Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 03:22 pm GMT

PDB ID	:	5NO2
EMDB ID	:	EMD-3661
Title	:	RsgA-GDPNP bound to the 30S ribosomal subunit (RsgA assembly intermediate)
Authors	:	Lopez-Alonso, J.P.; Kaminishi, T.; Kikuchi, T.; Hirata, Y.; Iturrioz, I.; Dhimole, N.; Schedlbauer, A.; Hase, Y.; Goto, S.; Kurita, D.; Muto, A.; Zhou, S.; Naoe, C.; Mills, D.J.; Gil-Carton, D.; Takemoto, C.; Himeno, H.; Fucini, P.; Connell, S.R.
Deposited on	:	2017-04-10
Resolution	:	5.16 Å(reported)

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

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

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

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

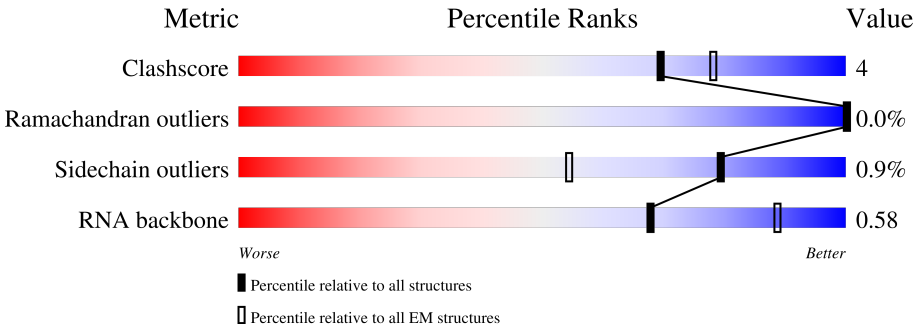
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.16 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	A	1534	73% 24%
2	D	205	8% 80% 20%
3	E	155	88% 12%
4	F	106	6% 92% 8%
5	G	130	75% 74% 8% 18%
6	H	129	93% 7%

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Mol	Chain	Length	Quality of chain
7	I	127	23% 82% 16%
8	J	99	44% 82% 18%
9	K	117	7% 85% 15%
10	L	14	79% 71% 29%
11	M	114	11% 91% 9%
12	N	100	45% 83% 17%
13	O	88	95% 5%
14	P	82	89% 11%
15	Q	80	5% 89% 11%
16	R	55	93% 7%
17	S	79	9% 84% 16%
18	T	86	86% 14%
19	Z	313	10% 85% 14%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 49225 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1534	32930	14694	6041	10661	1534	0	0

- Molecule 2 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	205	1643	1026	315	298	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	155	1144	711	216	211	6	0	0

- Molecule 4 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	106	862	545	156	154	7	0	0

- Molecule 5 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	107	841	525	160	153	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	129	979	616	173	184	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 8 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	99	Total	C	N	O	S	0	0
			796	498	152	145	1		

- Molecule 9 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	14	Total	C	N	O	0	0
			114	70	27	17		

- Molecule 11 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 12 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 13 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 14 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 15 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 16 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	R	55	Total	C	N	O	0	0
			456	288	86	82		

- Molecule 17 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 18 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 19 is a protein called Small ribosomal subunit biogenesis GTPase RsgA.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	313	Total	C	N	O	S	0	0
			2448	1538	432	468	10		

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
20	A	67	Total	Mg	0
			67	67	
20	N	1	Total	Mg	0
			1	1	
20	P	1	Total	Mg	0
			1	1	

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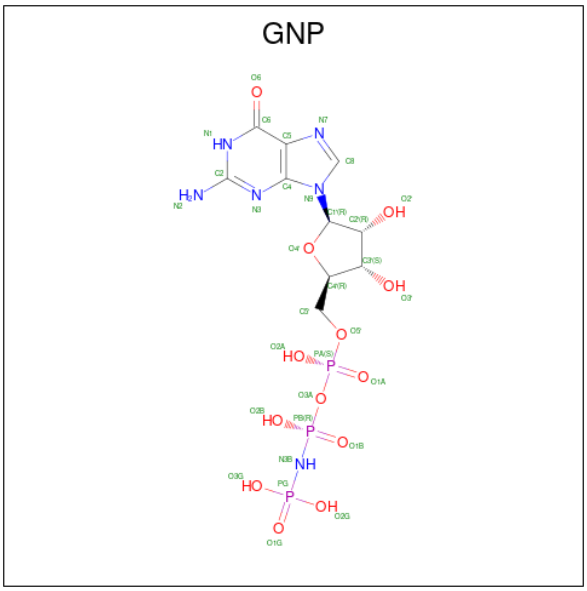
Mol	Chain	Residues	Atoms	AltConf
20	T	1	Total Mg 1 1	0
20	Z	1	Total Mg 1 1	0

- Molecule 21 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	Z	1	Total Zn 1 1	0

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



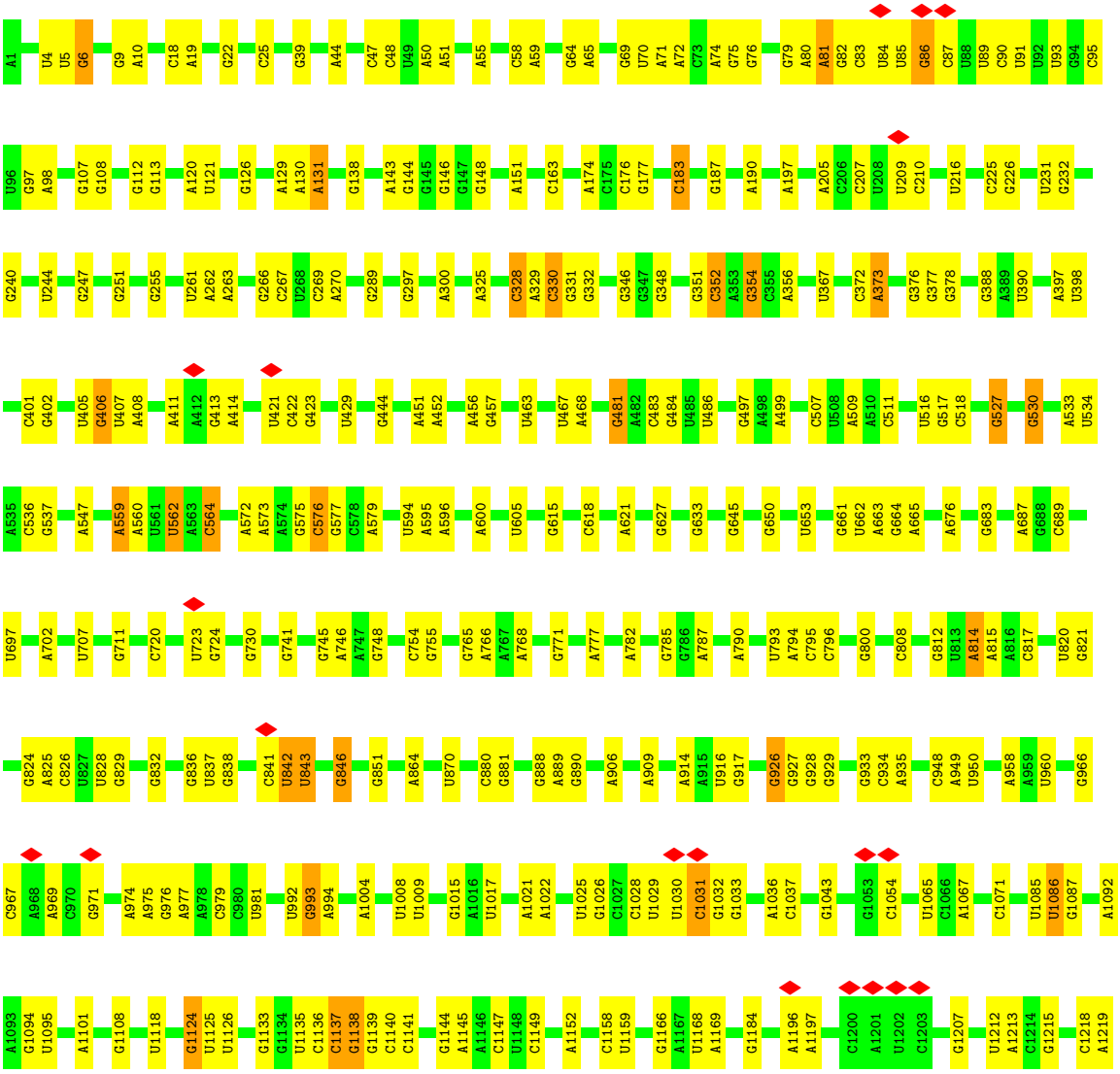
Mol	Chain	Residues	Atoms	AltConf
22	Z	1	Total C N O P 32 10 6 13 3	0

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.

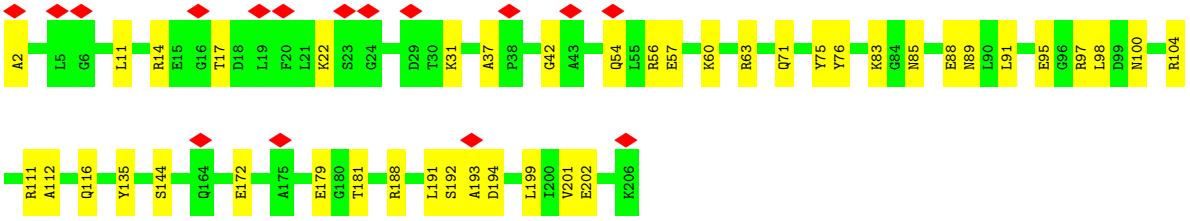
- Molecule 1: 16S ribosomal RNA

Chain A:



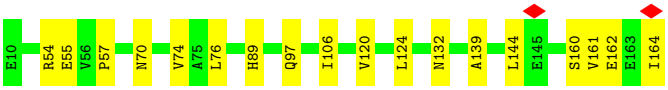
• Molecule 2: 30S ribosomal protein S4

Chain D:



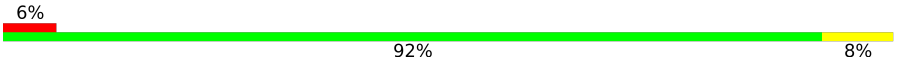
• Molecule 3: 30S ribosomal protein S5

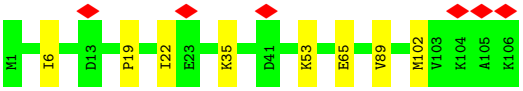
Chain E:



• Molecule 4: 30S ribosomal protein S6

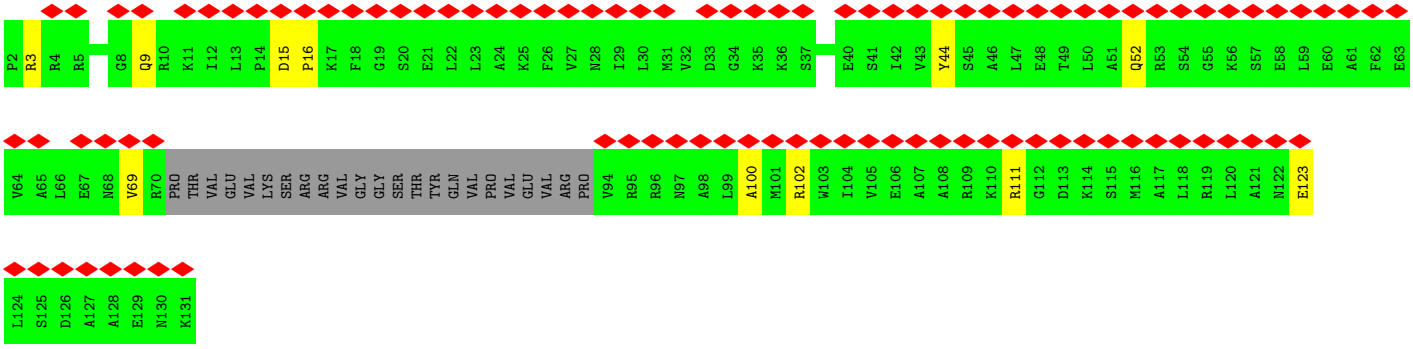
Chain F:





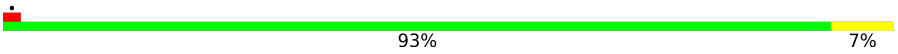
• Molecule 5: 30S ribosomal protein S7

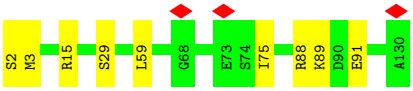
Chain G:



• Molecule 6: 30S ribosomal protein S8

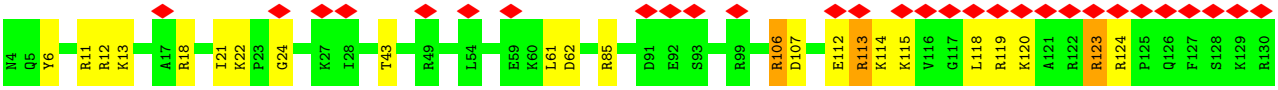
Chain H:





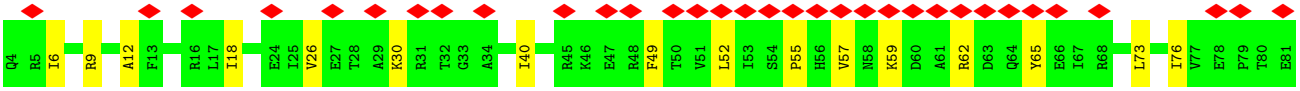
• Molecule 7: 30S ribosomal protein S9

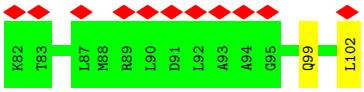
Chain I:



• Molecule 8: 30S ribosomal protein S10

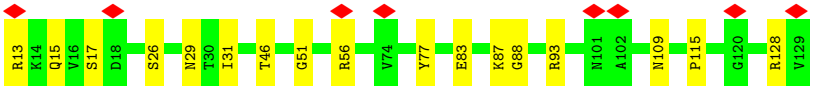
Chain J:





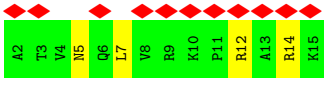
• Molecule 9: 30S ribosomal protein S11

Chain K:



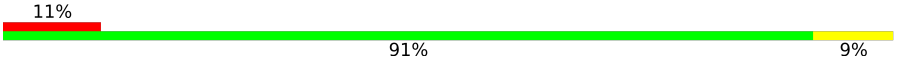
• Molecule 10: 30S ribosomal protein S12

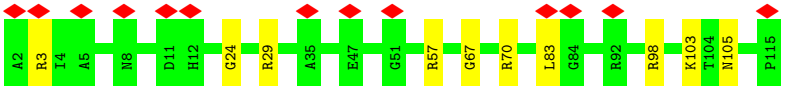
Chain L:



• Molecule 11: 30S ribosomal protein S13

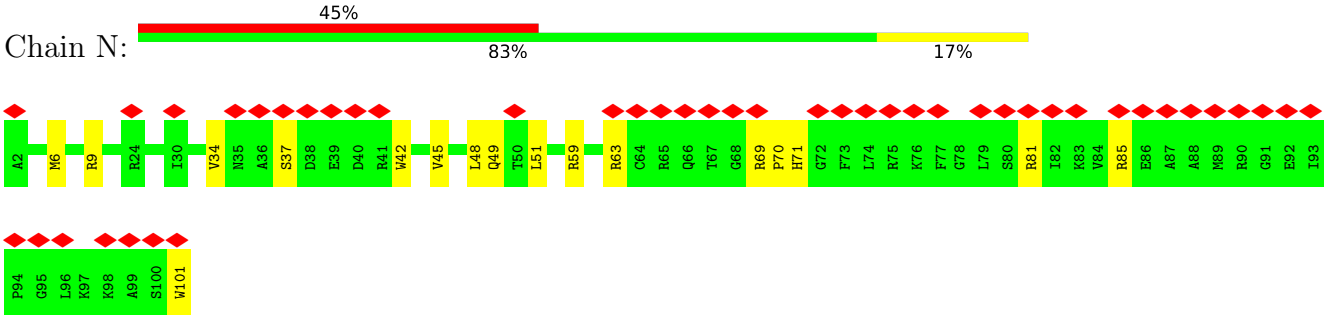
Chain M:





• Molecule 12: 30S ribosomal protein S14

Chain N:

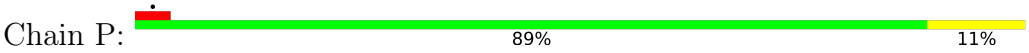


• Molecule 13: 30S ribosomal protein S15

Chain O:

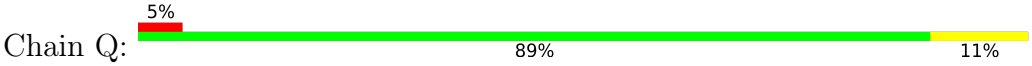
• Molecule 14: 30S ribosomal protein S16

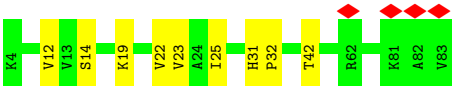
Chain P:



• Molecule 15: 30S ribosomal protein S17

Chain Q:



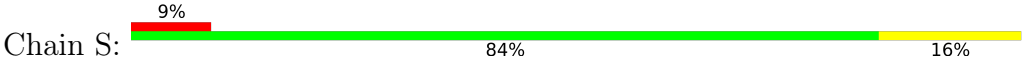


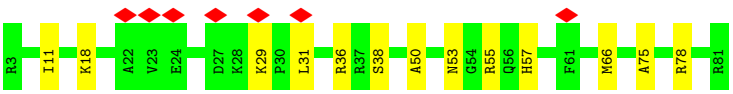
• Molecule 16: 30S ribosomal protein S18

Chain R:

• Molecule 17: 30S ribosomal protein S19

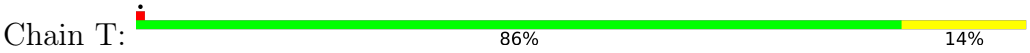
Chain S:

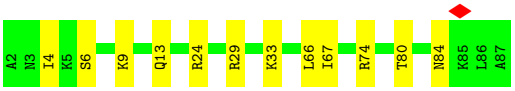




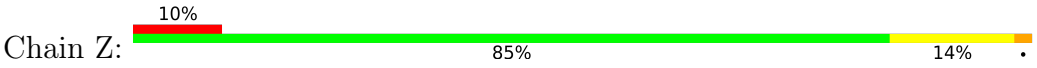
• Molecule 18: 30S ribosomal protein S20

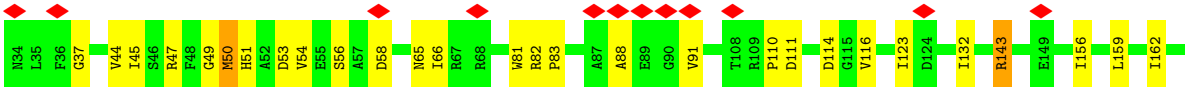
Chain T:

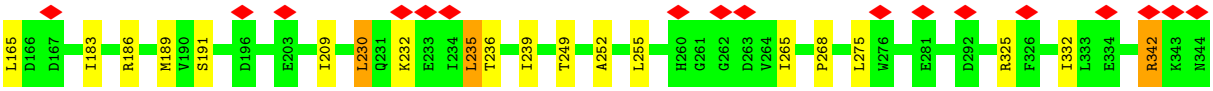




• Molecule 19: Small ribosomal subunit biogenesis GTPase RsgA







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.3	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	101000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.348	Depositor
Minimum map value	-0.126	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	355.84, 355.84, 355.84	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PSU, 2MG, 4OC, MG, 5MC, G7M, ZN, MA6, UR3, GNP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.19	0/36593	0.80	11/57081 (0.0%)
2	D	0.24	0/1665	0.43	0/2227
3	E	0.26	0/1157	0.51	0/1557
4	F	0.25	0/881	0.48	0/1189
5	G	0.25	0/848	0.47	0/1132
6	H	0.25	0/989	0.48	0/1326
7	I	0.26	0/1034	0.55	0/1375
8	J	0.24	0/806	0.50	0/1089
9	K	0.25	0/893	0.47	0/1205
10	L	0.22	0/114	0.41	0/151
11	M	0.25	0/893	0.50	0/1193
12	N	0.23	0/817	0.44	0/1088
13	O	0.23	0/722	0.47	0/964
14	P	0.24	0/659	0.47	0/884
15	Q	0.24	0/658	0.50	0/881
16	R	0.22	0/463	0.41	0/621
17	S	0.25	0/653	0.49	0/877
18	T	0.24	0/676	0.42	0/895
19	Z	0.26	0/2493	0.56	2/3376 (0.1%)
All	All	0.21	0/53014	0.72	13/79111 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	1
19	Z	0	2
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1158	C	N1-C2-O2	8.46	123.98	118.90
1	A	1158	C	C2-N1-C1'	8.43	128.07	118.80
19	Z	230	LEU	CA-CB-CG	6.92	131.22	115.30
1	A	754	C	C2-N1-C1'	6.85	126.34	118.80
1	A	1158	C	N3-C2-O2	-6.80	117.14	121.90
19	Z	235	LEU	CA-CB-CG	6.59	130.46	115.30
1	A	754	C	N1-C2-O2	6.30	122.68	118.90
1	A	1031	C	P-O3'-C3'	6.02	126.92	119.70
1	A	1158	C	C6-N1-C1'	-5.84	113.79	120.80
1	A	1158	C	C6-N1-C2	-5.41	118.14	120.30
1	A	183	C	N1-C2-O2	5.39	122.14	118.90
1	A	328	C	N1-C2-O2	5.15	121.99	118.90
1	A	754	C	N3-C2-O2	-5.12	118.32	121.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	J	57	VAL	Peptide
19	Z	235	LEU	Peptide
19	Z	342	ARG	Peptide

