W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

May 18, 2024 – 09:50 pm BST

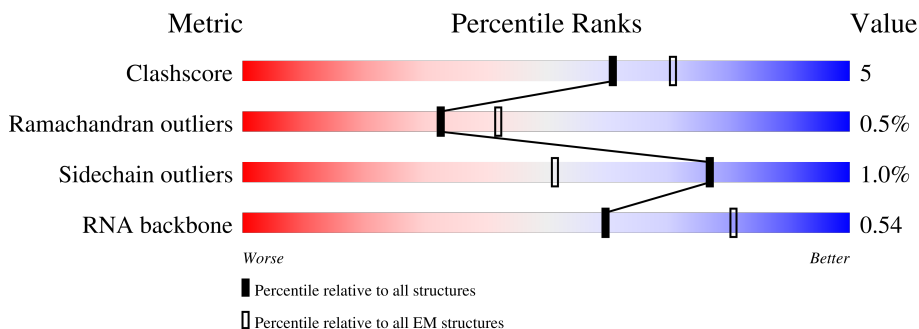|		
PDB ID	:	6TMF
EMDB ID	:	EMD-10519
Title	:	Structure of an archaeal ABCE1-bound ribosomal post-splitting complex
Authors	:	Kratzat, H.; Becker, T.; Tampe, R.; Beckmann, R.
Deposited on	:	2019-12-04
Resolution	:	2.80 Å(reported)

1   Overall quality at a glance   ⓘ

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

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0.5%
Sidechain outliers		1.0%
RNA backbone		0.54

Worse   *Better*

▮ Percentile relative to all structures

❏ Percentile relative to all EM structures

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	1485	64% 28% 7% ·
2	B	195	89% 11%
3	C	193	92% 8%
4	D	184	85% 14% ·
5	E	178	87% 11% ··
6	F	241	83% 17%
7	G	220	87% 12% ·

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Mol	Chain	Length	Quality of chain
8	H	125	6% / 87% / 13%
9	I	214	78% / 22%
10	J	129	92% / 8%
11	K	126	88% / 11%
12	L	132	80% / 19%
13	M	102	97%
14	N	133	10% / 86% / 14%
15	O	144	84% / 15%
16	P	136	85% / 15%
17	Q	56	14% / 79% / 20%
18	R	151	91% / 7%
19	S	111	5% / 91% / 9%
20	T	64	92% / 8%
21	U	115	76% / 24%
22	V	149	77% / 21%
23	W	56	89% / 9%
24	X	97	81% / 19%
25	Y	63	8% / 87% / 13%
26	Z	50	98% / 92% / 8%
27	a	66	8% / 95% / 5%
28	b	123	89% / 100%
29	c	37	8% / 89% / 11%
30	d	594	96%

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 65449 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	1485	31920	14202	5912	10321	1485	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	195	1571	1014	271	282	4	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	193	1526	970	284	268	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	184	1520	976	272	268	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	178	1476	923	291	260	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	241	1963	1257	362	339	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	220	Total 1721	C 1083	N 322	O 308	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	125	Total 961	C 601	N 185	O 172	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	214	Total 1704	C 1067	N 326	O 303	S 8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	129	Total 1022	C 661	N 176	O 182	S 3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	126	Total 997	C 625	N 199	O 173	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	132	Total 1040	C 648	N 202	O 184	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	102	Total 819	C 507	N 155	O 153	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	133	Total 1005	C 621	N 200	O 181	S 3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	144	Total 1131	C 718	N 218	O 193	S 2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total 1109	C 700	N 217	O 188	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	56	Total 459	C 291	N 94	O 68	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	151	Total 1225	C 776	N 235	O 208	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	111	Total 913	C 576	N 179	O 154	S 4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	64	Total 540	C 339	N 101	O 97	S 3	0	0

- Molecule 21 is a protein called 30S ribosomal protein S19P.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	115	Total 949	C 610	N 174	O 161	S 4	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
22	V	149	Total 1218	C 786	N 217	O 215	0	0

- Molecule 23 is a protein called RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	56	Total 435	C 275	N 76	O 76	S 8	0	0

- Molecule 24 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total 799	C 509	N 138	O 148	S 4	0	0

- Molecule 25 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	63	Total 475	C 303	N 82	O 85	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	50	Total 417	C 264	N 83	O 64	S 6	0	0

- Molecule 27 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	66	Total 514	C 316	N 101	O 96	S 1	0	0

- Molecule 28 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	123	Total	C	N	O	S	0	0
			936	594	157	182	3		

- Molecule 29 is a protein called LSU ribosomal protein L41E.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	37	Total	C	N	O	S	0	0
			351	224	85	40	2		

- Molecule 30 is a protein called ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	582	Total	C	N	O	S	0	0
			4622	2959	784	863	16		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
d	238	ALA	GLU	engineered mutation	UNP A0A0E3MFT8
d	485	ALA	GLU	engineered mutation	UNP A0A0E3MFT8

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	A	27	Total	Mg	0
			27	27	
31	d	2	Total	Mg	0
			2	2	

- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	Q	1	Total	Zn	0
			1	1	
32	W	2	Total	Zn	0
			2	2	
32	Y	1	Total	Zn	0
			1	1	

- Molecule 33 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

Mol	Chain	Residues	Atoms			AltConf
33	d	1	Total 8	Fe 4	S 4	0
33	d	1	Total 8	Fe 4	S 4	0

- Molecule 34 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).
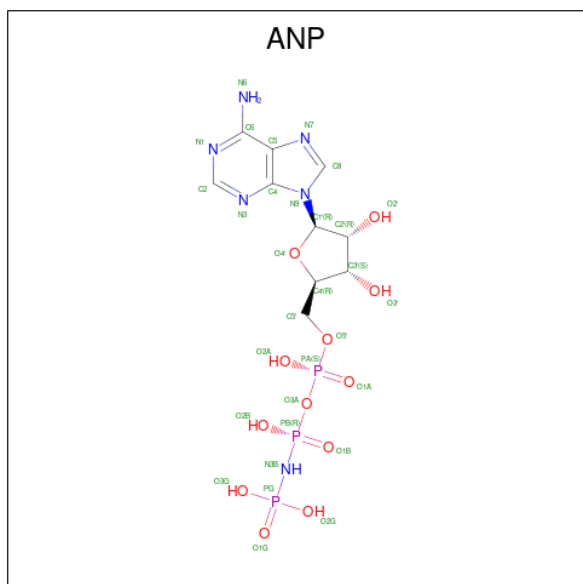
Mol	Chain	Residues	Atoms					AltConf
34	d	1	Total 31	C 10	N 6	O 12	P 3	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	d	1	31	10	6	12	3	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
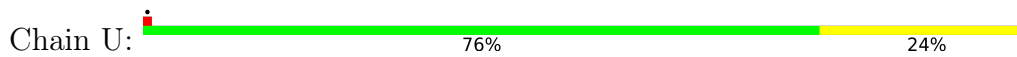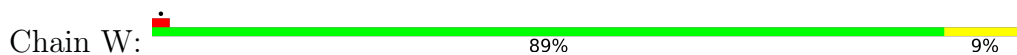
• Molecule 1: 16S ribosomal RNA
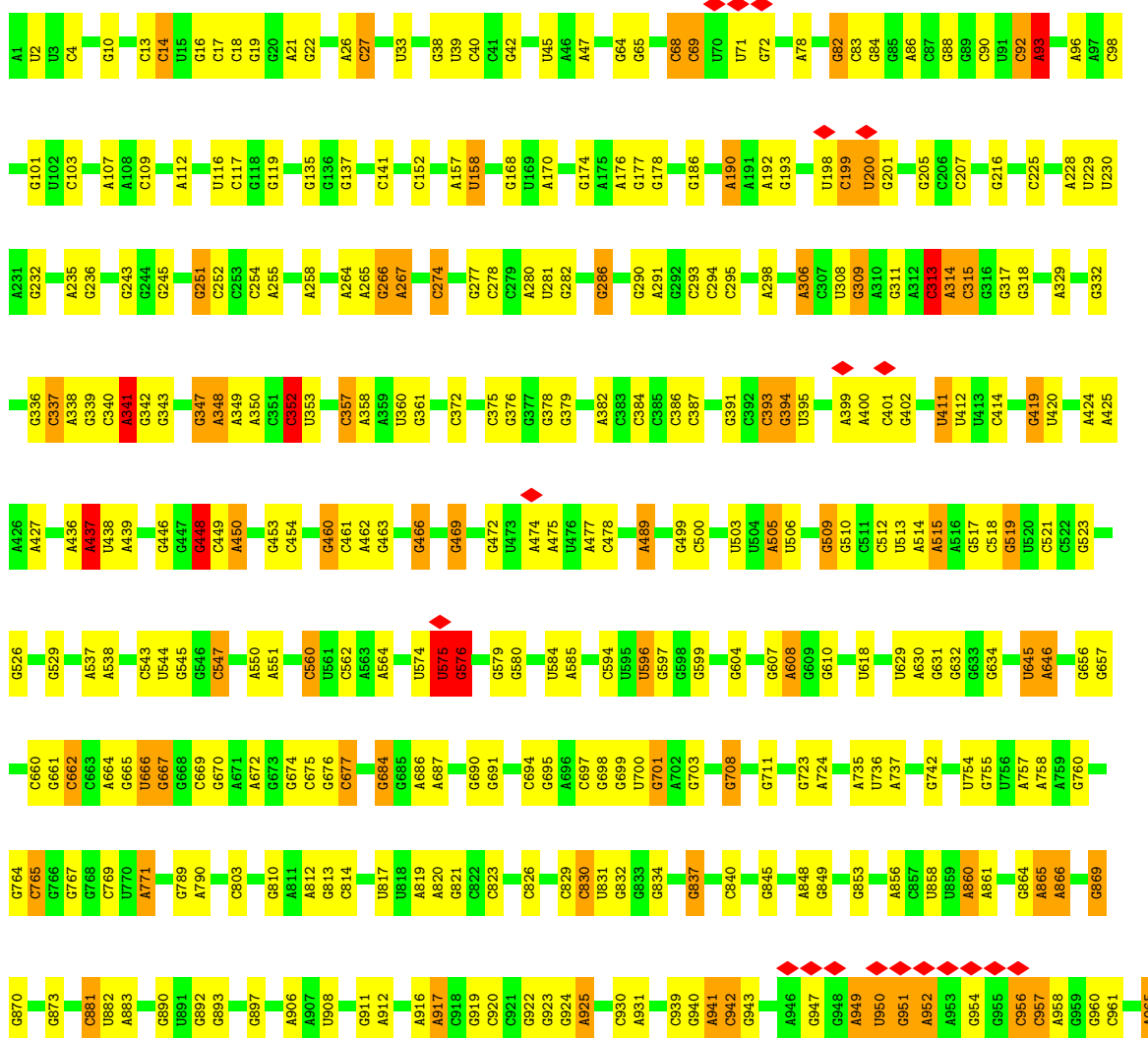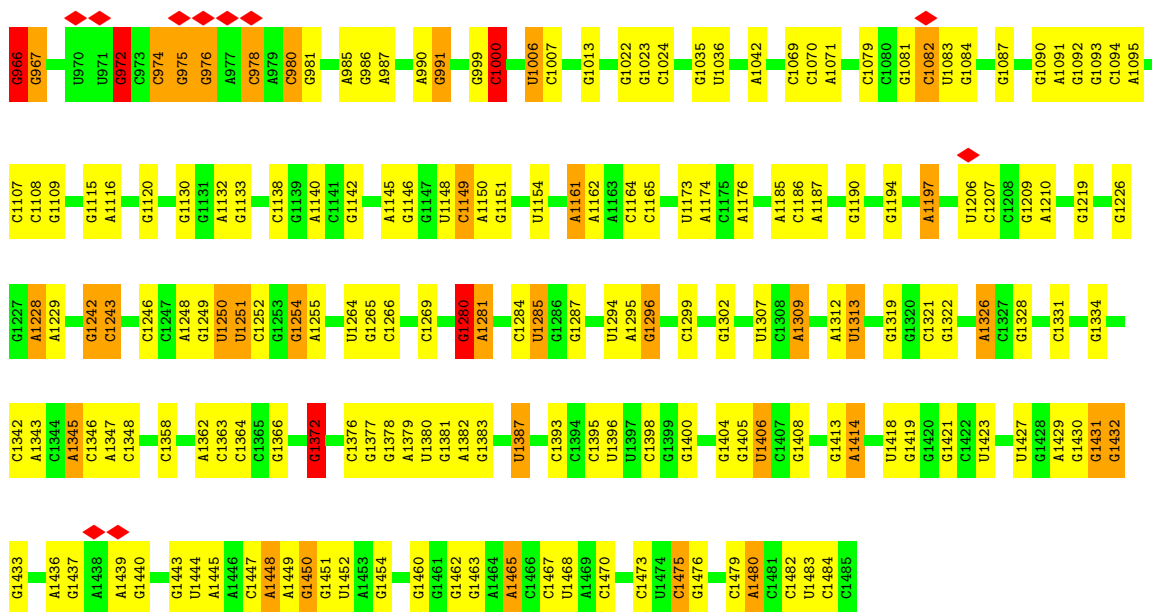
• Molecule 2: 30S ribosomal protein S2

