wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 08:40 am GMT

PDB ID	:	5LL6
EMDB ID	:	EMD-4071
Title	:	Structure of the 40S ABCE1 post-splitting complex in ribosome recycling and translation initiation
Authors	:	Heuer, A.; Gerovac, M.; Schmidt, C.; Trowitzsch, S.; Preis, A.; Koetter, P.; Berninghausen, O.; Becker, T.; Beckmann, R.; Tampe, R.
Deposited on	:	2016-07-26
Resolution	:	3.90 Å(reported)

This is a wwPDB EM Validation Summary 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:

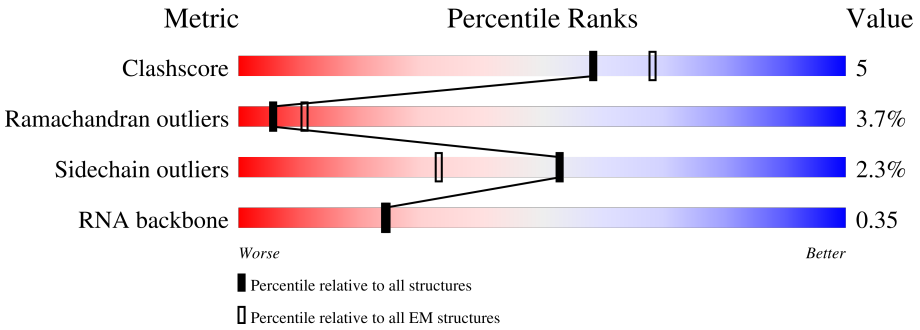
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	2	1798	5% 40% 30% · 26%
2	P	252	· 75% 6% · 18%
3	Q	255	11% 72% 11% 16%
4	R	254	6% 77% 11% · 11%
5	S	261	· 85% 14% ·
6	T	236	· 90% 6% ·
7	U	190	10% 86% 11% ·

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Mol	Chain	Length	Quality of chain
8	V	200	8% 82% 10% 6%
9	W	197	85% 7% 6%
10	X	156	13% 88% 10%
11	Y	151	91% 8%
12	Z	137	81% 9% 7%
13	a	87	94% 5%
14	b	130	92% 7%
15	c	145	91% 7%
16	d	135	91% 6%
17	e	119	76% 5% 18%
18	f	82	96%
19	g	63	8% 92% 5%
20	h	608	6% 87% 8% 5%

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 55262 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	1325	28237	12628	5001	9283	1325	0	0

- Molecule 2 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P	206	1577	1014	278	283	2	0	0

- Molecule 3 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	Q	214	1709	1084	310	311	4	0	0

- Molecule 4 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	R	226	1717	1098	305	312	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S4-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	T	226	1799	1129	346	321	3	0	0

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

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

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

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

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

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

- Molecule 10 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	155	Total	C	N	O	S	0	0
			1213	774	230	206	3		

- Molecule 11 is a protein called 40S ribosomal protein S13.

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

- Molecule 12 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Z	127	Total	C	N	O	S	0	0
			891	545	182	163	1		

- Molecule 13 is a protein called 40S ribosomal protein S21-A.

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

- Molecule 14 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 15 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 16 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	d	132	Total	C	N	O	0	0
			1060	669	206	185		

- Molecule 17 is a protein called 40S ribosomal protein S26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	e	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 18 is a protein called 40S ribosomal protein S27-A.

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

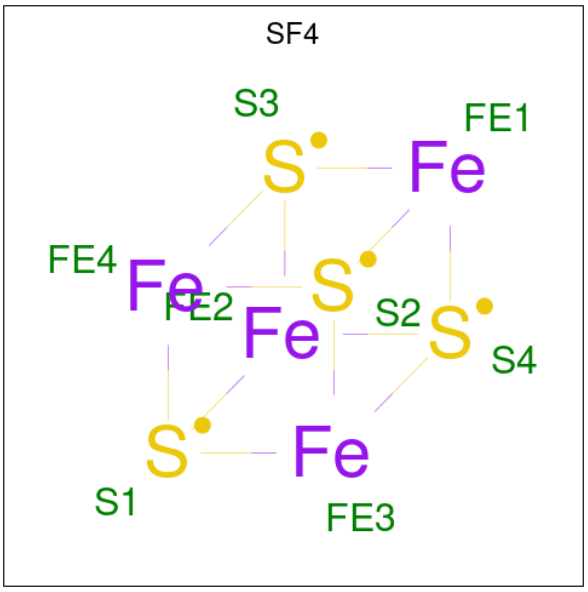
- Molecule 19 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	60	Total	C	N	O	S	0	0
			473	297	98	77	1		

- Molecule 20 is a protein called Translation initiation factor RLI1.

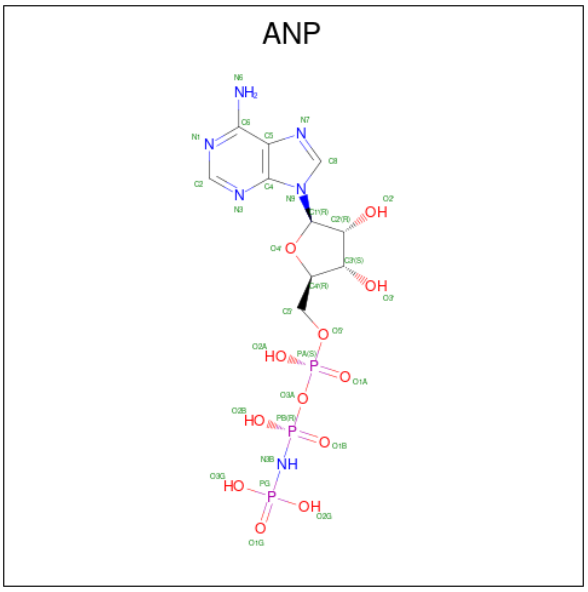
Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	578	Total	C	N	O	S	0	0
			4578	2933	791	831	23		

- Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
21	h	1	Total	Fe	S	0
			16	8	8	
21	h	1	Total	Fe	S	0
			16	8	8	

- Molecule 22 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
22	h	1	Total	C	N	O	P	0
			62	20	12	24	6	

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Mol	Chain	Residues	Atoms					AltConf
22	h	1	Total	C	N	O	P	0
			62	20	12	24	6	

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

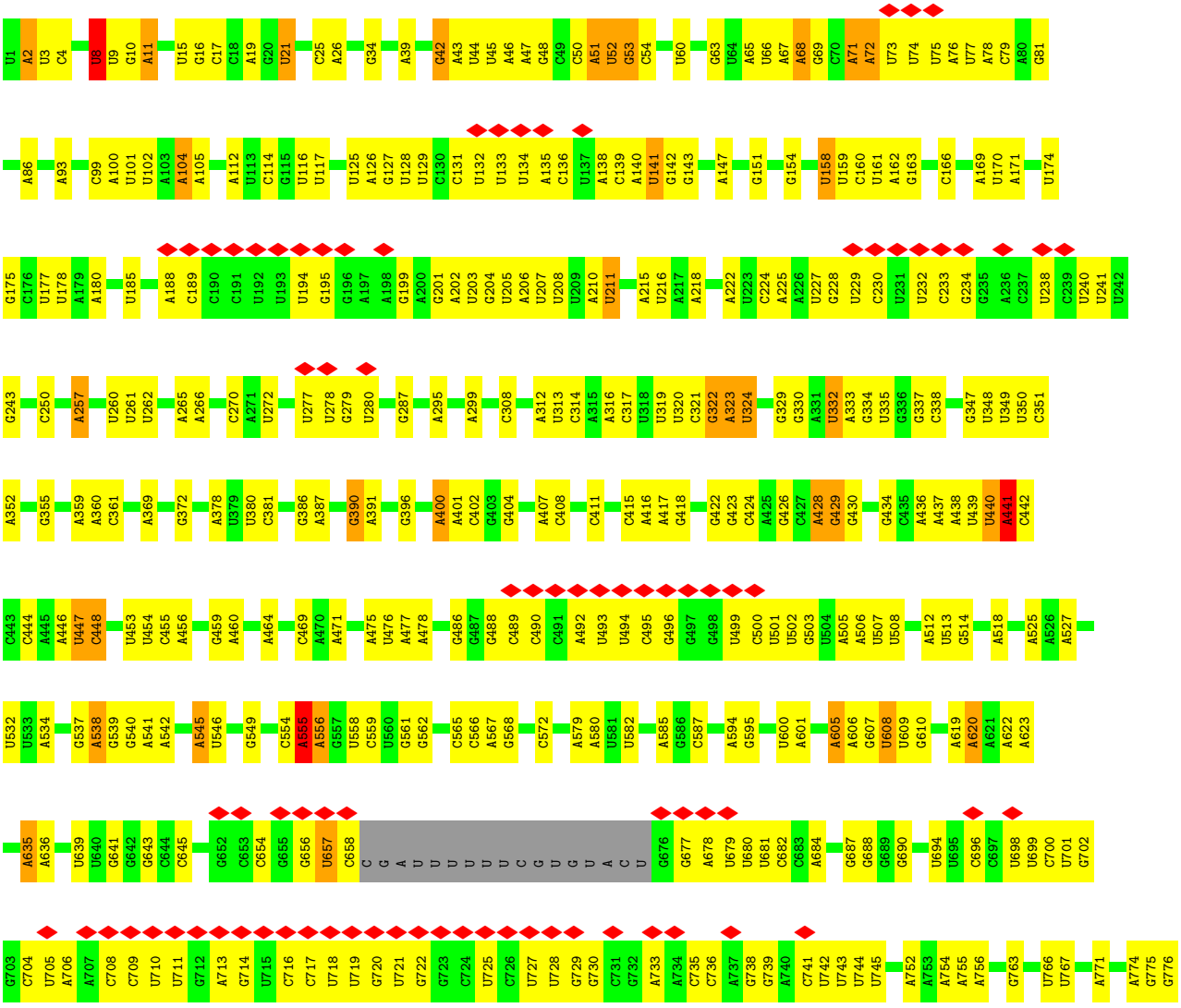
Mol	Chain	Residues	Atoms		AltConf
23	h	1	Total	Mg	0
			1	1	

