WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 12:26 am GMT

PDB ID	:	6ZXD
EMDB ID	:	EMD-11517
Title	:	Cryo-EM structure of a late human pre-40S ribosomal subunit - State F1
Authors	:	Ameismeier, M.; Zemp, I.; van den Heuvel, J.; Thoms, M.; Berninghausen, O.; Kutay, U.; Beckmann, R.
Deposited on	:	2020-07-29
Resolution	:	3.20 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:
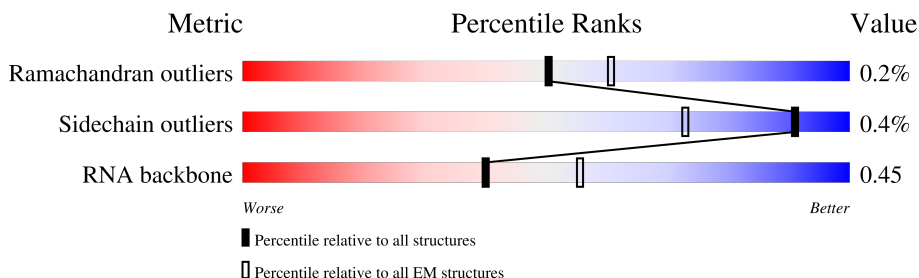
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.20 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.
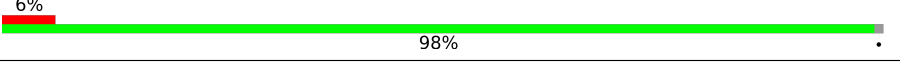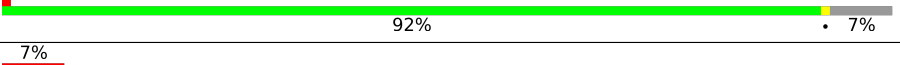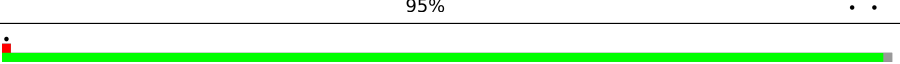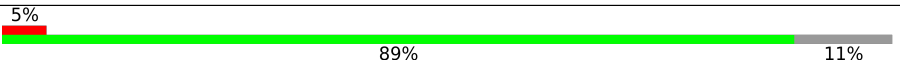
Metric	Percentile Ranks	Value
Ramachandran outliers		0.2%
Sidechain outliers		0.4%
RNA backbone		0.45

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures
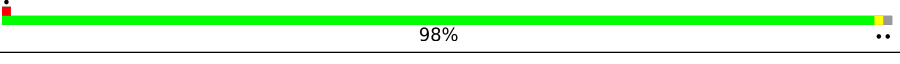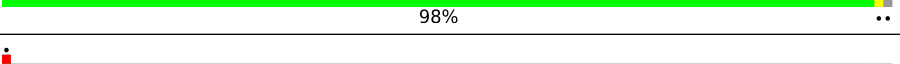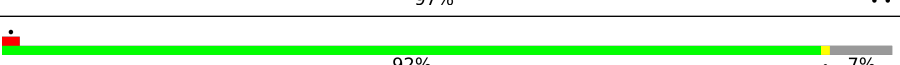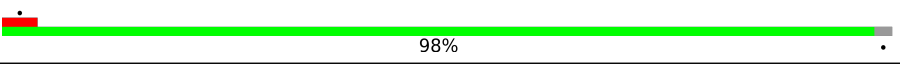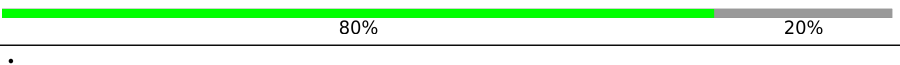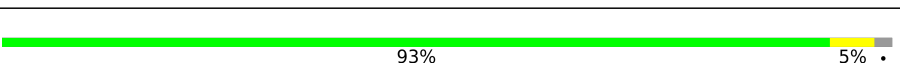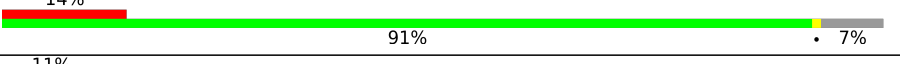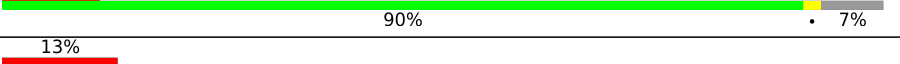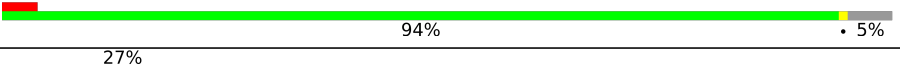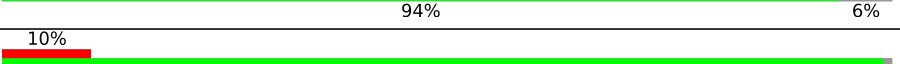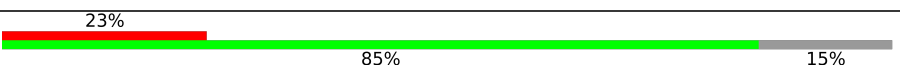
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1873	59% 25% 12%
2	R	135	8% / 87% 10%
3	A	295	73% 27%
4	B	264	80% 19%
5	C	293	74% 26%
6	E	263	99%
7	G	249	6% / 92% 8%
8	H	194	8% / 96%

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Mol	Chain	Length	Quality of chain
9	I	208	6% / 98%
10	J	194	92% / 7%
11	L	158	7% / 95%
12	N	151	99%
13	O	151	5% / 89% / 11%
14	V	83	98%
15	W	130	98%
16	X	143	97%
17	Y	133	92% / 7%
18	b	84	98%
19	e	59	80% / 20%
20	x	252	71% / 29%
21	y	412	16% / 78% / 21%
22	d	56	93% / 5%
23	D	243	14% / 91% / 7%
24	F	204	11% / 90% / 7%
25	K	165	13% / 58% / 42%
26	M	132	79% / 90% / 10%
27	P	145	21% / 83% / 17%
28	Q	146	94% / 5%
29	S	152	27% / 94% / 6%
30	T	145	10% / 99%
31	U	119	23% / 85% / 15%
32	Z	125	38% / 58% / 42%
33	c	69	20% / 88% / 12%

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Mol	Chain	Length	Quality of chain
34	f	156	24% 45% 55%
35	g	317	44% 98% ..
36	z	568	24% 51% 49%
37	k	583	36% 73% • 26%

2 Entry composition ⓘ

There are 38 unique types of molecules in this entry. The entry contains 80922 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 pre-18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1645	Total 35125	C 15677	N 6304	O 11499	P 1645	0	0

- Molecule 2 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	122	Total 990	C 621	N 184	O 182	S 3	0	0

- Molecule 3 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	216	Total 1705	C 1083	N 299	O 315	S 8	0	0

- Molecule 4 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	213	Total 1729	C 1098	N 309	O 308	S 14	0	0

- Molecule 5 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	218	Total 1690	C 1094	N 289	O 297	S 10	0	0

- Molecule 6 is a protein called 40S ribosomal protein S4, X isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	262	Total 2076	C 1324	N 386	O 358	S 8	0	0

- Molecule 7 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total	C	N	O	S	0	0
			1862	1164	371	320	7		

- Molecule 8 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	186	Total	C	N	O	S	0	0
			1501	957	276	267	1		

- Molecule 9 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1682	1056	331	290	5		

- Molecule 10 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	180	Total	C	N	O	S	0	0
			1499	955	300	242	2		

- Molecule 11 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	151	Total	C	N	O	S	0	0
			1229	782	230	211	6		

- Molecule 12 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 13 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	135	Total	C	N	O	S	0	0
			1009	618	198	187	6		

- Molecule 14 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	V	82	Total 625	C 384	N 116	O 120	S 5	0	0

- Molecule 15 is a protein called 40S ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	129	Total 1034	C 659	N 193	O 176	S 6	0	0

- Molecule 16 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	X	141	Total 1098	C 693	N 219	O 183	S 3	0	0

- Molecule 17 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	124	Total 1014	C 641	N 198	O 170	S 5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	b	82	Total 640	C 402	N 118	O 113	S 7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	e	47	Total 375	C 228	N 84	O 62	S 1	0	0

- Molecule 20 is a protein called RNA-binding protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	x	178	Total 1391	C 891	N 252	O 244	S 4	0	0

- Molecule 21 is a protein called RNA-binding protein NOB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	y	325	Total 2568	C 1622	N 473	O 463	S 10	0	0

- Molecule 22 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	d	55	Total 459	C 286	N 94	O 74	S 5	0	0

- Molecule 23 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	D	225	Total 1752	C 1117	N 315	O 313	S 7	0	0

- Molecule 24 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	189	Total 1495	C 934	N 284	O 270	S 7	0	0

- Molecule 25 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K	95	Total 800	C 522	N 142	O 131	S 5	0	0

- Molecule 26 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M	119	Total 588	C 350	N 119	O 119	0	0

- Molecule 27 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	P	120	Total 984	C 625	N 184	O 168	S 7	0	0

- Molecule 28 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	139	Total 1109	C 704	N 210	O 192	S 3	0	0

- Molecule 29 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	S	143	Total 1184	C 743	N 240	O 200	S 1	0	0

- Molecule 30 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	T	144	Total 1122	C 703	N 217	O 199	S 3	0	0

- Molecule 31 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	U	101	Total 803	C 504	N 153	O 142	S 4	0	0

- Molecule 32 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	72	Total 574	C 368	N 104	O 101	S 1	0	0

- Molecule 33 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	61	Total 479	C 292	N 95	O 90	S 2	0	0

- Molecule 34 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	f	70	Total 346	C 206	N 70	O 70	0	0

- Molecule 35 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	314	Total 2440	C 1537	N 425	O 466	S 12	0	0

- Molecule 36 is a protein called Serine/threonine-protein kinase RIO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	z	292	Total 1921	C 1186	N 372	O 353	S 10	0	0

