



wwPDB EM Validation Summary Report ⓘ

Nov 19, 2022 – 02:57 pm GMT

PDB ID : 5MY1
EMDB ID : EMD-3580
Title : E. coli expressome
Authors : Kohler, R.; Mooney, R.A.; Mills, D.J.; Kostrewa, D.; Landick, R.; Cramer, P.
Deposited on : 2017-01-25
Resolution : 7.60 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 ⓘ 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:

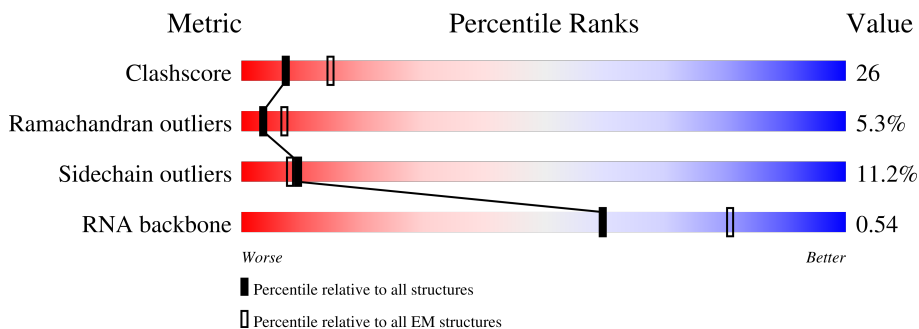
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 7.60 Å.

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



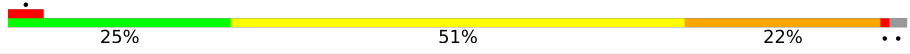
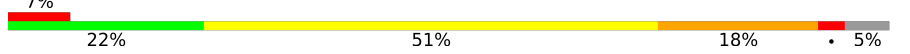
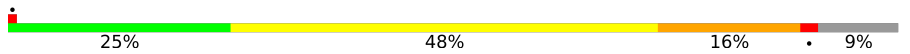
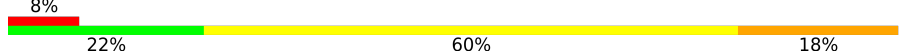
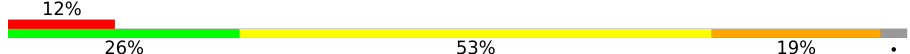
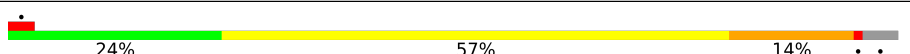
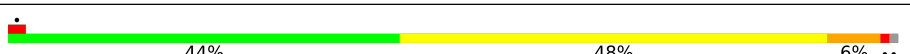
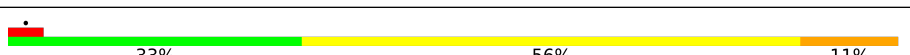
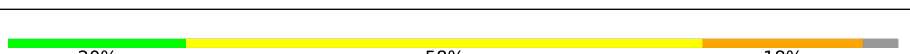
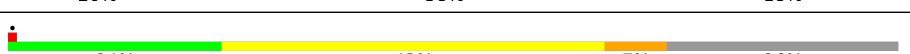
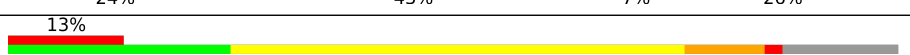
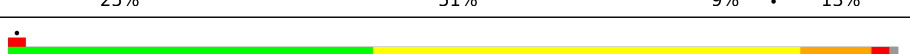
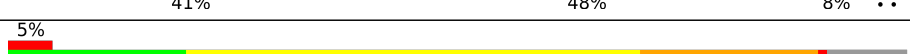
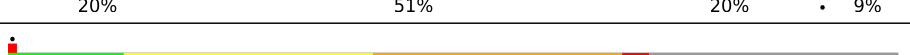
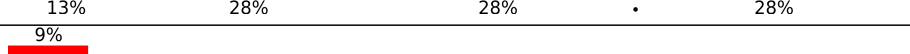
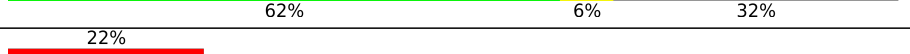
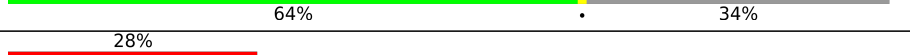
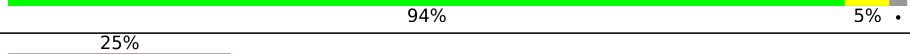
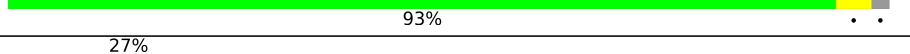
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	1542	
2	C	232	
3	D	205	
4	E	166	
5	F	135	
6	G	178	
7	H	129	

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Mol	Chain	Length	Quality of chain
8	I	129	
9	J	103	
10	K	128	
11	L	123	
12	M	117	
13	N	100	
14	O	89	
15	P	82	
16	Q	83	
17	R	74	
18	S	91	
19	T	86	
20	B	240	
21	U	71	
22	V	329	
22	W	329	
23	X	1342	
24	Y	1407	
25	Z	91	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 71071 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	1530	32831	14642	6024	10635	1530	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	206	1624	1028	305	288	3	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	150	1105	687	211	201	6	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	100	817	515	148	148	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	150	1174	730	226	214	4	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	J	98	786	493	150	142	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	L	123	955	590	196	165	4	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	M	114	883	546	178	156	3	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	N	96	774	483	160	128	3	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	O	88	716	440	146	129	1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	79	ARG	GLN	conflict	UNP P0ADZ4

- Molecule 15 is a protein called 30S ribosomal protein S16.

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

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Q	80	648	411	121	113	3	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	R	55	455	288	86	81	0	0

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	S	79	637	408	120	107	2	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	T	85	665	411	137	114	3	0	0

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	225	Total	C	N	O	S	0	0
			1422	884	254	280	4		
22	W	216	Total	C	N	O	S	0	0
			1485	917	271	292	5		

- Molecule 23 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	1319	Total	C	N	O	S	1	0
			8347	5174	1507	1642	24		

- Molecule 24 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	1372	Total	C	N	O	S	0	0
			7824	4771	1488	1552	13		

- Molecule 25 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	79	Total	C	N	O	S	0	0
			623	379	116	127	1		

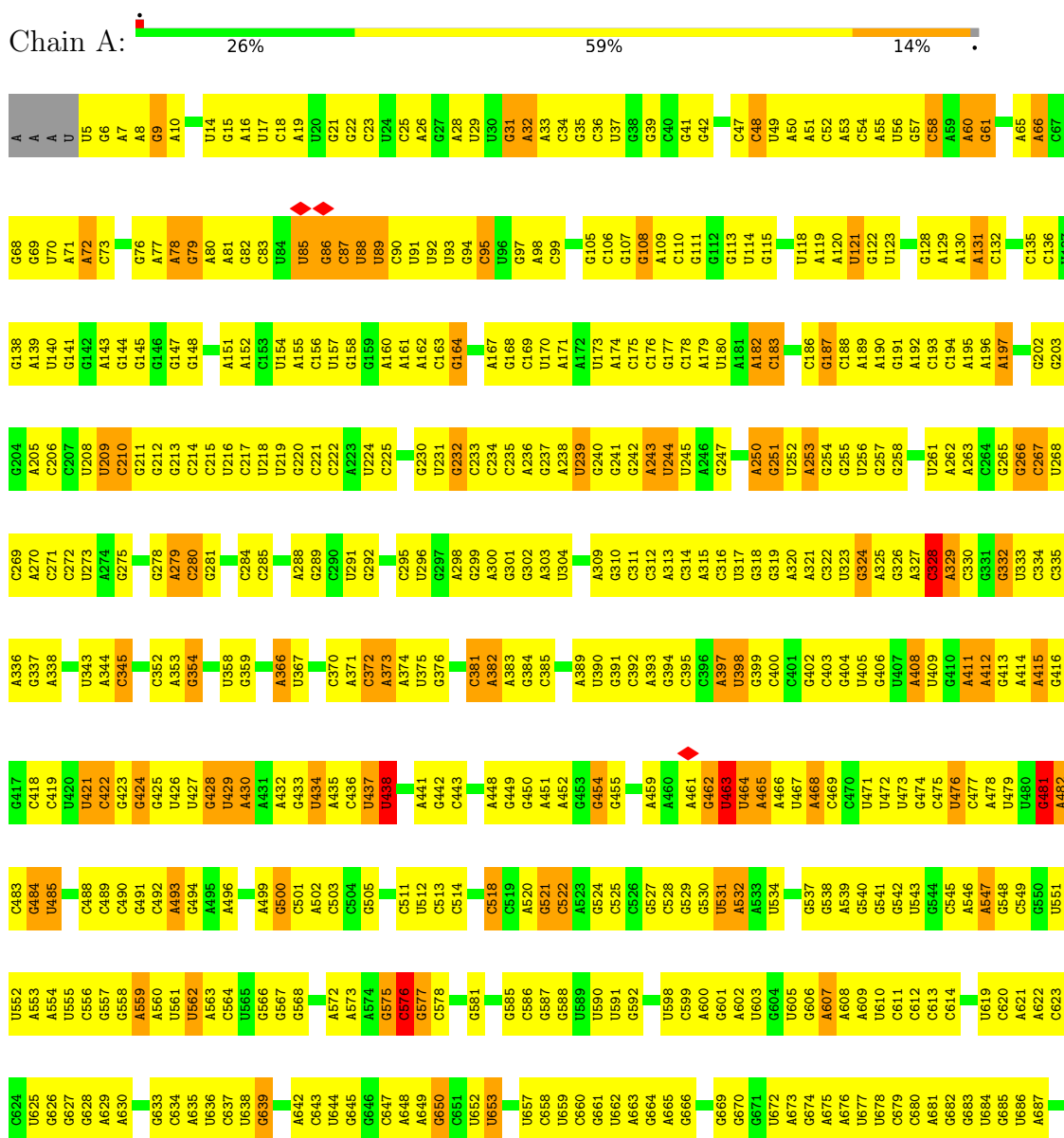
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

