W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 – 01:19 PM EST

PDB ID	:	7LXU
EMDB ID	:	EMD-23575
Title	:	Structure of Plasmodium falciparum 20S proteasome with bound MPI-5
Authors	:	Metcalfe, R.D.; Morton, C.J.; Xie, S.C.; Liu, B.; Hanssen, E.; Leis, A.P.; Tilley, L.; Griffin, M.D.W.
Deposited on	:	2021-03-05
Resolution	:	3.10 Å(reported)

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

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

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

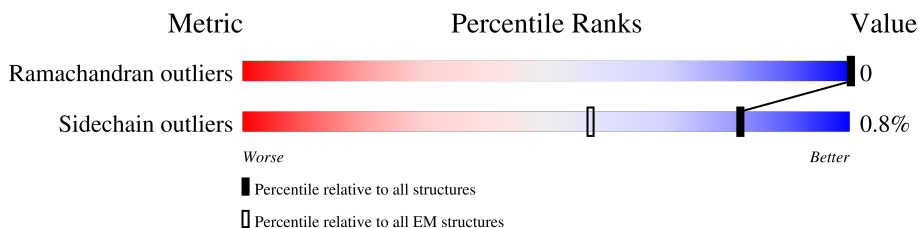The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
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)	:	2.31.2

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
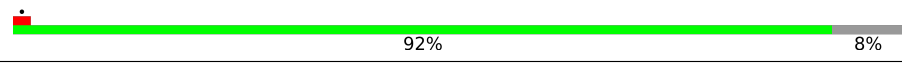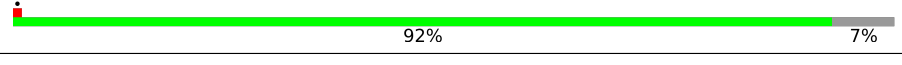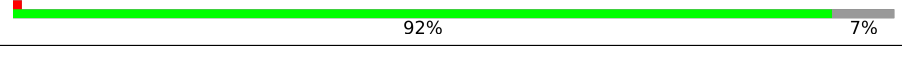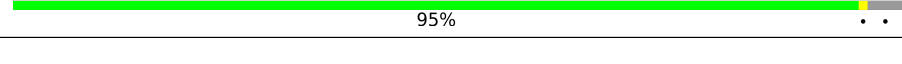
Metric	Percentile Ranks	Value
Ramachandran outliers		0
Sidechain outliers		0.8%

Worse   *Better*

▮ Percentile relative to all structures

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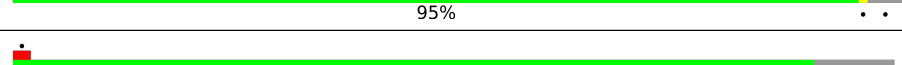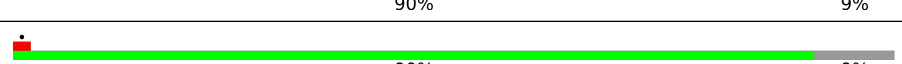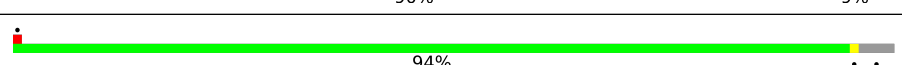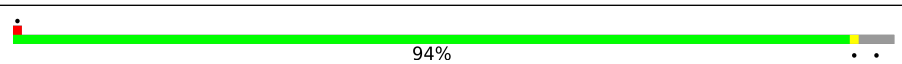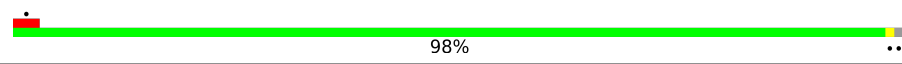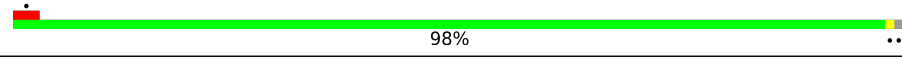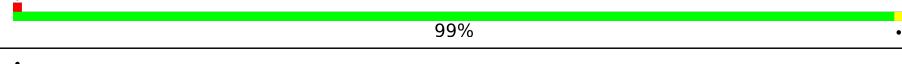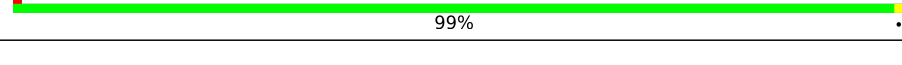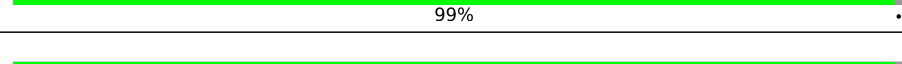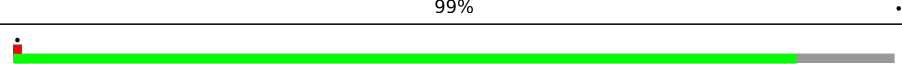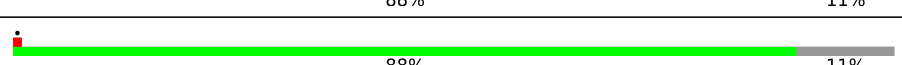
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	260	96% ·
1	O	260	96% ·
2	B	235	97% ·
2	P	235	97% ·
3	C	246	98% ·
3	Q	246	98% ·
4	D	241	95% · ·
4	R	241	95% · ·
5	E	256	92% 8%

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Mol	Chain	Length	Quality of chain
5	S	256	92% 8%
6	F	254	92% 7%
6	T	254	92% 7%
7	G	252	95%
7	U	252	95%
8	H	252	90% 9%
8	V	252	90% 9%
9	I	229	94%
9	W	229	94%
10	J	218	98%
10	X	218	98%
11	K	195	99%
11	Y	195	99%
12	L	211	99%
12	Z	211	99%
13	M	240	88% 11%
13	a	240	88% 11%
14	N	265	87% 12%
14	b	265	87% 12%

2   Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 50778 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 20S proteasome alpha-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	251	Total 1986	C 1248	N 332	O 391	S 15	0	0
1	O	251	Total 1986	C 1248	N 332	O 391	S 15	0	0

- Molecule 2 is a protein called 20S proteasome alpha-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total 1826	C 1175	N 298	O 347	S 6	0	0
2	P	229	Total 1826	C 1175	N 298	O 347	S 6	0	0

- Molecule 3 is a protein called 20S proteasome alpha-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	242	Total 1934	C 1237	N 315	O 378	S 4	0	0
3	Q	242	Total 1934	C 1237	N 315	O 378	S 4	0	0

- Molecule 4 is a protein called 20S proteasome alpha-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	233	Total 1845	C 1178	N 312	O 347	S 8	0	0
4	R	233	Total 1845	C 1178	N 312	O 347	S 8	0	0

- Molecule 5 is a protein called 20S proteasome alpha-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	236	Total 1830	C 1155	N 301	O 363	S 11	0	0
5	S	236	Total 1830	C 1155	N 301	O 363	S 11	0	0

- Molecule 6 is a protein called 20S proteasome alpha-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	235	Total 1866	C 1187	N 308	O 360	S 11	0	0
6	T	235	Total 1866	C 1187	N 308	O 360	S 11	0	0

- Molecule 7 is a protein called 20S proteasome alpha-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	242	Total 1979	C 1257	N 332	O 377	S 13	0	0
7	U	242	Total 1979	C 1257	N 332	O 377	S 13	0	0

- Molecule 8 is a protein called 20S proteasome beta-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total 1846	C 1170	N 317	O 347	S 12	0	0
8	V	229	Total 1846	C 1170	N 317	O 347	S 12	0	0

- Molecule 9 is a protein called 20S proteasome beta-2 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total 1676	C 1058	N 291	O 313	S 14	0	0
9	W	219	Total 1676	C 1058	N 291	O 313	S 14	0	0

- Molecule 10 is a protein called 20S proteasome beta-3 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	215	Total 1698	C 1082	N 275	O 327	S 14	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	X	215	1698	1082	275	327	14	0	0

- Molecule 11 is a protein called 20S proteasome beta-4 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	K	195	1614	1042	266	298	8	0	0
11	Y	195	1614	1042	266	298	8	0	0

- Molecule 12 is a protein called 20S proteasome beta-5 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	L	209	1647	1050	273	317	7	0	0
12	Z	209	1647	1050	273	317	7	0	0

- Molecule 13 is a protein called 20S proteasome beta-6 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	213	1696	1085	283	321	7	0	0
13	a	213	1696	1085	283	321	7	0	0

- Molecule 14 is a protein called 20S proteasome beta-7 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	234	1920	1225	324	363	8	0	0
14	b	234	1920	1225	324	363	8	0	0