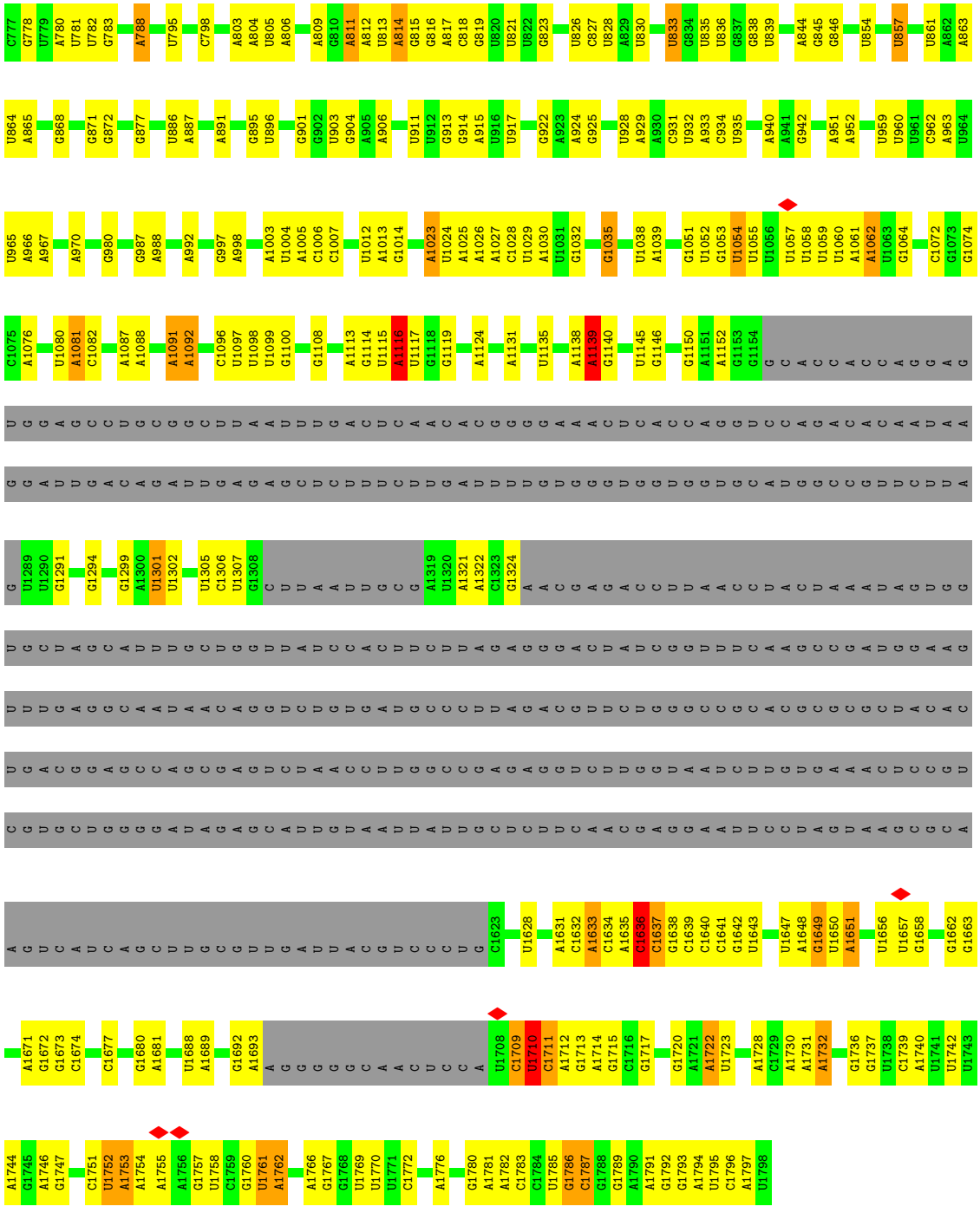
3 Residue-property plots (i)

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: 18S ribosomal RNA

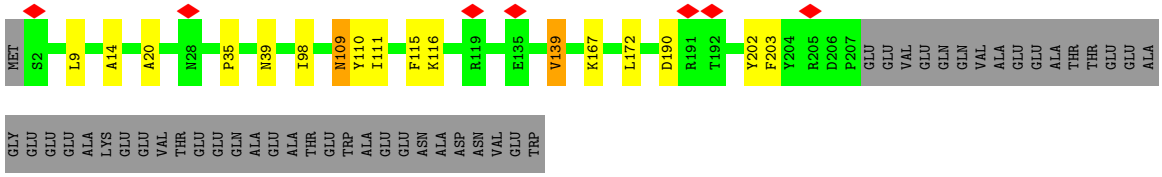
Chain 2:





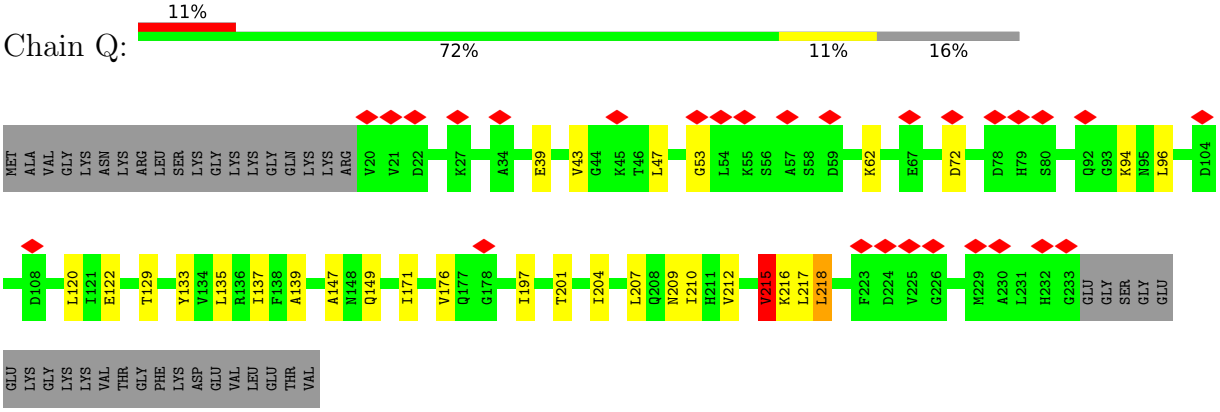
• Molecule 2: 40S ribosomal protein S0-A

Chain P:



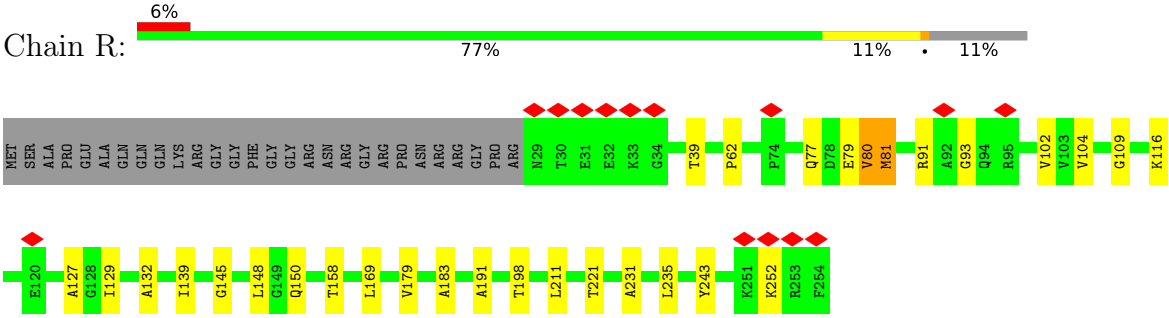
• Molecule 3: 40S ribosomal protein S1-A

Chain Q:



