wwPDB EM Validation Summary Report

Dec 22, 2024 – 06:36 PM JST

PDB ID	:	8XP3
EMDB ID	:	EMD-38549
Title	:	Cryo-EM structure of the human 40S ribosome with LARP1 and LRRC47
Authors	:	Huang, Z.; Ye, X.; Li, Y.; Cheng, J.
Deposited on	:	2024-01-02
Resolution	:	3.40 Å(reported)
Based on initial model	:	6Z6M

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

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

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

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

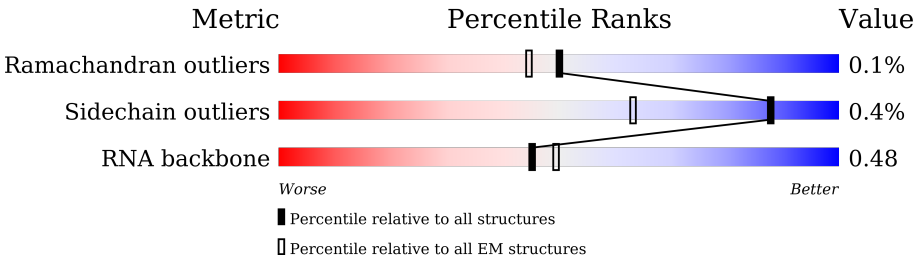
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	Ln	25	20% 96%
2	S2	1869	67% 24% 7%
3	SA	295	75% 25%
4	SB	264	81% 19%
5	SD	243	93% 7%
6	SE	263	99%
7	SF	204	85% 5% 10%
8	SH	194	95%

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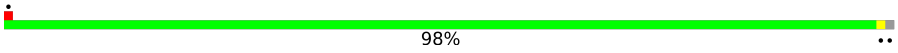
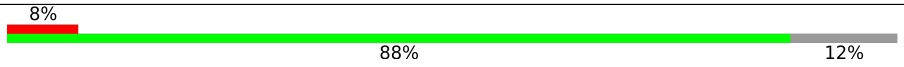
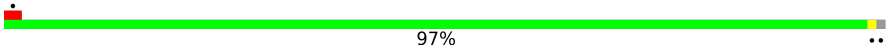
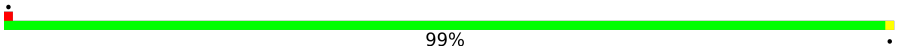
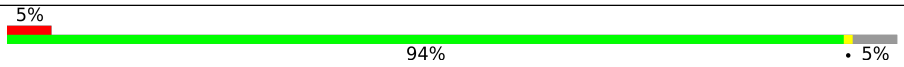
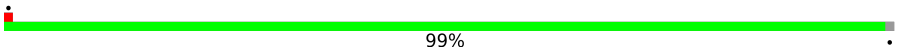
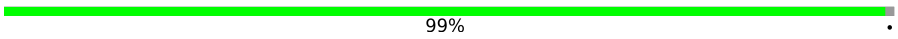
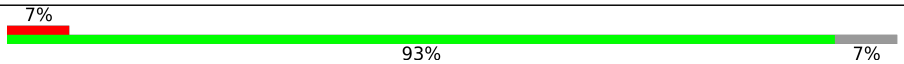
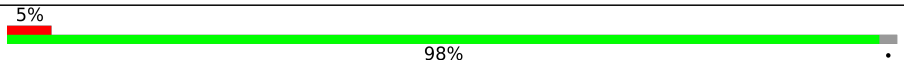
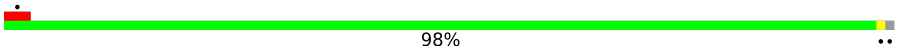
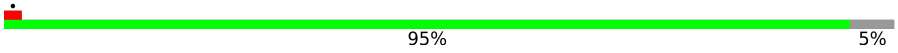
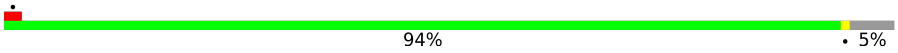
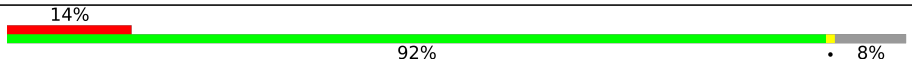
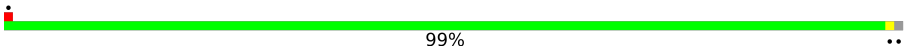
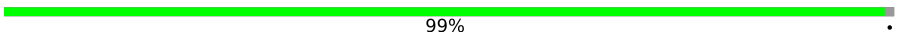
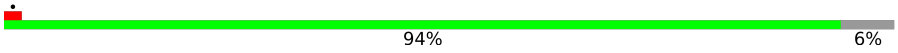
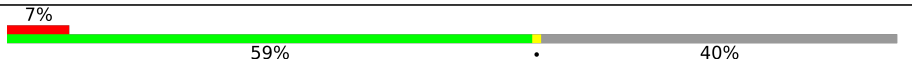
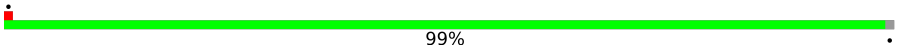
Mol	Chain	Length	Quality of chain
9	SI	208	
10	SK	165	
11	SL	158	
12	SP	145	
13	SQ	146	
14	SR	135	
15	SS	152	
16	ST	145	
17	SU	119	
18	SV	83	
19	SX	143	
20	Sa	115	
21	Sc	69	
22	Sd	56	
23	Sg	317	
24	SC	293	
25	SG	249	
26	SJ	194	
27	SM	132	
28	SN	151	
29	SO	151	
30	SW	130	
31	SY	133	
32	SZ	125	
33	Sb	84	

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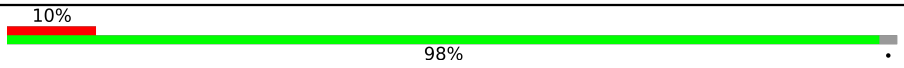
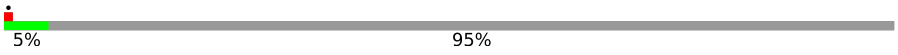
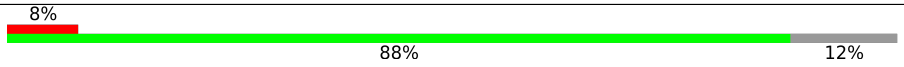
Mol	Chain	Length	Quality of chain
34	Se	59	
35	Sf	156	
36	JD	1096	
37	JC	583	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 80435 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 protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 2 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S2	1740	Total	C	N	O	P	0	0
			36896	16458	6597	12102	1739		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S2	582	C	U	conflict	GB 36162
S2	583	C	A	conflict	GB 36162
S2	584	G	A	conflict	GB 36162
S2	798	A	G	conflict	GB 36162
S2	1095	U	C	conflict	GB 36162

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	SA	222	Total	C	N	O	S	0	0
			1747	1109	306	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	SB	214	Total	C	N	O	S	0	0
			1738	1103	310	311	14		

- Molecule 5 is a protein called 40S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	SD	227	Total	C	N	O	S	0	0
			1765	1125	317	315	8		

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

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

- Molecule 7 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SF	184	Total	C	N	O	S	0	0
			1461	914	276	264	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	SH	186	Total	C	N	O	S	0	0
			1497	956	274	266	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SI	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

- Molecule 10 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	SK	98	Total	C	N	O	S	0	0
			827	539	148	134	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	SL	144	Total	C	N	O	S	0	0
			1182	752	224	200	6		

- Molecule 12 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	SP	127	Total	C	N	O	S	0	0
			1045	663	198	177	7		

- Molecule 13 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SQ	144	Total	C	N	O	S	0	0
			1142	726	216	197	3		

- Molecule 14 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SR	135	Total	C	N	O	S	0	0
			1090	685	202	198	5		

- Molecule 15 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 16 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 17 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 18 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	SV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 19 is a protein called 40S ribosomal protein S23.

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

- Molecule 20 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Sa	102	Total	C	N	O	S	0	0
			821	512	171	133	5		

- Molecule 21 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

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

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

- Molecule 23 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 24 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	SC	222	Total	C	N	O	S	0	0
			1725	1115	298	302	10		

- Molecule 25 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	SG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 26 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	SJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 27 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 28 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	SN	150	Total	C	N	O	S	0	0
			1208	773	229	205	1		

- Molecule 29 is a protein called 40S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	SO	135	Total	C	N	O	S	0	0
			1010	618	198	188	6		

- Molecule 30 is a protein called 40S ribosomal protein S15a.

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

- Molecule 31 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	SY	125	Total	C	N	O	S	0	0
			1022	645	200	172	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 33 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Sb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 34 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Se	58	Total	C	N	O	S	0	0
			459	284	100	74	1		

- Molecule 35 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Sf	61	Total	C	N	O	S	0	0
			497	312	94	84	7		

- Molecule 36 is a protein called La-related protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JD	52	Total	C	N	O	S	0	0
			429	269	75	83	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	JC	512	Total	C	N	O	S	0	0
			3941	2479	713	734	15		

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

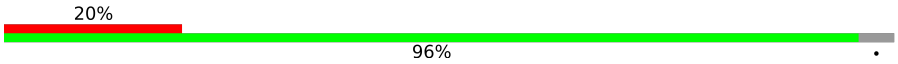
Mol	Chain	Residues	Atoms		AltConf
38	Sa	1	Total	Zn	0
			1	1	
38	Sd	1	Total	Zn	0
			1	1	
38	Sb	1	Total	Zn	0
			1	1	
38	Sf	1	Total	Zn	0
			1	1	

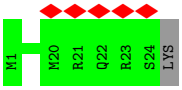
3 Residue-property plots (i)