- Molecule 15 is N-[(1R)-2-([1,1'-biphenyl]-4-yl)-1-boronoethyl]-1-methyl-L-prolinamide (three-letter code: YHD) (formula: $C_{20}H_{25}BN_2O_3$) (labeled as "Ligand of Interest" by depositor).
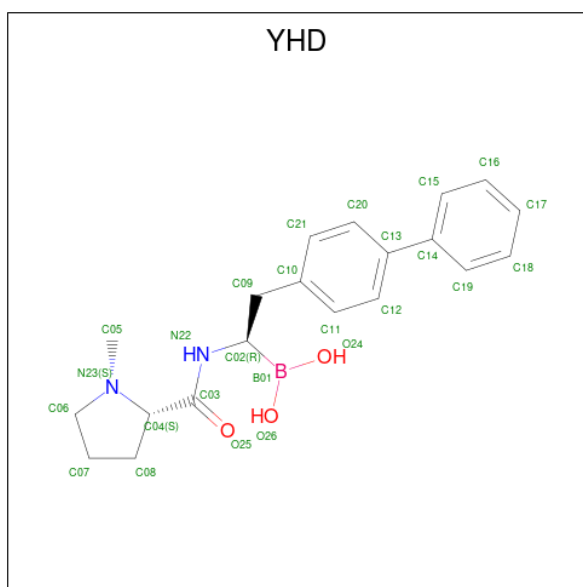
Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	B	C	N	O	0
			26	1	20	2	3	
15	Z	1	Total	B	C	N	O	0
			26	1	20	2	3	

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: 20S proteasome alpha-1 subunit

Chain A:

96%

- Molecule 1: 20S proteasome alpha-1 subunit

Chain O:

96%

- Molecule 2: 20S proteasome alpha-2 subunit

Chain B:

97%

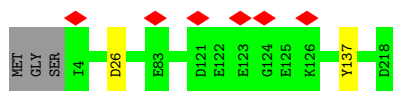- Molecule 2: 20S proteasome alpha-2 subunit

Chain P:

97%

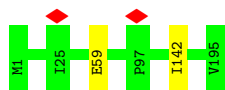- Molecule 3: 20S proteasome alpha-3 subunit

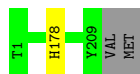Chain C:

98%

- Molecule 3: 20S proteasome alpha-3 subunit

Chain Q: 98%

M1   D41   N80   K242 TYR ILE LYS GLU

• Molecule 4: 20S proteasome alpha-4 subunit

Chain D: 95%

MET S2 K174 K183 D213 E232 R233 T234 LYS ASN ASN GLU GLN ASN GLU

• Molecule 4: 20S proteasome alpha-4 subunit

Chain R: 95%

MET S2 K174 K183 D213 E232 R233 T234 LYS ASN ASN GLU GLN ASN GLU

• Molecule 5: 20S proteasome alpha-5 subunit

Chain E: 92%   8%

MET PHE SER THR ARG SER E7 Y8 D9 L126 SER ASP SER LYS ARG LYS LYS I134 S246 P247 V248 Y249 PRO THR ILE ASP MET THR ALA

• Molecule 5: 20S proteasome alpha-5 subunit

Chain S: 92%   8%

MET PHE SER THR ARG SER E7 Y8 D9 L126 SER ASP SER LYS ARG LYS LYS I134 S246 P247 V248 Y249 PRO THR ILE ASP MET THR ALA

• Molecule 6: 20S proteasome alpha-6 subunit

Chain F: 92%   7%

MET TYR R3 R163 E201 S202 E203 M237 ASP ALA GLU GLN GLU GLN VAL GLU GLU ASN VAL GLN ASN GLU GLN ALA ASN GLU

• Molecule 6: 20S proteasome alpha-6 subunit

Chain T: 92%   7%

MET TYR R3 R163 E201 S202 E203 M237 ASP ALA GLU GLN GLU GLN VAL GLU GLU ASN VAL GLN ASN GLU GLN ALA ASN GLU

• Molecule 7: 20S proteasome alpha-7 subunit

Chain G:

95%

MET ALA GLY LEU S5 R20 K146 H206 K243 E246 TYR ILE GLU LYS LEU ASN

• Molecule 7: 20S proteasome alpha-7 subunit

Chain U:

95%

MET ALA GLY LEU S5 R20 K146 H206 K243 E246 TYR ILE GLU LYS LEU ASN

• Molecule 8: 20S proteasome beta-1 subunit

Chain H:

90%　　　　9%

T1 N28 I82 Y83 D84 GLU THR THR TYR ASP GLU GLU ILE ILE ASP ASP SER ILE ASN TYR LEU ASP TYR ASN ASN ASN ASN D107 N108 N109 L110 V111 N114 F250 Q251 TYR

• Molecule 8: 20S proteasome beta-1 subunit

Chain V:

90%　　　　9%

T1 N28 I82 Y83 D84 GLU THR THR TYR ASP GLU GLU ILE ILE ASP ASP SER ILE ASN TYR LEU ASP TYR ASN ASN ASN ASN D107 N108 N109 N114 F250 Q251 TYR

• Molecule 9: 20S proteasome beta-2 subunit

Chain I:

94%

T1 V26 D144 M194 H198 K216 Y219 ILE LYS LYS PHE ILE SER VAL GLU ASP ALA

• Molecule 9: 20S proteasome beta-2 subunit

Chain W:

94%

T1 V26 D144 M194 H198 K216 Y219 ILE LYS LYS PHE ILE SER VAL GLU ASP ALA

• Molecule 10: 20S proteasome beta-3 subunit

Chain J:

98%

• Molecule 10: 20S proteasome beta-3 subunit

Chain X:

• Molecule 11: 20S proteasome beta-4 subunit

Chain K:

• Molecule 11: 20S proteasome beta-4 subunit

Chain Y:

• Molecule 12: 20S proteasome beta-5 subunit

Chain L:

• Molecule 12: 20S proteasome beta-5 subunit
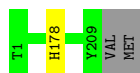
Chain Z:

• Molecule 13: 20S proteasome beta-6 subunit
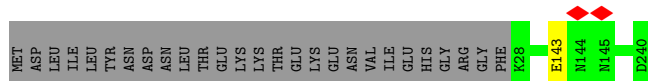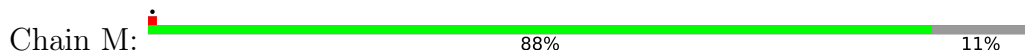
Chain M:

• Molecule 13: 20S proteasome beta-6 subunit

Chain a:

88%　　　　　　　　　　　　　11%

MET ASP LEU ILE LEU TYR ASN ASP ASN LEU THR GLU LYS LYS THR GLU LYS GLU ASN VAL ILE GLU HIS GLY ARG GLY PHE K28 R29 E143 N144 N145 D240
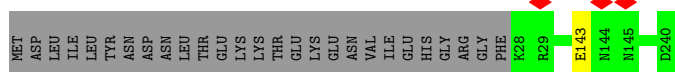
• Molecule 14: 20S proteasome beta-7 subunit

Chain N:

87%　　　　　　　　　　　　　12%

MET T2 N75 L109 L132 TYR THR ASN LYS ASN ASN ASP GLU GLN ASN GLU TYR LYS ASN ASN E149 L242 Y251 VAL TYR PRO SER THR LEU LEU PRO PRO ALA GLY CYS MET TRP

• Molecule 14: 20S proteasome beta-7 subunit

Chain b:

87%　　　　　　　　　　　　　12%

MET T2 N75 L109 L132 TYR THR ASN LYS ASN ASN ASP GLU GLN ASN GLU TYR LYS ASN ASN E149 L242 Y251 VAL TYR PRO SER THR LEU LEU PRO PRO ALA GLY CYS MET TRP
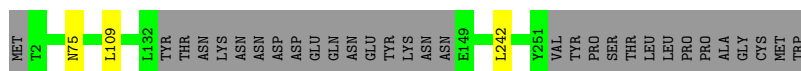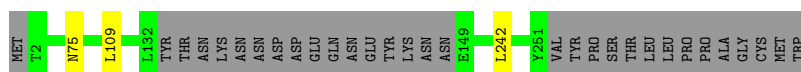
4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/Å^2)$	50	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	45.612	Depositor
Minimum map value	-22.978	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5.0	Depositor
Map size (Å)	524.0, 524.0, 524.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.31, 1.31, 1.31	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.34	0/2013	0.49	0/2715
1	O	0.34	0/2013	0.49	0/2715
2	B	0.34	0/1860	0.47	0/2512
2	P	0.34	0/1860	0.47	0/2512
3	C	0.35	0/1969	0.45	0/2665
3	Q	0.35	0/1969	0.45	0/2665
4	D	0.32	0/1875	0.44	0/2530
4	R	0.32	0/1875	0.44	0/2530
5	E	0.31	0/1856	0.46	0/2509
5	S	0.31	0/1856	0.46	0/2509
6	F	0.34	0/1900	0.45	0/2558
6	T	0.34	0/1900	0.45	0/2558
7	G	0.35	0/2022	0.47	0/2733
7	U	0.35	0/2022	0.47	0/2733
8	H	0.37	0/1877	0.51	0/2520
8	V	0.37	0/1877	0.51	0/2520
9	I	0.33	0/1712	0.52	0/2328
9	W	0.33	0/1712	0.52	0/2328
10	J	0.36	0/1727	0.49	0/2331
10	X	0.35	0/1727	0.49	0/2331
11	K	0.35	0/1649	0.48	0/2223
11	Y	0.35	0/1649	0.48	0/2223
12	L	0.35	0/1681	0.48	0/2266
12	Z	0.35	0/1681	0.48	0/2266
13	M	0.34	0/1728	0.46	0/2339
13	a	0.34	0/1728	0.46	0/2339
14	N	0.37	0/1959	0.52	2/2645 (0.1%)
14	b	0.37	0/1959	0.52	2/2645 (0.1%)
All	All	0.34	0/51656	0.48	4/69748 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	N	109	LEU	CA-CB-CG	6.63	130.56	115.30
14	b	109	LEU	CA-CB-CG	6.63	130.55	115.30
14	N	242	LEU	CA-CB-CG	5.26	127.39	115.30
14	b	242	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2　Too-close contacts ⓘ