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	A	32930	0	16591	127	0
2	D	1643	0	1707	24	0
3	E	1144	0	1185	10	0
4	F	862	0	864	4	0
5	G	841	0	886	7	0
6	H	979	0	1031	5	0
7	I	1022	0	1070	18	0
8	J	796	0	836	12	0
9	K	877	0	887	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	L	114	0	131	3	0
11	M	884	0	941	8	0
12	N	805	0	844	13	0
13	O	714	0	734	2	0
14	P	649	0	666	7	0
15	Q	649	0	691	5	0
16	R	456	0	478	3	0
17	S	638	0	665	9	0
18	T	670	0	719	9	0
19	Z	2448	0	2419	27	0
20	A	67	0	0	0	0
20	N	1	0	0	0	0
20	P	1	0	0	0	0
20	T	1	0	0	0	0
20	Z	1	0	0	0	0
21	Z	1	0	0	0	0
22	Z	32	0	13	0	0
All	All	49225	0	33358	249	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 (249) 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)
3:E:89:HIS:HB2	3:E:139:ALA:HB2	1.78	0.66
19:Z:252:ALA:HA	19:Z:268:PRO:HG3	1.79	0.65
1:A:376:G:H5"	14:P:5:ARG:HB2	1.81	0.62
8:J:6:ILE:HG22	8:J:102:LEU:HA	1.83	0.61
3:E:76:LEU:HD11	3:E:120:VAL:HG22	1.83	0.61
2:D:14:ARG:HG3	2:D:56:ARG:HH22	1.67	0.60
7:I:24:GLY:H	7:I:61:LEU:HA	1.67	0.59
17:S:18:LYS:HE3	17:S:31:LEU:HD23	1.84	0.59
19:Z:132:ILE:HG12	19:Z:165:LEU:HD11	1.83	0.59
1:A:579:A:H4'	13:O:54:ARG:HH22	1.68	0.59
1:A:1320:C:N3	17:S:36:ARG:NH1	2.50	0.59
1:A:1437:A:H5"	18:T:29:ARG:HH12	1.67	0.59
3:E:55:GLU:HG3	3:E:57:PRO:HD2	1.85	0.59
1:A:261:U:OP2	18:T:74:ARG:NH2	2.37	0.58
1:A:664:G:H22	1:A:741:G:H1	1.50	0.58
7:I:123:ARG:NH1	7:I:124:ARG:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:68:ASP:HB3	13:O:72:ARG:HH21	1.68	0.58
1:A:782:A:H62	1:A:800:G:H21	1.49	0.58
8:J:26:VAL:HG12	8:J:30:LYS:HE3	1.86	0.57
19:Z:159:LEU:HB3	19:Z:189:MET:HG3	1.87	0.57
1:A:1438:G:H1	1:A:1463:U:H3	1.53	0.57
7:I:114:LYS:NZ	7:I:118:LEU:O	2.38	0.57
11:M:67:GLY:HA2	11:M:70:ARG:HD3	1.86	0.56
1:A:1221:G:OP1	17:S:36:ARG:NH1	2.38	0.56
14:P:18:GLN:HE22	14:P:35:ARG:HE	1.53	0.56
1:A:618:C:O2'	14:P:14:ARG:NH2	2.38	0.56
17:S:50:ALA:HB1	17:S:57:HIS:HB3	1.86	0.56
1:A:683:G:H1	1:A:707:U:H3	1.51	0.56
3:E:160:SER:HA	3:E:164:ILE:HD12	1.87	0.56
1:A:1406:U:O2	1:A:1517:G:N2	2.39	0.56
8:J:40:ILE:HD11	8:J:73:LEU:HD23	1.88	0.56
19:Z:37:GLY:H	19:Z:82:ARG:HB3	1.72	0.55
19:Z:47:ARG:HH12	19:Z:66:ILE:HG21	1.72	0.55
1:A:787:A:N1	1:A:795:C:N4	2.53	0.55
2:D:22:LYS:HE3	2:D:31:LYS:HE2	1.87	0.55
1:A:979:C:OP1	1:A:1223:C:N4	2.40	0.55
1:A:981:U:OP1	12:N:9:ARG:NH1	2.40	0.55
2:D:188:ARG:HH12	2:D:193:ALA:HA	1.72	0.55
1:A:1071:C:OP1	3:E:54:ARG:NH2	2.40	0.55
1:A:1368:A:H5"	7:I:114:LYS:HB3	1.89	0.55
8:J:9:ARG:HB2	8:J:99:GLN:HB2	1.89	0.55
1:A:81:A:N1	1:A:86:G:N1	2.50	0.54
9:K:51:GLY:O	9:K:56:ARG:NH1	2.41	0.54
1:A:297:G:N2	1:A:300:A:OP2	2.39	0.53
1:A:1373:G:O6	7:I:13:LYS:NZ	2.41	0.53
1:A:627:G:OP1	14:P:35:ARG:NH1	2.42	0.53
1:A:974:A:OP1	12:N:69:ARG:NH2	2.42	0.53
1:A:1147:C:H1'	7:I:18:ARG:HH12	1.73	0.53
12:N:6:MET:HB3	12:N:63:ARG:HH12	1.72	0.53
8:J:52:LEU:HD23	8:J:62:ARG:HG2	1.91	0.53
1:A:1375:A:O2'	5:G:102:ARG:NH2	2.41	0.53
7:I:120:LYS:HB2	7:I:123:ARG:HB3	1.91	0.52
15:Q:12:VAL:HG22	15:Q:23:VAL:HG22	1.91	0.52
1:A:69:G:O6	1:A:98:A:N6	2.42	0.52
1:A:600:A:H5"	6:H:89:LYS:HD2	1.91	0.52
1:A:1377:A:OP2	5:G:9:GLN:NE2	2.42	0.52
19:Z:111:ASP:HB3	19:Z:114:ASP:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:ARG:O	2:D:56:ARG:NH2	2.42	0.52
12:N:49:GLN:NE2	17:S:11:ILE:O	2.42	0.52
5:G:16:PRO:HG3	7:I:43:THR:HG23	1.91	0.52
1:A:933:G:N7	5:G:3:ARG:NH1	2.58	0.52
1:A:401:C:O2'	1:A:621:A:N3	2.41	0.52
1:A:958:A:OP1	17:S:55:ARG:NH1	2.39	0.52
19:Z:123:ILE:HG13	19:Z:209:ILE:HB	1.91	0.52
1:A:187:G:N2	1:A:190:A:OP2	2.43	0.51
2:D:71:GLN:NE2	2:D:75:TYR:OH	2.43	0.51
19:Z:45:ILE:N	19:Z:53:ASP:O	2.42	0.51
7:I:112:GLU:OE2	7:I:115:LYS:NZ	2.42	0.51
19:Z:45:ILE:HG23	19:Z:255:LEU:HB3	1.93	0.51
1:A:771:G:N2	1:A:808:C:O2	2.43	0.51
1:A:950:U:O4	11:M:105:ASN:ND2	2.44	0.51
1:A:890:G:O2'	1:A:906:A:N6	2.43	0.51
12:N:42:TRP:HE1	12:N:45:VAL:HG23	1.76	0.51
1:A:768:A:N3	1:A:1512:U:O2'	2.43	0.50
1:A:618:C:N4	1:A:621:A:OP2	2.44	0.50
1:A:1118:U:H4'	7:I:85:ARG:HH22	1.76	0.50
12:N:69:ARG:HG3	12:N:71:HIS:H	1.76	0.50
2:D:192:SER:OG	2:D:194:ASP:OD1	2.30	0.50
1:A:1316:G:N1	1:A:1319:A:OP2	2.45	0.50
19:Z:143:ARG:HD2	19:Z:332:ILE:HG12	1.94	0.50
1:A:1137:C:O2	1:A:1138:G:N2	2.43	0.50
1:A:1418:A:N6	1:A:1482:G:O2'	2.44	0.50
1:A:59:A:H3'	1:A:331:G:H22	1.75	0.50
1:A:58:C:O2'	1:A:388:G:N7	2.43	0.49
5:G:111:ARG:NH1	5:G:123:GLU:OE2	2.39	0.49
11:M:83:LEU:HD21	17:S:66:MET:HG2	1.94	0.49
12:N:48:LEU:HD12	12:N:51:LEU:HD12	1.94	0.49
15:Q:25:ILE:HB	15:Q:42:THR:HB	1.94	0.49
1:A:846:G:OP1	16:R:48:ARG:NH2	2.45	0.49
1:A:107:G:OP1	1:A:325:A:N6	2.45	0.49
1:A:926:G:H1	19:Z:342:ARG:HH21	1.61	0.49
1:A:711:G:OP1	4:F:53:LYS:NZ	2.43	0.49
1:A:1147:C:O2	7:I:18:ARG:NH2	2.45	0.49
1:A:1309:G:OP2	11:M:98:ARG:NH2	2.46	0.49
7:I:106:ARG:NH1	7:I:107:ASP:O	2.45	0.49
9:K:15:GLN:HE21	9:K:17:SER:HB2	1.77	0.49
1:A:993:G:O2'	1:A:994:A:N7	2.46	0.49
1:A:1304:G:H21	1:A:1333:A:H62	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:A:H5”	9:K:115:PRO:HB3	1.94	0.48
18:T:4:ILE:HG22	18:T:6:SER:H	1.78	0.48
1:A:373:A:O2’	1:A:451:A:N7	2.46	0.48
1:A:255:G:H4’	15:Q:19:LYS:HD2	1.96	0.48
2:D:37:ALA:HB3	2:D:42:GLY:HA2	1.96	0.48
1:A:405:U:O4	2:D:2:ALA:N	2.46	0.48
8:J:52:LEU:HB2	12:N:81:ARG:HD2	1.95	0.48
19:Z:162:ILE:HG12	19:Z:191:SER:HB2	1.95	0.48
1:A:1402:4OC:HM22	1:A:1403:C:H5’	1.96	0.48
3:E:97:GLN:HB3	3:E:124:LEU:HB2	1.95	0.47
1:A:76:G:H22	1:A:93:U:H3	1.61	0.47
1:A:517:G:N2	1:A:530:G:O5’	2.46	0.47
1:A:766:A:OP2	1:A:812:G:N2	2.46	0.47
1:A:562:U:OP2	10:L:14:ARG:NH1	2.40	0.47
1:A:730:G:O2’	1:A:814:A:N6	2.47	0.47
1:A:979:C:O2	12:N:59:ARG:NH1	2.46	0.47
19:Z:56:SER:OG	19:Z:58:ASP:OD1	2.33	0.47
6:H:88:ARG:NH2	6:H:91:GLU:OE2	2.48	0.47
1:A:55:A:OP2	1:A:352:C:N4	2.40	0.47
1:A:888:G:H21	1:A:909:A:H62	1.62	0.47
2:D:76:TYR:HE1	2:D:201:VAL:HG13	1.80	0.47
1:A:1144:G:O6	1:A:1145:A:N6	2.48	0.47
1:A:1166:G:N1	1:A:1169:A:OP2	2.47	0.47
1:A:1439:G:OP2	18:T:33:LYS:NZ	2.45	0.47
5:G:15:ASP:OD1	5:G:44:TYR:OH	2.30	0.47
7:I:113:ARG:NH1	12:N:101:TRP:OXT	2.48	0.47
1:A:18:C:OP1	3:E:132:ASN:ND2	2.46	0.47
2:D:95:GLU:HA	2:D:100:ASN:HD22	1.80	0.47
1:A:25:C:H41	1:A:559:A:H61	1.63	0.46
1:A:231:U:H2’	1:A:232:G:H8	1.80	0.46
1:A:1008:U:H3	1:A:1021:A:H61	1.63	0.46
1:A:1238:A:H5’	1:A:1336:C:H41	1.80	0.46
11:M:3:ARG:O	11:M:57:ARG:NH2	2.39	0.46
1:A:263:A:OP1	18:T:74:ARG:NH1	2.49	0.46
1:A:948:C:H2’	1:A:949:A:H8	1.80	0.46
1:A:406:G:H21	2:D:116:GLN:HE22	1.64	0.46
1:A:407:U:H5”	2:D:112:ALA:HB1	1.98	0.46
1:A:451:A:H61	1:A:481:G:H5’	1.79	0.46
1:A:1086:U:H3’	1:A:1087:G:H8	1.79	0.46
2:D:75:TYR:OH	2:D:97:ARG:NH1	2.49	0.46
2:D:98:LEU:HB2	2:D:135:TYR:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:12:ARG:HG3	7:I:13:LYS:H	1.80	0.46
1:A:138:G:H1	1:A:225:C:H42	1.63	0.46
1:A:148:G:H1	1:A:174:A:H61	1.64	0.46
2:D:104:ARG:HH21	2:D:111:ARG:HH22	1.64	0.46
1:A:10:A:HO2'	1:A:507:C:HO2'	1.64	0.46
1:A:842:U:H3'	1:A:843:U:H4'	1.98	0.46
1:A:1308:U:OP2	11:M:98:ARG:NH1	2.48	0.46
2:D:57:GLU:HG2	2:D:199:LEU:HB2	1.98	0.46
1:A:86:G:H21	1:A:87:C:H41	1.63	0.45
19:Z:51:HIS:HA	19:Z:65:ASN:HA	1.98	0.45
1:A:407:U:H2'	1:A:408:A:H8	1.81	0.45
1:A:1124:G:H1	1:A:1149:C:H42	1.65	0.45
1:A:1126:U:O4	8:J:9:ARG:NH1	2.50	0.45
14:P:34:GLU:OE2	14:P:60:TRP:NE1	2.49	0.45
16:R:63:ARG:HB3	16:R:70:TYR:HE1	1.81	0.45
1:A:837:U:H2'	1:A:838:G:H8	1.82	0.45
9:K:88:GLY:O	9:K:93:ARG:NH1	2.49	0.45
18:T:9:LYS:HE3	18:T:13:GLN:HE21	1.81	0.45
2:D:11:LEU:HB3	2:D:63:ARG:HD3	1.99	0.45
5:G:69:VAL:HG23	5:G:100:ALA:HB1	2.00	0.45
10:L:7:LEU:HD21	10:L:12:ARG:HE	1.82	0.44
15:Q:14:SER:HB3	15:Q:22:VAL:HB	1.99	0.44
17:S:53:ASN:HB3	17:S:75:ALA:HB1	2.00	0.44
8:J:12:ALA:HB3	8:J:18:ILE:HB	1.98	0.44
1:A:64:G:H4'	1:A:65:A:H3'	1.99	0.44
2:D:91:LEU:HD13	2:D:191:LEU:HD12	1.99	0.44
1:A:928:G:O2'	1:A:1533:C:OP1	2.36	0.44
6:H:2:SER:OG	6:H:3:MET:N	2.49	0.44
7:I:22:LYS:HB3	7:I:62:ASP:HB2	1.99	0.44
1:A:594:U:H3	1:A:645:G:H1	1.65	0.44
1:A:662:U:H2'	1:A:663:A:H8	1.82	0.44
17:S:11:ILE:HG13	17:S:38:SER:HB2	2.00	0.44
1:A:390:U:O3'	14:P:28:ARG:NH1	2.51	0.43
9:K:13:ARG:NH2	9:K:77:TYR:OH	2.51	0.43
1:A:824:G:H2'	1:A:825:A:H8	1.83	0.43
1:A:916:U:H2'	1:A:917:G:H8	1.83	0.43
2:D:144:SER:HA	2:D:179:GLU:HA	2.00	0.43
19:Z:183:ILE:HD13	19:Z:325:ARG:HH12	1.81	0.43
1:A:880:C:H2'	1:A:881:G:H8	1.83	0.43
1:A:1118:U:OP1	7:I:11:ARG:NH1	2.45	0.43
19:Z:88:ALA:HB3	19:Z:91:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:6:ILE:HG12	4:F:89:VAL:HG12	2.01	0.43
11:M:24:GLY:O	11:M:29:ARG:NH1	2.51	0.43
19:Z:47:ARG:HE	19:Z:49:GLY:H	1.65	0.43
8:J:55:PRO:HA	12:N:81:ARG:HH22	1.83	0.43
19:Z:47:ARG:HH12	19:Z:66:ILE:HD13	1.84	0.43
7:I:6:TYR:HB2	7:I:21:ILE:HB	2.00	0.43
8:J:59:LYS:HE2	8:J:62:ARG:HH21	1.83	0.43
3:E:74:VAL:HG21	3:E:144:LEU:HB3	2.00	0.43
1:A:377:G:H2'	1:A:378:G:H8	1.83	0.42
1:A:481:G:O2'	1:A:483:C:N4	2.50	0.42
1:A:707:U:OP1	9:K:87:LYS:NZ	2.39	0.42
12:N:69:ARG:HD2	12:N:70:PRO:HD2	2.01	0.42
1:A:575:G:H4'	1:A:576:C:H5"	2.01	0.42
1:A:1452:C:O2	1:A:1453:G:N2	2.52	0.42
1:A:112:G:N2	1:A:330:C:N3	2.66	0.42
3:E:106:ILE:HD11	3:E:124:LEU:HD23	2.00	0.42
9:K:31:ILE:HG12	9:K:46:THR:HG22	2.00	0.42
18:T:80:THR:O	18:T:84:ASN:ND2	2.51	0.42
2:D:83:LYS:O	2:D:89:ASN:ND2	2.44	0.42
19:Z:110:PRO:HB3	19:Z:116:VAL:HG22	2.00	0.42
1:A:352:C:O2'	1:A:354:G:OP1	2.31	0.42
19:Z:156:ILE:HD12	19:Z:186:ARG:HB3	2.02	0.42
1:A:689:C:OP1	9:K:29:ASN:ND2	2.53	0.42
1:A:720:C:H5"	16:R:41:PRO:HB3	2.02	0.42
1:A:401:C:H2'	1:A:402:G:H8	1.84	0.42
1:A:765:G:N1	1:A:812:G:O2'	2.45	0.42
8:J:49:PHE:HB2	8:J:65:TYR:HB2	2.02	0.42
6:H:29:SER:HB2	6:H:59:LEU:HB2	2.02	0.42
1:A:928:G:H2'	1:A:929:G:H8	1.85	0.42
3:E:161:VAL:HG12	3:E:162:GLU:H	1.85	0.42
4:F:35:LYS:N	4:F:65:GLU:O	2.53	0.42
1:A:126:G:OP1	1:A:605:U:O2'	2.30	0.41
1:A:536:C:N4	1:A:537:G:O6	2.53	0.41
1:A:697:U:O2'	1:A:785:G:O2'	2.34	0.41
1:A:1234:C:OP1	7:I:119:ARG:NH2	2.51	0.41
2:D:172:GLU:HB2	2:D:181:THR:HB	2.01	0.41
1:A:745:G:H2'	1:A:746:A:H8	1.84	0.41
9:K:26:SER:OG	9:K:29:ASN:O	2.33	0.41
9:K:83:GLU:HG2	9:K:109:ASN:HB2	2.02	0.41
15:Q:31:HIS:HA	15:Q:32:PRO:HD3	1.96	0.41
19:Z:239:ILE:O	19:Z:249:THR:OG1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:C:OP2	10:L:12:ARG:NH2	2.53	0.41
8:J:6:ILE:HG13	8:J:76:ILE:HB	2.01	0.41
18:T:66:LEU:HD23	18:T:67:ILE:HG23	2.01	0.41
19:Z:143:ARG:HG2	19:Z:275:LEU:HD11	2.00	0.41
1:A:113:G:H1'	1:A:354:G:H5'	2.02	0.41
1:A:1342:C:H2'	1:A:1343:G:C8	2.56	0.41
12:N:34:VAL:HG12	12:N:37:SER:H	1.85	0.41
1:A:843:U:OP1	1:A:846:G:N1	2.38	0.41
6:H:15:ARG:NH2	6:H:75:ILE:O	2.43	0.41
14:P:40:ASN:HB3	14:P:43:ALA:HB2	2.03	0.41
19:Z:162:ILE:HG21	19:Z:189:MET:HG2	2.03	0.41
1:A:1239:A:H61	1:A:1296:C:H2'	1.86	0.41
1:A:1493:A:H62	19:Z:50:MET:HA	1.86	0.41
4:F:19:PRO:HA	4:F:22:ILE:HD12	2.02	0.41
1:A:131:A:O2'	1:A:262:A:O2'	2.36	0.41
1:A:269:C:H2'	1:A:270:A:C8	2.56	0.41
1:A:1067:A:N1	1:A:1108:G:O2'	2.52	0.41
1:A:1218:C:H2'	1:A:1219:A:C8	2.55	0.41
1:A:1226:C:H41	11:M:103:LYS:HE2	1.84	0.41
19:Z:44:VAL:HG22	19:Z:54:VAL:HG22	2.02	0.41
19:Z:123:ILE:HD12	19:Z:265:ILE:HD12	2.02	0.41
1:A:824:G:H2'	1:A:825:A:C8	2.56	0.41
19:Z:81:TRP:HZ3	19:Z:83:PRO:HB3	1.86	0.41
2:D:17:THR:HG21	2:D:60:LYS:HD2	2.03	0.40
1:A:4:U:O2'	1:A:6:G:OP1	2.37	0.40
1:A:176:C:H5"	18:T:24:ARG:HH22	1.86	0.40
2:D:54:GLN:NE2	2:D:202:GLU:OE1	2.55	0.40
2:D:85:ASN:HB3	2:D:88:GLU:HB2	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	
2	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
3	E	153/155 (99%)	147 (96%)	6 (4%)	0	100	100
4	F	104/106 (98%)	102 (98%)	2 (2%)	0	100	100
5	G	103/130 (79%)	100 (97%)	3 (3%)	0	100	100
6	H	127/129 (98%)	124 (98%)	3 (2%)	0	100	100
7	I	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
8	J	97/99 (98%)	92 (95%)	5 (5%)	0	100	100
9	K	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
10	L	12/14 (86%)	12 (100%)	0	0	100	100
11	M	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
12	N	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
13	O	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
14	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
15	Q	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
16	R	53/55 (96%)	51 (96%)	2 (4%)	0	100	100
17	S	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
18	T	84/86 (98%)	84 (100%)	0	0	100	100
19	Z	311/313 (99%)	294 (94%)	16 (5%)	1 (0%)	41	76
All	All	2018/2079 (97%)	1938 (96%)	79 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	Z	236	THR

