



wwPDB EM Validation Summary Report ⓘ

Nov 22, 2022 – 02:52 PM JST

PDB ID : 7EKQ
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 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:

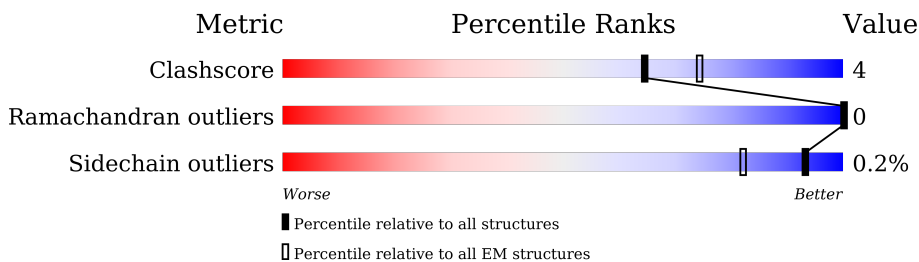
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
2	B	238	
2	D	238	
2	F	238	
3	C	296	
3	E	296	
3	G	296	
4	H	208	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 [i](#)

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
			Total	C	N	O	S		
1	A	227	1763	1115	293	341	14	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Chaperonin 11.

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

- Molecule 11 is a protein called Chaperonin 23.

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

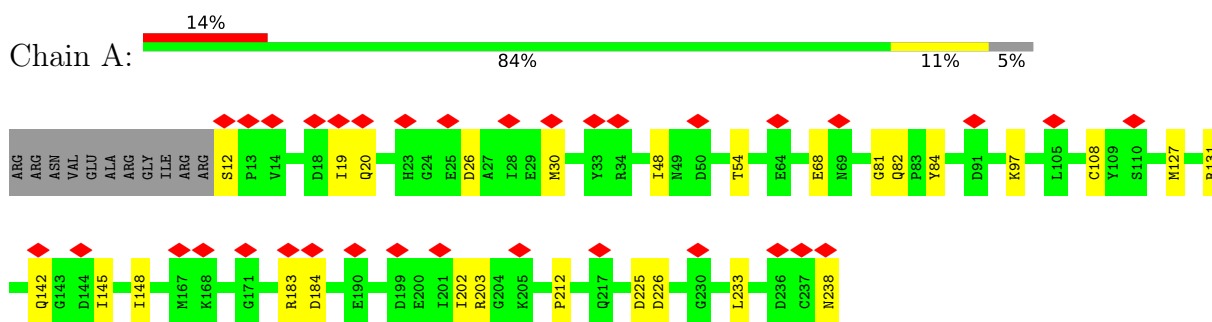
- Molecule 12 is a protein called Cpn20 co-chaperonin subunit.

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

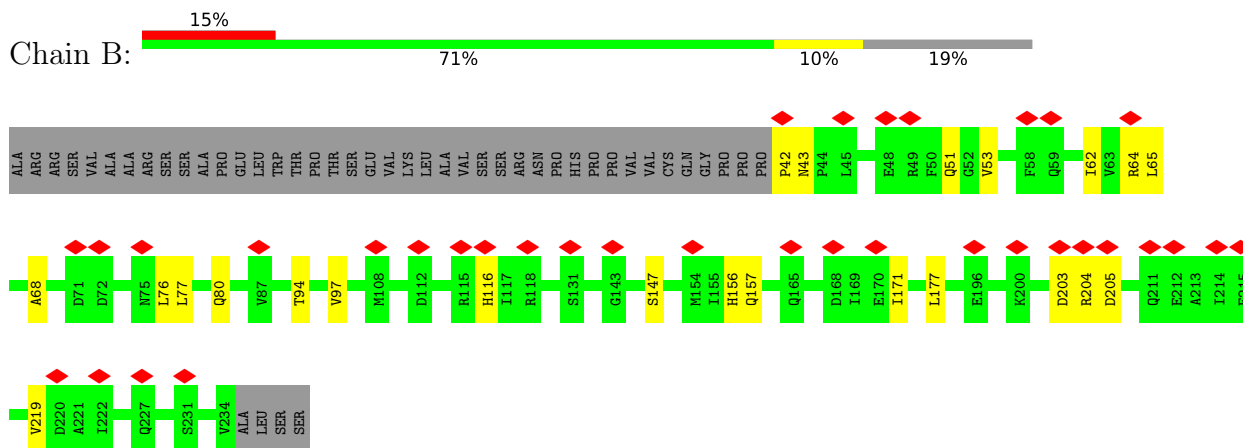
3 Residue-property plots [i](#)

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.

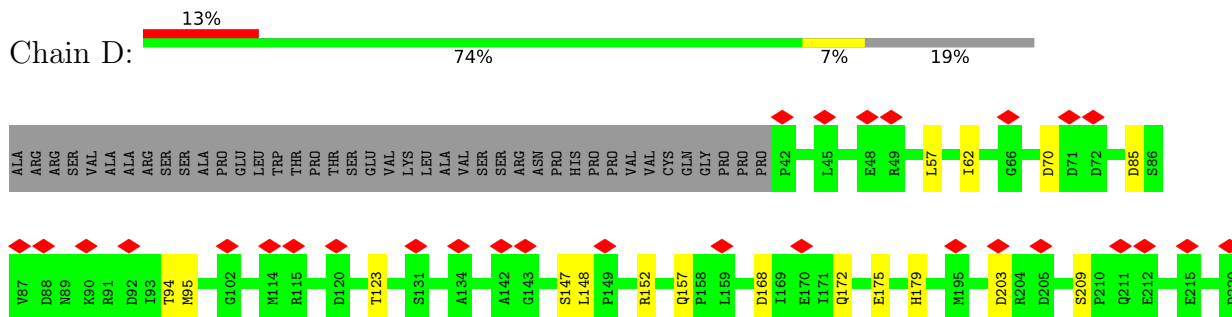
- Molecule 1: ATP-dependent Clp protease proteolytic subunit