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

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/260 (96%)	224 (90%)	25 (10%)	0	100	100
1	O	249/260 (96%)	224 (90%)	25 (10%)	0	100	100
2	B	227/235 (97%)	214 (94%)	13 (6%)	0	100	100
2	P	227/235 (97%)	213 (94%)	14 (6%)	0	100	100
3	C	240/246 (98%)	224 (93%)	16 (7%)	0	100	100
3	Q	240/246 (98%)	224 (93%)	16 (7%)	0	100	100
4	D	231/241 (96%)	216 (94%)	15 (6%)	0	100	100
4	R	231/241 (96%)	216 (94%)	15 (6%)	0	100	100
5	E	232/256 (91%)	221 (95%)	11 (5%)	0	100	100
5	S	232/256 (91%)	221 (95%)	11 (5%)	0	100	100
6	F	233/254 (92%)	214 (92%)	19 (8%)	0	100	100
6	T	233/254 (92%)	214 (92%)	19 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	240/252 (95%)	224 (93%)	16 (7%)	0	100	100
7	U	240/252 (95%)	224 (93%)	16 (7%)	0	100	100
8	H	225/252 (89%)	211 (94%)	14 (6%)	0	100	100
8	V	225/252 (89%)	211 (94%)	14 (6%)	0	100	100
9	I	217/229 (95%)	194 (89%)	23 (11%)	0	100	100
9	W	217/229 (95%)	194 (89%)	23 (11%)	0	100	100
10	J	213/218 (98%)	191 (90%)	22 (10%)	0	100	100
10	X	213/218 (98%)	191 (90%)	22 (10%)	0	100	100
11	K	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
11	Y	193/195 (99%)	181 (94%)	12 (6%)	0	100	100
12	L	207/211 (98%)	186 (90%)	21 (10%)	0	100	100
12	Z	207/211 (98%)	186 (90%)	21 (10%)	0	100	100
13	M	211/240 (88%)	194 (92%)	17 (8%)	0	100	100
13	a	211/240 (88%)	194 (92%)	17 (8%)	0	100	100
14	N	230/265 (87%)	208 (90%)	22 (10%)	0	100	100
14	b	230/265 (87%)	208 (90%)	22 (10%)	0	100	100
All	All	6296/6708 (94%)	5803 (92%)	493 (8%)	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	222/231 (96%)	221 (100%)	1 (0%)	88	94
1	O	222/231 (96%)	221 (100%)	1 (0%)	88	94
2	B	201/205 (98%)	200 (100%)	1 (0%)	88	94
2	P	201/205 (98%)	200 (100%)	1 (0%)	88	94
3	C	209/213 (98%)	208 (100%)	1 (0%)	88	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Q	209/213 (98%)	208 (100%)	1 (0%)	88	94
4	D	199/207 (96%)	195 (98%)	4 (2%)	55	80
4	R	199/207 (96%)	195 (98%)	4 (2%)	55	80
5	E	204/223 (92%)	204 (100%)	0	100	100
5	S	204/223 (92%)	204 (100%)	0	100	100
6	F	210/227 (92%)	209 (100%)	1 (0%)	88	94
6	T	210/227 (92%)	209 (100%)	1 (0%)	88	94
7	G	221/229 (96%)	218 (99%)	3 (1%)	67	86
7	U	221/229 (96%)	218 (99%)	3 (1%)	67	86
8	H	208/231 (90%)	207 (100%)	1 (0%)	88	94
8	V	208/231 (90%)	207 (100%)	1 (0%)	88	94
9	I	185/194 (95%)	182 (98%)	3 (2%)	62	84
9	W	185/194 (95%)	182 (98%)	3 (2%)	62	84
10	J	189/191 (99%)	187 (99%)	2 (1%)	73	89
10	X	189/191 (99%)	187 (99%)	2 (1%)	73	89
11	K	174/174 (100%)	172 (99%)	2 (1%)	73	89
11	Y	174/174 (100%)	172 (99%)	2 (1%)	73	89
12	L	174/176 (99%)	173 (99%)	1 (1%)	86	94
12	Z	174/176 (99%)	173 (99%)	1 (1%)	86	94
13	M	191/216 (88%)	190 (100%)	1 (0%)	88	94
13	a	191/216 (88%)	190 (100%)	1 (0%)	88	94
14	N	210/239 (88%)	209 (100%)	1 (0%)	88	94
14	b	210/239 (88%)	209 (100%)	1 (0%)	88	94
All	All	5594/5912 (95%)	5550 (99%)	44 (1%)	82	92

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	233	ARG
9	W	144	ASP
6	T	163	ARG
7	U	243	LYS
10	X	26	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
6	T	138	HIS
8	V	38	ASN
14	b	89	GLN
10	X	80	GLN
7	G	74	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
15	YHD	Z	301	12	24,28,28	1.89	6 (25%)	33,38,38	2.91	19 (57%)
15	YHD	L	301	12	24,28,28	1.89	6 (25%)	33,38,38	2.91	20 (60%)

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
15	YHD	Z	301	12	-	9/15/30/30	0/3/3/3
15	YHD	L	301	12	-	9/15/30/30	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	301	YHD	C14-C13	5.51	1.62	1.49
15	Z	301	YHD	C14-C13	5.50	1.62	1.49
15	Z	301	YHD	C09-C02	2.87	1.58	1.53
15	L	301	YHD	C09-C02	2.86	1.58	1.53
15	Z	301	YHD	O25-C03	2.32	1.28	1.23

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	301	YHD	C21-C10-C11	-5.84	108.99	118.17
15	Z	301	YHD	C21-C10-C11	-5.82	109.01	118.17
15	L	301	YHD	C20-C13-C12	-5.35	106.93	117.59
15	Z	301	YHD	C20-C13-C12	-5.33	106.95	117.59
15	L	301	YHD	C18-C19-C14	4.56	126.29	120.56

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	301	YHD	B01-C02-C09-C10
15	Z	301	YHD	B01-C02-C09-C10
15	L	301	YHD	C20-C13-C14-C19
15	Z	301	YHD	C20-C13-C14-C19
15	L	301	YHD	C12-C13-C14-C19

There are no ring outliers.

No monomer is involved in short contacts.

