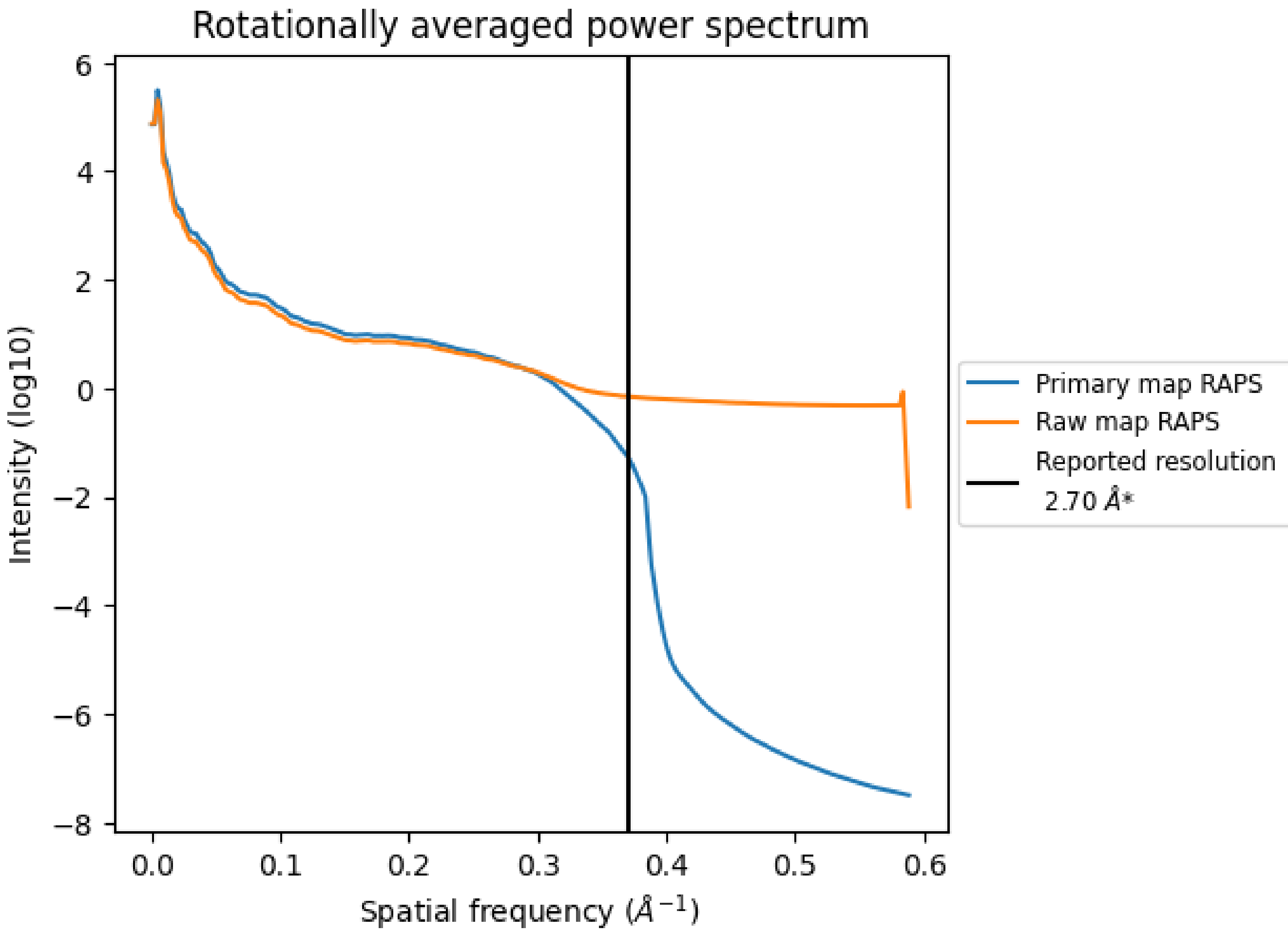
7.2 Volume estimate (i)



The volume at the recommended contour level is 834 nm^3; this corresponds to an approximate mass of 753 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)

