wwPDB EM Validation Summary Report (i)

Aug 27, 2026 – 05:41 am BST

PDB ID	:	7ARC / pdb_00007arc
EMDB ID	:	EMD-11879
Title	:	Cryo-EM structure of Polytomella Complex-I (peripheral arm)
Authors	:	Klusch, N.; Kuehlbrandt, W.; Yildiz, O.
Deposited on	:	2020-10-23
Resolution	:	2.88 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:

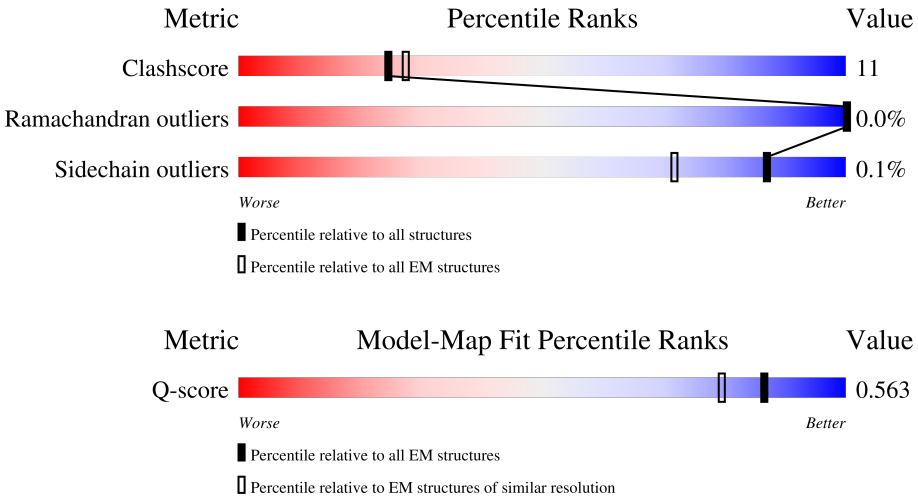
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.88 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12111 (2.38 - 3.38)

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	B	164	18% 73% 21% 6%
2	C	217	6% 71% 28%
3	D	395	8% 66% 34%
4	E	276	14% 63% 22% 15%

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Mol	Chain	Length	Quality of chain
5	F	469	8% 70% 22% 8%
6	G	720	5% 74% 21% 5%
7	I	229	27% 68% 19% 13%
8	P	370	12% 73% 21% 6%
9	Q	185	7% 64% 23% 12%
10	R	132	20% 69% 13% 18%
11	S	98	10% 64% 33%
12	U	122	46% 41% 28% 31%
13	V	159	16% 71% 13% 16%
14	W	137	26% 65% 28% 7%
15	q	155	15% 82%
16	r	121	31% 38% 12% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	F	501	-	-	X	-

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 27699 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 PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	154	Total	C	N	O	S	0	0
			1206	774	208	211	13		

- Molecule 2 is a protein called ND9.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	216	Total	C	N	O	S	0	0
			1808	1169	302	332	5		

- Molecule 3 is a protein called ND7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	395	Total	C	N	O	S	0	0
			3178	2029	557	569	23		

- Molecule 4 is a protein called 24 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	235	Total	C	N	O	S	0	0
			1806	1135	306	350	15		

- Molecule 5 is a protein called 51 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	430	Total	C	N	O	S	0	0
			3322	2088	594	617	23		

- Molecule 6 is a protein called 75 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	682	Total	C	N	O	S	0	0
			5166	3243	919	980	24		

- Molecule 7 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	199	Total	C	N	O	S	0	0
			1602	1000	274	317	11		

- Molecule 8 is a protein called 39 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	347	Total	C	N	O	S	0	0
			2701	1713	464	514	10		

- Molecule 9 is a protein called 18 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	162	Total	C	N	O	S	0	0
			1276	812	227	233	4		

- Molecule 10 is a protein called 13 kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	108	Total	C	N	O	S	0	0
			812	510	138	159	5		

- Molecule 11 is a protein called B8.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	S	95	Total	C	N	O	0	0
			716	450	124	142		

- Molecule 12 is a protein called SDAP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	84	Total	C	N	O	0	0
			655	414	103	138		

- Molecule 13 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	V	134	Total	C	N	O	S	0	0
			1052	671	170	209	2		

- Molecule 14 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	W	127	Total	C	N	O	S	0	0
			1074	695	185	188	6		

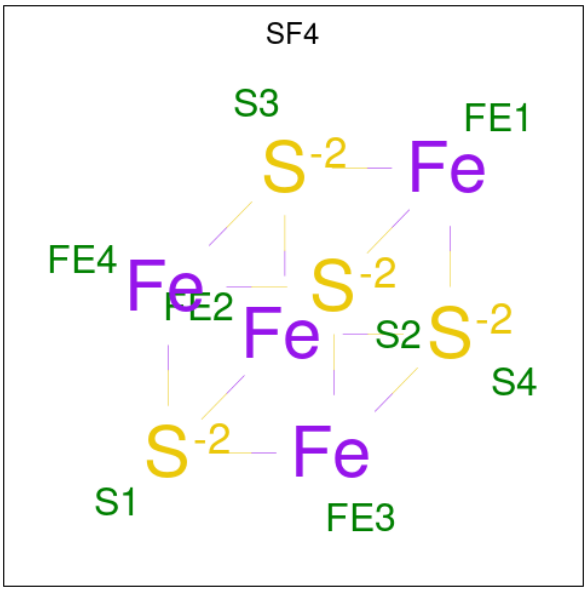
- Molecule 15 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	q	28	Total	C	N	O	S	0	0
			243	160	43	39	1		

- Molecule 16 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	r	60	Total	C	N	O	S	0	0
			493	317	88	87	1		

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



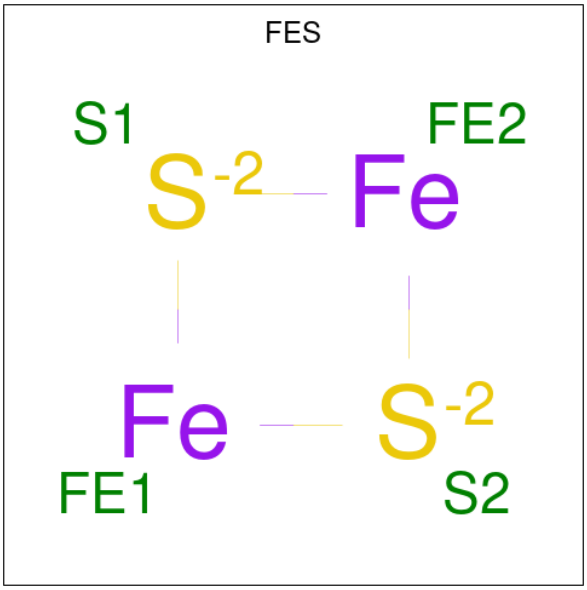
Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	Fe	S	0
			8	4	4	
17	F	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	
17	G	1	Total	Fe	S	0
			8	4	4	

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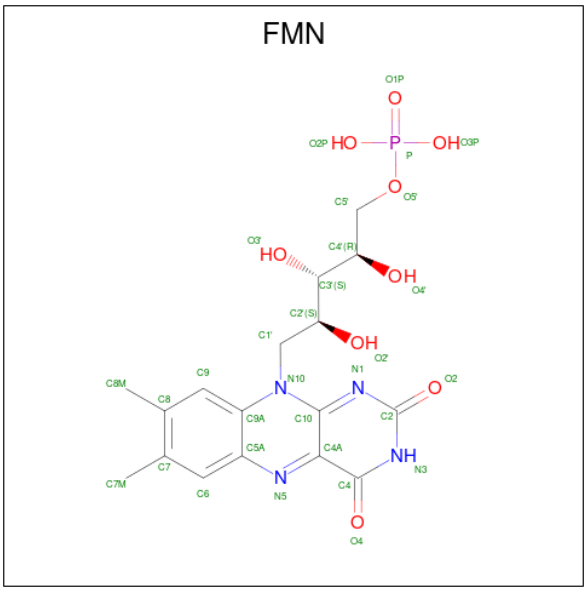
Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total Fe S 8 4 4	0
17	I	1	Total Fe S 8 4 4	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



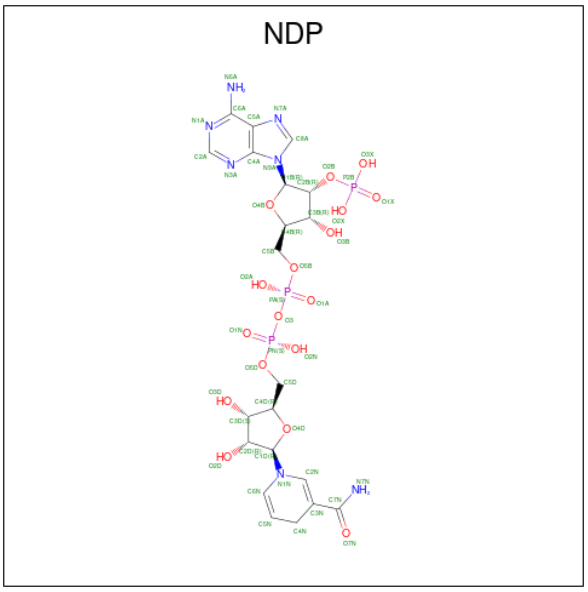
Mol	Chain	Residues	Atoms	AltConf
18	E	1	Total Fe S 4 2 2	0
18	G	1	Total Fe S 4 2 2	0

- Molecule 19 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 20 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

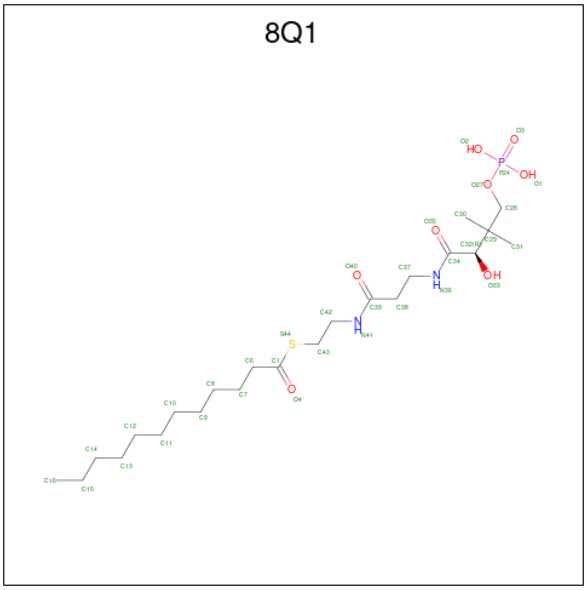


Mol	Chain	Residues	Atoms					AltConf
20	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 21 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
21	R	1	Total Zn 1 1	0

- Molecule 22 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms	AltConf
22	W	1	Total C N O P S 35 23 2 8 1 1	0

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	AltConf
23	B	14	Total O 14 14	0
23	C	36	Total O 36 36	0
23	D	44	Total O 44 44	0
23	E	12	Total O 12 12	0
23	F	17	Total O 17 17	0
23	G	113	Total O 113 113	0
23	I	36	Total O 36 36	0

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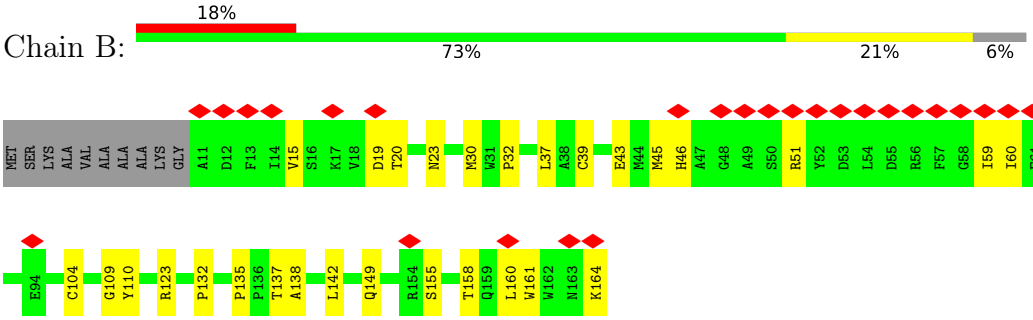
Mol	Chain	Residues	Atoms	AltConf
23	P	56	Total O 56 56	0
23	Q	36	Total O 36 36	0
23	R	9	Total O 9 9	0
23	S	8	Total O 8 8	0
23	V	10	Total O 10 10	0
23	W	12	Total O 12 12	0
23	q	8	Total O 8 8	0
23	r	7	Total O 7 7	0

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.