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	D	172/172 (100%)	172 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	E	118/118 (100%)	117 (99%)	1 (1%)	81 89
4	F	92/92 (100%)	91 (99%)	1 (1%)	73 84
5	G	88/109 (81%)	87 (99%)	1 (1%)	73 84
6	H	104/104 (100%)	104 (100%)	0	100 100
7	I	105/105 (100%)	102 (97%)	3 (3%)	42 64
8	J	87/87 (100%)	87 (100%)	0	100 100
9	K	90/90 (100%)	89 (99%)	1 (1%)	73 84
10	L	12/12 (100%)	11 (92%)	1 (8%)	11 36
11	M	92/92 (100%)	92 (100%)	0	100 100
12	N	83/83 (100%)	82 (99%)	1 (1%)	71 84
13	O	76/76 (100%)	75 (99%)	1 (1%)	69 82
14	P	65/65 (100%)	65 (100%)	0	100 100
15	Q	74/74 (100%)	74 (100%)	0	100 100
16	R	48/48 (100%)	48 (100%)	0	100 100
17	S	70/70 (100%)	68 (97%)	2 (3%)	42 64
18	T	65/65 (100%)	65 (100%)	0	100 100
19	Z	267/267 (100%)	263 (98%)	4 (2%)	65 80
All	All	1708/1729 (99%)	1692 (99%)	16 (1%)	79 87

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

Mol	Chain	Res	Type
3	E	70	ASN
4	F	102	MET
5	G	52	GLN
7	I	106	ARG
7	I	113	ARG
7	I	123	ARG
9	K	128	ARG
10	L	5	ASN
12	N	85	ARG
13	O	89	ARG
17	S	29	LYS
17	S	78	ARG
19	Z	50	MET
19	Z	143	ARG

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Mol	Chain	Res	Type
19	Z	230	LEU
19	Z	232	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	71	GLN
2	D	116	GLN
3	E	70	ASN
4	F	3	HIS
4	F	55	HIS
5	G	52	GLN
7	I	75	GLN
7	I	126	GLN
9	K	15	GLN
11	M	91	HIS
11	M	105	ASN
14	P	18	GLN
17	S	57	HIS
18	T	84	ASN
19	Z	242	ASN
19	Z	291	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1530/1534 (99%)	246 (16%)	2 (0%)

All (246) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	5	U
1	A	6	G
1	A	9	G
1	A	19	A
1	A	22	G
1	A	39	G
1	A	44	A
1	A	47	C
1	A	48	C

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Mol	Chain	Res	Type
1	A	50	A
1	A	51	A
1	A	70	U
1	A	71	A
1	A	72	A
1	A	74	A
1	A	75	G
1	A	79	G
1	A	80	A
1	A	81	A
1	A	82	G
1	A	83	C
1	A	84	U
1	A	85	U
1	A	86	G
1	A	89	U
1	A	90	C
1	A	91	U
1	A	95	C
1	A	97	G
1	A	108	G
1	A	120	A
1	A	121	U
1	A	129	A
1	A	130	A
1	A	131	A
1	A	143	A
1	A	144	G
1	A	146	G
1	A	151	A
1	A	163	C
1	A	177	G
1	A	183	C
1	A	197	A
1	A	205	A
1	A	207	C
1	A	210	C
1	A	216	U
1	A	226	G
1	A	240	G
1	A	244	U
1	A	247	G

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Mol	Chain	Res	Type
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	346	G
1	A	348	G
1	A	351	G
1	A	352	C
1	A	354	G
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	397	A
1	A	398	U
1	A	406	G
1	A	411	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	422	C
1	A	423	G
1	A	429	U
1	A	444	G
1	A	452	A
1	A	456	A
1	A	457	G
1	A	463	U
1	A	467	U
1	A	468	A
1	A	481	G
1	A	484	G
1	A	486	U
1	A	497	G
1	A	499	A
1	A	509	A
1	A	511	C
1	A	518	C