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

- Molecule 1: 60S ribosomal protein L41

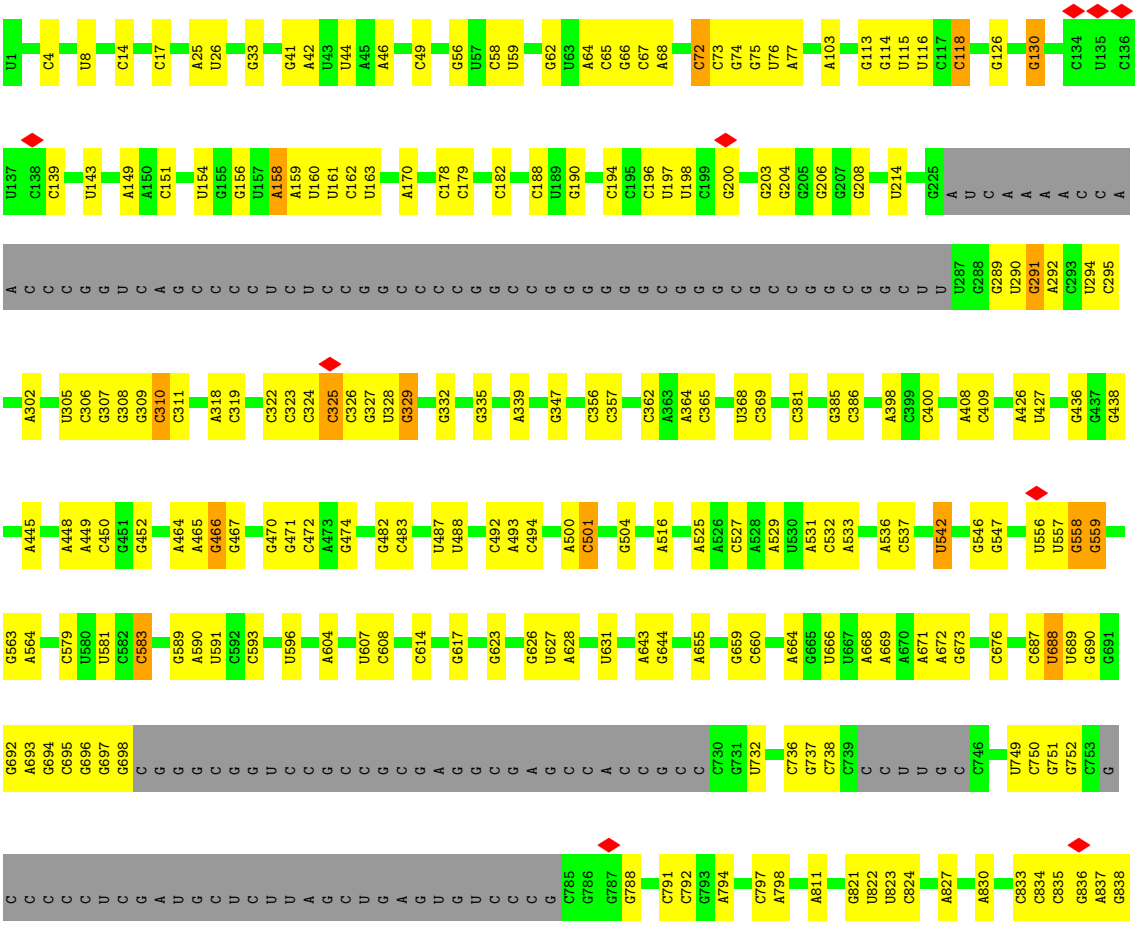
Chain Ln:

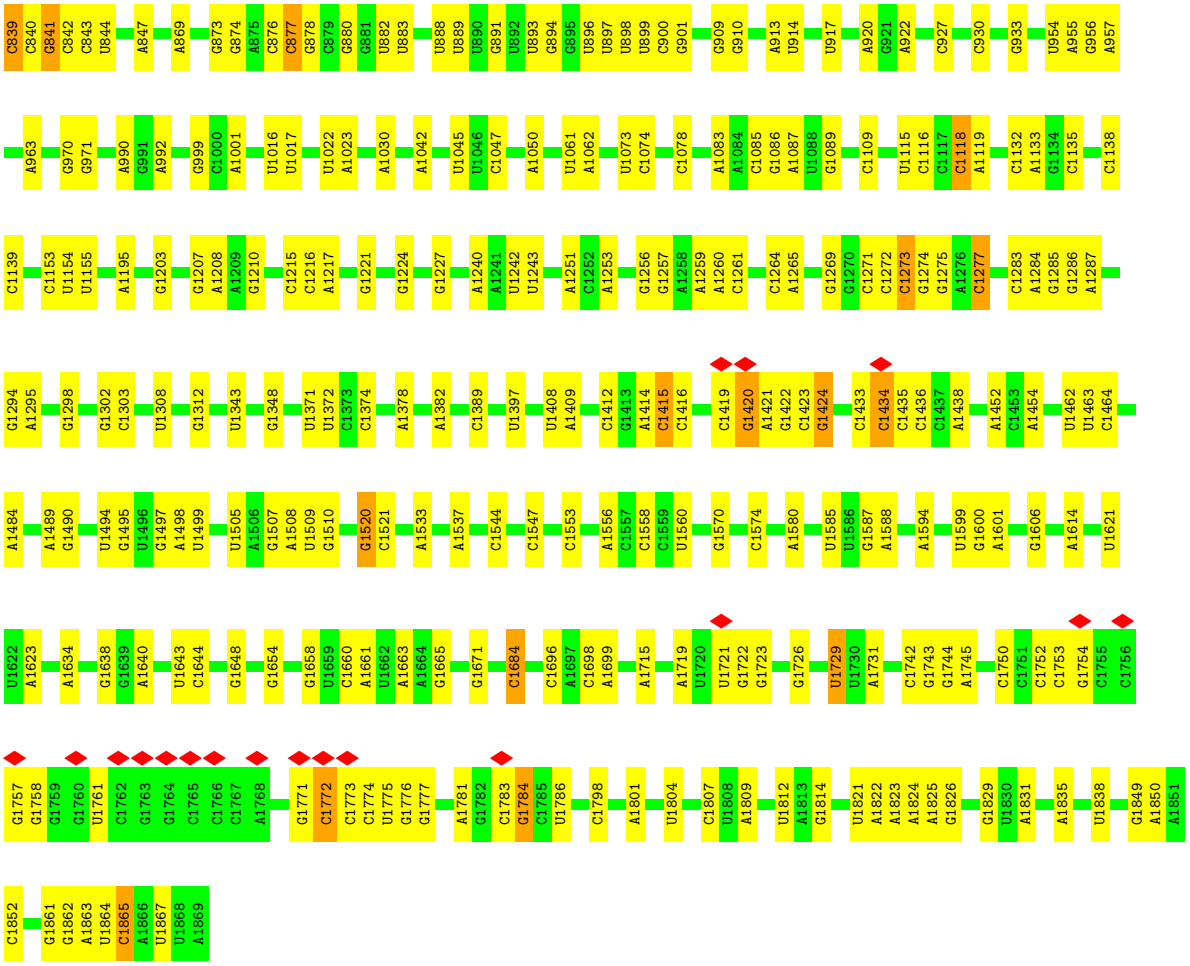




- Molecule 2: 18S rRNA

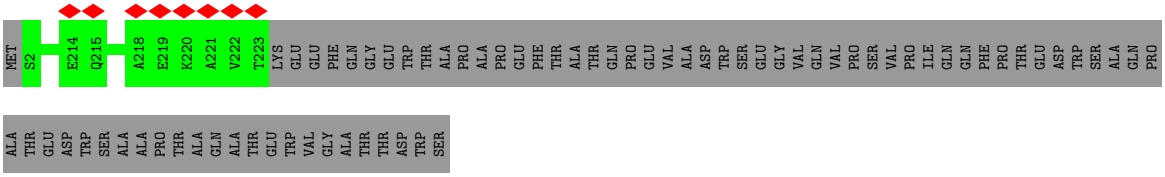
Chain S2:





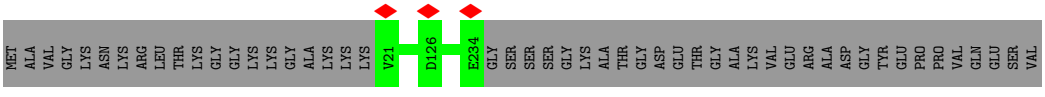
• Molecule 3: 40S ribosomal protein SA

Chain SA:



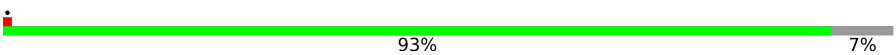
• Molecule 4: 40S ribosomal protein S3a

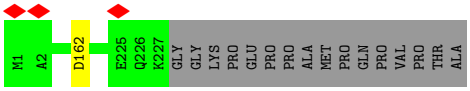
Chain SB:



• Molecule 5: 40S ribosomal protein S3

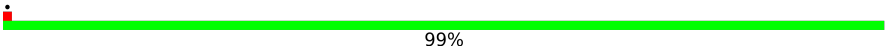
Chain SD:

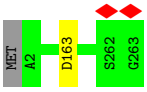




• Molecule 6: 40S ribosomal protein S4, X isoform

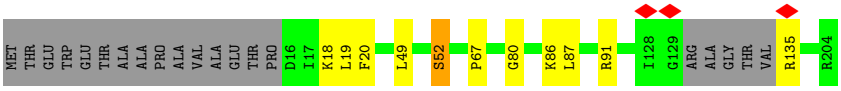
Chain SE:





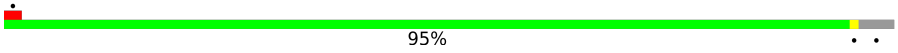
• Molecule 7: 40S ribosomal protein S5

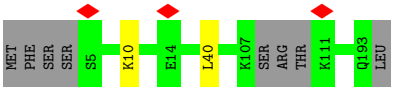
Chain SF:



• Molecule 8: 40S ribosomal protein S7

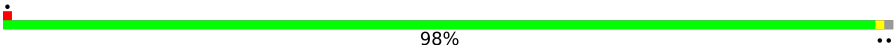
Chain SH:

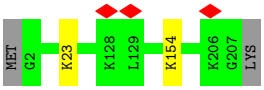




• Molecule 9: 40S ribosomal protein S8

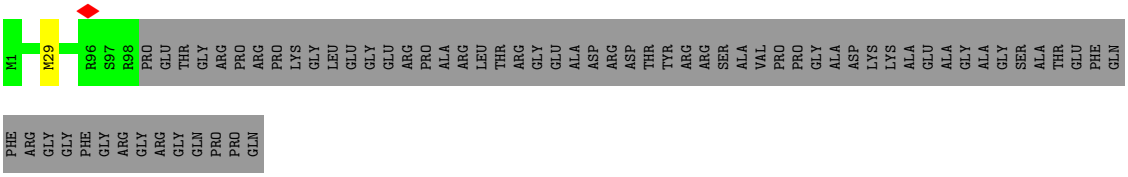
Chain SI:





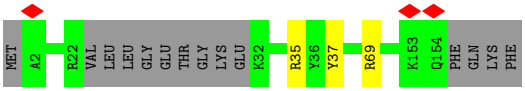
• Molecule 10: 40S ribosomal protein S10

Chain SK:

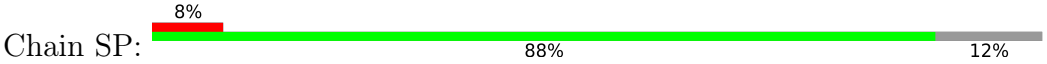


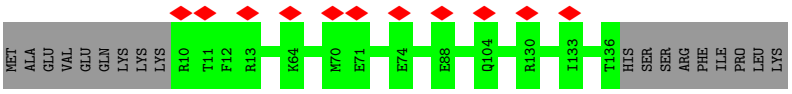
• Molecule 11: 40S ribosomal protein S11

Chain SL:

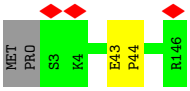


• Molecule 12: 40S ribosomal protein S15

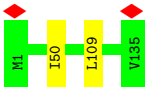




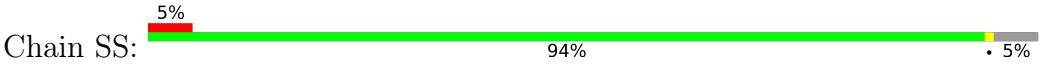
• Molecule 13: 40S ribosomal protein S16

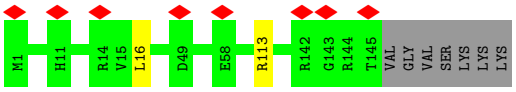


• Molecule 14: 40S ribosomal protein S17

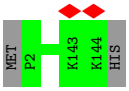


• Molecule 15: 40S ribosomal protein S18

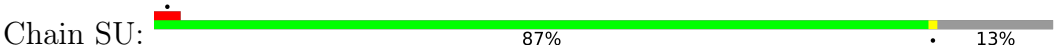


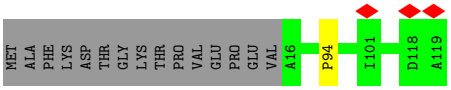


• Molecule 16: 40S ribosomal protein S19



• Molecule 17: 40S ribosomal protein S20





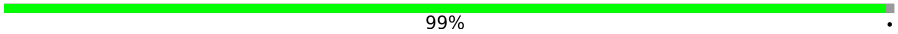
• Molecule 18: 40S ribosomal protein S21

Chain SV:

There are no outlier residues recorded for this chain.