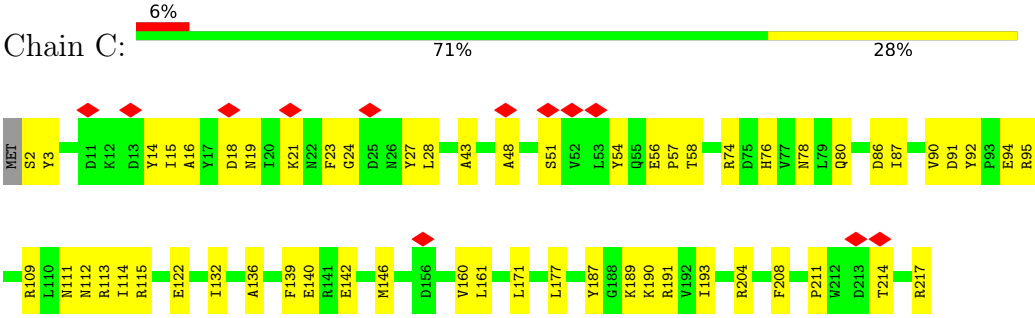
• Molecule 1: PSST

Chain B:



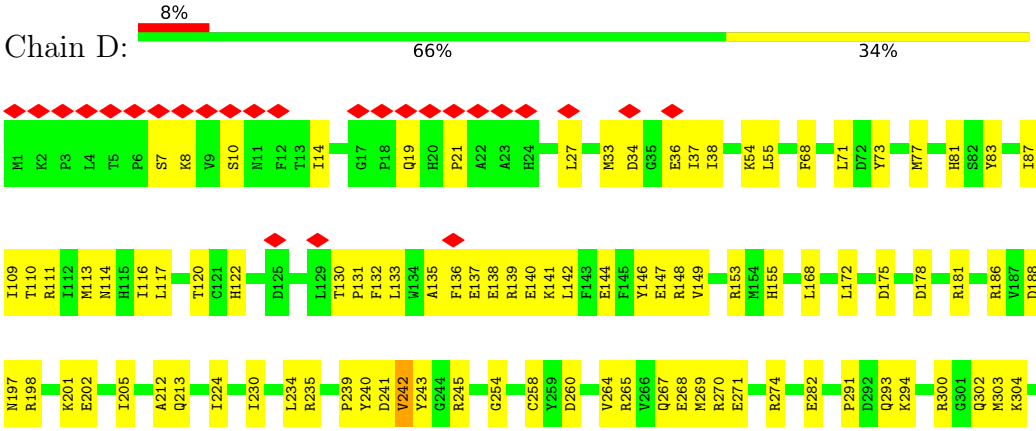
• Molecule 2: ND9

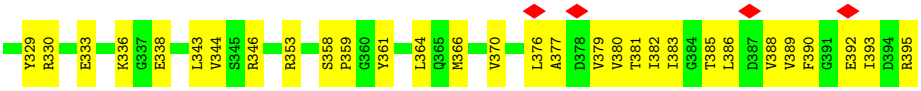
Chain C:



• Molecule 3: ND7

Chain D:

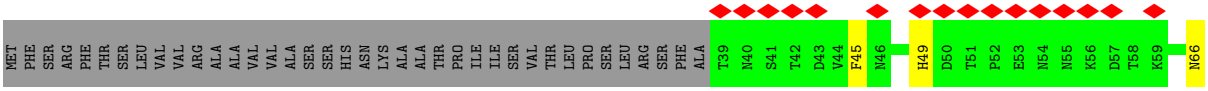


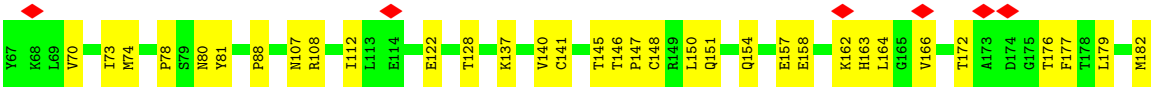


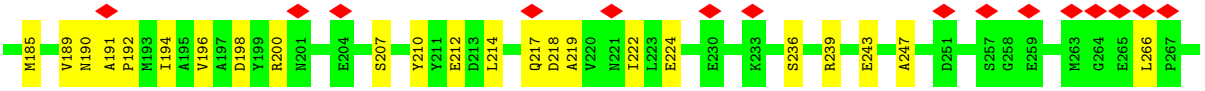
• Molecule 4: 24 kDa

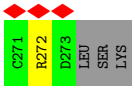
Chain E:







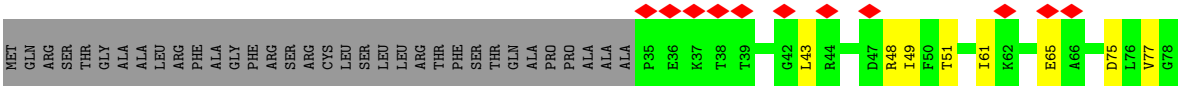




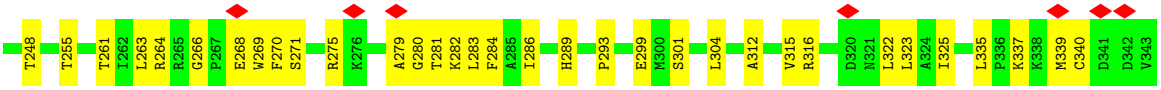
• Molecule 5: 51 kDa

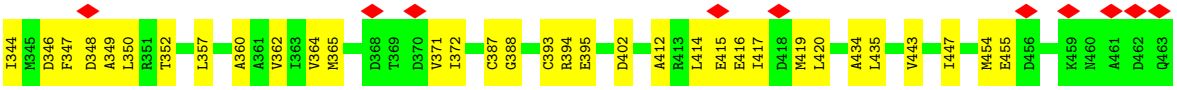
Chain F:

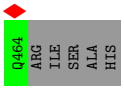








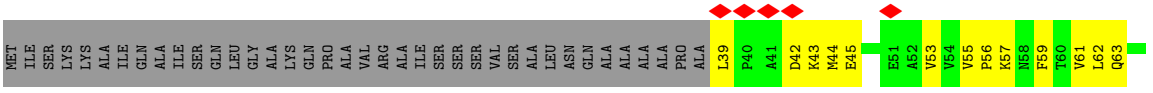


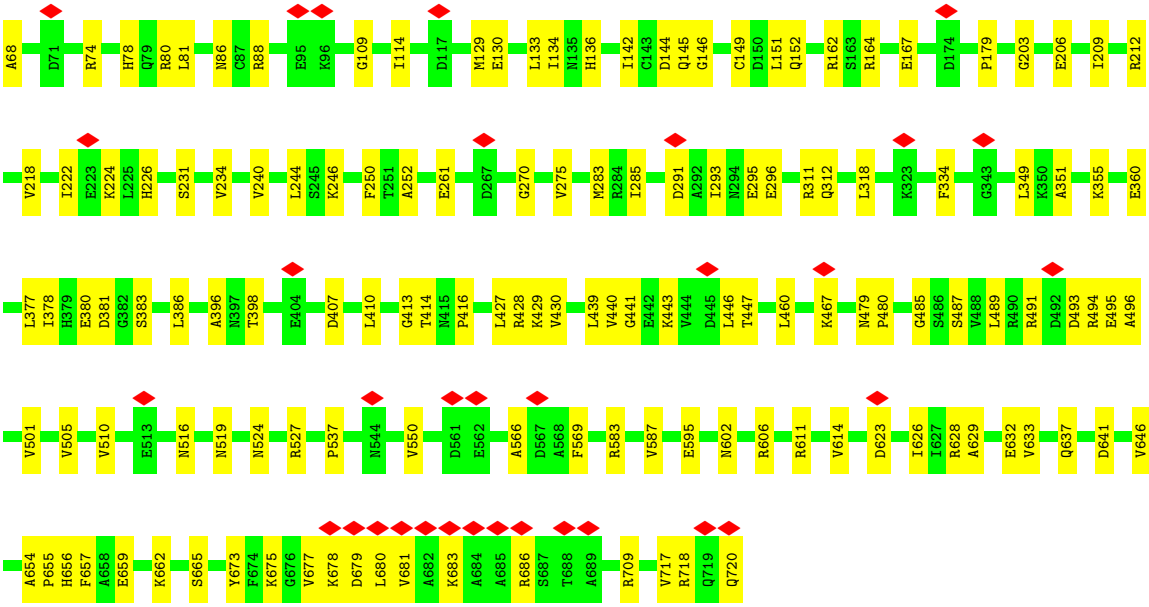


• Molecule 6: 75 kDa

Chain G:



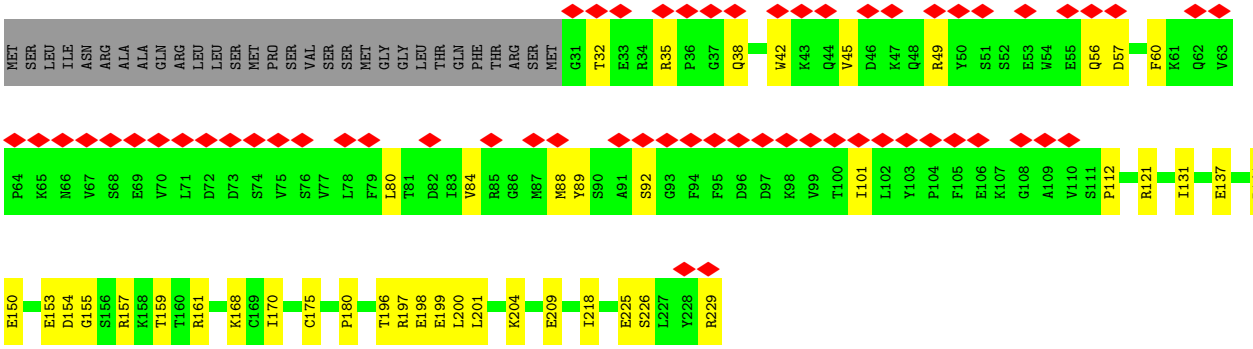




• Molecule 7: TYKY

Chain I:

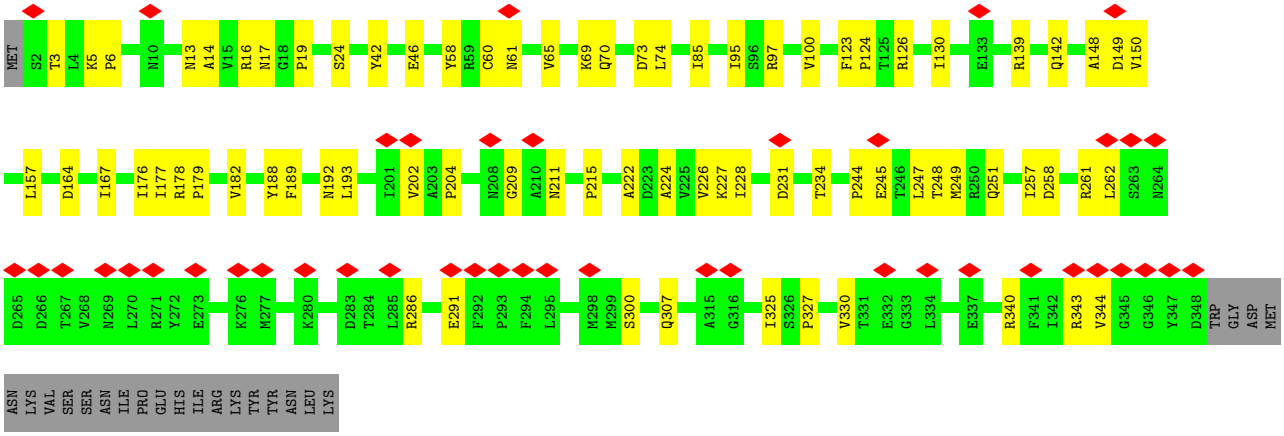




• Molecule 8: 39 kDa

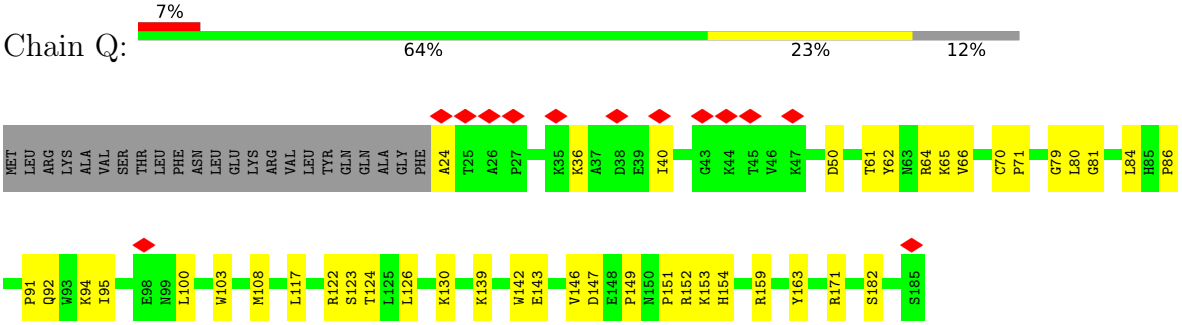
Chain P:





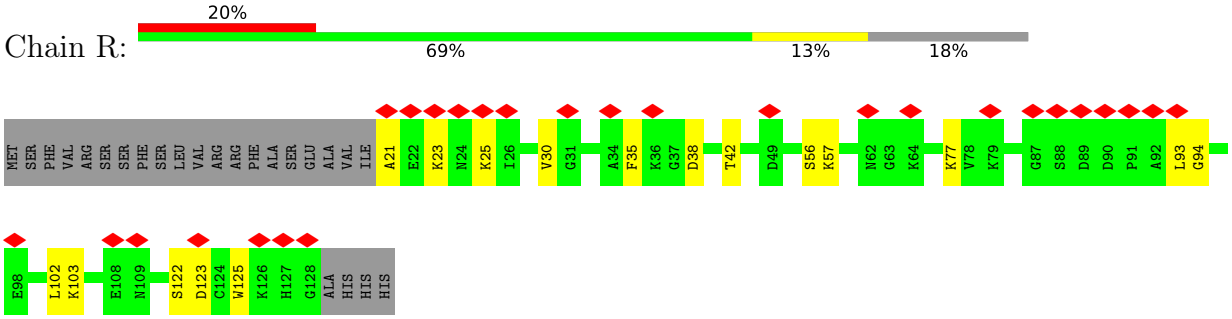
• Molecule 9: 18 kDa

Chain Q:



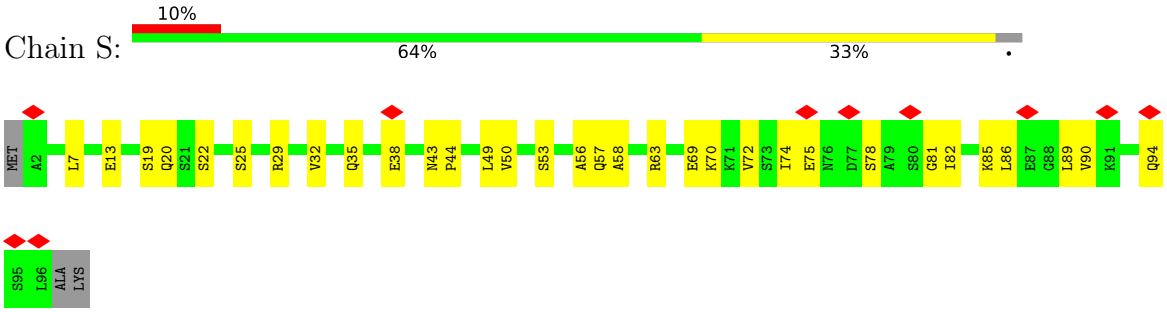
• Molecule 10: 13 kDa

Chain R:



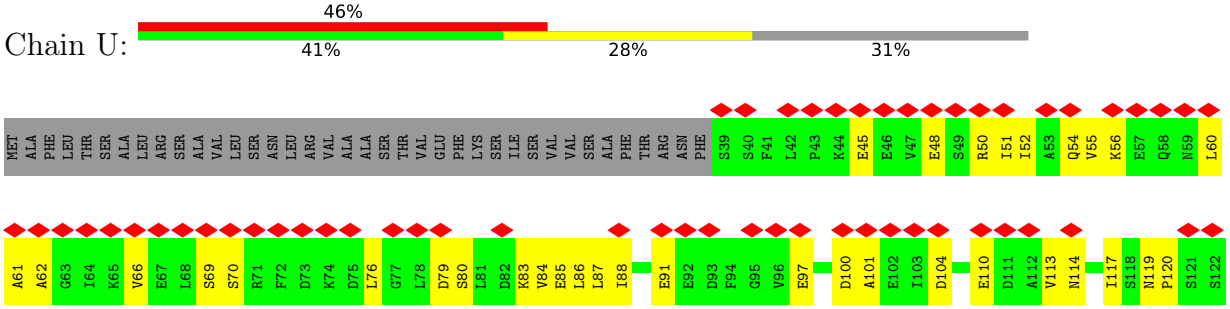
• Molecule 11: B8

Chain S:



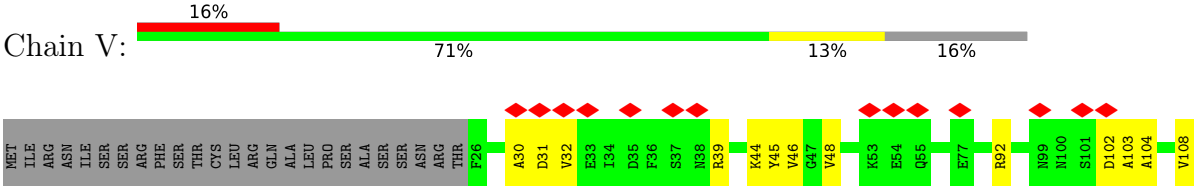
• Molecule 12: SDAP2

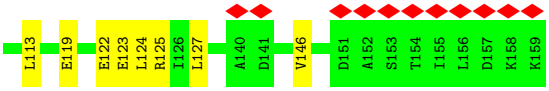
Chain U:



• Molecule 13: B13

Chain V:

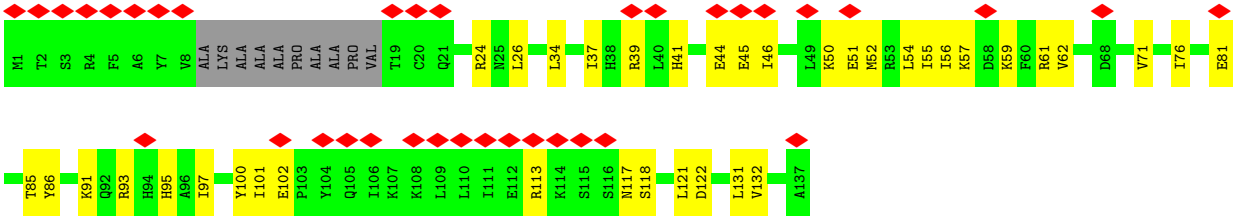




• Molecule 14: B14

Chain W:

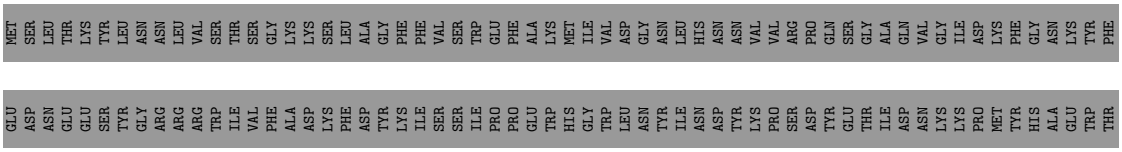


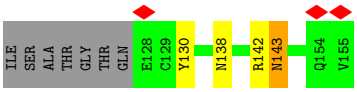


• Molecule 15: B17.2

Chain q:





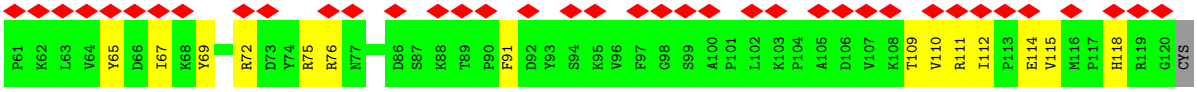


• Molecule 16: B14.5a

Chain r:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42350	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 ($e^-/Å^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, NDP, FMN, SF4, 8Q1, FES