Chain B:

89% 11%

• Molecule 3: 30S ribosomal protein S3

Chain C:

92% 8%
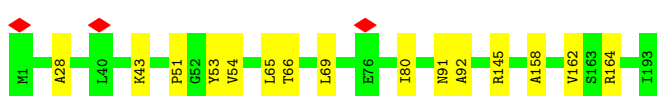
• Molecule 4: 30S ribosomal protein S3Ae

Chain D:

85% 14%
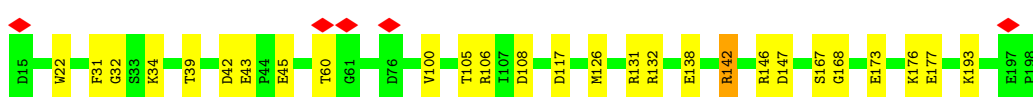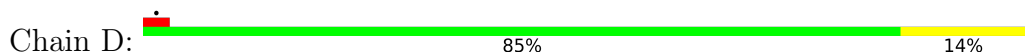
• Molecule 5: 30S ribosomal protein S4

Chain E:

87% 11%
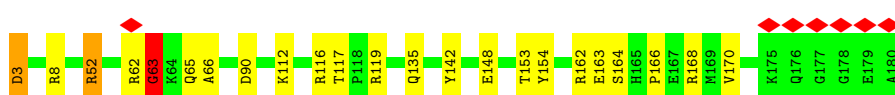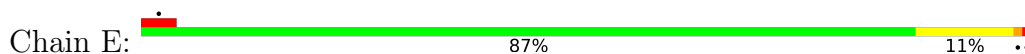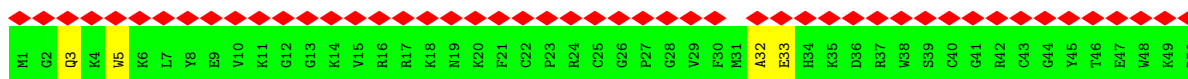
• Molecule 6: 30S ribosomal protein S4e

Chain F:　83%　17%

R3 R12 A15 R23 R33 H37 S42 T58 A59 R60 E68 G69 R70 D80 V85 M88 V102 L125 R126 I127 R131 N141 L142 H143 D144 G145 S146 K155 Y158 V164 L165 M166 K167 R171 E172 V173 I174 E175 I176 A183

Y184 V185 N192 R195 I199 F205 P206 D217 E221 A230 P243
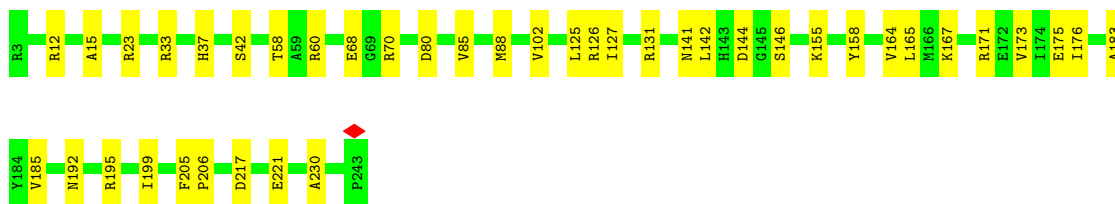
• Molecule 7: 30S ribosomal protein S5

Chain G:　87%　12%

S2 Q3 R4 E7 T13 K14 L15 I24 T25 D26 I27 I30 F31 E39 I42 V43 R53 E54 R66 N84 R85 D86 G87 Y88 K111 S133 I134 G143 S144 V145 R146 R154 A171 V176 W177 S178 F190 R220 E221

• Molecule 8: 30S ribosomal protein S6e

Chain H:　6%　87%　13%

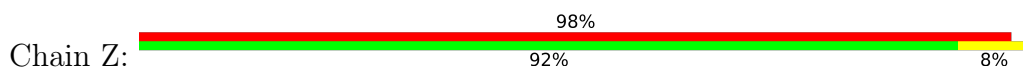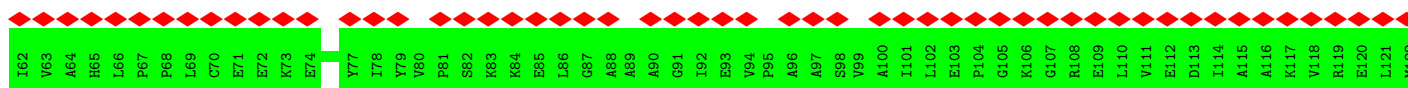M1 A2 T3 N13 G14 I15 E20 A26 L47 I50 E54 I55 P56 G57 D58 V59 G80 R99 R102 N110 T111 I112 S113 P114 E115 V124 F125
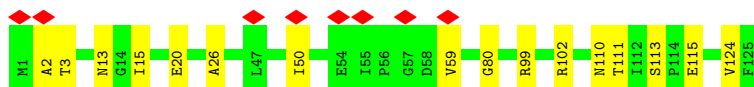
• Molecule 9: 30S ribosomal protein S7

Chain I:　78%　22%

A2 Y10 G19 V28 R34 S47 G57 K58 V61 V64 E65 R66 L67 I68 S74 S77 F85 M86 R87 R88 R91 S92 L93 M94 S95 K96 V104 K105 E106 A107 I111 E112 R113 R114 T115 K116 Q117 N118 P119 I120 S130 A131 P132 G142

G143 I144 R145 R156 R157 L158 D159 K172 R175 N176 K177 T178 A185 I188 A200 R215
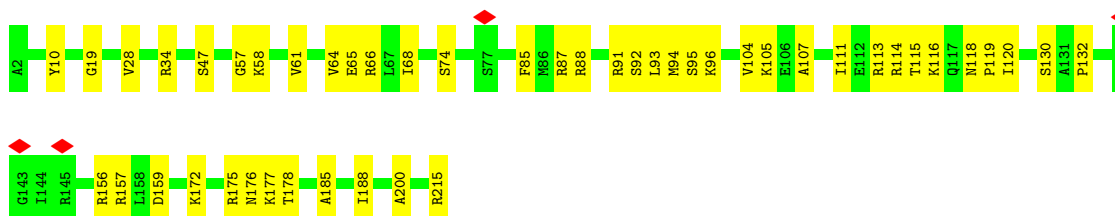
• Molecule 10: 30S ribosomal protein S8

Chain J:　92%　8%

T2 L3 L4 D5 K22 Y26 R62 R78 V104 S105 R124 L125 Y130

• Molecule 11: 30S ribosomal protein S8e

Chain K:　88%　11%

A2 I3 K25 G29 A33 E39 E40 K45 R57 I62 V77 V81 R87 I100 E104 A105 R113 P114 G115 E127

• Molecule 12: 30S ribosomal protein S9

Chain L:
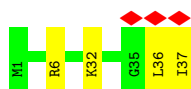
80%   19%

M1 R10 K11 T12 A13 R16 G24 R25 V26 R27 E34 I35 I36 E39 I40 A41 R42 F43 T44 E47 L51 V60 D61 G68 R79 T90 N91 D92 M93 N94 F99 P116 H117 K118 K132
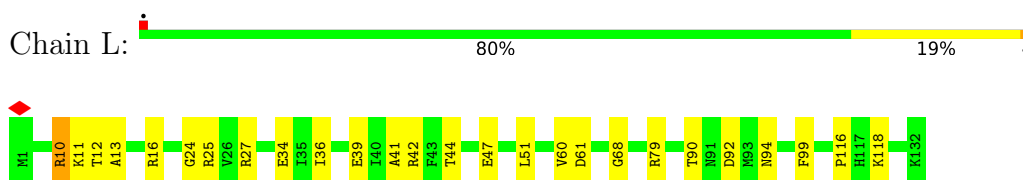
• Molecule 13: 30S ribosomal protein S10