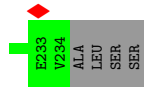


- Molecule 2: ATP-dependent Clp protease proteolytic subunit

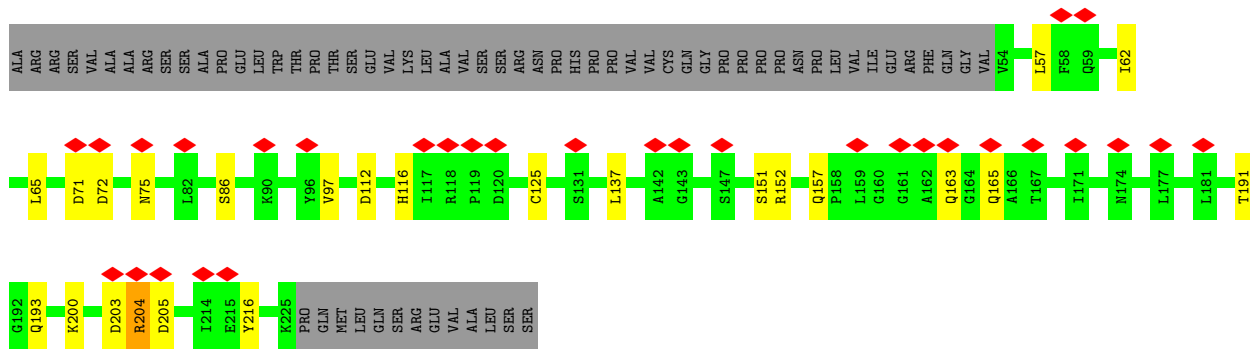


- Molecule 2: ATP-dependent Clp protease proteolytic subunit

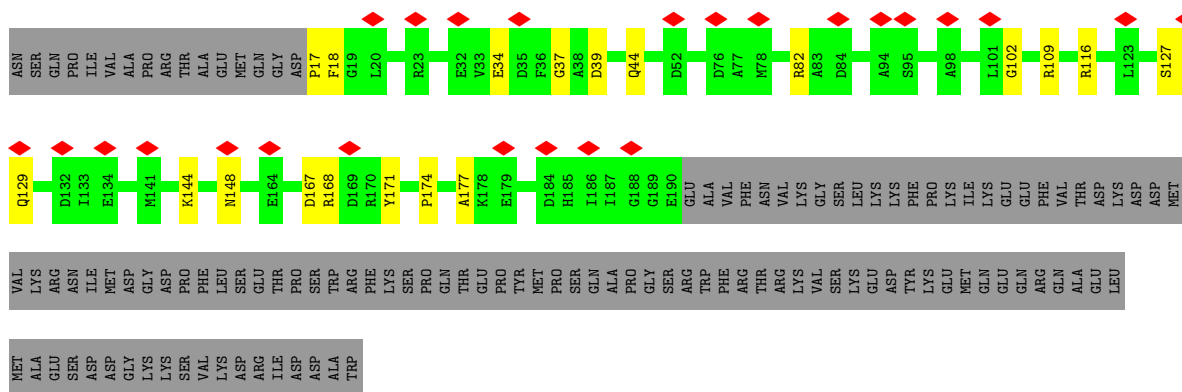




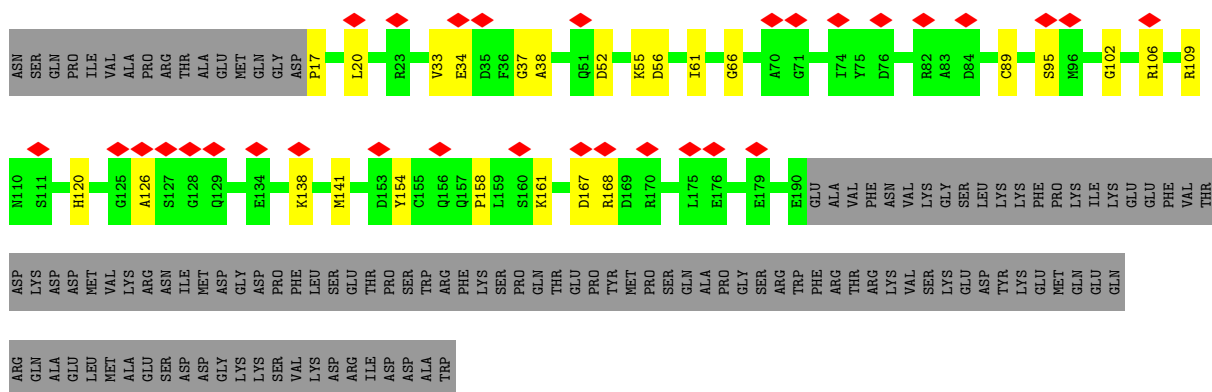
• Molecule 2: ATP-dependent Clp protease proteolytic subunit



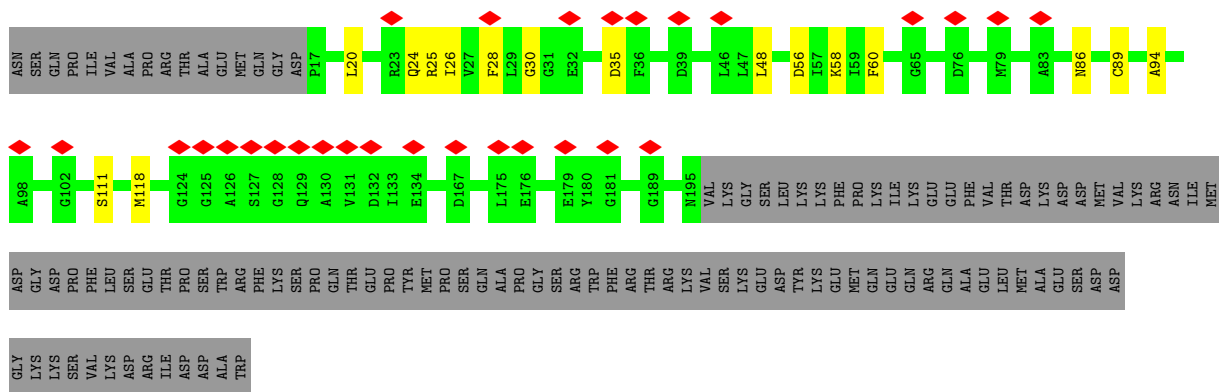
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



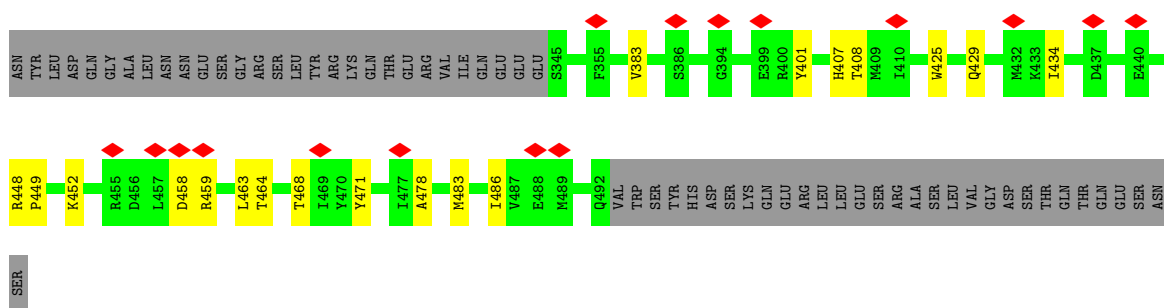
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



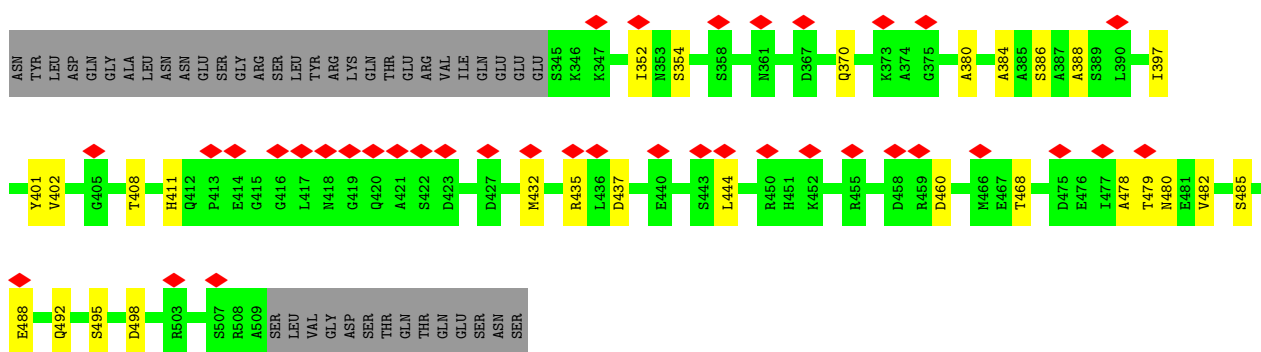
• Molecule 3: ATP-dependent Clp protease proteolytic subunit



