



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 11:26 PM UTC

PDB ID : 7EKQ / pdb_00007ekq
EMDB ID : EMD-31173
Title : CrClpP-S2c
Authors : Wang, N.; Wang, Y.F.; Cong, Y.; Liu, C.M.
Deposited on : 2021-04-06
Resolution : 3.60 Å(reported)

This is a Full wwPDB EM Validation 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:

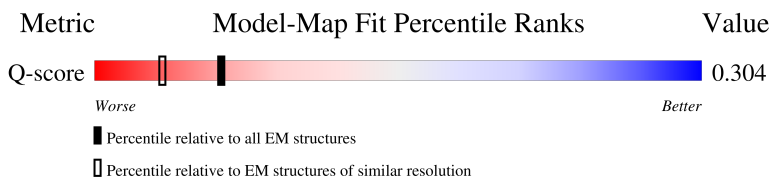
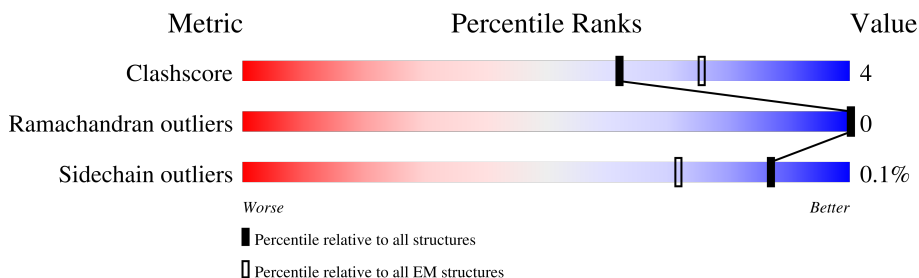
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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

Mol	Chain	Length	Quality of chain
1	A	238	14% 82% 13% 5%
2	B	238	15% 70% 11% 19%
2	D	238	13% 74% 7% 19%
2	F	238	13% 62% 10% 28%

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Mol	Chain	Length	Quality of chain
3	C	296	
3	E	296	
3	G	296	
4	H	208	
4	J	208	
4	M	208	
5	I	246	
6	K	251	
7	L	250	
8	N	383	
9	O	180	
10	P	103	
11	Q	212	
12	R	194	
12	S	194	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 27663 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 ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	227	Total	C	N	O	S	0	0
			1763	1115	293	341	14		

- Molecule 2 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	193	Total	C	N	O	S	0	0
			1477	925	258	283	11		
2	D	193	Total	C	N	O	S	0	0
			1477	925	258	283	11		
2	F	172	Total	C	N	O	S	0	0
			1307	817	227	253	10		

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	174	Total	C	N	O	S	0	0
			1329	836	229	252	12		
3	E	174	Total	C	N	O	S	0	0
			1329	836	229	252	12		
3	G	179	Total	C	N	O	S	0	0
			1369	862	235	260	12		

- Molecule 4 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	148	Total	C	N	O	S	0	0
			1131	713	192	219	7		
4	J	165	Total	C	N	O	S	0	0
			1279	805	220	247	7		
4	M	133	Total	C	N	O	S	0	0
			1014	644	172	193	5		

- Molecule 5 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	217	Total	C	N	O	S	0	0
			1745	1123	300	315	7		

- Molecule 6 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	233	Total	C	N	O	S	0	0
			1841	1179	308	342	12		

- Molecule 7 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	187	Total	C	N	O	S	0	0
			1494	950	256	275	13		

- Molecule 8 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	338	Total	C	N	O	S	0	0
			2691	1699	474	504	14		

- Molecule 9 is a protein called ATP-dependent Clp protease ATP-binding subunit CLPT4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	162	Total	C	N	O	S	0	0
			1259	807	207	239	6		

- Molecule 10 is a protein called Chaperonin 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	95	Total	C	N	O	S	0	0
			713	455	118	136	4		

- Molecule 11 is a protein called Chaperonin 23.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	205	Total	C	N	O	S	0	0
			1567	993	267	302	5		

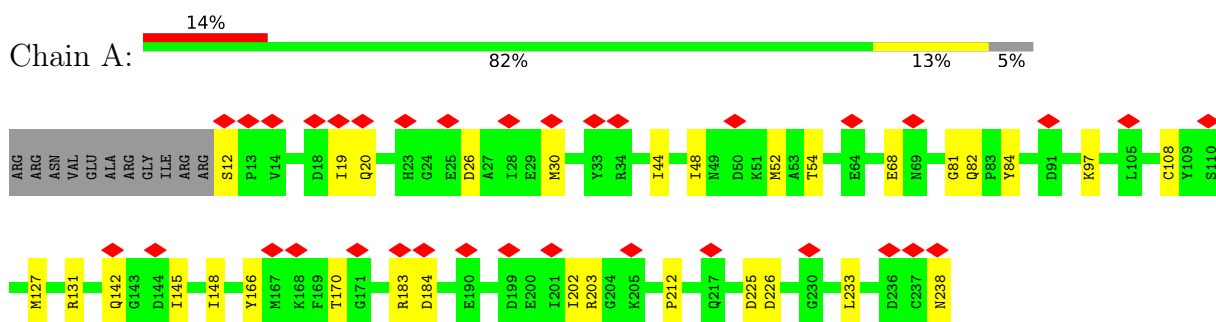
- Molecule 12 is a protein called Cpn20 co-chaperonin subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	194	Total	C	N	O	S	0	0
			1439	909	238	291	1		
12	S	194	Total	C	N	O	S	0	0
			1439	909	238	291	1		

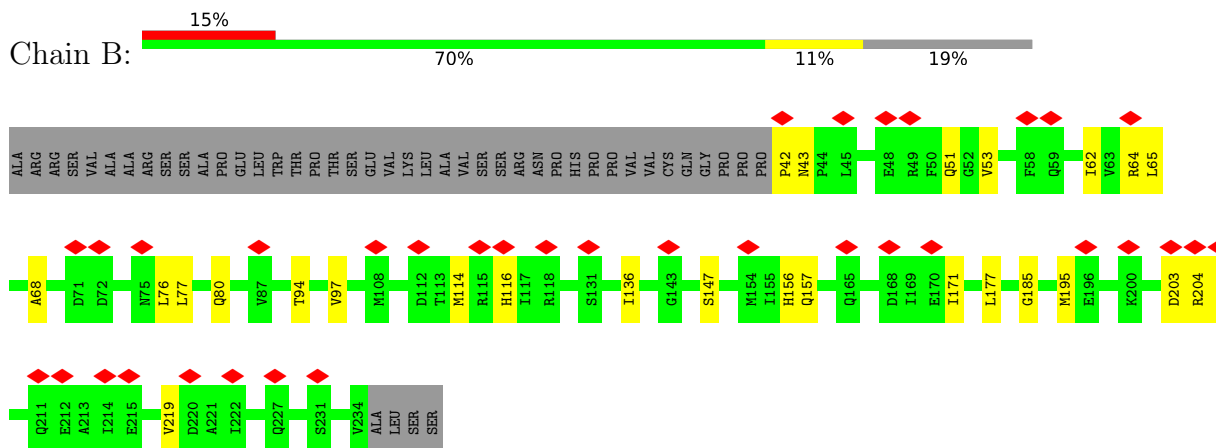
3 Residue-property plots

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

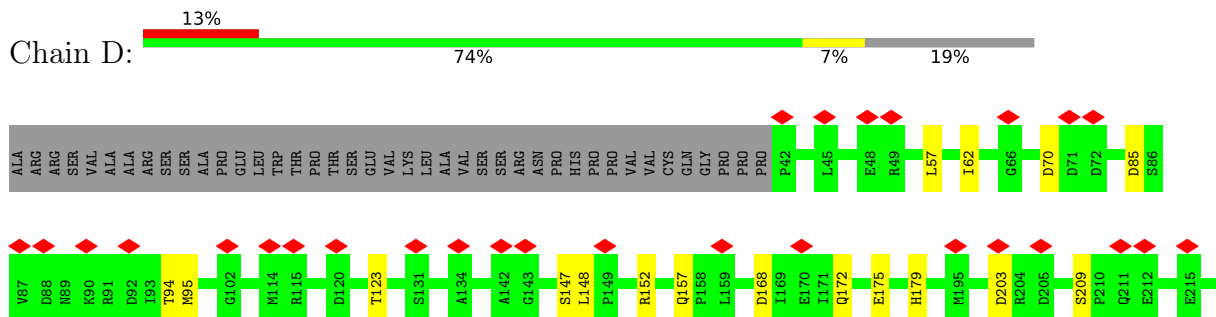
- Molecule 1: ATP-dependent Clp protease proteolytic subunit



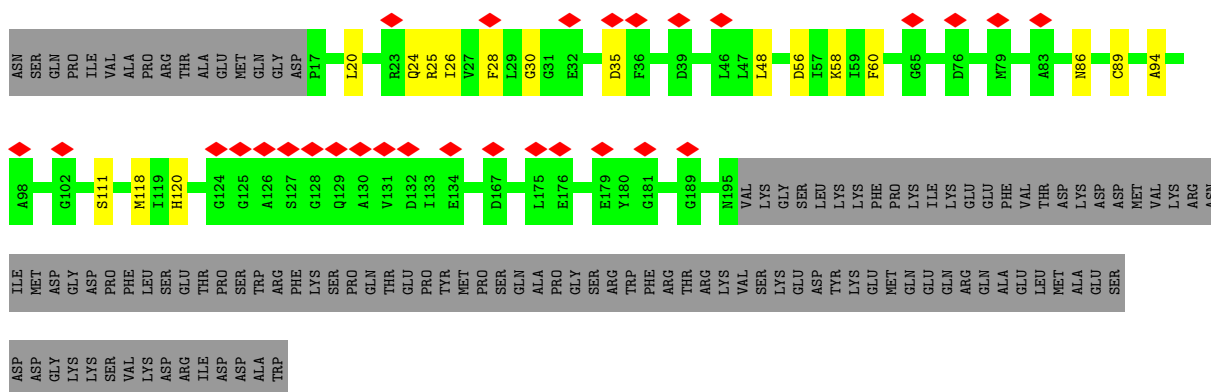
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