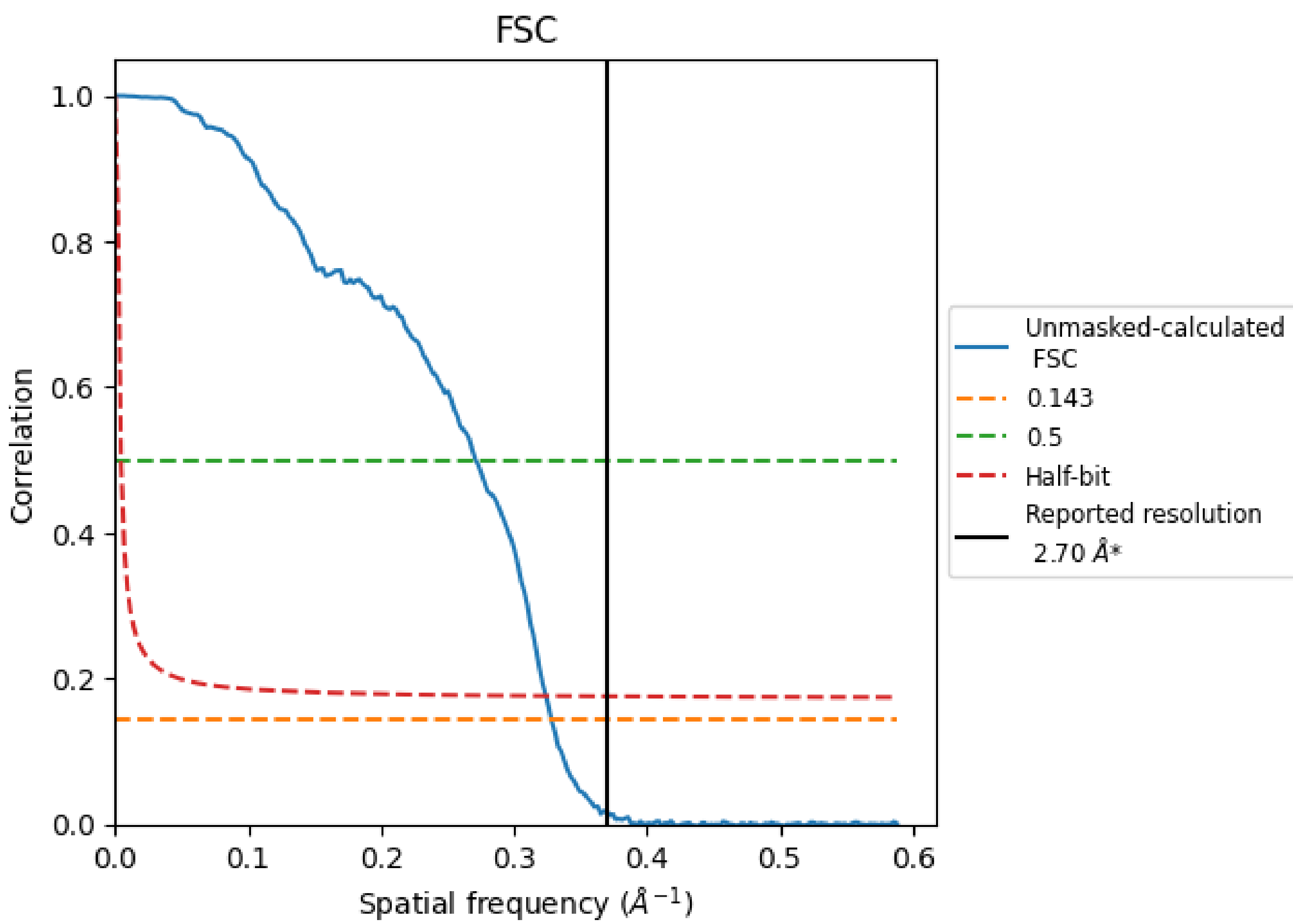


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

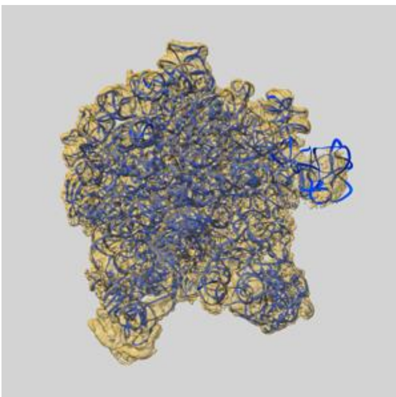
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.05	3.69	3.08

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.05 differs from the reported value 2.7 by more than 10 %

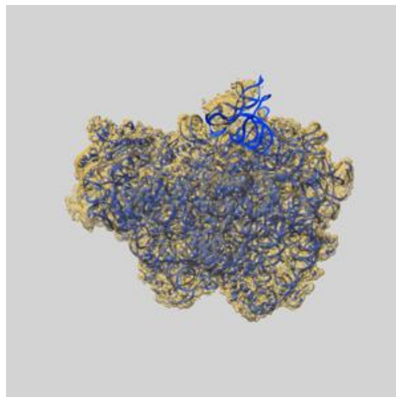
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-42577 and PDB model 8UUA. Per-residue inclusion information can be found in section 3 on page 11.