- Molecule 37 is a protein called Leucine-rich repeat-containing protein 47.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	430	Total 2820	C 1743	N 543	O 527	S 7	0	0

- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
38	2	1	Total 1	Zn 1	0
38	y	1	Total 1	Zn 1	0

3   Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
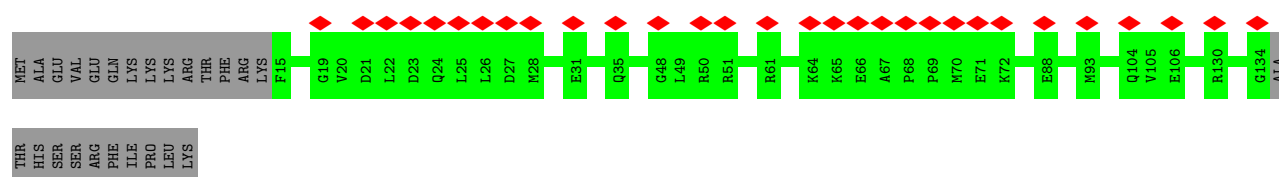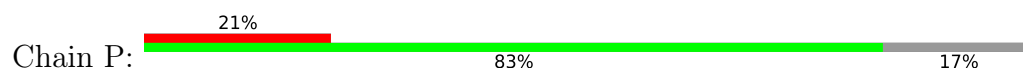
- Molecule 1: pre-18S ribosomal RNA

- Molecule 2: 40S ribosomal protein S17
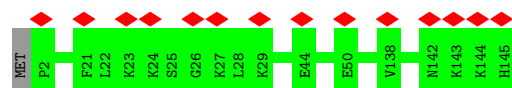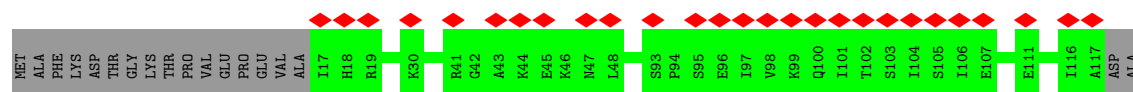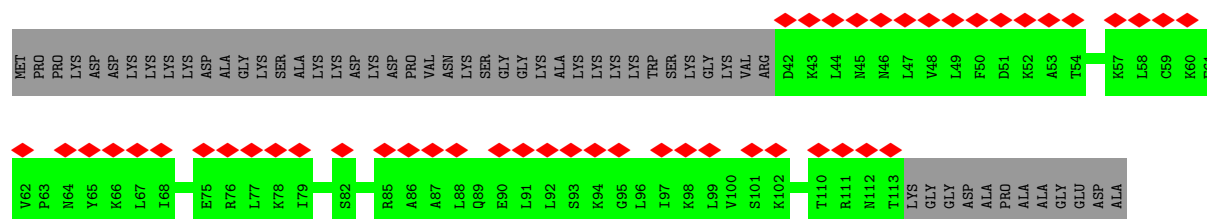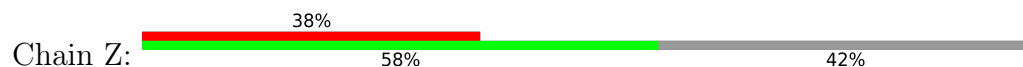

Chain R:
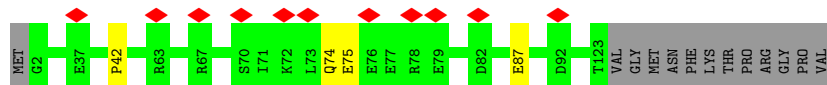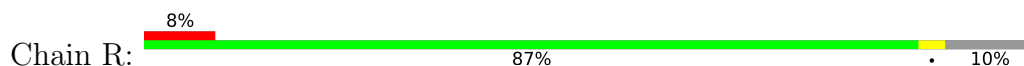
- Molecule 3: 40S ribosomal protein SA

Chain A:

MET S2 A114 E192 H193 A217 ALA GLU LYS ALA VAL THR LYS GLU GLU PHE GLN GLU TRP THR ALA PRO PRO GLU PHE THR ALA THR GLN PRO GLU VAL ALA ASP TRP SER GLU GLY VAL GLN VAL PRO SER VAL PRO ILE GLN GLN PHE PRO THR GLU ASP TRP SER

ALA GLN PRO ALA THR GLU ASP TRP SER ALA ALA PRO THR ALA GLN ALA THR GLU THR GLU TRP VAL GLY THR ALA THR THR ASP TRP SER
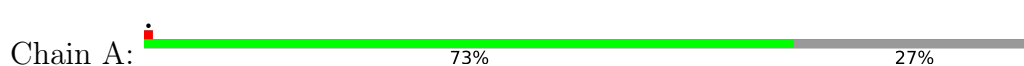
• Molecule 4: 40S ribosomal protein S3a

Chain B: 80% 19%

MET ALA VAL GLY LYS ASN LYS ARG LEU THR LYS GLY GLY LYS LYS GLY ALA LYS LYS LYS V21 V22 D23 Q53 G54 T55 K56 L62 E68 N76 D77 T88 D180 G233 GLU GLY SER SER GLY LYS SER ALA THR GLY ASP GLU THR GLY ALA LYS VAL GLU ARG

ALA ASP GLY TYR GLU PRO PRO VAL GLN GLU SER VAL
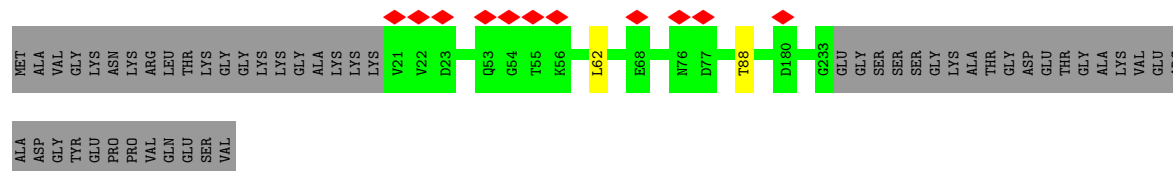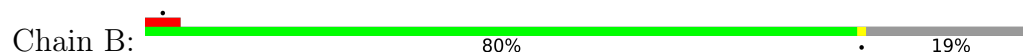
• Molecule 5: 40S ribosomal protein S2

Chain C: 74% 26%

MET ALA ASP ASP ALA GLY ALA ALA GLY GLY PRO GLY GLY PRO GLY GLY PRO GLY MET GLY ASN ARG GLY GLY PHE ARG GLY GLY PHE GLY SER GLY ILE ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ARG GLY ALA ARG GLY GLY LYS ALA GLU ASP LYS E59

R68 T116 R117 Y248 T276 HIS THR ARG VAL SER VAL GLN ARG THR GLN ALA PRO ALA VAL ALA THR THR
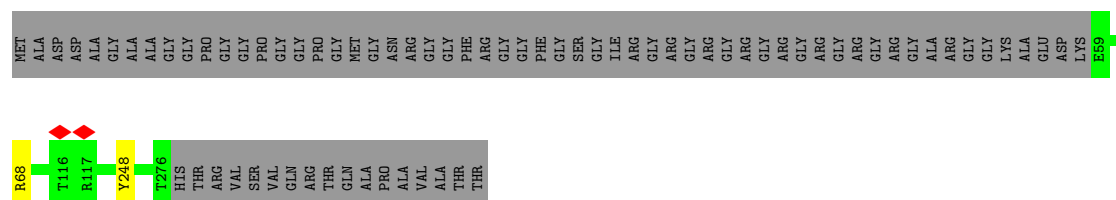
• Molecule 6: 40S ribosomal protein S4, X isoform

Chain E: 99%

MET A2 L38 Q260 S261 S262 G263
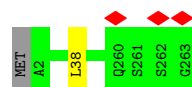
• Molecule 7: 40S ribosomal protein S6

Chain G: 6% 92% 8%

M1 D19 D20 E21 R22 D39 E43 R92 K115 K116 G117 T128 L147 D151 E165 R224 Q225 E226 Q227 I228 A229 K230 ARG ARG ARG LEU SER SER LEU ARG ALA ALA SER THR SER LYS SER GLU SER SER GLN LYS
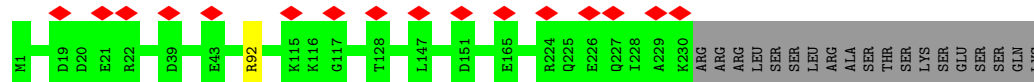
• Molecule 8: 40S ribosomal protein S7

Chain H: 8% 96%

MET PHE SER SER SER ALA LYS I8 E14 K15 P16 D17 E18 L27 N32 N33 S34 D35 E52 V53 G54 G55 G56 S88 G89 K111 Q193 LEU
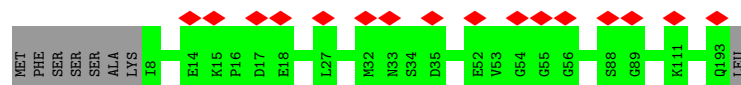
• Molecule 9: 40S ribosomal protein S8

Chain I:

6%

98%

MET G2 K124 K125 G126 A127 K128 L129 E133 E134 K139 K140 R141 K144 D150 K206 GLY LYS
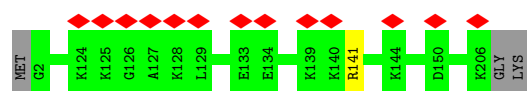
• Molecule 10: 40S ribosomal protein S9

Chain J:

92%

7%

MET P2 L161 G181 GLN GLY GLY ALA GLY ALA GLY ASP ASP GLU GLU GLU ASP
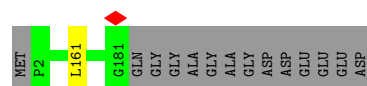
• Molecule 11: 40S ribosomal protein S11

Chain L:

7%

95%

MET A2 R22 V23 L24 L25 G26 E27 T28 G29 K30 E31 R69 K152 LYS GLN PHE GLN LYS PHE

• Molecule 12: 40S ribosomal protein S13

Chain N:

99%

MET G2 D83 V150 ALA
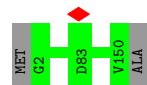
• Molecule 13: 40S ribosomal protein S14