• Molecule 4: ATP-dependent Clp protease proteolytic subunit

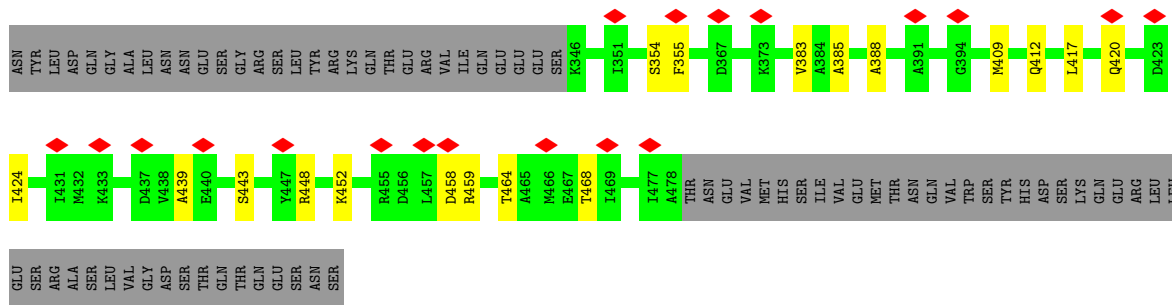


• Molecule 4: ATP-dependent Clp protease proteolytic subunit

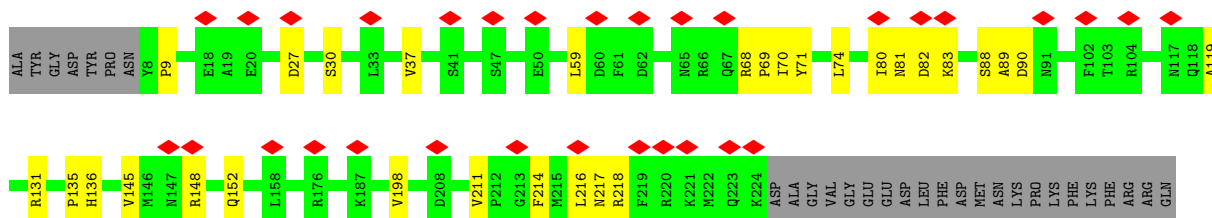
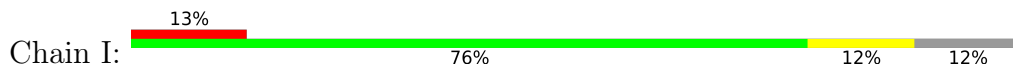


• Molecule 4: ATP-dependent Clp protease proteolytic subunit

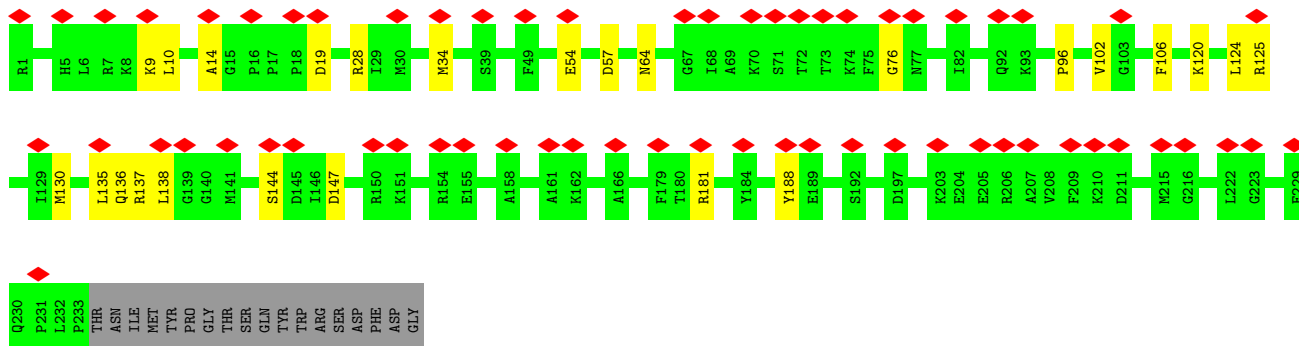
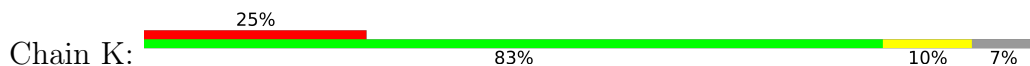




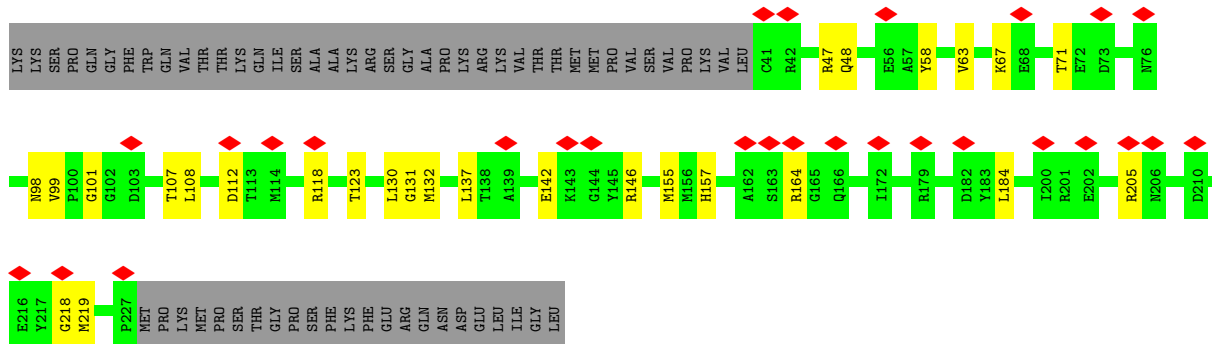
• Molecule 5: ATP-dependent Clp protease proteolytic subunit



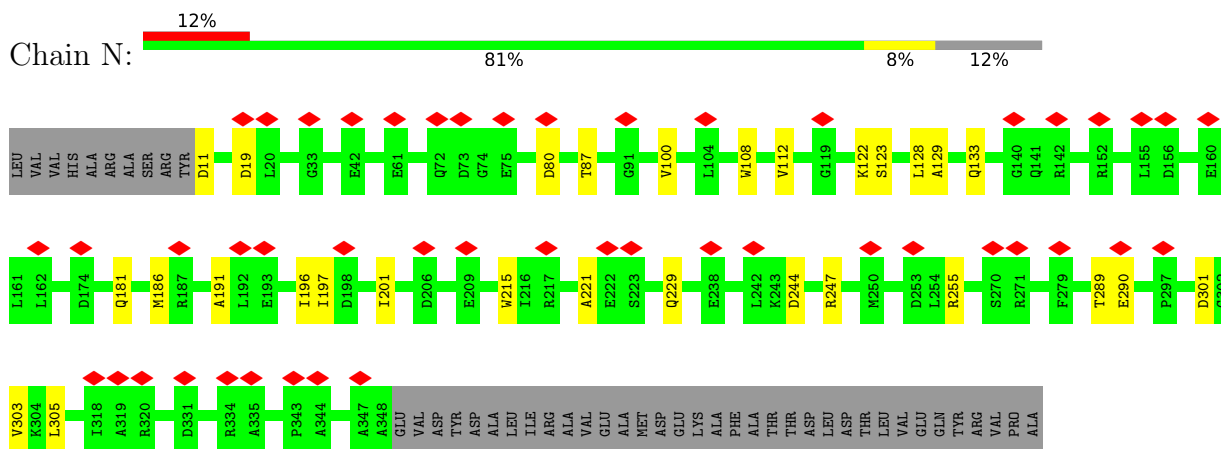
• Molecule 6: ATP-dependent Clp protease proteolytic subunit



