WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 12:10 am GMT

PDB ID	:	6TCZ
EMDB ID	:	EMD-10462
Title	:	Leishmania tarentolae proteasome 20S subunit complexed with LXE408
Authors	:	Srinivas, H.
Deposited on	:	2019-11-07
Resolution	:	3.40 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.dev43
Mogul	:	1.8.4, 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)	:	2.31.3

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
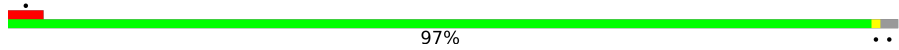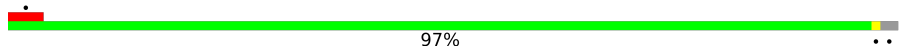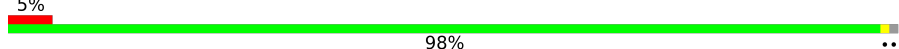*ELECTRON MICROSCOPY*
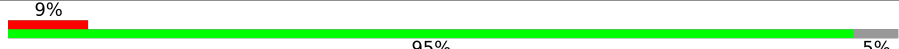
The reported resolution of this entry is 3.40 Å.

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

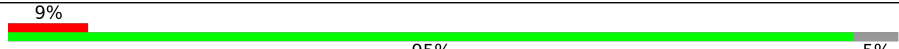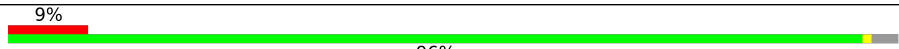| Metric	Percentile Ranks	Value
Ramachandran outliers		0.0%
Sidechain outliers		1.1%

Worse   *Better*

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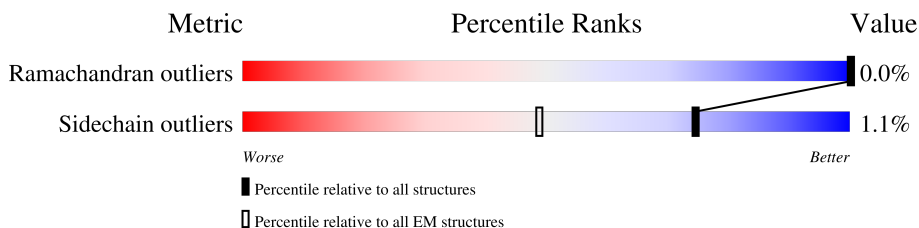
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	250	97% ··
1	a	250	97% ··
2	B	231	5% 98% ··
2	b	231	5% 98% ··
3	C	285	9% 95% 5%
3	c	285	9% 95% 5%
4	D	248	9% 96% ··
4	d	248	9% 96% ··
5	E	344	67% · 32%

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Mol	Chain	Length	Quality of chain
5	e	344	5% / 67% / 32%
6	F	428	55% / 44%
6	f	428	55% / 44%
7	G	238	5% / 96%
7	g	238	96%
8	H	283	80% / 19%
8	h	283	80% / 19%
9	I	254	8% / 85% / 14%
9	i	254	6% / 85% / 14%
10	J	205	99%
10	j	205	99%
11	K	206	100%
11	k	206	100%
12	L	302	67% / 33%
12	l	302	67% / 33%
13	M	339	63% / 37%
13	m	339	63% / 37%
14	N	220	99%
14	n	220	99%

2 Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 49248 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 Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		
1	a	245	Total	C	N	O	S	0	0
			1861	1171	324	354	12		

- Molecule 2 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		
2	b	229	Total	C	N	O	S	0	0
			1753	1112	292	341	8		

- Molecule 3 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		
3	c	272	Total	C	N	O	S	0	0
			2155	1357	371	415	12		

- Molecule 4 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		
4	d	240	Total	C	N	O	S	0	0
			1882	1186	324	364	8		

- Molecule 5 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	235	Total 1802	C 1119	N 315	O 356	S 12	0	0
5	e	235	Total 1802	C 1119	N 315	O 356	S 12	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total 1869	C 1173	N 325	O 359	S 12	0	0
6	f	238	Total 1869	C 1173	N 325	O 359	S 12	0	0

- Molecule 7 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	230	Total 1741	C 1085	N 308	O 338	S 10	0	0
7	g	230	Total 1741	C 1085	N 308	O 338	S 10	0	0

- Molecule 8 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	229	Total 1709	C 1062	N 295	O 340	S 12	0	0
8	h	229	Total 1709	C 1062	N 295	O 340	S 12	0	0

- Molecule 9 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	219	Total 1659	C 1037	N 292	O 318	S 12	0	0
9	i	219	Total 1659	C 1037	N 292	O 318	S 12	0	0

- Molecule 10 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	204	Total 1557	C 980	N 259	O 302	S 16	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total 1557	C 980	N 259	O 302	S 16	0	0

- Molecule 11 is a protein called Proteasome subunit family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total 1612	C 1012	N 280	O 304	S 16	0	0
11	k	206	Total 1612	C 1012	N 280	O 304	S 16	0	0

- Molecule 12 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	202	Total 1577	C 997	N 277	O 296	S 7	0	0
12	l	202	Total 1577	C 997	N 277	O 296	S 7	0	0

- Molecule 13 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	214	Total 1702	C 1079	N 287	O 324	S 12	0	0
13	m	214	Total 1702	C 1079	N 287	O 324	S 12	0	0

- Molecule 14 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	218	Total 1712	C 1083	N 292	O 323	S 14	0	0
14	n	218	Total 1712	C 1083	N 292	O 323	S 14	0	0

- Molecule 15 is {N}-[4-fluoranyl-3-[6-(3-methylpyridin-2-yl)-[1,2,4]triazolo[1,5-a]pyrimidin-2-yl]phenyl]-2,4-dimethyl-1,3-oxazole-5-carboxamide (three-letter code: N2E) (formula: $C_{23}H_{18}FN_7O_2$) (labeled as "Ligand of Interest" by depositor).
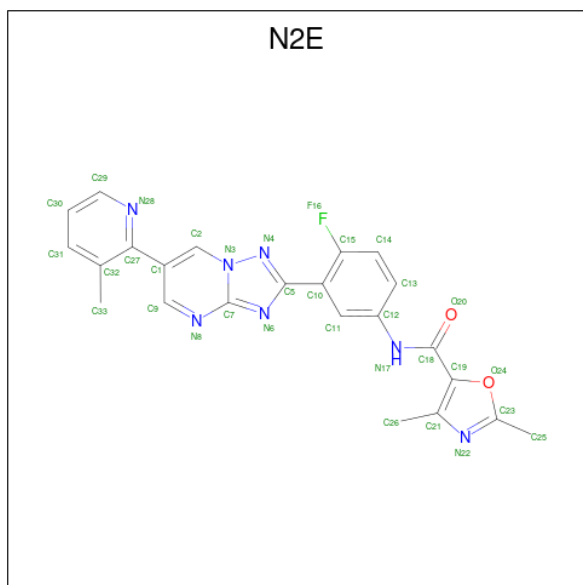
N2E