Chain M:

97%

M1 A27 T30 E79 E92 S102
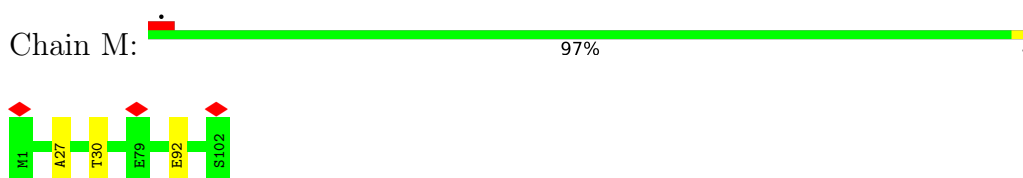
• Molecule 14: 30S ribosomal protein S11

Chain N:

10%

86%   14%

Q7 V8 N9 L10 K11 K12 K13 E14 I21 Y25 N26 N27 G46 V50 K51 Y60 A61 A62 M63 I64 A70 M74 V85 S95 I104 R105 A106 L107 A108 R109 L112 D126 G127 R138 V139
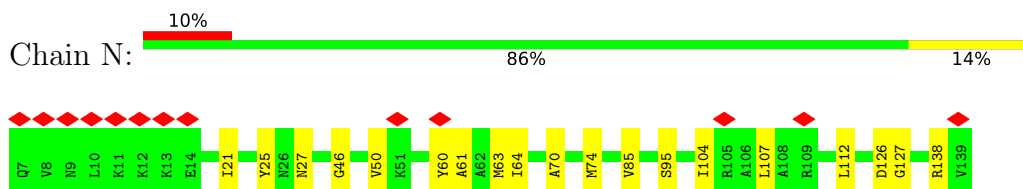
• Molecule 15: 30S ribosomal protein S12

Chain O:

84%   15%

G3 K4 K5 A6 P7 R14 L18 R32 P43 Q49 V60 E61 A62 K63 Q64 P65 M69 R70 K71 N80 D91 V103 P111 I119 I122 R123 V126 R146
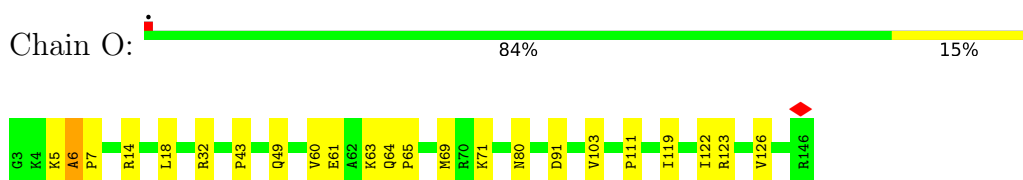
• Molecule 16: 30S ribosomal protein S13

Chain P:

85%   15%

D3 E4 F5 R6 R10 G13 V14 D15 L16 N19 K20 Q21 G31 R42 V43 A44 L55 I66 K84 K90 D91 M92 H93 L94 I95 T96 A97 N135 H138
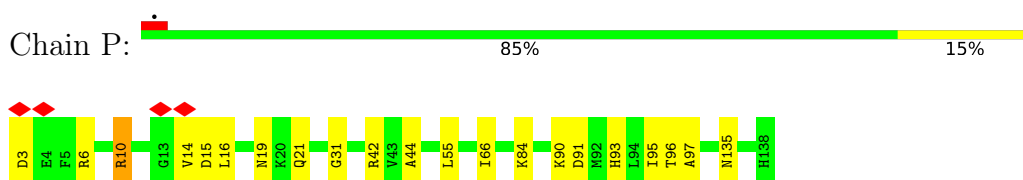
• Molecule 17: 30S ribosomal protein S14 type Z

Chain Q:

14%

79%   20%

M1 A2 K3 A4 D5 Y6 N7 K8 R9 R19 R23 C24 G28 P29 V30 L36 M37 L38 C42 F43 R44 E56
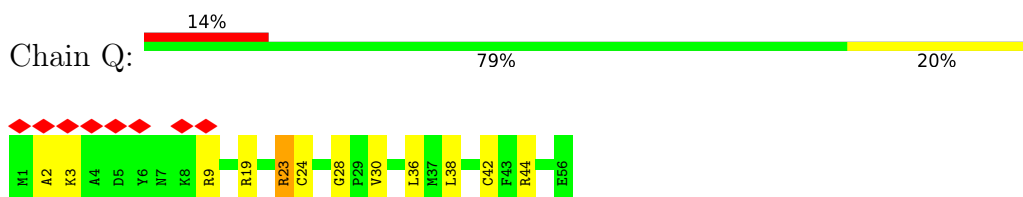
• Molecule 18: 30S ribosomal protein S15

Chain R:

91%   7%

M1 A2 A6 E34 V38 R55 V63 D87 L88 R99 E119 R124 R131 K138 R151
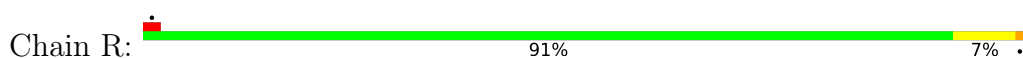
• Molecule 19: 30S ribosomal protein S17

Chain S:
5%
91%
9%

M1 L6 D16 H23 D40 Y59 E60 R61 V69 V104 T105 A108 G109 E110 R111
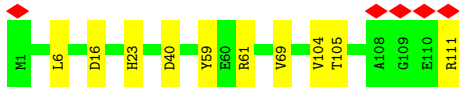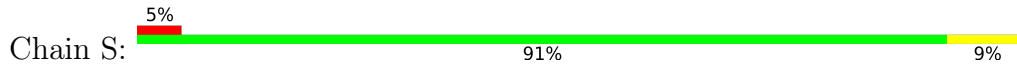
• Molecule 20: 30S ribosomal protein S17e

Chain T:
92%
8%

M1 F24 S25 R26 I54 G64
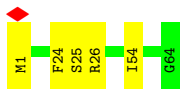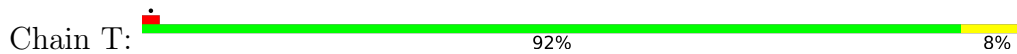
• Molecule 21: 30S ribosomal protein S19P

Chain U:
76%
24%

E6 R10 G11 Y12 E15 D24 F25 L28 L29 R34 R35 S36 L37 G40 K47 L48 I52 R53 L54 A55 R56 K57 K61 E76 M77 I80 H83 F90 I95 K112 V113 V114 Q115 G120
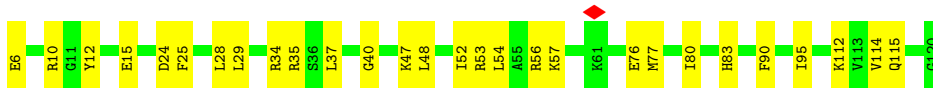
• Molecule 22: 30S ribosomal protein S19e

Chain V:
77%
21%

A2 D6 D10 L11 L12 T16 E22 V23 E24 K27 F34 V35 R39 H40 K41 P45 D49 R54 V55 A56 S57 R60 K61 I62 G66 P67 V68 Y77 K81 H89 R99 L102 Q103 Q104 L105 E106 R119 K137 L140 E141

E142 Q143 L147 Y150
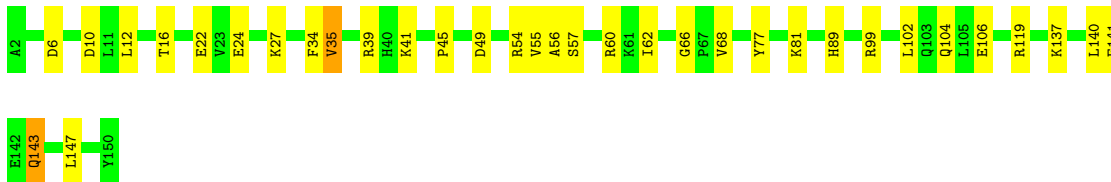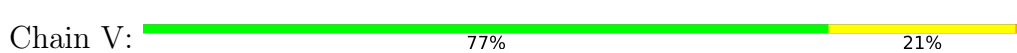
• Molecule 23: RNA-binding protein

Chain W:
89%
9%

K4 V7 E16 R38 C51 C54 P59
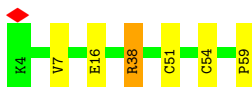
• Molecule 24: 30S ribosomal protein S24e

Chain X:
81%
19%

M1 E2 I3 R6 D22 V23 I24 H25 T30 P31 S32 R33 A34 D35 V41 L44 D45 L46 I53 I56 F60 S65 E84 V88 K95 E96 E97
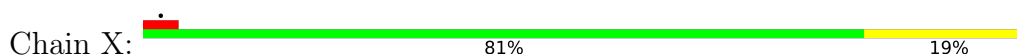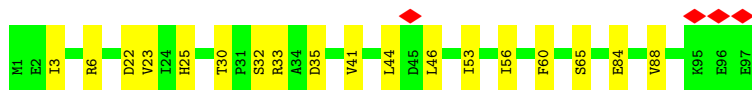
• Molecule 25: 30S ribosomal protein S27e

Chain Y:

8%
87%
13%

L3 P4 K5 N6 L16 C20 G24 V37 V47 L56 V60 L61 E62 V63 L64 E65
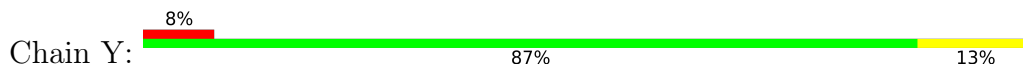
• Molecule 26: 30S ribosomal protein S27ae

Chain Z:

98%
92%
8%

M1 G2 Q3 K4 W5 K6 L7 Y8 E9 V10 K11 G12 G13 K14 V15 R16 R17 K18 N19 K20 F21 C22 P23 R24 C25 G26 P27 G28 V29 F30 M31 A32 E33 H34 K35 D36 R37 W38 S39 C40 G41 R42 C43 G44 Y45 T46 E47 W48 K49 R50

• Molecule 27: 30S ribosomal protein S28e

Chain a:

8%
95%
5%

M1 S2 D3 E4 R34 V48 E60 R64 E65 I66
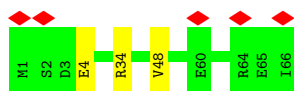
• Molecule 28: 50S ribosomal protein L7Ae