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 YHD Z 301

Bond lengths

Bond angles

Torsions

Rings

Ligand YHD L 301

Bond lengths

Bond angles

Torsions

Rings
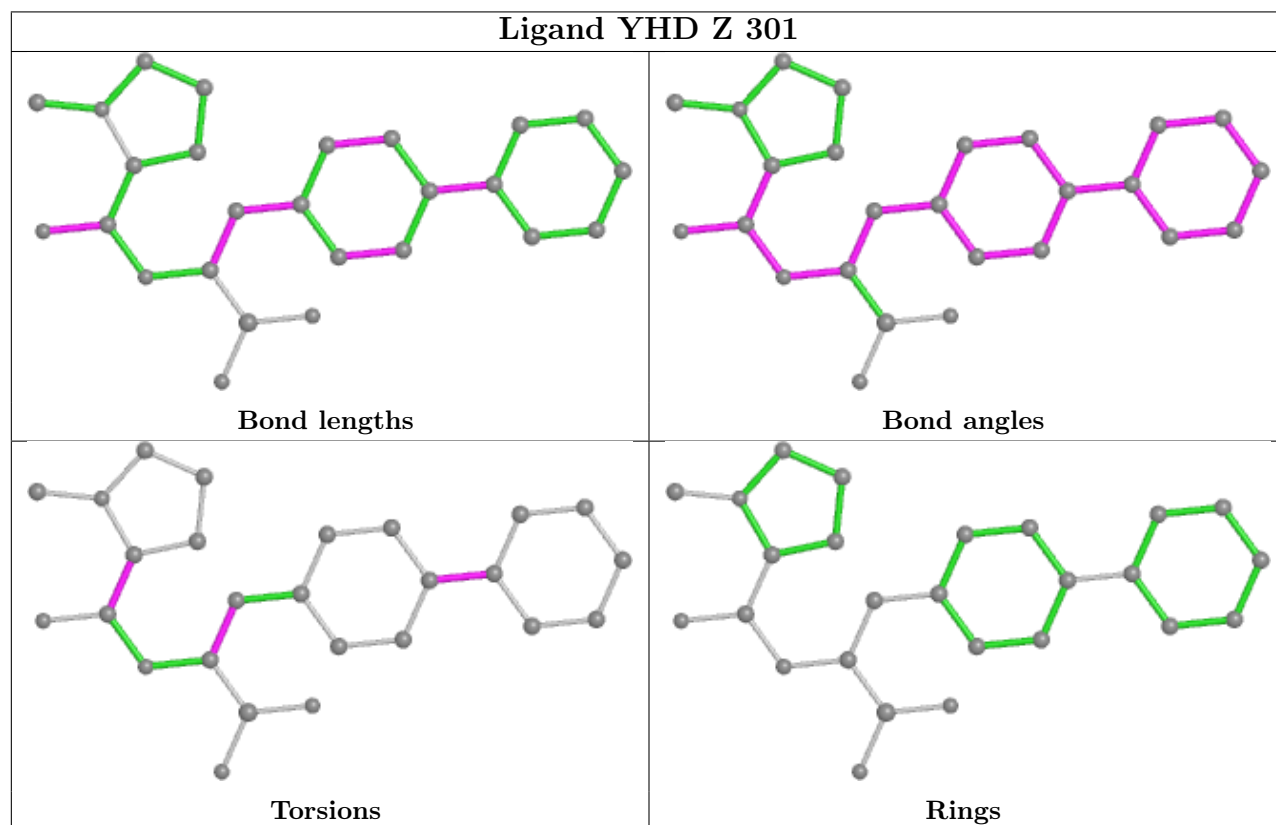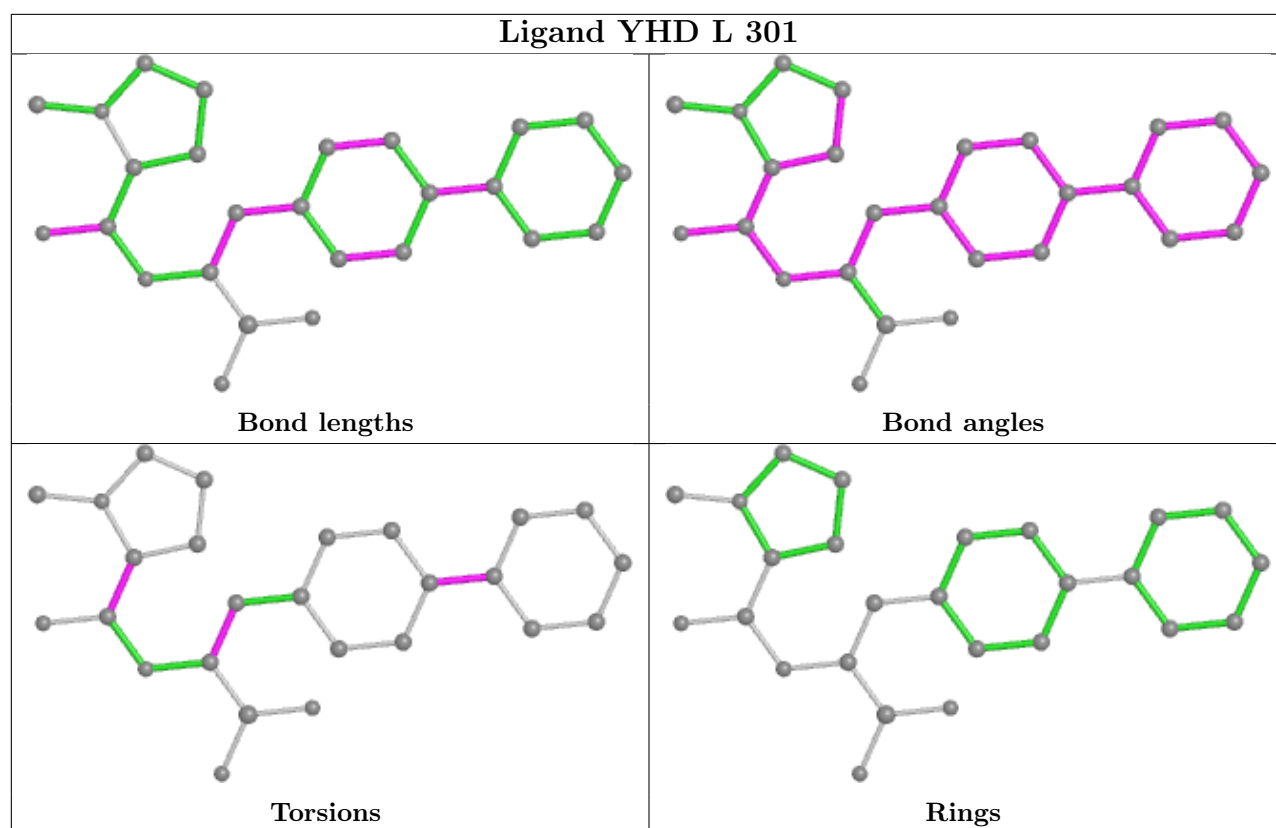
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23575. 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 (i)

6.1.1   Primary map
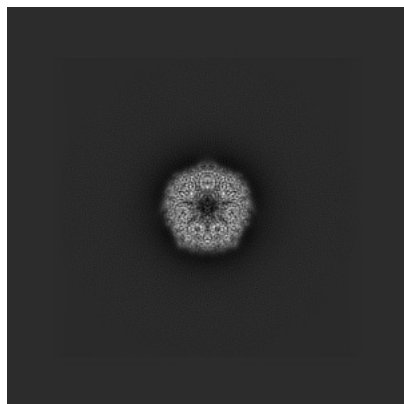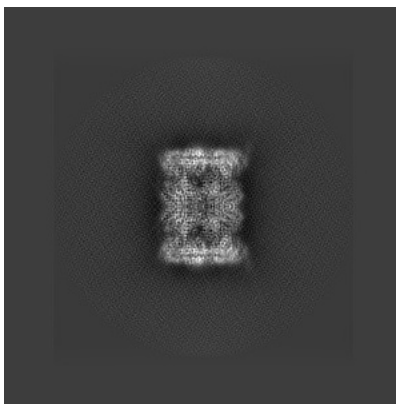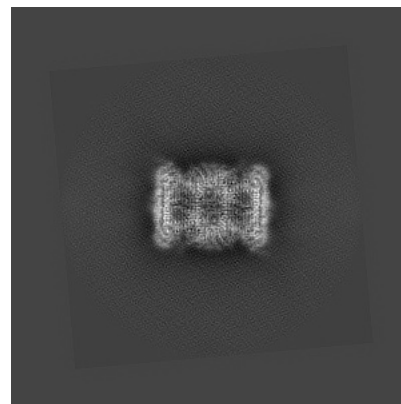
| X | Y | Z |