Mol	Chain	Residues	Atoms					AltConf
15	L	1	Total	C	F	N	O	0
			33	23	1	7	2	
15	l	1	Total	C	F	N	O	0
			33	23	1	7	2	

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: Proteasome subunit alpha type

Chain A:

- Molecule 1: Proteasome subunit alpha type

Chain a:

- Molecule 2: Proteasome subunit alpha type

Chain B:

- Molecule 2: Proteasome subunit alpha type

Chain b:

- Molecule 3: Proteasome subunit alpha type

Chain C:

• Molecule 3: Proteasome subunit alpha type

Chain c:

• Molecule 4: Proteasome endopeptidase complex

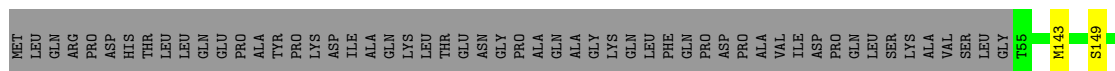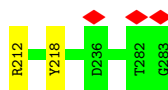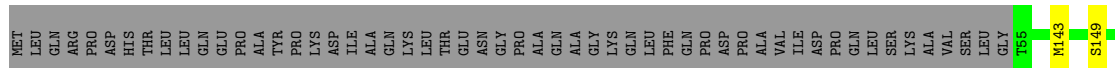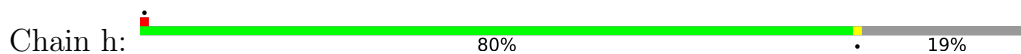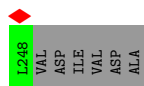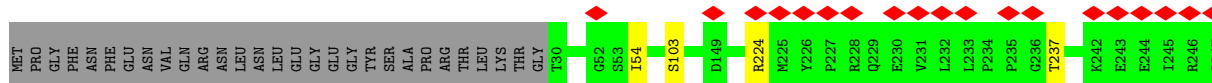Chain D:

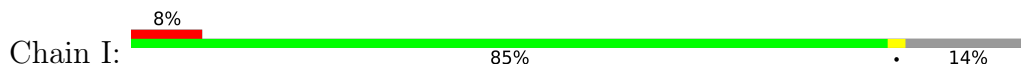• Molecule 4: Proteasome endopeptidase complex

Chain d:

• Molecule 5: Proteasome subunit alpha type

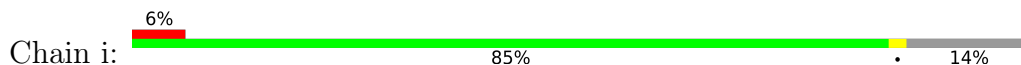Chain E:

• Molecule 5: Proteasome subunit alpha type

Chain e:

• Molecule 6: Proteasome subunit alpha type

Chain F:

55%   44%

MET GLN SER GLU LYS GLY GLU GLY TRP ARG ASP THR GLY THR ASP SER SER LEU PRO PRO PHE SER PHE CYS CYS SER PRO ALA PHE SER SER PRO LEU ALA PHE GLY GLU GLY GLY ALA ASP GLY CYS ALA TYR ILE LEU LEU THR HIS VAL CYS ARG TYR ALA CYS ILE ALA ALA LEU THR LEU

HIS SER GLU ALA GLU HIS MET ARG VAL CYS VAL CYS VAL ARG ARG CYS ALA TYR ASN GLU MET VAL LEU HIS GLN VAL VAL ALA PHE ALA SER LEU ALA PRO ALA LEU HIS PRO LEU SER PRO LEU PRO LEU PRO CYS MET ALA THR THR HIS ALA CYS CYS GLY LEU ARG VAL

ARG SER PHE LEU LYS LYS SER GLU LYS LYS ASN GLN GLN ARG ARG LEU GLN GLN ALA PRO ASP LEU SER GLN LYS THR ARG ARG THR GLN LYS GLU LYS GLN THR LEU GLN ILE TYR LEU ARG CYS VAL MET PHE LYS **N168** **R215** **A219** **D245** **G289** **S365** **E366** **G367**

E390 **E391** **G400** **M403** **R404** **P405** GLU ASP ARG VAL ALA VAL ALA GLU GLU GLU ASP GLU GLU GLU MET LEU HIS GLU GLN PRO LEU ASP GLU GLU

• Molecule 6: Proteasome subunit alpha type

Chain f:

55%   44%

MET GLN SER LYS GLY GLU GLY TRP ARG ASP THR GLY THR ASP SER SER LEU PRO PRO PHE SER PHE CYS CYS SER PRO ALA PHE SER SER PRO LEU ALA PHE GLY GLU GLY GLY ALA ASP GLY CYS ALA TYR ILE LEU LEU THR HIS VAL CYS ARG TYR ALA CYS ILE ALA ALA LEU THR LEU

HIS SER GLU ALA GLU HIS MET ARG VAL CYS VAL CYS VAL ARG ARG CYS ALA TYR ASN GLU MET VAL LEU HIS GLN VAL VAL ALA PHE ALA SER LEU ALA PRO ALA LEU HIS PRO LEU SER PRO LEU PRO LEU PRO CYS MET ALA THR THR HIS ALA CYS CYS GLY LEU ARG VAL

ARG SER PHE LEU LYS LYS SER GLU LYS LYS ASN GLN GLN ARG ARG LEU GLN GLN ALA PRO ASP LEU SER GLN LYS THR ARG ARG THR GLN LYS GLU LYS GLN THR LEU GLN ILE TYR LEU ARG CYS VAL MET PHE LYS **N168** **R215** **A219** **D245** **G289** **S365** **E366** **G367**

I368 **E390** **E391** **G400** **M403** **R404** **P405** GLU ASP ARG VAL ALA VAL ALA GLU GLU GLU ASP GLU GLU GLU MET LEU HIS GLU GLN PRO LEU ASP GLU GLU

• Molecule 7: Proteasome endopeptidase complex

Chain G:

5%
96%

MET ALA GLY THR GLY **S6** **K43** **S174** **S182** **E188** **K203** **Q204** **K205** **D206** **K207** **D221** **P228** **A229** **D230** **A234** **E235** THR SER HIS

• Molecule 7: Proteasome endopeptidase complex

Chain g:

96%

MET ALA GLY THR GLY **S6** **K43** **S174** **D202** **K203** **Q204** **K205** **D206** **K207** **P228** **A229** **D230** **A234** **E235** THR SER HIS

• Molecule 8: Proteasome subunit beta

Chain H:

80%   19%

MET LEU GLN ARG PRO ASP HIS THR LEU LEU GLN GLU PRO ALA TYR PRO LYS ASP ILE ALA GLN LYS LEU THR GLU ASN GLY PRO ALA GLN ALA GLY LYS LEU GLN LEU PHE GLN PRO ASP PRO ALA VAL ILE ASP PRO GLN LEU SER LYS ALA VAL SER LEU GLY T55 M143 S149

R212 Y218 D236 T282 G283

• Molecule 8: Proteasome subunit beta

Chain h:

80% 19%

MET LEU GLN ARG PRO ASP HIS THR LEU LEU GLN GLU PRO ALA TYR PRO LYS ASP ILE ALA GLN LYS LEU THR GLU ASN GLY PRO ALA GLN ALA GLY LYS LEU GLN LEU PHE GLN PRO ASP PRO ALA VAL ILE ASP PRO GLN LEU SER LYS ALA VAL SER LEU GLY T55 M143 S149

R212 Y218 D236 T282 G283

• Molecule 9: Proteasome subunit beta

Chain I:

8%

85% 14%

MET PRO GLY PHE ASN PHE GLU ASN VAL GLN ARG ASN LEU ASN LEU GLU GLY GLU GLY TYR SER ALA PRO ARG THR LEU LYS THR GLY T30 G52 S53 I54 S103 D149 R224 M225 Y226 P227 R228 Q229 E230 V231 L232 L233 P234 P235 G236 T237 K242 E243 E244 I245 R246 Q247

L248 VAL ASP ILE VAL ASP ALA

• Molecule 9: Proteasome subunit beta

Chain i:

6%

85% 14%

MET PRO GLY PHE ASN PHE GLU ASN VAL GLN ARG ASN LEU ASN LEU GLU GLY GLU GLY TYR SER ALA PRO ARG THR LEU LYS THR GLY T30 D39 I54 S103 D149 R224 M225 Y226 P227 R228 Q229 E230 V231 L232 G236 T237 E243 R246 Q247 L248 VAL ASP ILE

VAL ASP ALA

• Molecule 10: Proteasome subunit beta

Chain J:

99%

MET S2 R99 F100 G101 D205

• Molecule 10: Proteasome subunit beta

Chain j:

99%

MET S2 R99 F100 G101 D205

• Molecule 11: Proteasome subunit family protein

Chain K: 100%

M1 Y26 E50 E98 D118 D119 T203 H206

• Molecule 11: Proteasome subunit family protein

Chain k: 100%

M1 Y26 E50 E98 D117 D118 D119 T203 H206

• Molecule 12: Proteasome subunit beta

Chain L: 67% 33%

MET PHE ALA ASP PHE GLU ALA VAL THR SER SER ASN PHE THR LEU ASP CYS PRO ARG VAL GLY PRO PHE THR TYR HIS ASN MET ASP GLU ASP THR LEU GLU GLU PRO LEU SER LEU CYS SER TYR ARG ARG ALA PRO GLN GLN THR ASP GLU ARG SER PRO ALA SER CYS ASP ALA

VAL THR ALA ASP PRO LEU ASP SER SER ARG TYR LEU HIS GLY GLU ASN ARG CYS TRP THR LEU LYS VAL SER CYS PRO VAL PRO ARG ALA ILE PRO LYS LEU ASP MET LYS LYS GLY T100 D245 D250 S301 GLN

• Molecule 12: Proteasome subunit beta

Chain l: 67% 33%

MET PHE ALA ASP PHE GLU ALA VAL THR SER SER ASN PHE THR LEU ASP CYS PRO ARG VAL GLY PRO PHE THR TYR HIS ASN MET ASP GLU ASP THR LEU GLU GLU PRO LEU SER LEU CYS SER TYR ARG ARG ALA PRO GLN GLN THR ASP GLU ARG SER PRO ALA SER CYS ASP ALA

VAL THR ALA ASP PRO LEU ASP SER SER ARG TYR LEU HIS GLY GLU ASN ARG CYS TRP THR LEU LYS VAL SER CYS PRO VAL PRO ARG ALA ILE PRO LYS LEU ASP MET LYS LYS GLY T100 T121 D250 S301 GLN

• Molecule 13: Proteasome subunit beta

Chain M: 63% 37%

MET ALA SER SER PRO PRO LEU LEU PRO PHE SER SER PHE VAL VAL ALA VAL VAL ALA ILE HIS LEU SER PHE ARG VAL PHE CYS VAL GLY ALA GLN SER LEU CYS LYS CYS SER CYS CYS VAL PRO ALA CYS ALA LEU PRO LEU CYS PHE SER SER PRO SER VAL SER ALA GLU

ASP VAL ALA LEU ALA LEU PHE ALA HIS PRO LYS VAL LEU THR HIS ARG PRO THR ALA ARG TYR SER PRO ILE LEU LEU HIS TYR ALA VAL MET ILE GLU ASP HIS ALA GLU TYR GLY HIS ASN TYR TYR PRO GLN LYS LEU ALA SER SER THR LEU THR LEU PRO GLN GLN GLY

ALA LYS GLN GLN GLN W126 R226 E242 Q282 H283 M284 T285 S286 Q287 A288 P289 P290 E291 D339

• Molecule 13: Proteasome subunit beta

Chain m:

63%   37%

MET ALA SER SER PRO PRO LEU LEU PRO PHE SER SER PHE VAL VAL ALA VAL VAL ALA ILE HIS LEU SER PHE ARG VAL PHE CYS VAL GLY ALA GLN SER LEU CYS LYS CYS CYS SER CYS VAL PRO ALA CYS ALA LEU PRO LEU CYS SER PHE SER SER PRO SER VAL SER ALA GLU

ASP VAL ALA LEU ALA LEU PHE ALA HIS PRO LYS VAL LEU THR HIS ARG PRO THR ALA ARG TYR SER PRO ILE LEU SER LEU LEU HIS TYR ALA VAL MET ILE GLU ASP HIS ALA GLU TYR GLY HIS ASN TYR TYR PRO GLN LYS LEU ALA SER SER THR LEU THR LEU PRO GLN GLN GLY

ALA LYS GLN GLN GLN **W126** **R226** E242 Q282 H283 M284 T285 S286 Q287 A288 P289 P290 E291 D327 D339

• Molecule 14: Proteasome subunit beta

Chain N:

99%

MET A2 D65 I219 ARG

• Molecule 14: Proteasome subunit beta

Chain n:

99%

MET A2 I219 ARG

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	38000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0154	Depositor
Map size (Å)	255.6, 255.6, 255.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.852, 0.852, 0.852	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: N2E

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	0.38	0/1893	0.48	0/2567
1	a	0.38	0/1893	0.48	0/2567
2	B	0.42	0/1786	0.50	0/2421
2	b	0.42	0/1786	0.50	0/2421
3	C	0.35	0/2202	0.46	0/2982
3	c	0.35	0/2202	0.46	0/2982
4	D	0.37	0/1911	0.47	0/2573
4	d	0.37	0/1911	0.47	0/2573
5	E	0.35	0/1831	0.49	0/2476
5	e	0.35	0/1831	0.49	0/2476
6	F	0.37	0/1907	0.47	0/2575
6	f	0.37	0/1907	0.46	0/2575
7	G	0.39	0/1773	0.46	0/2398
7	g	0.38	0/1773	0.46	0/2398
8	H	0.44	0/1741	0.51	0/2359
8	h	0.44	0/1741	0.51	0/2359
9	I	0.38	0/1685	0.51	0/2284
9	i	0.38	0/1685	0.51	0/2284
10	J	0.43	0/1583	0.49	0/2135
10	j	0.43	0/1583	0.49	0/2135
11	K	0.42	0/1643	0.49	0/2222
11	k	0.42	0/1643	0.49	0/2222
12	L	0.44	0/1611	0.49	0/2180
12	l	0.44	0/1611	0.49	0/2180
13	M	0.43	0/1743	0.49	0/2354
13	m	0.43	0/1743	0.49	0/2354
14	N	0.43	0/1748	0.50	0/2363
14	n	0.43	0/1748	0.50	0/2363
All	All	0.40	0/50114	0.49	0/67778