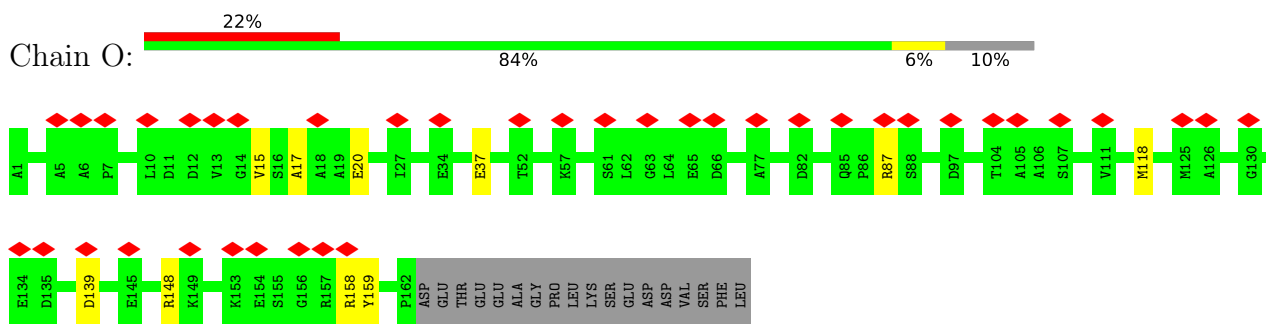
• Molecule 7: ATP-dependent Clp protease proteolytic subunit



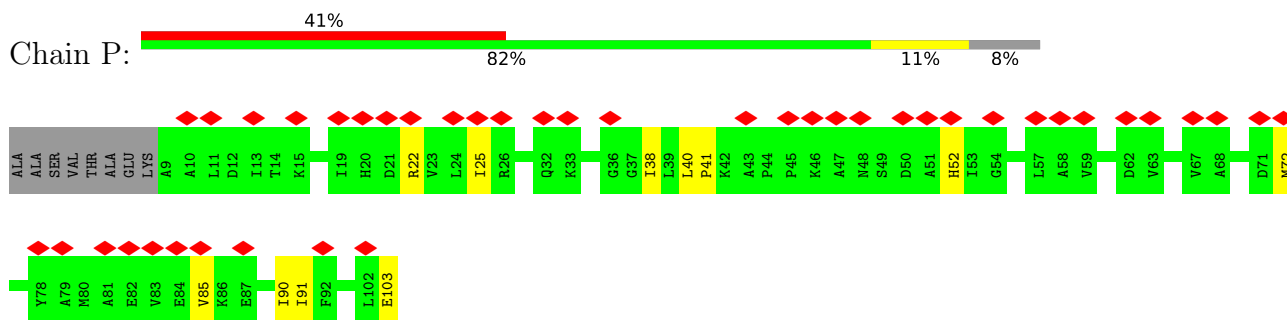
- Molecule 8: ATP-dependent Clp protease proteolytic subunit



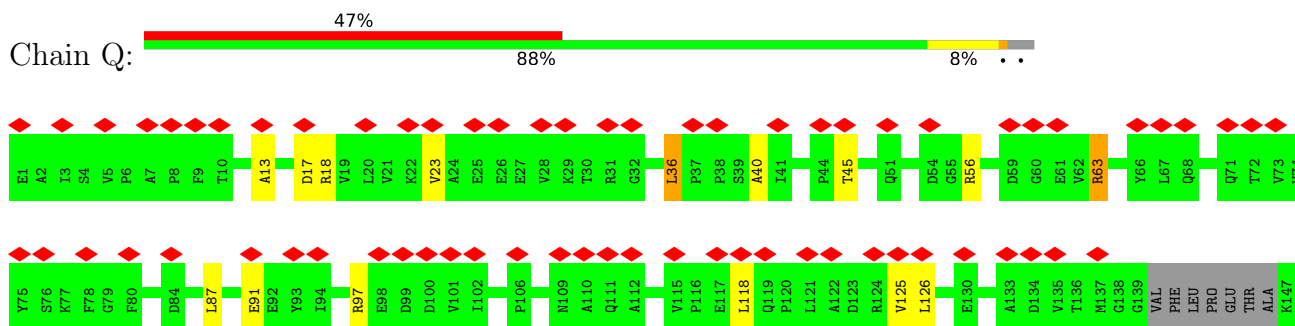
- Molecule 9: ATP-dependent Clp protease ATP-binding subunit CLPT4, chloroplastic

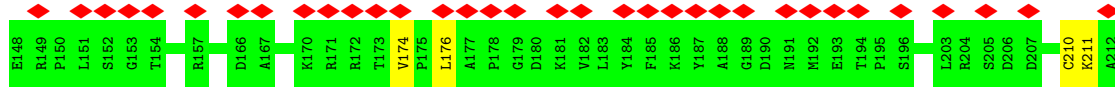


- Molecule 10: Chaperonin 11

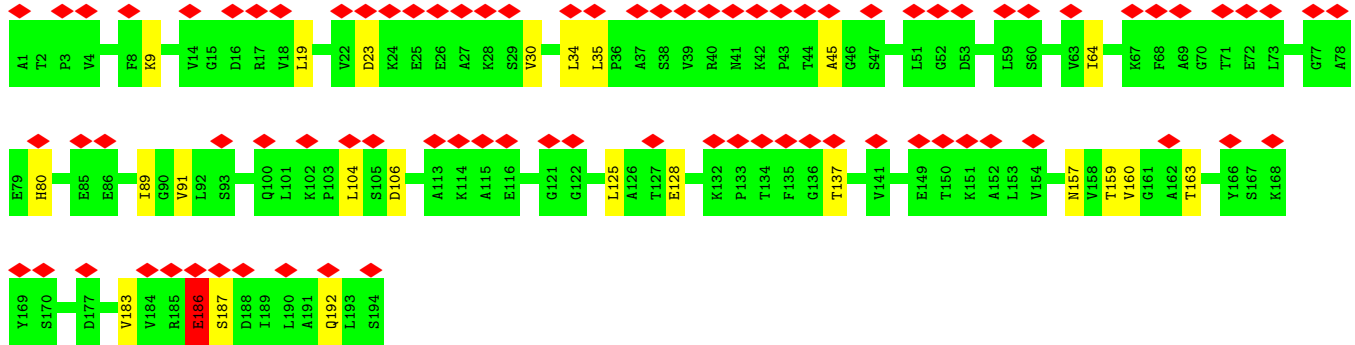
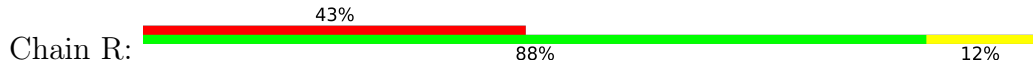


- Molecule 11: Chaperonin 23

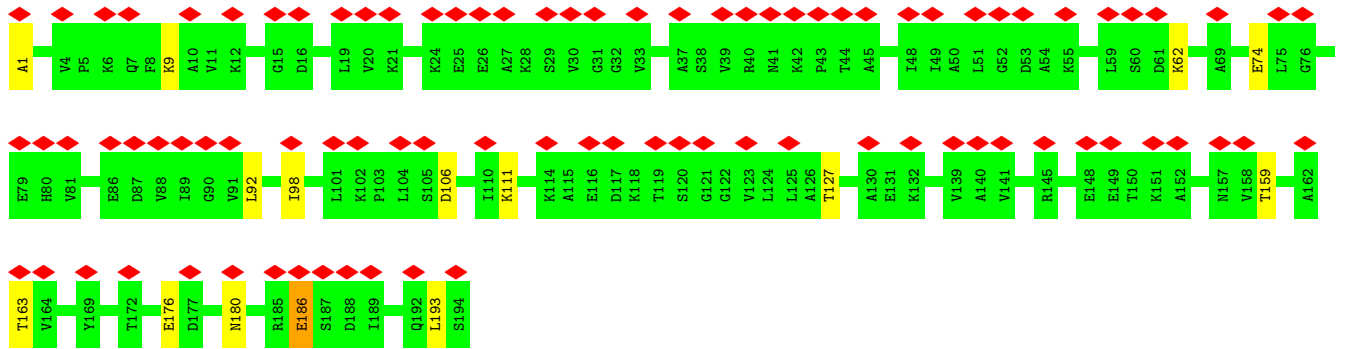
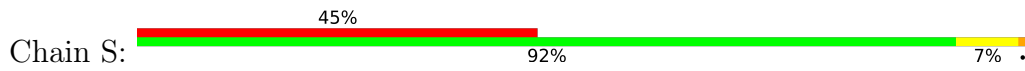