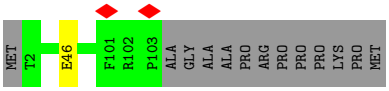
• Molecule 19: 40S ribosomal protein S23

Chain SX:



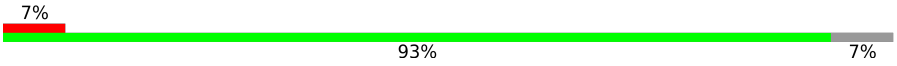
• Molecule 20: 40S ribosomal protein S26

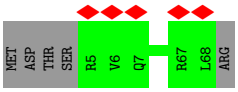
Chain Sa:



• Molecule 21: 40S ribosomal protein S28

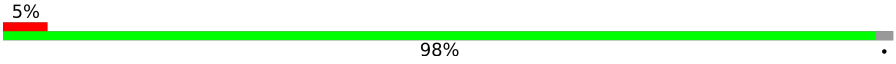
Chain Sc:

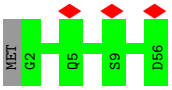




• Molecule 22: 40S ribosomal protein S29

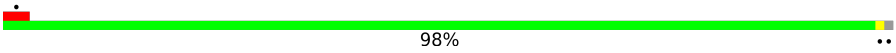
Chain Sd:

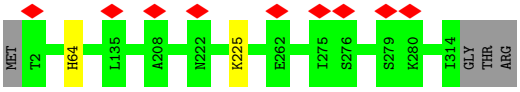




• Molecule 23: Receptor of activated protein C kinase 1

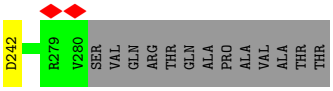
Chain Sg:





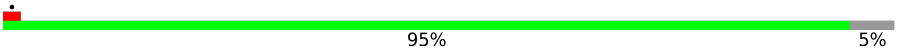
• Molecule 24: 40S ribosomal protein S2

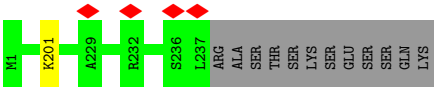
Chain SC:



• Molecule 25: 40S ribosomal protein S6

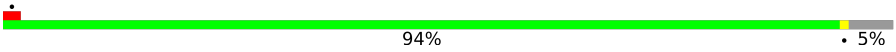
Chain SG:

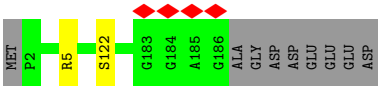




• Molecule 26: 40S ribosomal protein S9

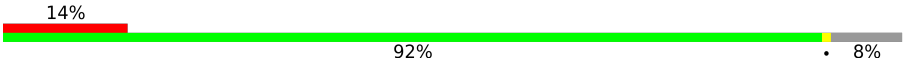
Chain SJ:

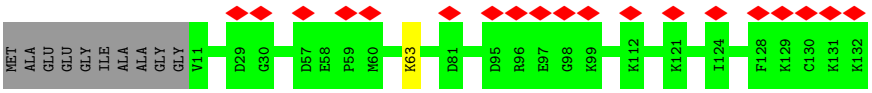




• Molecule 27: 40S ribosomal protein S12

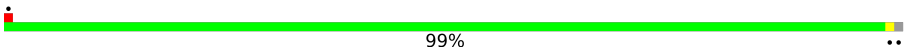
Chain SM:

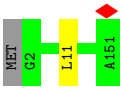




• Molecule 28: 40S ribosomal protein S13

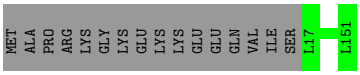
Chain SN:





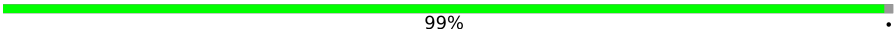
• Molecule 29: 40S ribosomal protein S14

Chain SO:



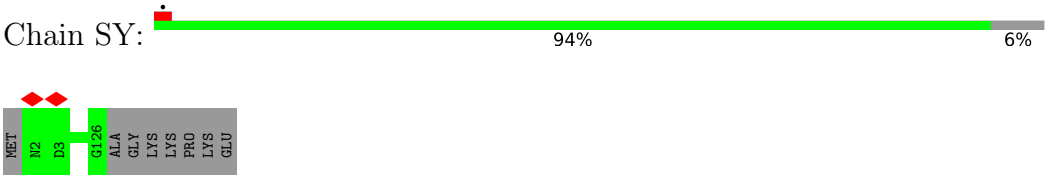
• Molecule 30: 40S ribosomal protein S15a

Chain SW:



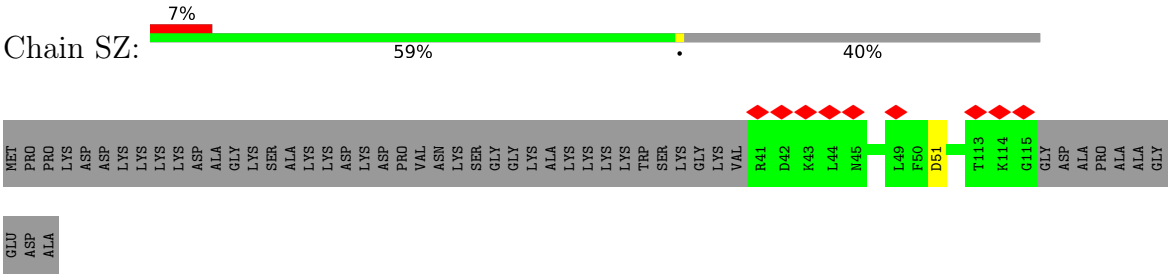
• Molecule 31: 40S ribosomal protein S24

Chain SY:



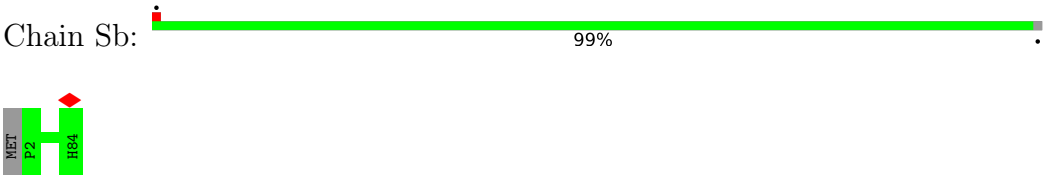
• Molecule 32: 40S ribosomal protein S25

Chain SZ:



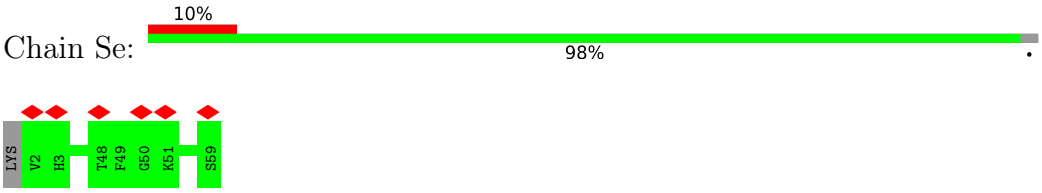
• Molecule 33: 40S ribosomal protein S27

Chain Sb:



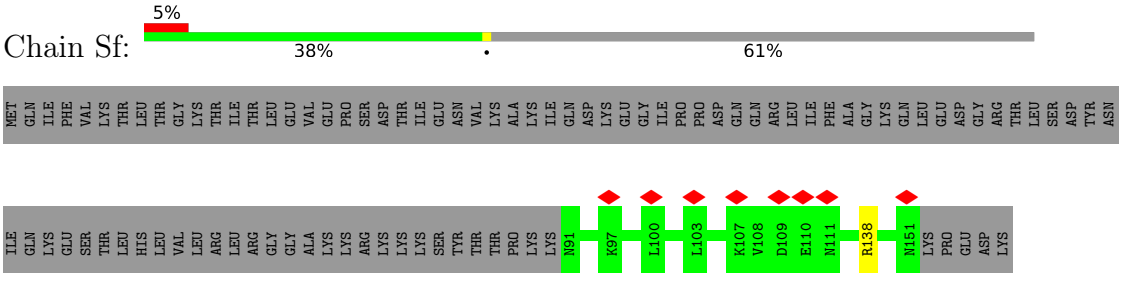
• Molecule 34: 40S ribosomal protein S30

Chain Se:



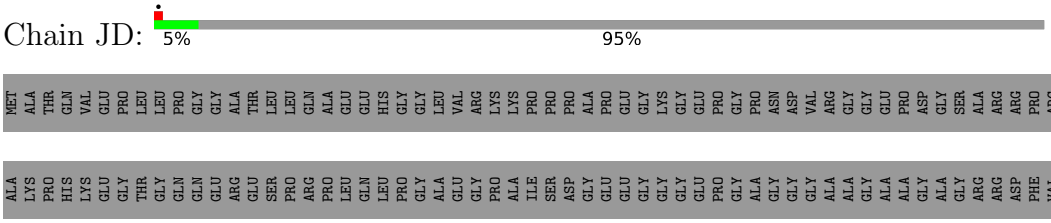
• Molecule 35: Ubiquitin-40S ribosomal protein S27a