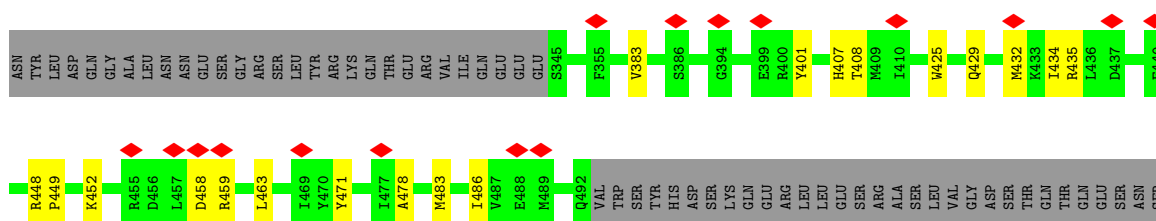
- Molecule 2: ATP-dependent Clp protease proteolytic subunit



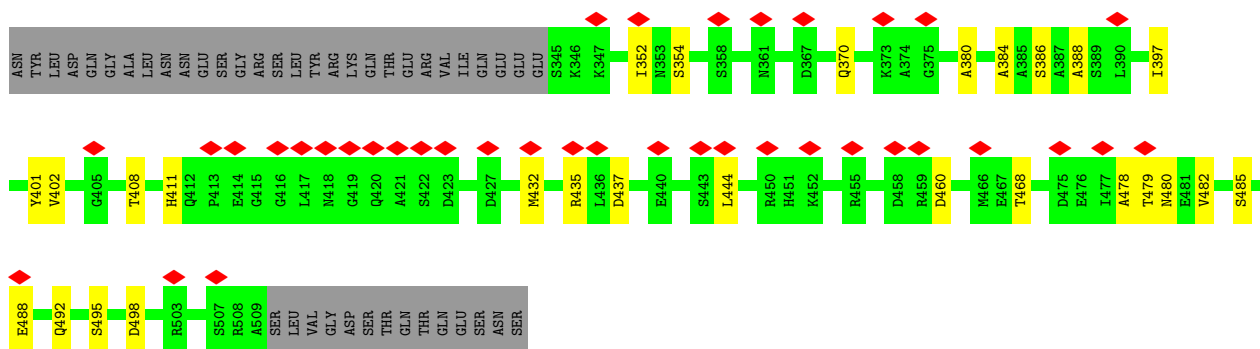
Chain G:



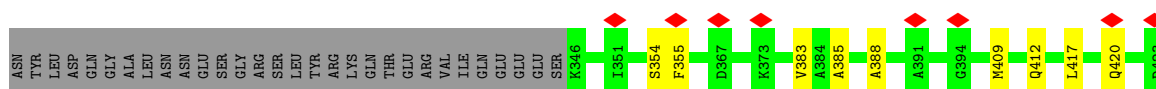
Chain H:

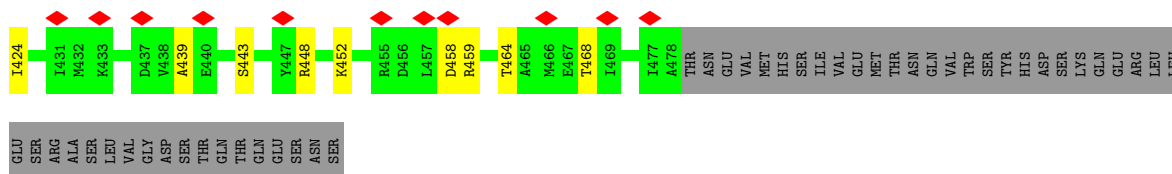


Chain J:

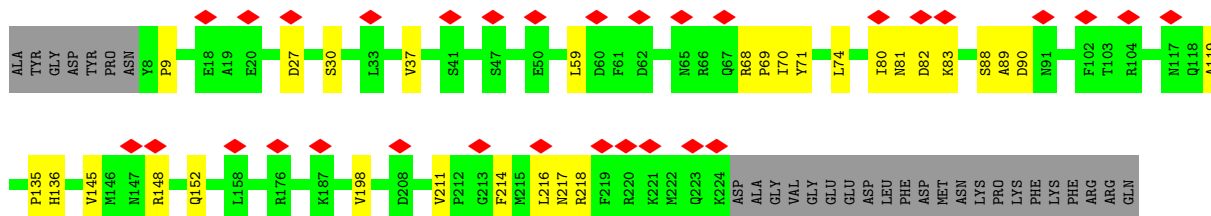
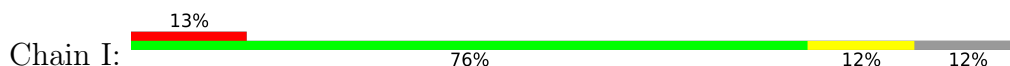


Chain M:

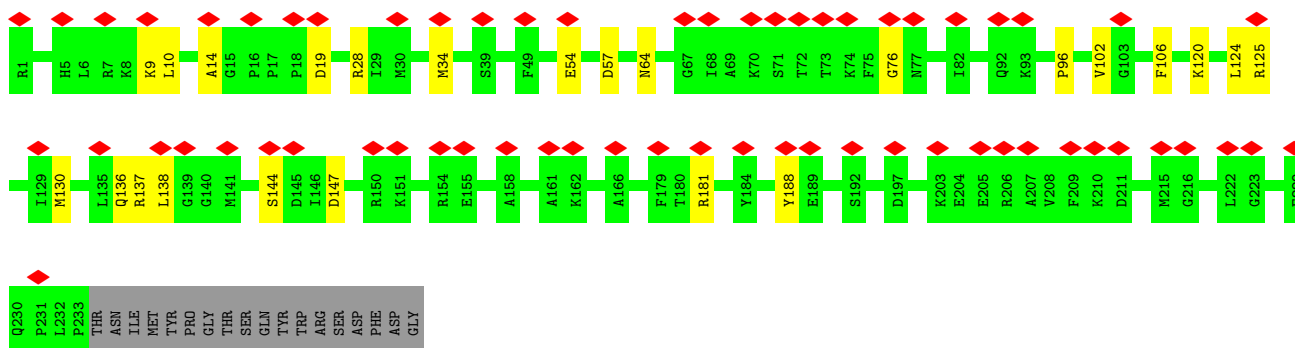
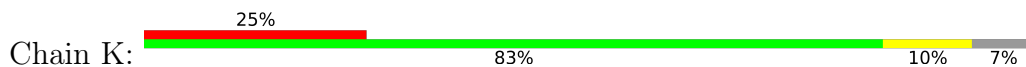




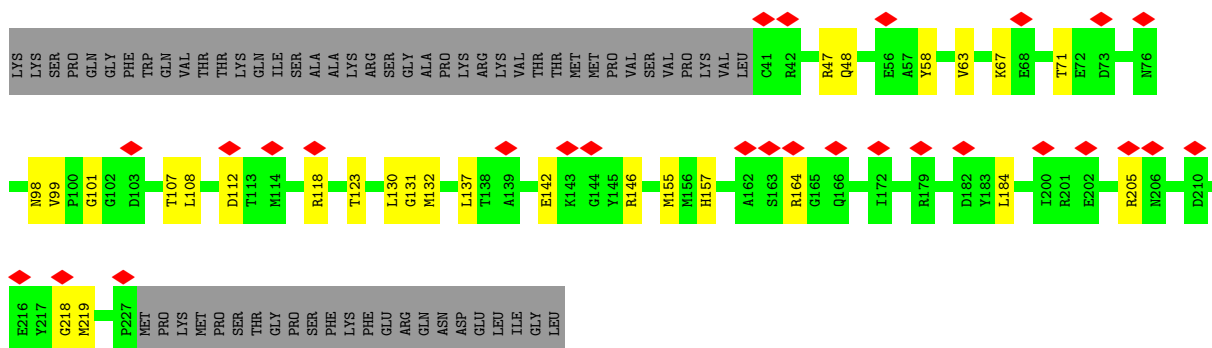
• Molecule 5: ATP-dependent Clp protease proteolytic subunit



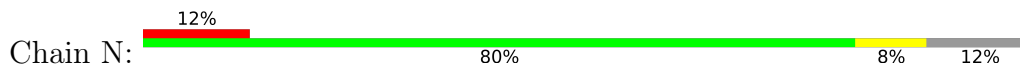
• Molecule 6: ATP-dependent Clp protease proteolytic subunit

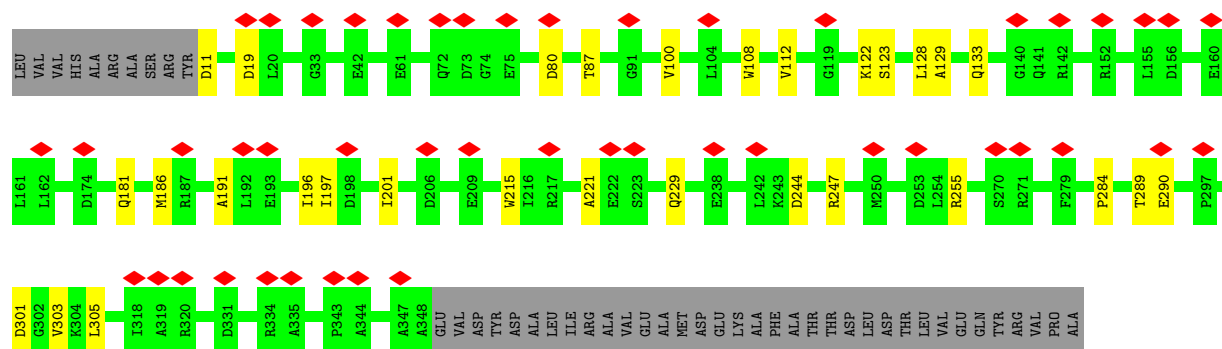


• Molecule 7: ATP-dependent Clp protease proteolytic subunit

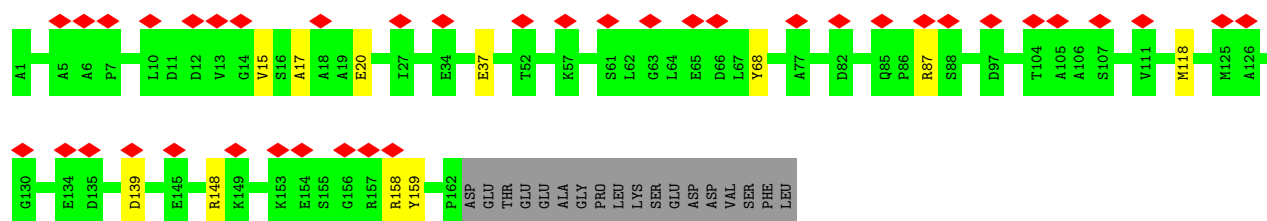
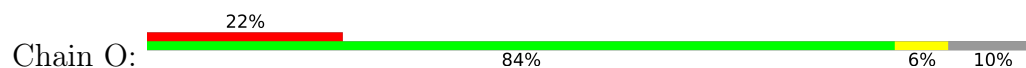