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Mol	Chain	Res	Type
1	A	527	G7M
1	A	530	G
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	A
1	A	562	U
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	595	A
1	A	596	A
1	A	615	G
1	A	633	G
1	A	650	G
1	A	653	U
1	A	661	G
1	A	665	A
1	A	687	A
1	A	702	A
1	A	723	U
1	A	724	G
1	A	748	G
1	A	755	G
1	A	777	A
1	A	790	A
1	A	793	U
1	A	794	A
1	A	796	C
1	A	814	A
1	A	815	A
1	A	817	C
1	A	820	U
1	A	821	G
1	A	826	C
1	A	828	U
1	A	829	G
1	A	832	G
1	A	836	G

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Mol	Chain	Res	Type
1	A	841	C
1	A	842	U
1	A	843	U
1	A	846	G
1	A	851	G
1	A	864	A
1	A	870	U
1	A	889	A
1	A	914	A
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	969	A
1	A	971	G
1	A	975	A
1	A	976	G
1	A	977	A
1	A	992	U
1	A	993	G
1	A	1004	A
1	A	1009	U
1	A	1015	G
1	A	1017	U
1	A	1022	A
1	A	1025	U
1	A	1026	G
1	A	1028	C
1	A	1029	U
1	A	1030	U
1	A	1032	G
1	A	1033	G
1	A	1036	A
1	A	1037	C
1	A	1043	G
1	A	1054	C
1	A	1065	U
1	A	1085	U
1	A	1086	U
1	A	1092	A
1	A	1094	G

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Mol	Chain	Res	Type
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1133	G
1	A	1135	U
1	A	1136	C
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1141	C
1	A	1152	A
1	A	1159	U
1	A	1168	U
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1212	U
1	A	1213	A
1	A	1215	G
1	A	1224	U
1	A	1225	A
1	A	1238	A
1	A	1239	A
1	A	1257	A
1	A	1260	G
1	A	1275	A
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1300	G
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1323	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1364	U
1	A	1368	A

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Mol	Chain	Res	Type
1	A	1370	G
1	A	1377	A
1	A	1394	A
1	A	1397	C
1	A	1398	A
1	A	1400	C
1	A	1432	G
1	A	1441	A
1	A	1446	A
1	A	1451	U
1	A	1452	C
1	A	1454	G
1	A	1455	G
1	A	1491	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1503	A
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1529	G
1	A	1530	G
1	A	1533	C
1	A	1534	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	209	U
1	A	1031	C

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

11 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	2MG	A	966	1	18,26,27	0.89	1 (5%)	16,38,41	1.12	2 (12%)
1	MA6	A	1519	1	19,26,27	0.97	1 (5%)	18,38,41	1.90	6 (33%)
1	PSU	A	516	1,20	18,21,22	1.36	2 (11%)	22,30,33	1.83	3 (13%)
1	2MG	A	1207	1	18,26,27	0.90	1 (5%)	16,38,41	1.11	2 (12%)
1	UR3	A	1498	1,20	19,22,23	0.97	0	26,32,35	1.42	1 (3%)
1	G7M	A	527	1	20,26,27	1.10	2 (10%)	17,39,42	0.88	0
1	5MC	A	967	1	18,22,23	0.97	2 (11%)	26,32,35	1.13	3 (11%)
1	5MC	A	1407	1	18,22,23	0.93	2 (11%)	26,32,35	1.13	3 (11%)
1	MA6	A	1518	1	19,26,27	1.01	1 (5%)	18,38,41	1.93	6 (33%)
1	4OC	A	1402	1	20,23,24	0.76	0	26,32,35	1.01	2 (7%)
1	2MG	A	1516	1	18,26,27	0.90	1 (5%)	16,38,41	1.12	2 (12%)

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	2MG	A	966	1	-	0/5/27/28	0/3/3/3
1	MA6	A	1519	1	-	4/7/29/30	0/3/3/3
1	PSU	A	516	1,20	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	1	-	0/5/27/28	0/3/3/3
1	UR3	A	1498	1,20	-	2/7/25/26	0/2/2/2
1	G7M	A	527	1	-	3/3/25/26	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	MA6	A	1518	1	-	4/7/29/30	0/3/3/3
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	2MG	A	1516	1	-	0/5/27/28	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	516	PSU	C6-C5	3.29	1.39	1.35
1	A	527	G7M	C5-C4	2.88	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	5MC	C6-C5	2.77	1.39	1.34
1	A	1407	5MC	C6-C5	2.64	1.38	1.34
1	A	516	PSU	C4-N3	-2.61	1.34	1.38
1	A	1518	MA6	C5-C4	2.51	1.47	1.40
1	A	1207	2MG	C6-N1	-2.45	1.34	1.37
1	A	1519	MA6	C5-C4	2.43	1.47	1.40
1	A	1516	2MG	C6-N1	-2.39	1.34	1.37
1	A	527	G7M	C6-N1	-2.33	1.34	1.37
1	A	966	2MG	C6-N1	-2.32	1.34	1.37
1	A	967	5MC	C6-N1	-2.21	1.34	1.38
1	A	1407	5MC	C6-N1	-2.06	1.34	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1498	UR3	C4-N3-C2	-5.89	119.02	124.56
1	A	516	PSU	N1-C2-N3	5.79	121.69	115.13
1	A	1518	MA6	N1-C6-N6	4.84	122.15	117.06
1	A	516	PSU	C4-N3-C2	-3.69	121.03	126.34
1	A	1519	MA6	C10-N6-C6	-3.58	108.68	119.51
1	A	1519	MA6	C9-N6-C6	-3.51	108.87	119.51
1	A	967	5MC	C5-C6-N1	-3.36	119.89	123.34
1	A	1519	MA6	N3-C2-N1	-3.30	123.53	128.68
1	A	1518	MA6	C9-N6-C6	-3.30	109.53	119.51
1	A	516	PSU	O2-C2-N1	-3.28	119.18	122.79
1	A	1518	MA6	C10-N6-C6	-3.13	110.04	119.51
1	A	1519	MA6	C4-C5-N7	-3.11	106.16	109.40
1	A	1518	MA6	N3-C2-N1	-3.04	123.93	128.68
1	A	1407	5MC	C5-C6-N1	-2.98	120.28	123.34
1	A	1407	5MC	C5-C4-N3	-2.62	118.85	121.67
1	A	1519	MA6	N1-C6-N6	2.60	119.79	117.06
1	A	1519	MA6	C10-N6-C9	-2.56	107.88	116.12
1	A	967	5MC	C5-C4-N3	-2.46	119.02	121.67
1	A	1402	4OC	O2-C2-N3	-2.39	118.45	122.33
1	A	1518	MA6	C4-C5-N7	-2.38	106.92	109.40
1	A	1207	2MG	C8-N7-C5	2.36	107.49	102.99
1	A	966	2MG	C8-N7-C5	2.35	107.47	102.99
1	A	1407	5MC	O2-C2-N3	-2.35	118.51	122.33
1	A	1516	2MG	C8-N7-C5	2.35	107.46	102.99
1	A	1518	MA6	C10-N6-C9	-2.35	108.56	116.12
1	A	1516	2MG	C5-C6-N1	2.33	118.07	113.95
1	A	1207	2MG	C5-C6-N1	2.32	118.05	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	966	2MG	C5-C6-N1	2.29	118.00	113.95
1	A	967	5MC	O2-C2-N3	-2.13	118.87	122.33
1	A	1402	4OC	C6-C5-C4	2.01	119.42	116.96

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1518	MA6	C5-C6-N6-C9
1	A	1518	MA6	C5-C6-N6-C10
1	A	1518	MA6	N1-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C9
1	A	1519	MA6	C5-C6-N6-C10
1	A	1519	MA6	N1-C6-N6-C9
1	A	1519	MA6	N1-C6-N6-C10
1	A	1518	MA6	N1-C6-N6-C10
1	A	527	G7M	C4'-C5'-O5'-P
1	A	1498	UR3	O4'-C4'-C5'-O5'
1	A	1498	UR3	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1402	4OC	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 73 ligands modelled in this entry, 72 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	$\#\|Z\| > 2$
22	GNP	Z	402	20	29,34,34	1.70	6 (20%)	33,54,54	2.35	9 (27%)

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
22	GNP	Z	402	20	-	6/14/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	Z	402	GNP	PB-O3A	-4.80	1.53	1.59
22	Z	402	GNP	C6-N1	3.79	1.39	1.33
22	Z	402	GNP	PB-O2B	-3.09	1.48	1.56
22	Z	402	GNP	PG-O1G	3.01	1.50	1.46
22	Z	402	GNP	C8-N7	-2.22	1.30	1.34
22	Z	402	GNP	PG-O3G	-2.05	1.51	1.56

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	Z	402	GNP	C5-C6-N1	-8.60	111.67	123.43
22	Z	402	GNP	C2-N1-C6	5.56	124.77	115.93
22	Z	402	GNP	O2B-PB-O1B	3.68	117.63	109.92
22	Z	402	GNP	O3G-PG-O1G	-3.63	104.33	113.45
22	Z	402	GNP	C2-N3-C4	-3.12	111.80	115.36
22	Z	402	GNP	O2G-PG-O3G	2.95	115.50	107.64
22	Z	402	GNP	O1B-PB-N3B	-2.41	108.22	111.77
22	Z	402	GNP	PB-O3A-PA	-2.38	124.23	132.62
22	Z	402	GNP	N3-C2-N1	-2.29	124.16	127.22

There are no chirality outliers.

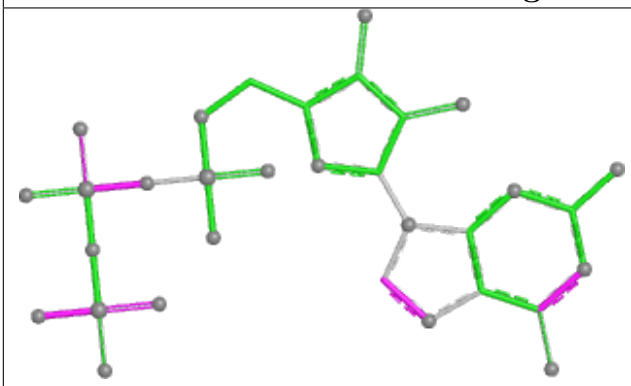
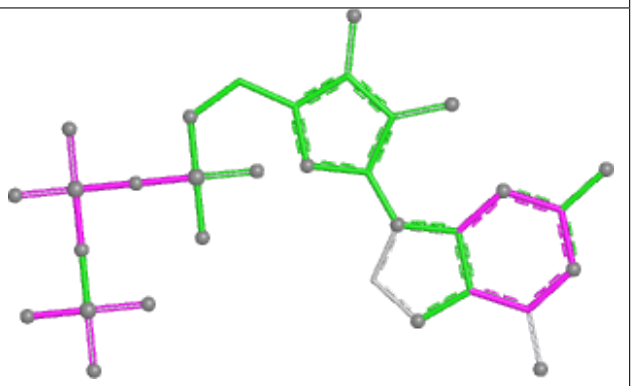
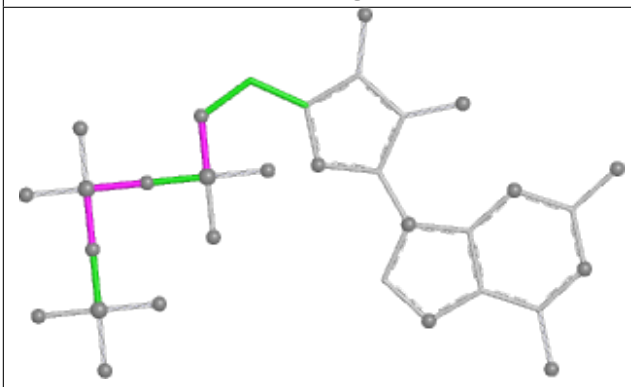
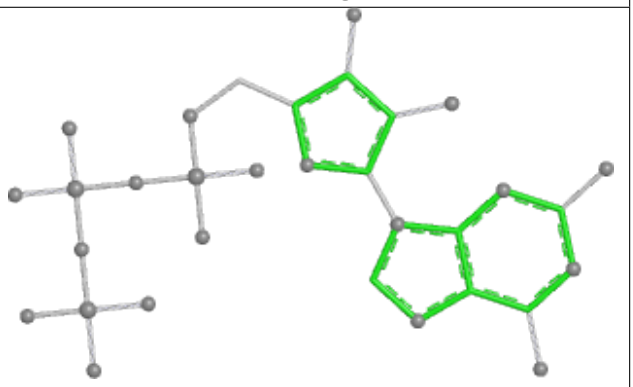
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	Z	402	GNP	PG-N3B-PB-O1B
22	Z	402	GNP	PG-N3B-PB-O3A
22	Z	402	GNP	PA-O3A-PB-O1B
22	Z	402	GNP	PA-O3A-PB-O2B
22	Z	402	GNP	C5'-O5'-PA-O1A
22	Z	402	GNP	C5'-O5'-PA-O3A

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.