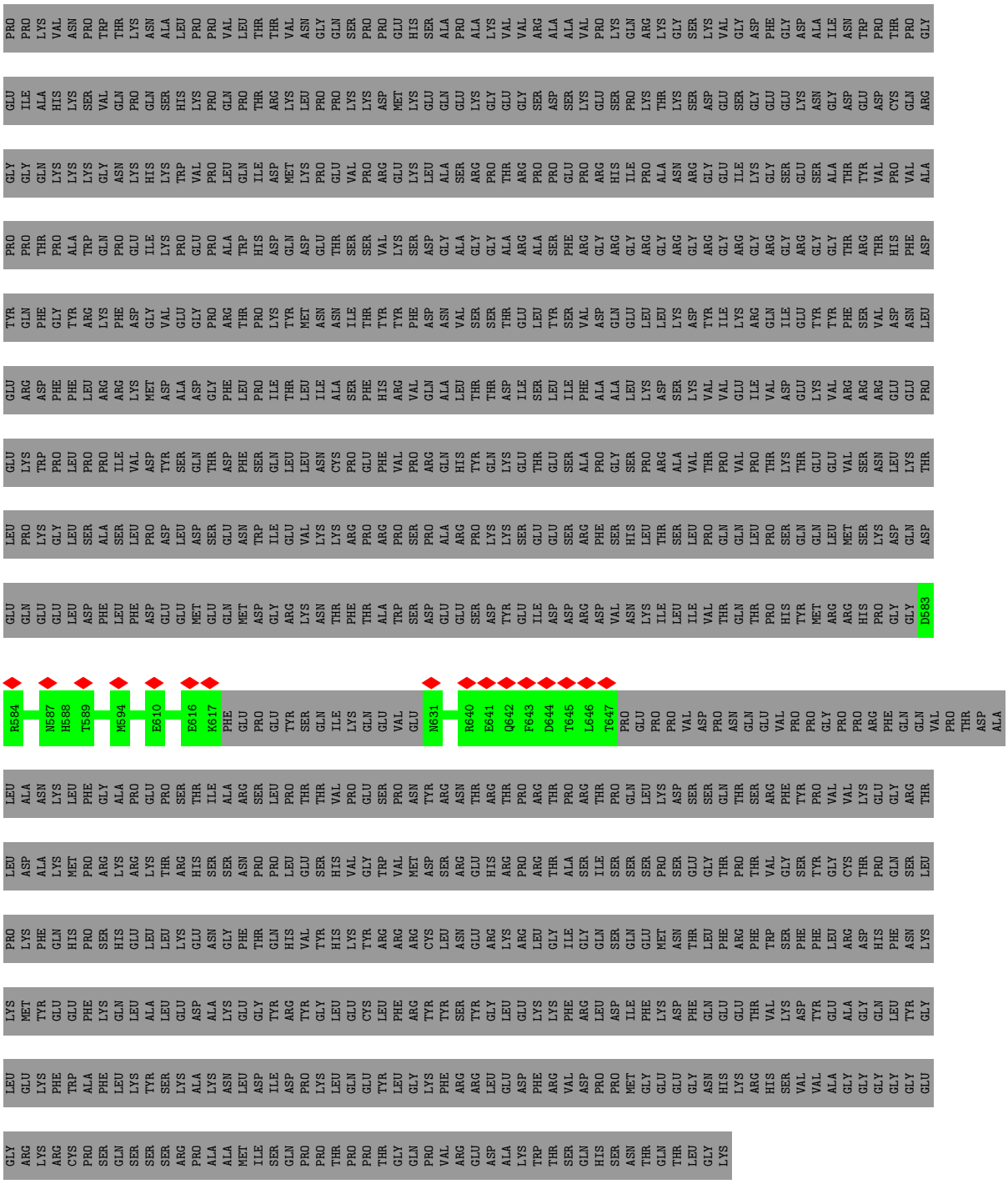
Chain Sf:



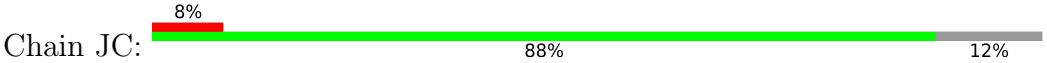
• Molecule 36: La-related protein 1

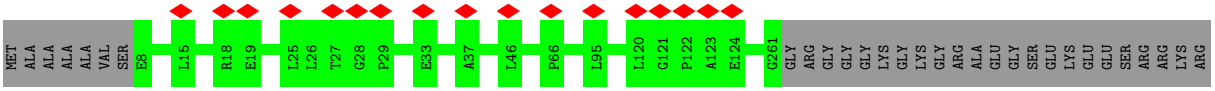
Chain JD:

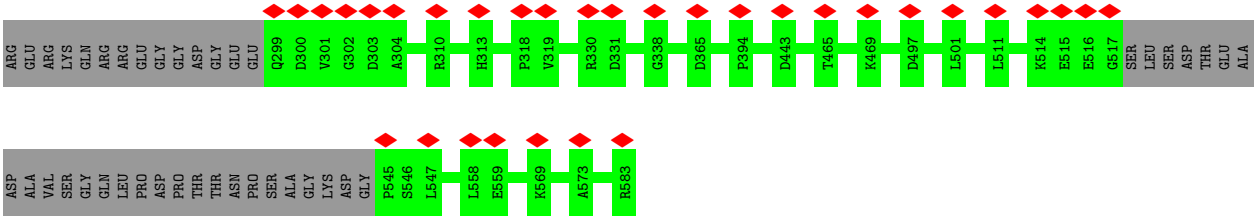




• Molecule 37: Leucine-rich repeat-containing protein 47






ARG GLU ARG LYS GLN ARG ARG GLU GLY GLY ASP GLY GLU GLU
Q299 D300 V301 G302 D303 A304 R310 H313 P318 V319 R330 D331 G338 D365 P394 D443 T465 K469 D497 L501 L511 K514 E515 E516 G517
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
P545 S546 L547 L558 E559 K569 A573 R583

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9897	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.072	Depositor
Minimum map value	-0.026	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	481.32, 481.32, 481.32	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.146, 1.146, 1.146	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	Ln	0.34	0/231	0.78	0/294
2	S2	0.47	0/41241	0.99	143/64258 (0.2%)
3	SA	0.30	0/1784	0.57	0/2424
4	SB	0.27	0/1765	0.62	0/2362
5	SD	0.29	0/1793	0.64	1/2414 (0.0%)
6	SE	0.31	0/2118	0.62	1/2849 (0.0%)
7	SF	0.33	0/1481	0.68	1/1988 (0.1%)
8	SH	0.28	0/1519	0.62	1/2033 (0.0%)
9	SI	0.29	0/1715	0.64	0/2287
10	SK	0.27	0/851	0.57	0/1147
11	SL	0.33	0/1202	0.64	1/1606 (0.1%)
12	SP	0.27	0/1065	0.63	0/1423
13	SQ	0.30	0/1160	0.62	0/1553
14	SR	0.32	0/1105	0.62	1/1484 (0.1%)
15	SS	0.27	0/1216	0.67	1/1628 (0.1%)
16	ST	0.27	0/1131	0.59	0/1515
17	SU	0.27	0/831	0.64	0/1115
18	SV	0.29	0/643	0.54	0/860
19	SX	0.29	0/1116	0.59	0/1490
20	Sa	0.30	0/836	0.62	0/1121
21	Sc	0.28	0/508	0.68	0/680
22	Sd	0.30	0/470	0.68	0/623
23	Sg	0.28	0/2493	0.59	0/3394
24	SC	0.32	0/1762	0.58	1/2381 (0.0%)
25	SG	0.29	0/1946	0.64	0/2590
26	SJ	0.30	0/1550	0.63	0/2069
27	SM	0.26	0/950	0.56	0/1275
28	SN	0.29	0/1232	0.65	1/1656 (0.1%)
29	SO	0.29	0/1023	0.60	0/1372
30	SW	0.30	0/1051	0.58	0/1406
31	SY	0.27	0/1039	0.60	0/1381
32	SZ	0.28	0/604	0.68	1/810 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	Sb	0.31	0/665	0.65	0/891
34	Se	0.28	0/465	0.62	0/612
35	Sf	0.26	0/507	0.63	0/673
36	JD	0.25	0/435	0.48	0/581
37	JC	0.25	0/4006	0.56	0/5429
All	All	0.39	0/85509	0.83	153/123674 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	SK	0	1
13	SQ	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 153 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	S2	1772	C	N1-C2-O2	13.45	126.97	118.90
2	S2	1772	C	N3-C2-O2	-12.87	112.89	121.90
2	S2	839	C	N1-C2-O2	10.99	125.50	118.90
2	S2	322	C	N3-C2-O2	-10.79	114.35	121.90
2	S2	839	C	N3-C2-O2	-9.78	115.05	121.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	SK	29	MET	Peptide
13	SQ	43	GLU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Ln	22/25 (88%)	22 (100%)	0	0	100 100
3	SA	220/295 (75%)	214 (97%)	6 (3%)	0	100 100
4	SB	212/264 (80%)	206 (97%)	6 (3%)	0	100 100
5	SD	225/243 (93%)	219 (97%)	6 (3%)	0	100 100
6	SE	260/263 (99%)	249 (96%)	11 (4%)	0	100 100
7	SF	180/204 (88%)	165 (92%)	12 (7%)	3 (2%)	7 28
8	SH	182/194 (94%)	173 (95%)	9 (5%)	0	100 100
9	SI	204/208 (98%)	194 (95%)	10 (5%)	0	100 100
10	SK	96/165 (58%)	90 (94%)	6 (6%)	0	100 100
11	SL	140/158 (89%)	134 (96%)	6 (4%)	0	100 100
12	SP	125/145 (86%)	122 (98%)	3 (2%)	0	100 100
13	SQ	142/146 (97%)	131 (92%)	10 (7%)	1 (1%)	19 47
14	SR	133/135 (98%)	130 (98%)	3 (2%)	0	100 100
15	SS	143/152 (94%)	137 (96%)	6 (4%)	0	100 100
16	ST	141/145 (97%)	138 (98%)	3 (2%)	0	100 100
17	SU	102/119 (86%)	93 (91%)	8 (8%)	1 (1%)	13 39
18	SV	81/83 (98%)	78 (96%)	3 (4%)	0	100 100
19	SX	139/143 (97%)	133 (96%)	6 (4%)	0	100 100
20	Sa	100/115 (87%)	97 (97%)	2 (2%)	1 (1%)	13 39
21	Sc	62/69 (90%)	59 (95%)	3 (5%)	0	100 100
22	Sd	53/56 (95%)	49 (92%)	4 (8%)	0	100 100
23	Sg	311/317 (98%)	289 (93%)	22 (7%)	0	100 100
24	SC	220/293 (75%)	213 (97%)	7 (3%)	0	100 100
25	SG	235/249 (94%)	228 (97%)	7 (3%)	0	100 100
26	SJ	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	25 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	SM	120/132 (91%)	112 (93%)	8 (7%)	0	100	100
28	SN	148/151 (98%)	144 (97%)	4 (3%)	0	100	100
29	SO	133/151 (88%)	125 (94%)	8 (6%)	0	100	100
30	SW	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
31	SY	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
32	SZ	73/125 (58%)	67 (92%)	6 (8%)	0	100	100
33	Sb	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
34	Se	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
35	Sf	59/156 (38%)	55 (93%)	4 (7%)	0	100	100
36	JD	48/1096 (4%)	48 (100%)	0	0	100	100
37	JC	506/583 (87%)	488 (96%)	18 (4%)	0	100	100
All	All	5385/7180 (75%)	5141 (96%)	237 (4%)	7 (0%)	50	78