Chain O:

5%

89%

11%

MET ALA PRO ARG LYS GLY LYS GLU LYS LYS GLU GLN GLN VAL ILE SER L17 Q20 V21 A22 E23 G24 E25 L151
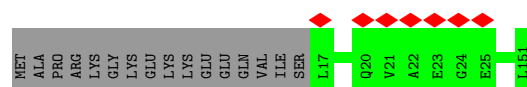
• Molecule 14: 40S ribosomal protein S21

Chain V:

98%

M1 R60 N82 PHE
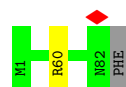
• Molecule 15: 40S ribosomal protein S15a

Chain W:

98%

MET V2 L104 F130
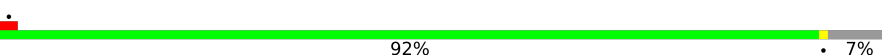
• Molecule 16: 40S ribosomal protein S23

Chain X:

• Molecule 17: 40S ribosomal protein S24

Chain Y:
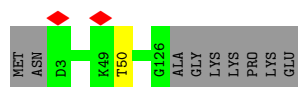
• Molecule 18: 40S ribosomal protein S27

Chain b:
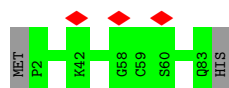
• Molecule 19: 40S ribosomal protein S30

Chain e:
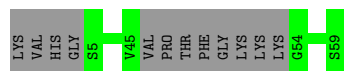
• Molecule 20: RNA-binding protein PNO1

Chain x:
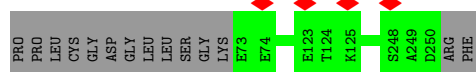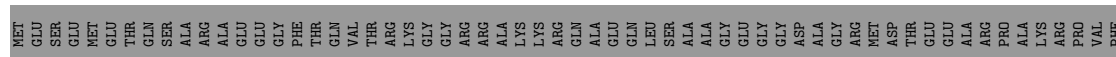
• Molecule 21: RNA-binding protein NOB1

Chain y:
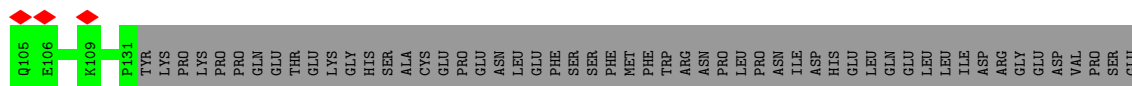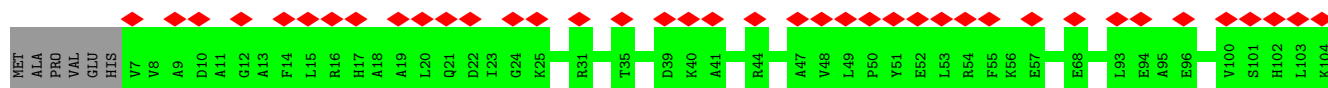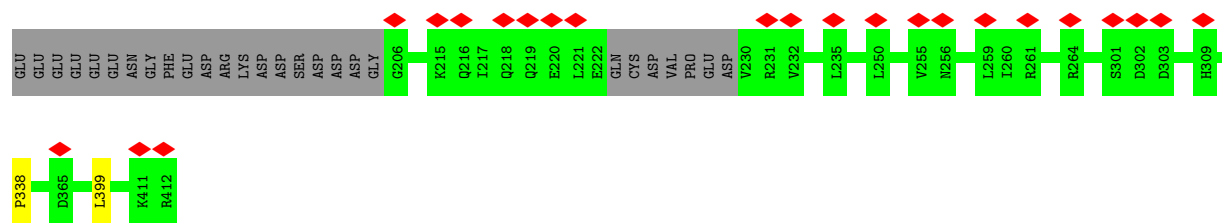
• Molecule 22: 40S ribosomal protein S29

Chain d:

• Molecule 23: 40S ribosomal protein S3

Chain D:
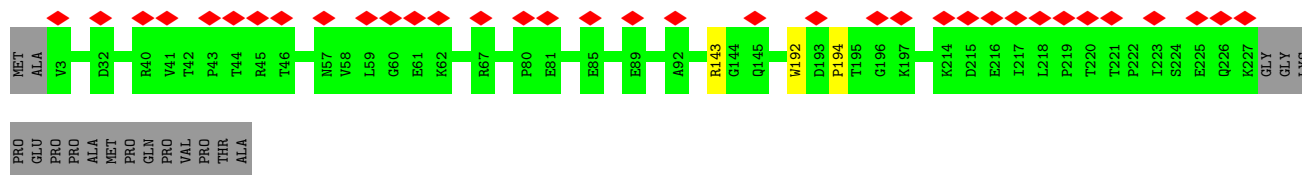
• Molecule 24: 40S ribosomal protein S5

Chain F:
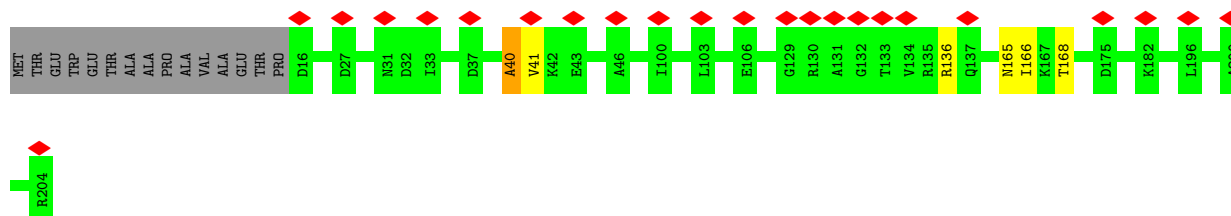
• Molecule 25: 40S ribosomal protein S10

Chain K:
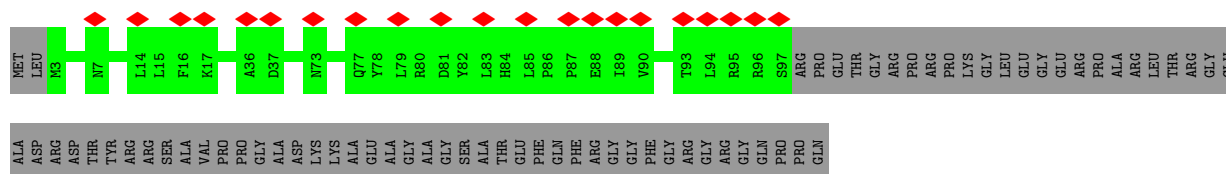
• Molecule 26: 40S ribosomal protein S12

Chain M:

MET ALA GLU GLU GLY ILE ALA ALA GLY G10 V11 M12 D13 V14 N15 T16 A17 L18 Q19 E20 V21 L22 K23 T24 A25 H28 D29 G30 L31 A32 R36 A39 K40 A41 K44 R45 Q46 A47 H48 L49 C50 V51 L52 A53 S54 N55 C56 D57 E58 P59 M60 Y61 V62 K63 L64 V65

E66 A67 A70 E71 H72 Q73 I74 N75 L76 I77 K78 V79 D80 D81 N82 K83 K84 L85 G86 E87 W88 V89 G90 L91 C92 K93 I94 ASP ARG GLY K99 P100 R101 K102 V103 V104 G105 C106 S107 C108 V109 V110 V111 K112 D113 Y114 G115 K116 E117 S118 Q119 A120 K121 D122 V123 I124 E125 E126

Y127 F128 K129 C130 K131 K132

• Molecule 27: 40S ribosomal protein S15

Chain P:

21%

83%   17%

MET ALA GLU VAL GLU GLN LYS LYS LYS ARG THR PHE ARG LYS F15 G19 V20 D21 L22 D23 Q24 L25 L26 D27 M28 E31 Q35 G48 L49 R50 R51 R61 K64 K65 E66 A67 P68 P69 M70 E71 K72 E88 M93 Q104 V105 E106 R130 G134 ALA

THR HIS SER ARG PHE ILE PRO LEU LYS

• Molecule 28: 40S ribosomal protein S16

Chain Q:

94%   • 5%

MET PRO SER LYS GLY PRO LEU Q8 E43 K60 E61 R62 F63 A64 R146
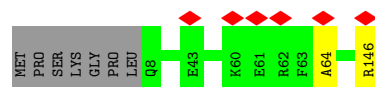
• Molecule 29: 40S ribosomal protein S18

Chain S:

27%

94%   6%

MET SER L3 V4 I5 P6 E7 K8 F9 Q10 H11 I12 L13 R14 V15 L16 N17 T18 N19 I20 D21 G22 I26 D49 I50 D51 L52 A56 G57 E58 L59 T60 E61 D62 E63 V64 E65 R75 Q76 Y77 K78 D92 N101 D104 R108 K115 R142 G143 R144 T145

VAL GLY VAL SER LYS LYS LYS
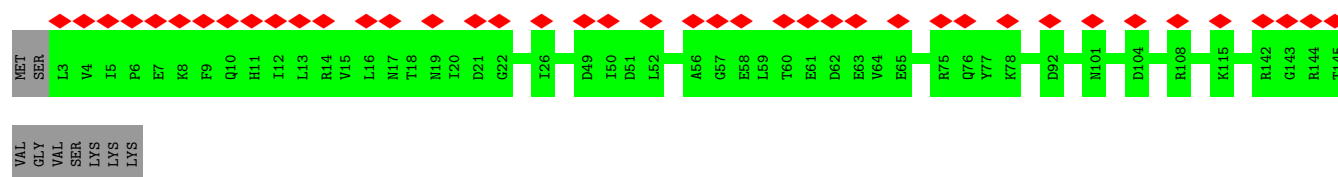
• Molecule 30: 40S ribosomal protein S19

Chain T:

10%

99%   •

MET P2 F21 L22 K23 K24 S25 G26 K27 L28 K29 E44 E50 V138 N142 K143 K144 H145

• Molecule 31: 40S ribosomal protein S20

Chain U:

23%

85%   15%
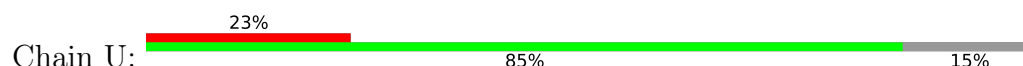
• Molecule 32: 40S ribosomal protein S25

Chain Z:

• Molecule 33: 40S ribosomal protein S28

Chain c:
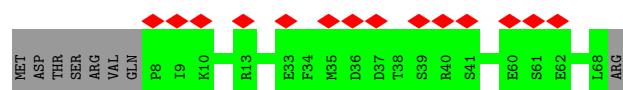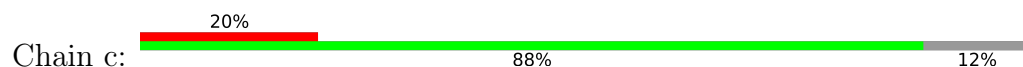
• Molecule 34: Ubiquitin-40S ribosomal protein S27a

Chain f:
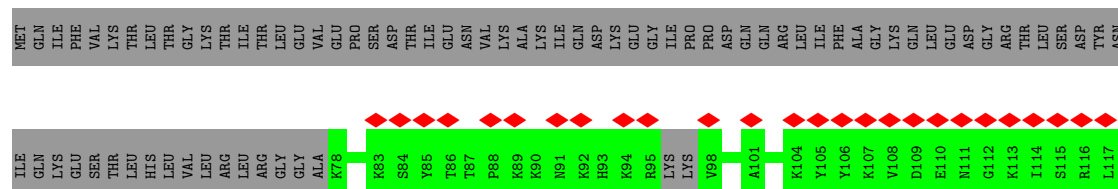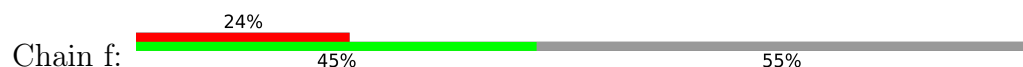
• Molecule 35: Receptor of activated protein C kinase 1

Chain g:

ARG

• Molecule 36: Serine/threonine-protein kinase RIO1

Chain z:

24%

51%   49%

• Molecule 37: Leucine-rich repeat-containing protein 47

Chain k:

36%

73%   26%

I399 V400 P401 L402 G403 R404 K405 E406 A407 K408 A409 K410 E411 Q415 E419 A420 E421 GLU GLN R424 S433 G434 Y438 L439 H440 L441 L442 ASP GLY N445 E446 N447 Y448 P449 C450 L451 V452 D453 A454 D455 G456 D457 V458 I459 S460 F461 P462 P463 I464 T465 N466 S467 E468 K469 T470 K471

V472 K473 K474 T475 T476 S477 D478 L479 F480 L481 E482 V483 T484 S485 ALA THR S488 L489 Q490 I491 C492 K493 D494 V495 M496 D497 A498 L499 I500 L501 K502 M503 A504 E505 M506 LYS LYS TYR THR LEU GLU ASN LYS GLU GLU GLY GLY SER LEU SER ASP THR GLU ALA ASP ALA VAL SER GLY GLN LEU

PRO ASP PRO THR THR ASN PRO SER ALA GLY LYS ASP GLY PRO SER LEU LEU VAL VAL GLU GLN VAL ARG VAL VAL ASP LEU GLU GLY SER LEU LYS VAL VAL TYR PRO SER LYS ALA ASP LEU ALA THR ALA PRO PRO HIS VAL THR VAL VAL ARG

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16876	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 $(e^-/\text{Å}^2)$	48	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	0.591	Depositor
Minimum map value	-0.304	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	381.24, 381.24, 381.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	2	0.76	1/39273 (0.0%)	1.10	209/61196 (0.3%)
2	R	0.37	0/1002	0.54	0/1345
3	A	0.43	0/1742	0.56	0/2367
4	B	0.41	0/1756	0.56	1/2350 (0.0%)
5	C	0.46	0/1726	0.57	0/2332
6	E	0.42	0/2118	0.55	1/2849 (0.0%)
7	G	0.37	0/1885	0.52	0/2510
8	H	0.36	0/1524	0.56	0/2042
9	I	0.42	0/1711	0.54	0/2282
10	J	0.44	0/1524	0.56	0/2035
11	L	0.47	0/1250	0.55	0/1673
12	N	0.41	0/1226	0.52	0/1649
13	O	0.37	0/1022	0.56	0/1372
14	V	0.40	0/631	0.54	0/844
15	W	0.48	0/1051	0.57	0/1406
16	X	0.43	0/1116	0.55	0/1490
17	Y	0.43	0/1031	0.56	1/1370 (0.1%)
18	b	0.39	0/653	0.54	0/876
19	e	0.39	0/377	0.52	0/493
20	x	0.41	0/1413	0.59	0/1906
21	y	0.36	0/2618	0.54	1/3536 (0.0%)
22	d	0.40	0/470	0.57	0/623
23	D	0.37	0/1780	0.56	0/2397
24	F	0.32	0/1516	0.53	0/2037
25	K	0.35	0/824	0.58	0/1112
26	M	0.25	0/586	0.49	0/813
27	P	0.36	0/1003	0.51	0/1341
28	Q	0.39	0/1126	0.59	0/1506
29	S	0.32	0/1202	0.53	0/1610
30	T	0.36	0/1142	0.50	0/1530
31	U	0.34	0/813	0.56	0/1092
32	Z	0.30	0/580	0.57	0/780

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
33	c	0.32	0/481	0.58	0/643
34	f	0.26	0/344	0.57	0/476
35	g	0.31	0/2497	0.57	0/3399
36	z	0.31	0/1933	0.53	0/2616
37	k	0.29	0/2851	0.57	1/3888 (0.0%)
All	All	0.59	1/85797 (0.0%)	0.87	214/123786 (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
2	R	0	1
16	X	0	1
23	D	0	1
24	F	0	2
37	k	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	1254	C	O3'-P	-6.41	1.53	1.61

The worst 5 of 214 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	501	C	N1-C2-O2	13.98	127.28	118.90
1	2	501	C	C2-N1-C1'	12.30	132.33	118.80
1	2	501	C	N3-C2-O2	-11.76	113.67	121.90
1	2	293	C	N1-C2-O2	11.12	125.57	118.90
1	2	427	U	N3-C2-O2	-9.91	115.26	122.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	D	194	PRO	Peptide
24	F	165	ASN	Peptide
24	F	40	ALA	Peptide

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Mol	Chain	Res	Type	Group
2	R	74	GLN	Peptide
16	X	60	LYS	Peptide

5.2   Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	R	120/135 (89%)	109 (91%)	8 (7%)	3 (2%)	5	32
3	A	214/295 (72%)	202 (94%)	12 (6%)	0	100	100
4	B	211/264 (80%)	199 (94%)	12 (6%)	0	100	100
5	C	216/293 (74%)	206 (95%)	10 (5%)	0	100	100
6	E	260/263 (99%)	243 (94%)	17 (6%)	0	100	100
7	G	228/249 (92%)	213 (93%)	15 (7%)	0	100	100
8	H	184/194 (95%)	171 (93%)	13 (7%)	0	100	100
9	I	203/208 (98%)	192 (95%)	11 (5%)	0	100	100
10	J	178/194 (92%)	166 (93%)	11 (6%)	1 (1%)	25	64
11	L	149/158 (94%)	143 (96%)	6 (4%)	0	100	100
12	N	147/151 (97%)	144 (98%)	3 (2%)	0	100	100
13	O	133/151 (88%)	120 (90%)	13 (10%)	0	100	100
14	V	80/83 (96%)	77 (96%)	3 (4%)	0	100	100
15	W	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
16	X	139/143 (97%)	133 (96%)	5 (4%)	1 (1%)	22	61
17	Y	122/133 (92%)	115 (94%)	7 (6%)	0	100	100
18	b	80/84 (95%)	72 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	e	43/59 (73%)	41 (95%)	2 (5%)	0	100	100
20	x	176/252 (70%)	168 (96%)	8 (4%)	0	100	100
21	y	319/412 (77%)	288 (90%)	30 (9%)	1 (0%)	41	74
22	d	53/56 (95%)	48 (91%)	4 (8%)	1 (2%)	8	39
23	D	223/243 (92%)	210 (94%)	12 (5%)	1 (0%)	34	69
24	F	187/204 (92%)	165 (88%)	19 (10%)	3 (2%)	9	43
25	K	93/165 (56%)	89 (96%)	4 (4%)	0	100	100
26	M	115/132 (87%)	102 (89%)	13 (11%)	0	100	100
27	P	118/145 (81%)	113 (96%)	5 (4%)	0	100	100
28	Q	137/146 (94%)	123 (90%)	13 (10%)	1 (1%)	22	61
29	S	141/152 (93%)	131 (93%)	10 (7%)	0	100	100
30	T	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
31	U	99/119 (83%)	93 (94%)	6 (6%)	0	100	100
32	Z	70/125 (56%)	67 (96%)	3 (4%)	0	100	100
33	c	59/69 (86%)	55 (93%)	4 (7%)	0	100	100
34	f	66/156 (42%)	51 (77%)	15 (23%)	0	100	100
35	g	312/317 (98%)	280 (90%)	32 (10%)	0	100	100
36	z	282/568 (50%)	255 (90%)	27 (10%)	0	100	100
37	k	418/583 (72%)	374 (90%)	44 (10%)	0	100	100
All	All	5844/7176 (81%)	5411 (93%)	421 (7%)	12 (0%)	50	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
24	F	166	ILE
28	Q	64	ALA
2	R	87	GLU
10	J	161	LEU
21	y	338	PRO