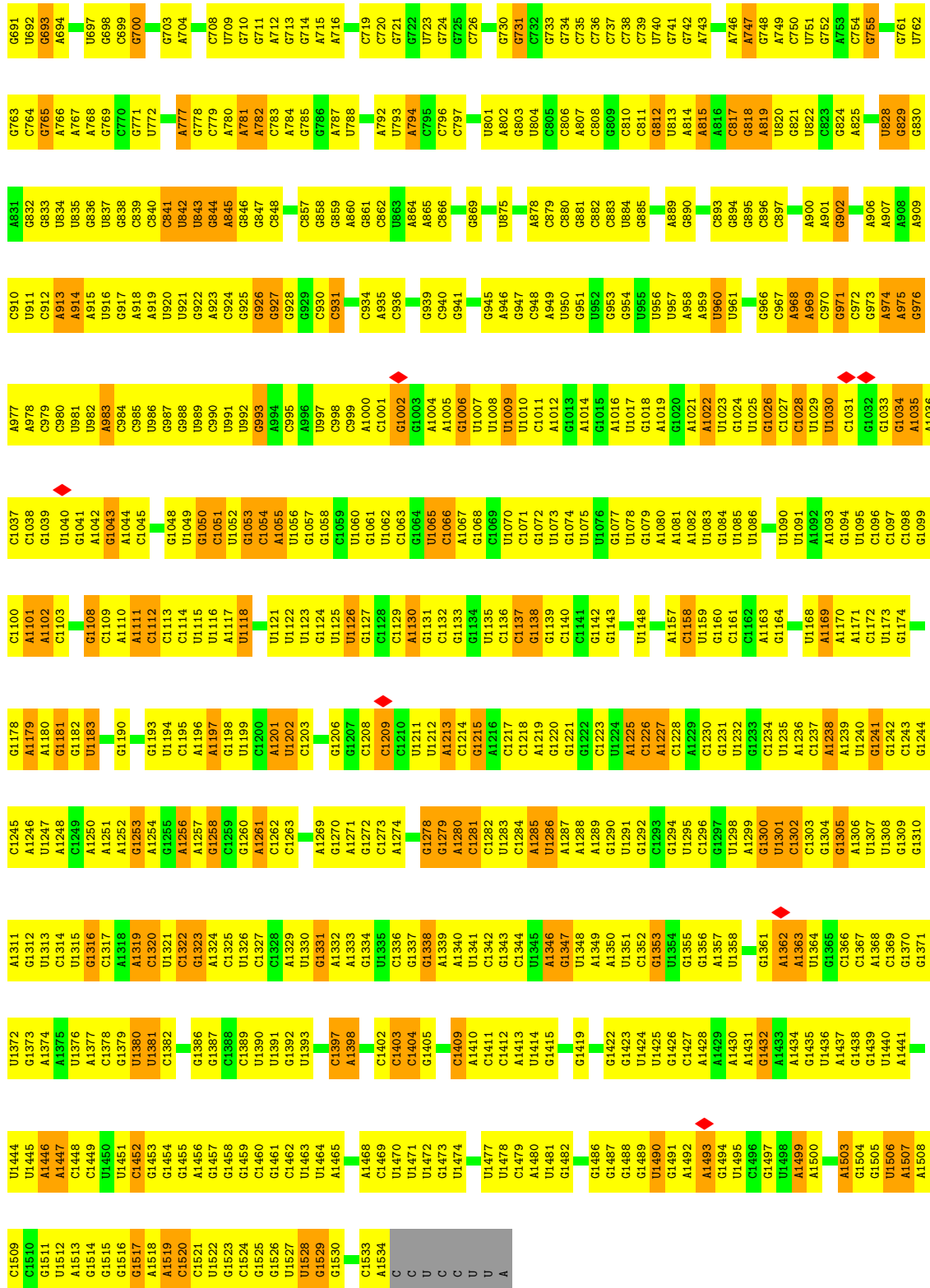
Mol	Chain	Residues	Atoms		AltConf
26	Y	1	Total	Zn	0
			1	1	

3 Residue-property plots i

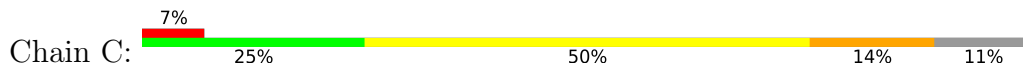
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