6.1.2   Raw map

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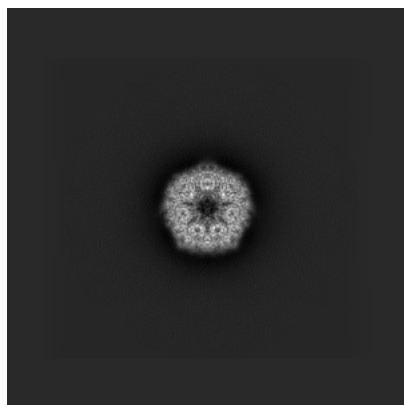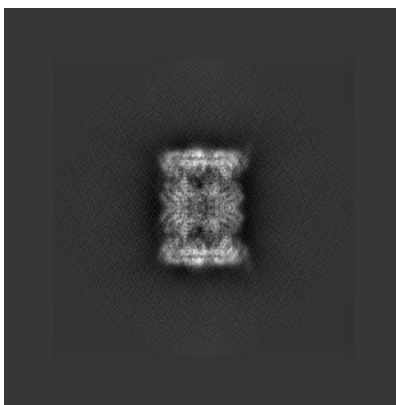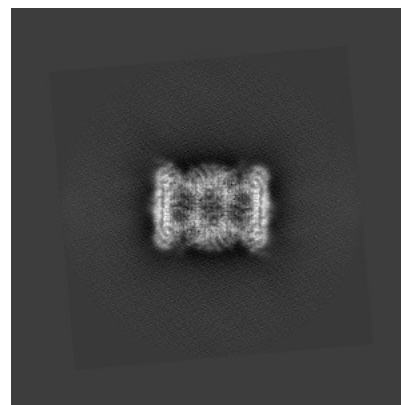
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
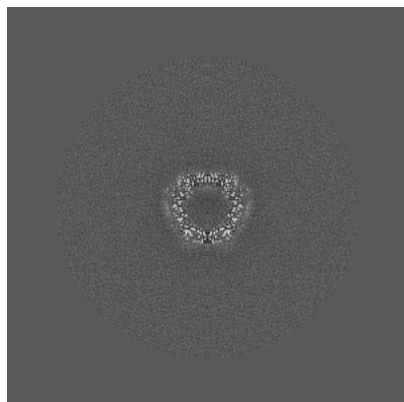
6.2.1   Primary map
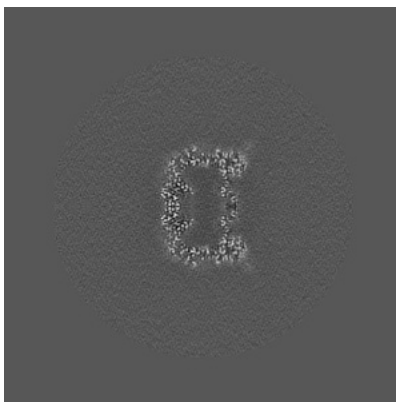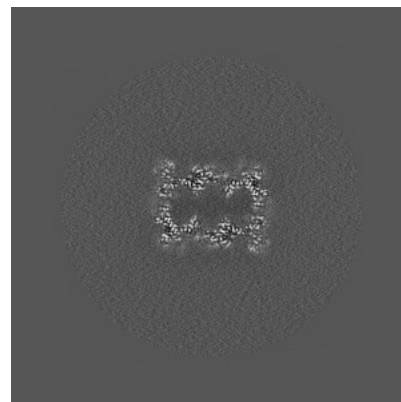
| X Index: 200 | Y Index: 200 | Z Index: 200 |

6.2.2   Raw map
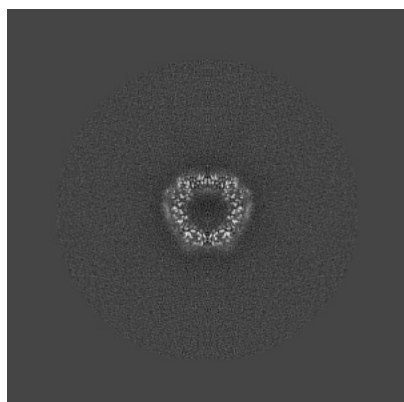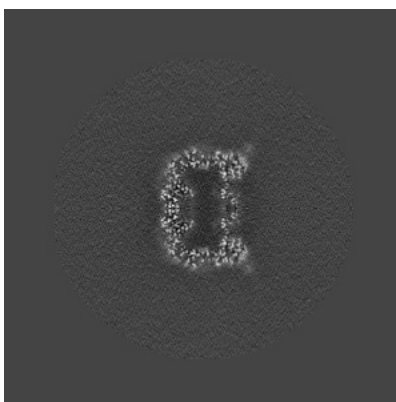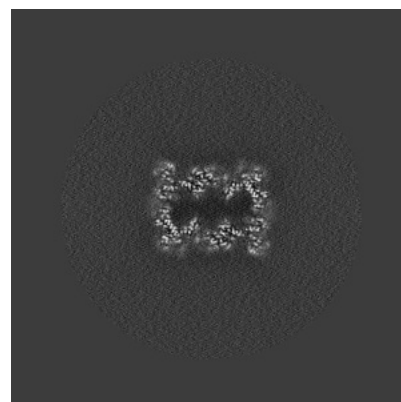
| X Index: 200 | Y Index: 200 | Z Index: 200 |

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

6.3 Largest variance slices (i)

6.3.1 Primary map
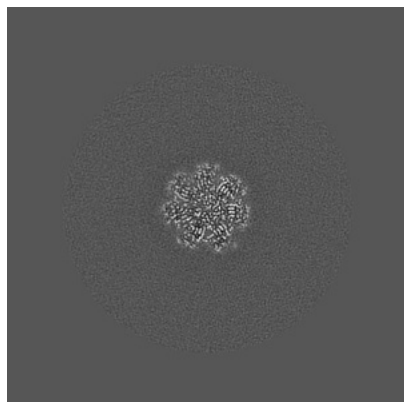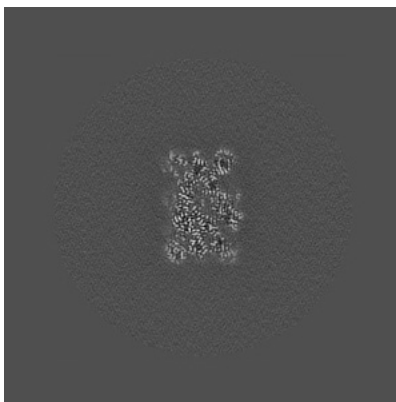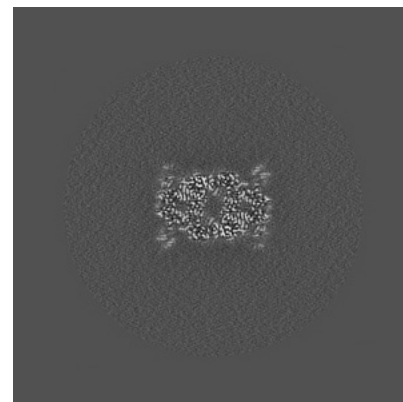
| X Index: 244 | Y Index: 222 | Z Index: 181 |

6.3.2 Raw map
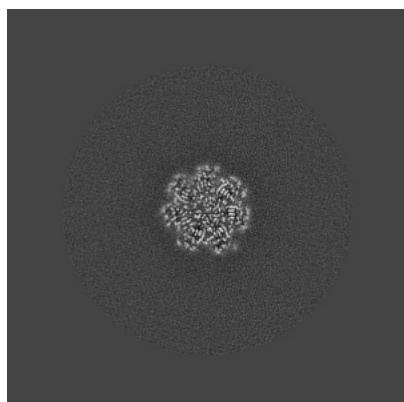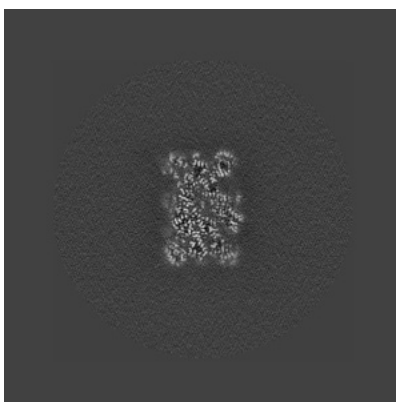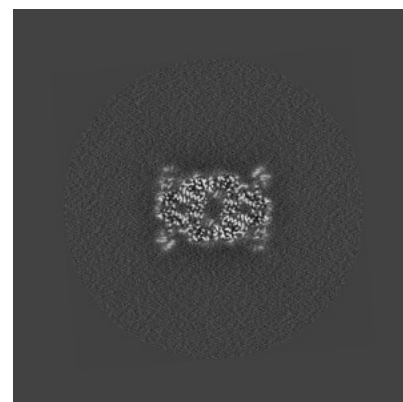
| X Index: 244 | Y Index: 222 | Z Index: 181 |