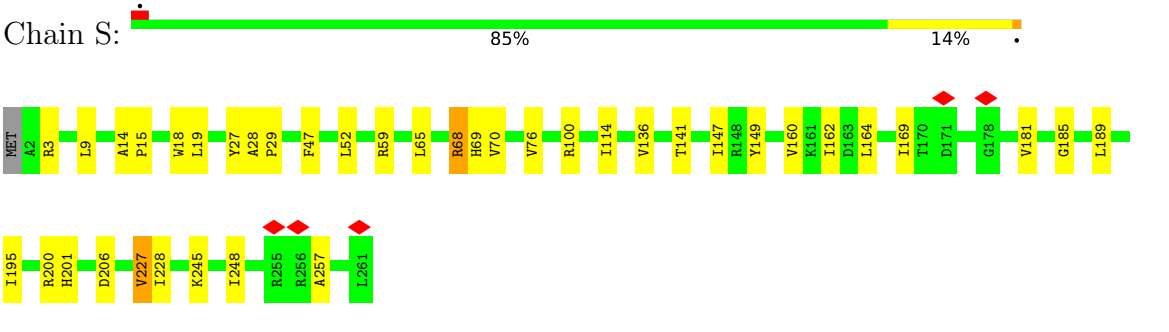
• Molecule 4: 40S ribosomal protein S2

Chain R:



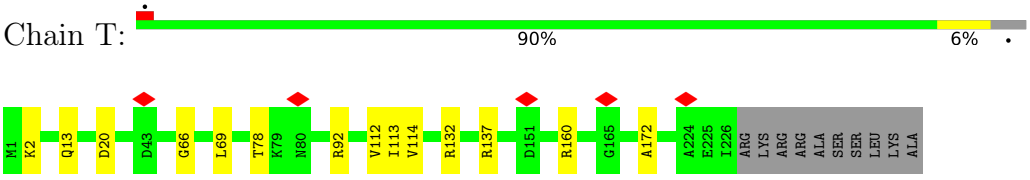
• Molecule 5: 40S ribosomal protein S4-A

Chain S:



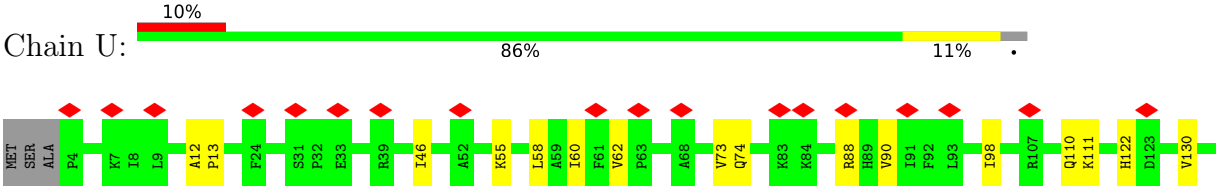
• Molecule 6: 40S ribosomal protein S6-A

Chain T:



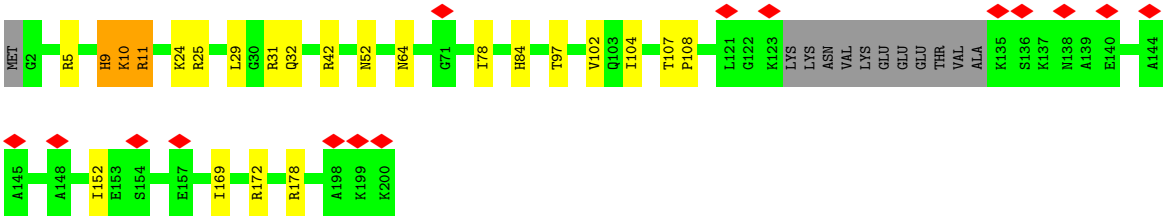
• Molecule 7: 40S ribosomal protein S7-A

Chain U:



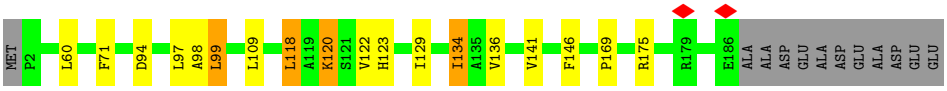
• Molecule 8: 40S ribosomal protein S8-A

Chain V:



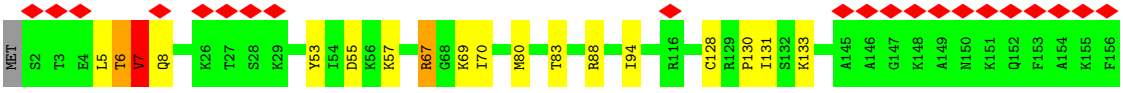
• Molecule 9: 40S ribosomal protein S9-A

Chain W:



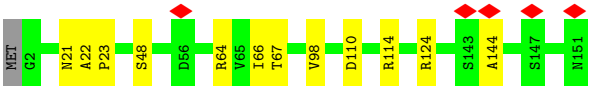
• Molecule 10: 40S ribosomal protein S11-A

Chain X:



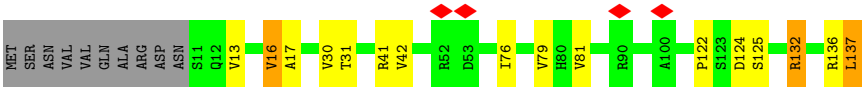
• Molecule 11: 40S ribosomal protein S13

Chain Y:



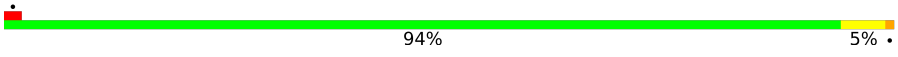
• Molecule 12: 40S ribosomal protein S14-A

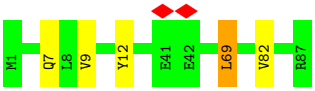
Chain Z:



• Molecule 13: 40S ribosomal protein S21-A

Chain a:





• Molecule 14: 40S ribosomal protein S22-A

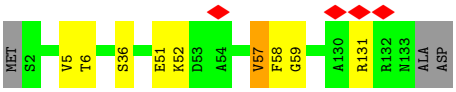
Chain b:

• Molecule 15: 40S ribosomal protein S23-A

Chain c:

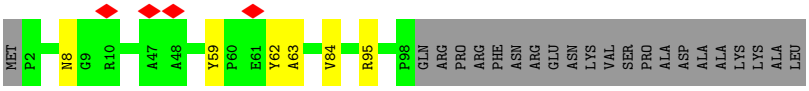
• Molecule 16: 40S ribosomal protein S24-A

Chain d:



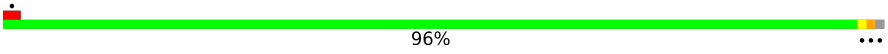
• Molecule 17: 40S ribosomal protein S26-A

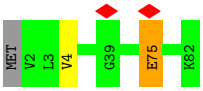
Chain e:



• Molecule 18: 40S ribosomal protein S27-A

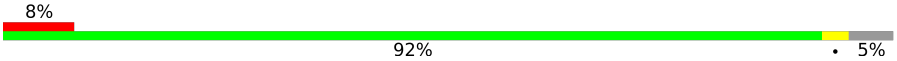
Chain f:

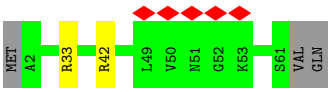




• Molecule 19: 40S ribosomal protein S30-A

Chain g:

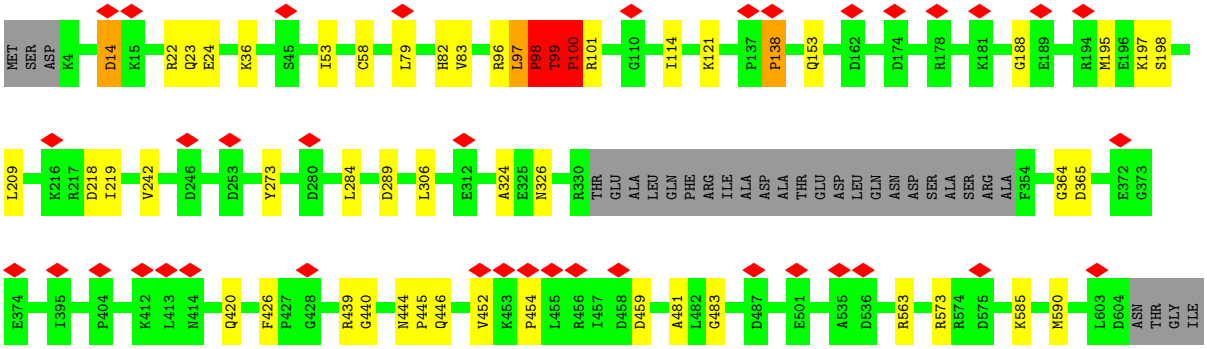




• Molecule 20: Translation initiation factor RLI1

Chain h:


6%
87%
8%
5%


MET SER ASP K4 D14 K15 R22 Q23 E24 K36 S45 I53 C58 L79 H82 V83 R96 L97 P98 T99 P100 R101 G110 I114 K121 P137 P138 Q153 D162 D174 R178 K181 G188 E189 R194 M195 E196 K197 S198
L209 K216 R217 D218 I219 V242 D246 D263 Y273 D280 L284 D289 L306 E312 A324 E325 N326 R330 THR GLU ALA LEU GLN PHE ARG ILE ALA ASP ALA THR GLU ASP LEU GLN ASN ASP SER ALA SER ARG ALA F354 G364 D365 E372 G373
E374 I395 P404 K412 L413 N414 Q420 F426 P427 G428 R439 G440 N444 P445 Q446 V452 K453 P454 L455 R456 I457 D458 D459 A481 L482 G483 D487 E501 A535 D536 R563 R573 R574 D575 K585 M590 L603 D604 ASN THR GLY ILE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	102000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	2.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.472	Depositor
Minimum map value	-0.195	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.038	Depositor
Map size (Å)	416.25598, 416.25598, 416.25598	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SF4, ANP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	2	0.50	7/31584 (0.0%)	0.75	30/49203 (0.1%)
2	P	0.47	0/1617	0.66	0/2215
3	Q	0.44	0/1735	0.67	0/2335
4	R	0.50	0/1748	0.68	0/2371
5	S	0.47	0/2109	0.76	3/2839 (0.1%)
6	T	0.45	0/1823	0.71	1/2439 (0.0%)
7	U	0.47	0/1506	0.68	0/2028
8	V	0.46	0/1514	0.69	0/2021
9	W	0.49	0/1519	0.73	0/2035
10	X	0.51	0/1239	0.73	2/1673 (0.1%)
11	Y	0.47	0/1215	0.70	0/1638
12	Z	0.45	0/901	0.76	2/1217 (0.2%)
13	a	0.47	0/693	0.73	1/935 (0.1%)
14	b	0.50	0/1038	0.76	1/1395 (0.1%)
15	c	0.54	0/1139	0.81	3/1518 (0.2%)
16	d	0.49	0/1074	0.68	0/1431
17	e	0.64	2/782 (0.3%)	0.82	1/1047 (0.1%)
18	f	0.43	0/620	0.64	0/838
19	g	0.49	0/481	0.82	2/640 (0.3%)
20	h	1.25	6/4665 (0.1%)	1.78	12/6294 (0.2%)
All	All	0.59	15/59002 (0.0%)	0.86	58/86112 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	2	0	2
7	U	0	2
20	h	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	14	ASP	CG-OD1	55.27	2.52	1.25
20	h	14	ASP	CG-OD2	50.09	2.40	1.25
1	2	1761	U	O3'-P	-44.73	1.07	1.61
1	2	1636	C	O3'-P	-30.52	1.24	1.61
1	2	1139	A	C6-N1	-12.73	1.26	1.35

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	h	14	ASP	CB-CG-OD2	-93.77	33.91	118.30
20	h	14	ASP	CB-CG-OD1	-73.93	51.77	118.30
20	h	14	ASP	OD1-CG-OD2	-37.02	52.95	123.30
20	h	99	THR	CA-C-N	-15.15	74.68	117.10
1	2	1761	U	P-O3'-C3'	-15.02	101.68	119.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	1139	A	Sidechain
1	2	8	U	Sidechain
7	U	55	LYS	Peptide
7	U	88	ARG	Peptide
20	h	14	ASP	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	28237	0	14200	162	0
2	P	1577	0	1567	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1709	0	1784	8	0
4	R	1717	0	1809	16	0
5	S	2068	0	2154	19	0
6	T	1799	0	1878	9	0
7	U	1481	0	1572	9	0
8	V	1489	0	1525	19	0
9	W	1494	0	1573	7	0
10	X	1213	0	1257	9	0
11	Y	1192	0	1255	8	0
12	Z	891	0	883	11	0
13	a	684	0	672	0	0
14	b	1021	0	1060	0	0
15	c	1121	0	1196	0	0
16	d	1060	0	1123	0	0
17	e	769	0	818	0	0
18	f	610	0	633	0	0
19	g	473	0	518	0	0
20	h	4578	0	4727	0	0
21	h	16	0	0	0	0
22	h	62	0	26	0	0
23	h	1	0	0	0	0
All	All	55262	0	42230	239	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 5.

The worst 5 of 239 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)
1:2:1636:C:C2'	1:2:1637:C:OP2	1.67	1.30
1:2:1636:C:O2'	1:2:1637:C:OP2	1.55	1.21
1:2:1636:C:N4	1:2:1638:G:N2	1.93	1.17
1:2:1080:U:O4	1:2:1091:A:N1	1.81	1.12
1:2:1636:C:N4	1:2:1638:G:C2	2.18	1.11

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	P	204/252 (81%)	175 (86%)	19 (9%)	10 (5%)	2	24
3	Q	212/255 (83%)	163 (77%)	35 (16%)	14 (7%)	1	19
4	R	224/254 (88%)	192 (86%)	21 (9%)	11 (5%)	2	24
5	S	258/261 (99%)	226 (88%)	22 (8%)	10 (4%)	3	28
6	T	224/236 (95%)	207 (92%)	13 (6%)	4 (2%)	8	42
7	U	182/190 (96%)	161 (88%)	15 (8%)	6 (3%)	4	31
8	V	184/200 (92%)	158 (86%)	21 (11%)	5 (3%)	5	35
9	W	183/197 (93%)	162 (88%)	14 (8%)	7 (4%)	3	28
10	X	153/156 (98%)	133 (87%)	14 (9%)	6 (4%)	3	28
11	Y	148/151 (98%)	134 (90%)	13 (9%)	1 (1%)	22	60
12	Z	125/137 (91%)	105 (84%)	18 (14%)	2 (2%)	9	44
13	a	85/87 (98%)	73 (86%)	8 (9%)	4 (5%)	2	24
14	b	127/130 (98%)	115 (91%)	8 (6%)	4 (3%)	4	32
15	c	142/145 (98%)	116 (82%)	20 (14%)	6 (4%)	3	26
16	d	130/135 (96%)	112 (86%)	10 (8%)	8 (6%)	1	20
17	e	95/119 (80%)	78 (82%)	13 (14%)	4 (4%)	3	26
18	f	79/82 (96%)	70 (89%)	7 (9%)	2 (2%)	5	36
19	g	58/63 (92%)	51 (88%)	7 (12%)	0	100	100
20	h	574/608 (94%)	472 (82%)	82 (14%)	20 (4%)	3	30
All	All	3387/3658 (93%)	2903 (86%)	360 (11%)	124 (4%)	6	29

5 of 124 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	111	ILE
3	Q	215	VAL

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Mol	Chain	Res	Type
3	Q	216	LYS
7	U	110	GLN
9	W	98	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	164/210 (78%)	164 (100%)	0	100	100
3	Q	191/224 (85%)	186 (97%)	5 (3%)	46	68
4	R	185/205 (90%)	183 (99%)	2 (1%)	73	84
5	S	221/222 (100%)	219 (99%)	2 (1%)	78	87
6	T	188/201 (94%)	187 (100%)	1 (0%)	88	93
7	U	165/170 (97%)	164 (99%)	1 (1%)	86	91
8	V	150/161 (93%)	150 (100%)	0	100	100
9	W	158/166 (95%)	154 (98%)	4 (2%)	47	69
10	X	129/137 (94%)	127 (98%)	2 (2%)	62	79
11	Y	127/128 (99%)	127 (100%)	0	100	100
12	Z	81/105 (77%)	78 (96%)	3 (4%)	34	60
13	a	74/74 (100%)	73 (99%)	1 (1%)	67	81
14	b	110/111 (99%)	106 (96%)	4 (4%)	35	61
15	c	119/120 (99%)	113 (95%)	6 (5%)	24	53
16	d	111/113 (98%)	109 (98%)	2 (2%)	59	77
17	e	83/101 (82%)	82 (99%)	1 (1%)	71	83
18	f	70/71 (99%)	69 (99%)	1 (1%)	67	81
19	g	50/54 (93%)	50 (100%)	0	100	100
20	h	513/537 (96%)	482 (94%)	31 (6%)	19	49
All	All	2889/3110 (93%)	2823 (98%)	66 (2%)	53	71

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	h	365	ASP
20	h	426	PHE
20	h	590	MET
14	b	103	ILE
14	b	93	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
16	d	107	GLN
20	h	95	HIS
20	h	78	ASN
20	h	210	GLN
6	T	190	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1319/1798 (73%)	501 (37%)	65 (4%)

5 of 501 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	3	U
1	2	4	C
1	2	8	U
1	2	9	U

5 of 65 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1097	U
1	2	1114	G
1	2	380	U
1	2	322	G
1	2	1633	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 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	ANP	h	703	23	29,33,33	1.42	6 (20%)	31,52,52	2.14	7 (22%)
21	SF4	h	701	20	0,12,12	-	-	-		
22	ANP	h	705	-	29,33,33	1.92	10 (34%)	31,52,52	2.07	9 (29%)
21	SF4	h	702	20	0,12,12	-	-	-		