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	243/250 (97%)	228 (94%)	15 (6%)	0	100	100
1	a	243/250 (97%)	228 (94%)	15 (6%)	0	100	100
2	B	227/231 (98%)	212 (93%)	15 (7%)	0	100	100
2	b	227/231 (98%)	212 (93%)	15 (7%)	0	100	100
3	C	270/285 (95%)	251 (93%)	19 (7%)	0	100	100
3	c	270/285 (95%)	251 (93%)	19 (7%)	0	100	100
4	D	238/248 (96%)	221 (93%)	17 (7%)	0	100	100
4	d	238/248 (96%)	221 (93%)	17 (7%)	0	100	100
5	E	233/344 (68%)	220 (94%)	13 (6%)	0	100	100
5	e	233/344 (68%)	220 (94%)	13 (6%)	0	100	100
6	F	236/428 (55%)	220 (93%)	16 (7%)	0	100	100
6	f	236/428 (55%)	220 (93%)	16 (7%)	0	100	100
7	G	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
7	g	228/238 (96%)	220 (96%)	8 (4%)	0	100	100
8	H	227/283 (80%)	215 (95%)	12 (5%)	0	100	100
8	h	227/283 (80%)	215 (95%)	12 (5%)	0	100	100
9	I	217/254 (85%)	203 (94%)	14 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	i	217/254 (85%)	203 (94%)	14 (6%)	0	100	100
10	J	202/205 (98%)	184 (91%)	18 (9%)	0	100	100
10	j	202/205 (98%)	184 (91%)	18 (9%)	0	100	100
11	K	204/206 (99%)	195 (96%)	8 (4%)	1 (0%)	29	61
11	k	204/206 (99%)	196 (96%)	7 (3%)	1 (0%)	29	61
12	L	200/302 (66%)	194 (97%)	6 (3%)	0	100	100
12	l	200/302 (66%)	196 (98%)	4 (2%)	0	100	100
13	M	212/339 (62%)	203 (96%)	9 (4%)	0	100	100
13	m	212/339 (62%)	203 (96%)	9 (4%)	0	100	100
14	N	216/220 (98%)	200 (93%)	16 (7%)	0	100	100
14	n	216/220 (98%)	200 (93%)	16 (7%)	0	100	100
All	All	6306/7666 (82%)	5935 (94%)	369 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	26	TYR
11	k	26	TYR

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	193/197 (98%)	190 (98%)	3 (2%)	62	81
1	a	193/197 (98%)	190 (98%)	3 (2%)	62	81
2	B	188/190 (99%)	185 (98%)	3 (2%)	62	81
2	b	188/190 (99%)	185 (98%)	3 (2%)	62	81
3	C	229/241 (95%)	228 (100%)	1 (0%)	91	95
3	c	229/241 (95%)	228 (100%)	1 (0%)	91	95
4	D	201/208 (97%)	198 (98%)	3 (2%)	65	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	201/208 (97%)	198 (98%)	3 (2%)	65	82
5	E	197/301 (65%)	192 (98%)	5 (2%)	47	72
5	e	197/301 (65%)	192 (98%)	5 (2%)	47	72
6	F	200/363 (55%)	199 (100%)	1 (0%)	88	94
6	f	200/363 (55%)	199 (100%)	1 (0%)	88	94
7	G	185/190 (97%)	183 (99%)	2 (1%)	73	86
7	g	185/190 (97%)	183 (99%)	2 (1%)	73	86
8	H	184/229 (80%)	180 (98%)	4 (2%)	52	75
8	h	184/229 (80%)	180 (98%)	4 (2%)	52	75
9	I	180/209 (86%)	176 (98%)	4 (2%)	52	75
9	i	180/209 (86%)	176 (98%)	4 (2%)	52	75
10	J	167/168 (99%)	166 (99%)	1 (1%)	86	94
10	j	167/168 (99%)	166 (99%)	1 (1%)	86	94
11	K	172/172 (100%)	172 (100%)	0	100	100
11	k	172/172 (100%)	172 (100%)	0	100	100
12	L	162/253 (64%)	162 (100%)	0	100	100
12	l	162/253 (64%)	162 (100%)	0	100	100
13	M	181/288 (63%)	180 (99%)	1 (1%)	86	94
13	m	181/288 (63%)	180 (99%)	1 (1%)	86	94
14	N	181/183 (99%)	181 (100%)	0	100	100
14	n	181/183 (99%)	181 (100%)	0	100	100
All	All	5240/6384 (82%)	5184 (99%)	56 (1%)	74	86

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	97	ASP
1	A	144	ASP
2	B	14	SER
2	B	18	ILE
2	B	25	THR
3	C	181	LEU
4	D	58	THR
4	D	105	ASP

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Mol	Chain	Res	Type
4	D	170	GLU
5	E	110	ARG
5	E	118	GLU
5	E	178	MET
5	E	231	LYS
5	E	233	MET
6	F	245	ASP
7	G	43	LYS
7	G	174	SER
8	H	143	MET
8	H	149	SER
8	H	212	ARG
8	H	218	TYR
9	I	54	ILE
9	I	103	SER
9	I	224	ARG
9	I	237	THR
10	J	99	ARG
13	M	226	ARG
1	a	29	VAL
1	a	97	ASP
1	a	144	ASP
2	b	14	SER
2	b	18	ILE
2	b	25	THR
3	c	181	LEU
4	d	58	THR
4	d	105	ASP
4	d	170	GLU
5	e	110	ARG
5	e	118	GLU
5	e	178	MET
5	e	231	LYS
5	e	233	MET
6	f	245	ASP
7	g	43	LYS
7	g	174	SER
8	h	143	MET
8	h	149	SER
8	h	212	ARG
8	h	218	TYR
9	i	54	ILE

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Mol	Chain	Res	Type
9	i	103	SER
9	i	224	ARG
9	i	237	THR
10	j	99	ARG
13	m	226	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	50	GLN
1	A	142	GLN
1	A	195	GLN
1	A	207	GLN
1	A	228	ASN
2	B	143	HIS
3	C	103	HIS
3	C	108	GLN
3	C	175	GLN
3	C	228	ASN
3	C	257	HIS
4	D	18	GLN
5	E	252	GLN
6	F	190	ASN
6	F	225	GLN
6	F	259	ASN
6	F	305	GLN
6	F	331	GLN
6	F	355	HIS
8	H	63	ASN
8	H	107	GLN
8	H	266	GLN
9	I	64	HIS
9	I	174	ASN
10	J	169	GLN
11	K	38	GLN
11	K	72	GLN
11	K	136	GLN
12	L	279	HIS
13	M	180	ASN
13	M	280	ASN
13	M	282	GLN