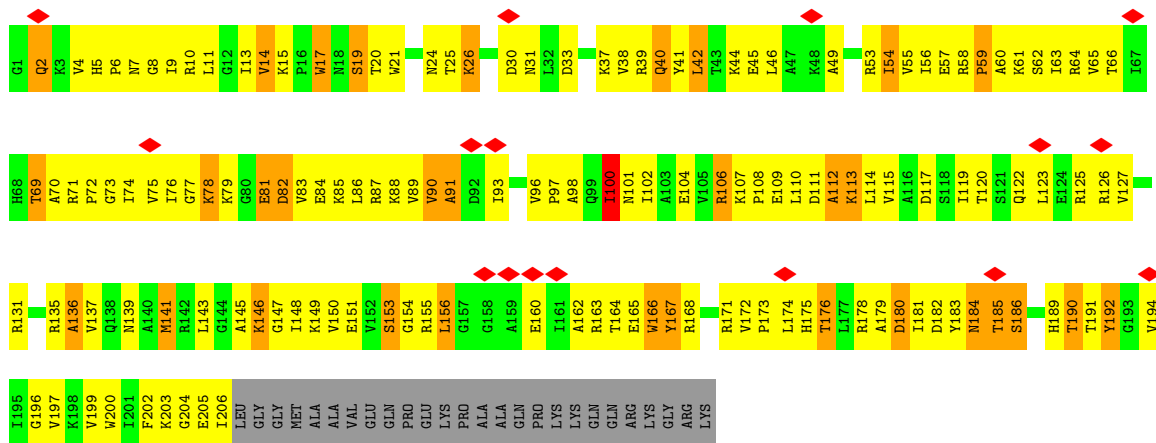
• Molecule 1: 16S ribosomal RNA



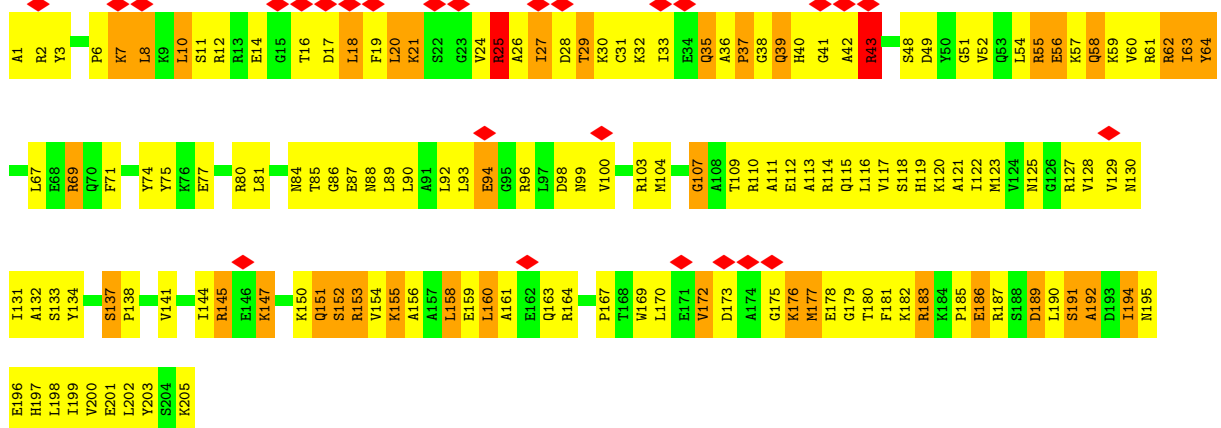


• Molecule 2: 30S ribosomal protein S3

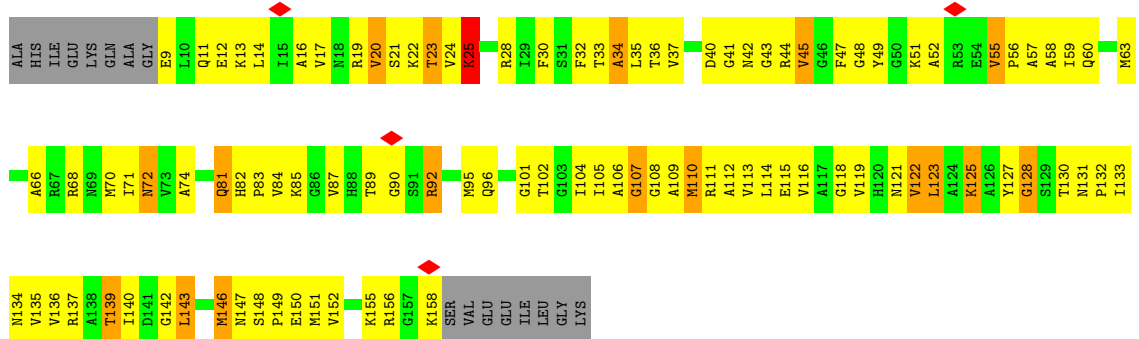




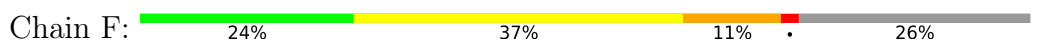
• Molecule 3: 30S ribosomal protein S4

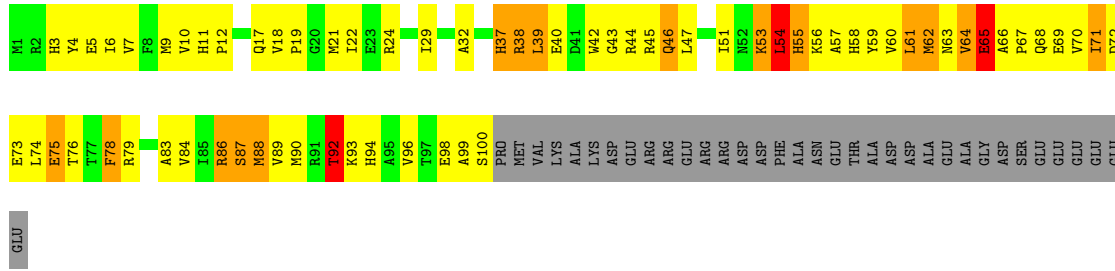


• Molecule 4: 30S ribosomal protein S5

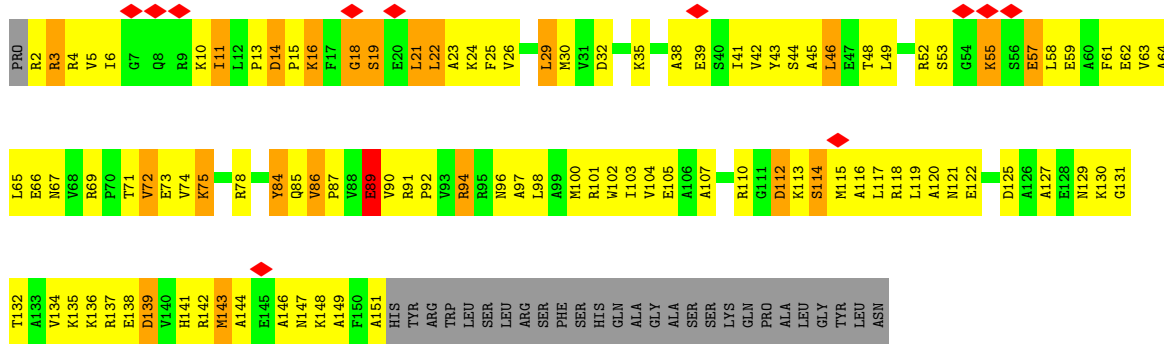


• Molecule 5: 30S ribosomal protein S6

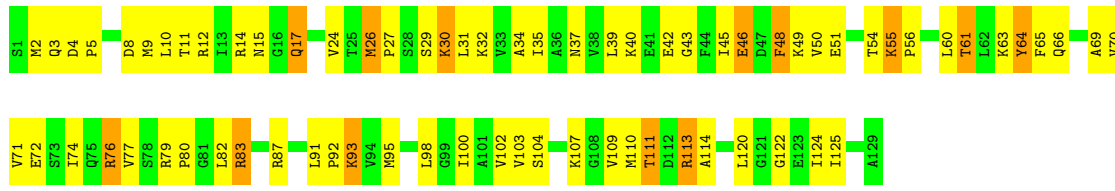
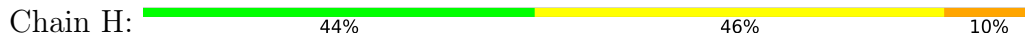




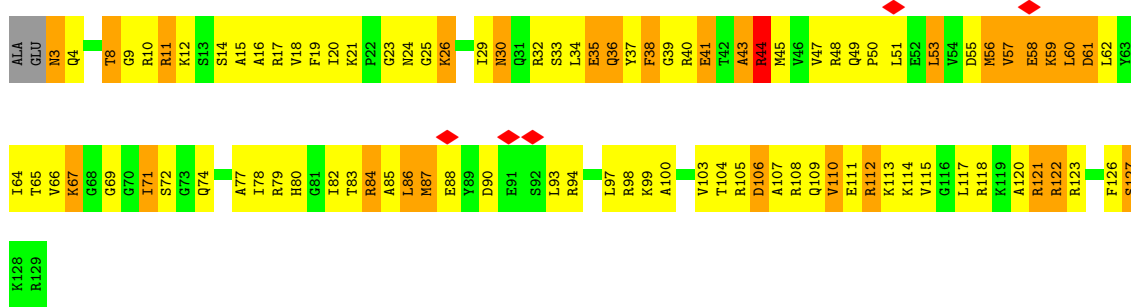
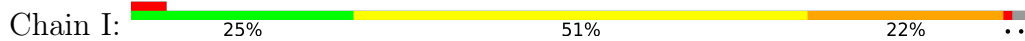
• Molecule 6: 30S ribosomal protein S7



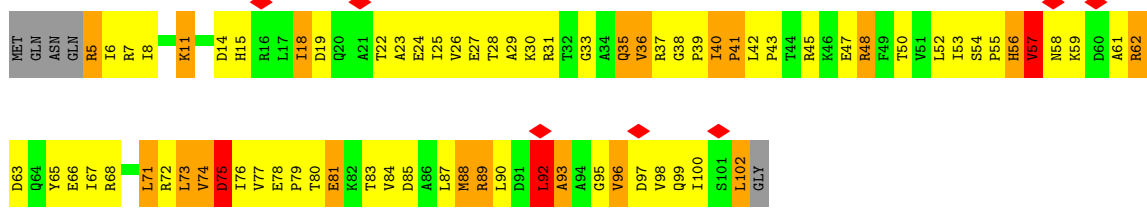
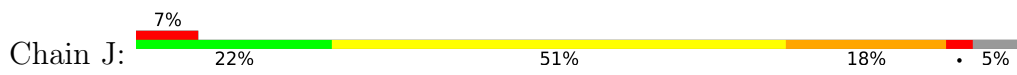
• Molecule 7: 30S ribosomal protein S8



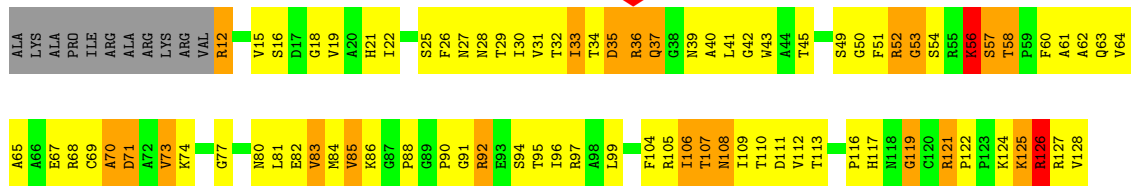
• Molecule 8: 30S ribosomal protein S9



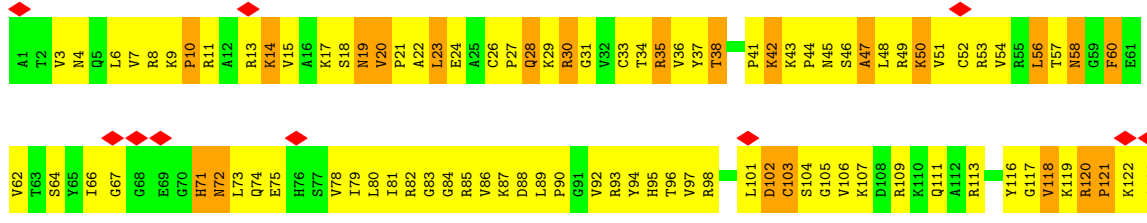
• Molecule 9: 30S ribosomal protein S10



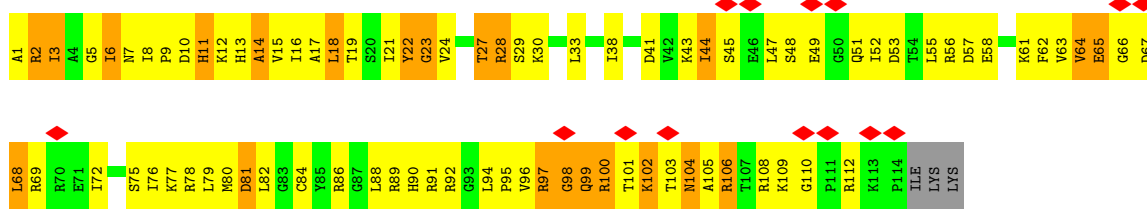
• Molecule 10: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S12