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	SQ	44	PRO
7	SF	80	GLY
7	SF	20	PHE
7	SF	52	SER
20	Sa	46	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Ln	23/24 (96%)	23 (100%)	0	100	100
3	SA	184/243 (76%)	184 (100%)	0	100	100
4	SB	195/231 (84%)	195 (100%)	0	100	100
5	SD	190/202 (94%)	190 (100%)	0	100	100
6	SE	224/225 (100%)	224 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	SF	156/170 (92%)	148 (95%)	8 (5%)	20 46
8	SH	166/174 (95%)	165 (99%)	1 (1%)	84 90
9	SI	178/180 (99%)	176 (99%)	2 (1%)	70 81
10	SK	89/136 (65%)	89 (100%)	0	100 100
11	SL	130/142 (92%)	128 (98%)	2 (2%)	60 76
12	SP	113/130 (87%)	113 (100%)	0	100 100
13	SQ	119/121 (98%)	119 (100%)	0	100 100
14	SR	122/122 (100%)	121 (99%)	1 (1%)	79 87
15	SS	126/132 (96%)	125 (99%)	1 (1%)	79 87
16	ST	113/115 (98%)	113 (100%)	0	100 100
17	SU	94/107 (88%)	94 (100%)	0	100 100
18	SV	67/67 (100%)	67 (100%)	0	100 100
19	SX	113/115 (98%)	113 (100%)	0	100 100
20	Sa	89/98 (91%)	89 (100%)	0	100 100
21	Sc	57/62 (92%)	57 (100%)	0	100 100
22	Sd	48/49 (98%)	48 (100%)	0	100 100
23	Sg	272/275 (99%)	270 (99%)	2 (1%)	81 88
24	SC	188/225 (84%)	188 (100%)	0	100 100
25	SG	207/218 (95%)	206 (100%)	1 (0%)	86 91
26	SJ	161/168 (96%)	160 (99%)	1 (1%)	84 90
27	SM	102/108 (94%)	101 (99%)	1 (1%)	73 83
28	SN	130/131 (99%)	130 (100%)	0	100 100
29	SO	105/119 (88%)	105 (100%)	0	100 100
30	SW	112/113 (99%)	112 (100%)	0	100 100
31	SY	109/115 (95%)	109 (100%)	0	100 100
32	SZ	66/103 (64%)	66 (100%)	0	100 100
33	Sb	75/76 (99%)	75 (100%)	0	100 100
34	Se	47/48 (98%)	47 (100%)	0	100 100
35	Sf	54/140 (39%)	53 (98%)	1 (2%)	52 71
36	JD	46/948 (5%)	46 (100%)	0	100 100
37	JC	437/487 (90%)	437 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4707/6119 (77%)	4686 (100%)	21 (0%)	88 93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	SS	113	ARG
25	SG	201	LYS
35	Sf	138	ARG
26	SJ	5	ARG
23	Sg	225	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
4	SB	40	ASN
4	SB	75	GLN
14	SR	48	ASN
26	SJ	154	GLN
32	SZ	103	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	S2	1717/1869 (91%)	437 (25%)	8 (0%)

5 of 437 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	S2	4	C
2	S2	8	U
2	S2	14	C
2	S2	17	C
2	S2	25	A

5 of 8 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	S2	1434	C
2	S2	954	U
2	S2	500	A

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Mol	Chain	Res	Type
2	S2	466	G
2	S2	688	U

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

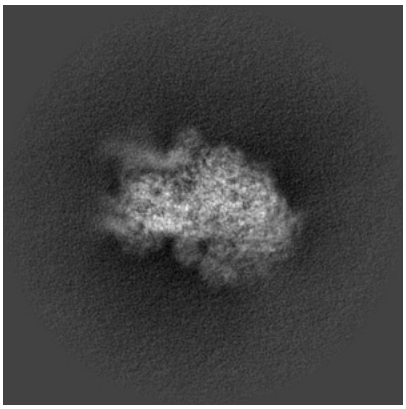
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38549. These allow visual inspection of the internal detail of the map and identification of artifacts.

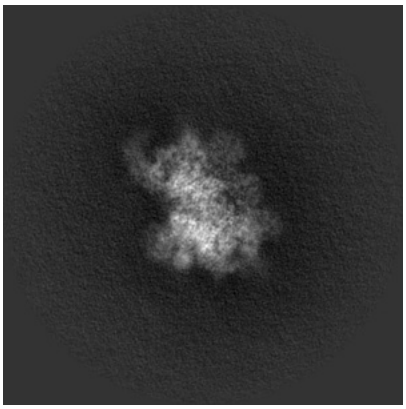
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

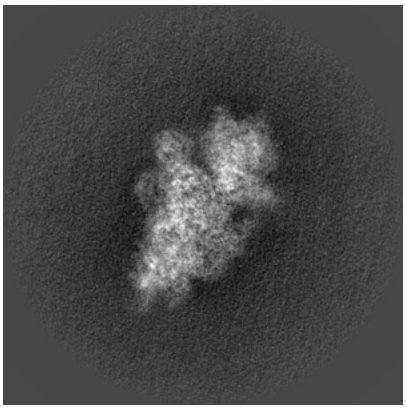
6.1.1 Primary map



X

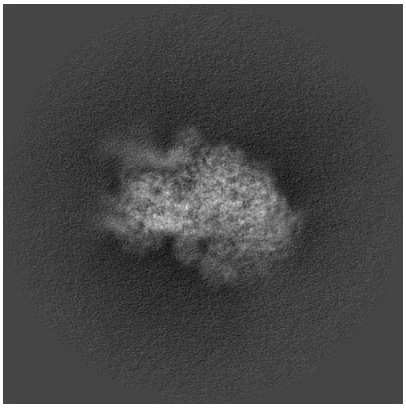


Y

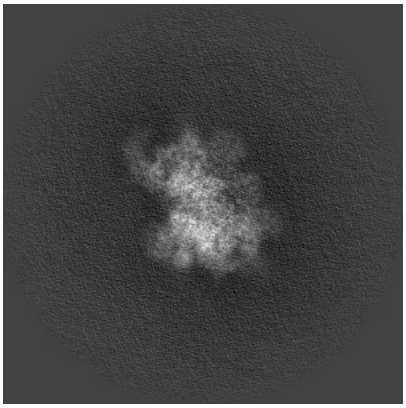


Z

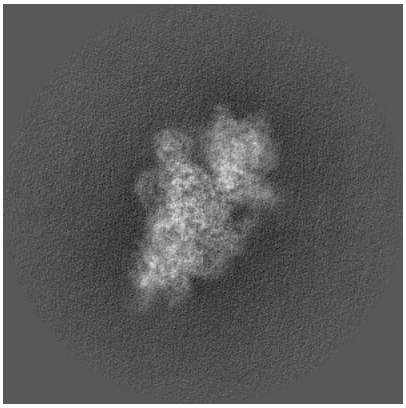
6.1.2 Raw map



X



Y

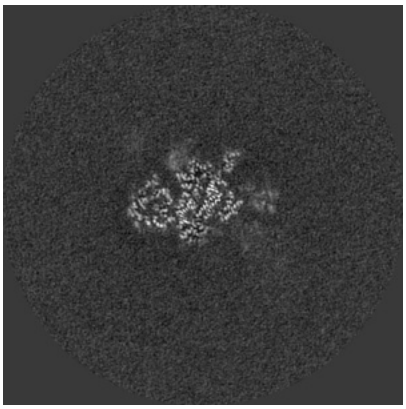


Z

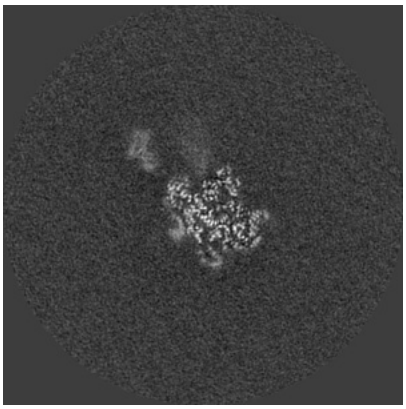
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

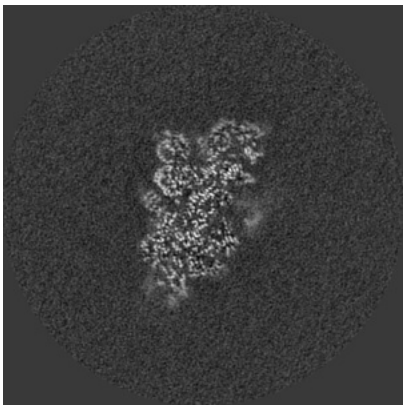
6.2.1 Primary map



X Index: 210

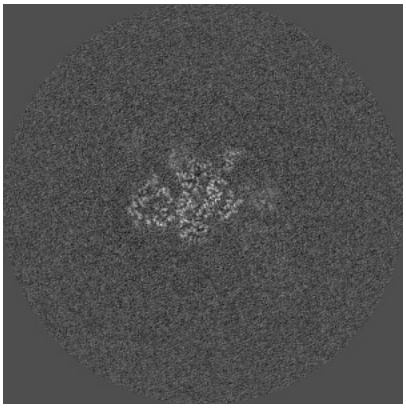


Y Index: 210

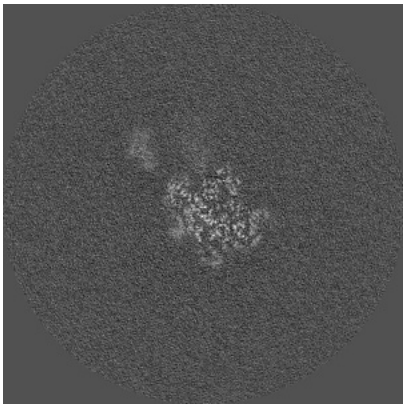


Z Index: 210

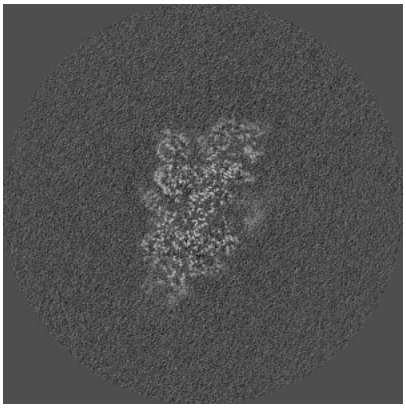
6.2.2 Raw map



X Index: 210



Y Index: 210

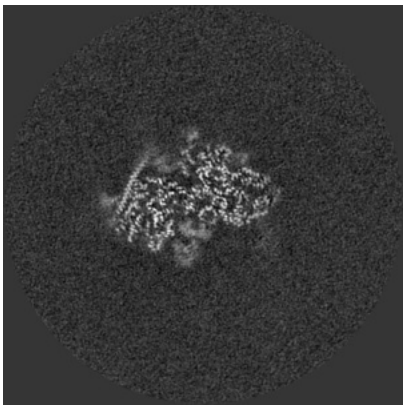


Z Index: 210

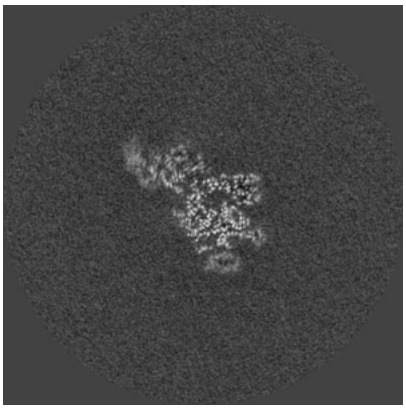
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