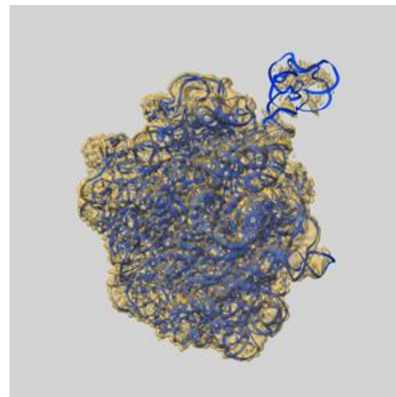
9.1 Map-model overlay (i)



X



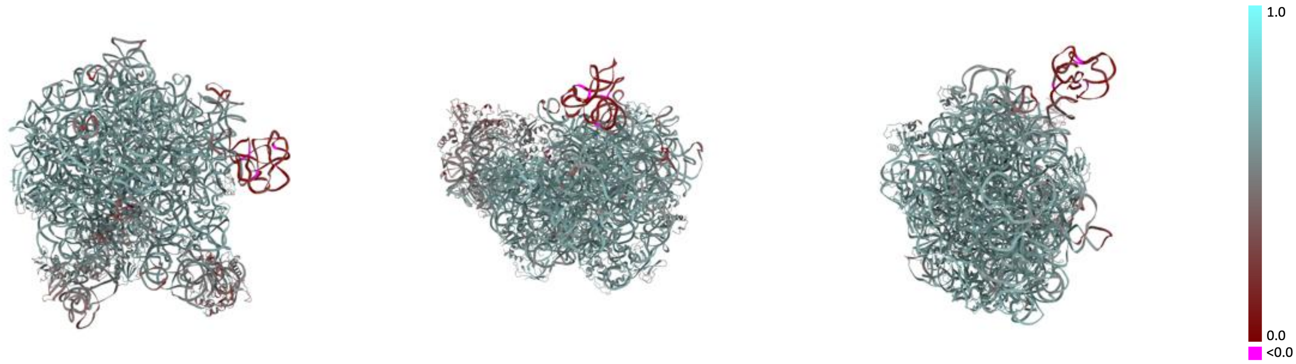
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

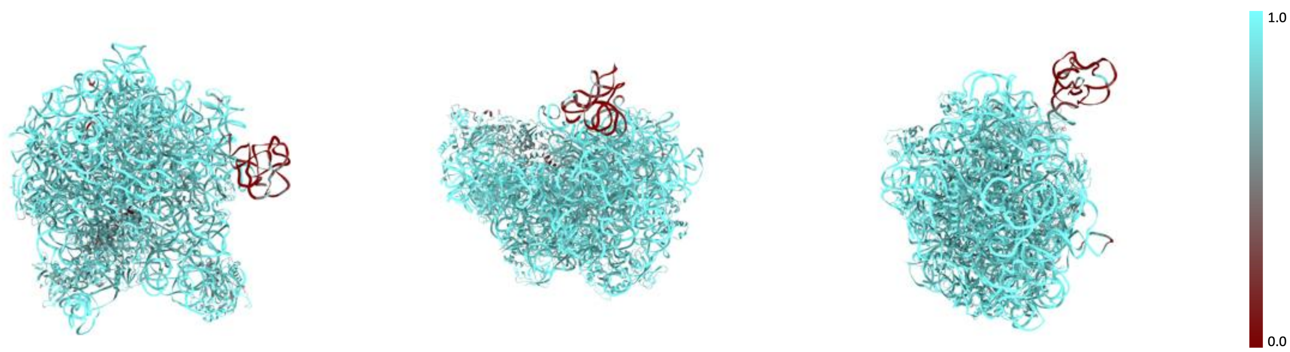
9.2 Q-score mapped to coordinate model (i)



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.