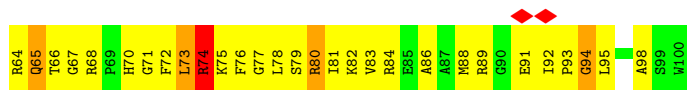


• Molecule 12: 30S ribosomal protein S13

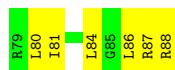
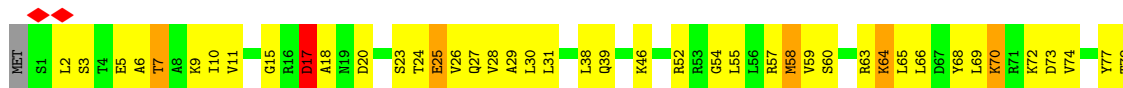


• Molecule 13: 30S ribosomal protein S14

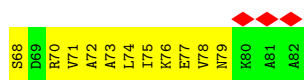
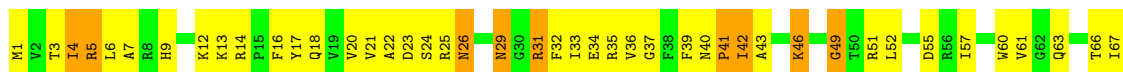




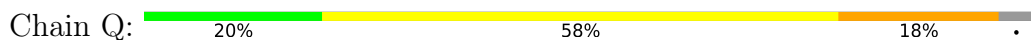
- Molecule 14: 30S ribosomal protein S15



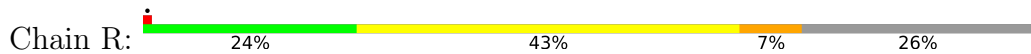
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

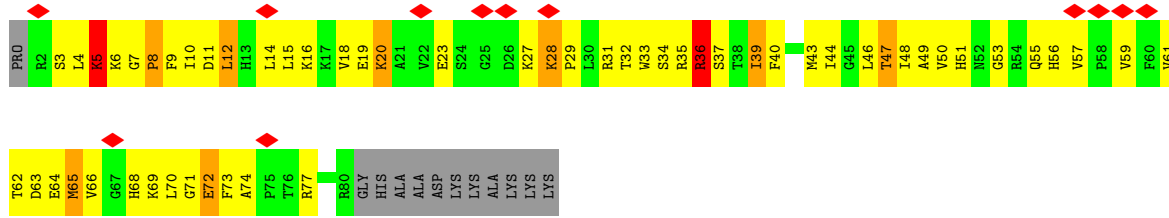


- Molecule 17: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S19

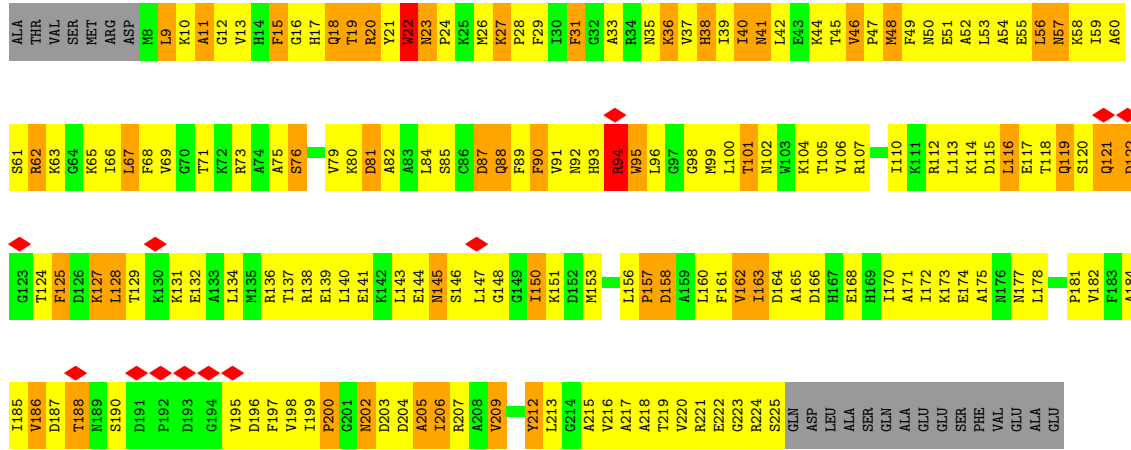
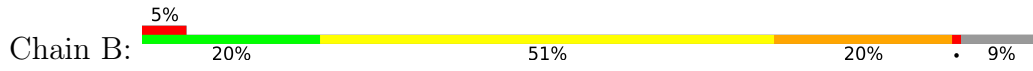




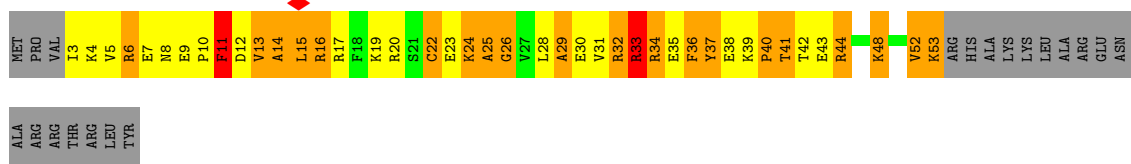
• Molecule 19: 30S ribosomal protein S20



• Molecule 20: 30S ribosomal protein S2

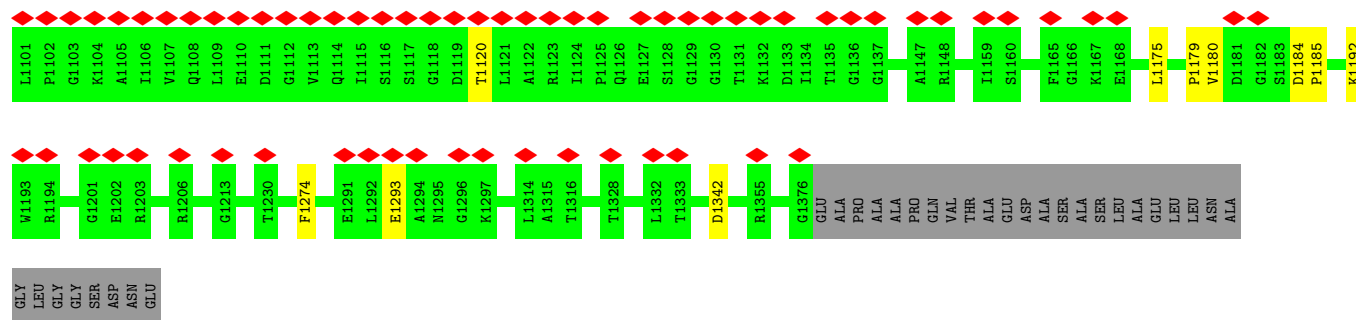


• Molecule 21: 30S ribosomal protein S21

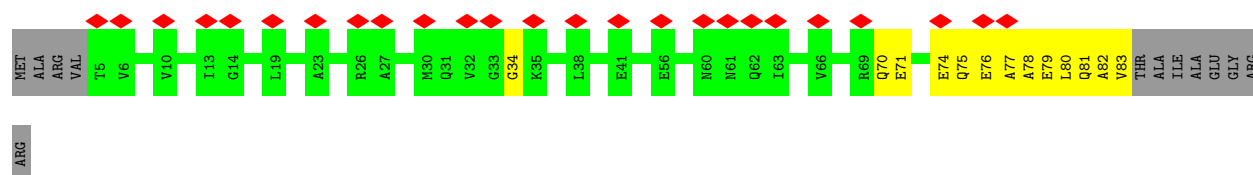
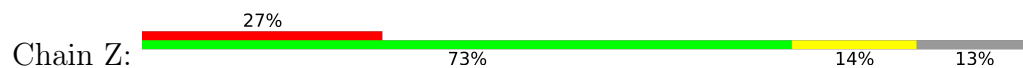


• Molecule 22: DNA-directed RNA polymerase subunit alpha





● Molecule 25: DNA-directed RNA polymerase subunit omega



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	15085	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	16	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	478.4, 478.4, 478.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.84, 1.84, 1.84	Depositor