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
22	ANP	h	703	23	-	5/14/38/38	0/3/3/3
21	SF4	h	701	20	-	-	0/6/5/5
22	ANP	h	705	-	-	2/14/38/38	0/3/3/3
21	SF4	h	702	20	-	-	0/6/5/5

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	705	ANP	PG-N3B	4.44	1.75	1.63
22	h	705	ANP	PB-N3B	3.98	1.73	1.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	h	705	ANP	PB-O3A	3.18	1.63	1.59
22	h	705	ANP	PB-O1B	3.18	1.51	1.46
22	h	703	ANP	PG-O1G	2.71	1.50	1.46

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	h	703	ANP	O1G-PG-N3B	-6.89	101.62	111.77
22	h	705	ANP	O1G-PG-N3B	-5.43	103.77	111.77
22	h	703	ANP	O2B-PB-O1B	4.44	119.23	109.92
22	h	705	ANP	O2B-PB-O1B	4.35	119.04	109.92
22	h	703	ANP	N3-C2-N1	-3.92	122.56	128.68

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

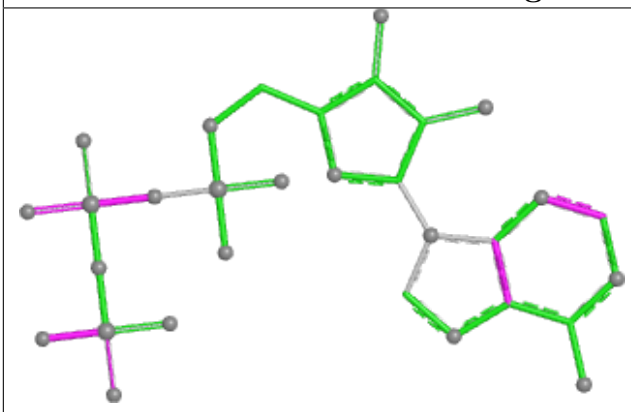
Mol	Chain	Res	Type	Atoms
22	h	703	ANP	PB-N3B-PG-O1G
22	h	703	ANP	PG-N3B-PB-O1B
22	h	703	ANP	C5'-O5'-PA-O1A
22	h	703	ANP	C5'-O5'-PA-O3A
22	h	705	ANP	C4'-C5'-O5'-PA

There are no ring outliers.

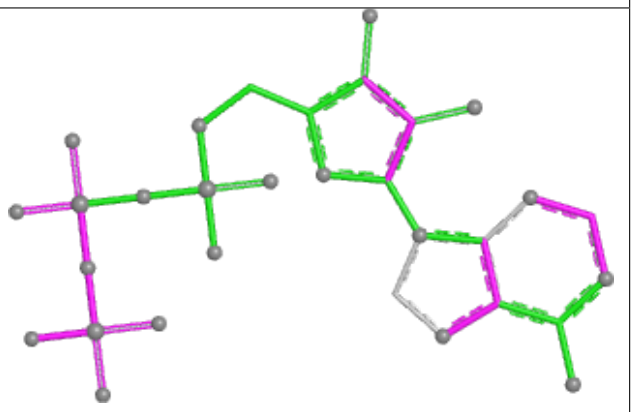
No monomer is involved in short contacts.

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.

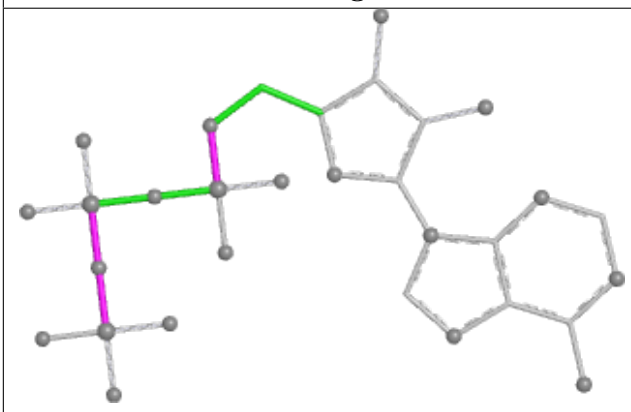
Ligand ANP h 703



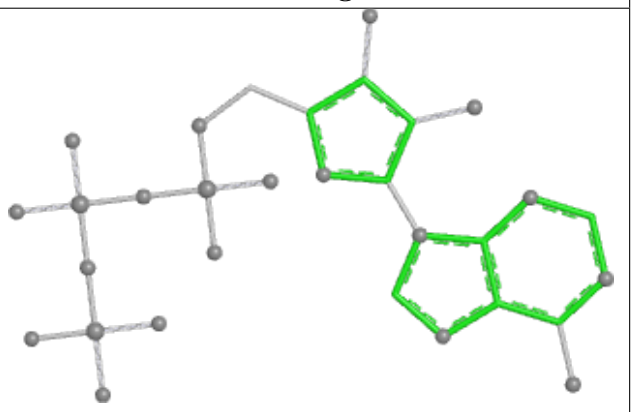
Bond lengths



Bond angles

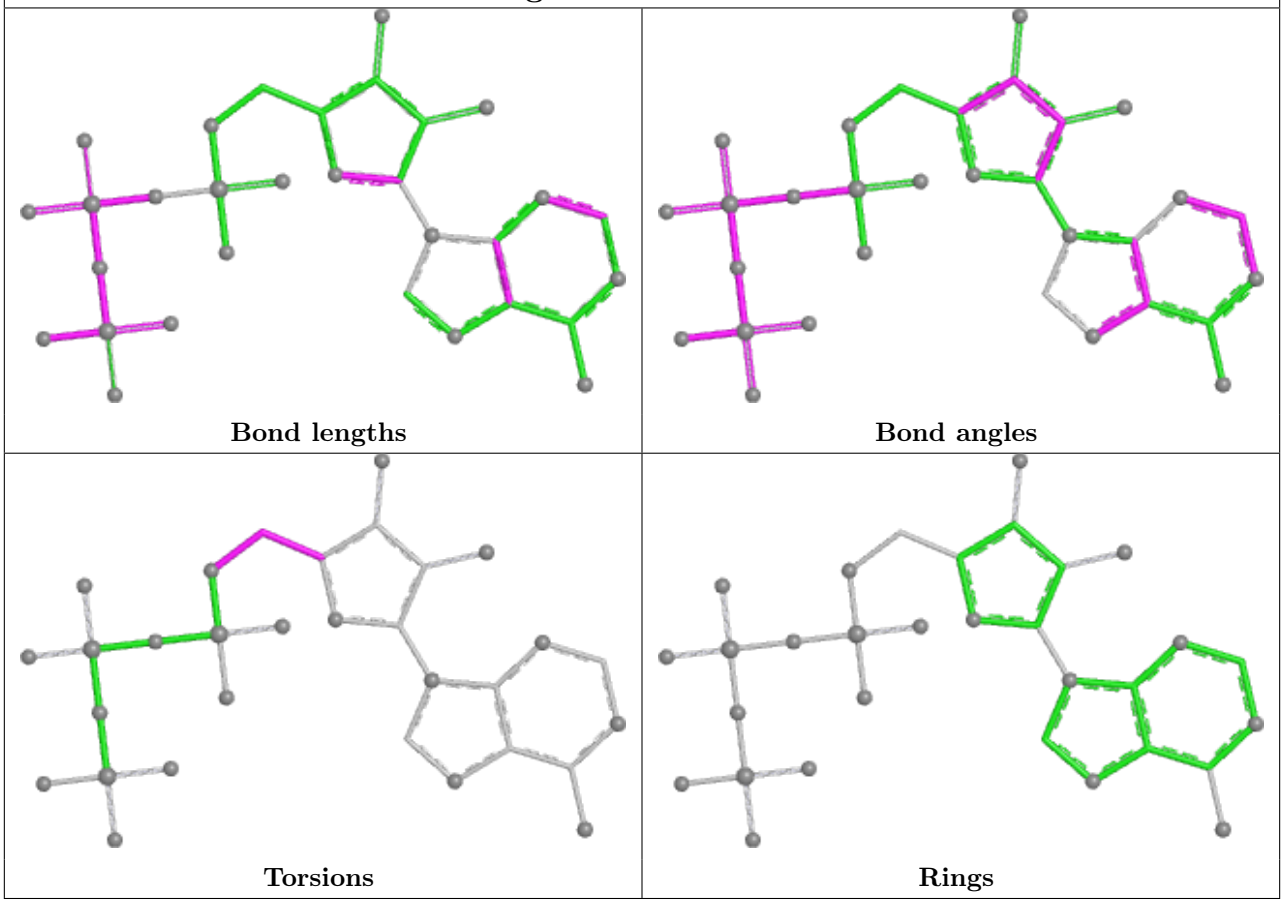


Torsions



Rings

Ligand ANP h 705



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	2	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	1636:C	O3'	1637:C	P	1.24
1	2	1761:U	O3'	1762:A	P	1.07

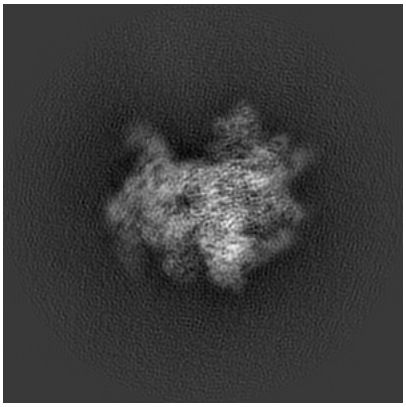
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4071. These allow visual inspection of the internal detail of the map and identification of artifacts.