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Mol	Chain	Res	Type
1	a	21	GLN
1	a	50	GLN
1	a	142	GLN
1	a	165	HIS
1	a	195	GLN
1	a	207	GLN
1	a	228	ASN
2	b	143	HIS
3	c	103	HIS
3	c	108	GLN
3	c	175	GLN
3	c	228	ASN
3	c	257	HIS
4	d	18	GLN
5	e	252	GLN
6	f	190	ASN
6	f	225	GLN
6	f	259	ASN
6	f	305	GLN
6	f	331	GLN
6	f	355	HIS
8	h	63	ASN
8	h	107	GLN
8	h	135	ASN
8	h	264	GLN
8	h	266	GLN
9	i	64	HIS
9	i	174	ASN
10	j	26	ASN
10	j	169	GLN
11	k	38	GLN
11	k	72	GLN
11	k	136	GLN
12	l	279	HIS
13	m	180	ASN
13	m	280	ASN
13	m	282	GLN
14	n	66	ASN

5.3.3 RNA (i)

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	N2E	l	401	-	30,37,37	2.27	8 (26%)	34,54,54	3.84	12 (35%)
15	N2E	L	401	-	30,37,37	2.26	8 (26%)	34,54,54	3.83	13 (38%)

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	N2E	l	401	-	-	2/12/16/16	0/5/5/5
15	N2E	L	401	-	-	2/12/16/16	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	l	401	N2E	C7-N6	-7.53	1.24	1.35
15	L	401	N2E	C7-N6	-7.49	1.24	1.35
15	l	401	N2E	C5-N6	5.39	1.42	1.35
15	L	401	N2E	C5-N6	5.39	1.42	1.35
15	l	401	N2E	C9-C1	4.80	1.48	1.39
15	L	401	N2E	C9-C1	4.75	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	401	N2E	C9-N8	-3.06	1.26	1.31
15	l	401	N2E	C9-N8	-3.04	1.26	1.31
15	L	401	N2E	C5-N4	-2.86	1.27	1.34
15	l	401	N2E	C5-N4	-2.83	1.28	1.34
15	l	401	N2E	C2-C1	-2.82	1.34	1.39
15	L	401	N2E	C2-C1	-2.78	1.34	1.39
15	l	401	N2E	C7-N8	2.28	1.43	1.33
15	L	401	N2E	C7-N8	2.27	1.43	1.33
15	L	401	N2E	C19-C21	-2.02	1.33	1.39
15	l	401	N2E	C19-C21	-2.02	1.33	1.39

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	L	401	N2E	N4-C5-N6	-17.57	102.93	114.56
15	l	401	N2E	N4-C5-N6	-17.56	102.94	114.56
15	l	401	N2E	C1-C9-N8	-9.52	116.74	125.55
15	L	401	N2E	C1-C9-N8	-9.49	116.77	125.55
15	l	401	N2E	C19-C18-N17	3.78	117.78	113.74
15	L	401	N2E	C19-C18-N17	3.76	117.77	113.74
15	l	401	N2E	C9-N8-C7	3.23	119.98	116.58
15	L	401	N2E	C9-N8-C7	3.18	119.93	116.58
15	L	401	N2E	C2-C1-C9	3.14	120.27	115.38
15	l	401	N2E	C2-C1-C9	3.12	120.25	115.38
15	l	401	N2E	C14-C15-C10	-3.01	119.62	123.30
15	L	401	N2E	C14-C15-C10	-3.00	119.63	123.30
15	L	401	N2E	C32-C27-N28	-2.99	120.46	123.05
15	l	401	N2E	C32-C27-N28	-2.96	120.48	123.05
15	l	401	N2E	C11-C10-C15	2.94	120.25	116.15
15	L	401	N2E	C11-C10-C15	2.91	120.21	116.15
15	L	401	N2E	C29-N28-C27	2.90	122.49	116.81
15	l	401	N2E	C29-N28-C27	2.87	122.43	116.81
15	l	401	N2E	C10-C5-N6	2.69	127.11	123.67
15	L	401	N2E	C10-C5-N6	2.68	127.09	123.67
15	L	401	N2E	C31-C32-C27	2.27	117.86	117.04
15	l	401	N2E	C31-C32-C27	2.27	117.86	117.04
15	L	401	N2E	C30-C29-N28	-2.22	119.80	123.43
15	l	401	N2E	C30-C29-N28	-2.21	119.82	123.43
15	L	401	N2E	C25-C23-N22	2.01	129.08	123.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	L	401	N2E	C2-C1-C27-N28
15	L	401	N2E	C9-C1-C27-N28
15	l	401	N2E	C9-C1-C27-N28
15	l	401	N2E	C2-C1-C27-N28

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 N2E l 401

Bond lengths

Bond angles

Torsions

Rings

Ligand N2E L 401

Bond lengths

Bond angles

Torsions

Rings
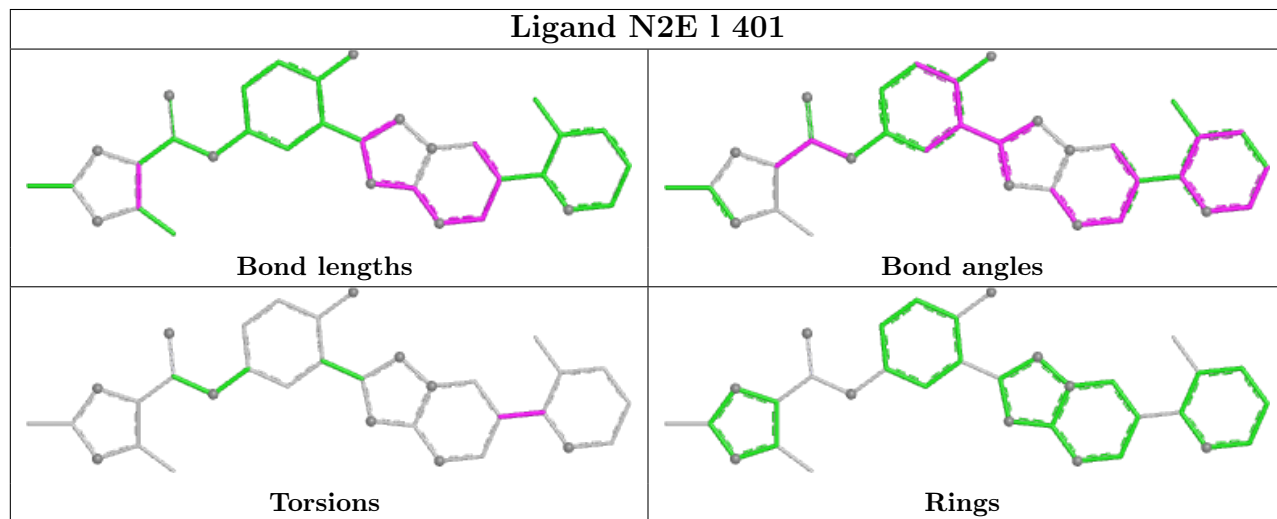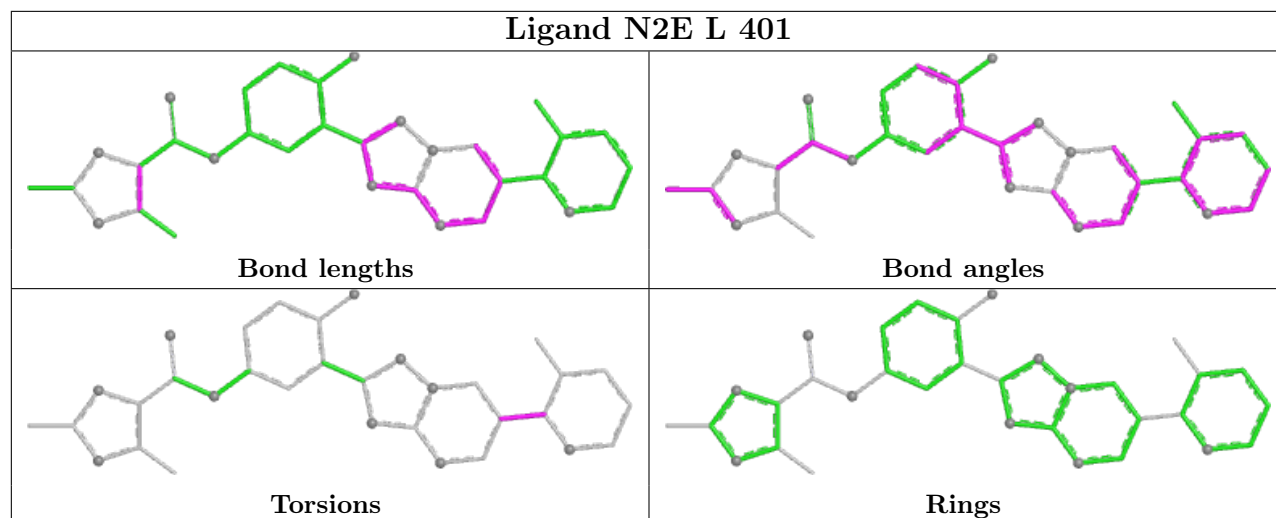
5.7 Other polymers ⓘ