5 Model quality i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	1/36762 (0.0%)	0.75	7/57350 (0.0%)
2	C	0.23	0/1651	0.45	0/2225
3	D	0.23	0/1665	0.46	0/2227
4	E	0.23	0/1118	0.45	0/1504
5	F	0.25	0/835	0.47	0/1128
6	G	0.23	0/1187	0.45	0/1591
7	H	0.24	0/989	0.45	0/1326
8	I	0.24	0/1034	0.45	0/1375
9	J	0.23	0/796	0.49	0/1077
10	K	0.24	0/893	0.46	0/1205
11	L	0.22	0/969	0.47	0/1300
12	M	0.21	0/892	0.48	0/1193
13	N	0.25	0/785	0.46	0/1043
14	O	0.23	0/724	0.45	0/966
15	P	0.26	0/659	0.44	0/884
16	Q	0.24	0/657	0.46	0/881
17	R	0.23	0/462	0.46	0/621
18	S	0.26	0/652	0.46	0/877
19	T	0.24	0/671	0.41	0/888
20	B	0.25	0/1735	0.47	0/2338
21	U	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
22	V	0.36	0/1438	0.57	0/1982
22	W	0.37	0/1502	0.57	0/2052
23	X	0.35	0/8473	0.54	2/11640 (0.0%)
24	Y	0.34	0/7889	0.52	0/10883
25	Z	0.36	0/625	0.52	0/842
All	All	0.29	5/75493 (0.0%)	0.64	11/109968 (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
1	A	0	16
21	U	0	1
23	X	0	1
All	All	0	18

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	U	15	LEU	C-N	-15.10	0.99	1.34
21	U	25	ALA	C-N	-9.37	1.16	1.33
1	A	463	U	O3'-P	-6.66	1.53	1.61
21	U	29	ALA	C-N	6.60	1.49	1.34
21	U	11	PHE	C-N	-5.38	1.21	1.34

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	765	G	N9-C1'-C2'	-8.19	102.99	112.00
1	A	438	U	N1-C1'-C2'	-6.31	105.06	112.00
1	A	232	G	C5'-C4'-C3'	-6.22	106.04	116.00
1	A	66	A	N9-C1'-C2'	-5.95	105.45	112.00
21	U	15	LEU	C-N-CA	5.74	136.05	121.70

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	187	G	Sidechain
1	A	281	G	Sidechain
1	A	437	U	Sidechain
1	A	438	U	Sidechain
1	A	58	C	Sidechain

5.2 Too-close contacts

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	32831	0	16521	1126	0
2	C	1624	0	1697	268	0
3	D	1643	0	1707	213	0
4	E	1105	0	1148	112	0
5	F	817	0	808	75	0
6	G	1174	0	1230	104	0
7	H	979	0	1034	79	0
8	I	1022	0	1070	143	0
9	J	786	0	828	129	0
10	K	877	0	887	109	0
11	L	955	0	1019	101	0
12	M	883	0	944	85	0
13	N	774	0	827	94	0
14	O	716	0	742	49	0
15	P	649	0	666	78	0
16	Q	648	0	691	77	0
17	R	455	0	478	40	0
18	S	637	0	665	76	0
19	T	665	0	714	52	0
20	B	1704	0	1725	314	0
21	U	425	0	447	102	0
22	V	1422	0	1178	38	0
22	W	1485	0	1322	0	0
23	X	8347	0	6484	136	0
24	Y	7824	0	5280	17	0
25	Z	623	0	617	126	0
26	Y	1	0	0	0	0
All	All	71071	0	50729	3201	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 26.

The worst 5 of 3201 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)
9:J:89:ARG:HG3	22:V:116:THR:CB	1.15	1.56
2:C:126:ARG:HB2	23:X:904:ALA:CB	1.15	1.55
20:B:63:LYS:NZ	25:Z:34:GLY:CA	1.70	1.50
2:C:126:ARG:CB	23:X:904:ALA:CB	1.89	1.49
9:J:89:ARG:CG	22:V:116:THR:CB	1.85	1.49

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	C	204/232 (88%)	135 (66%)	50 (24%)	19 (9%)	0	10
3	D	203/205 (99%)	131 (64%)	54 (27%)	18 (9%)	1	11
4	E	148/166 (89%)	107 (72%)	34 (23%)	7 (5%)	2	21
5	F	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	1	17
6	G	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	2	19
7	H	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	6	33
8	I	125/129 (97%)	86 (69%)	28 (22%)	11 (9%)	1	11
9	J	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	0	5
10	K	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	0	7
11	L	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	4
12	M	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	0	9
13	N	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	0	9
14	O	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	6	34
15	P	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	1	17
16	Q	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	2	19
17	R	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	4
18	S	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	13
19	T	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	1	14
20	B	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	12
21	U	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
22	V	223/329 (68%)	193 (86%)	23 (10%)	7 (3%)	4	27
22	W	212/329 (64%)	186 (88%)	23 (11%)	3 (1%)	11	46
23	X	1312/1342 (98%)	1106 (84%)	173 (13%)	33 (2%)	5	32
24	Y	1368/1407 (97%)	1155 (84%)	159 (12%)	54 (4%)	3	23
25	Z	77/91 (85%)	72 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5503/6059 (91%)	4299 (78%)	910 (16%)	294 (5%)	3	19

5 of 294 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	2	GLN
2	C	91	ALA
2	C	153	SER
3	D	18	LEU
3	D	31	CYS

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	C	170/189 (90%)	142 (84%)	28 (16%)	2	12
3	D	172/172 (100%)	140 (81%)	32 (19%)	1	9
4	E	113/125 (90%)	92 (81%)	21 (19%)	1	9
5	F	87/116 (75%)	68 (78%)	19 (22%)	1	6
6	G	123/146 (84%)	102 (83%)	21 (17%)	2	11
7	H	104/104 (100%)	87 (84%)	17 (16%)	2	13
8	I	105/106 (99%)	83 (79%)	22 (21%)	1	6
9	J	86/90 (96%)	66 (77%)	20 (23%)	1	4
10	K	90/98 (92%)	70 (78%)	20 (22%)	1	6
11	L	103/103 (100%)	88 (85%)	15 (15%)	3	15
12	M	92/95 (97%)	70 (76%)	22 (24%)	0	4
13	N	79/83 (95%)	67 (85%)	12 (15%)	3	14
14	O	76/77 (99%)	69 (91%)	7 (9%)	9	29
15	P	65/65 (100%)	56 (86%)	9 (14%)	3	17
16	Q	74/77 (96%)	60 (81%)	14 (19%)	1	8
17	R	48/64 (75%)	45 (94%)	3 (6%)	18	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	S	70/78 (90%)	60 (86%)	10 (14%)	3	16
19	T	65/65 (100%)	56 (86%)	9 (14%)	3	17
20	B	180/198 (91%)	142 (79%)	38 (21%)	1	6
21	U	44/61 (72%)	36 (82%)	8 (18%)	1	10
22	V	106/286 (37%)	104 (98%)	2 (2%)	57	75
22	W	130/286 (46%)	129 (99%)	1 (1%)	81	89
23	X	567/1157 (49%)	567 (100%)	0	100	100
24	Y	332/1168 (28%)	330 (99%)	2 (1%)	86	92
25	Z	66/75 (88%)	66 (100%)	0	100	100
All	All	3147/5084 (62%)	2795 (89%)	352 (11%)	9	21

5 of 352 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	M	97	ARG
18	S	28	LYS
13	N	27	LYS
15	P	31	ARG
19	T	85	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
19	T	20	ASN
19	T	60	GLN
20	B	121	GLN
6	G	85	GLN
6	G	67	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1529/1542 (99%)	277 (18%)	25 (1%)

5 of 277 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	A
1	A	9	G
1	A	14	U
1	A	31	G
1	A	32	A

5 of 25 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1025	U
1	A	1101	A
1	A	1528	U
1	A	1065	U
1	A	1181	G

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
23	X	2
21	U	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	967:LEU	C	968:GLU	N	4.69
1	X	941:LYS	C	942:ASP	N	3.24
1	U	25:ALA	C	26:GLY	N	1.16
1	U	15:LEU	C	16:ARG	N	0.99

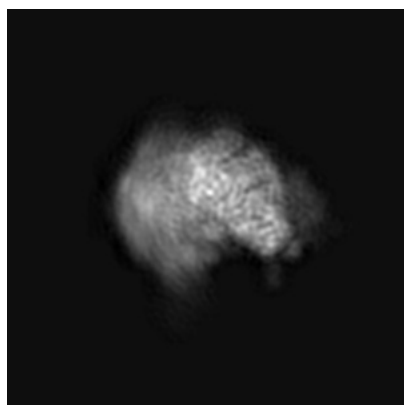
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3580. These allow visual inspection of the internal detail of the map and identification of artifacts.