• Molecule 12: Cpn20 co-chaperonin subunit



• Molecule 12: Cpn20 co-chaperonin subunit



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	0.25	0/1794	0.45	0/2427
2	B	0.25	0/1500	0.44	0/2028
2	D	0.24	0/1500	0.47	0/2028
2	F	0.24	0/1326	0.46	0/1792
3	C	0.25	0/1350	0.45	0/1814
3	E	0.25	0/1350	0.47	0/1814
3	G	0.25	0/1391	0.45	0/1870
4	H	0.24	0/1149	0.43	0/1553
4	J	0.23	0/1301	0.45	0/1758
4	M	0.24	0/1031	0.43	0/1393
5	I	0.25	0/1790	0.45	0/2428
6	K	0.25	0/1881	0.48	1/2542 (0.0%)
7	L	0.23	0/1529	0.46	0/2072
8	N	0.24	0/2746	0.43	0/3718
9	O	0.24	0/1285	0.41	0/1743
10	P	0.25	0/722	0.57	0/973
11	Q	0.27	0/1594	0.52	1/2154 (0.0%)
12	R	0.28	0/1455	0.62	2/1963 (0.1%)
12	S	0.27	0/1455	0.58	1/1963 (0.1%)
All	All	0.25	0/28149	0.48	5/38033 (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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	186	GLU	C-N-CA	6.96	139.10	121.70
12	S	186	GLU	C-N-CA	6.15	137.08	121.70
11	Q	36	LEU	CA-CB-CG	6.07	129.26	115.30
12	R	34	LEU	CA-CB-CG	5.96	129.01	115.30
6	K	135	LEU	CA-CB-CG	5.24	127.36	115.30

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 [i](#)

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	22	0
2	B	1477	0	1477	19	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	9	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	20	0
9	O	1259	0	1246	6	0
10	P	713	0	748	7	0
11	Q	1567	0	1599	13	0
12	R	1439	0	1498	15	0
12	S	1439	0	1498	8	0
All	All	27663	0	27810	230	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.

The worst 5 of 230 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: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

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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	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%)	140 (99%)	1 (1%)	84	93
3	C	140/250 (56%)	140 (100%)	0	100	100
3	E	140/250 (56%)	139 (99%)	1 (1%)	84	93
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%)	182 (100%)	1 (0%)	88	95
6	K	197/213 (92%)	197 (100%)	0	100	100
7	L	161/217 (74%)	160 (99%)	1 (1%)	86	94
8	N	290/327 (89%)	290 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	86	94
12	R	157/157 (100%)	157 (100%)	0	100	100
12	S	157/157 (100%)	156 (99%)	1 (1%)	86	94
All	All	2960/3753 (79%)	2954 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	L	71	THR
11	Q	63	ARG
12	S	159	THR
2	F	204	ARG
3	E	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
6	K	92	GLN
12	R	192	GLN
6	K	136	GLN
8	N	237	GLN
3	E	148	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 monosaccharides 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.

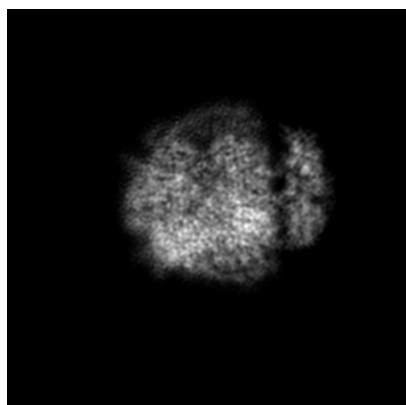
6 Map visualisation [i](#)

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.

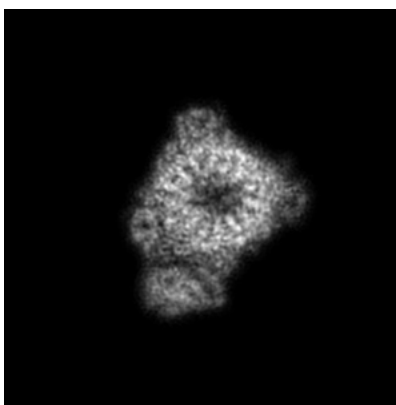
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

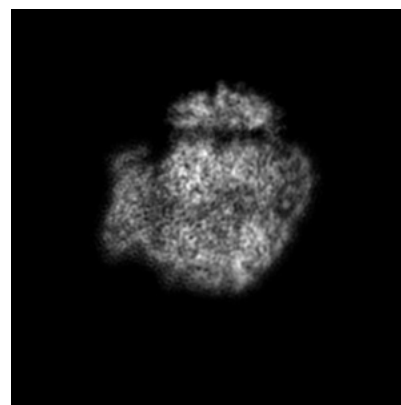
6.1.1 Primary map



X



Y

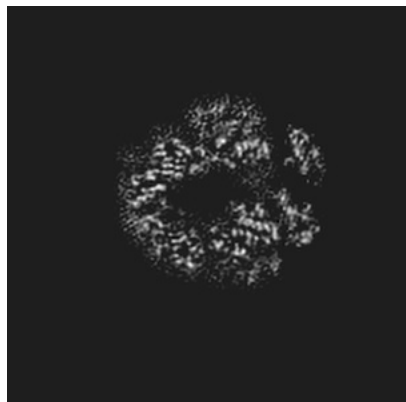


Z

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

6.2 Central slices [i](#)

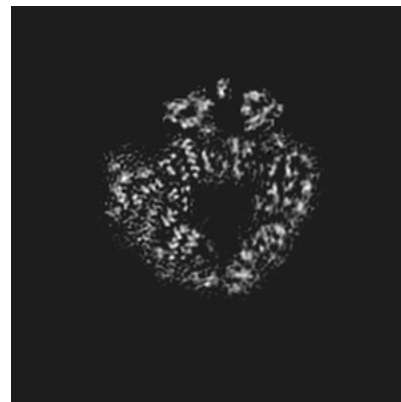
6.2.1 Primary map



X Index: 108



Y Index: 108

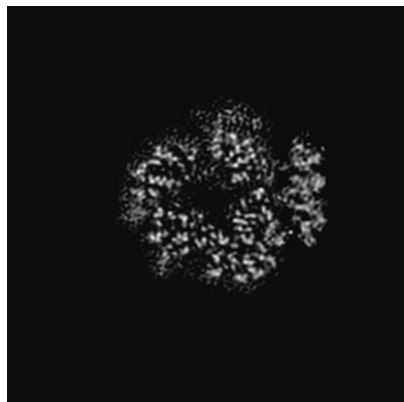


Z Index: 108

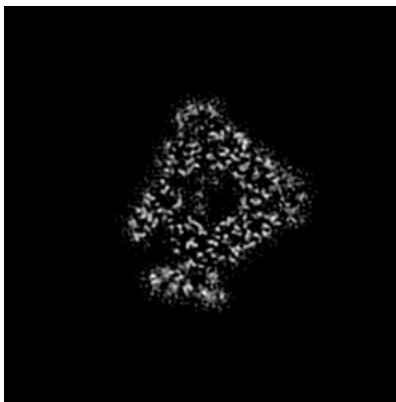
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