• Molecule 8: ATP-dependent Clp protease proteolytic subunit

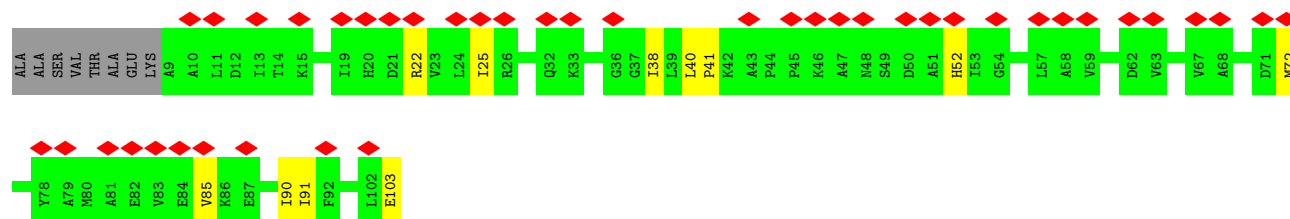
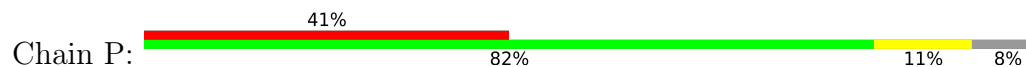




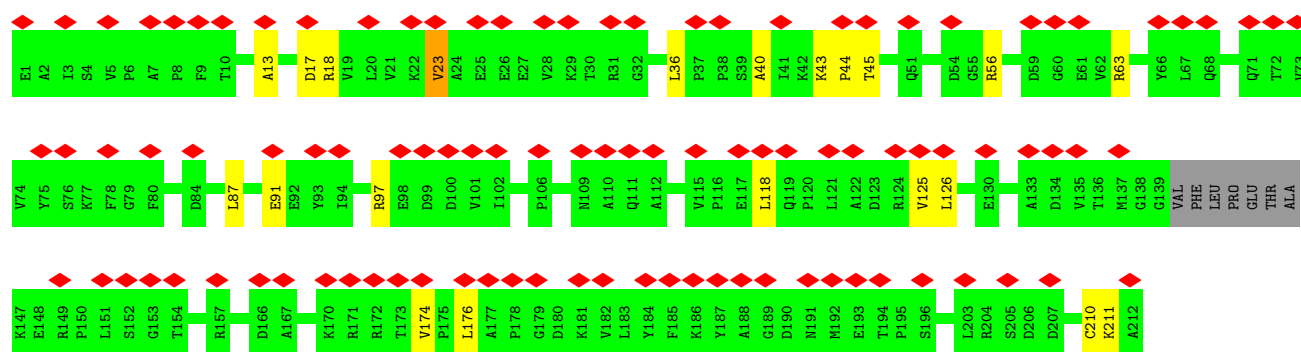
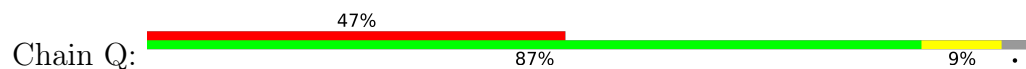
- Molecule 9: ATP-dependent Clp protease ATP-binding subunit CLPT4, chloroplastic



- Molecule 10: Chaperonin 11

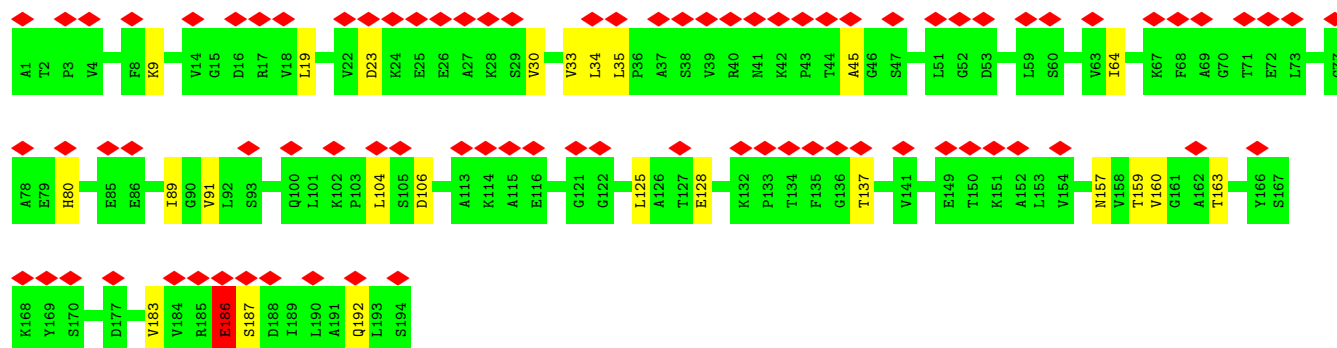


- Molecule 11: Chaperonin 23



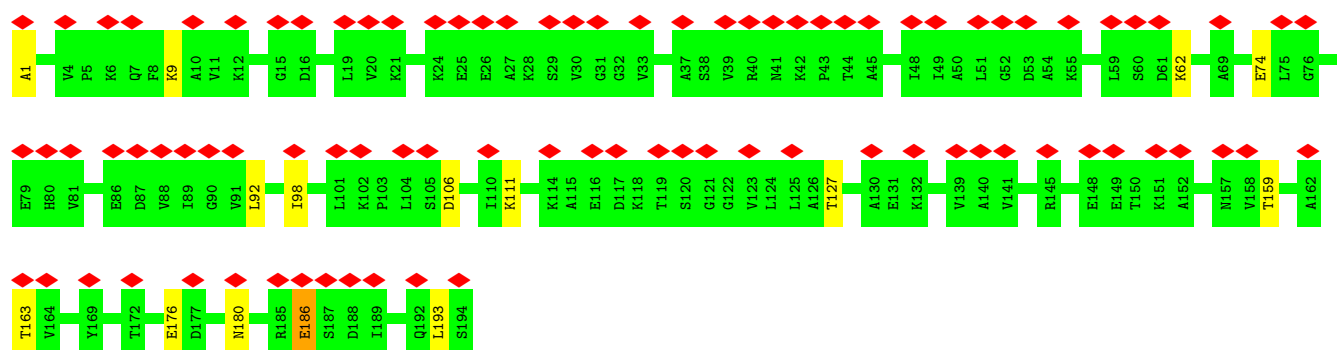
- Molecule 12: Cpn20 co-chaperonin subunit

Chain R:  43% 87% 12%



• Molecule 12: Cpn20 co-chaperonin subunit

Chain S:  45% 92% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	49759	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.736	Depositor
Minimum map value	-0.540	Depositor
Average map value	0.021	Depositor
Map value standard deviation	0.138	Depositor
Recommended contour level	0.852	Depositor
Map size (Å)	284.688, 284.688, 284.688	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/1794	0.38	0/2427
2	B	0.13	0/1500	0.37	0/2028
2	D	0.14	0/1500	0.39	0/2028
2	F	0.13	0/1326	0.38	0/1792
3	C	0.14	0/1350	0.37	0/1814
3	E	0.13	0/1350	0.36	0/1814
3	G	0.13	0/1391	0.38	0/1870
4	H	0.12	0/1149	0.32	0/1553
4	J	0.13	0/1301	0.33	0/1758
4	M	0.13	0/1031	0.33	0/1393
5	I	0.15	0/1790	0.39	0/2428
6	K	0.15	0/1881	0.40	0/2542
7	L	0.14	0/1529	0.37	0/2072
8	N	0.13	0/2746	0.35	0/3718
9	O	0.14	0/1285	0.33	0/1743
10	P	0.17	0/722	0.48	0/973
11	Q	0.20	0/1594	0.45	0/2154
12	R	0.23	0/1455	0.65	4/1963 (0.2%)
12	S	0.21	0/1455	0.60	2/1963 (0.1%)
All	All	0.15	0/28149	0.41	6/38033 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	R	0	1
12	S	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	186	GLU	CA-C-N	9.67	139.10	121.70
12	R	186	GLU	C-N-CA	9.67	139.10	121.70
12	S	186	GLU	CA-C-N	8.54	137.08	121.70
12	S	186	GLU	C-N-CA	8.54	137.08	121.70
12	R	33	VAL	CA-C-N	5.17	131.41	121.54
12	R	33	VAL	C-N-CA	5.17	131.41	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	R	186	GLU	Peptide
12	S	186	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1754	24	0
2	B	1477	0	1477	21	0
2	D	1477	0	1477	12	0
2	F	1307	0	1301	17	0
3	C	1329	0	1330	14	0
3	E	1329	0	1330	14	0
3	G	1369	0	1365	10	0
4	H	1131	0	1123	14	0
4	J	1279	0	1263	17	0
4	M	1014	0	1013	11	0
5	I	1745	0	1731	20	0
6	K	1841	0	1867	18	0
7	L	1494	0	1481	16	0
8	N	2691	0	2709	21	0
9	O	1259	0	1246	7	0
10	P	713	0	748	7	0
11	Q	1567	0	1599	14	0
12	R	1439	0	1498	15	0
12	S	1439	0	1498	8	0
All	All	27663	0	27810	237	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 4.