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	R	110/122 (90%)	110 (100%)	0	100	100
3	A	180/243 (74%)	180 (100%)	0	100	100
4	B	194/231 (84%)	193 (100%)	1 (0%)	88	95
5	C	184/225 (82%)	182 (99%)	2 (1%)	73	88
6	E	224/225 (100%)	224 (100%)	0	100	100
7	G	200/218 (92%)	199 (100%)	1 (0%)	88	95
8	H	167/174 (96%)	167 (100%)	0	100	100
9	I	178/180 (99%)	177 (99%)	1 (1%)	86	94
10	J	160/168 (95%)	160 (100%)	0	100	100
11	L	135/142 (95%)	134 (99%)	1 (1%)	84	94
12	N	130/131 (99%)	130 (100%)	0	100	100
13	O	105/119 (88%)	105 (100%)	0	100	100
14	V	66/67 (98%)	65 (98%)	1 (2%)	65	85
15	W	112/113 (99%)	111 (99%)	1 (1%)	78	91
16	X	113/115 (98%)	112 (99%)	1 (1%)	78	91
17	Y	108/115 (94%)	108 (100%)	0	100	100
18	b	74/76 (97%)	74 (100%)	0	100	100
19	e	38/48 (79%)	38 (100%)	0	100	100
20	x	150/208 (72%)	150 (100%)	0	100	100
21	y	285/367 (78%)	285 (100%)	0	100	100
22	d	48/49 (98%)	46 (96%)	2 (4%)	30	65
23	D	189/202 (94%)	188 (100%)	1 (0%)	88	95
24	F	159/170 (94%)	157 (99%)	2 (1%)	69	87
25	K	86/136 (63%)	86 (100%)	0	100	100
27	P	107/130 (82%)	107 (100%)	0	100	100
28	Q	115/121 (95%)	114 (99%)	1 (1%)	78	91
29	S	124/132 (94%)	124 (100%)	0	100	100
30	T	114/115 (99%)	114 (100%)	0	100	100
31	U	93/107 (87%)	93 (100%)	0	100	100
32	Z	64/103 (62%)	64 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	c	54/62 (87%)	54 (100%)	0	100	100
35	g	272/275 (99%)	270 (99%)	2 (1%)	84	94
36	z	135/512 (26%)	135 (100%)	0	100	100
37	k	215/487 (44%)	212 (99%)	3 (1%)	67	86
All	All	4688/5888 (80%)	4668 (100%)	20 (0%)	91	95

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	Q	146	ARG
37	k	150	ARG
37	k	263	ARG
37	k	242	LEU
14	V	60	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
35	g	76	GLN
35	g	237	ASN
37	k	156	GLN
11	L	112	HIS
11	L	83	GLN

5.3.3   RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1632/1873 (87%)	469 (28%)	41 (2%)

5 of 469 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	3	C
1	2	11	A
1	2	23	G
1	2	25	A
1	2	33	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	1403	C
1	2	1520	G
1	2	1425	G
1	2	1464	C
1	2	1606	G

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 2 ligands modelled in this entry, 2 are 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 ⓘ

There are no such residues in this entry.

5.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-11517. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections ⓘ
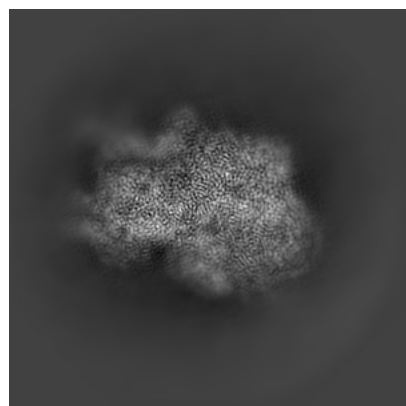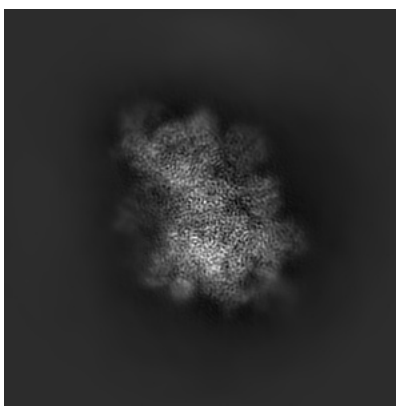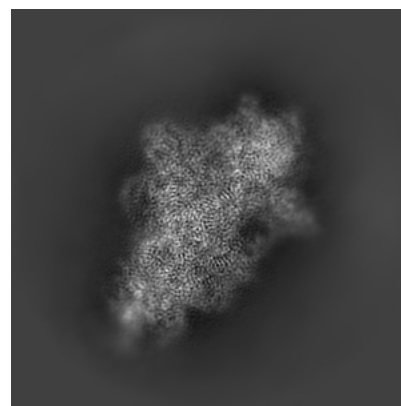
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
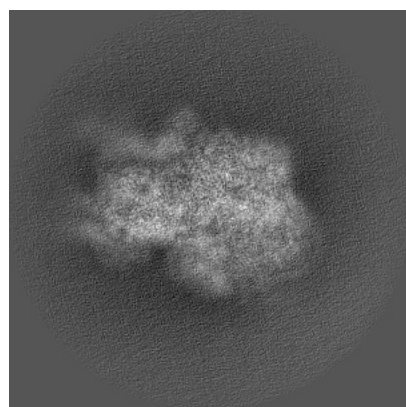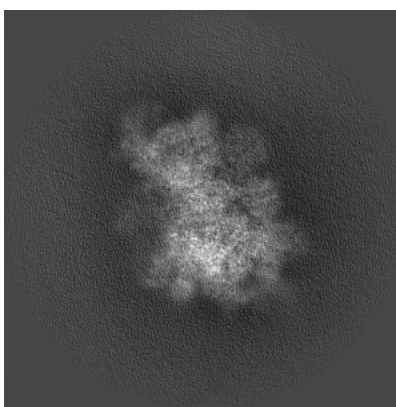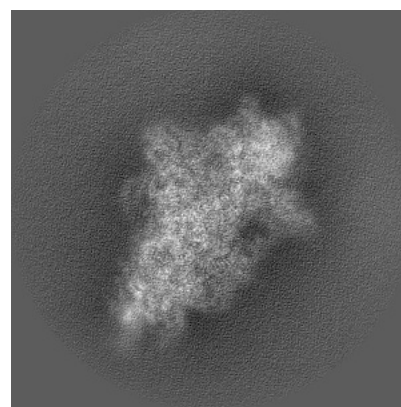
The images above show the map projected in three orthogonal directions.

6.2   Central slices (i)

6.2.1   Primary map
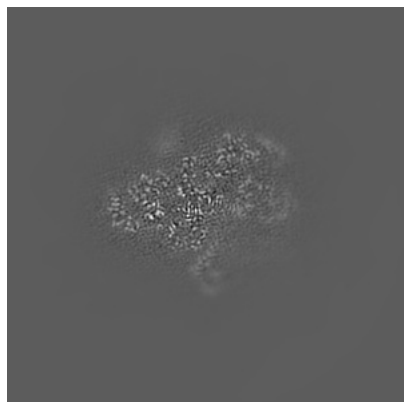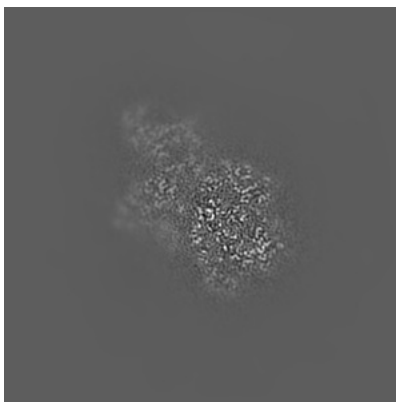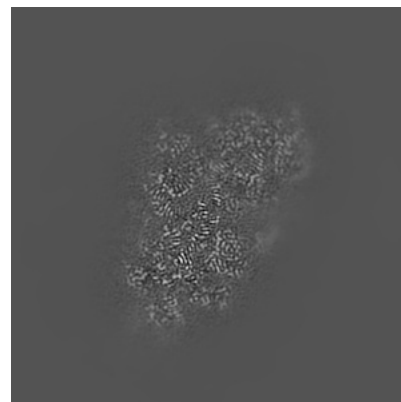
X Index: 180   Y Index: 180   Z Index: 180

6.2.2   Raw map
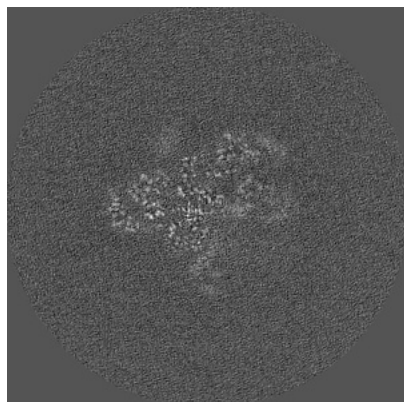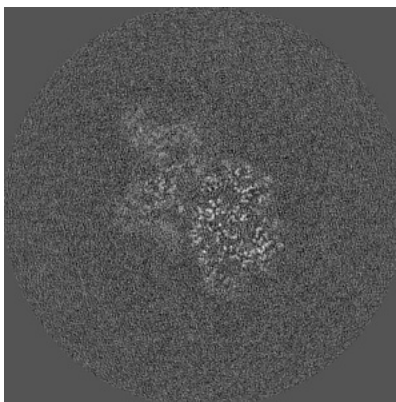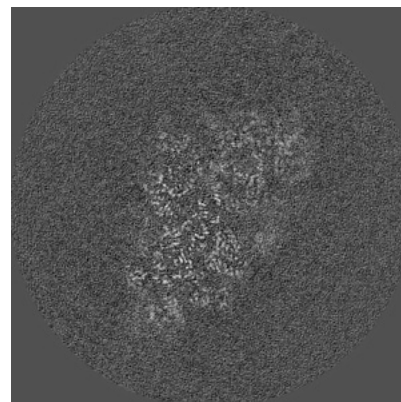
X Index: 180   Y Index: 180   Z Index: 180