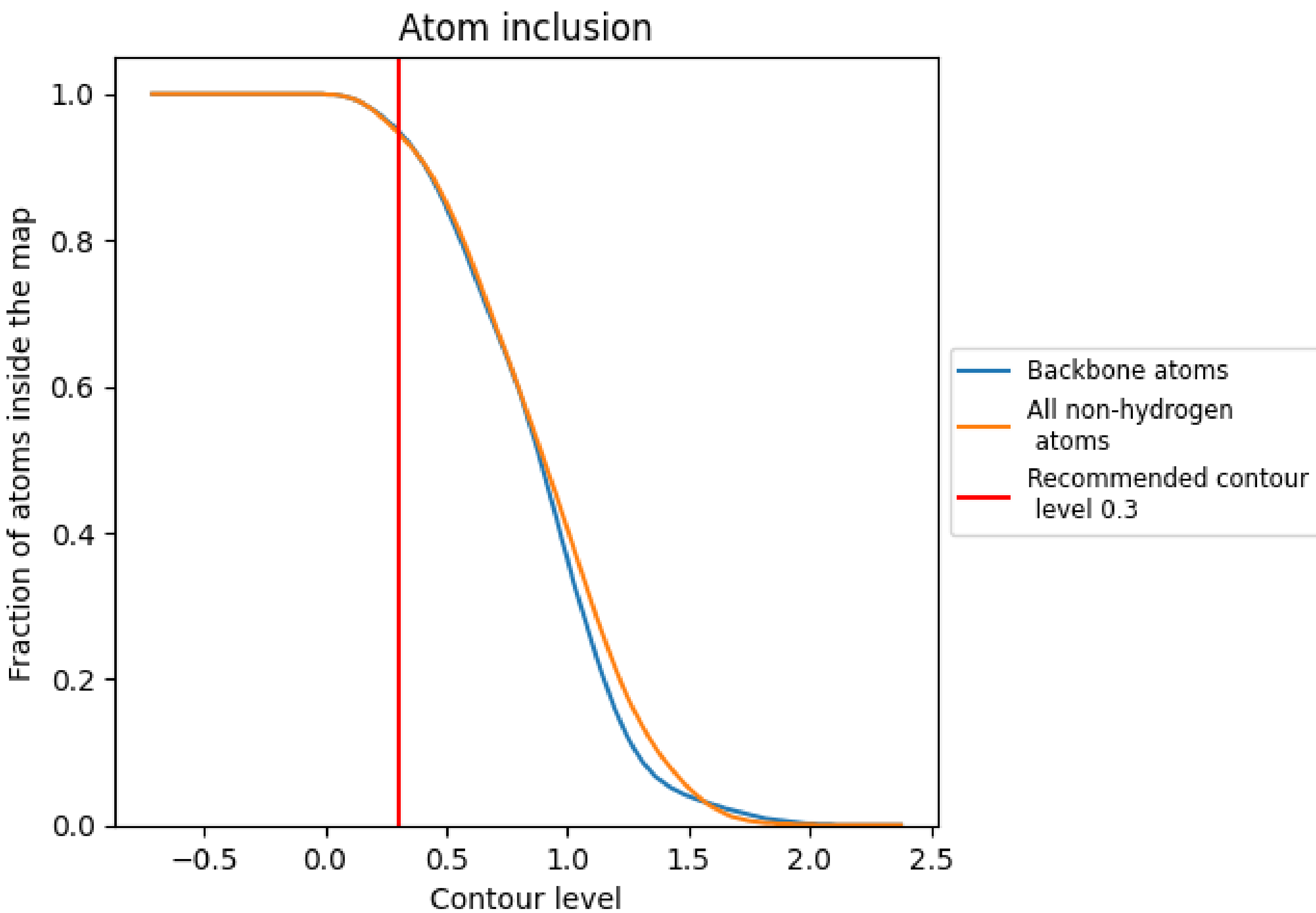
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9470	0.5830
1	0.9380	0.5630
2	0.9320	0.6020
3	0.7840	0.3990
4	0.9390	0.6110
5	0.9310	0.6080
6	0.9680	0.6350
7	0.9660	0.6350
8	0.9300	0.6190
A	0.9650	0.5890
B	0.9860	0.5260
C	0.9490	0.6170
D	0.9510	0.6140
E	0.9340	0.5940
F	0.8210	0.4180
G	0.8590	0.5170
L	0.9580	0.6140
M	0.9180	0.6040
N	0.9270	0.5920
O	0.9360	0.6040
P	0.9490	0.6120
Q	0.8790	0.5060
R	0.9420	0.6050
S	0.9710	0.6160
T	0.9640	0.6120
U	0.9450	0.6120
V	0.9390	0.5960
W	0.9380	0.5710
Y	0.9550	0.6240
Z	0.9360	0.5990
v	0.7170	0.4820