All (237) 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)
3:G:118:MET:HE2	3:G:120:HIS:HB2	1.79	0.64
1:A:184:ASP:HB3	2:B:171:ILE:HG21	1.78	0.63
11:Q:13:ALA:HB3	12:R:192:GLN:H	1.64	0.62
2:F:125:CYS:HB2	2:F:137:LEU:HD21	1.82	0.62
10:P:22:ARG:HE	11:Q:210:CYS:HB2	1.65	0.60
2:F:86:SER:HB3	12:R:128:GLU:HB3	1.85	0.59
2:B:62:ILE:HG12	2:B:94:THR:HB	1.85	0.59
11:Q:18:ARG:HD2	11:Q:97:ARG:HA	1.84	0.59
3:E:34:GLU:HG3	3:E:37:GLY:H	1.69	0.58
7:L:58:TYR:HB3	7:L:63:VAL:HB	1.84	0.58
1:A:203:ARG:O	2:B:116:HIS:ND1	2.37	0.57
3:E:33:VAL:HB	3:E:66:GLY:HA3	1.87	0.57
3:G:94:ALA:HA	3:G:118:MET:HB3	1.87	0.57
3:C:34:GLU:HG3	3:C:37:GLY:H	1.69	0.56
4:H:448:ARG:HH21	4:H:471:TYR:HA	1.69	0.56
8:N:303:VAL:HG12	8:N:305:LEU:H	1.70	0.56
4:J:488:GLU:O	4:J:492:GLN:NE2	2.39	0.56
5:I:74:LEU:HD13	5:I:119:ALA:HB1	1.88	0.56
2:F:65:LEU:HD22	2:F:97:VAL:HG13	1.88	0.55
5:I:216:LEU:HD21	4:J:444:LEU:HD13	1.89	0.55
11:Q:23:VAL:HG21	11:Q:45:THR:HB	1.88	0.55
5:I:37:VAL:HG22	5:I:71:TYR:HB2	1.87	0.55
7:L:108:LEU:HD21	7:L:184:LEU:HD21	1.89	0.55
3:G:20:LEU:O	3:G:24:GLN:NE2	2.40	0.55
12:R:19:LEU:HD11	12:R:80:HIS:HB3	1.89	0.55
4:M:412:GLN:NE2	4:M:458:ASP:O	2.40	0.54
4:J:384:ALA:HB3	4:J:408:THR:HA	1.87	0.54
2:B:185:GLY:HA2	2:B:195:MET:HE1	1.89	0.54
7:L:107:THR:HG21	7:L:132:MET:HB3	1.89	0.54
11:Q:36:LEU:HB3	11:Q:40:ALA:HB2	1.89	0.54
4:M:354:SER:HB3	4:M:388:ALA:HB2	1.89	0.54
6:K:96:PRO:HB3	6:K:120:LYS:HE3	1.89	0.54
1:A:68:GLU:HB3	1:A:97:LYS:HD2	1.90	0.53
2:B:114:MET:HE1	2:B:136:ILE:HG23	1.90	0.53
6:K:76:GLY:O	6:K:136:GLN:NE2	2.42	0.53
11:Q:174:VAL:HG12	11:Q:176:LEU:H	1.72	0.53
3:C:168:ARG:NH2	4:M:458:ASP:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:100:VAL:HG22	8:N:122:LYS:HB2	1.91	0.53
3:E:167:ASP:OD1	6:K:181:ARG:NH2	2.41	0.53
11:Q:210:CYS:SG	11:Q:211:LYS:N	2.82	0.53
8:N:244:ASP:HA	8:N:247:ARG:HD3	1.89	0.53
2:F:200:LYS:O	2:F:204:ARG:NH1	2.42	0.52
8:N:122:LYS:HD3	8:N:201:ILE:HD11	1.92	0.52
4:J:495:SER:HA	4:J:498:ASP:HB2	1.90	0.52
12:R:157:ASN:O	12:R:192:GLN:NE2	2.43	0.52
5:I:217:ASN:H	4:J:370:GLN:HE22	1.58	0.52
12:R:45:ALA:HB2	12:R:64:ILE:HG13	1.91	0.52
1:A:12:SER:N	2:B:68:ALA:O	2.43	0.52
2:D:57:LEU:HD22	2:D:62:ILE:HD12	1.92	0.52
2:F:57:LEU:HB3	2:F:62:ILE:HB	1.91	0.52
3:G:25:ARG:HG2	3:G:48:LEU:HD22	1.91	0.51
6:K:19:ASP:OD2	6:K:19:ASP:N	2.43	0.51
7:L:99:VAL:HG12	7:L:101:GLY:H	1.73	0.51
10:P:40:LEU:HD12	10:P:41:PRO:HD2	1.91	0.51
2:B:53:VAL:HG11	3:C:44:GLN:HG2	1.91	0.51
3:G:56:ASP:OD2	3:G:86:ASN:ND2	2.43	0.51
8:N:301:ASP:HB2	8:N:303:VAL:HG23	1.92	0.51
4:J:401:TYR:HB3	4:J:478:ALA:HB2	1.92	0.51
12:R:23:ASP:N	12:R:23:ASP:OD1	2.42	0.51
1:A:44:ILE:HG23	1:A:52:MET:HE1	1.92	0.51
1:A:142:GLN:OE1	5:I:148:ARG:NH2	2.43	0.51
2:D:175:GLU:O	2:D:179:HIS:ND1	2.44	0.51
4:H:459:ARG:NH1	5:I:152:GLN:OE1	2.43	0.51
5:I:135:PRO:HA	5:I:198:VAL:HG11	1.92	0.51
2:F:151:SER:OG	2:F:152:ARG:N	2.44	0.51
2:F:191:THR:HG23	2:F:193:GLN:H	1.76	0.51
2:B:147:SER:HB2	2:B:219:VAL:HG11	1.93	0.51
3:E:95:SER:HB3	3:E:120:HIS:HB3	1.93	0.51
1:A:26:ASP:OD1	1:A:26:ASP:N	2.44	0.50
3:E:126:ALA:O	7:L:164:ARG:NH1	2.44	0.50
4:M:448:ARG:HH21	4:M:452:LYS:HD2	1.76	0.50
2:F:165:GLN:OE1	6:K:137:ARG:NH1	2.44	0.50
2:D:147:SER:OG	2:D:148:LEU:N	2.43	0.50
2:B:64:ARG:NH1	3:C:39:ASP:OD2	2.45	0.50
5:I:27:ASP:O	5:I:30:SER:OG	2.29	0.50
6:K:34:MET:SD	6:K:34:MET:N	2.85	0.50
1:A:225:ASP:OD2	8:N:255:ARG:NH1	2.45	0.50
5:I:80:ILE:HD12	5:I:145:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:411:HIS:ND1	4:J:460:ASP:OD2	2.45	0.49
4:J:432:MET:SD	4:J:435:ARG:NH2	2.81	0.49
9:O:158:ARG:NH1	9:O:159:TYR:O	2.45	0.49
5:I:218:ARG:NH1	4:J:444:LEU:O	2.46	0.49
4:J:352:ILE:HB	4:J:380:ALA:HA	1.94	0.49
7:L:67:LYS:HA	7:L:98:ASN:HB2	1.93	0.49
4:H:449:PRO:HG2	4:H:452:LYS:HB2	1.94	0.49
8:N:80:ASP:HB2	8:N:108:TRP:HE1	1.76	0.49
12:S:111:LYS:O	12:S:180:ASN:ND2	2.45	0.49
3:C:129:GLN:OE1	8:N:133:GLN:NE2	2.45	0.49
2:B:204:ARG:NH2	8:N:181:GLN:O	2.45	0.49
5:I:90:ASP:OD2	5:I:90:ASP:N	2.42	0.49
4:H:483:MET:HG3	4:H:486:ILE:HD12	1.94	0.49
2:F:163:GLN:HE22	6:K:138:LEU:HD23	1.78	0.48
3:G:26:ILE:HG12	3:G:58:LYS:HB2	1.95	0.48
1:A:238:ASN:OXT	4:H:429:GLN:NE2	2.46	0.48
3:E:106:ARG:HH22	3:E:154:TYR:HA	1.78	0.48
5:I:82:ASP:OD1	5:I:82:ASP:N	2.45	0.48
2:D:70:ASP:N	2:D:70:ASP:OD1	2.46	0.48
7:L:47:ARG:NH1	7:L:48:GLN:OE1	2.44	0.48
1:A:127:MET:HA	1:A:202:ILE:HB	1.94	0.48
2:B:156:HIS:ND1	2:B:157:GLN:O	2.44	0.47
12:S:106:ASP:N	12:S:106:ASP:OD1	2.43	0.47
12:S:163:THR:OG1	12:S:193:LEU:O	2.33	0.47
2:D:57:LEU:HB3	2:D:62:ILE:HB	1.97	0.47
7:L:130:LEU:HA	7:L:155:MET:HB3	1.95	0.47
11:Q:43:LYS:NZ	11:Q:44:PRO:O	2.45	0.47
4:J:402:VAL:HG21	4:J:468:THR:HG21	1.97	0.47
8:N:289:THR:OG1	8:N:290:GLU:N	2.46	0.47
4:H:434:ILE:HD11	8:N:128:LEU:HD21	1.97	0.47
12:R:30:VAL:HB	12:R:35:LEU:HD12	1.97	0.47
1:A:183:ARG:NH2	4:H:458:ASP:OD1	2.47	0.47
3:G:89:CYS:HB3	3:G:111:SER:HB2	1.97	0.47
1:A:20:GLN:HE21	2:B:51:GLN:HE22	1.63	0.46
2:B:65:LEU:HD23	2:B:97:VAL:HG13	1.97	0.46
5:I:88:SER:OG	5:I:89:ALA:N	2.48	0.46
3:E:138:LYS:HA	3:E:141:MET:HB2	1.98	0.46
8:N:191:ALA:HB1	8:N:196:ILE:HB	1.97	0.46
10:P:52:HIS:HD2	10:P:72:MET:HB2	1.81	0.46
10:P:103:GLU:HB3	12:S:9:LYS:HG2	1.96	0.46
4:M:355:PHE:HB3	4:M:383:VAL:HG11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:139:ASP:N	9:O:139:ASP:OD1	2.46	0.46
2:B:157:GLN:NE2	2:B:203:ASP:O	2.48	0.46
6:K:64:ASN:HB2	6:K:102:VAL:HG23	1.97	0.46
3:C:167:ASP:O	4:M:459:ARG:NH2	2.49	0.46
4:H:408:THR:HB	4:H:463:LEU:HB2	1.96	0.46
2:B:177:LEU:HD11	4:H:425:TRP:HB2	1.98	0.46
2:F:112:ASP:OD2	2:F:112:ASP:N	2.46	0.46
9:O:148:ARG:HH22	9:O:158:ARG:HH12	1.64	0.46
1:A:226:ASP:OD1	1:A:226:ASP:N	2.49	0.46
2:F:191:THR:OG1	2:F:216:TYR:O	2.34	0.46
4:H:401:TYR:HB3	4:H:478:ALA:HB2	1.98	0.46
11:Q:118:LEU:HB3	11:Q:126:LEU:HD22	1.98	0.46
8:N:301:ASP:OD1	8:N:301:ASP:N	2.43	0.45
3:C:167:ASP:OD1	3:C:167:ASP:N	2.48	0.45
2:D:152:ARG:NH1	2:D:209:SER:OG	2.47	0.45
2:F:205:ASP:OD1	2:F:205:ASP:N	2.45	0.45
12:S:1:ALA:HB1	12:S:74:GLU:HG3	1.98	0.45
6:K:28:ARG:NH2	6:K:57:ASP:O	2.49	0.45
8:N:19:ASP:OD1	8:N:19:ASP:N	2.46	0.45
11:Q:125:VAL:HG21	11:Q:176:LEU:HD23	1.98	0.45
3:E:33:VAL:HG13	3:E:38:ALA:HB2	1.98	0.45
5:I:218:ARG:HH21	4:J:397:ILE:HD13	1.82	0.45
12:R:89:ILE:HG23	12:R:183:VAL:HG21	1.96	0.45
2:B:116:HIS:HD2	10:P:38:ILE:HG21	1.82	0.45
6:K:10:LEU:HA	6:K:14:ALA:HB3	1.98	0.45
10:P:25:ILE:HD11	10:P:91:ILE:HB	1.98	0.45
7:L:142:GLU:HG2	7:L:146:ARG:HH12	1.82	0.45