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

6.3 Largest variance slices (i)

6.3.1 Primary map
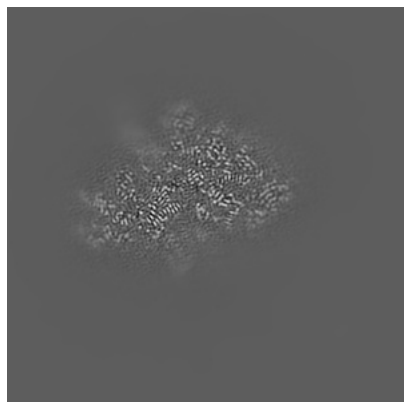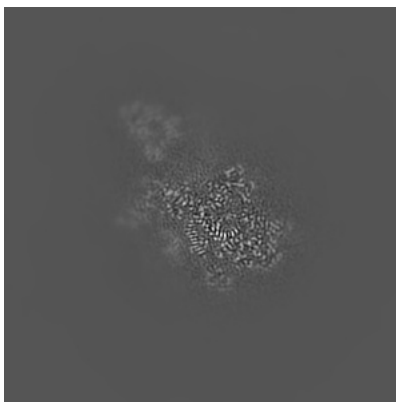
| X Index: 148 | Y Index: 172 | Z Index: 182 |
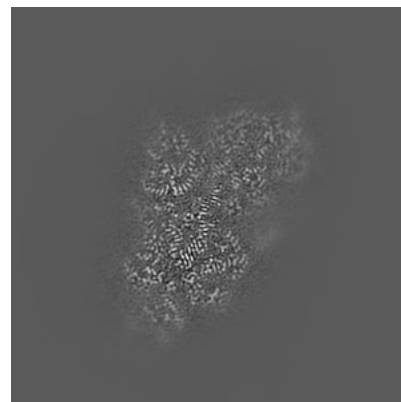
6.3.2 Raw map
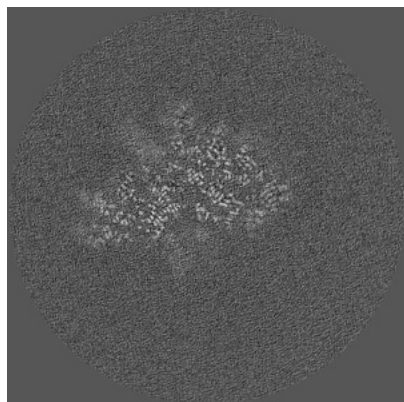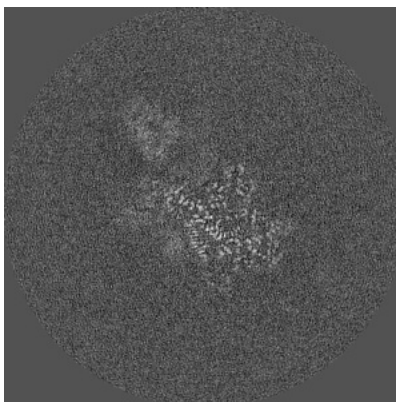
| X Index: 148 | Y Index: 173 | Z Index: 182 |
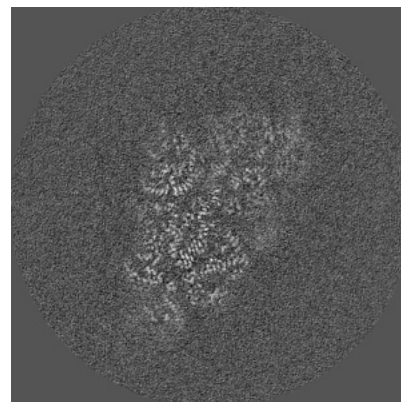
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal surface views ⓘ

6.4.1   Primary map

X   Y   Z
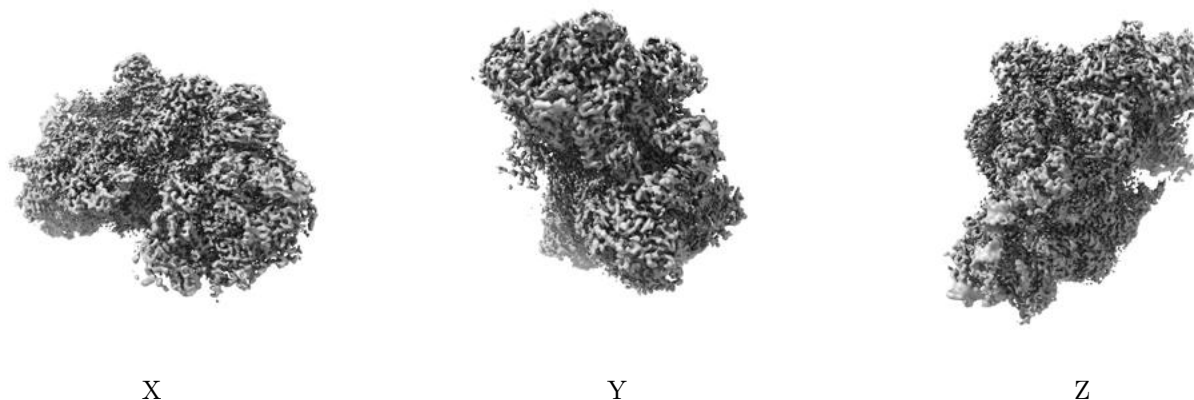
The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2   Raw map

X   Y   Z
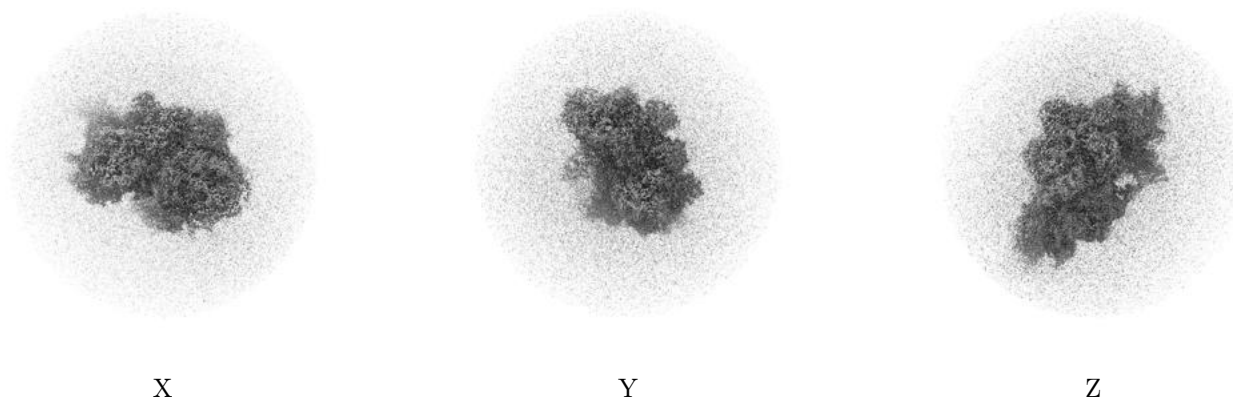
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5   Mask visualisation ⓘ

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

A mask typically either:

- Encompasses the whole structure

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

6.5.1   emd_11517_msk_1.map ⓘ

X   Y   Z
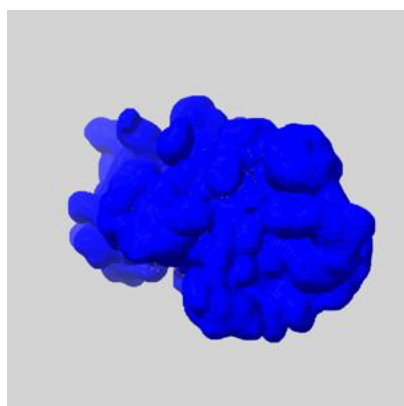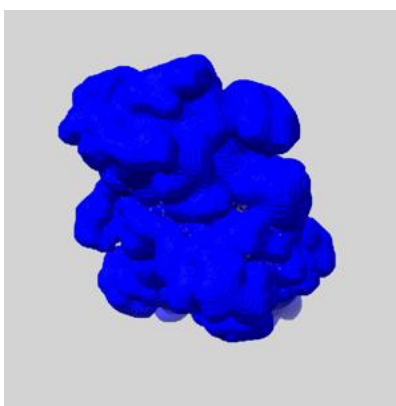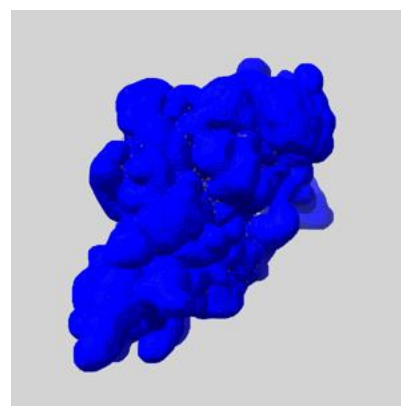
7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