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-10462. 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
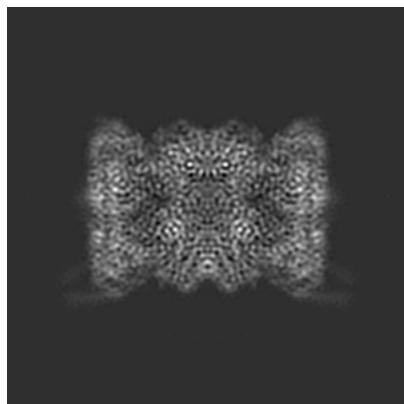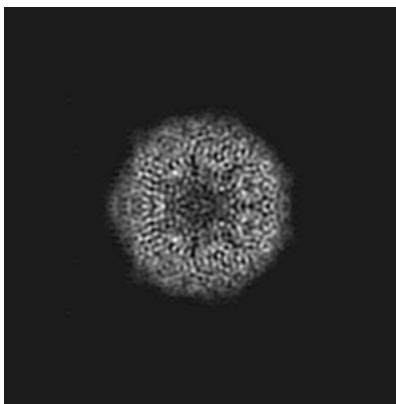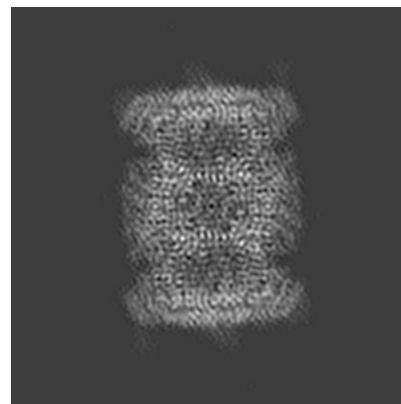
X Y Z

6.1.2 Raw map

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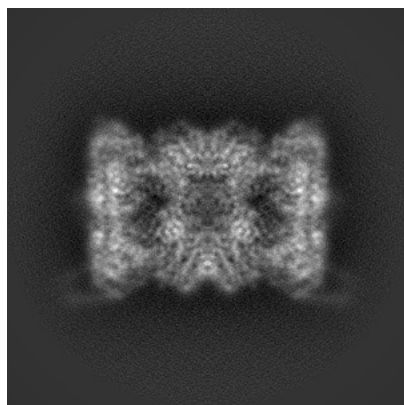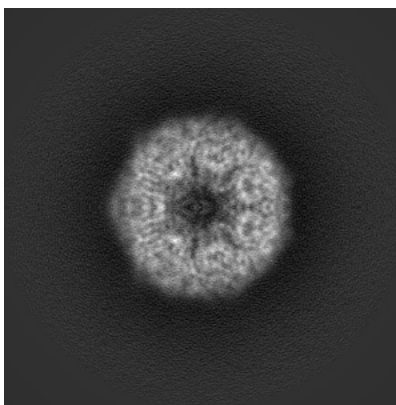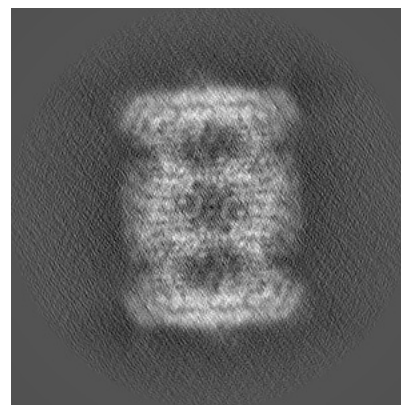
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
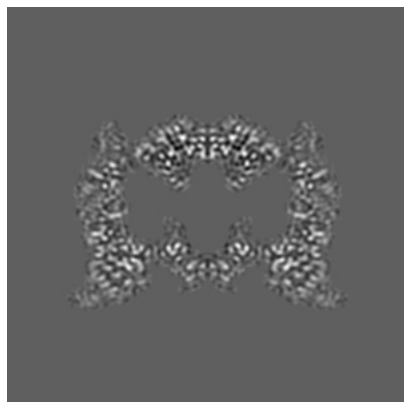
6.2.1 Primary map
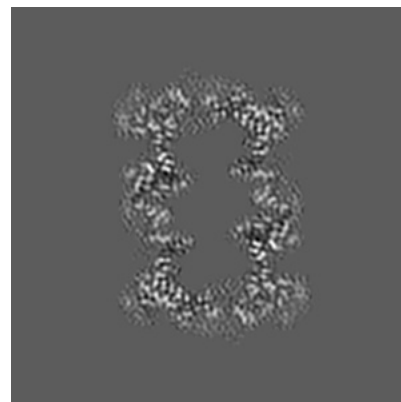
X Index: 150 Y Index: 150 Z Index: 150