Chain b:

89%
100%

M1 A2 K3 P4 S5 Y6 V7 K8 F9 E10 V11 P12 A13 E14 L15 A16 E17 K18 A19 L20 E21 A22 V23 E24 R27 D28 T29 G30 R31 I32 R33 K34 G35 T36 N37 E38 T39 T40 K41 A42 V43 E44 R45 G46 Q47 A48 K49 L50 V51 V52 I53 A54 E55 D56 V57 D58 P59 E60 E61

I62 V63 A64 H65 L66 P67 P68 L69 C70 E71 E72 K73 E74 Y77 I78 Y79 V80 P81 S82 K83 K84 E85 L86 G87 A88 A89 A90 G91 I92 E93 V94 P95 A96 A97 S98 V99 A100 I101 L102 E103 P104 G105 K106 G107 R108 E109 L110 V111 E112 D113 I114 A115 A116 K117 V118 R119 E120 L121 M122

K123

• Molecule 29: LSU ribosomal protein L41E

Chain c:

8%
89%
11%

M1 R6 K32 G35 L36 I37
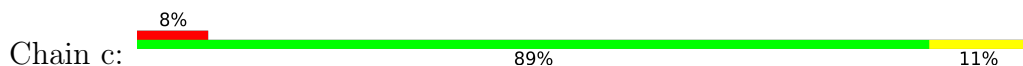
• Molecule 30: ATPase

Chain d:

96%

M1 E38 I39 V40 K41 C54 V69 N70 L71 L75 N98 G106 K133 V134 R246 L277 K329 GLU VAL SER ASP LEU ASP LEU SER LYS ASP LEU LYS T342 N362 K366 E369 Q411 R412 S594
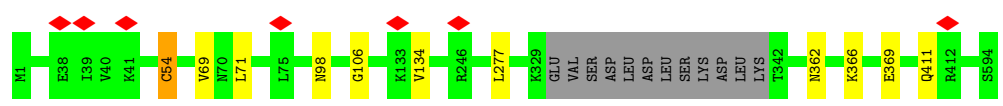
4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	293010	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 $(e^-/\text{Å}^2)$	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	49.493	Depositor
Minimum map value	-24.478	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.121	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	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, ZN, 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	A	1.61	104/35726 (0.3%)	1.32	233/55763 (0.4%)
2	B	0.74	0/1602	0.66	0/2167
3	C	0.76	0/1548	0.68	0/2076
4	D	0.65	0/1547	0.69	1/2076 (0.0%)
5	E	0.80	0/1499	0.75	2/2011 (0.1%)
6	F	0.90	0/2007	0.71	0/2708
7	G	0.91	0/1747	0.74	2/2351 (0.1%)
8	H	0.61	0/974	0.72	0/1306
9	I	0.90	2/1734 (0.1%)	0.69	1/2326 (0.0%)
10	J	0.94	0/1042	0.71	0/1399
11	K	0.79	0/1007	0.73	0/1342
12	L	0.91	0/1053	0.73	1/1408 (0.1%)
13	M	0.71	0/826	0.69	0/1107
14	N	0.61	0/1024	0.66	0/1377
15	O	0.89	0/1148	0.74	0/1529
16	P	0.88	1/1131 (0.1%)	0.74	0/1524
17	Q	0.82	0/469	0.64	0/618
18	R	0.74	0/1248	0.71	2/1672 (0.1%)
19	S	0.90	0/936	0.64	0/1260
20	T	0.72	0/547	0.57	0/726
21	U	0.91	0/968	0.67	0/1292
22	V	1.01	1/1250 (0.1%)	0.78	2/1688 (0.1%)
23	W	0.86	0/449	0.66	0/610
24	X	0.80	0/811	0.65	0/1085
25	Y	0.73	0/481	0.72	0/648
26	Z	0.32	0/429	0.62	0/568
27	a	0.74	0/516	0.72	0/692
28	b	0.34	0/949	0.60	0/1282
29	c	1.05	0/357	0.84	0/462
30	d	0.77	1/4701 (0.0%)	0.64	0/6338
All	All	1.28	109/69726 (0.2%)	1.09	244/101411 (0.2%)

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	3
2	B	0	1
All	All	0	4

The worst 5 of 109 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	19	ASN	CA-CB	-10.17	1.26	1.53
1	A	830	C	C2-O2	-8.92	1.16	1.24
9	I	96	LYS	CA-CB	-8.45	1.35	1.53
1	A	352	C	C2-O2	-7.93	1.17	1.24
1	A	379	G	N3-C4	-7.63	1.30	1.35

The worst 5 of 244 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	966	G	N1-C6-O6	-21.94	106.73	119.90
1	A	966	G	C5-C6-O6	20.78	141.07	128.60
1	A	956	C	N3-C4-N4	-19.90	104.07	118.00
1	A	956	C	C5-C4-N4	18.06	132.84	120.20
1	A	466	G	C4-N9-C1'	12.11	142.24	126.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1000	C	Sidechain
1	A	352	C	Sidechain
1	A	830	C	Sidechain
2	B	6	VAL	Peptide

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	31920	0	16102	146	0
2	B	1571	0	1624	12	0
3	C	1526	0	1611	7	0
4	D	1520	0	1583	19	0
5	E	1476	0	1545	16	0
6	F	1963	0	2043	25	0
7	G	1721	0	1780	20	0
8	H	961	0	1010	11	0
9	I	1704	0	1754	34	0
10	J	1022	0	1053	6	0
11	K	997	0	1078	10	0
12	L	1040	0	1101	17	0
13	M	819	0	871	2	0
14	N	1005	0	1029	11	0
15	O	1131	0	1225	22	0
16	P	1109	0	1137	14	0
17	Q	459	0	483	8	0
18	R	1225	0	1314	8	0
19	S	913	0	933	6	0
20	T	540	0	559	4	0
21	U	949	0	1000	19	0
22	V	1218	0	1231	22	0
23	W	435	0	414	4	0
24	X	799	0	823	13	0
25	Y	475	0	512	5	0
26	Z	417	0	421	5	0
27	a	514	0	547	0	0
28	b	936	0	978	0	0
29	c	351	0	418	0	0
30	d	4622	0	4729	0	0
31	A	27	0	0	0	0
31	d	2	0	0	0	0
32	Q	1	0	0	0	0
32	W	2	0	0	0	0
32	Y	1	0	0	0	0
33	d	16	0	0	0	0
34	d	62	0	24	0	0
All	All	65449	0	50932	397	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 397 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)
15:O:6:ALA:CB	15:O:7:PRO:HD3	1.39	1.41
15:O:6:ALA:CB	15:O:7:PRO:CD	2.17	1.21
15:O:6:ALA:HB3	15:O:7:PRO:HD3	1.37	1.04
15:O:6:ALA:HB1	15:O:7:PRO:CD	1.83	1.02
15:O:6:ALA:HB3	15:O:7:PRO:CD	1.90	1.00

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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	B	193/195 (99%)	174 (90%)	18 (9%)	1 (0%)	29	61
3	C	191/193 (99%)	182 (95%)	9 (5%)	0	100	100
4	D	182/184 (99%)	161 (88%)	20 (11%)	1 (0%)	29	61
5	E	176/178 (99%)	157 (89%)	17 (10%)	2 (1%)	14	41
6	F	239/241 (99%)	211 (88%)	26 (11%)	2 (1%)	19	49
7	G	218/220 (99%)	201 (92%)	16 (7%)	1 (0%)	29	61
8	H	123/125 (98%)	109 (89%)	14 (11%)	0	100	100
9	I	212/214 (99%)	199 (94%)	12 (6%)	1 (0%)	29	61
10	J	127/129 (98%)	113 (89%)	14 (11%)	0	100	100
11	K	124/126 (98%)	110 (89%)	14 (11%)	0	100	100
12	L	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
13	M	100/102 (98%)	91 (91%)	9 (9%)	0	100	100
14	N	131/133 (98%)	117 (89%)	14 (11%)	0	100	100
15	O	142/144 (99%)	128 (90%)	10 (7%)	4 (3%)	5	17
16	P	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
17	Q	54/56 (96%)	44 (82%)	10 (18%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	R	149/151 (99%)	139 (93%)	9 (6%)	1 (1%)	22	53
19	S	109/111 (98%)	101 (93%)	8 (7%)	0	100	100
20	T	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
21	U	113/115 (98%)	103 (91%)	10 (9%)	0	100	100
22	V	147/149 (99%)	138 (94%)	6 (4%)	3 (2%)	7	24
23	W	54/56 (96%)	44 (82%)	10 (18%)	0	100	100
24	X	95/97 (98%)	87 (92%)	8 (8%)	0	100	100
25	Y	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
26	Z	48/50 (96%)	38 (79%)	10 (21%)	0	100	100
27	a	64/66 (97%)	51 (80%)	12 (19%)	1 (2%)	9	31
28	b	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
29	c	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
30	d	578/594 (97%)	501 (87%)	73 (13%)	4 (1%)	22	53
All	All	4112/4184 (98%)	3700 (90%)	391 (10%)	21 (0%)	32	61

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	O	6	ALA
15	O	63	LYS
22	V	35	VAL
5	E	63	GLY
7	G	85	ARG

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	169/169 (100%)	169 (100%)	0	100	100
3	C	155/155 (100%)	153 (99%)	2 (1%)	69	91
4	D	159/159 (100%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	157/157 (100%)	155 (99%)	2 (1%)	69	91
6	F	212/212 (100%)	212 (100%)	0	100	100
7	G	182/182 (100%)	177 (97%)	5 (3%)	44	78
8	H	103/105 (98%)	103 (100%)	0	100	100
9	I	178/178 (100%)	177 (99%)	1 (1%)	86	96
10	J	105/105 (100%)	105 (100%)	0	100	100
11	K	102/102 (100%)	101 (99%)	1 (1%)	76	93
12	L	108/108 (100%)	108 (100%)	0	100	100
13	M	91/91 (100%)	91 (100%)	0	100	100
14	N	100/100 (100%)	99 (99%)	1 (1%)	76	93
15	O	118/118 (100%)	117 (99%)	1 (1%)	81	94
16	P	114/114 (100%)	111 (97%)	3 (3%)	46	79
17	Q	46/46 (100%)	44 (96%)	2 (4%)	29	62
18	R	130/130 (100%)	129 (99%)	1 (1%)	81	94
19	S	98/98 (100%)	97 (99%)	1 (1%)	76	93
20	T	59/59 (100%)	59 (100%)	0	100	100
21	U	103/103 (100%)	103 (100%)	0	100	100
22	V	124/124 (100%)	124 (100%)	0	100	100
23	W	50/50 (100%)	49 (98%)	1 (2%)	55	84
24	X	86/86 (100%)	86 (100%)	0	100	100
25	Y	56/56 (100%)	56 (100%)	0	100	100
26	Z	42/42 (100%)	42 (100%)	0	100	100
27	a	55/55 (100%)	53 (96%)	2 (4%)	35	69
28	b	98/98 (100%)	98 (100%)	0	100	100
29	c	35/35 (100%)	31 (89%)	4 (11%)	5	18
30	d	504/519 (97%)	497 (99%)	7 (1%)	67	90
All	All	3539/3556 (100%)	3505 (99%)	34 (1%)	77	93