Ligand GNP Z 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

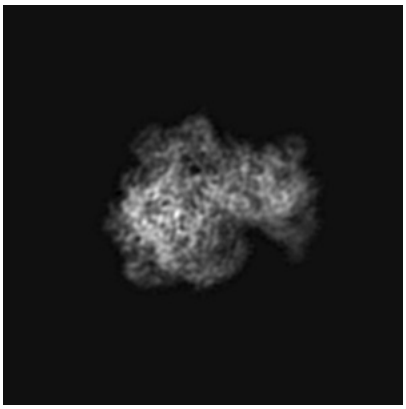
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3661. These allow visual inspection of the internal detail of the map and identification of artifacts.

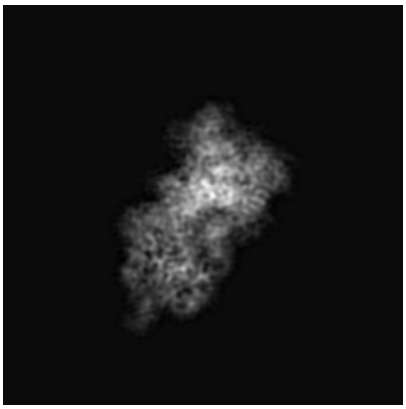
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

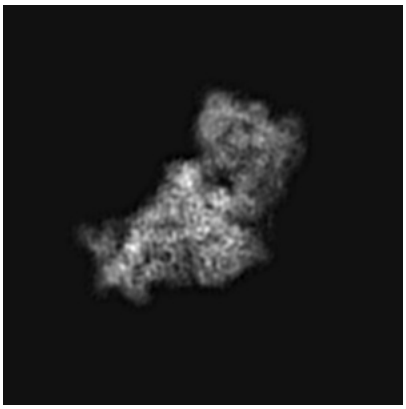
6.1.1 Primary map



X

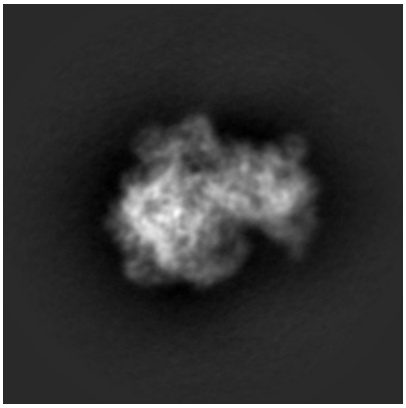


Y

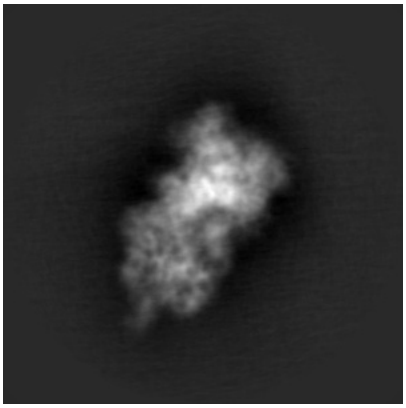


Z

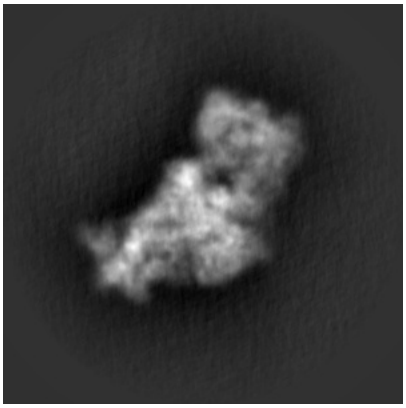
6.1.2 Raw map



X



Y



Z

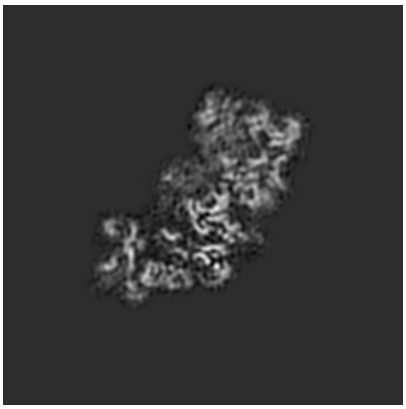
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

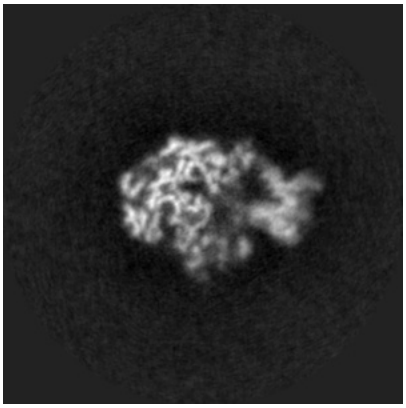
X Index: 128

Y Index: 128

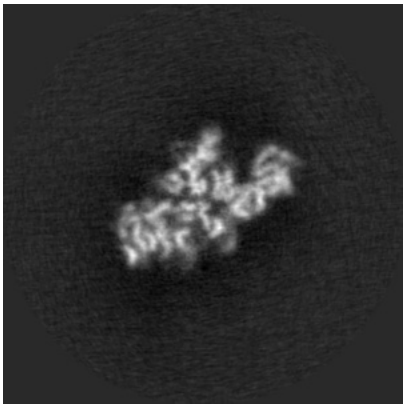


Z Index: 128

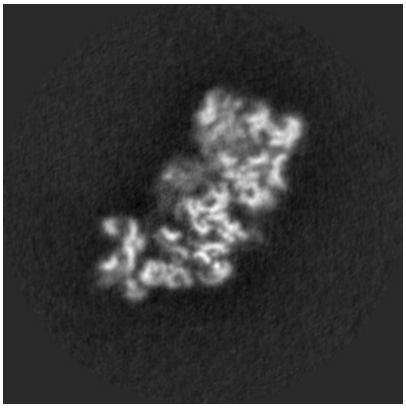
6.2.2 Raw map



X Index: 128



Y Index: 128

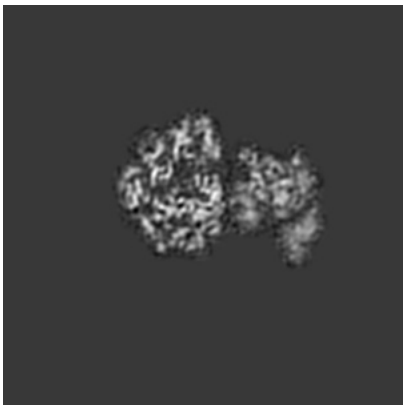


Z Index: 128

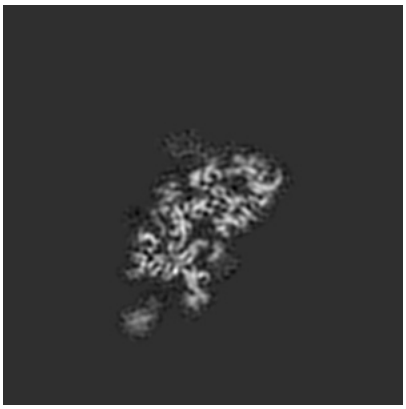
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

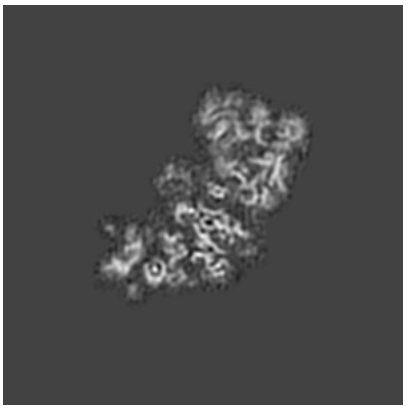
6.3.1 Primary map



X Index: 140

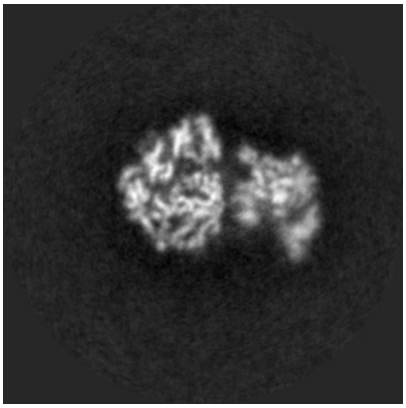


Y Index: 111

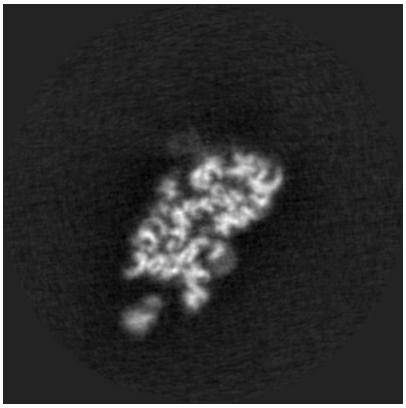


Z Index: 131

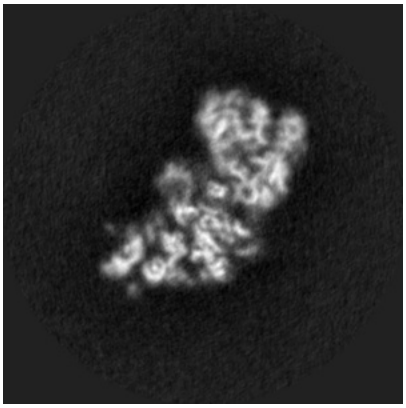
6.3.2 Raw map



X Index: 139



Y Index: 110

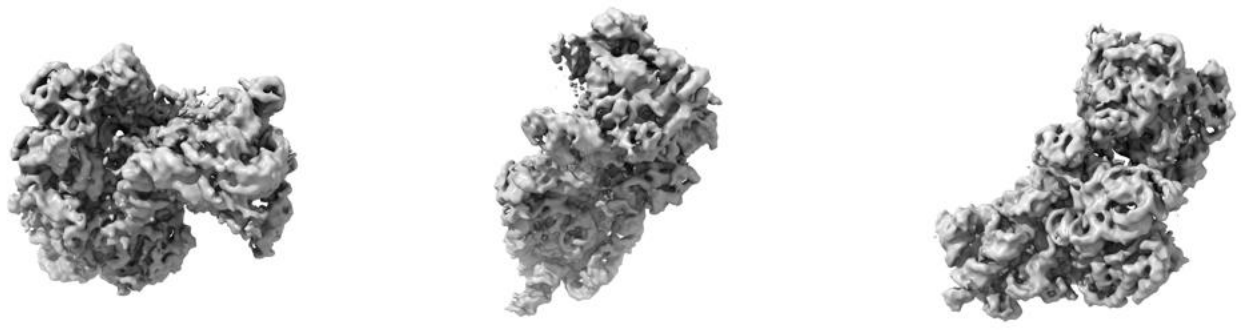


Z Index: 132

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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.