6.2.2 Raw map
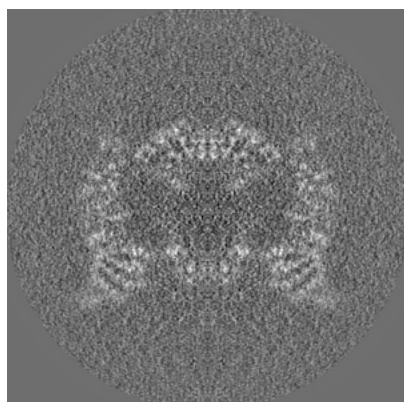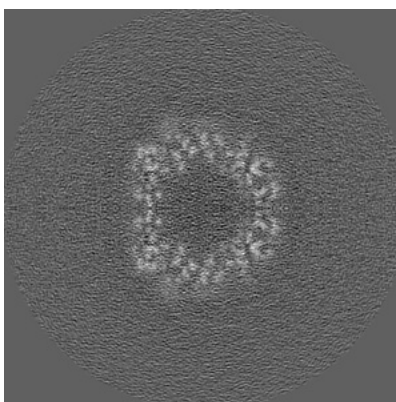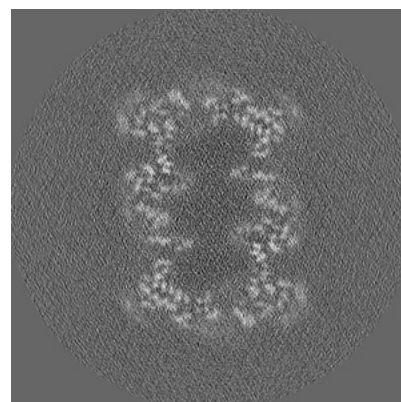
X Index: 150 Y Index: 150 Z Index: 150

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

6.3   Largest variance slices ⓘ
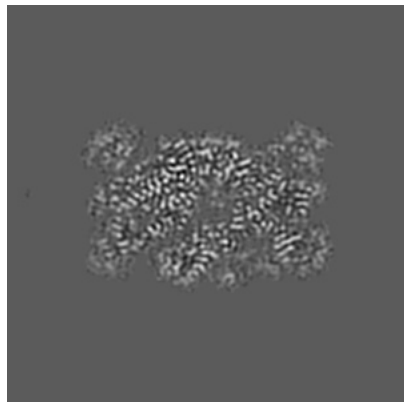
6.3.1   Primary map
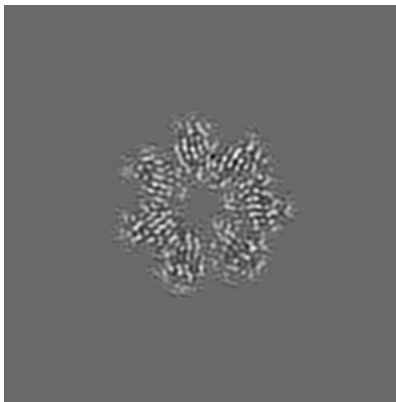
| X Index: 183 | Y Index: 129 | Z Index: 177 |
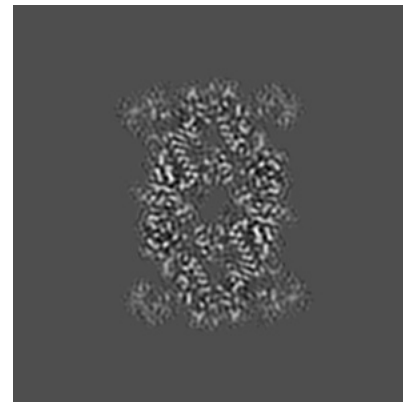
6.3.2   Raw map
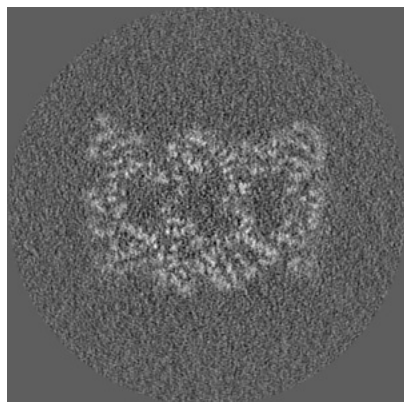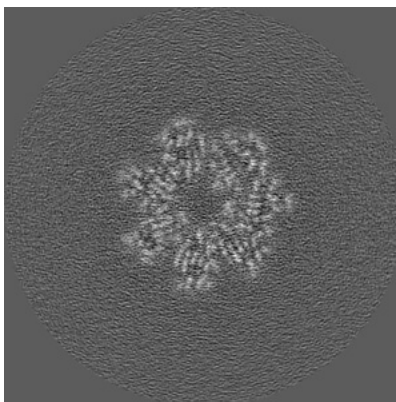
| X Index: 127 | Y Index: 171 | Z Index: 177 |
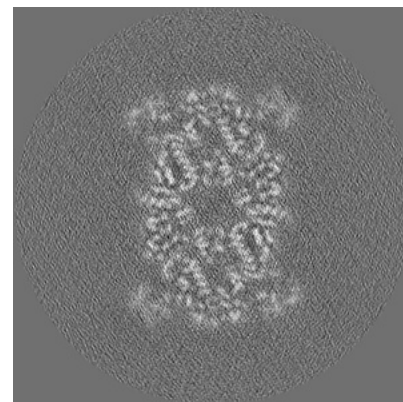
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
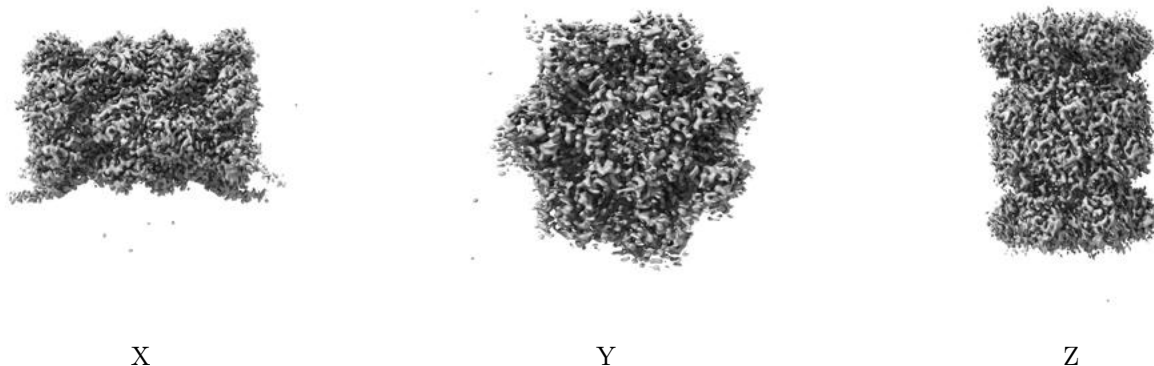
The images above show the 3D surface view of the map at the recommended contour level 0.0154. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