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	B	0.19	0/1240	0.42	0/1685
2	C	0.19	0/1862	0.37	0/2537
3	D	0.20	0/3257	0.42	0/4406
4	E	0.15	0/1843	0.39	0/2497
5	F	0.17	0/3394	0.38	0/4577
6	G	0.16	0/5254	0.34	0/7114
7	I	0.17	0/1634	0.41	0/2204
8	P	0.16	0/2750	0.37	0/3726
9	Q	0.16	0/1311	0.33	0/1774
10	R	0.13	0/832	0.33	0/1125
11	S	0.15	0/725	0.35	0/979
12	U	0.15	0/663	0.40	0/895
13	V	0.13	0/1069	0.31	0/1448
14	W	0.15	0/1097	0.34	0/1472
15	q	0.16	0/254	0.40	0/346
16	r	0.11	0/507	0.30	0/685
All	All	0.17	0/27692	0.37	0/37470

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1206	0	1193	34	0
2	C	1808	0	1750	51	0
3	D	3178	0	3148	105	0
4	E	1806	0	1769	50	0
5	F	3322	0	3278	75	0
6	G	5166	0	5193	109	0
7	I	1602	0	1534	38	0
8	P	2701	0	2719	61	0
9	Q	1276	0	1264	32	0
10	R	812	0	781	16	0
11	S	716	0	730	23	0
12	U	655	0	647	24	0
13	V	1052	0	1059	18	0
14	W	1074	0	1101	27	0
15	q	243	0	233	5	0
16	r	493	0	498	17	0
17	B	8	0	0	1	0
17	F	8	0	0	2	0
17	G	16	0	0	0	0
17	I	16	0	0	1	0
18	E	4	0	0	0	0
18	G	4	0	0	0	0
19	F	31	0	19	2	0
20	P	48	0	26	1	0
21	R	1	0	0	0	0
22	W	35	0	0	1	0
23	B	14	0	0	0	0
23	C	36	0	0	3	0
23	D	44	0	0	2	0
23	E	12	0	0	2	0
23	F	17	0	0	1	0
23	G	113	0	0	2	0
23	I	36	0	0	2	0
23	P	56	0	0	4	0
23	Q	36	0	0	2	0
23	R	9	0	0	1	0
23	S	8	0	0	1	0
23	V	10	0	0	1	0
23	W	12	0	0	0	0
23	q	8	0	0	0	0
23	r	7	0	0	0	0
All	All	27699	0	26942	576	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 576 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ARG:HE	1:B:63:PRO:HD2	1.35	0.92
5:F:271:SER:HA	5:F:279:ALA:HB1	1.58	0.85
3:D:101:TYR:OH	3:D:245:ARG:NH1	2.10	0.83
3:D:201:LYS:HE2	3:D:205:ILE:HD11	1.60	0.81
5:F:120:TYR:HB2	5:F:248:THR:HG22	1.64	0.80

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	152/164 (93%)	146 (96%)	6 (4%)	0	100	100
2	C	214/217 (99%)	211 (99%)	3 (1%)	0	100	100
3	D	393/395 (100%)	386 (98%)	6 (2%)	1 (0%)	36	62
4	E	233/276 (84%)	226 (97%)	7 (3%)	0	100	100
5	F	428/469 (91%)	415 (97%)	13 (3%)	0	100	100
6	G	680/720 (94%)	664 (98%)	16 (2%)	0	100	100
7	I	197/229 (86%)	195 (99%)	2 (1%)	0	100	100
8	P	345/370 (93%)	333 (96%)	12 (4%)	0	100	100
9	Q	160/185 (86%)	154 (96%)	6 (4%)	0	100	100
10	R	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
11	S	93/98 (95%)	92 (99%)	1 (1%)	0	100	100
12	U	82/122 (67%)	71 (87%)	11 (13%)	0	100	100
13	V	132/159 (83%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	W	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
15	q	26/155 (17%)	26 (100%)	0	0	100	100
16	r	58/121 (48%)	58 (100%)	0	0	100	100
All	All	3422/3949 (87%)	3330 (97%)	91 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	242	VAL

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	B	129/134 (96%)	129 (100%)	0	100	100
2	C	199/200 (100%)	199 (100%)	0	100	100
3	D	339/339 (100%)	339 (100%)	0	100	100
4	E	197/232 (85%)	196 (100%)	1 (0%)	81	93
5	F	343/372 (92%)	343 (100%)	0	100	100
6	G	544/570 (95%)	544 (100%)	0	100	100
7	I	175/201 (87%)	175 (100%)	0	100	100
8	P	296/318 (93%)	296 (100%)	0	100	100
9	Q	134/154 (87%)	134 (100%)	0	100	100
10	R	86/107 (80%)	86 (100%)	0	100	100
11	S	77/79 (98%)	77 (100%)	0	100	100
12	U	76/108 (70%)	76 (100%)	0	100	100
13	V	116/139 (84%)	116 (100%)	0	100	100
14	W	119/123 (97%)	119 (100%)	0	100	100
15	q	26/138 (19%)	25 (96%)	1 (4%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	r	55/109 (50%)	55 (100%)	0	100 100
All	All	2911/3323 (88%)	2909 (100%)	2 (0%)	87 97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	49	HIS
15	q	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
12	U	58	GLN
13	V	50	HIS
15	q	143	ASN
6	G	519	ASN
6	G	502	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	SF4	G	803	6	0,12,12	-	-	-		
17	SF4	B	500	1	0,12,12	-	-	-		
17	SF4	F	501	5	0,12,12	-	-	-		
20	NDP	P	500	-	49,52,52	2.15	6 (12%)	66,80,80	1.64	13 (19%)
18	FES	E	500	4	0,4,4	-	-	-		
22	8Q1	W	200	-	31,34,34	1.68	6 (19%)	40,43,43	1.56	5 (12%)
17	SF4	G	802	6	0,12,12	-	-	-		
18	FES	G	801	6	0,4,4	-	-	-		
19	FMN	F	500	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
17	SF4	I	500	7	0,12,12	-	-	-		
17	SF4	I	501	7	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SF4	G	803	6	-	-	0/6/5/5
17	SF4	B	500	1	-	-	0/6/5/5
17	SF4	F	501	5	-	-	0/6/5/5
20	NDP	P	500	-	-	10/34/77/77	0/5/5/5
18	FES	E	500	4	-	-	0/1/1/1
22	8Q1	W	200	-	-	11/41/41/41	-
17	SF4	G	802	6	-	-	0/6/5/5
18	FES	G	801	6	-	-	0/1/1/1
19	FMN	F	500	-	-	9/18/18/18	0/3/3/3
17	SF4	I	500	7	-	-	0/6/5/5
17	SF4	I	501	7	-	-	0/6/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	500	NDP	P2B-O2B	12.13	1.82	1.59
22	W	200	8Q1	C34-N36	5.48	1.45	1.33
22	W	200	8Q1	C39-N41	5.26	1.45	1.33
20	P	500	NDP	PN-O5D	3.89	1.75	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	F	500	FMN	C4A-N5	3.74	1.38	1.30

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	P	500	NDP	PN-O3-PA	-7.01	108.77	132.83
22	W	200	8Q1	C6-C1-S44	5.77	120.17	113.46
22	W	200	8Q1	O4-C1-C6	-3.35	120.04	123.99
20	P	500	NDP	O2B-P2B-O1X	-3.30	96.65	109.39
19	F	500	FMN	C4-N3-C2	-3.22	119.69	125.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	F	500	FMN	N10-C1'-C2'-O2'
19	F	500	FMN	N10-C1'-C2'-C3'
19	F	500	FMN	C1'-C2'-C3'-O3'
19	F	500	FMN	C1'-C2'-C3'-C4'
19	F	500	FMN	C5'-O5'-P-O2P

There are no ring outliers.

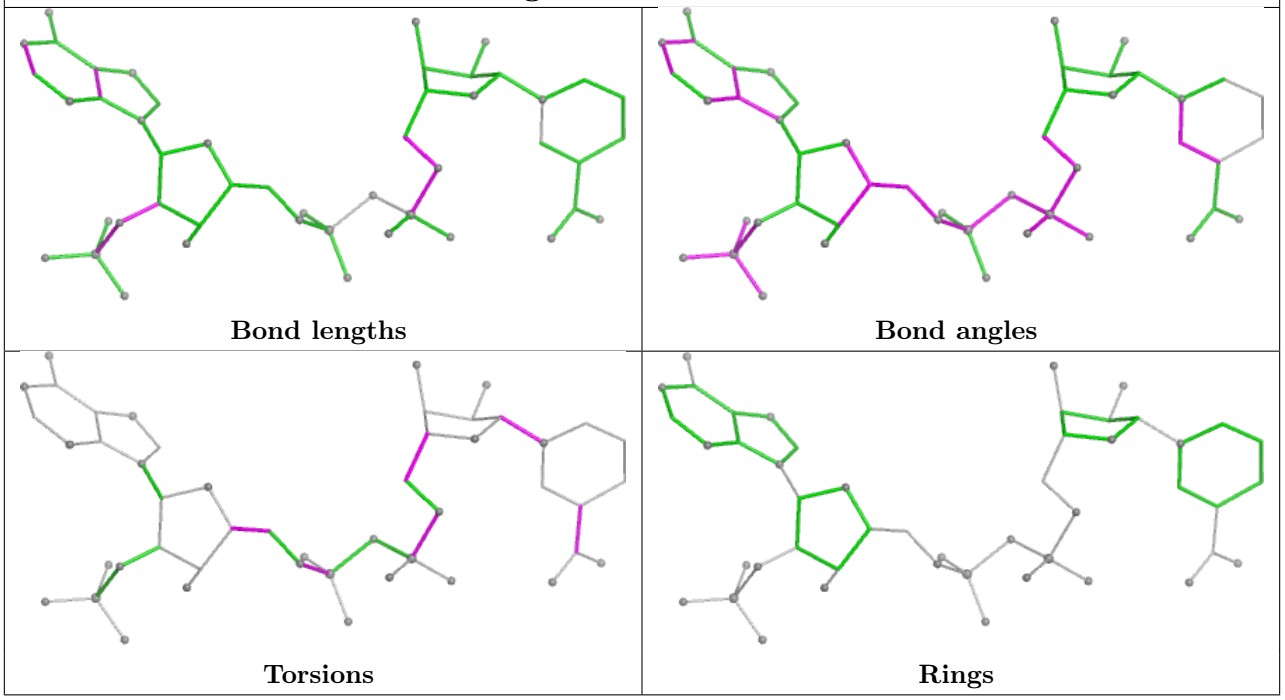
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	500	SF4	1	0
17	F	501	SF4	2	0
20	P	500	NDP	1	0
22	W	200	8Q1	1	0
19	F	500	FMN	2	0
17	I	500	SF4	1	0