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

7.2   Volume estimate ⓘ
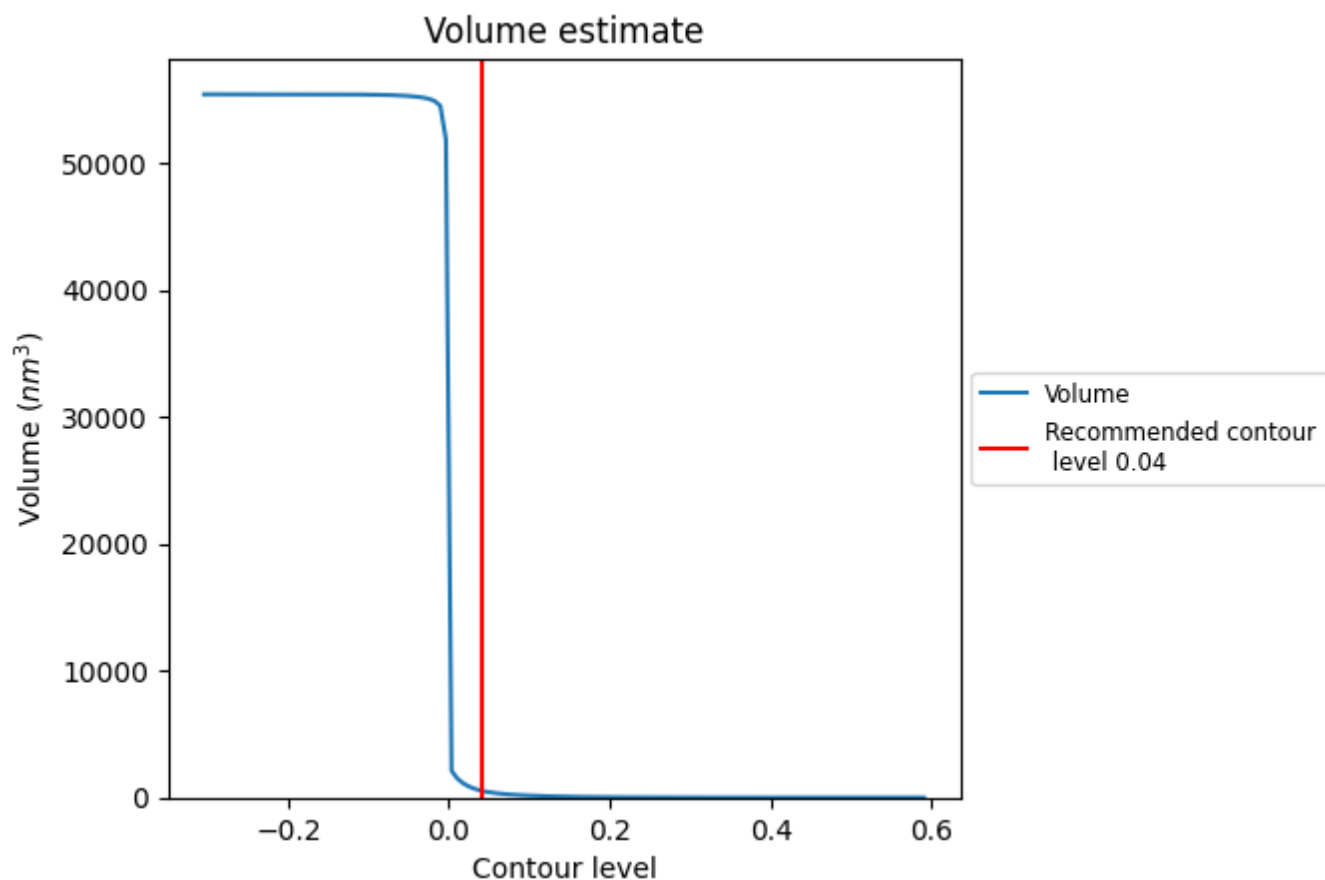
The volume at the recommended contour level is 547 nm^3; this corresponds to an approximate mass of 494 kDa.

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 ⓘ
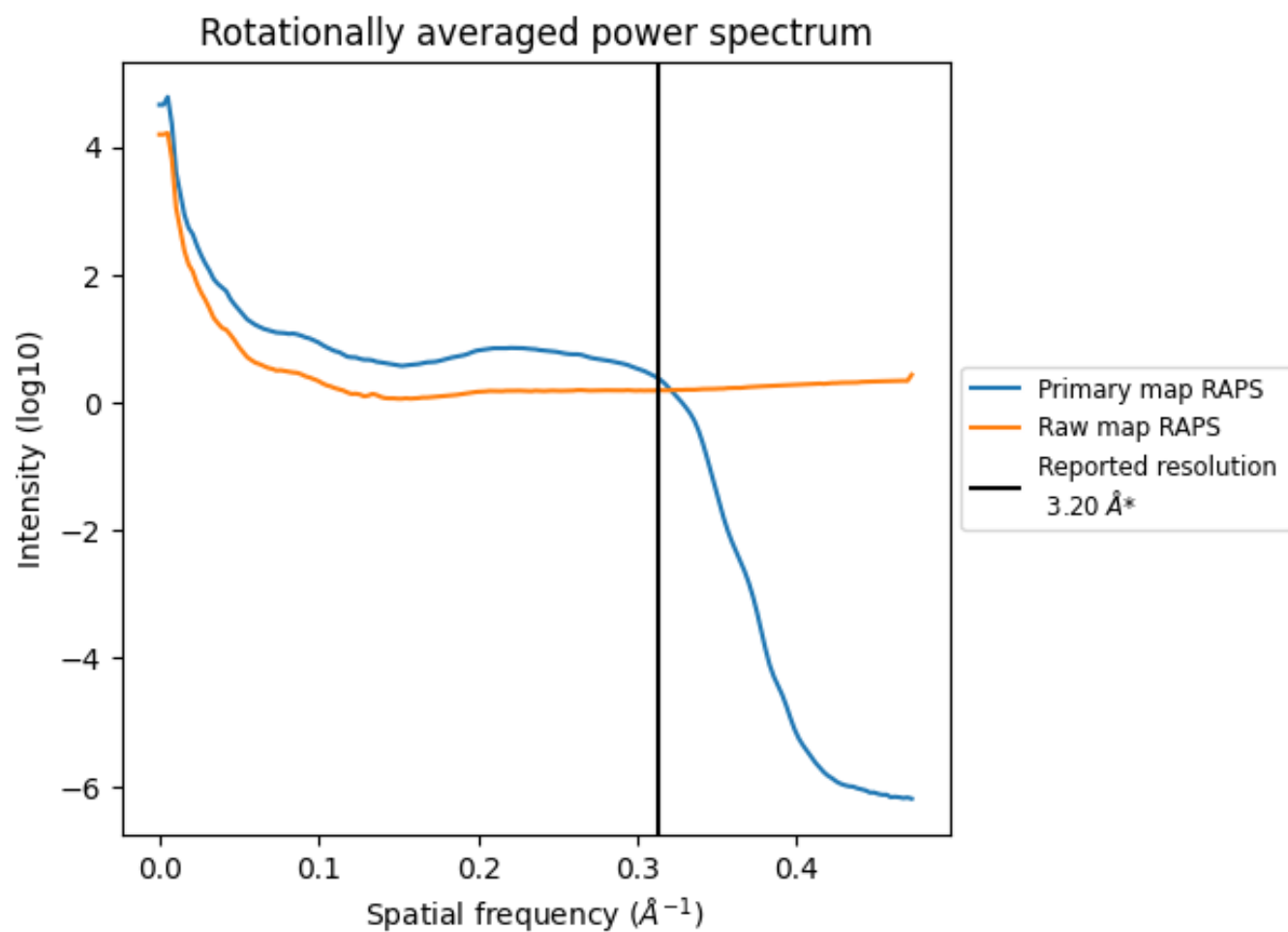
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)
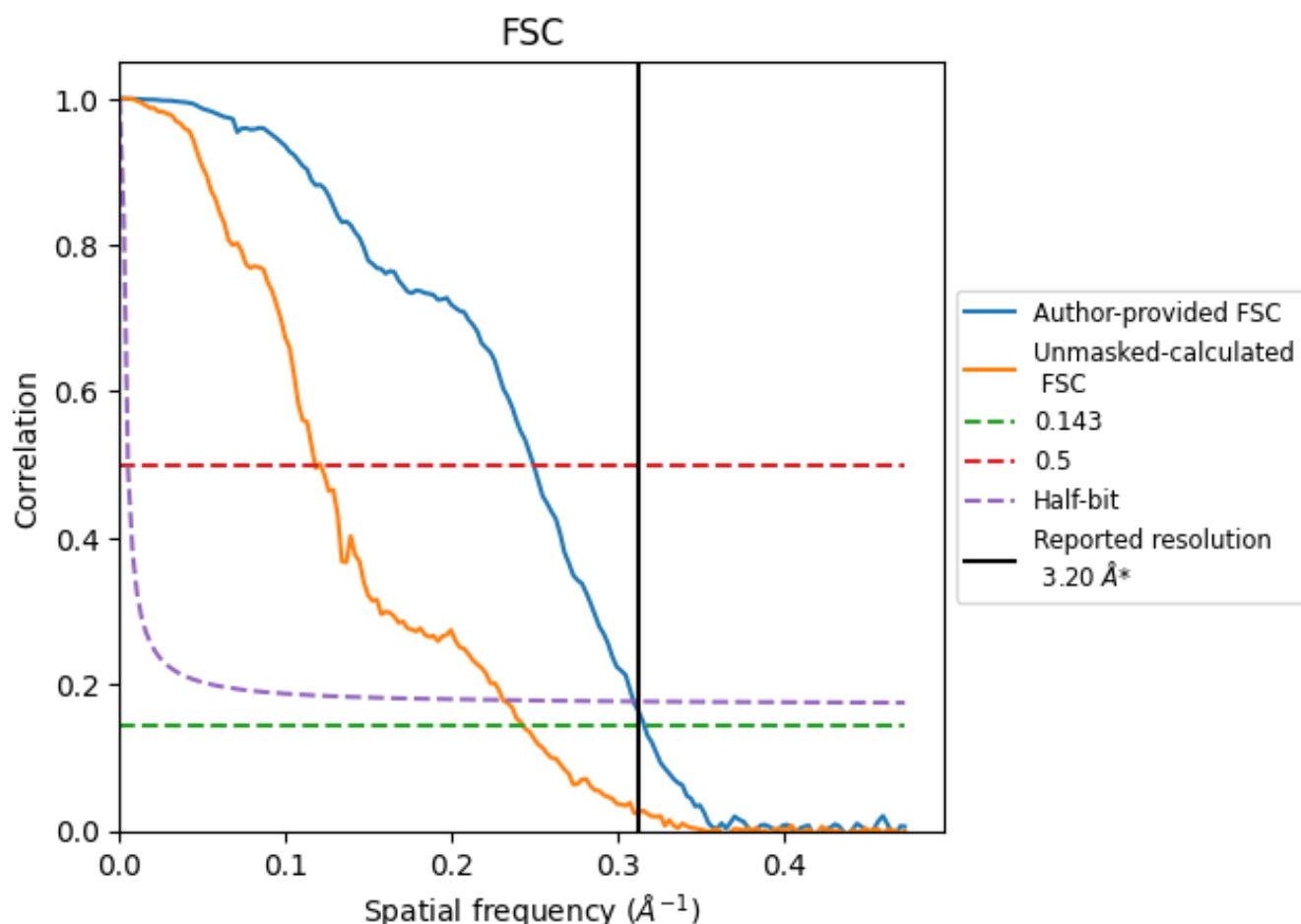
*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2   Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.17	4.02	3.24
Unmasked-calculated*	4.12	8.50	4.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.12 differs from the reported value 3.2 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11517 and PDB model 6ZXD. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ
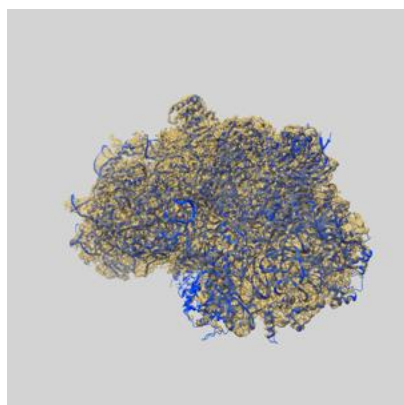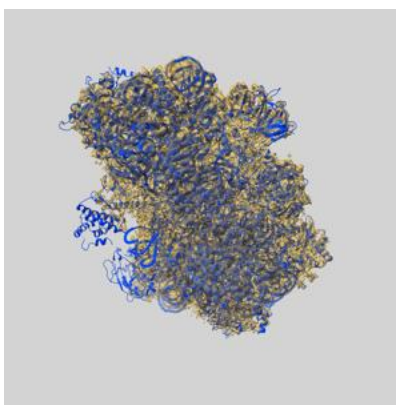
| X | Y | Z |
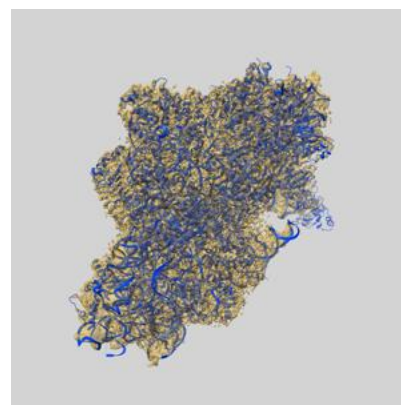
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