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	d	69	VAL
30	d	71	LEU

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Mol	Chain	Res	Type
30	d	369	GLU
15	O	5	LYS
14	N	138	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
26	Z	3	GLN
30	d	450	HIS
30	d	70	ASN
30	d	456	ASN
30	d	164	HIS

5.3.3　RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1484/1485 (99%)	303 (20%)	34 (2%)

5 of 303 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	C
1	A	14	C
1	A	33	U
1	A	39	U
1	A	40	C

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1242	G
1	A	1249	G
1	A	1431	G
1	A	438	U
1	A	437	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 37 ligands modelled in this entry, 33 are 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	#$|Z| > 2$
34	ANP	d	603	31	29,33,33	4.61	15 (51%)	31,52,52	2.25	5 (16%)
33	SF4	d	601	30	0,12,12	-	-	-		
33	SF4	d	602	30	0,12,12	-	-	-		
34	ANP	d	605	31	29,33,33	4.61	15 (51%)	31,52,52	2.12	3 (9%)

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
34	ANP	d	603	31	-	7/14/38/38	0/3/3/3
33	SF4	d	601	30	-	-	0/6/5/5
33	SF4	d	602	30	-	-	0/6/5/5
34	ANP	d	605	31	-	4/14/38/38	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	d	603	ANP	C2'-C1'	-15.95	1.29	1.53
34	d	605	ANP	C2'-C1'	-15.66	1.30	1.53
34	d	605	ANP	O4'-C1'	14.69	1.61	1.41
34	d	603	ANP	O4'-C1'	14.50	1.61	1.41
34	d	603	ANP	O4'-C4'	-6.68	1.30	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	d	605	ANP	C5-C6-N6	7.37	131.55	120.35
34	d	603	ANP	C5-C6-N6	7.10	131.14	120.35
34	d	603	ANP	N3-C2-N1	-5.71	119.75	128.68
34	d	605	ANP	N3-C2-N1	-5.23	120.51	128.68
34	d	605	ANP	N6-C6-N1	-4.78	108.66	118.57

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	d	603	ANP	PB-N3B-PG-O1G
34	d	603	ANP	PG-N3B-PB-O1B
34	d	603	ANP	C5'-O5'-PA-O1A
34	d	603	ANP	C5'-O5'-PA-O2A
34	d	603	ANP	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 ANP d 603

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP d 605

Bond lengths

Bond angles

Torsions

Rings
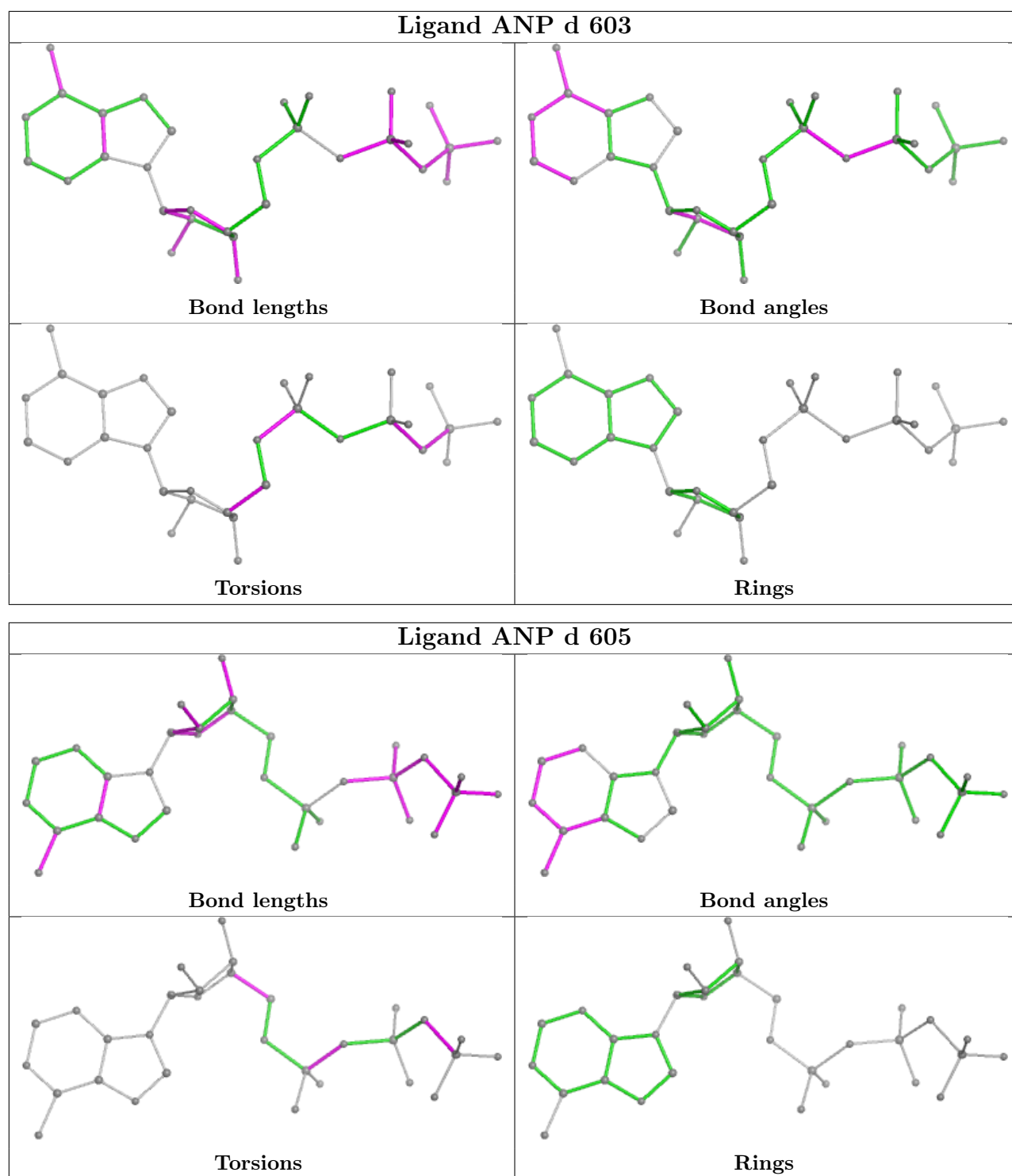
5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-10519. 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 |
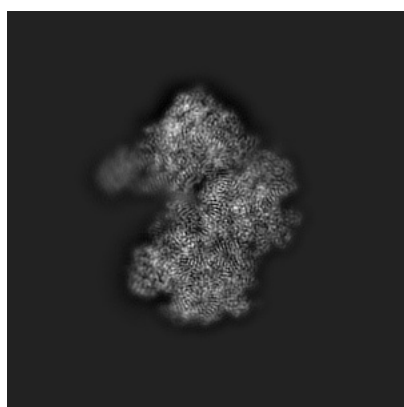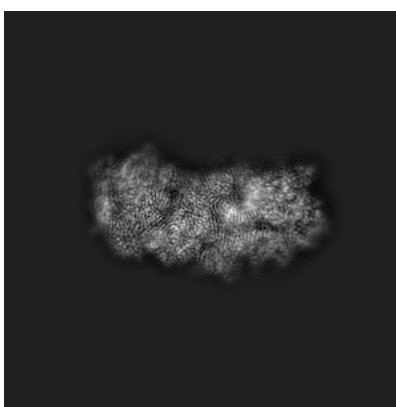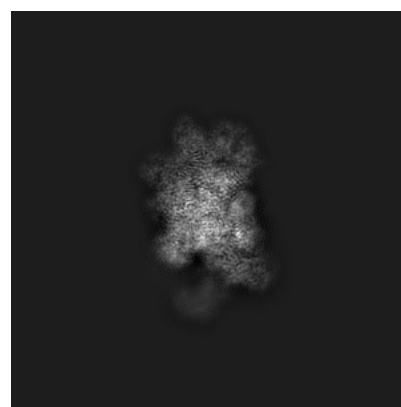
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
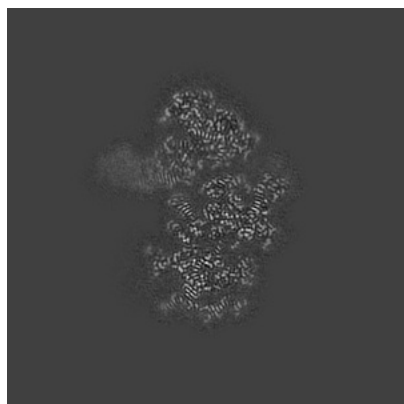
6.2.1   Primary map
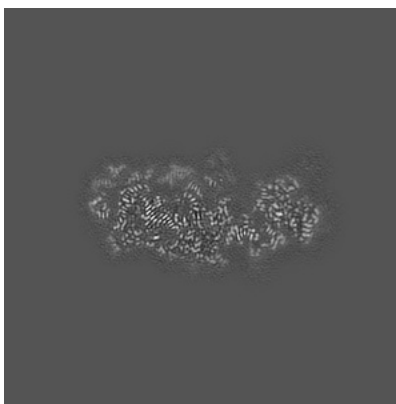
| X Index: 180 | Y Index: 180 | Z Index: 180 |
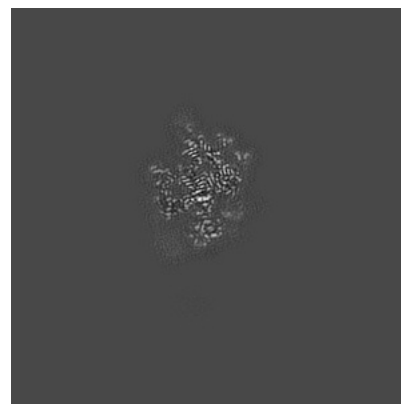
The images above show central slices of the map in three orthogonal directions.