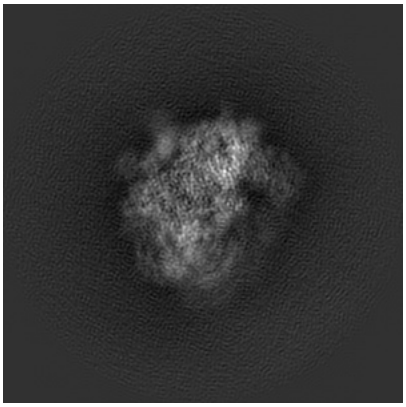
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

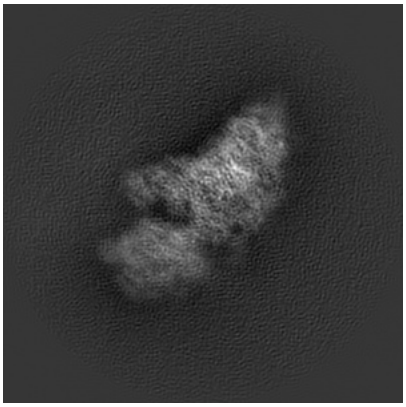
6.1.1 Primary map



X



Y

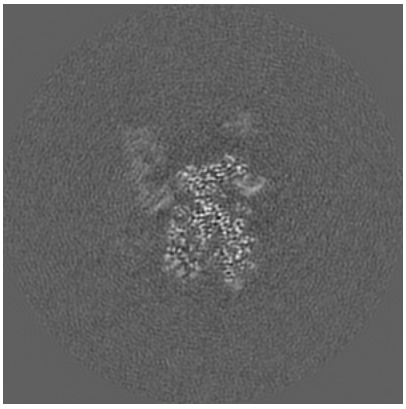


Z

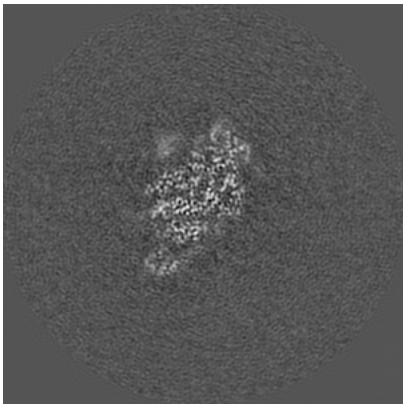
The images above show the map projected in three orthogonal directions.

6.2 Central slices

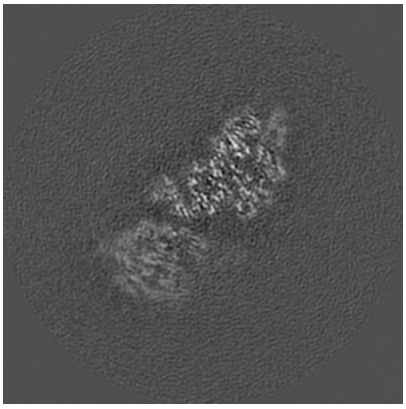
6.2.1 Primary map



X Index: 192



Y Index: 192

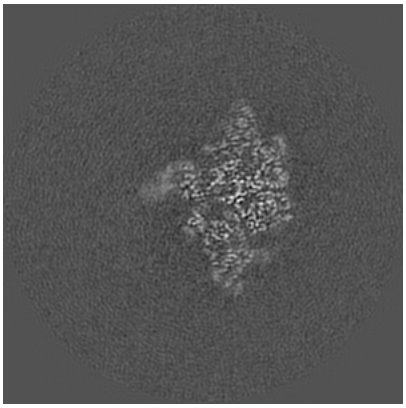


Z Index: 192

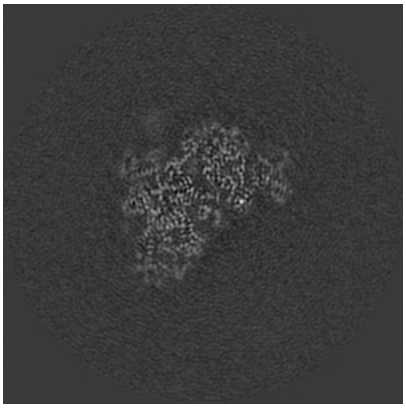
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

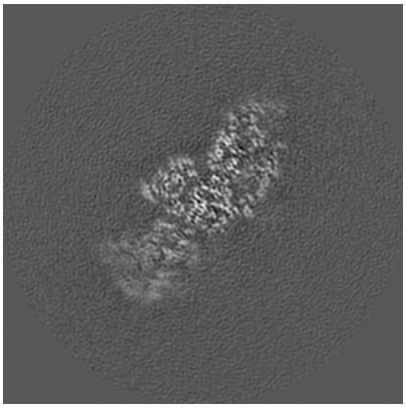
6.3.1 Primary map



X Index: 223



Y Index: 216

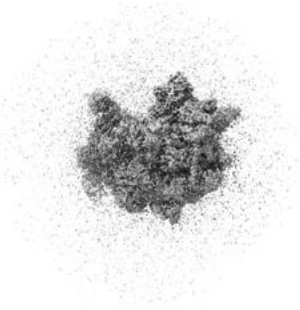


Z Index: 181

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 0.038. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

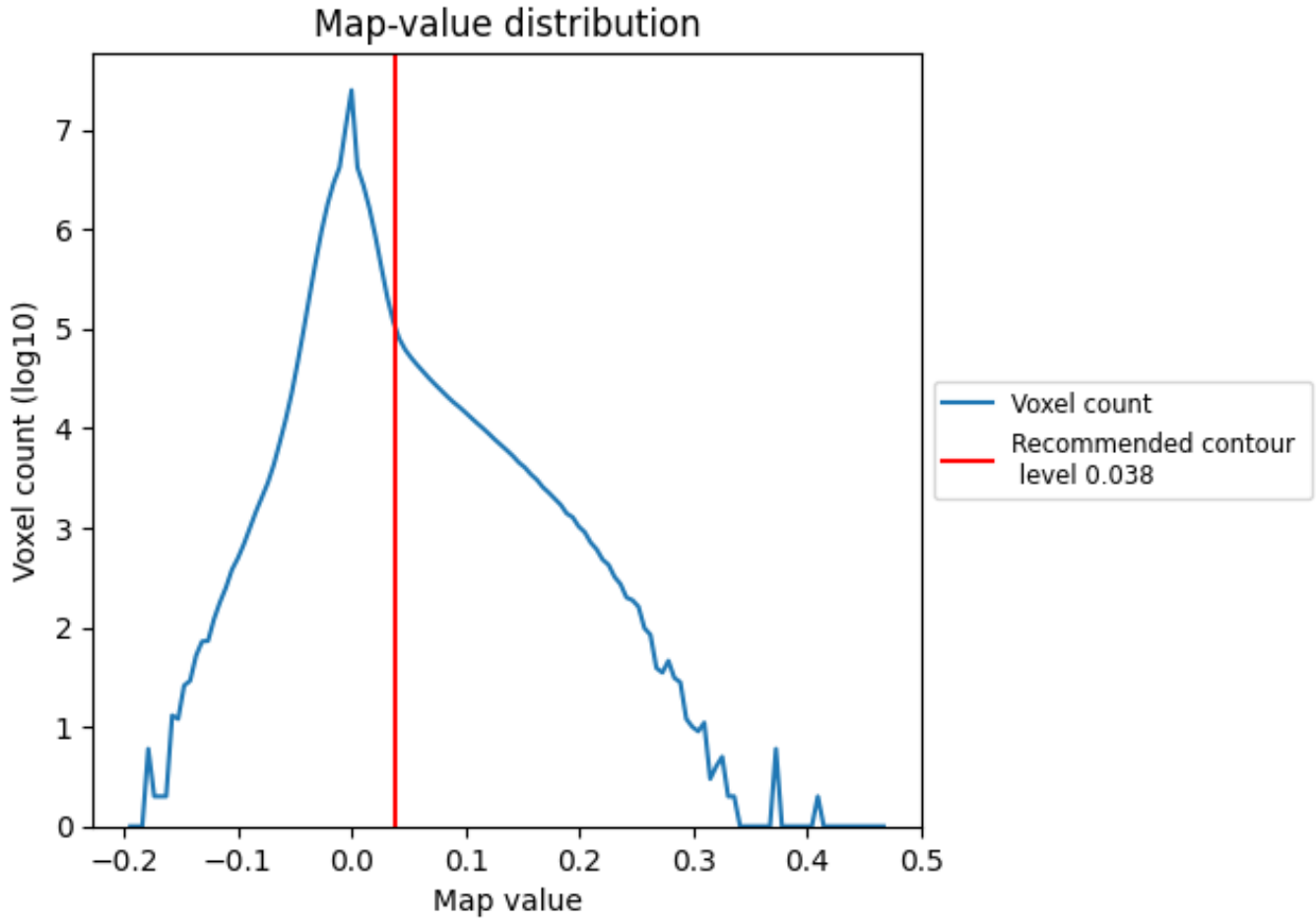
6.5 Mask visualisation (i)