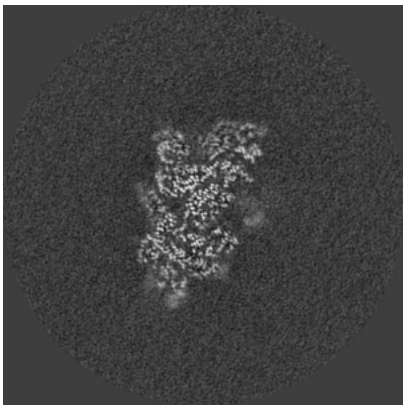
6.3.1 Primary map



X Index: 179

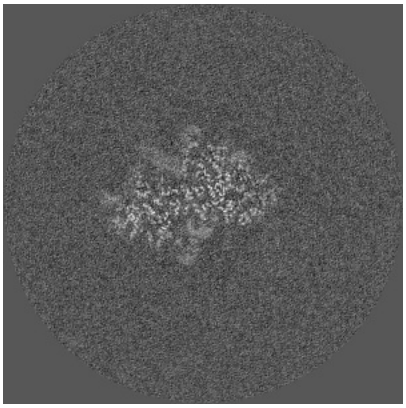


Y Index: 232

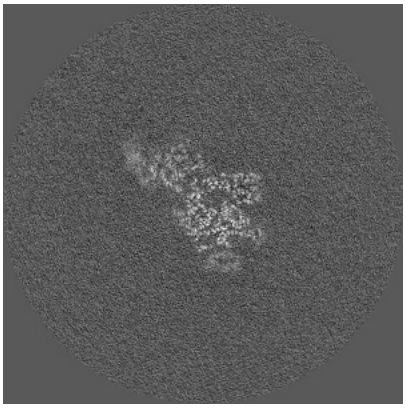


Z Index: 212

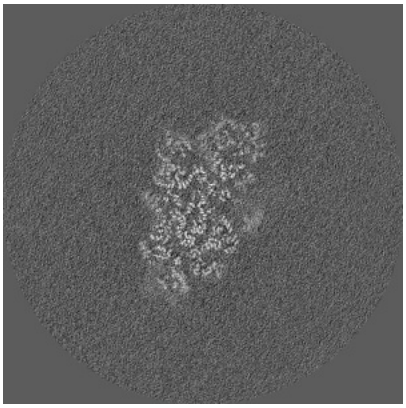
6.3.2 Raw map



X Index: 182



Y Index: 232

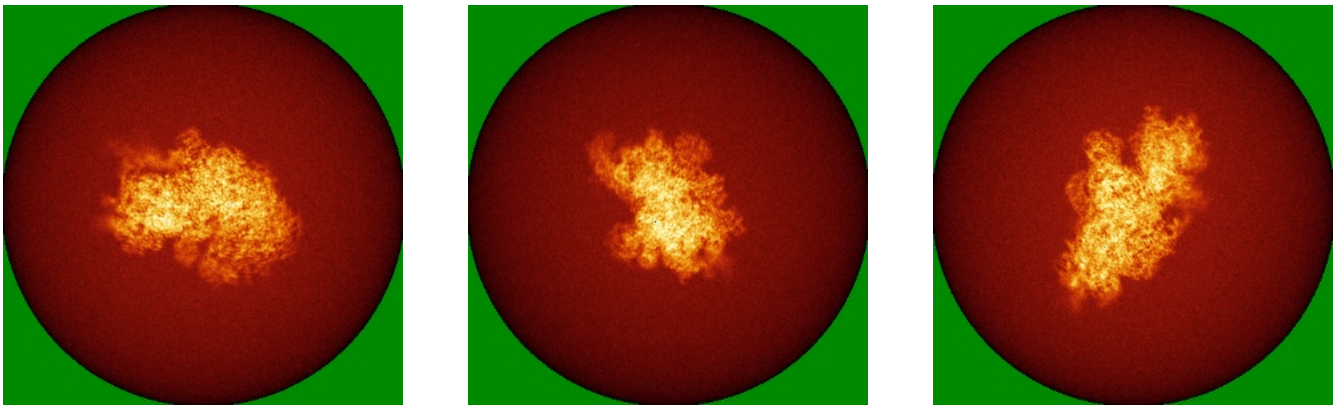


Z Index: 208

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

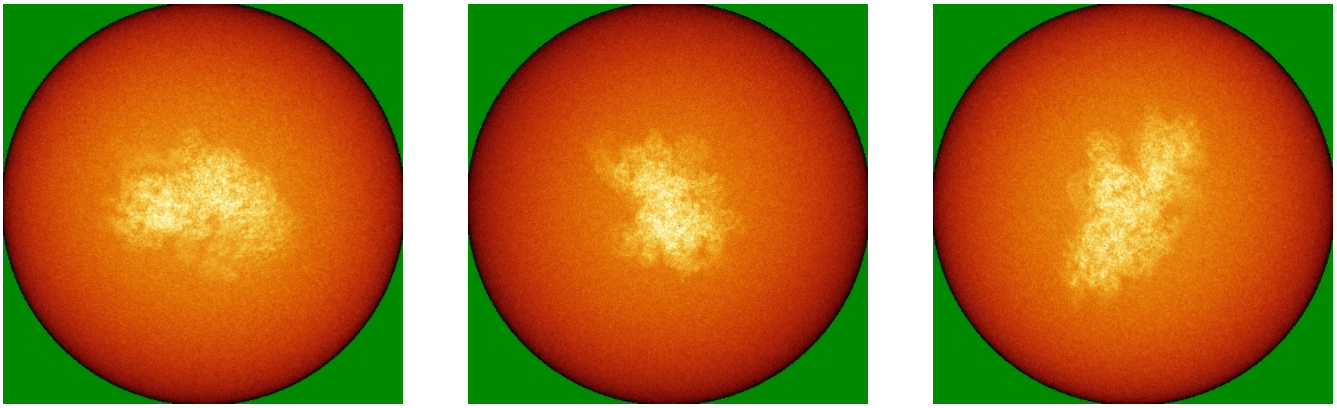
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw 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.

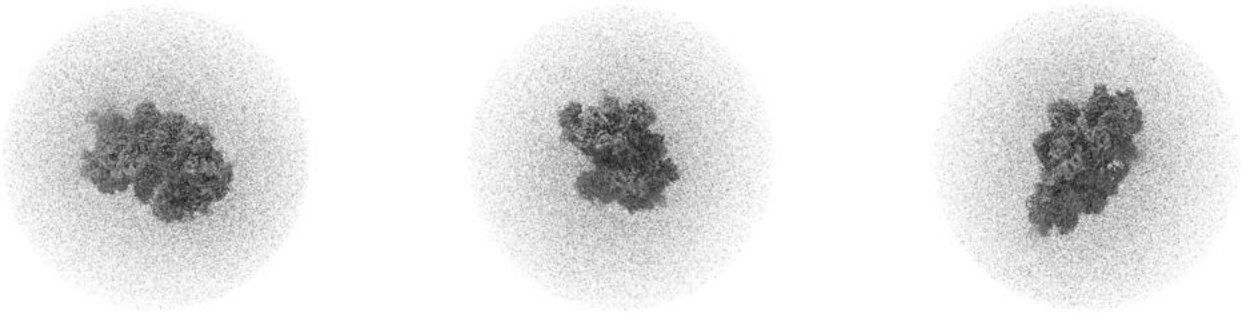
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

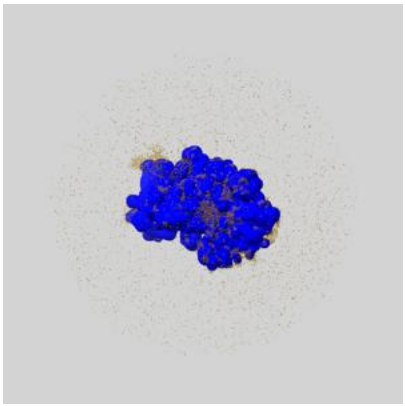
6.6 Mask visualisation (i)

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

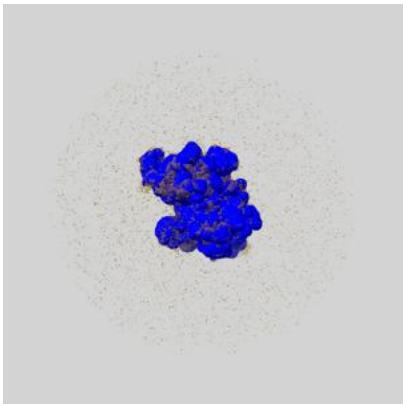
A mask typically either:

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

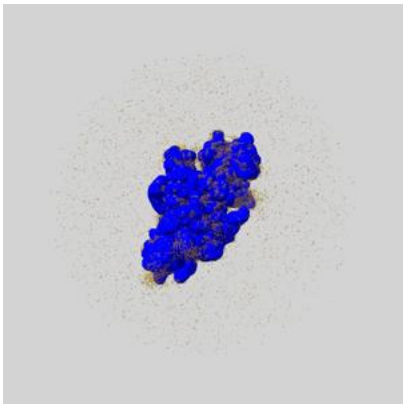
6.6.1 emd_38549_msk_1.map (i)