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
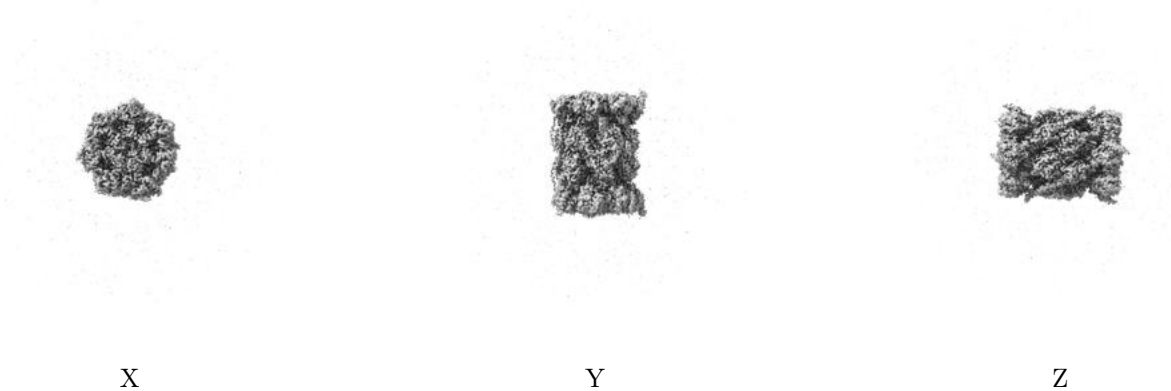
The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

| X | Y | Z |

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

6.5 Mask visualisation ⓘ

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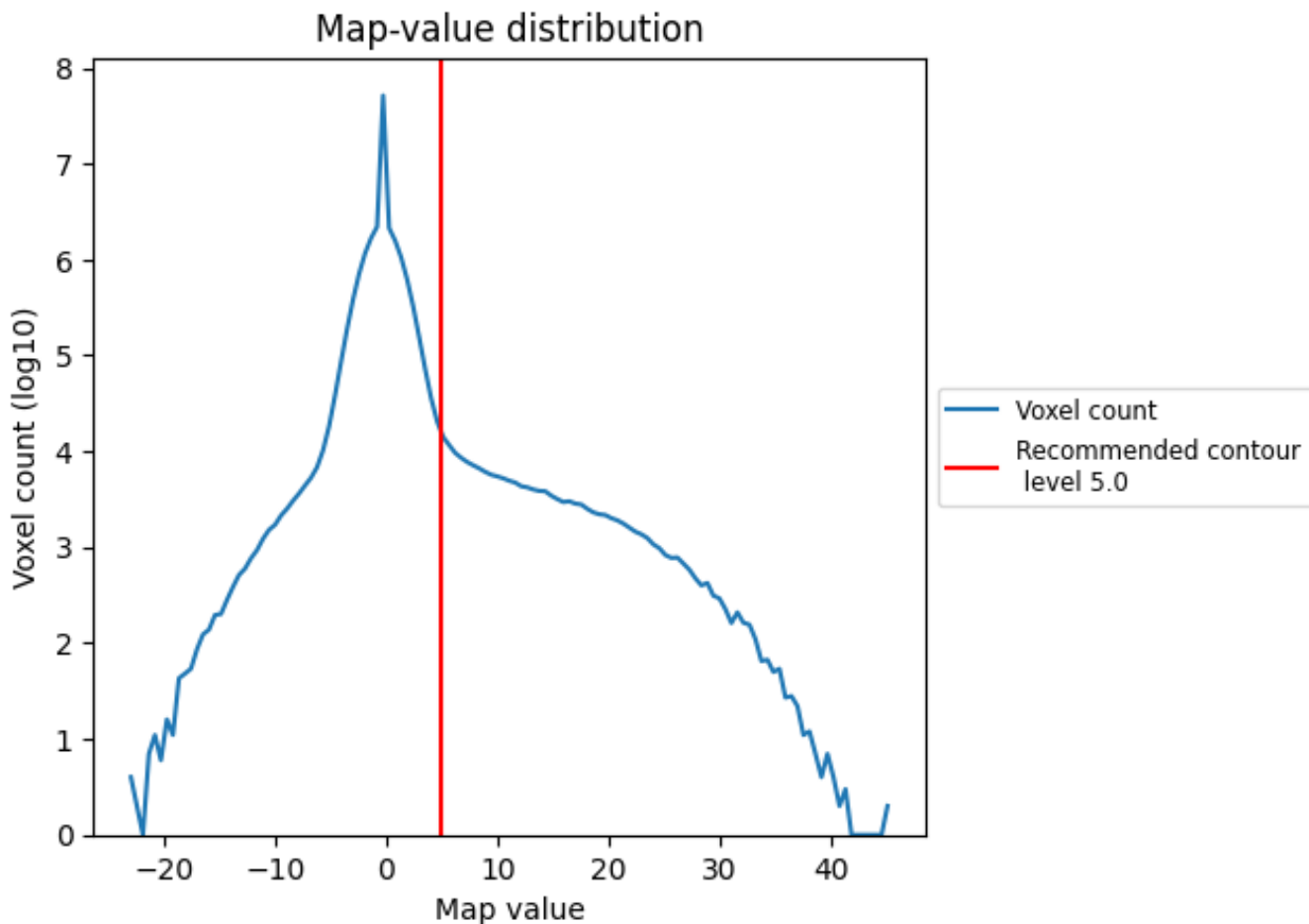
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2   Volume estimate ⓘ
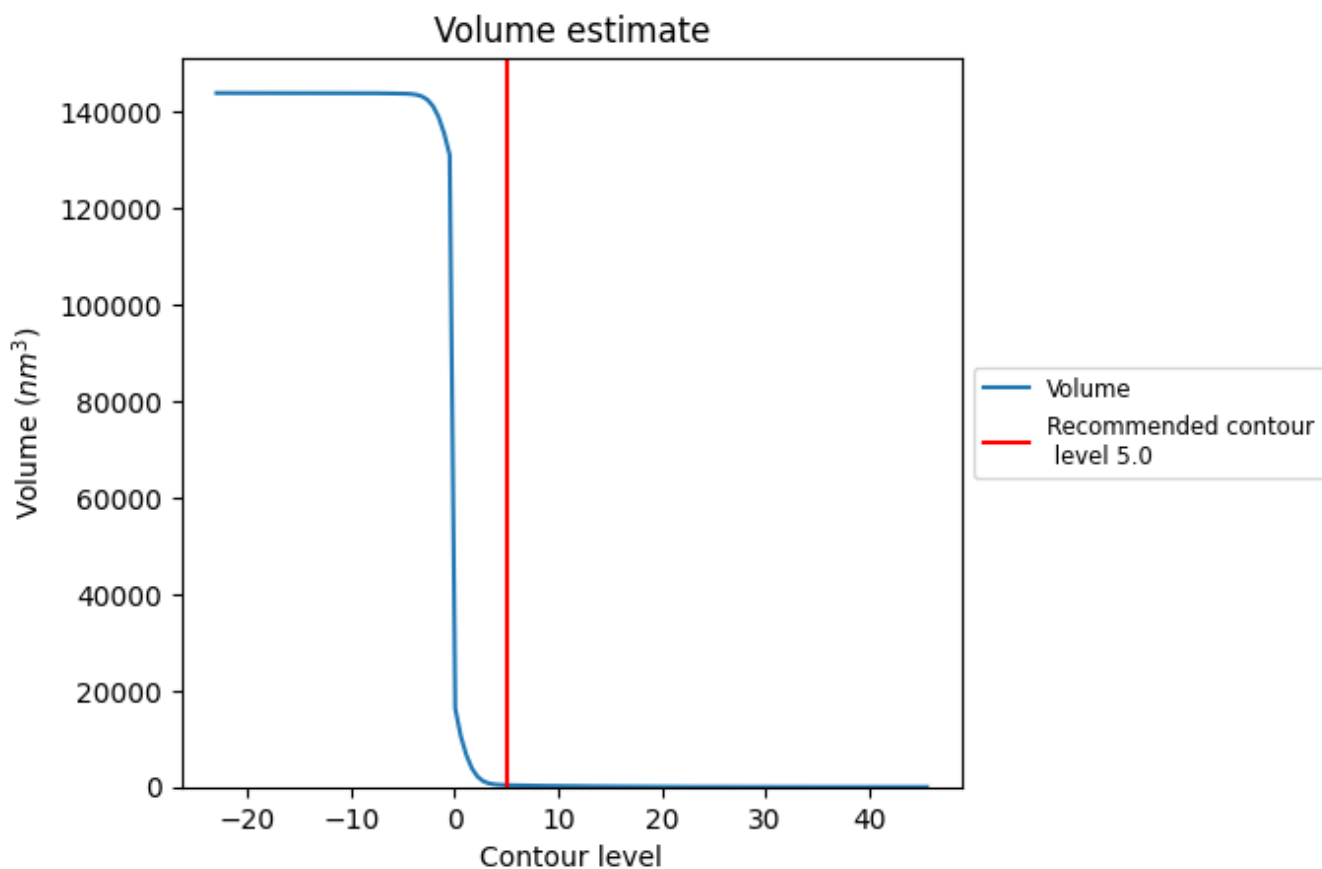
The volume at the recommended contour level is 381 nm^3; this corresponds to an approximate mass of 344 kDa.