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

7 Map analysis

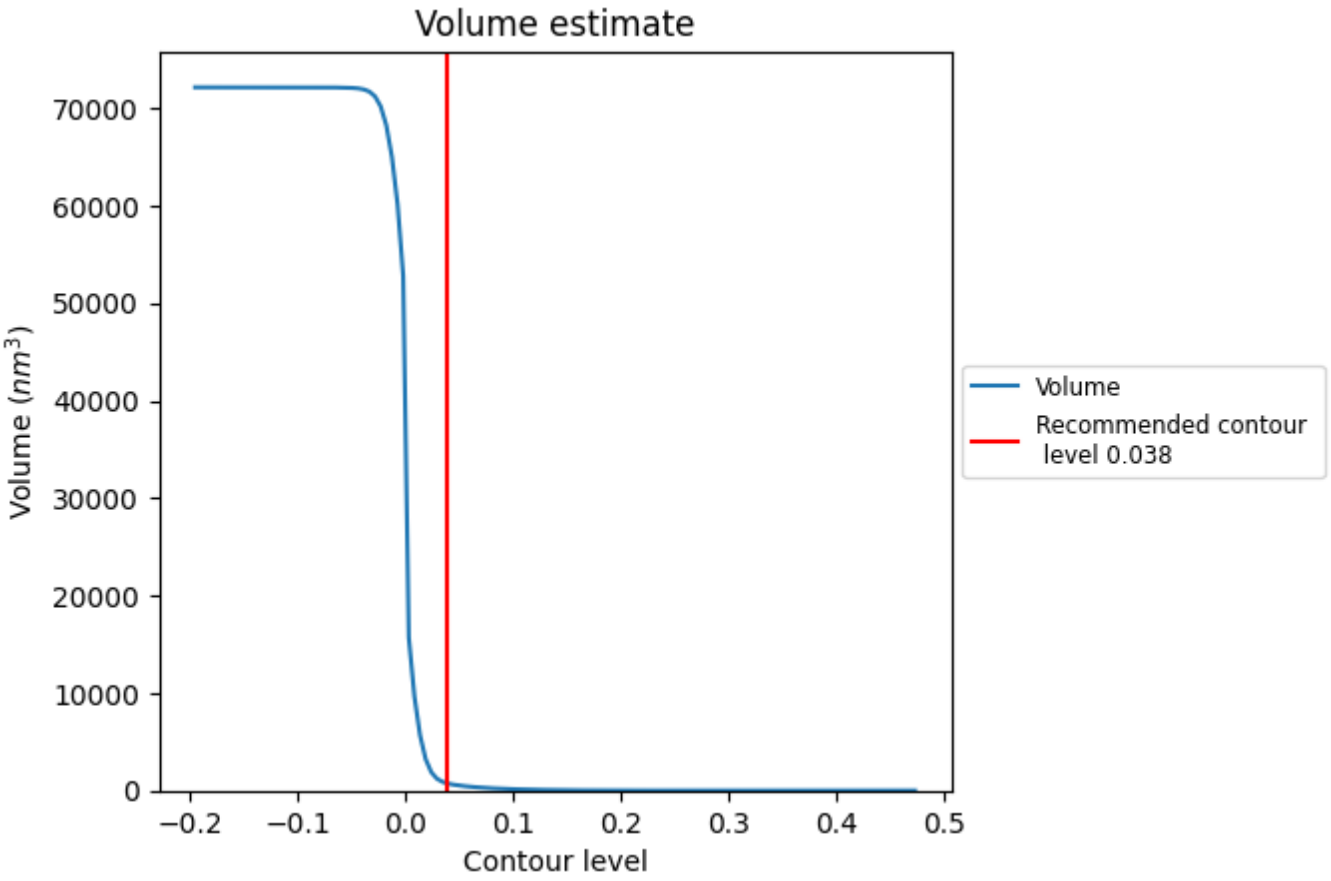
This section contains the results of statistical analysis of the map.

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.

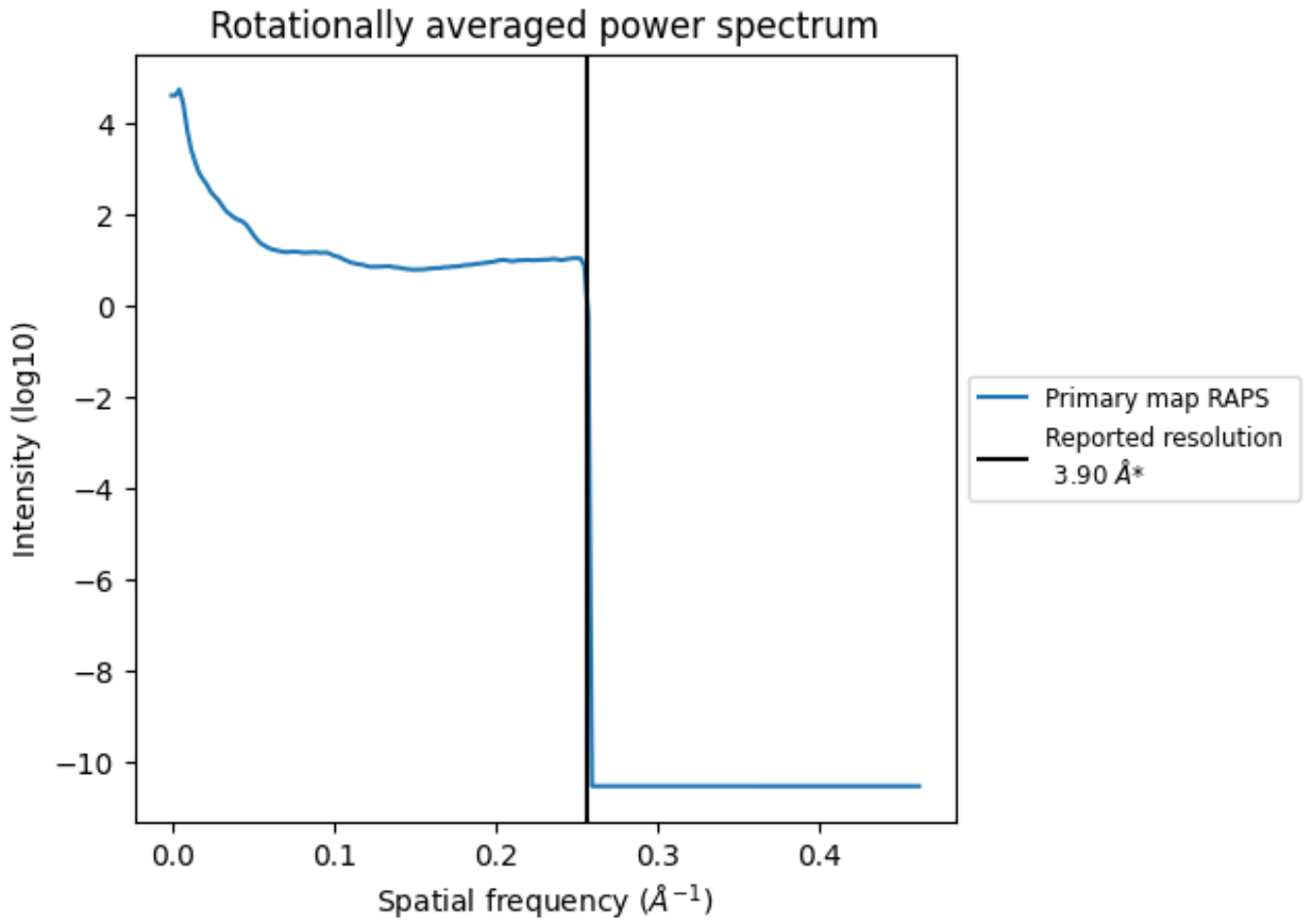
7.2 Volume estimate (i)



The volume at the recommended contour level is 774 nm^3; this corresponds to an approximate mass of 699 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 0.256 Å^{-1}

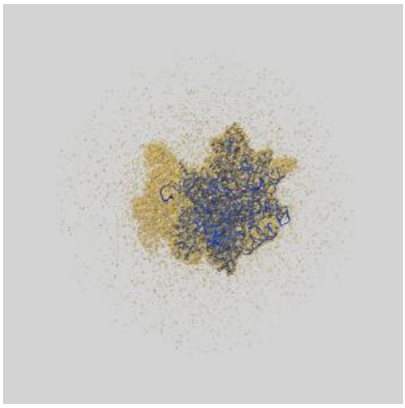
8 Fourier-Shell correlation (i)

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

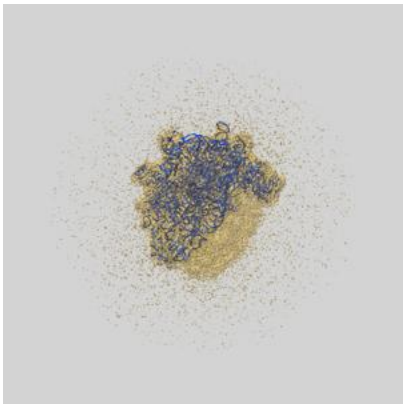
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4071 and PDB model 5LL6. Per-residue inclusion information can be found in section 3 on page 9.