4:M:417:LEU:HD23	4:M:424:ILE:HG23	1.99	0.45
1:A:19:ILE:HB	2:B:76:LEU:HD12	1.99	0.45
1:A:212:PRO:HB3	1:A:233:LEU:HD11	1.99	0.45
2:B:156:HIS:HB3	2:B:205:ASP:HA	1.98	0.45
3:G:35:ASP:OD1	3:G:35:ASP:N	2.50	0.45
1:A:48:ILE:HB	1:A:81:GLY:HA3	1.99	0.44
2:B:77:LEU:HA	2:B:80:GLN:HE21	1.82	0.44
5:I:211:VAL:HG23	5:I:214:PHE:HB2	2.00	0.44
8:N:87:THR:HG22	8:N:112:VAL:HG12	1.98	0.44
11:Q:56:ARG:HB2	11:Q:63:ARG:HB2	1.99	0.44
4:J:386:SER:HB2	4:J:411:HIS:HB3	2.00	0.44
12:R:106:ASP:OD1	12:R:106:ASP:N	2.45	0.44
2:D:157:GLN:HE21	4:M:420:GLN:HE22	1.66	0.44
9:O:37:GLU:OE1	9:O:87:ARG:NH1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:95:MET:HB3	2:D:123:THR:HA	2.00	0.44
11:Q:87:LEU:HD12	11:Q:91:GLU:HB2	1.99	0.44
3:E:52:ASP:OD2	3:E:55:LYS:NZ	2.50	0.44
4:M:464:THR:O	4:M:468:THR:OG1	2.28	0.44
12:R:9:LYS:HE3	12:R:9:LYS:HB3	1.88	0.44
1:A:183:ARG:NH2	4:H:458:ASP:O	2.49	0.43
7:L:146:ARG:NH2	7:L:218:GLY:O	2.51	0.43
1:A:54:THR:HG21	3:G:30:GLY:HA3	2.00	0.43
6:K:9:LYS:O	6:K:14:ALA:N	2.51	0.43
4:M:385:ALA:HA	4:M:409:MET:HB3	1.99	0.43
2:D:203:ASP:HB2	7:L:205:ARG:HH21	1.82	0.43
6:K:102:VAL:HA	6:K:124:LEU:HD12	2.01	0.43
12:R:159:THR:OG1	12:R:160:VAL:N	2.51	0.43
12:R:186:GLU:H	12:R:187:SER:HB3	1.84	0.43
3:C:17:PRO:HB2	3:C:18:PHE:H	1.72	0.43
5:I:9:PRO:HD3	8:N:11:ASP:HB3	2.00	0.43
3:C:127:SER:OG	3:C:128:GLY:N	2.51	0.43
2:F:116:HIS:HD2	12:R:125:LEU:HD13	1.83	0.43
2:F:72:ASP:OD1	2:F:72:ASP:N	2.49	0.43
1:A:30:MET:SD	1:A:30:MET:N	2.83	0.43
4:H:383:VAL:HG12	4:H:407:HIS:HB2	2.01	0.43
7:L:146:ARG:NE	7:L:219:MET:O	2.52	0.43
11:Q:97:ARG:HE	11:Q:97:ARG:HB3	1.68	0.43
3:E:61:ILE:HB	3:E:89:CYS:HA	2.01	0.43
4:J:354:SER:HB3	4:J:388:ALA:HB2	2.00	0.42
4:J:482:VAL:O	4:J:485:SER:OG	2.33	0.42
1:A:108:CYS:N	1:A:131:ARG:O	2.52	0.42
5:I:136:HIS:ND1	4:J:437:ASP:OD1	2.53	0.42
6:K:28:ARG:NH1	6:K:54:GLU:OE2	2.53	0.42
1:A:166:TYR:O	1:A:170:THR:OG1	2.37	0.42
1:A:225:ASP:OD1	1:A:225:ASP:N	2.53	0.42
8:N:284:PRO:O	9:O:68:TYR:OH	2.36	0.42
1:A:145:ILE:HD12	1:A:148:ILE:HB	2.01	0.42
9:O:17:ALA:HA	9:O:20:GLU:HG2	2.02	0.42
2:B:42:PRO:HB2	2:B:43:ASN:H	1.72	0.41
3:C:116:ARG:HH21	3:C:171:TYR:HB3	1.85	0.41
2:D:62:ILE:HG12	2:D:94:THR:HB	2.01	0.41
2:B:203:ASP:OD1	2:B:203:ASP:N	2.53	0.41
3:C:174:PRO:HA	3:C:177:ALA:HB3	2.02	0.41
3:E:102:GLY:HA2	3:E:109:ARG:HD2	2.02	0.41
12:R:91:VAL:HG13	12:R:104:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:102:GLY:HA2	3:C:109:ARG:HD2	2.01	0.41
3:E:56:ASP:OD1	3:E:56:ASP:N	2.45	0.41
4:M:439:ALA:O	4:M:443:SER:OG	2.32	0.41
3:G:28:PHE:HD1	3:G:60:PHE:HB2	1.86	0.41
4:J:479:THR:OG1	4:J:480:ASN:N	2.53	0.41
7:L:131:GLY:HA2	7:L:157:HIS:CD2	2.56	0.41
2:D:168:ASP:OD1	2:D:172:GLN:NE2	2.53	0.41
4:H:432:MET:HE1	4:H:435:ARG:HH21	1.85	0.41
4:H:448:ARG:NH1	8:N:229:GLN:OE1	2.53	0.41
2:D:85:ASP:HB2	12:S:127:THR:HG21	2.03	0.41
11:Q:17:ASP:OD1	11:Q:17:ASP:N	2.47	0.41
12:R:137:THR:HA	12:R:163:THR:HA	2.02	0.41
6:K:124:LEU:HD13	7:L:112:ASP:HB3	2.03	0.41
2:F:71:ASP:O	2:F:75:ASN:ND2	2.44	0.41
2:F:203:ASP:N	2:F:203:ASP:OD2	2.47	0.41
1:A:82:GLN:HE22	1:A:84:TYR:HD2	1.69	0.41
3:E:158:PRO:HG2	3:E:161:LYS:HG2	2.02	0.41
5:I:81:ASN:HD21	5:I:83:LYS:HB2	1.85	0.41
7:L:118:ARG:H	7:L:118:ARG:HG2	1.68	0.41
8:N:123:SER:HB2	8:N:197:ILE:HG21	2.03	0.41
8:N:129:ALA:HB3	8:N:186:MET:HB3	2.02	0.41
12:S:62:LYS:HG2	12:S:92:LEU:HD12	2.03	0.41
3:C:82:ARG:H	3:C:82:ARG:HG2	1.58	0.41
3:E:17:PRO:HD2	3:E:20:LEU:HD13	2.02	0.41
10:P:85:VAL:HB	10:P:90:ILE:HD12	2.02	0.41
3:C:144:LYS:O	3:C:148:ASN:ND2	2.44	0.40
6:K:147:ASP:OD2	6:K:147:ASP:N	2.54	0.40
2:F:157:GLN:HE22	6:K:144:SER:HB3	1.86	0.40
5:I:59:LEU:HD13	5:I:70:ILE:HD12	2.03	0.40
6:K:125:ARG:NH1	6:K:188:TYR:OH	2.54	0.40
9:O:15:VAL:HG13	9:O:118:MET:HB2	2.03	0.40
6:K:106:PHE:HA	6:K:130:MET:HB3	2.03	0.40
7:L:123:THR:HG21	7:L:137:LEU:HA	2.03	0.40
12:S:98:ILE:HG22	12:S:176:GLU:HB2	2.02	0.40
5:I:68:ARG:HA	5:I:69:PRO:HD3	1.96	0.40
8:N:215:TRP:HB3	8:N:221:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/238 (94%)	218 (97%)	7 (3%)	0	100	100
2	B	191/238 (80%)	191 (100%)	0	0	100	100
2	D	191/238 (80%)	187 (98%)	4 (2%)	0	100	100
2	F	170/238 (71%)	166 (98%)	4 (2%)	0	100	100
3	C	172/296 (58%)	169 (98%)	3 (2%)	0	100	100
3	E	172/296 (58%)	169 (98%)	3 (2%)	0	100	100
3	G	177/296 (60%)	175 (99%)	2 (1%)	0	100	100
4	H	146/208 (70%)	143 (98%)	3 (2%)	0	100	100
4	J	163/208 (78%)	161 (99%)	2 (1%)	0	100	100
4	M	131/208 (63%)	131 (100%)	0	0	100	100
5	I	215/246 (87%)	206 (96%)	9 (4%)	0	100	100
6	K	231/251 (92%)	222 (96%)	9 (4%)	0	100	100
7	L	185/250 (74%)	181 (98%)	4 (2%)	0	100	100
8	N	336/383 (88%)	325 (97%)	11 (3%)	0	100	100
9	O	160/180 (89%)	154 (96%)	6 (4%)	0	100	100
10	P	93/103 (90%)	88 (95%)	5 (5%)	0	100	100
11	Q	201/212 (95%)	191 (95%)	10 (5%)	0	100	100
12	R	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
12	S	192/194 (99%)	169 (88%)	23 (12%)	0	100	100
All	All	3543/4477 (79%)	3424 (97%)	119 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/200 (96%)	191 (100%)	0	100	100
2	B	161/199 (81%)	161 (100%)	0	100	100
2	D	161/199 (81%)	161 (100%)	0	100	100
2	F	141/199 (71%)	141 (100%)	0	100	100
3	C	140/250 (56%)	140 (100%)	0	100	100
3	E	140/250 (56%)	140 (100%)	0	100	100
3	G	144/250 (58%)	144 (100%)	0	100	100
4	H	120/175 (69%)	120 (100%)	0	100	100
4	J	136/175 (78%)	136 (100%)	0	100	100
4	M	105/175 (60%)	105 (100%)	0	100	100
5	I	183/207 (88%)	183 (100%)	0	100	100
6	K	197/213 (92%)	197 (100%)	0	100	100
7	L	161/217 (74%)	160 (99%)	1 (1%)	78	79
8	N	290/327 (89%)	290 (100%)	0	100	100
9	O	130/146 (89%)	130 (100%)	0	100	100
10	P	76/81 (94%)	76 (100%)	0	100	100
11	Q	170/176 (97%)	169 (99%)	1 (1%)	78	79
12	R	157/157 (100%)	156 (99%)	1 (1%)	78	79
12	S	157/157 (100%)	156 (99%)	1 (1%)	78	79
All	All	2960/3753 (79%)	2956 (100%)	4 (0%)	87	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	L	71	THR
11	Q	23	VAL
12	R	34	LEU
12	S	159	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	39	ASN
1	A	69	ASN
1	A	94	GLN
1	A	129	ASN
1	A	156	ASN
1	A	217	GLN
2	B	51	GLN
2	B	59	GLN
2	B	75	ASN
2	B	80	GLN
2	B	174	ASN
2	B	178	HIS
3	C	24	GLN
2	D	43	ASN
2	D	157	GLN
3	E	129	GLN
3	E	136	GLN
3	E	148	ASN
2	F	59	GLN
2	F	116	HIS
2	F	179	HIS
2	F	184	ASN
3	G	146	ASN
3	G	148	ASN
5	I	55	GLN
5	I	81	ASN
5	I	118	GLN
5	I	147	ASN
5	I	157	GLN
5	I	161	ASN
4	J	361	ASN
4	J	366	HIS
4	J	370	GLN
4	J	429	GLN
4	J	451	HIS
4	J	492	GLN
6	K	92	GLN
6	K	136	GLN
7	L	77	ASN
7	L	166	GLN