6.3   Largest variance slices ⓘ
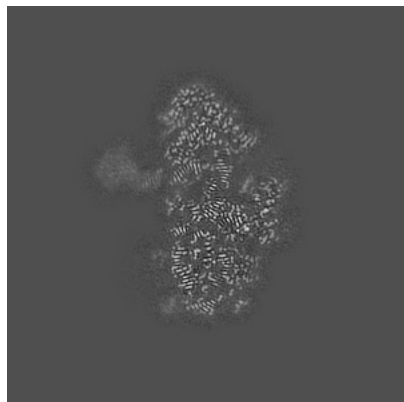
6.3.1   Primary map
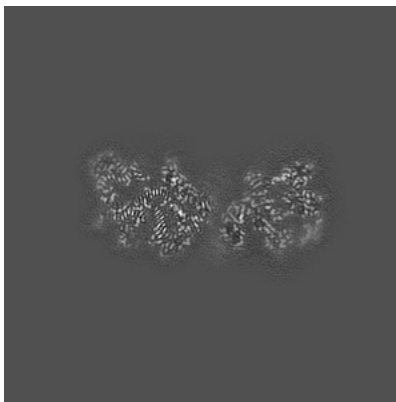
| X Index: 173 | Y Index: 159 | Z Index: 182 |
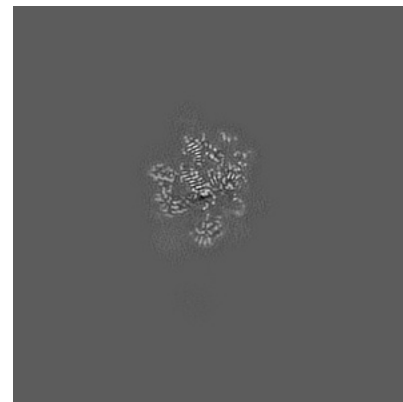
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1   Primary map

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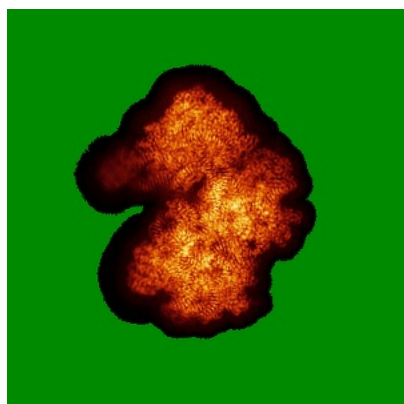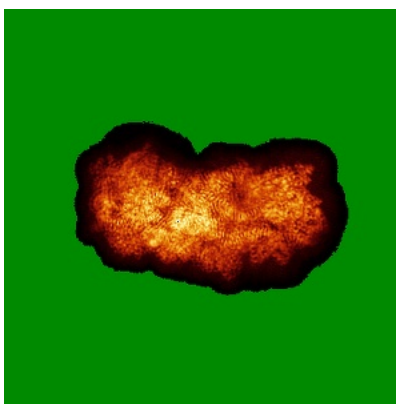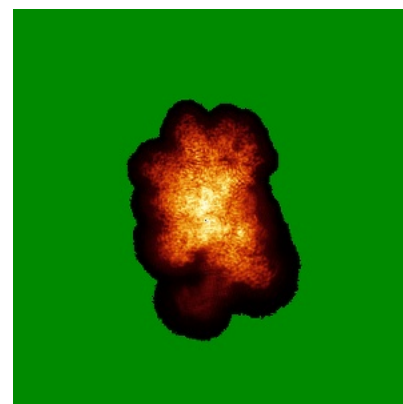
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5　Orthogonal surface views　ⓘ

6.5.1　Primary map

| X | Y | Z |
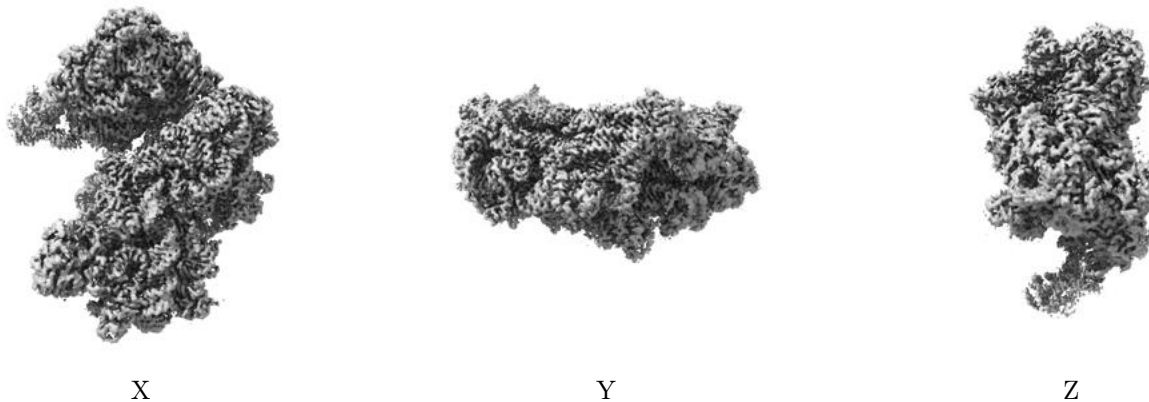
The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6　Mask visualisation　ⓘ

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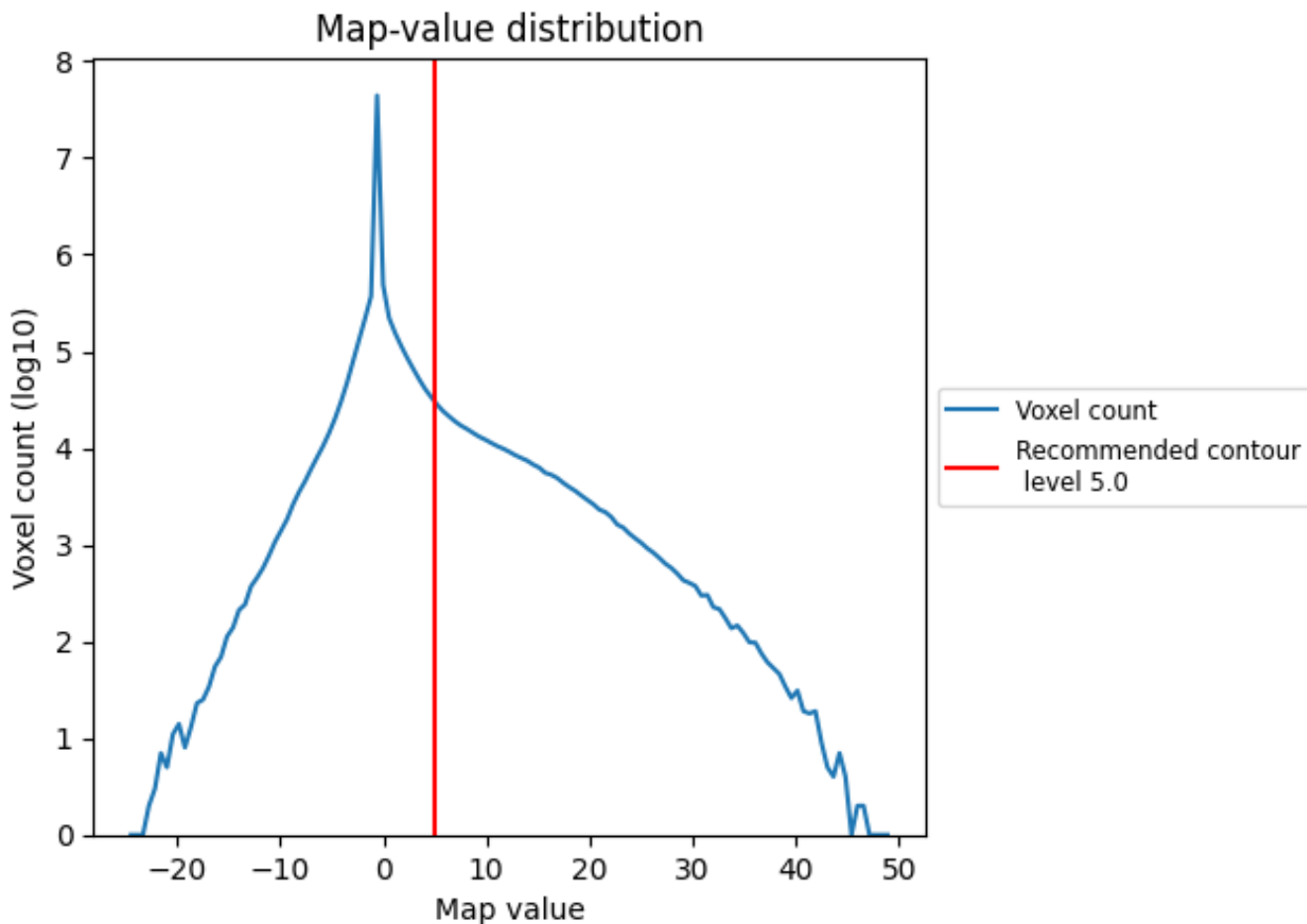
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
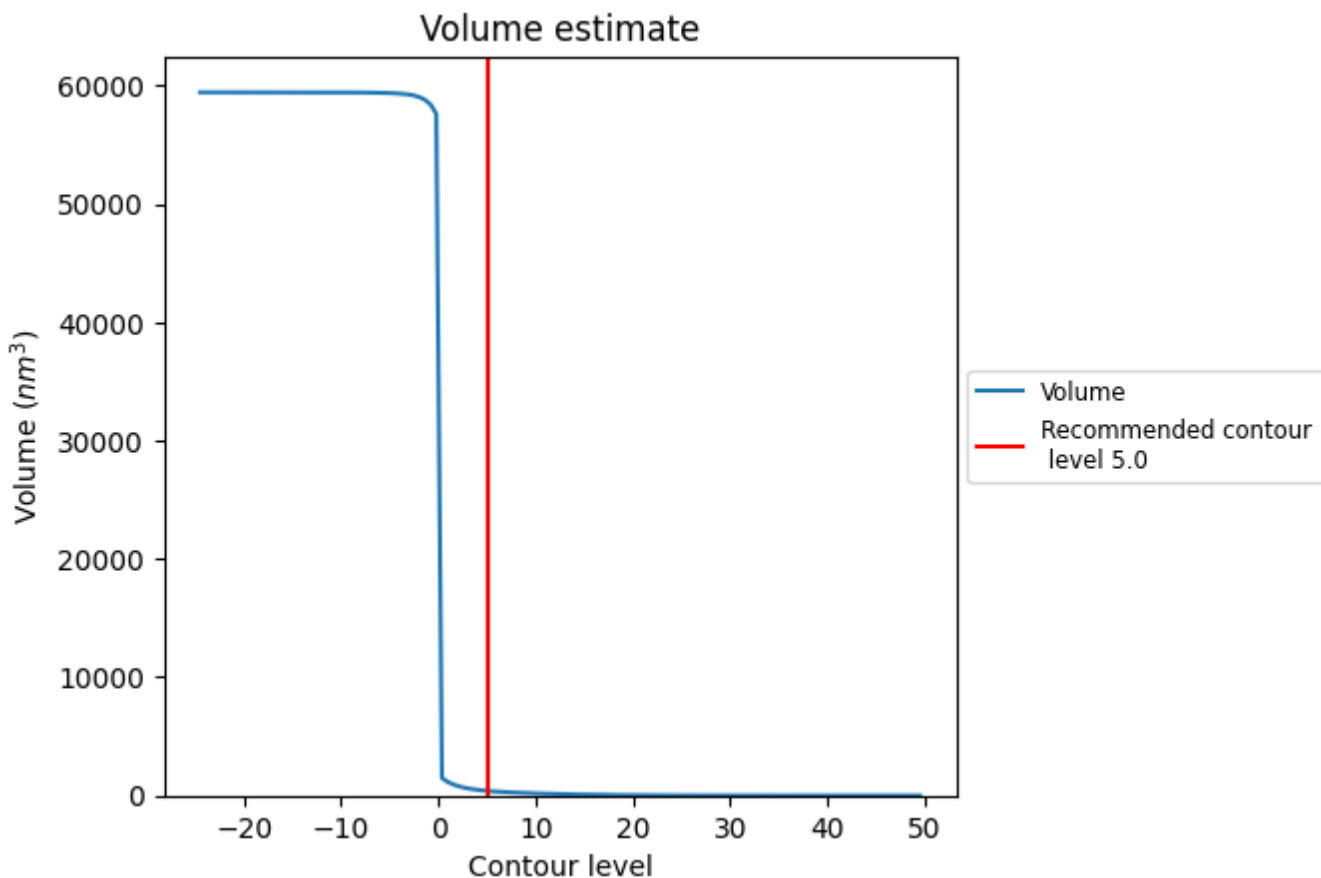
The volume at the recommended contour level is 397 nm^3; this corresponds to an approximate mass of 358 kDa.