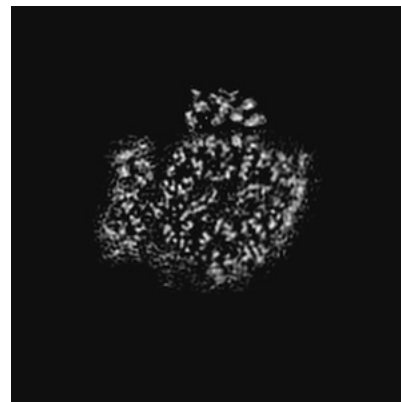
6.3.1 Primary map



X Index: 101



Y Index: 122



Z Index: 95

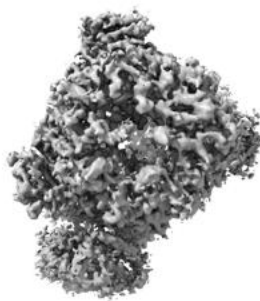
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

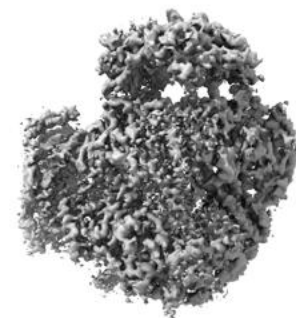
6.4.1 Primary map



X



Y



Z

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

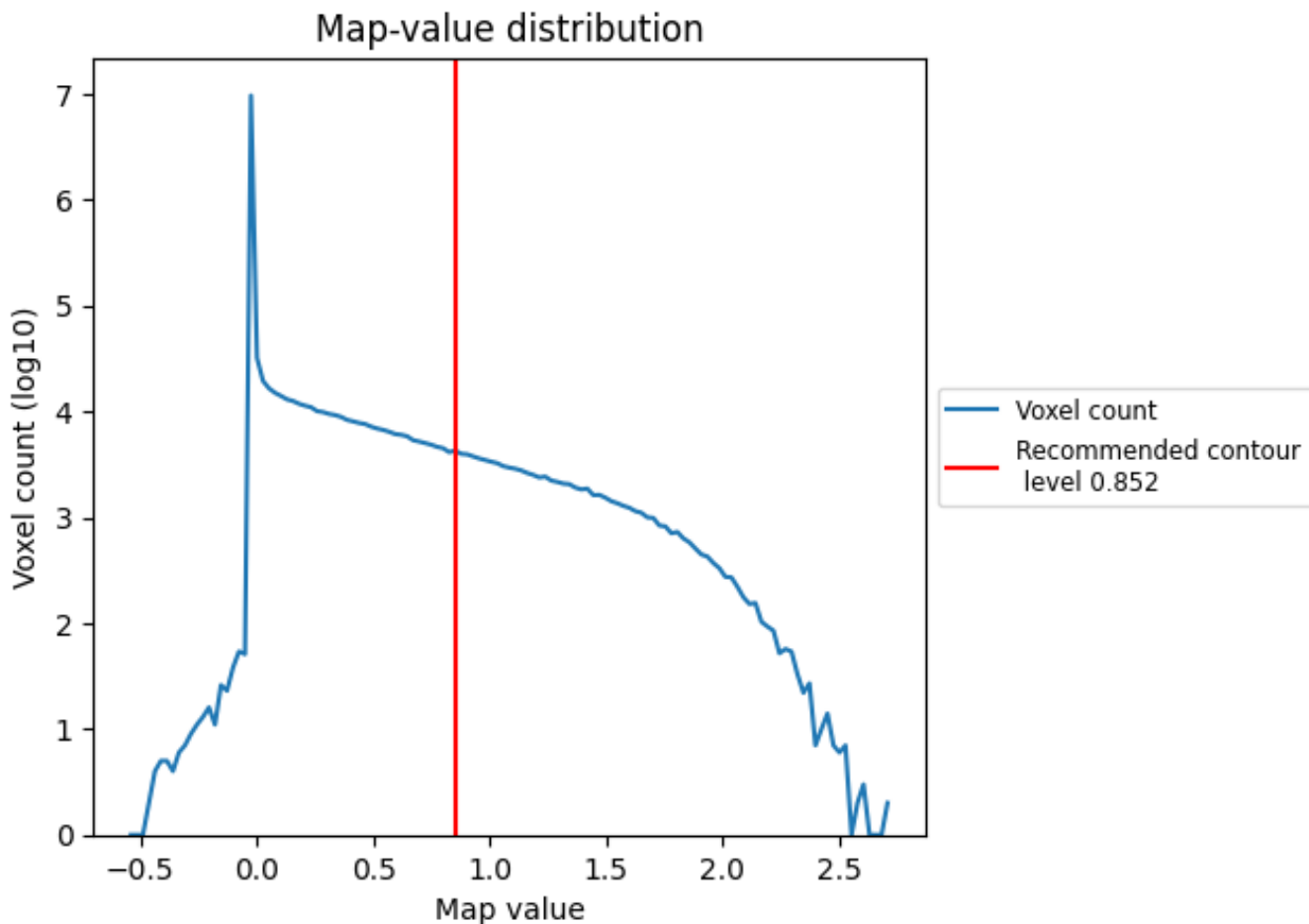
6.5 Mask visualisation

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

7 Map analysis [i](#)

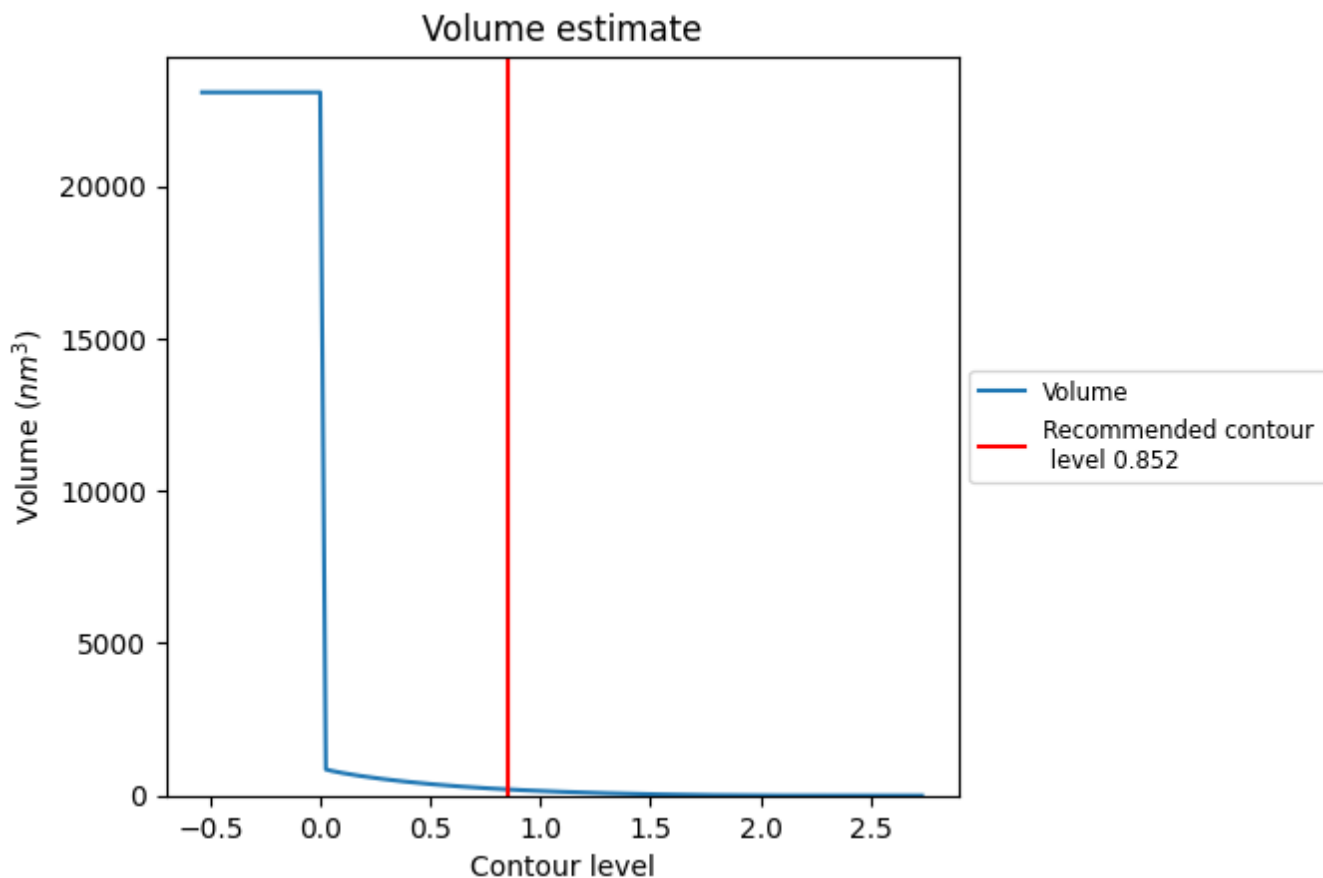
This section contains the results of statistical analysis of the map.