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Mol	Chain	Res	Type
4	M	370	GLN
4	M	429	GLN
8	N	141	GLN
8	N	237	GLN
8	N	272	ASN
9	O	72	ASN
10	P	52	HIS
11	Q	83	GLN
11	Q	109	ASN
12	R	100	GLN
12	R	192	GLN
12	S	7	GLN

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](#)

There are no ligands in this entry.

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.

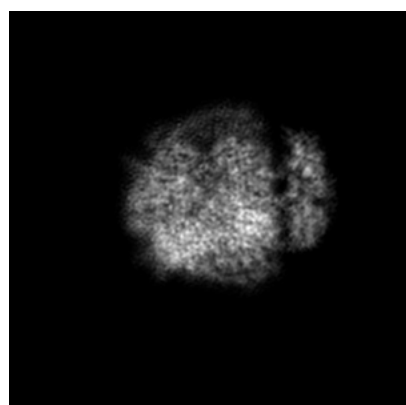
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31173. These allow visual inspection of the internal detail of the map and identification of artifacts.

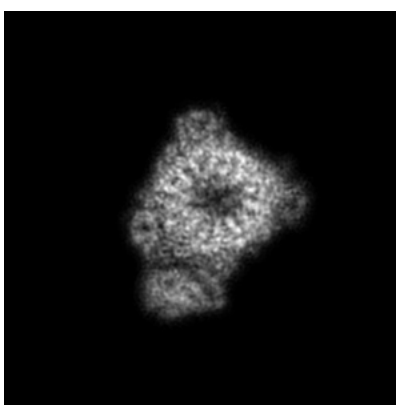
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

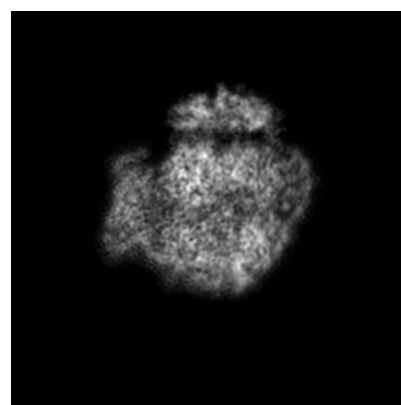
6.1.1 Primary map



X



Y

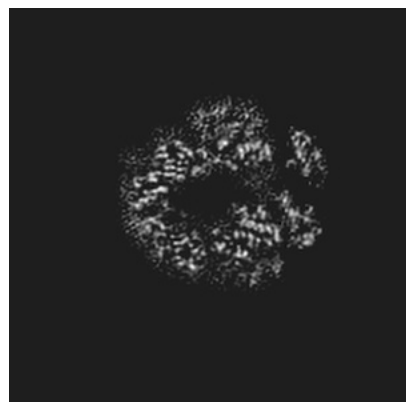


Z

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

6.2 Central slices [i](#)

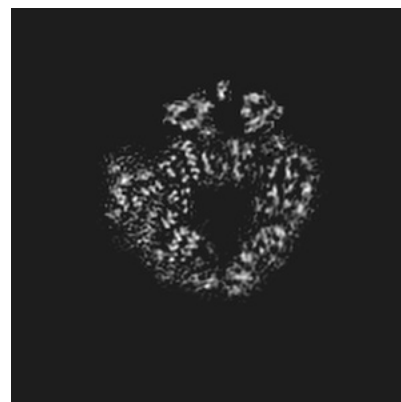
6.2.1 Primary map



X Index: 108



Y Index: 108

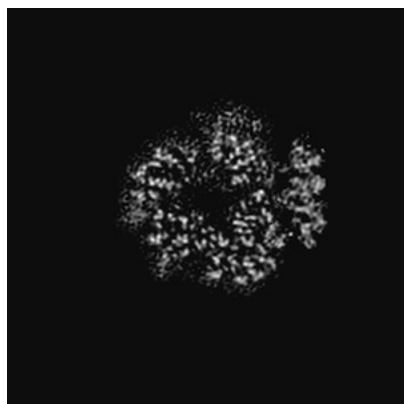


Z Index: 108

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

6.3 Largest variance slices [i](#)

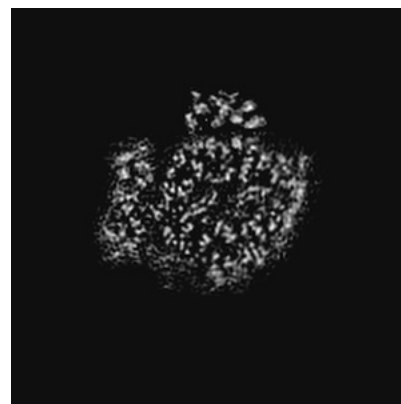
6.3.1 Primary map



X Index: 101



Y Index: 122

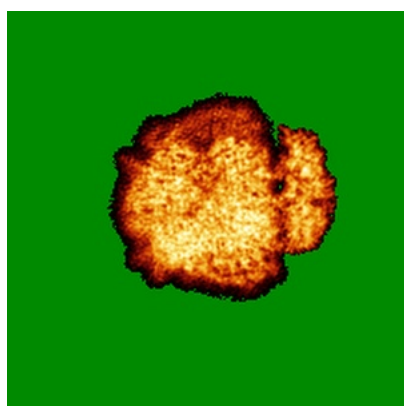


Z Index: 95

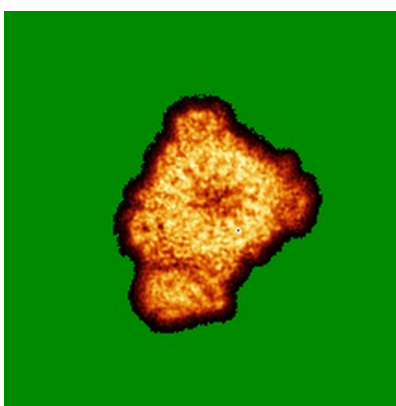
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

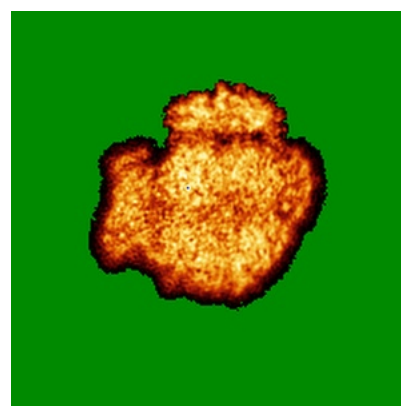
6.4.1 Primary map



X



Y

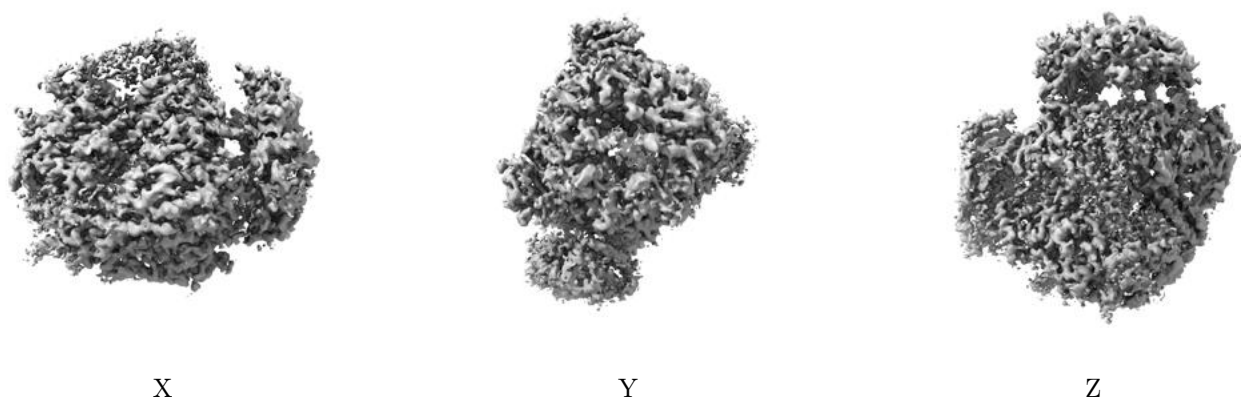


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.852. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