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 ⓘ
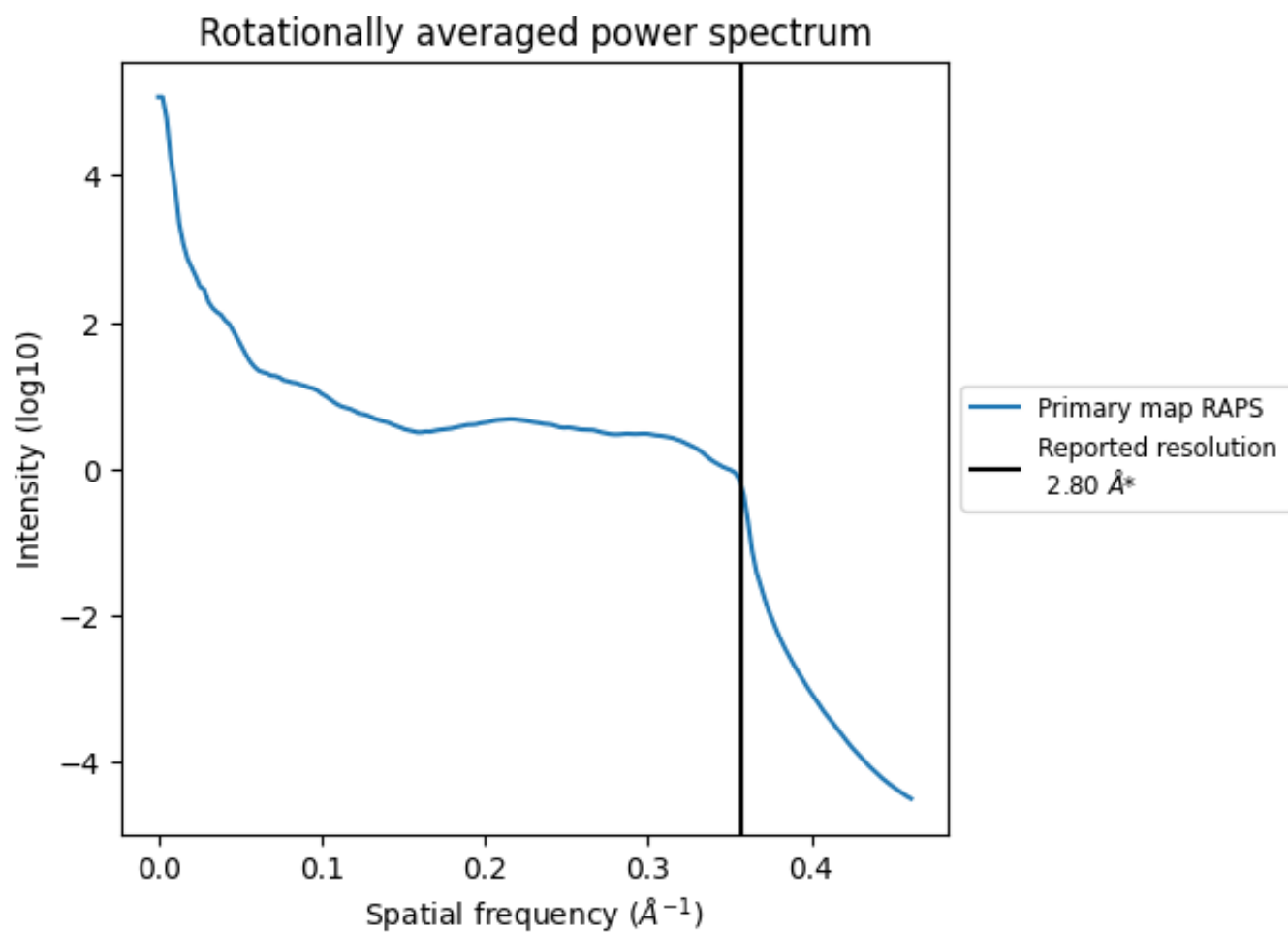
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 ⓘ
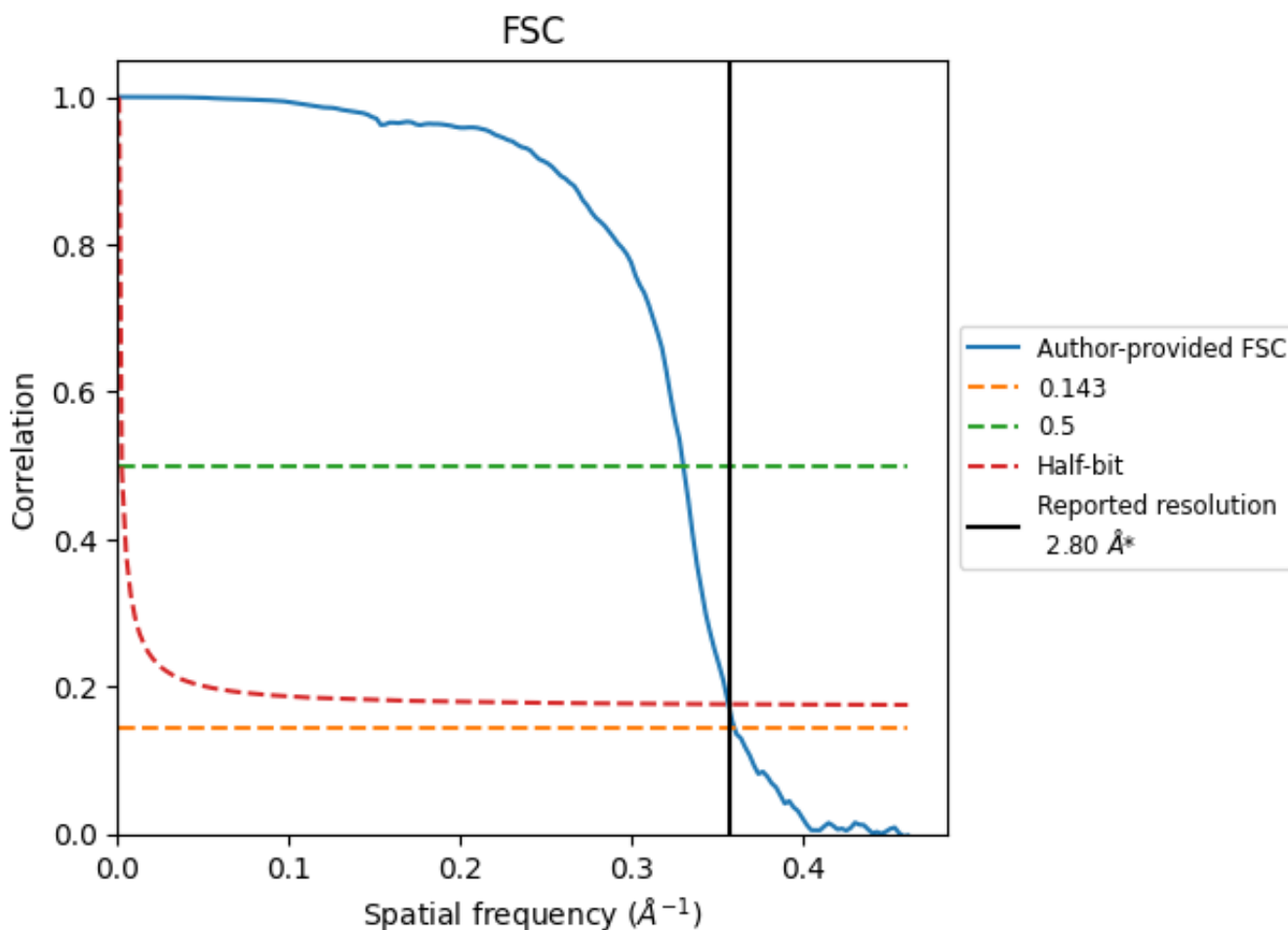
*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.78	3.03	2.80
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-10519 and PDB model 6TMF. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