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 ⓘ
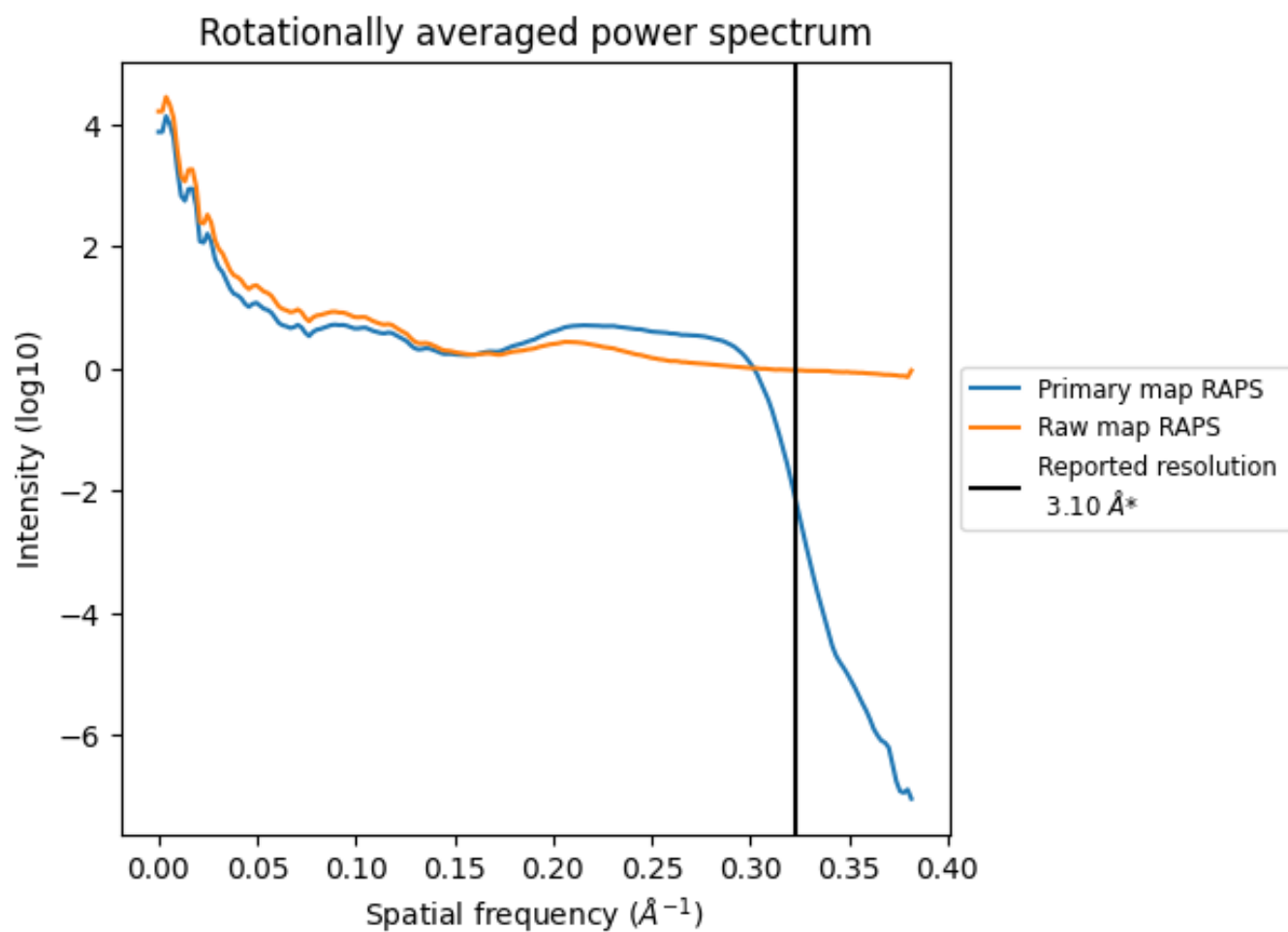
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 ⓘ
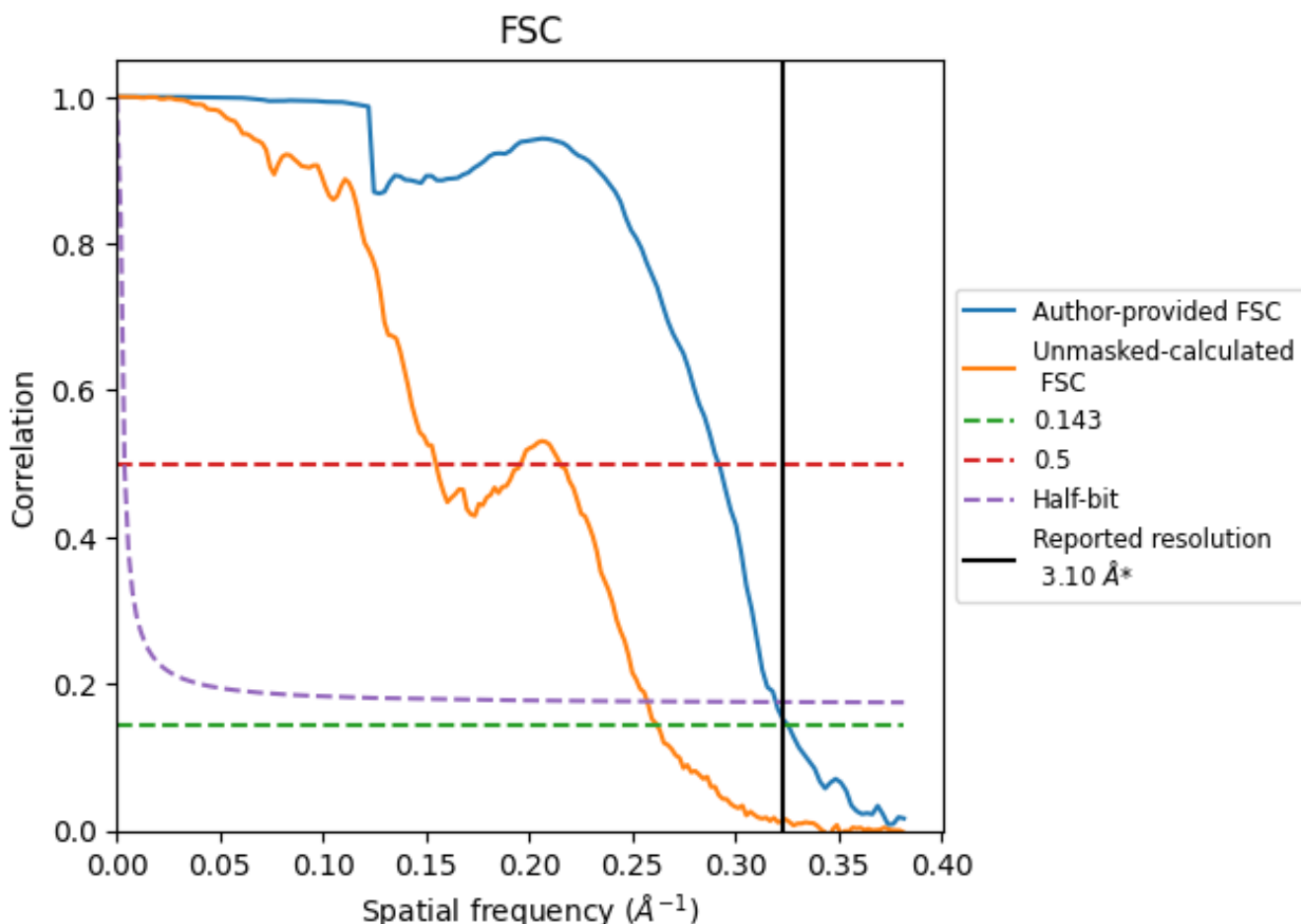
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2   Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.43	3.13
Unmasked-calculated*	3.82	6.46	3.89

*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 3.82 differs from the reported value 3.1 by more than 10 %

9   Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-23575 and PDB model 7LXU. Per-residue inclusion information can be found in section 3 on page 8.