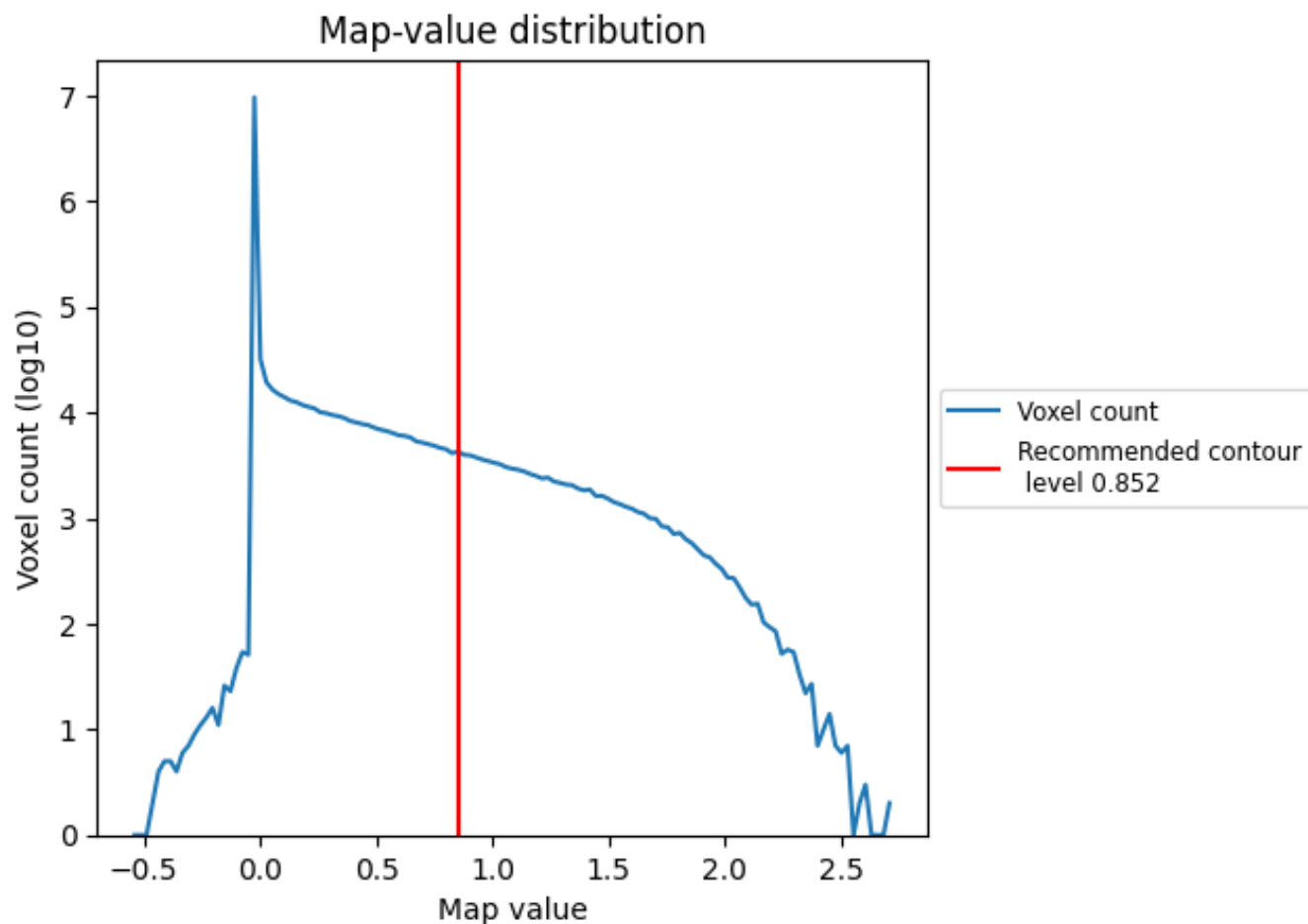
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

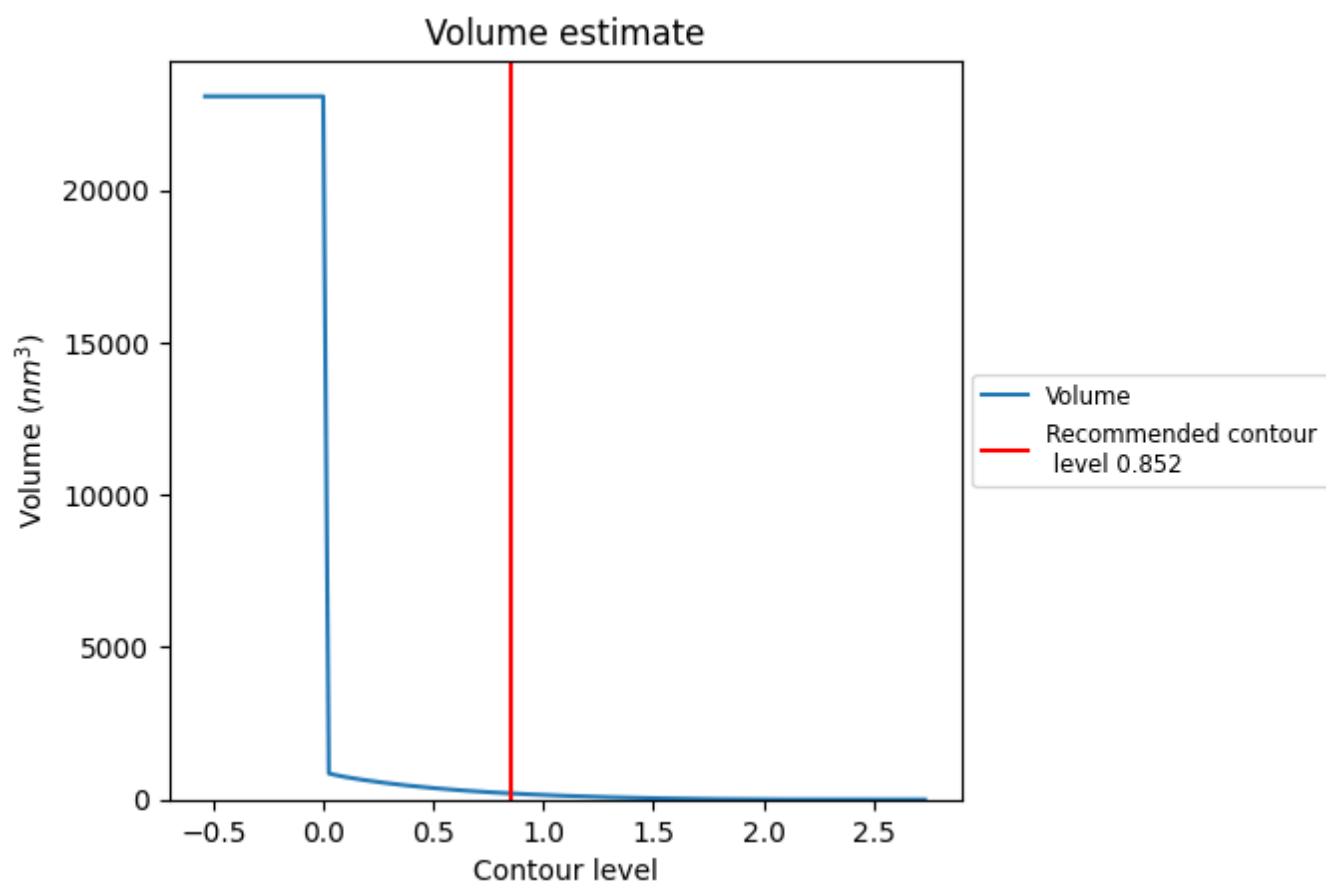
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

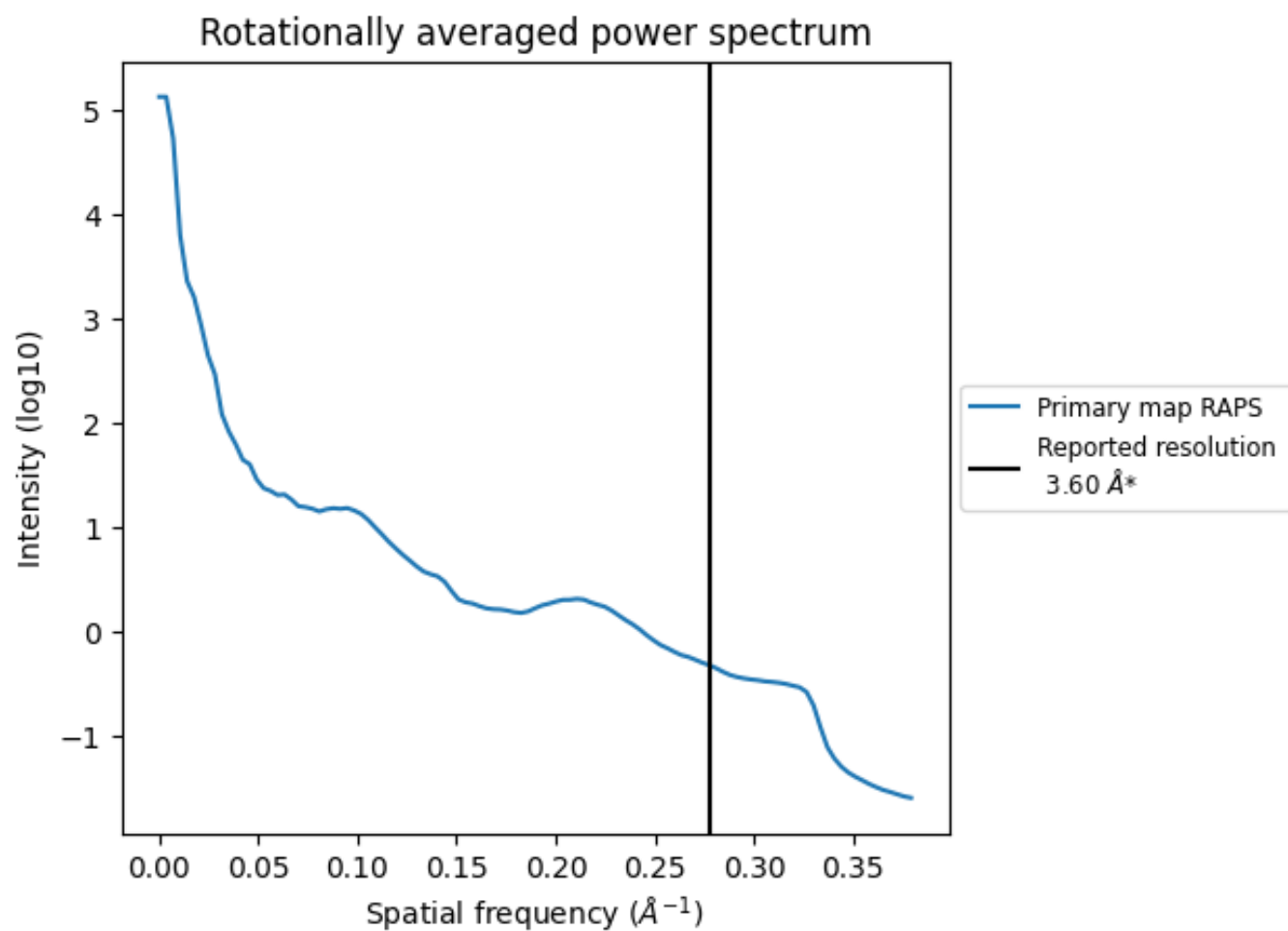
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 201 nm^3 ; this corresponds to an approximate mass of 182 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