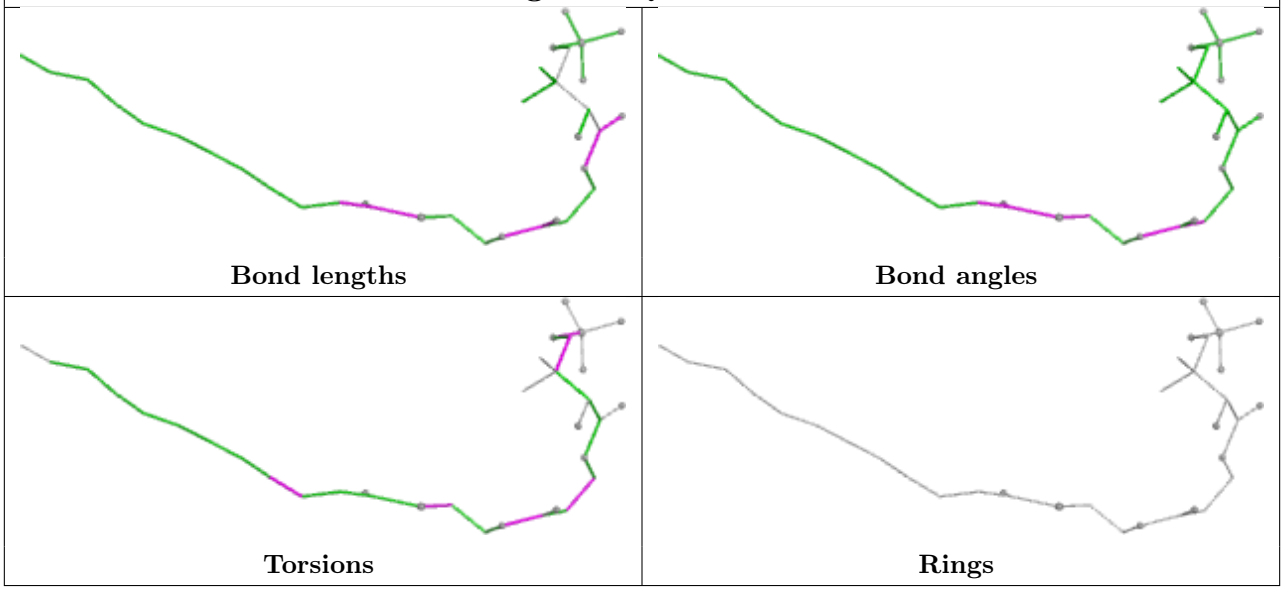
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

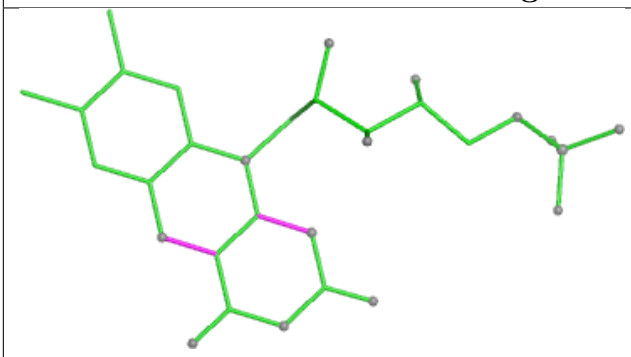
Ligand NDP P 500



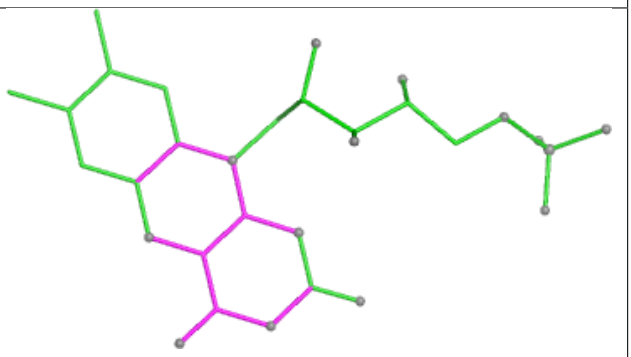
Ligand 8Q1 W 200



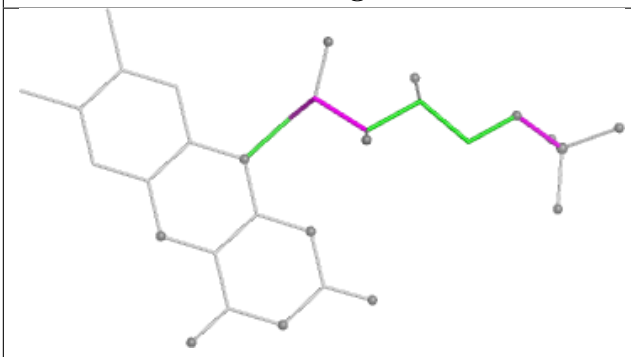
Ligand FMN F 500



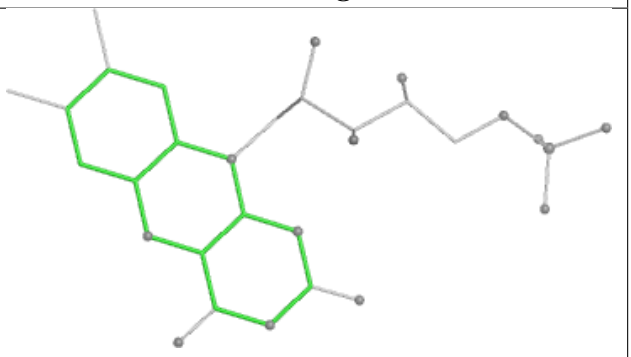
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

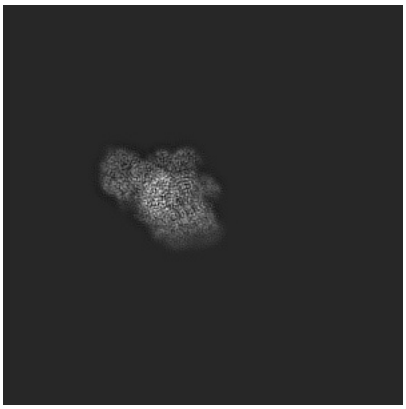
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11879. These allow visual inspection of the internal detail of the map and identification of artifacts.

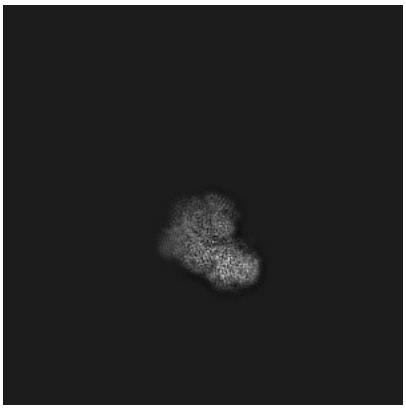
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

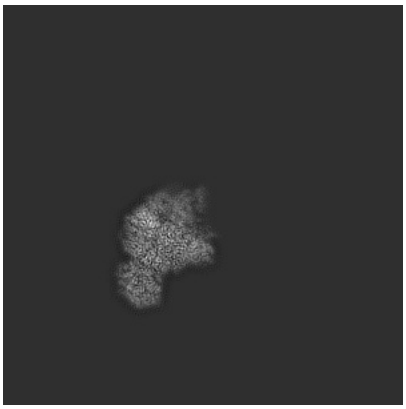
6.1.1 Primary map



X

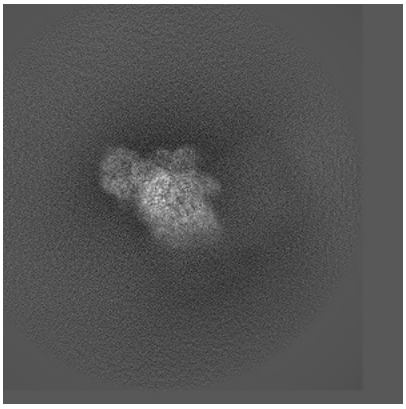


Y

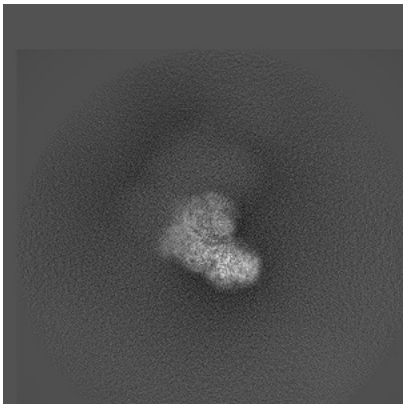


Z

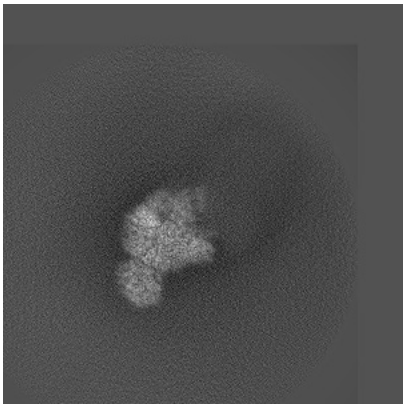
6.1.2 Raw map



X



Y



Z

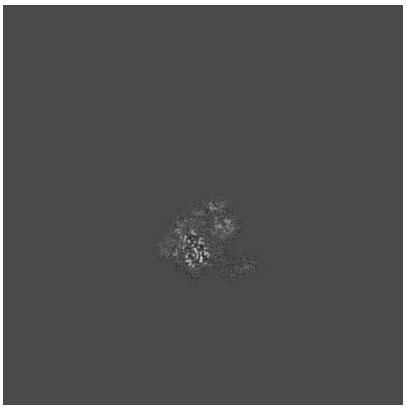
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

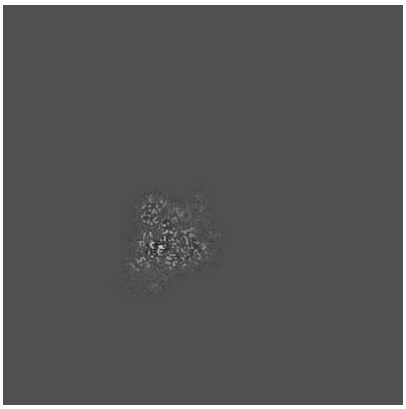
6.2.1 Primary map



X Index: 300

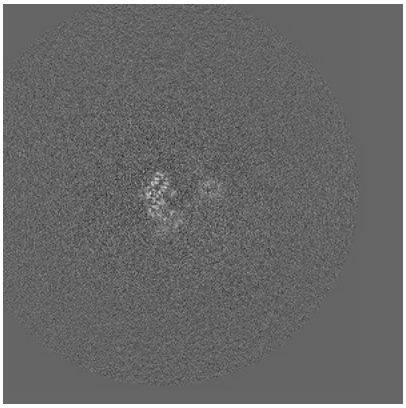


Y Index: 300

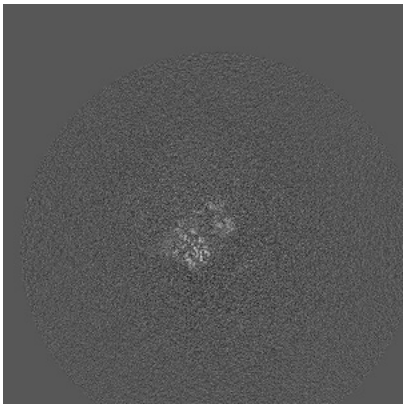


Z Index: 300

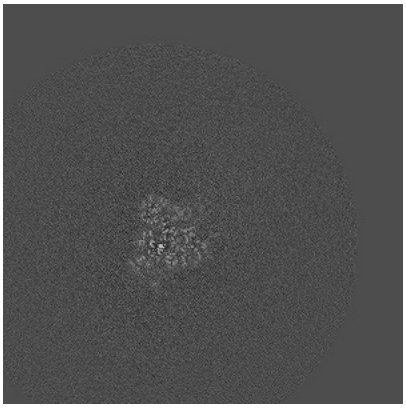
6.2.2 Raw map



X Index: 300



Y Index: 300

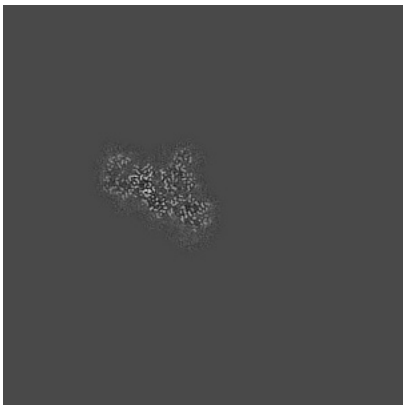


Z Index: 300

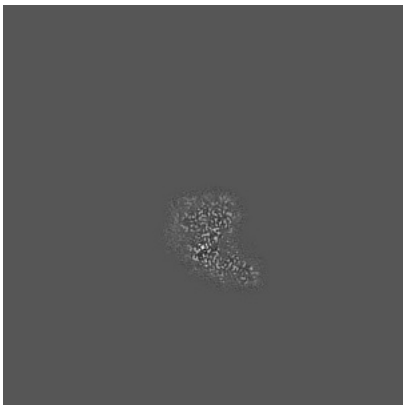
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