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.

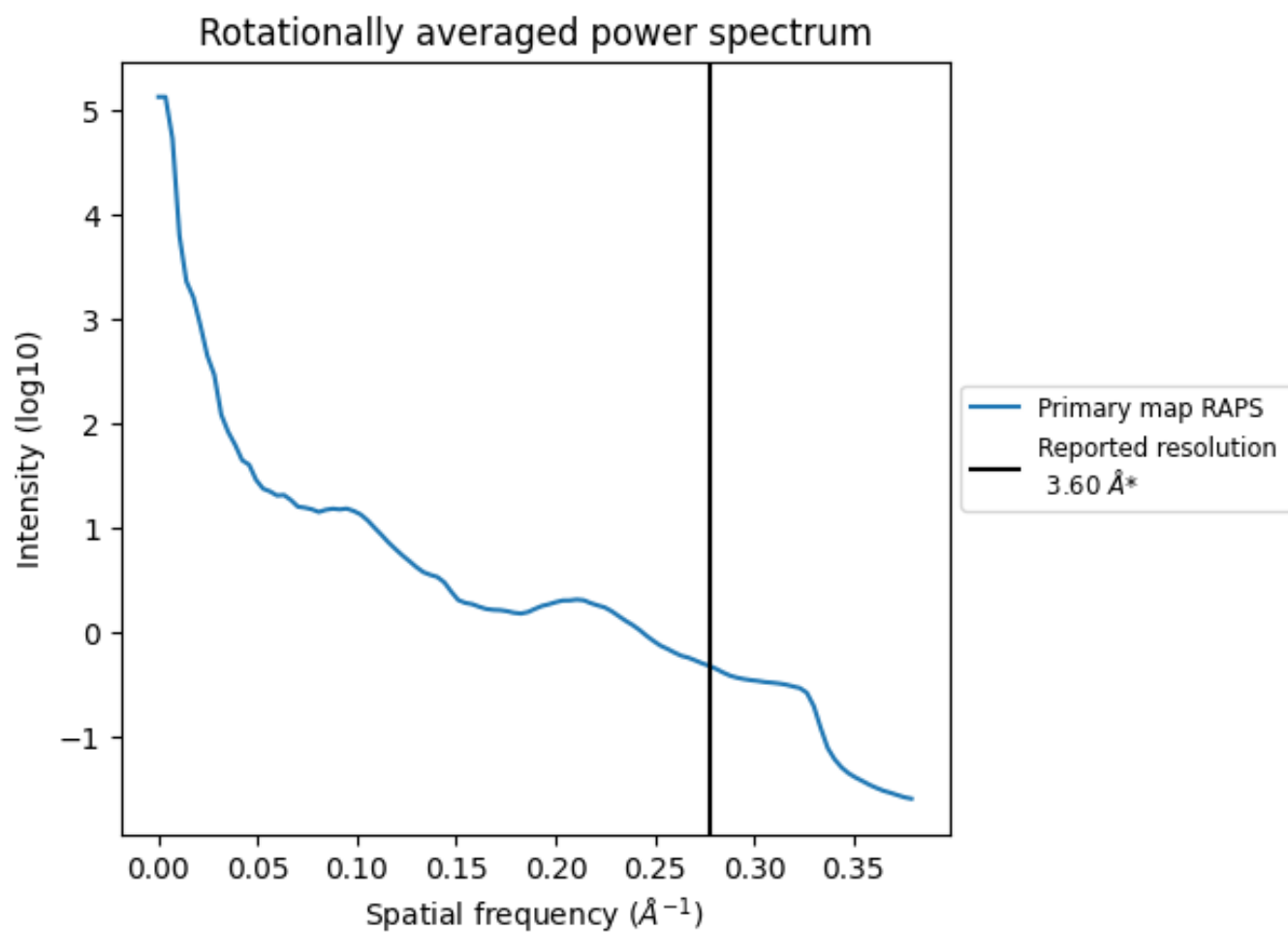
7.2 Volume estimate [i](#)



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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

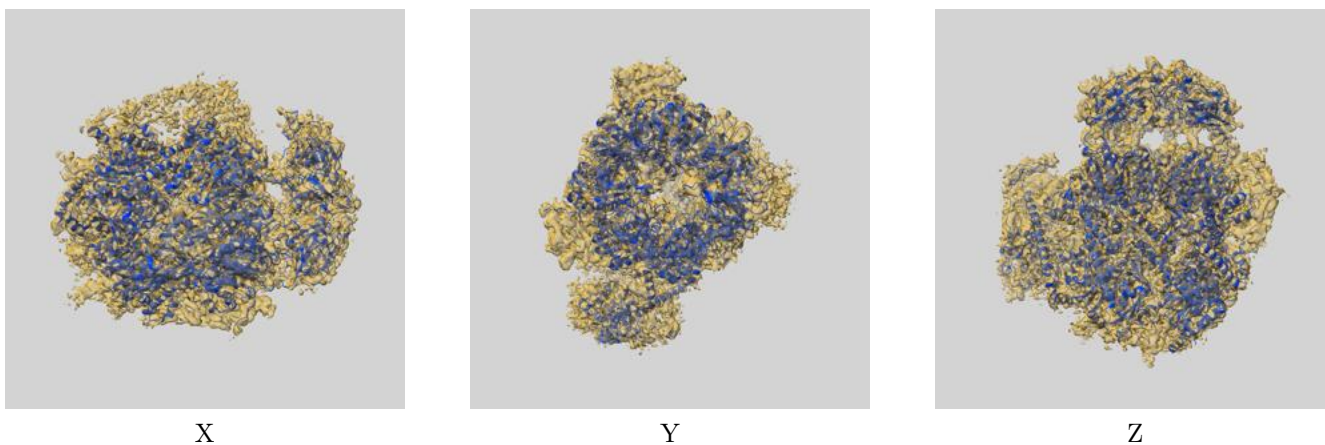
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