X   Y   Z
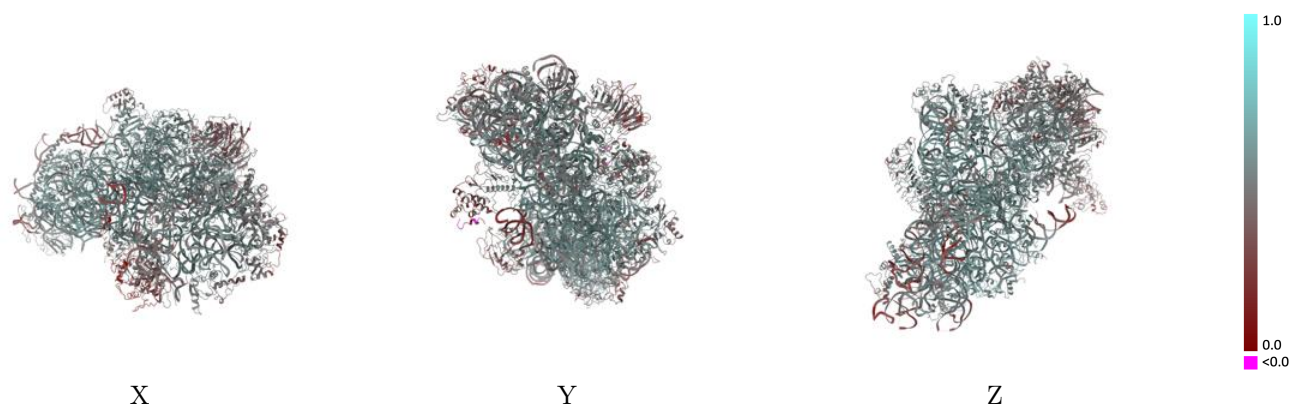
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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
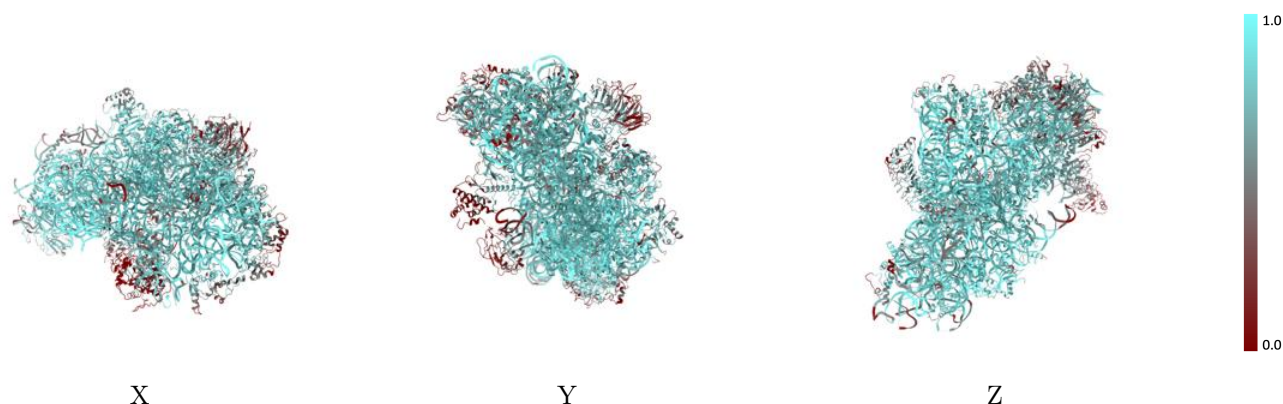
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

9.4 Atom inclusion ⓘ
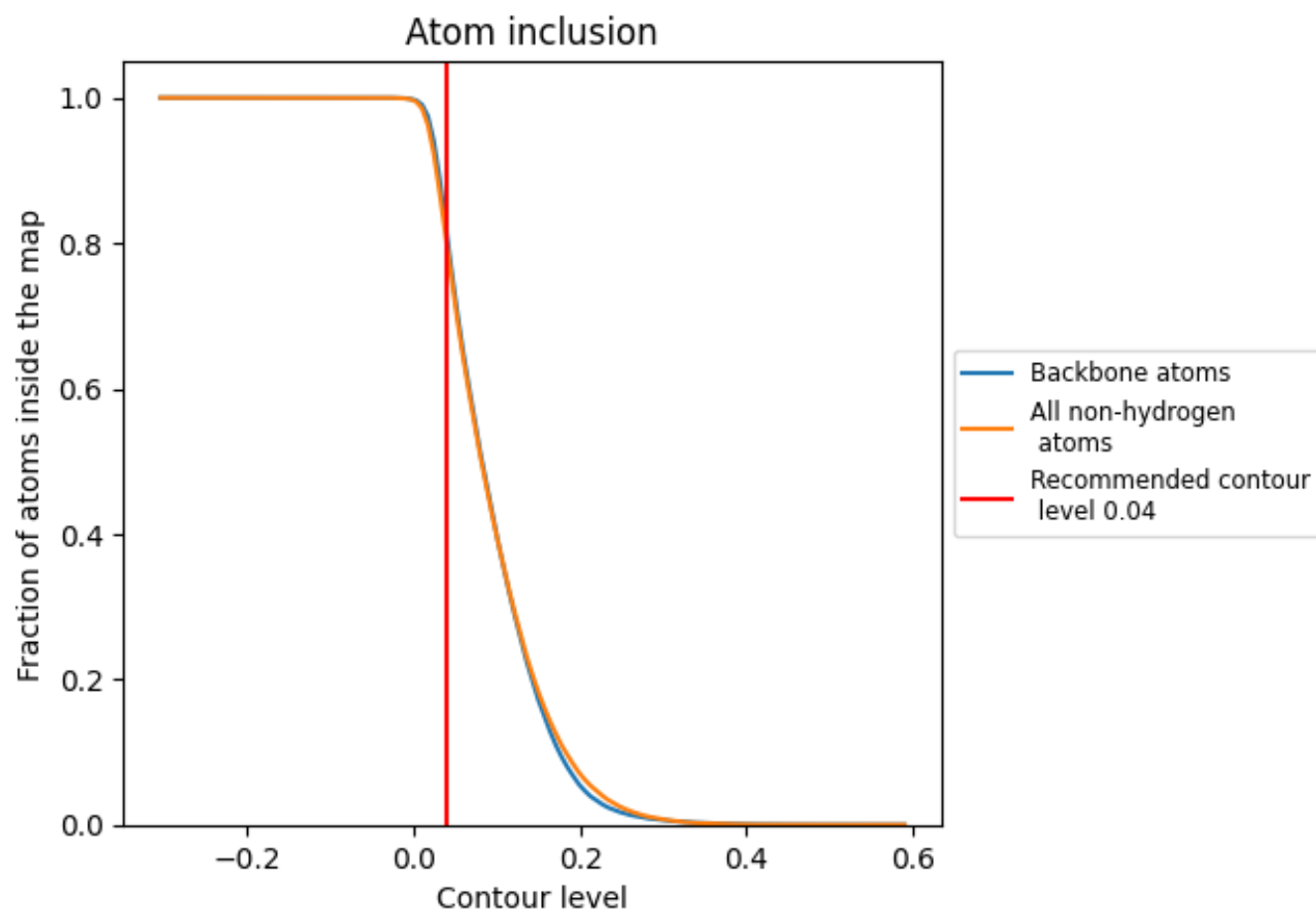
At the recommended contour level, 81% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7978	0.5200
2	0.8957	0.5340
A	0.8816	0.5690
B	0.8040	0.5440
C	0.9005	0.5730
D	0.6706	0.4880
E	0.8958	0.5780
F	0.6891	0.4800
G	0.7328	0.5010
H	0.7296	0.4950
I	0.8189	0.5390
J	0.8909	0.5730
K	0.6026	0.4620
L	0.8593	0.5600
M	0.1276	0.3010
N	0.8834	0.5680
O	0.7878	0.5330
P	0.6279	0.4990
Q	0.7735	0.5140
R	0.7401	0.4950
S	0.5478	0.4560
T	0.7106	0.5130
U	0.6138	0.4920
V	0.8871	0.5670
W	0.9446	0.6010
X	0.9244	0.5940
Y	0.8791	0.5660
Z	0.3422	0.3910
b	0.8503	0.5560
c	0.6204	0.4690
d	0.9161	0.5750
e	0.8889	0.5810
f	0.3873	0.3320
g	0.4597	0.3990
k	0.4691	0.4620

1.0

0.0

<0.0

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Continued from previous page...

Chain	Atom inclusion	Q-score
x	0.8700	0.5610
y	0.6911	0.4770
z	0.5079	0.4350