X



Y

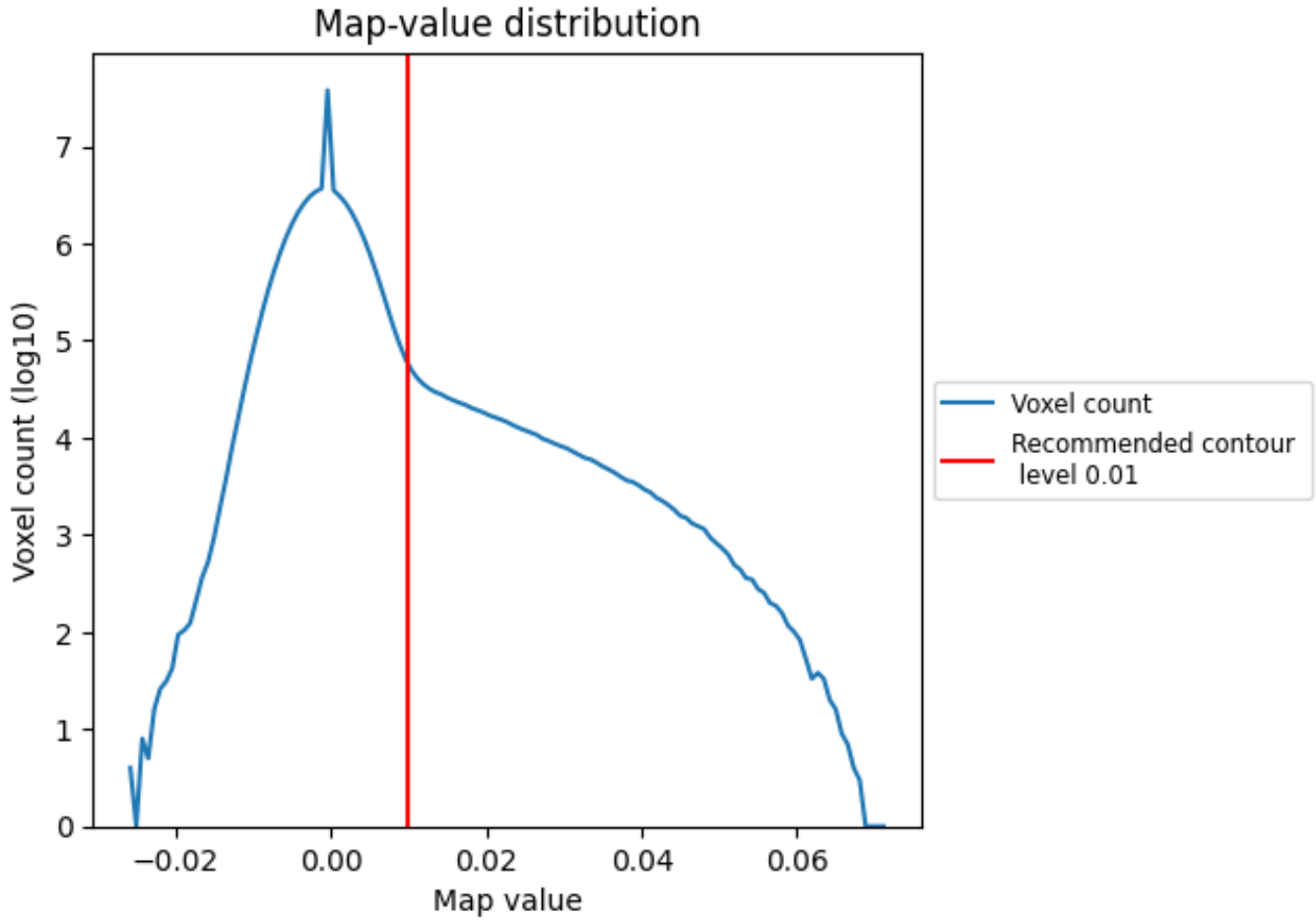


Z

7 Map analysis

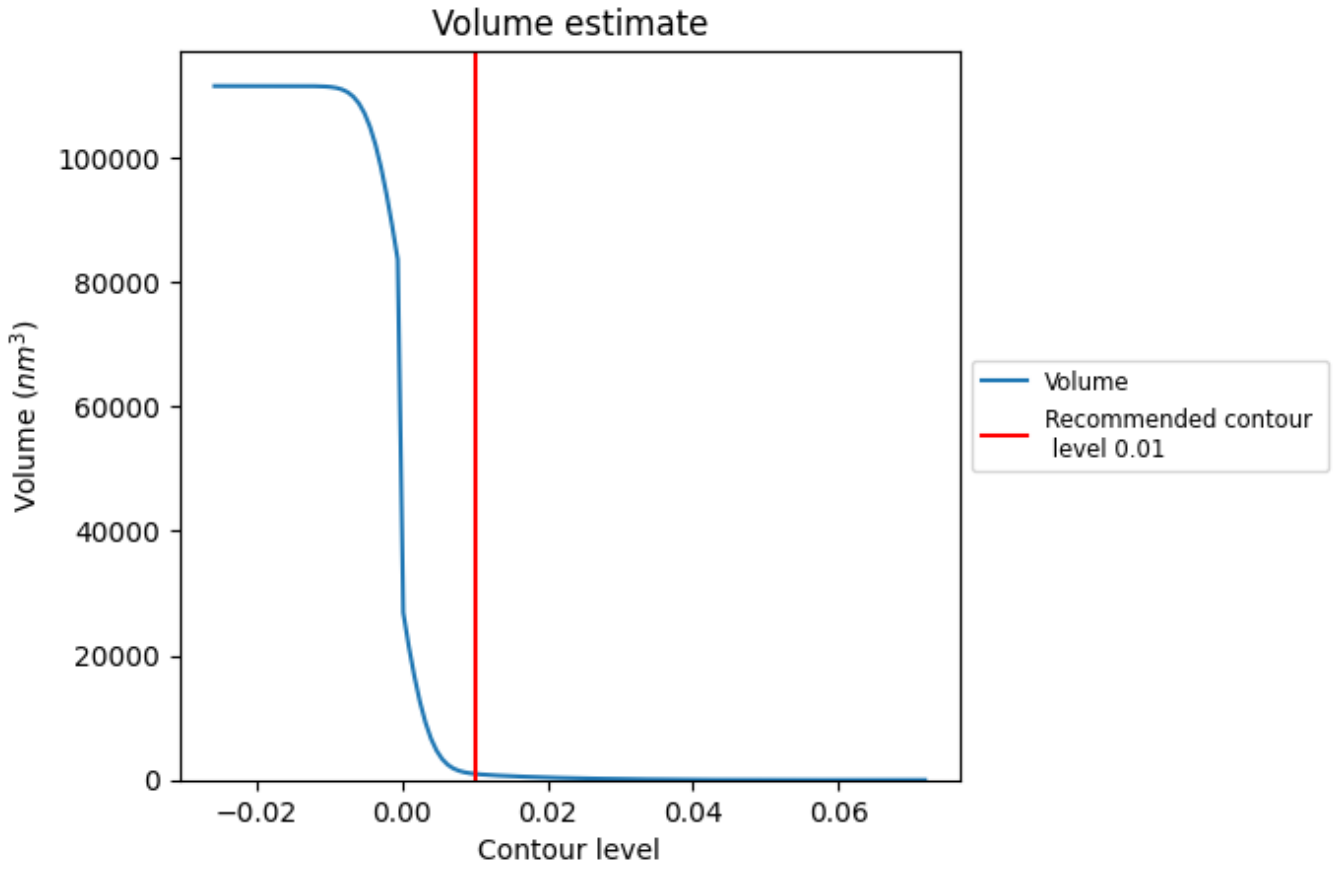
This section contains the results of statistical analysis of the map.

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.

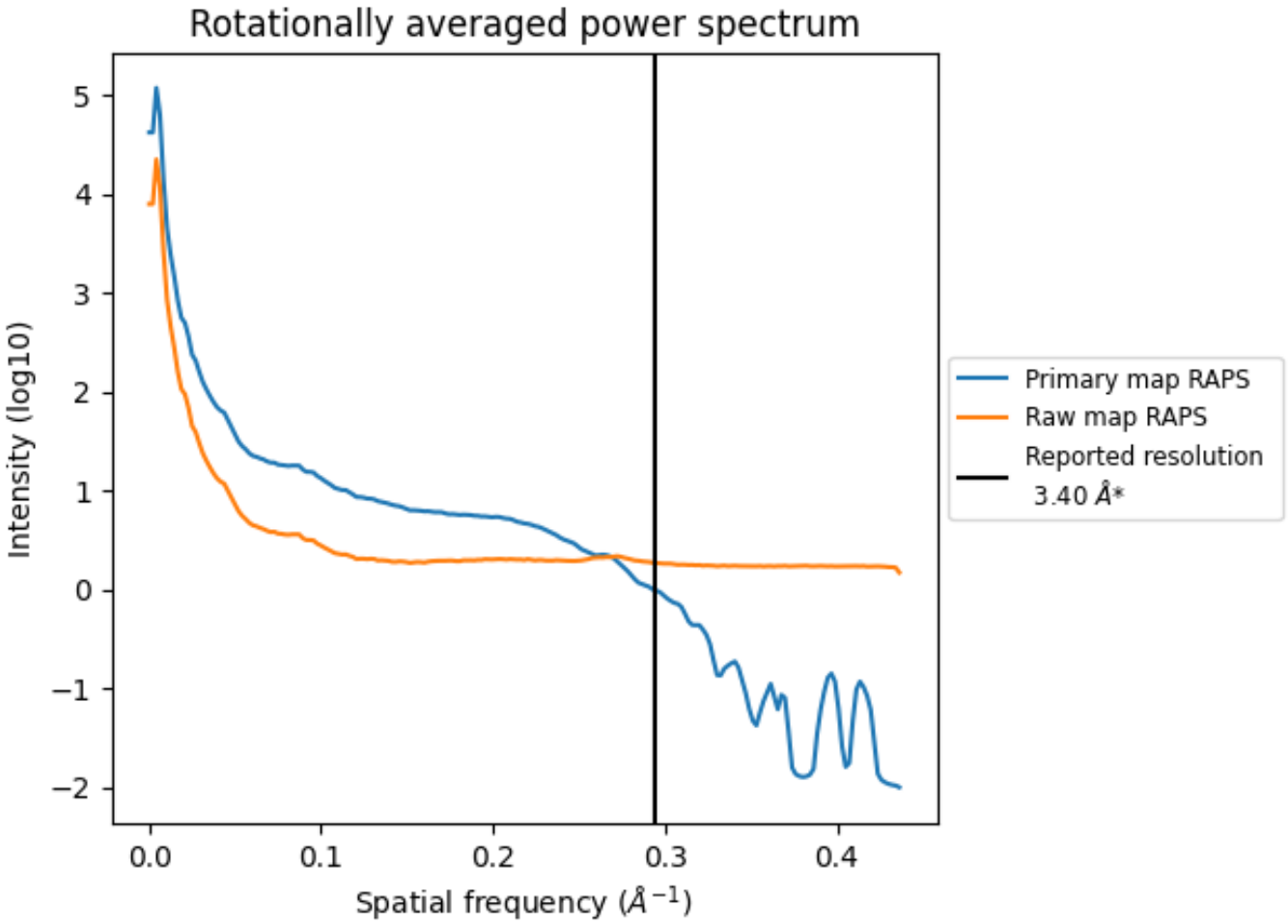
7.2 Volume estimate (i)



The volume at the recommended contour level is 985 nm^3; this corresponds to an approximate mass of 890 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