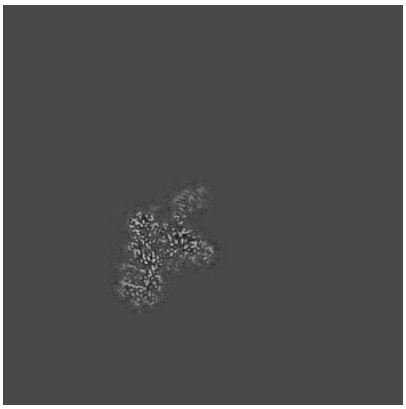
6.3.1 Primary map



X Index: 220

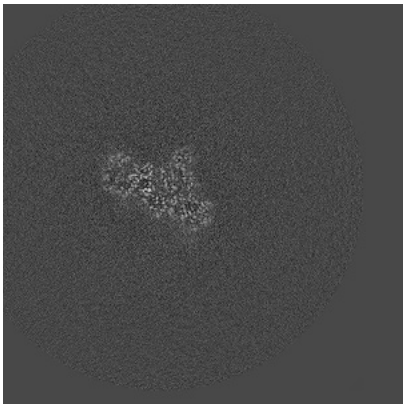


Y Index: 236

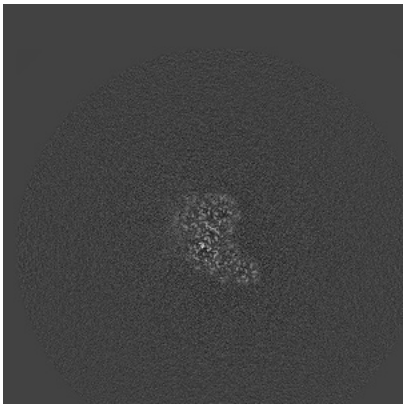


Z Index: 326

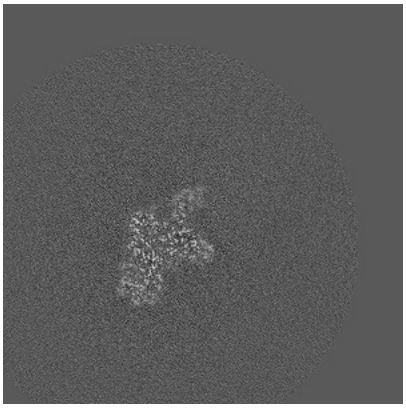
6.3.2 Raw map



X Index: 220



Y Index: 235

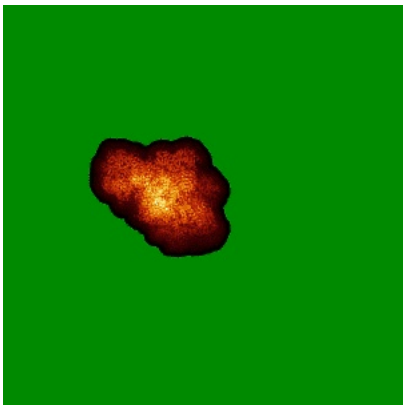


Z Index: 326

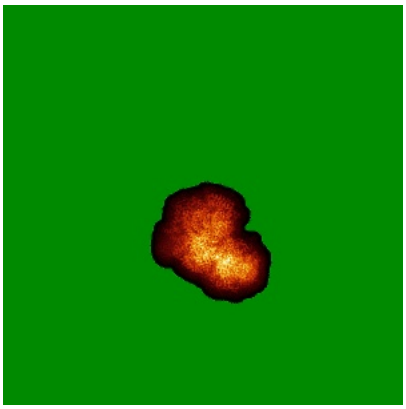
The images above show the largest variance slices of the map in three orthogonal directions.

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

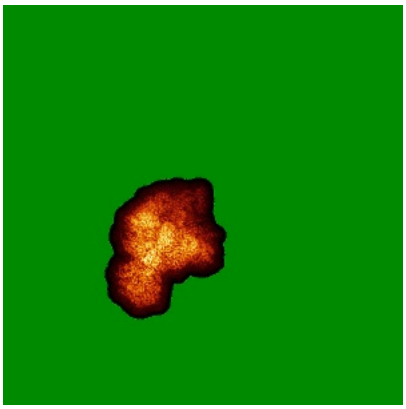
6.4.1 Primary map



X

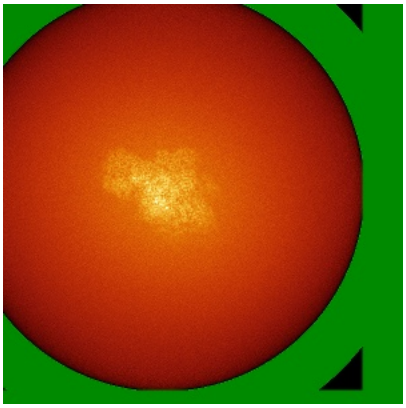


Y

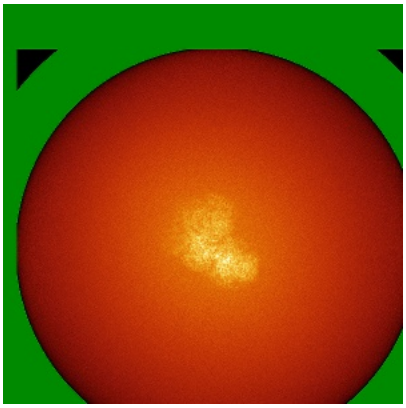


Z

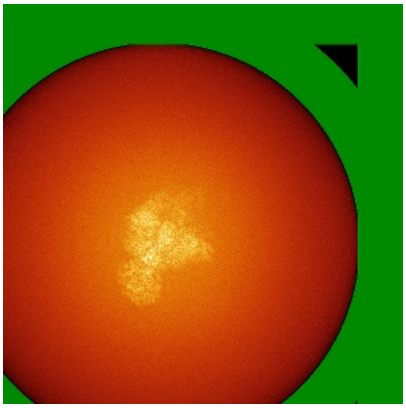
6.4.2 Raw map



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)

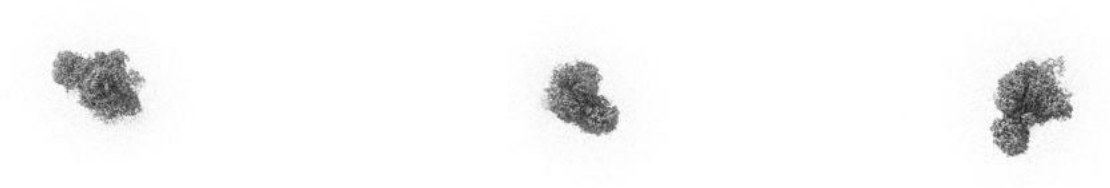
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

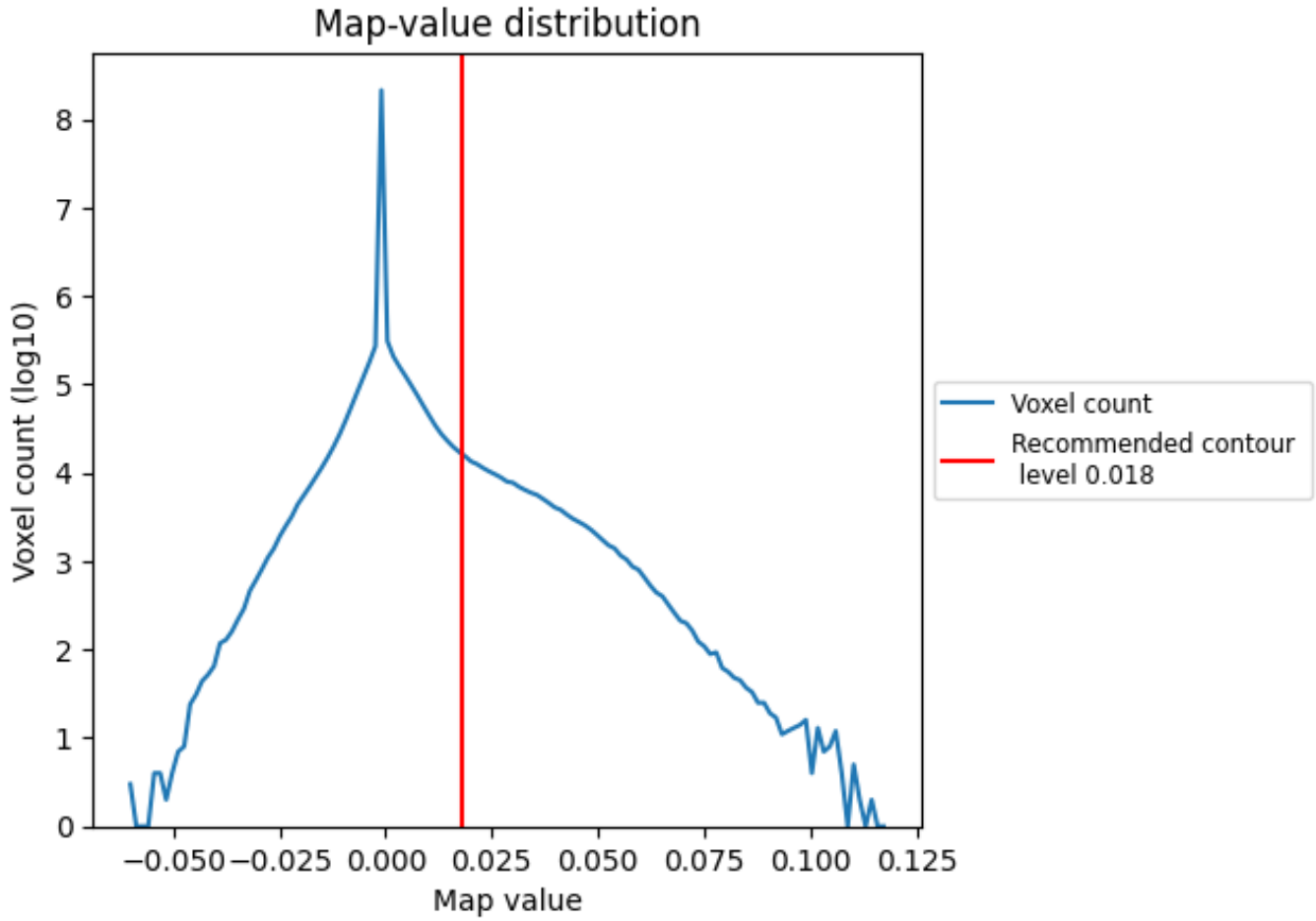
6.6 Mask visualisation (i)