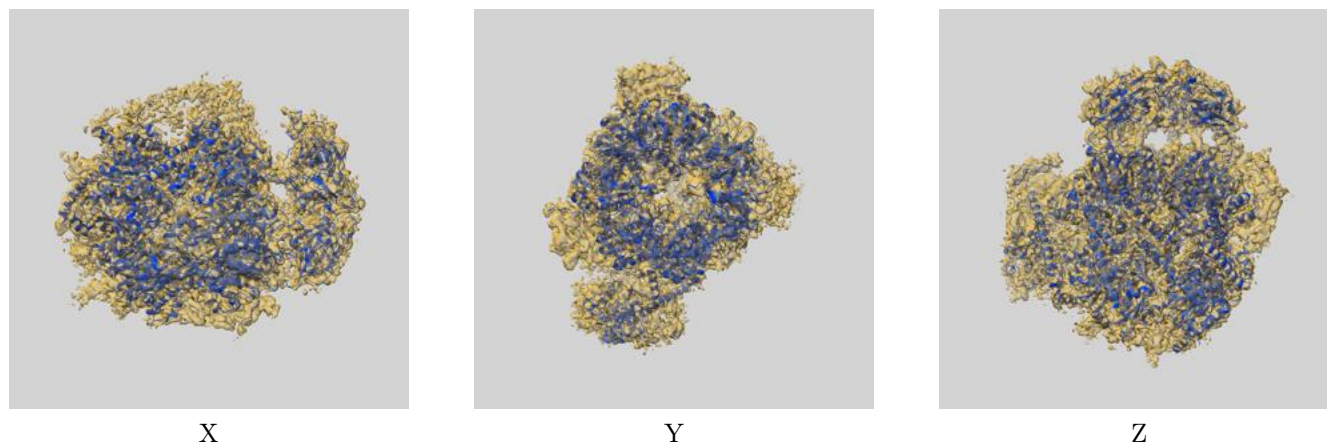
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

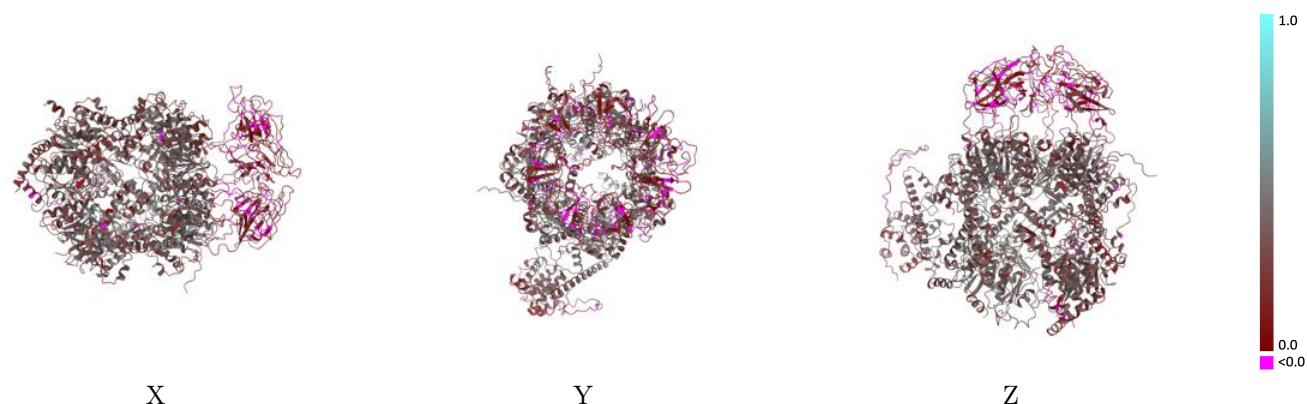
This section contains information regarding the fit between EMDB map EMD-31173 and PDB model 7EKQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



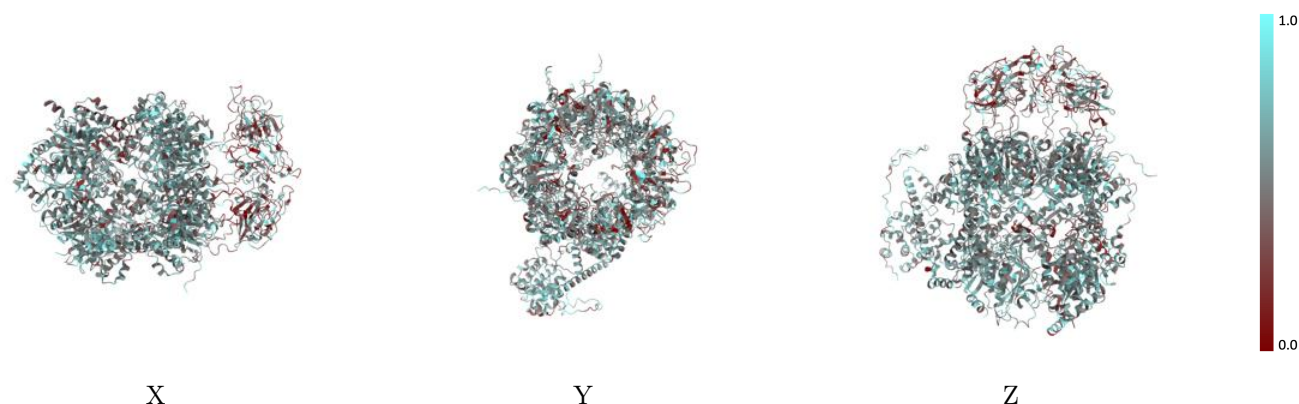
The images above show the 3D surface view of the map at the recommended contour level 0.852 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



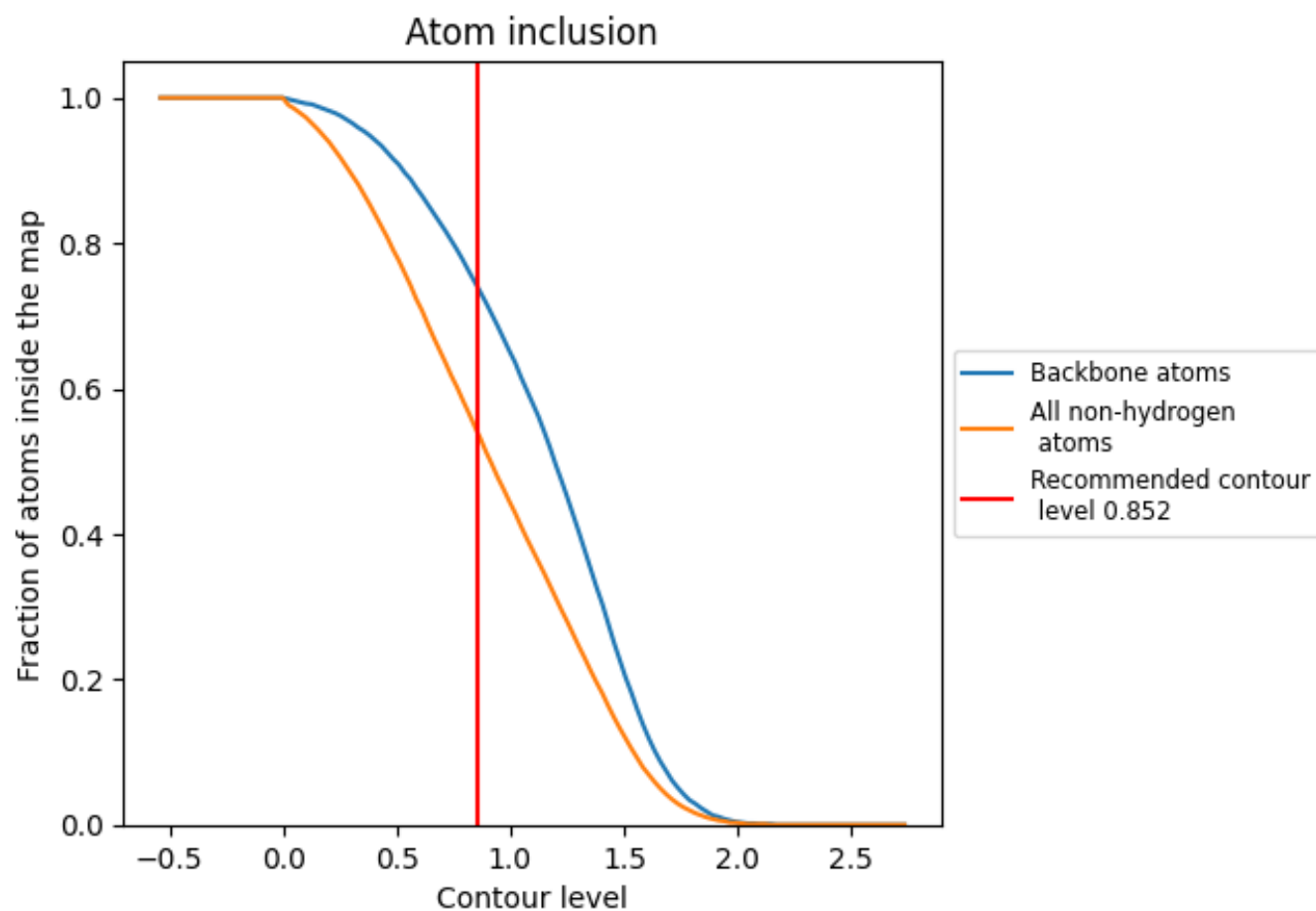
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.852).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 54% 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 (0.852) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5420	 0.3040
A	 0.5640	 0.3620
B	 0.5610	 0.3910
C	 0.5660	 0.3790
D	 0.5610	 0.3680
E	 0.5710	 0.3590
F	 0.5660	 0.3380
G	 0.5810	 0.3480
H	 0.6020	 0.3890
I	 0.5900	 0.3630
J	 0.5550	 0.3200
K	 0.5240	 0.2690
L	 0.5810	 0.3440
M	 0.5840	 0.3870
N	 0.5870	 0.3440
O	 0.5610	 0.2790
P	 0.4290	 0.1150
Q	 0.4130	 0.0940
R	 0.4200	 0.1400
S	 0.4270	 0.1190