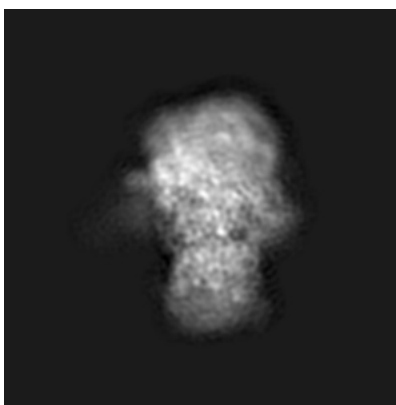
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

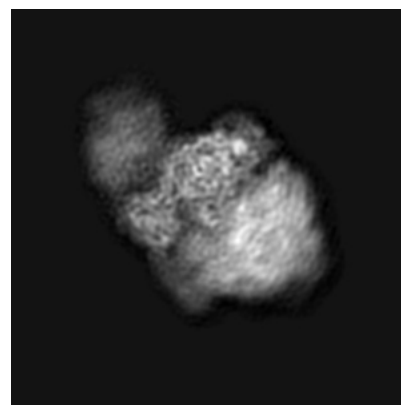
6.1.1 Primary map



X



Y

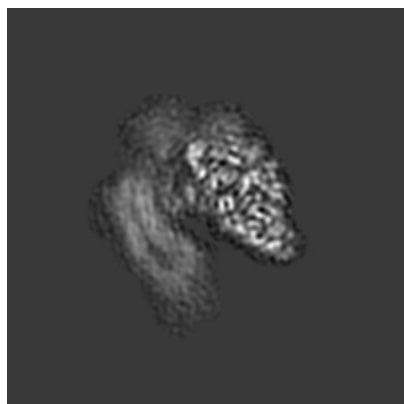


Z

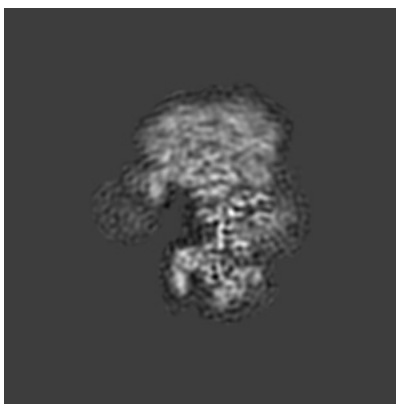
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

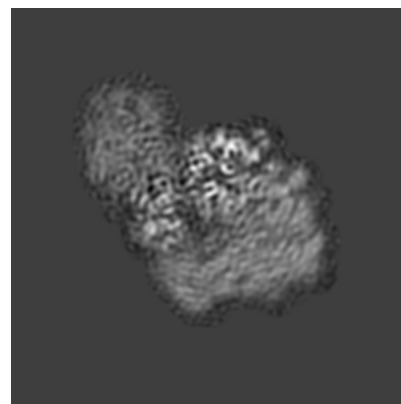
6.2.1 Primary map



X Index: 130



Y Index: 130

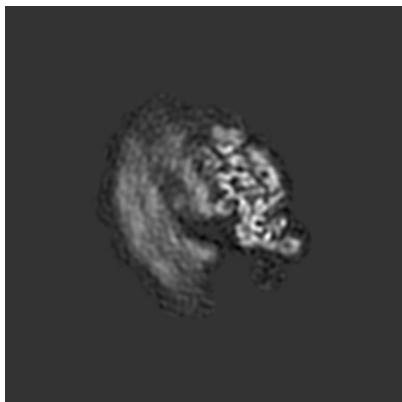


Z Index: 130

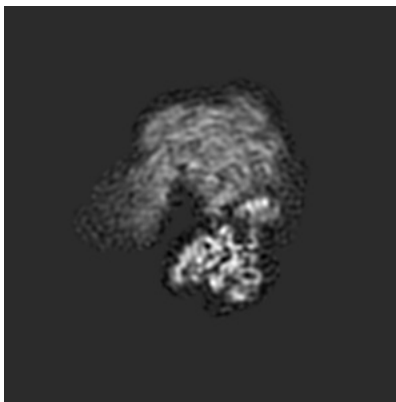
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

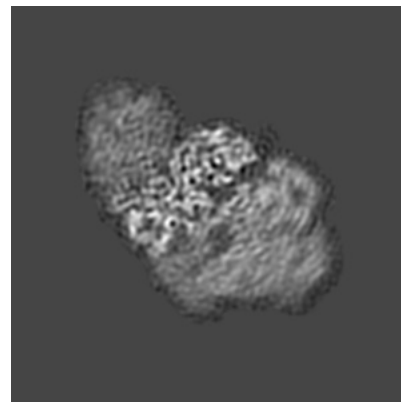
6.3.1 Primary map



X Index: 139



Y Index: 121

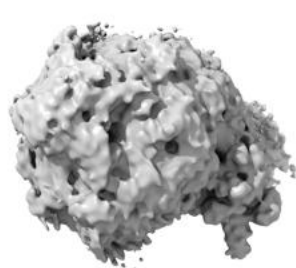


Z Index: 139

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

6.4 Orthogonal surface views [i](#)

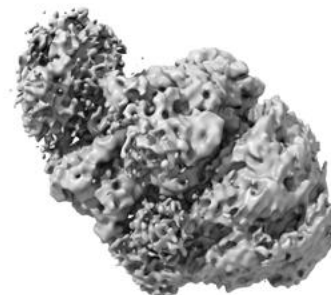
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