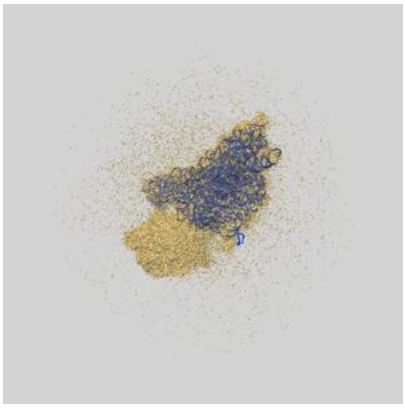
9.1 Map-model overlay



X



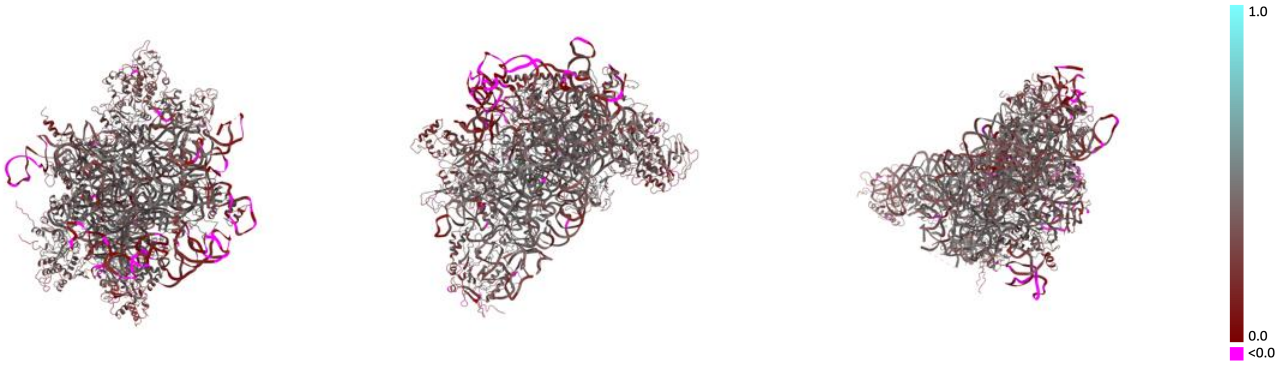
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.038 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.

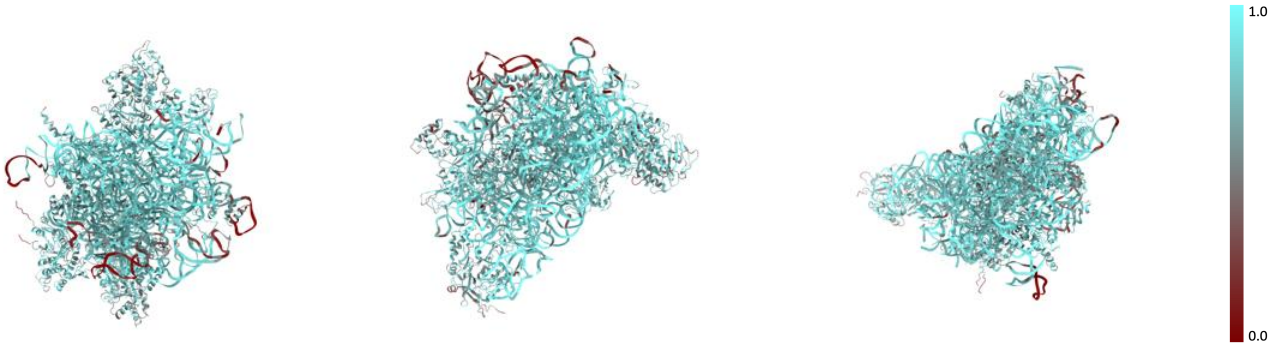
9.2 Q-score mapped to coordinate model



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.

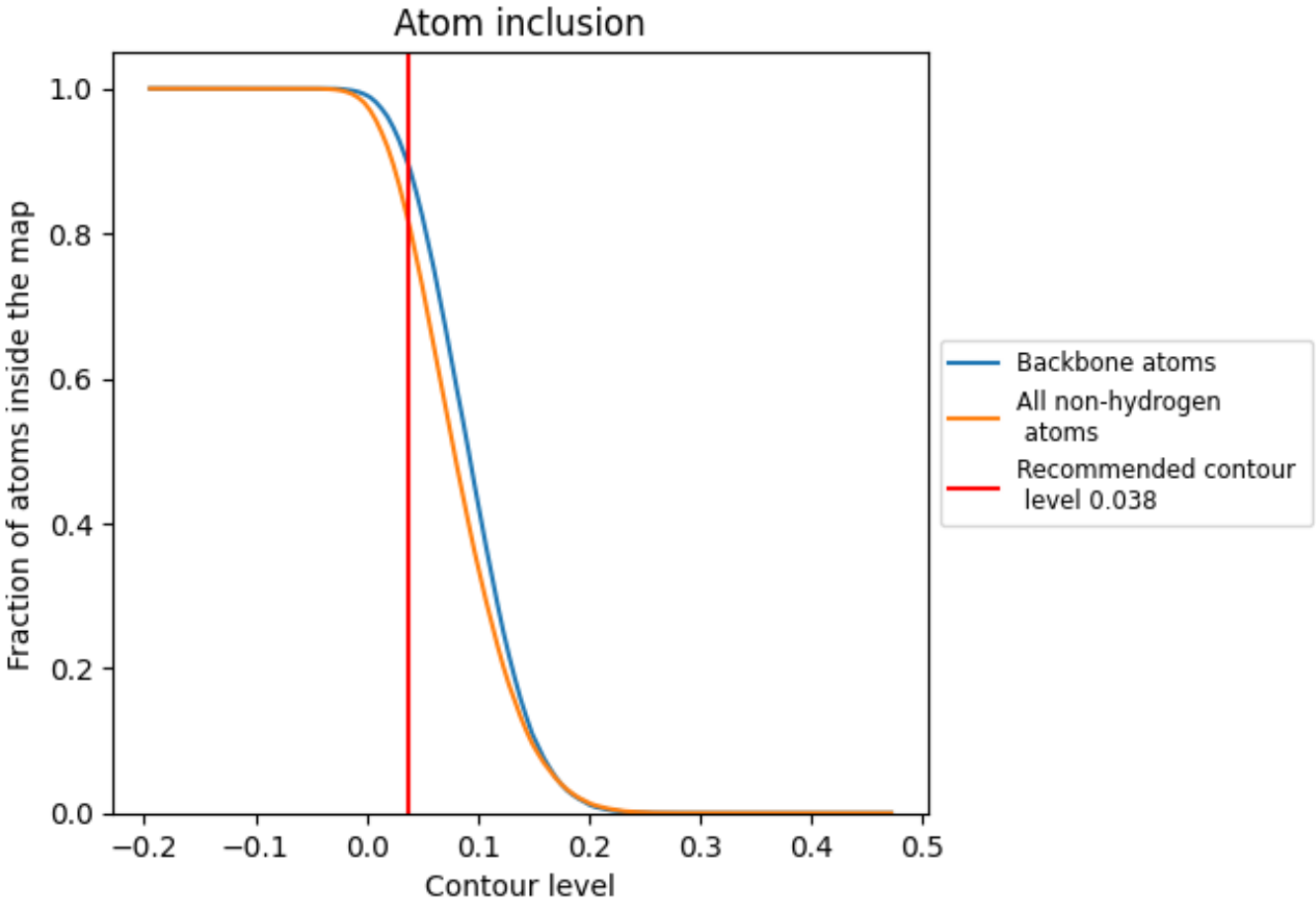
9.3 Atom inclusion mapped to coordinate model



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 (0.038).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.038) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8153	0.3480
2	0.8582	0.3360
P	0.7900	0.3560
Q	0.6754	0.2900
R	0.7494	0.3770
S	0.8143	0.3970
T	0.8064	0.3540
U	0.6701	0.2800
V	0.7939	0.3660
W	0.8079	0.3860
X	0.7648	0.3960
Y	0.8251	0.3680
Z	0.7749	0.3470
a	0.7967	0.3800
b	0.8317	0.4310
c	0.7824	0.4090
d	0.8025	0.3700
e	0.7821	0.3880
f	0.7704	0.3740
g	0.7571	0.3570
h	0.7396	0.3380