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

7 Map analysis

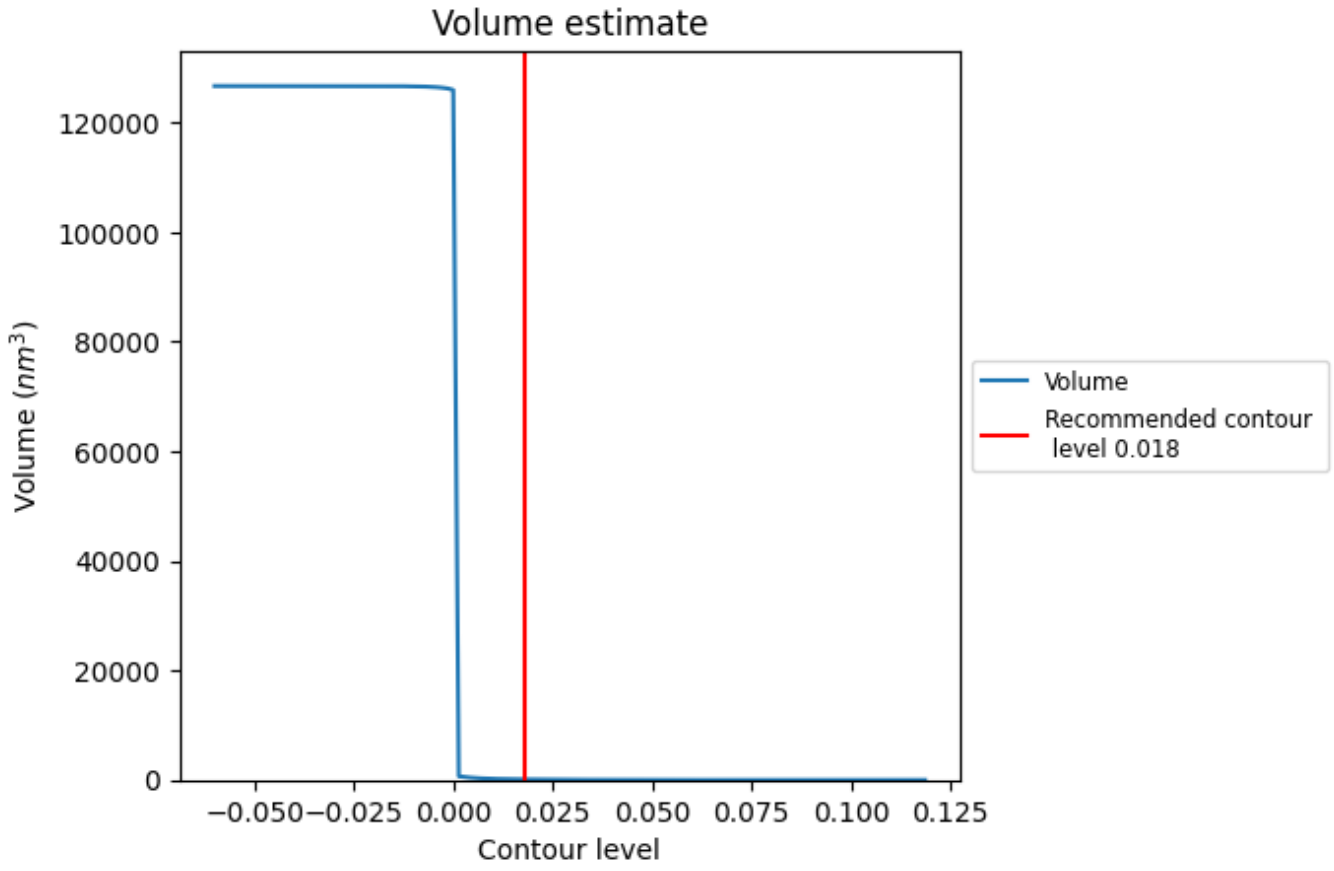
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

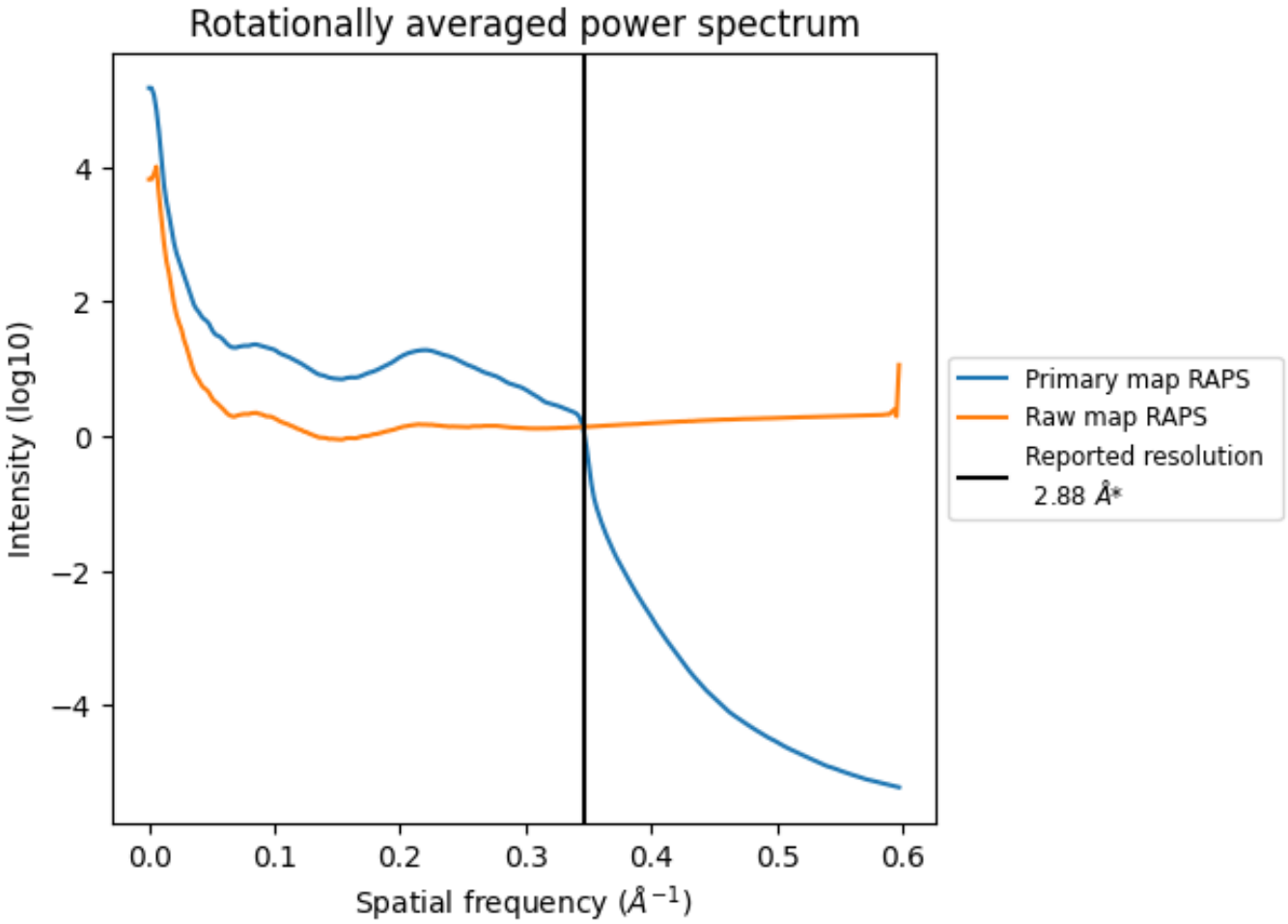
7.2 Volume estimate (i)



The volume at the recommended contour level is 104 nm^3; this corresponds to an approximate mass of 94 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)