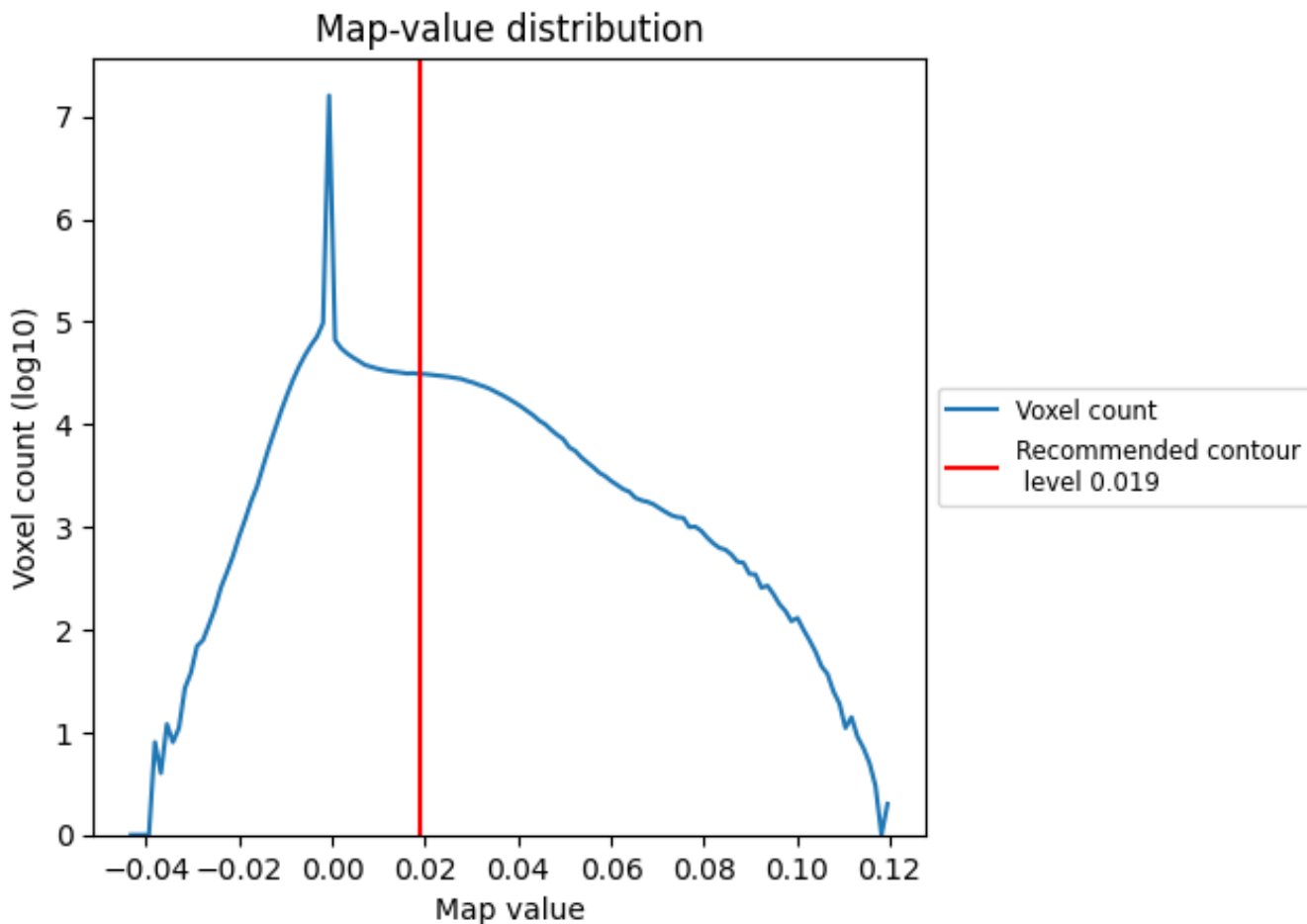
6.5 Mask visualisation

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

7 Map analysis [i](#)

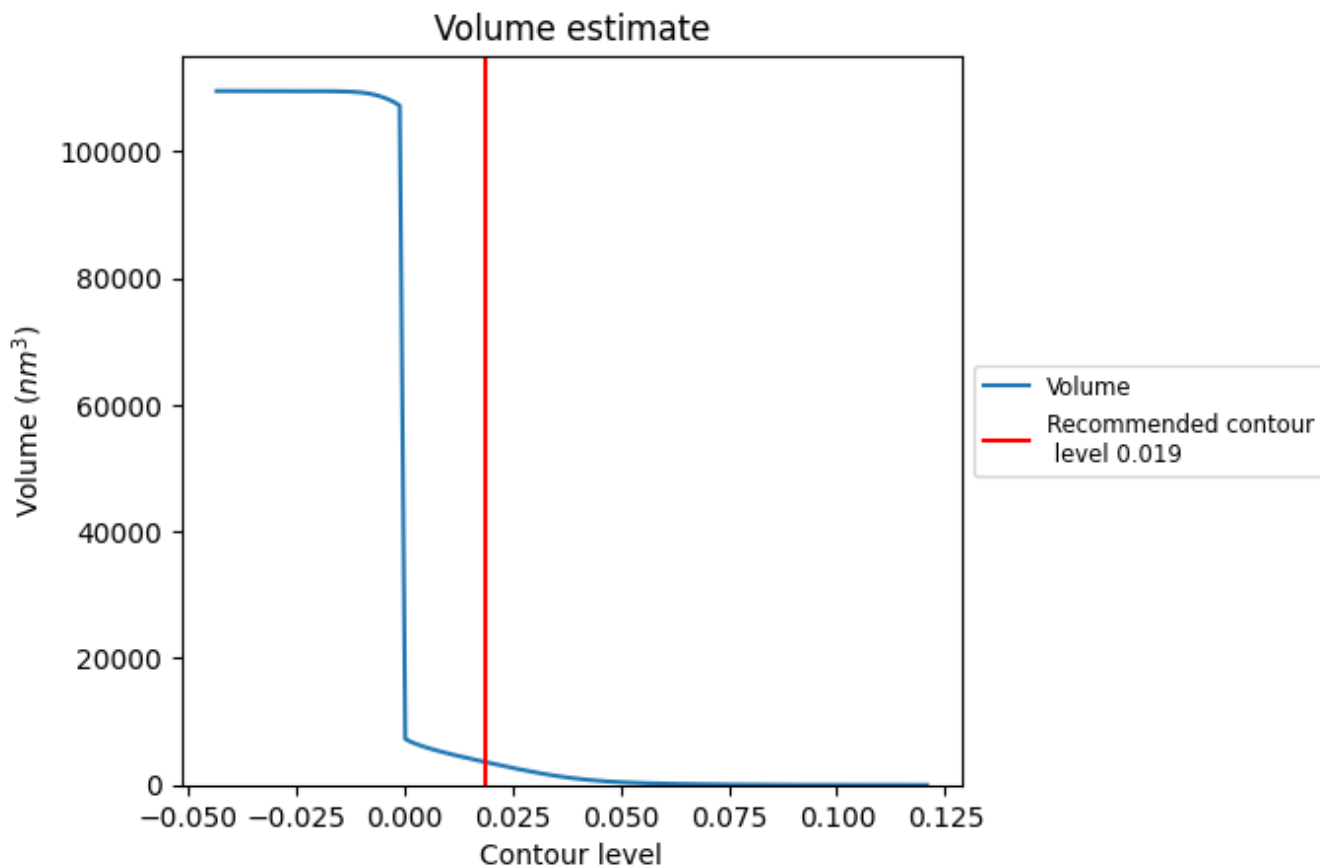
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

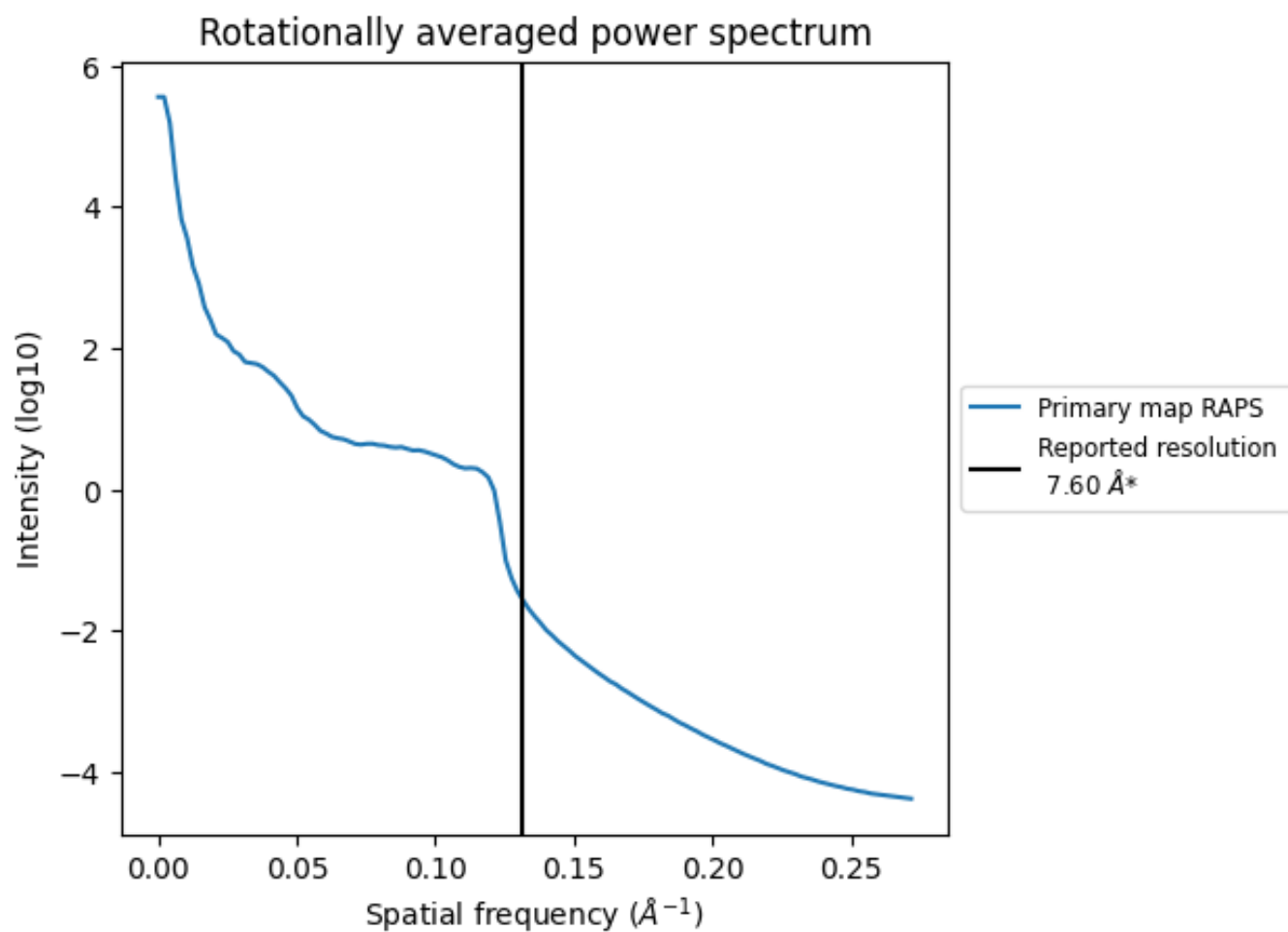
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3584 nm³; this corresponds to an approximate mass of 3238 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 0.132\AA^{-1}

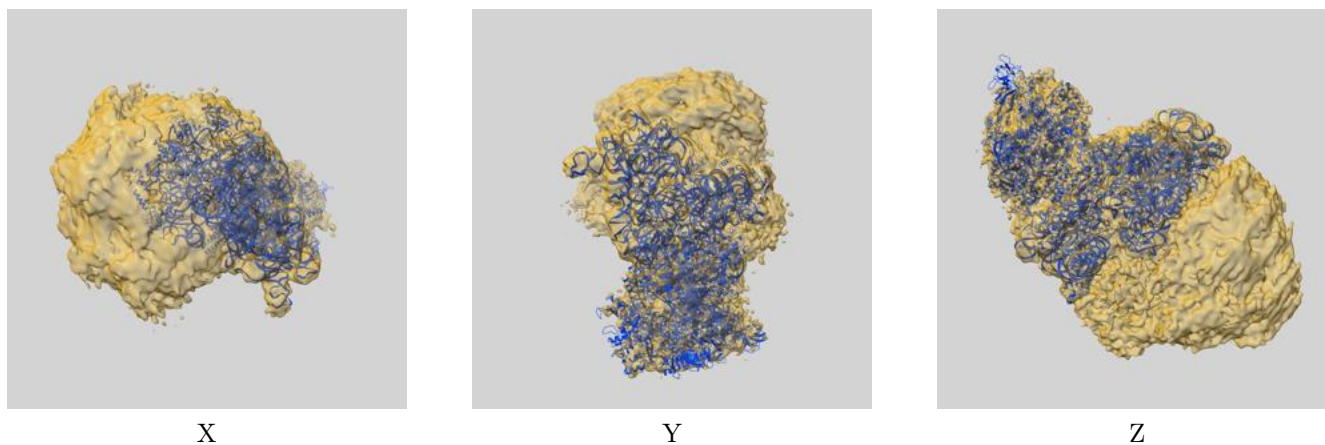
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