9.1   Map-model overlay ⓘ

| X | Y | Z |
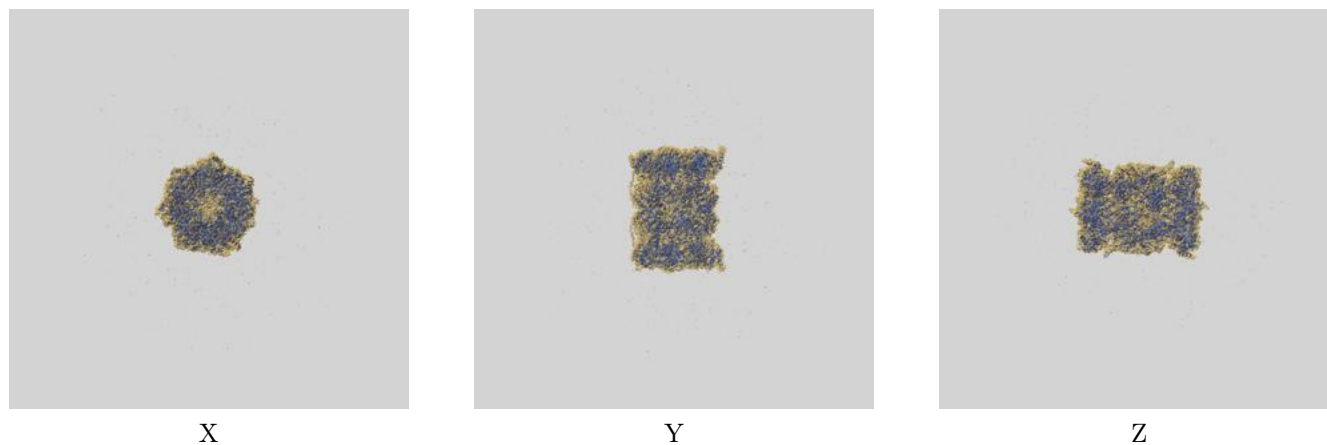
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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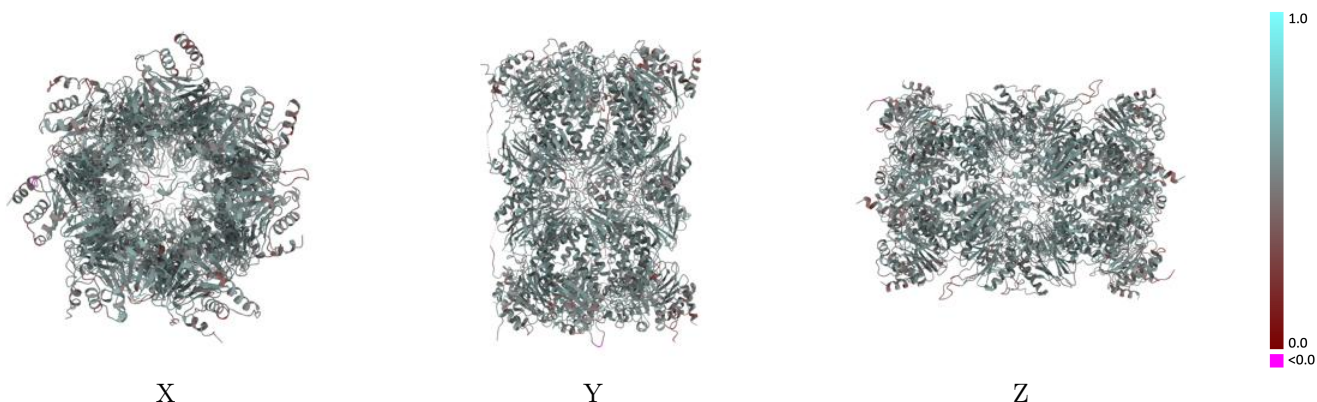
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3   Atom inclusion mapped to coordinate model ⓘ

| X | Y | Z |
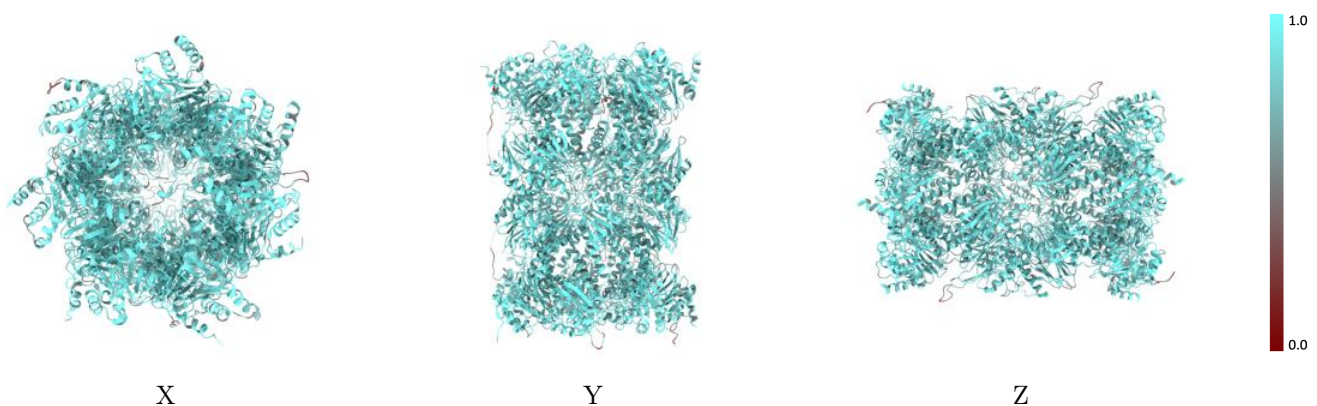
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (5.0).

9.4   Atom inclusion ⓘ
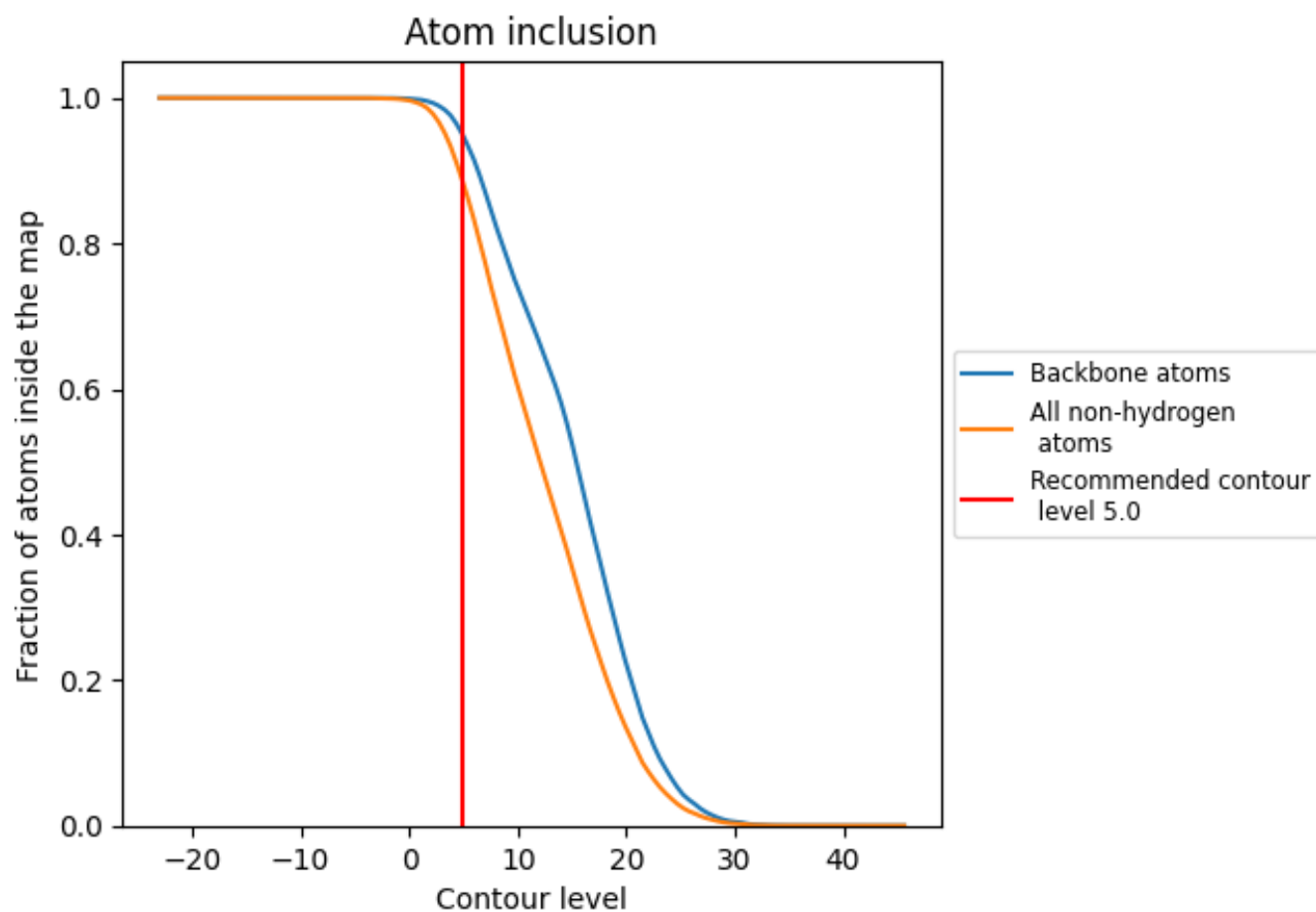
At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (5.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8821	0.5240
A	0.8664	0.5140
B	0.9081	0.5300
C	0.8878	0.5130
D	0.8732	0.5090
E	0.8594	0.5060
F	0.8717	0.5180
G	0.9032	0.5270
H	0.8856	0.5320
I	0.8758	0.5150
J	0.8573	0.5260
K	0.8658	0.5370
L	0.8771	0.5320
M	0.8925	0.5380
N	0.9142	0.5400
O	0.8654	0.5150
P	0.9058	0.5300
Q	0.8915	0.5150
R	0.8716	0.5070
S	0.8605	0.5050
T	0.8707	0.5170
U	0.9047	0.5270
V	0.8878	0.5320
W	0.8818	0.5150
X	0.8639	0.5240
Y	0.8690	0.5350
Z	0.8734	0.5340
a	0.8907	0.5370
b	0.9142	0.5390

1.0

0.0
<0.0