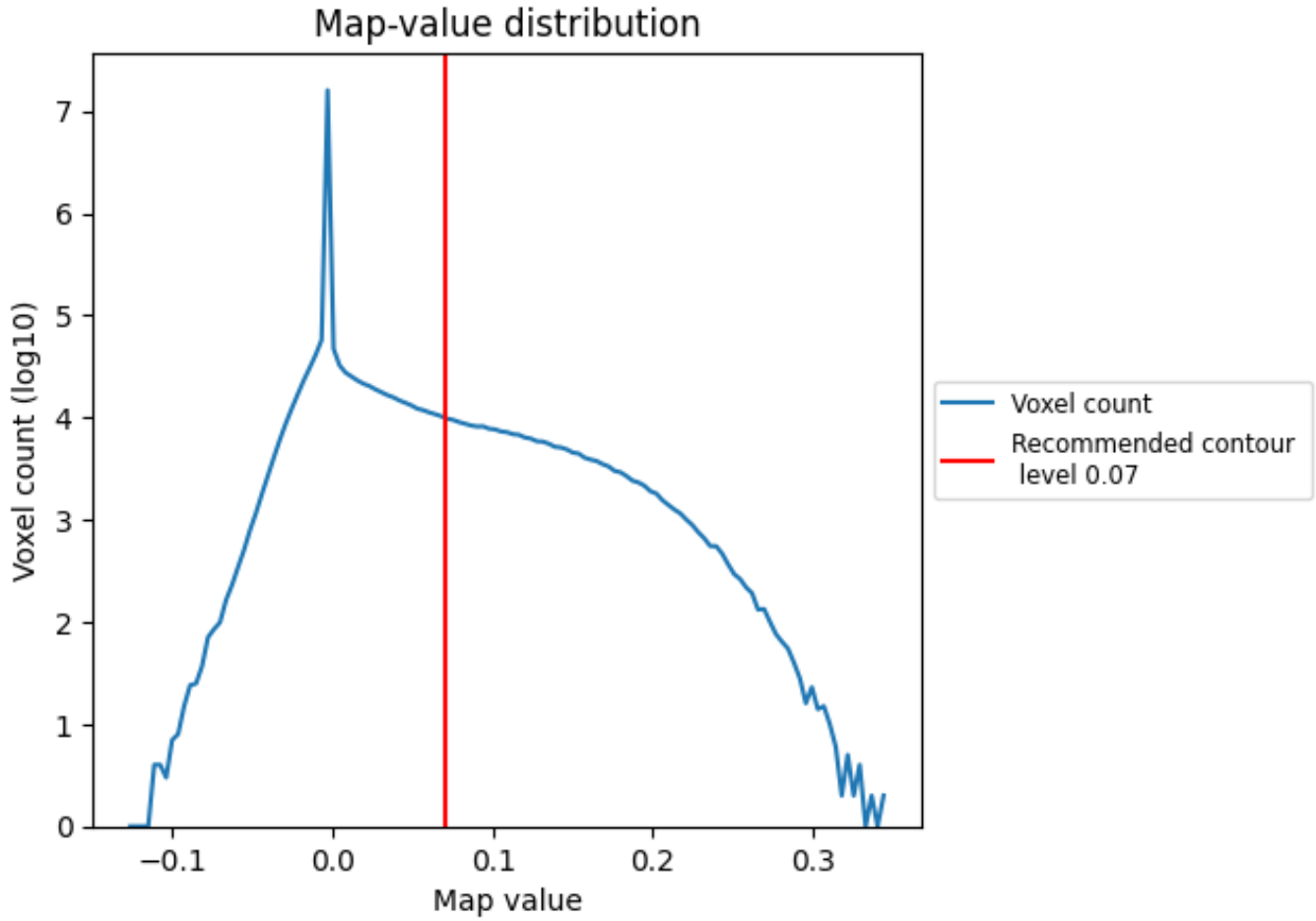
6.5 Mask visualisation (i)

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

7 Map analysis

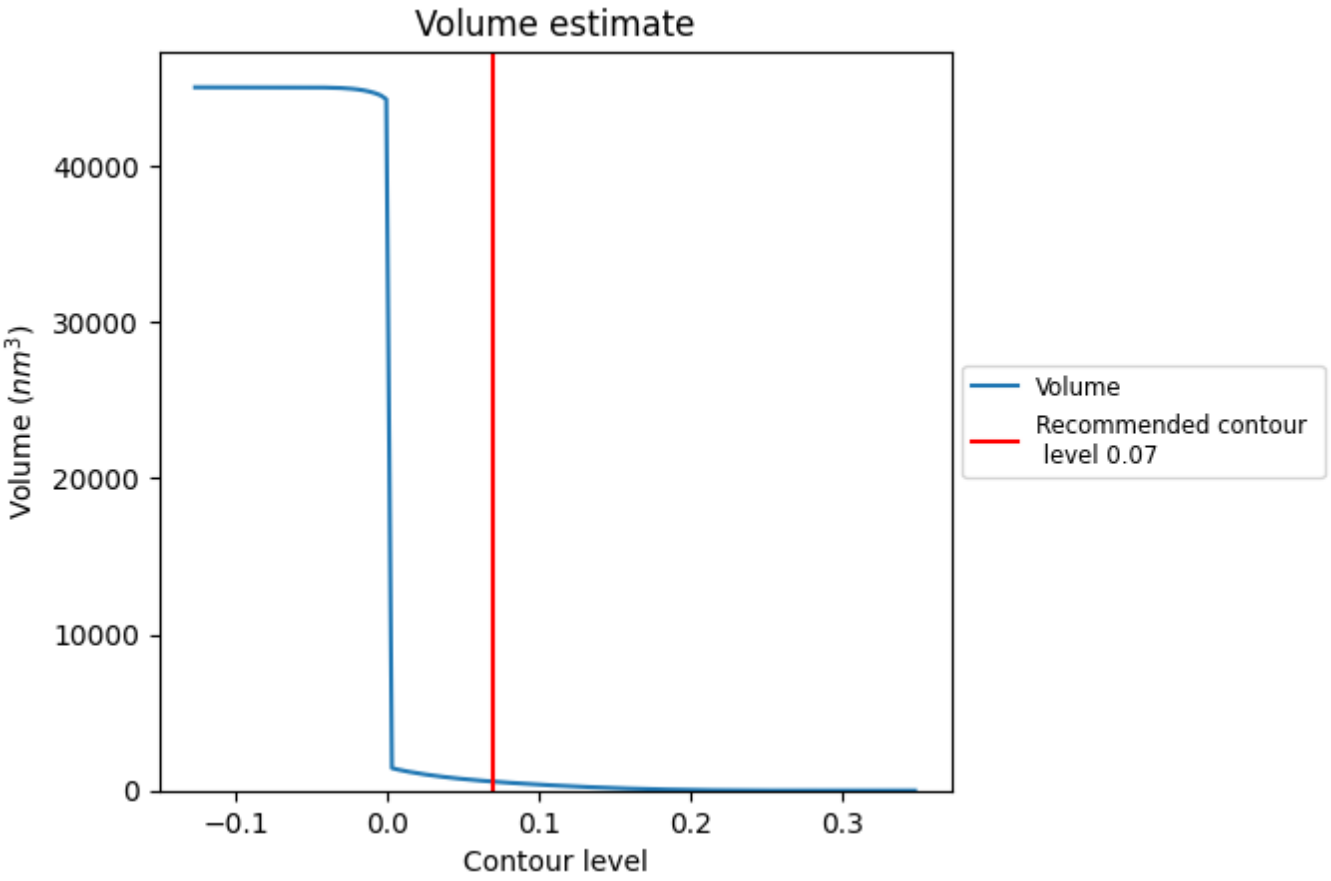
This section contains the results of statistical analysis of the map.

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.

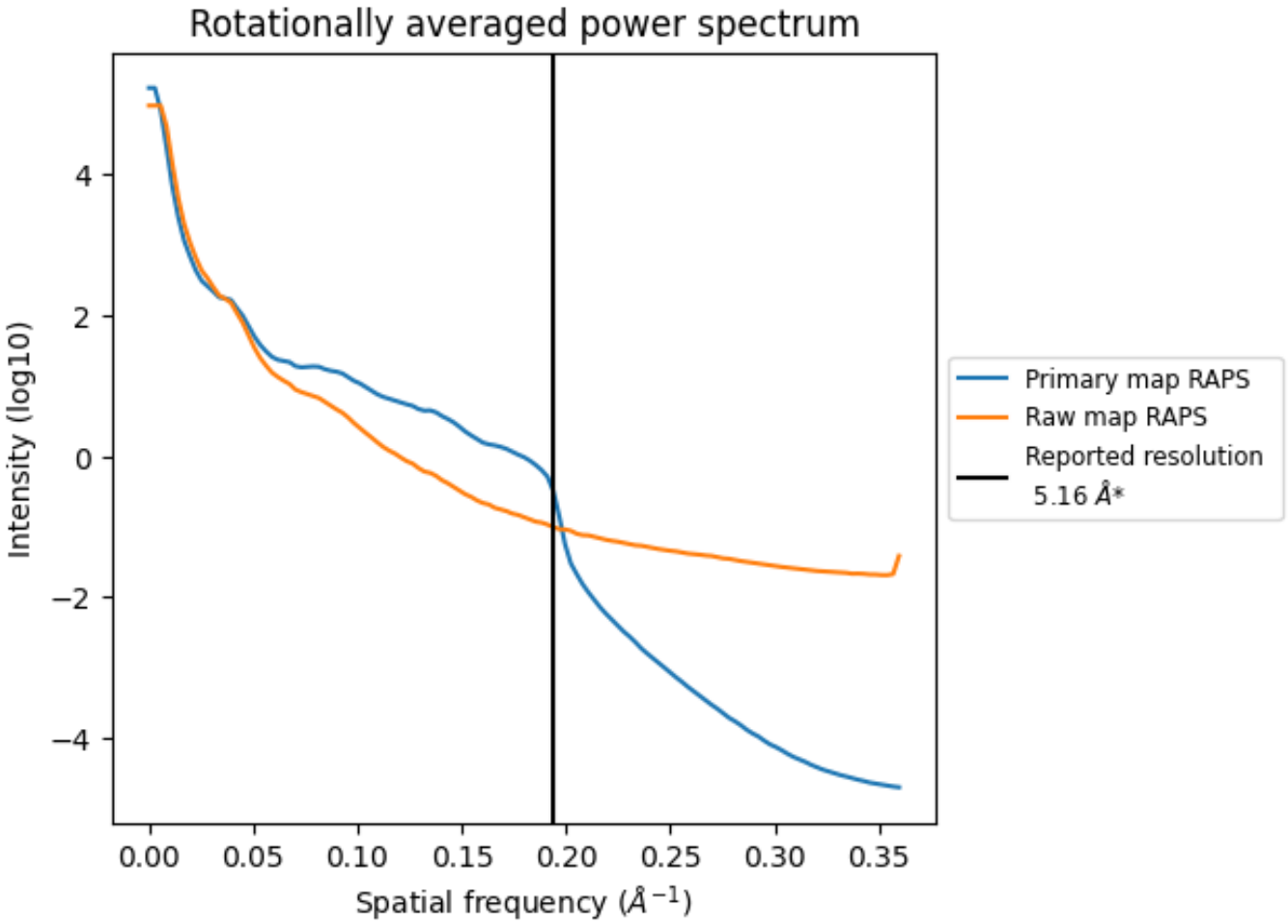
7.2 Volume estimate



The volume at the recommended contour level is 573 nm^3; this corresponds to an approximate mass of 517 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)