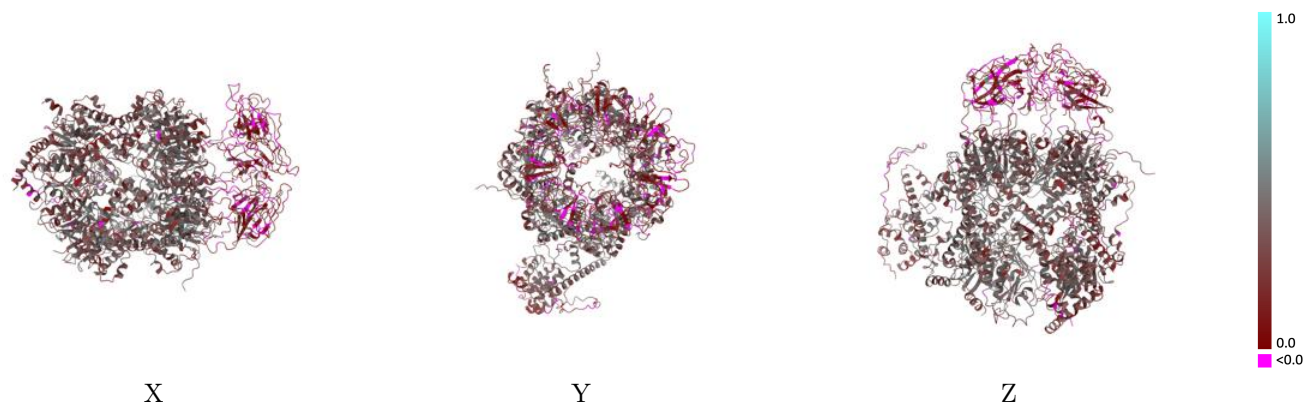
This section contains information regarding the fit between EMDB map EMD-31173 and PDB model 7EKQ. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



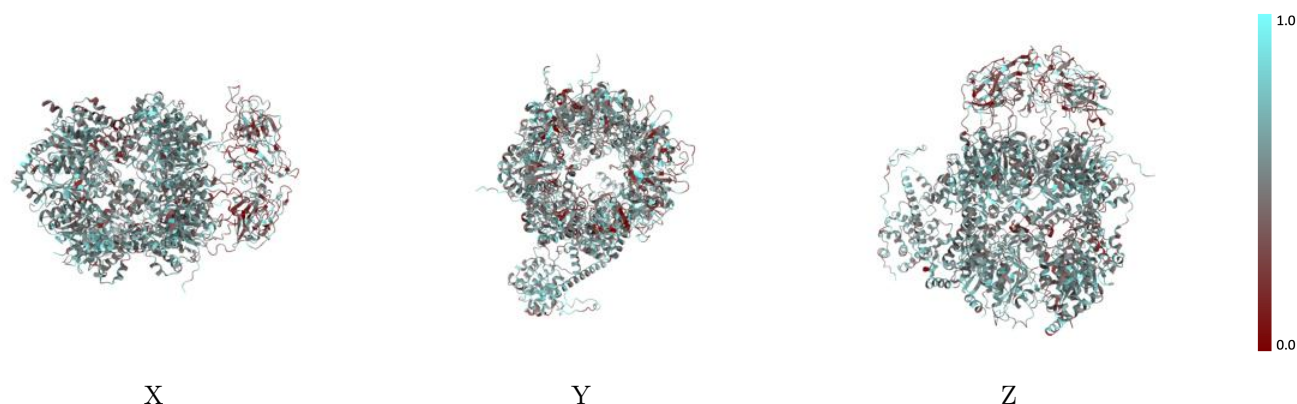
The images above show the 3D surface view of the map at the recommended contour level 0.852 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



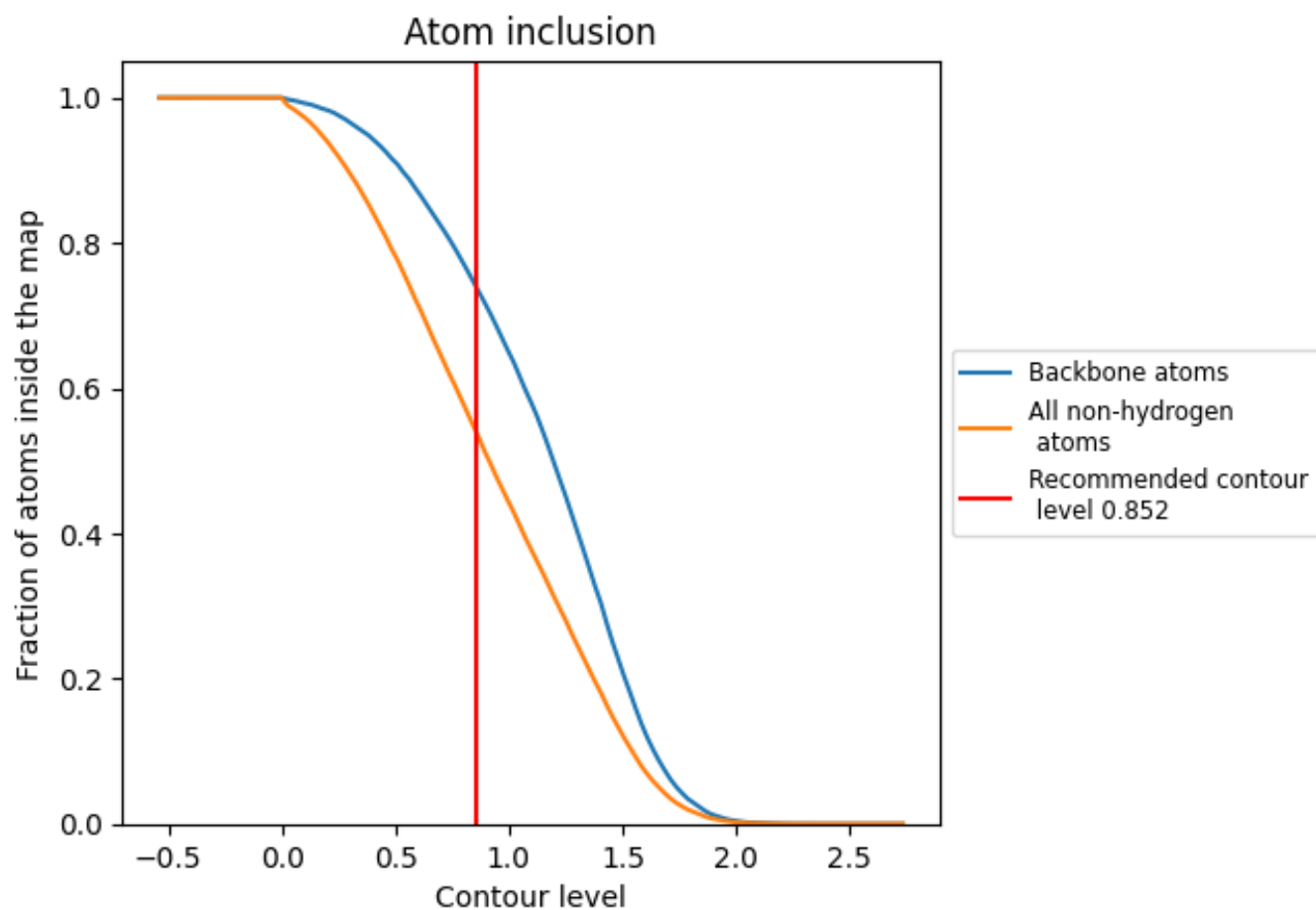
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 [i](#)

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	 0.5421	 0.3040
A	 0.5642	 0.3620
B	 0.5606	 0.3910
C	 0.5655	 0.3790
D	 0.5606	 0.3680
E	 0.5709	 0.3590
F	 0.5661	 0.3380
G	 0.5814	 0.3480
H	 0.6016	 0.3890
I	 0.5900	 0.3630
J	 0.5550	 0.3200
K	 0.5244	 0.2690
L	 0.5805	 0.3440
M	 0.5839	 0.3870
N	 0.5870	 0.3440
O	 0.5611	 0.2790
P	 0.4294	 0.1150
Q	 0.4134	 0.0940
R	 0.4204	 0.1400
S	 0.4274	 0.1190