| X | Y | Z |
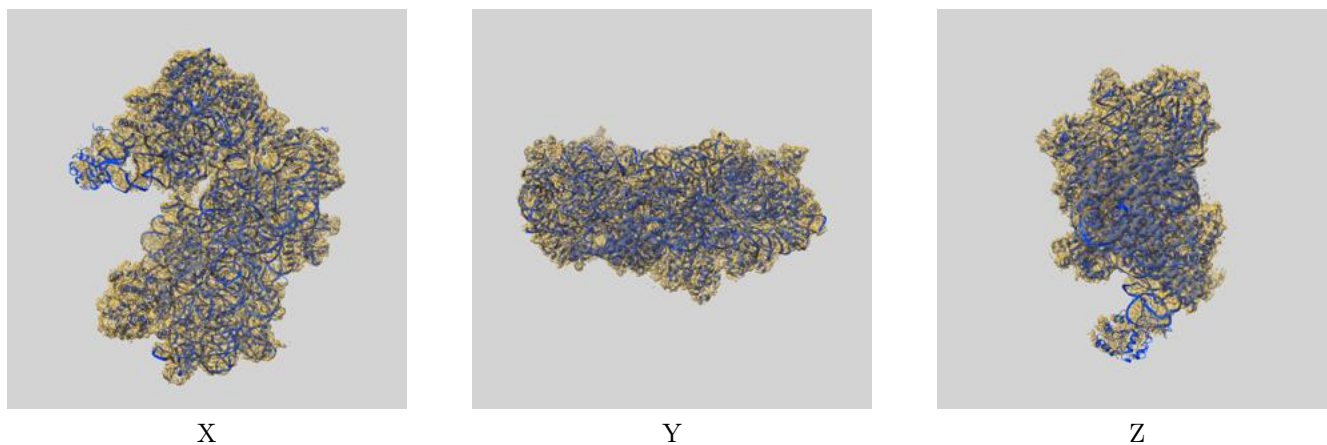
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
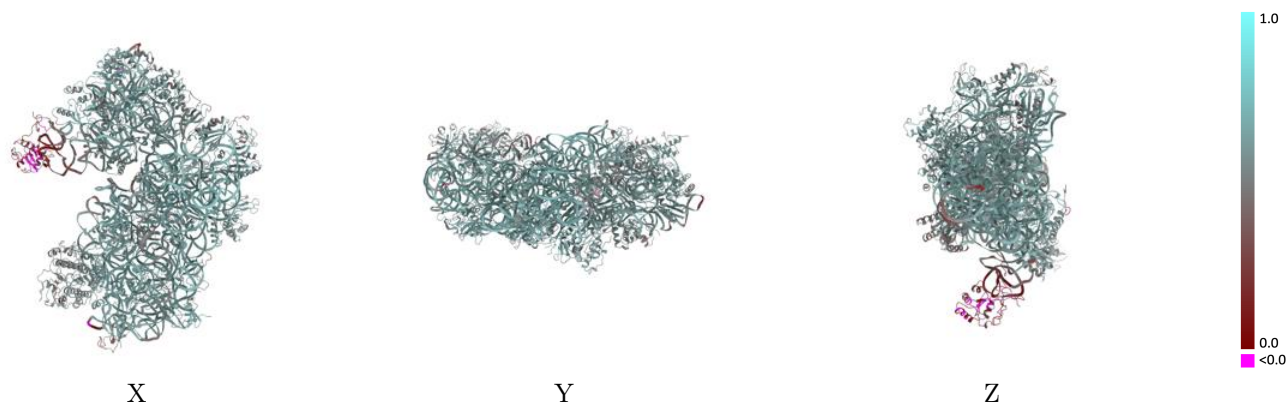
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
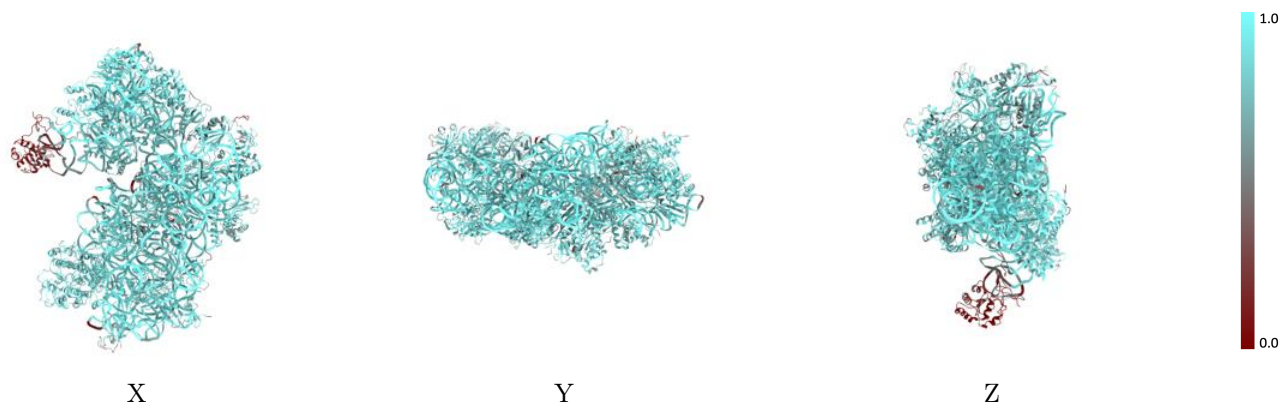
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).

9.4 Atom inclusion ⓘ
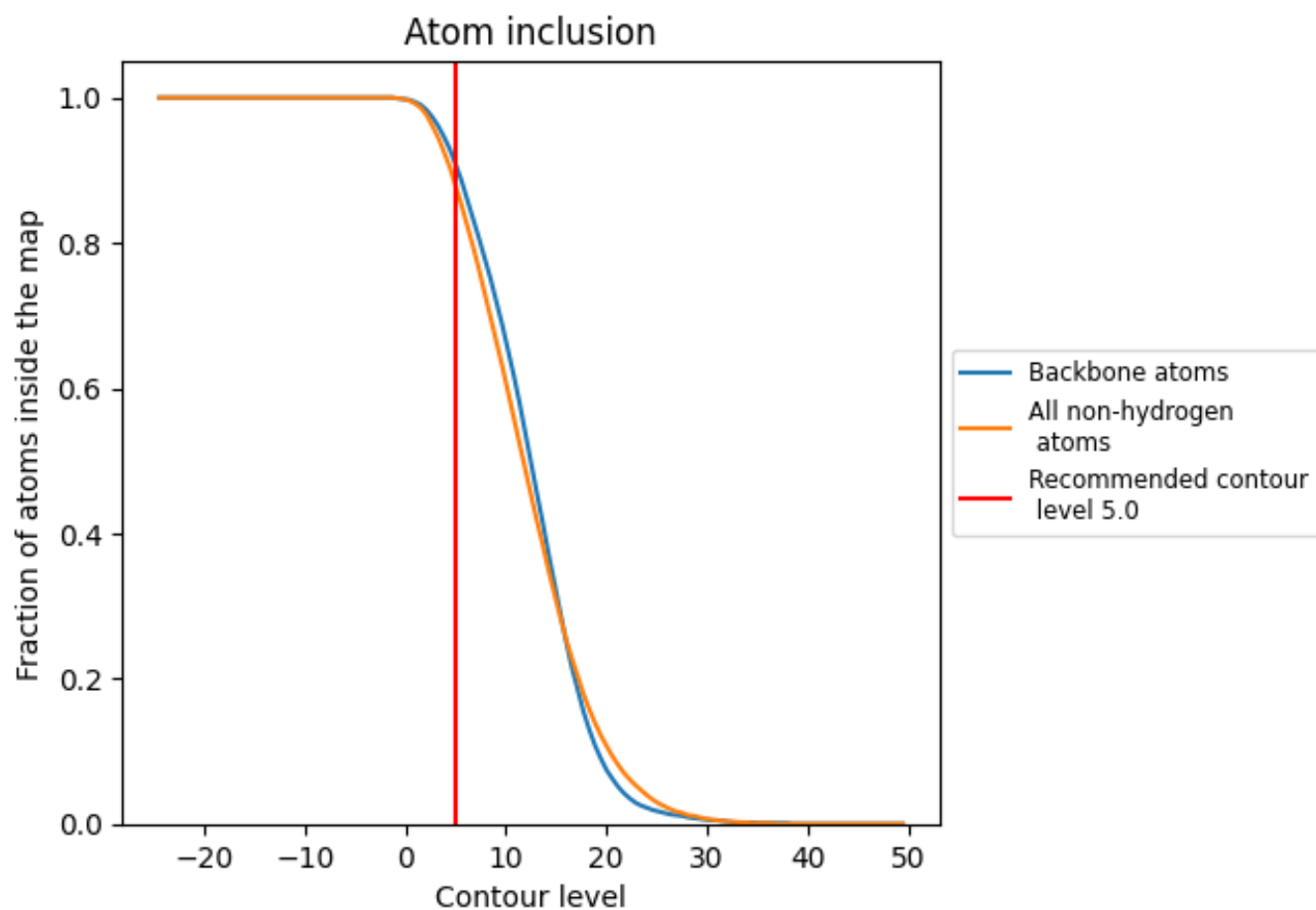
At the recommended contour level, 91% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5830
A	0.9430	0.6100
B	0.8350	0.5900
C	0.8270	0.5380
D	0.7900	0.5580
E	0.8350	0.5960
F	0.8870	0.6140
G	0.8670	0.6190
H	0.7700	0.5410
I	0.8770	0.5710
J	0.8890	0.6280
K	0.8500	0.5990
L	0.9030	0.5970
M	0.8020	0.5180
N	0.7290	0.5510
O	0.8480	0.6160
P	0.8970	0.5660
Q	0.7730	0.5410
R	0.8450	0.5930
S	0.8530	0.6000
T	0.8380	0.5450
U	0.8910	0.5730
V	0.9100	0.5880
W	0.8780	0.6120
X	0.8020	0.5870
Y	0.7700	0.5530
Z	0.0680	0.1720
a	0.8010	0.5280
b	0.1220	0.1360
c	0.8370	0.6170
d	0.8380	0.5340

1.0

0.0
<0.0