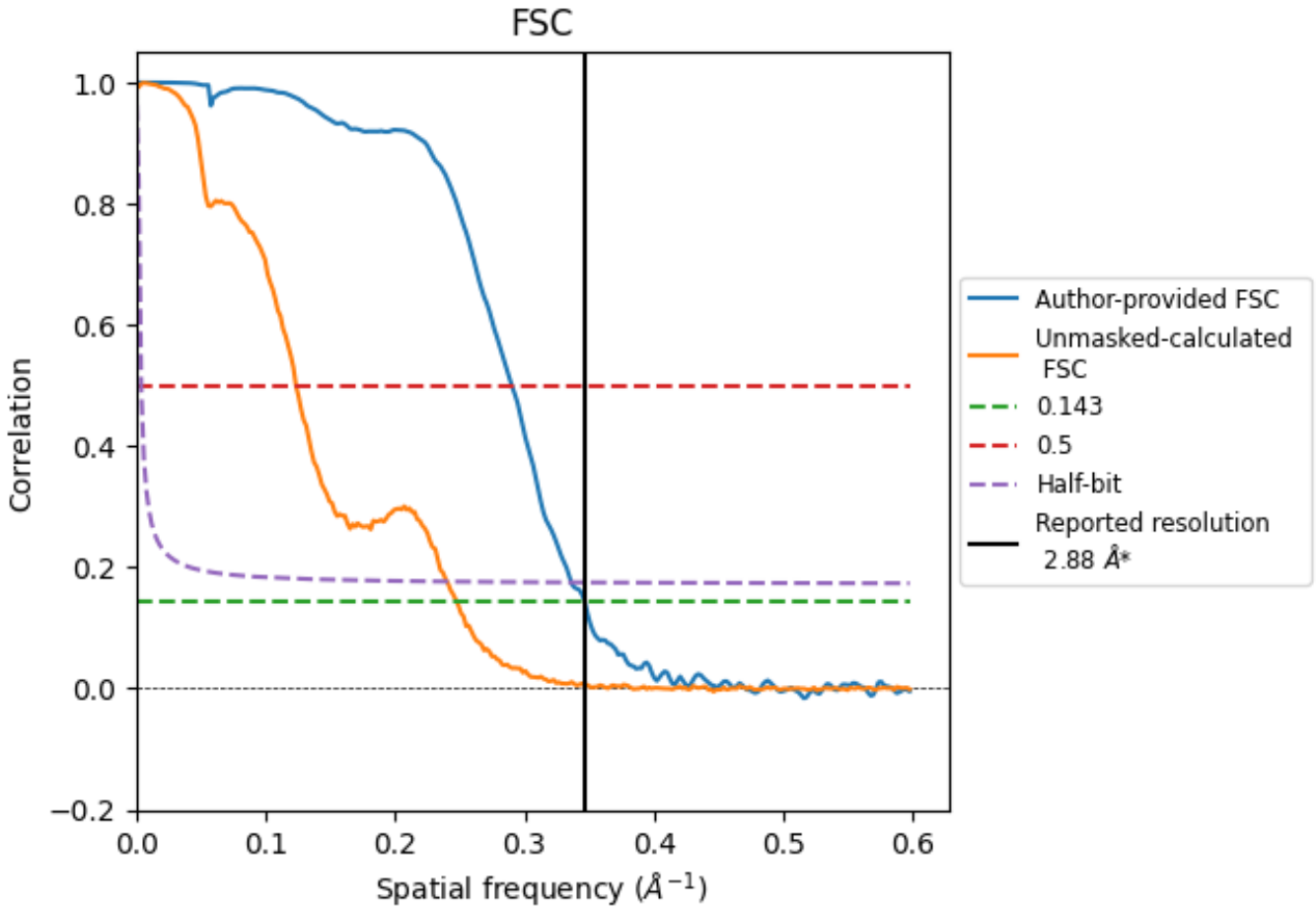


*Reported resolution corresponds to spatial frequency of 0.347 Å^{-1}

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 0.347 Å^{-1}

8.2 Resolution estimates (i)

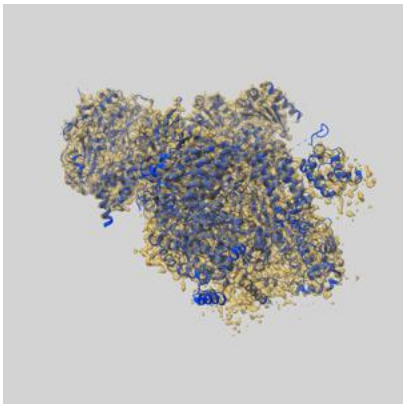
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.89	3.45	2.98
Unmasked-calculated*	4.04	8.10	4.16

*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 4.04 differs from the reported value 2.88 by more than 10 %

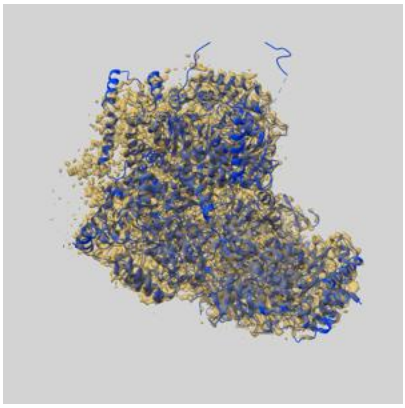
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11879 and PDB model 7ARC. Per-residue inclusion information can be found in section 3 on page 11.

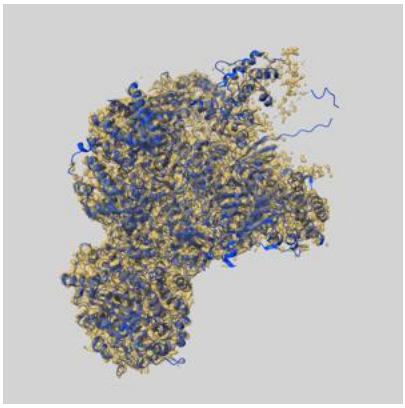
9.1 Map-model overlay



X



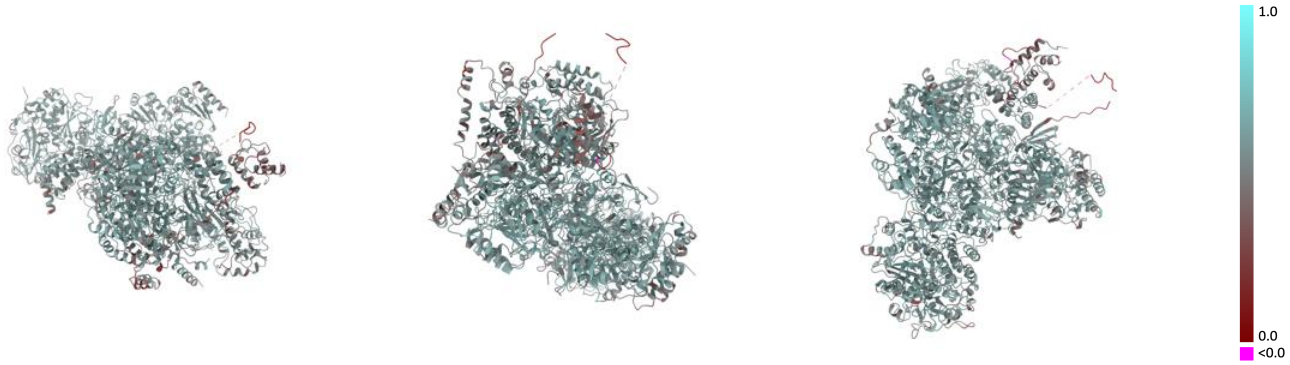
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

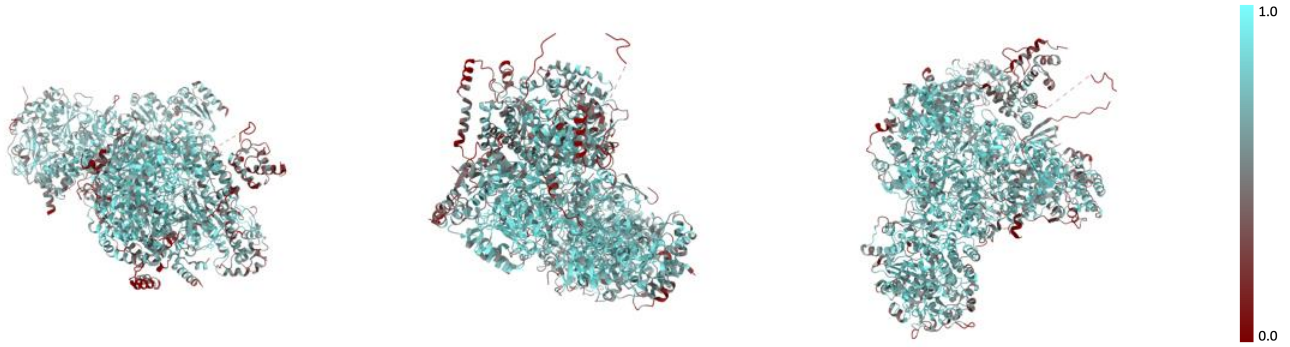
9.2 Q-score mapped to coordinate model (i)



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.

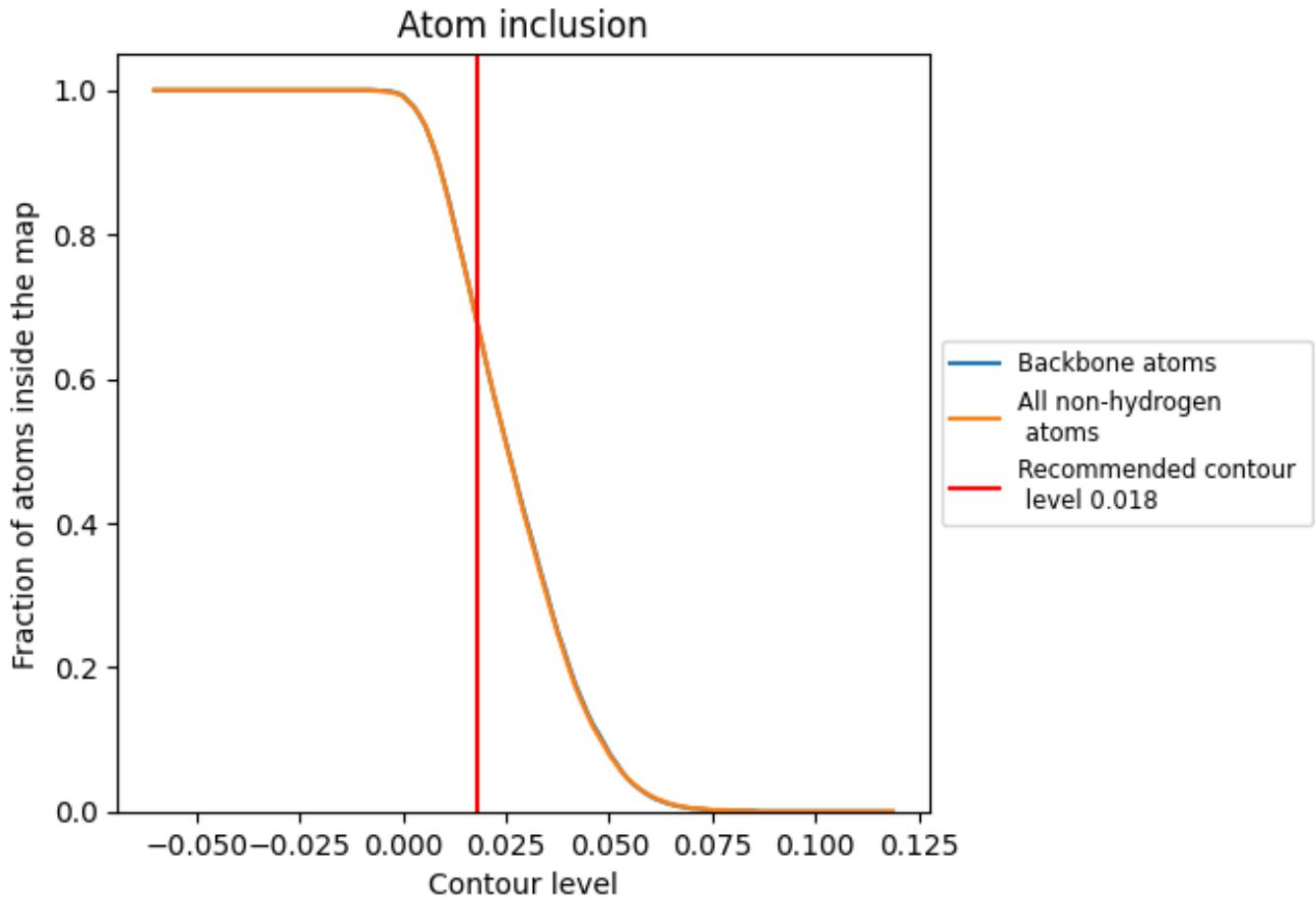
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 68% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6780	0.5630
B	0.6900	0.5560
C	0.8000	0.6040
D	0.7530	0.5750
E	0.6500	0.5490
F	0.7060	0.5660
G	0.7680	0.5940
I	0.6070	0.5440
P	0.6770	0.5580
Q	0.7170	0.5900
R	0.5940	0.5410
S	0.6610	0.5540
U	0.3070	0.3960
V	0.5870	0.5320
W	0.5620	0.5080
q	0.7340	0.5870
r	0.3170	0.5150