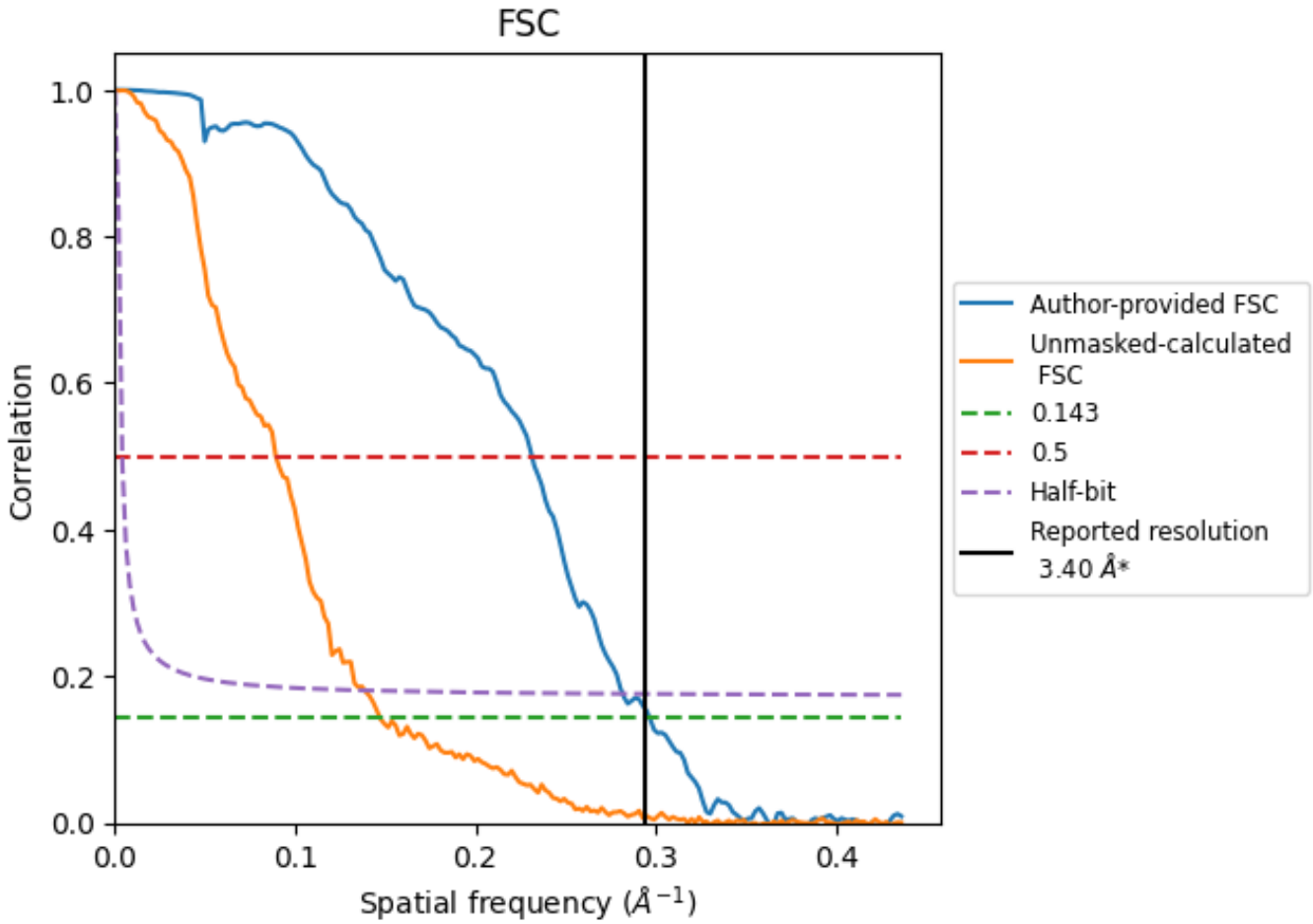


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

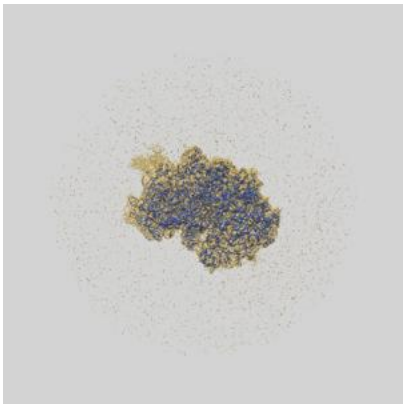
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	4.32	3.55
Unmasked-calculated*	6.79	11.19	7.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.79 differs from the reported value 3.4 by more than 10 %

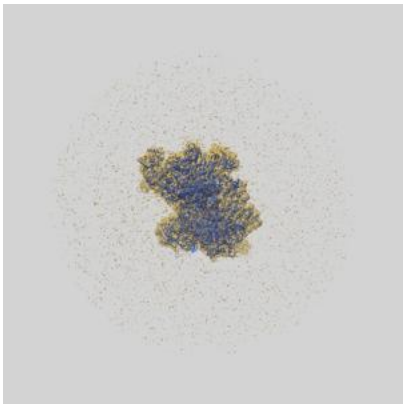
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38549 and PDB model 8XP3. Per-residue inclusion information can be found in section 3 on page 11.

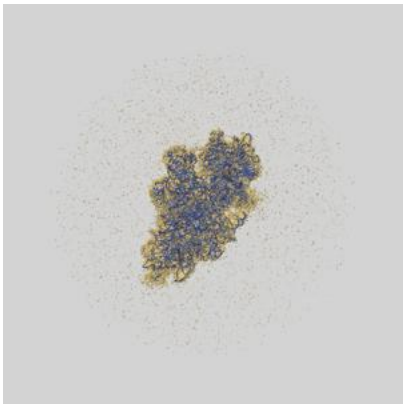
9.1 Map-model overlay



X



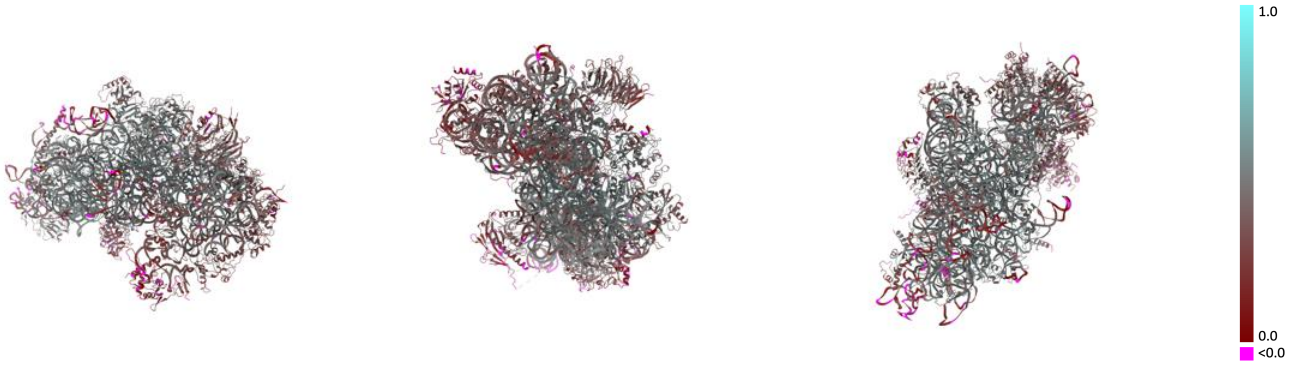
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

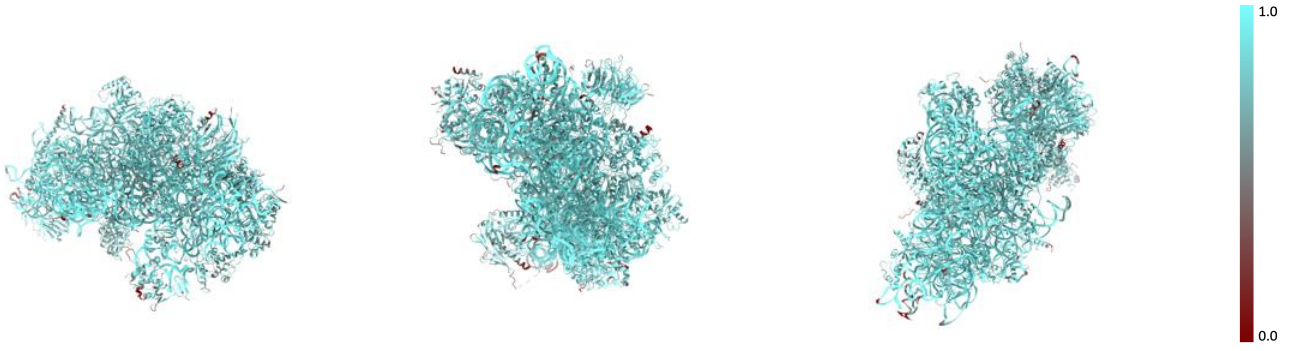
9.2 Q-score mapped to coordinate model



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.

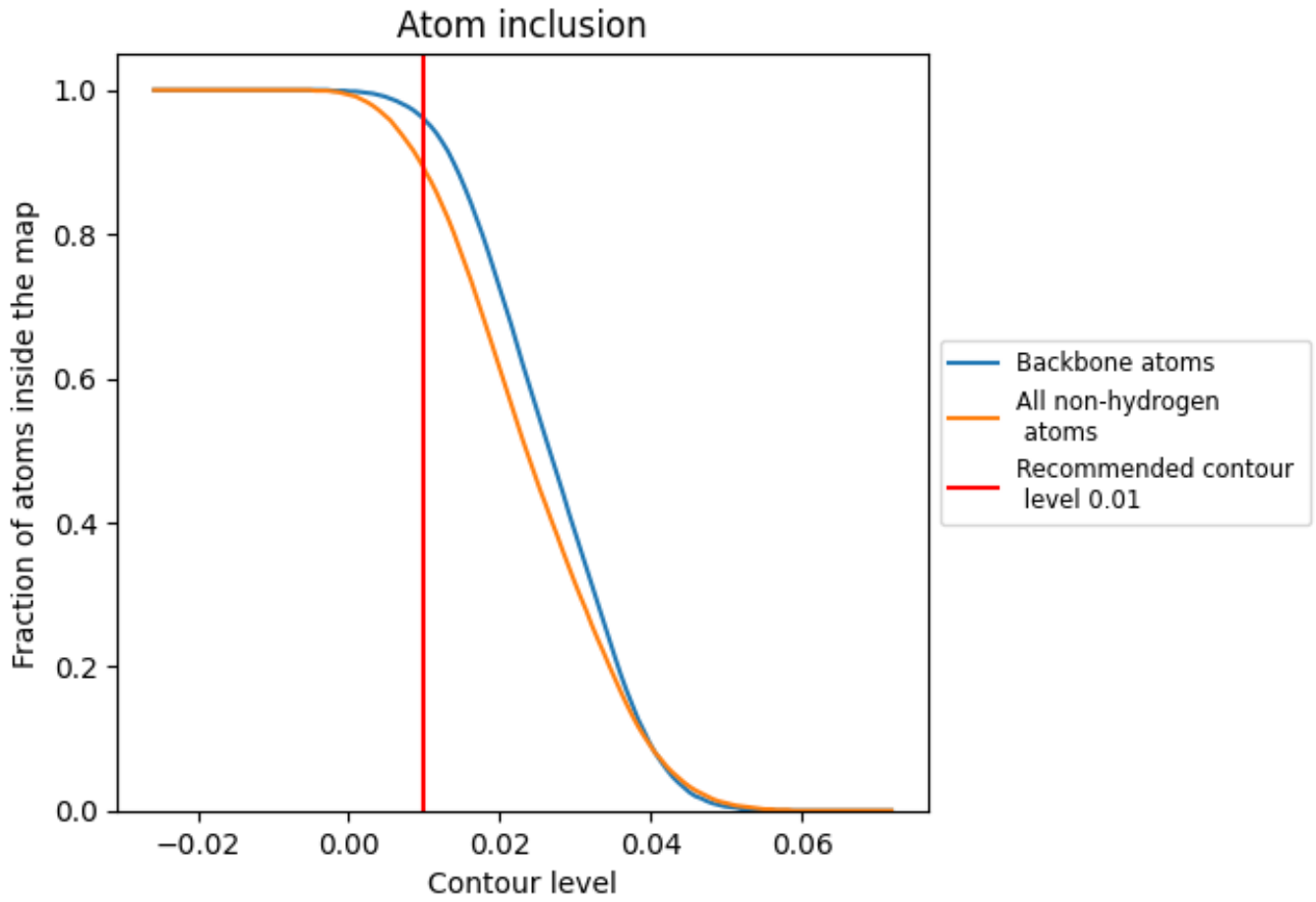
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8910	0.4130
JC	0.7490	0.2460
JD	0.4830	0.2700
Ln	0.6510	0.3420
S2	0.9600	0.4400
SA	0.8750	0.4570
SB	0.8680	0.4400
SC	0.8910	0.4880
SD	0.7890	0.3590
SE	0.9010	0.4910
SF	0.8070	0.3640
SG	0.8720	0.3990
SH	0.8500	0.3900
SI	0.8920	0.4420
SJ	0.8850	0.4730
SK	0.7970	0.3010
SL	0.8940	0.4860
SM	0.6630	0.1520
SN	0.8870	0.4600
SO	0.8540	0.4270
SP	0.7330	0.2940
SQ	0.8290	0.4140
SR	0.8260	0.4230
SS	0.7420	0.3090
ST	0.8210	0.3730
SU	0.7970	0.3740
SV	0.9070	0.4850
SW	0.9080	0.5120
SX	0.9040	0.4930
SY	0.8900	0.4530
SZ	0.7080	0.2750
Sa	0.8760	0.4650
Sb	0.8770	0.4590
Sc	0.7650	0.3410
Sd	0.8530	0.4100

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Chain	Atom inclusion	Q-score
Se	0.8150	0.4040
Sf	0.6900	0.1820
Sg	0.8330	0.3370