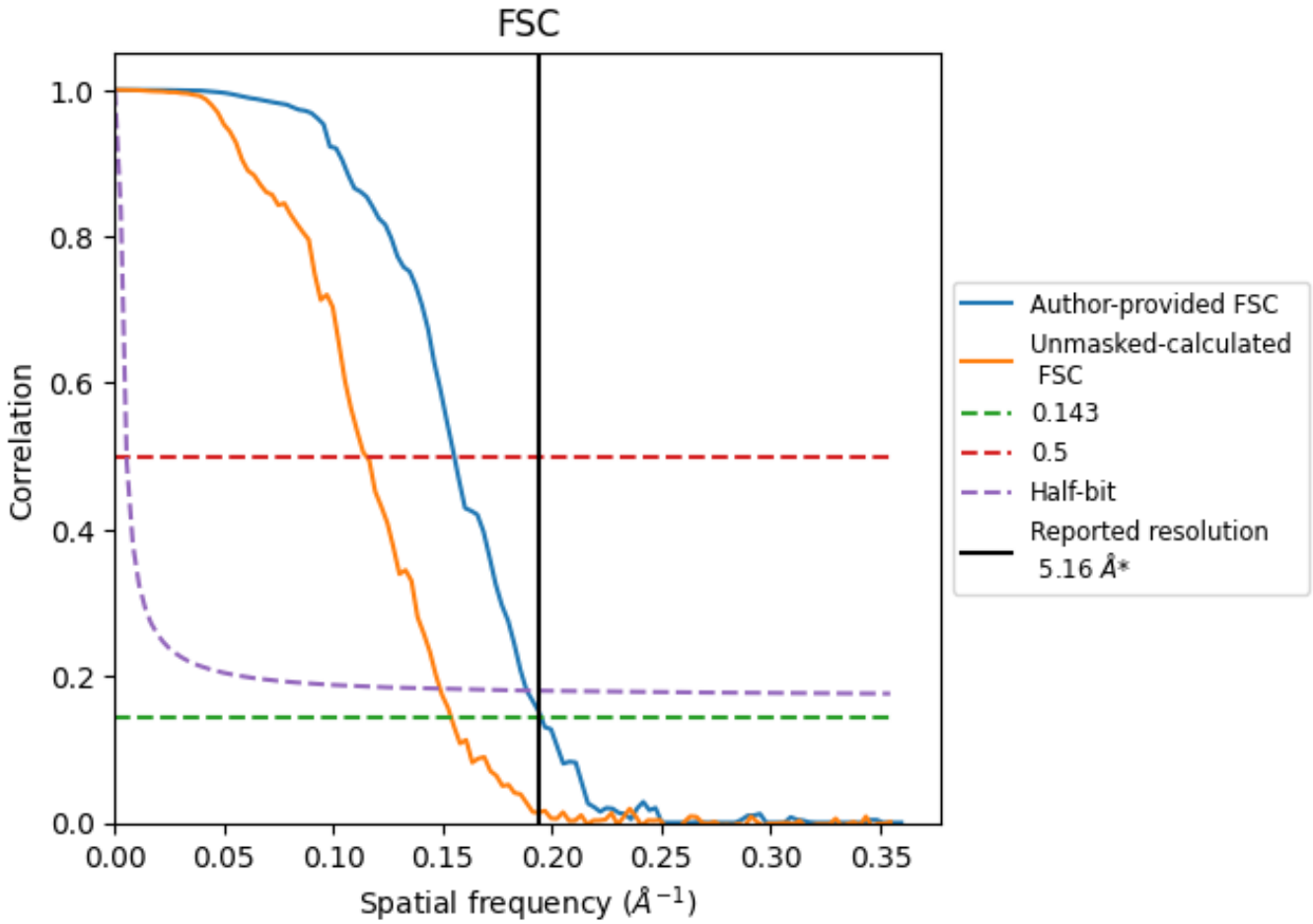


*Reported resolution corresponds to spatial frequency of 0.194 Å^{-1}

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 0.194 Å^{-1}

8.2 Resolution estimates (i)

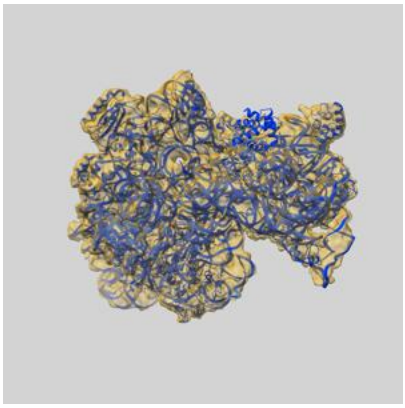
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.16	-	-
Author-provided FSC curve	5.13	6.44	5.31
Unmasked-calculated*	6.50	8.70	6.72

*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 6.50 differs from the reported value 5.16 by more than 10 %

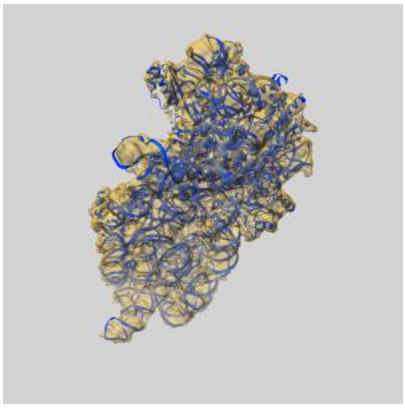
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3661 and PDB model 5NO2. Per-residue inclusion information can be found in section 3 on page 8.

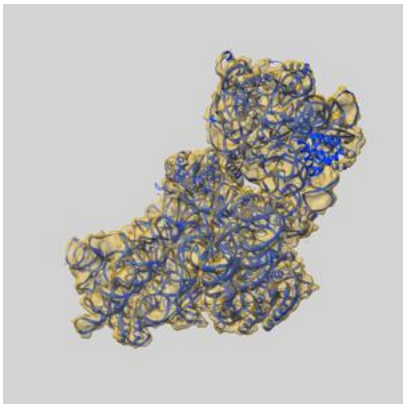
9.1 Map-model overlay



X



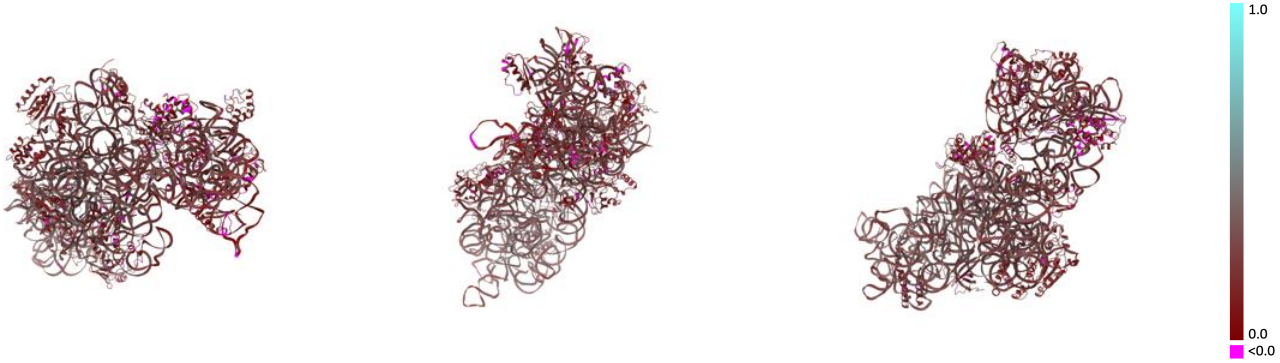
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

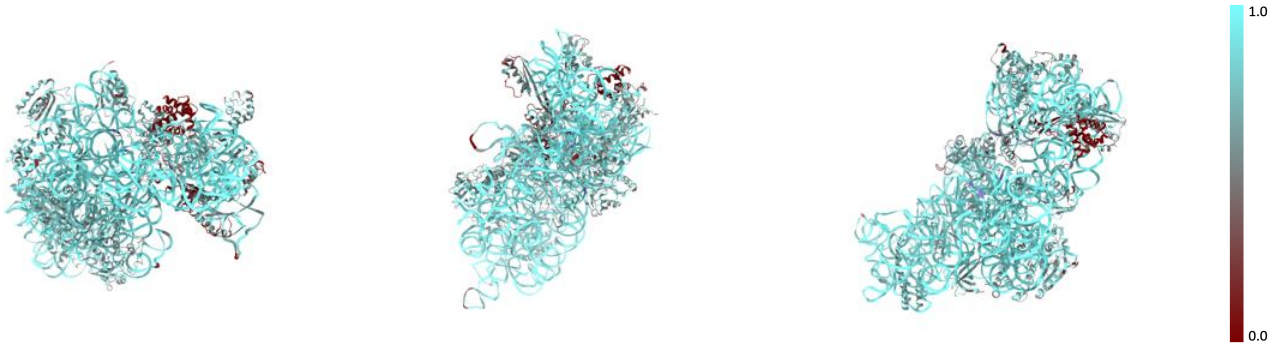
9.2 Q-score mapped to coordinate model (i)



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.

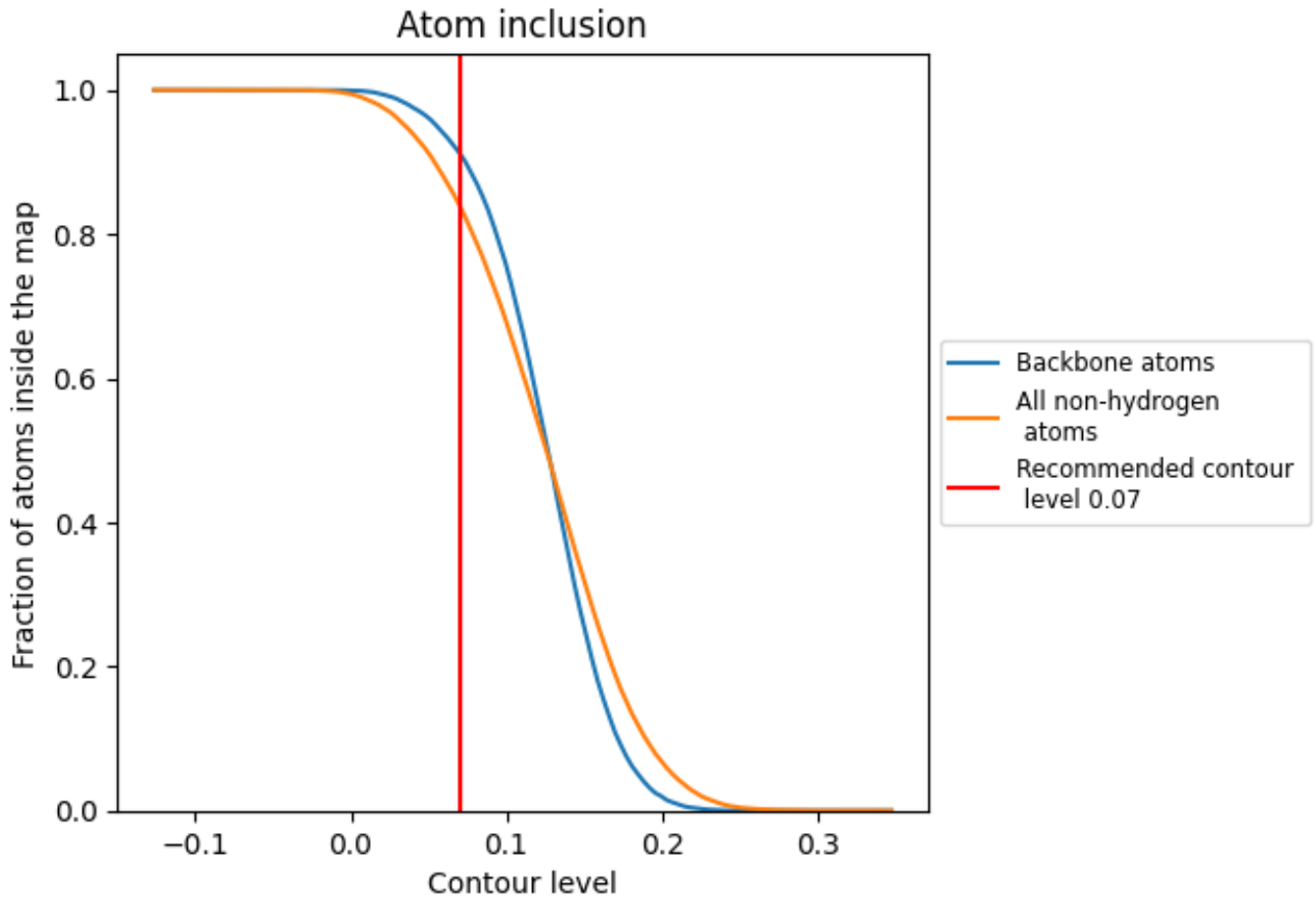
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 84% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8396	0.2460
A	0.9451	0.2730
D	0.6428	0.1880
E	0.7166	0.2310
F	0.6659	0.2140
G	0.0834	0.1020
H	0.7031	0.2140
I	0.5832	0.1490
J	0.4073	0.1590
K	0.6835	0.2100
L	0.1944	0.1190
M	0.6678	0.1810
N	0.4013	0.1370
O	0.7087	0.1970
P	0.7245	0.2440
Q	0.7077	0.2440
R	0.7391	0.2180
S	0.7219	0.1920
T	0.7424	0.2040
Z	0.6604	0.2030