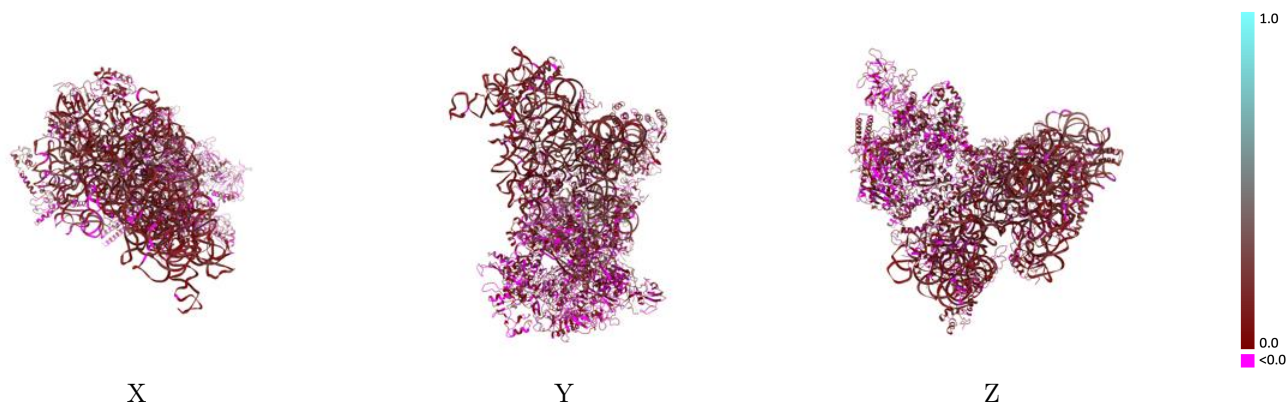
This section contains information regarding the fit between EMDB map EMD-3580 and PDB model 5MY1. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



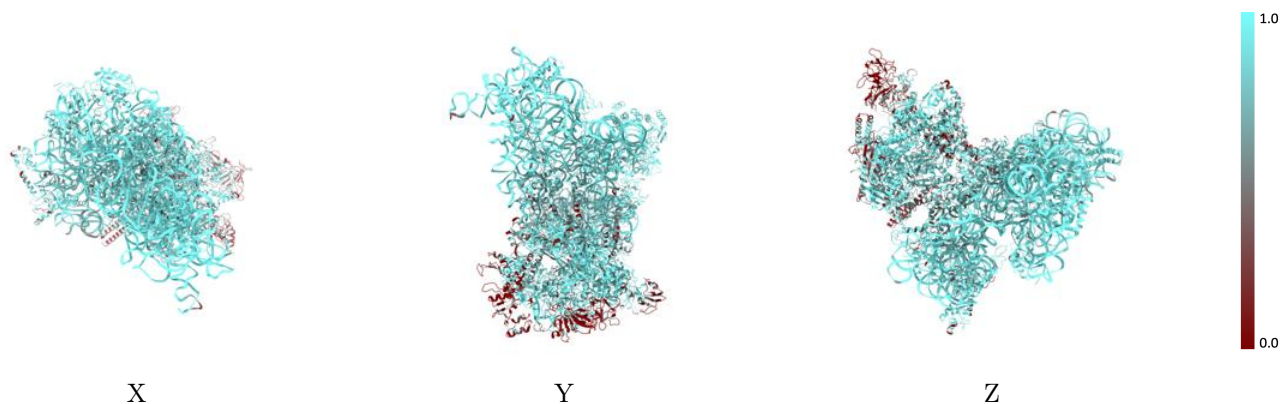
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



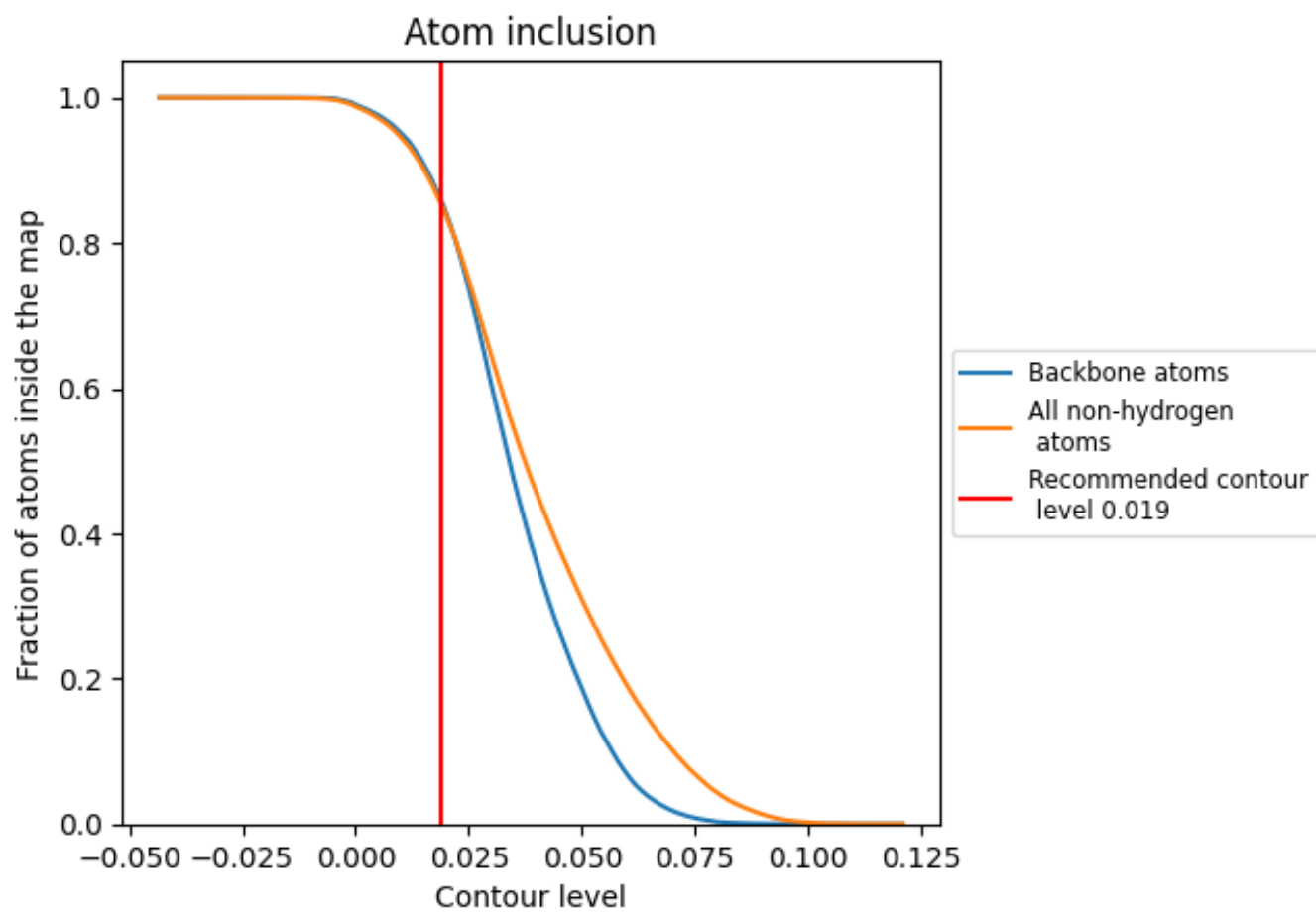
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).























































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 85% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8520	 0.1130
A	 0.9604	 0.1450
B	 0.8299	 0.1310
C	 0.7719	 0.0880
D	 0.7635	 0.1130
E	 0.8504	 0.1160
F	 0.9259	 0.1300
G	 0.8329	 0.1100
H	 0.8958	 0.1380
I	 0.8866	 0.0660
J	 0.8200	 0.0810
K	 0.9004	 0.1180
L	 0.8165	 0.0910
M	 0.7955	 0.0830
N	 0.8964	 0.0620
O	 0.8797	 0.1080
P	 0.8868	 0.1230
Q	 0.9367	 0.1210
R	 0.9220	 0.1100
S	 0.8148	 0.0410
T	 0.9000	 0.1420
U	 0.8251	 0.1100
V	 0.7847	 0.0870
W	 0.5988	 0.0610
X	 0.6739	 0.0660
Y	 0.6779	 0.0760
Z	 0.5813	 0.0160