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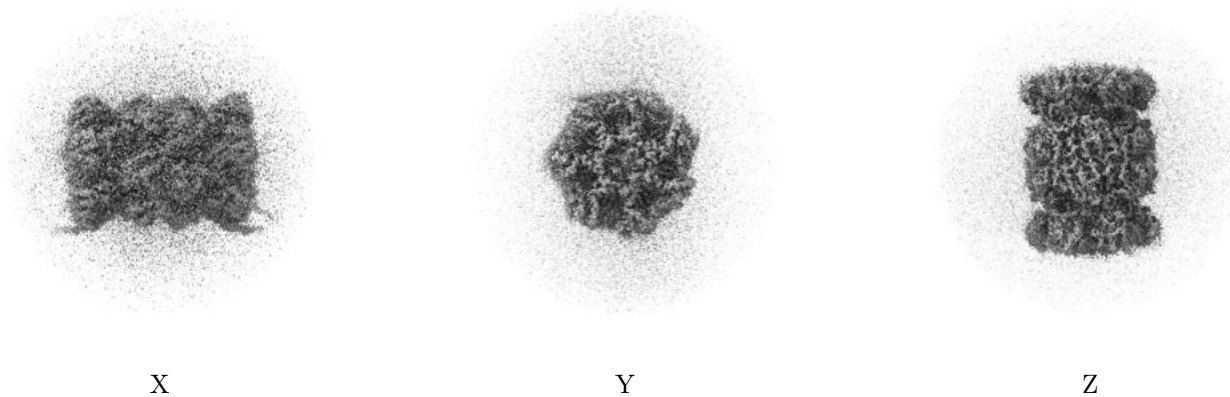
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.5 Mask visualisation (i)

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

A mask typically either:

- Encompasses the whole structure

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

6.5.1 emd_10462_msk_1.map (i)

| X | Y | Z |
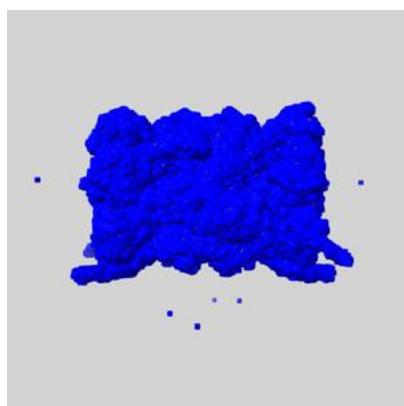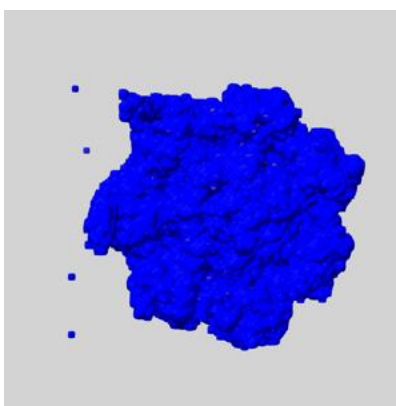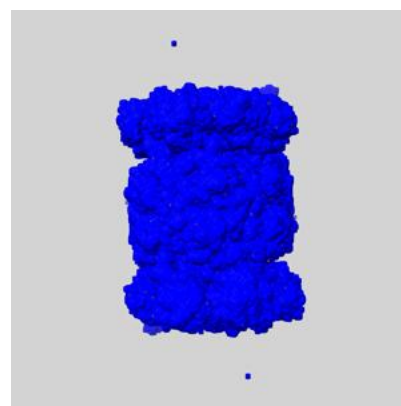
7 Map analysis ⓘ

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

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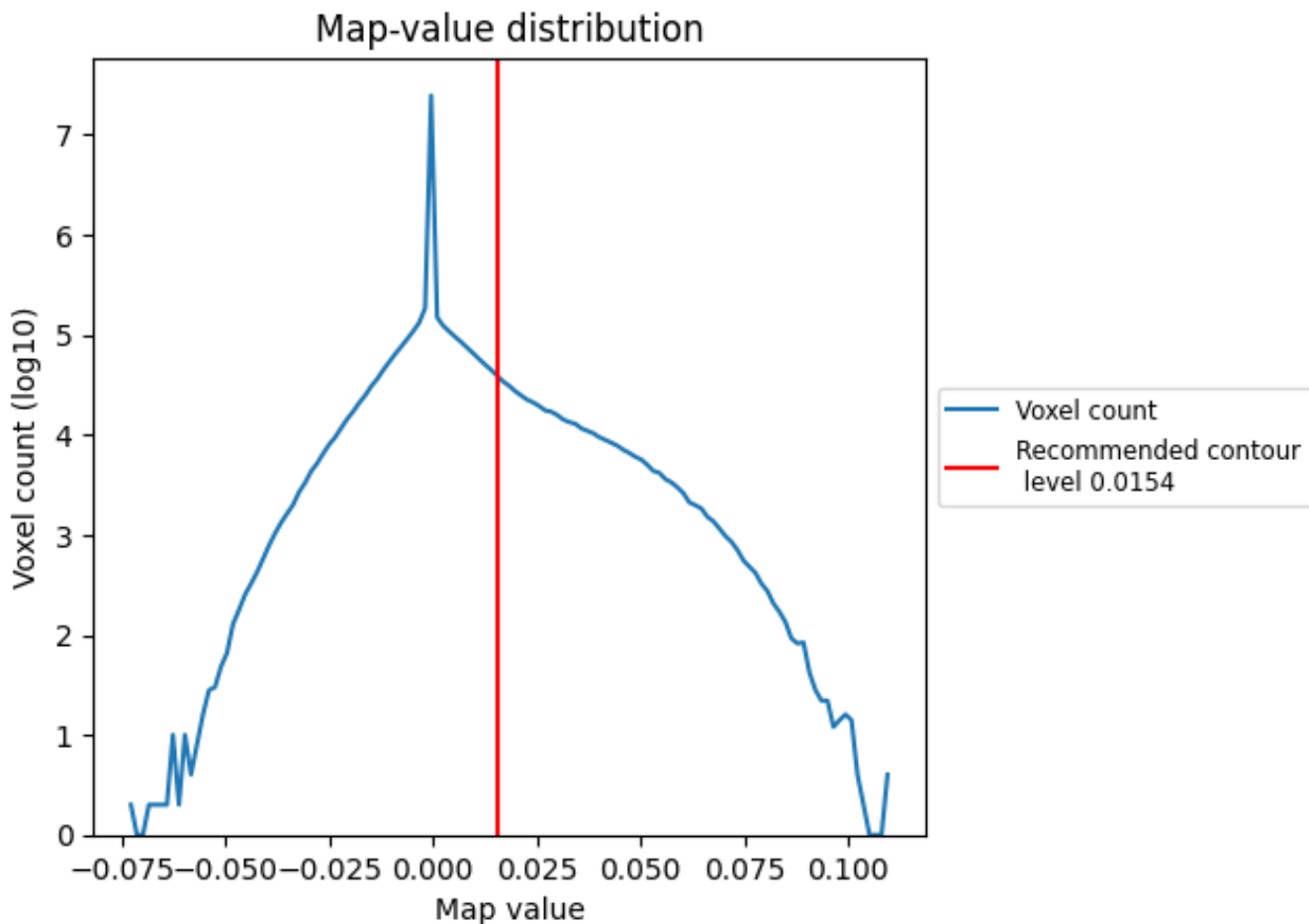
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
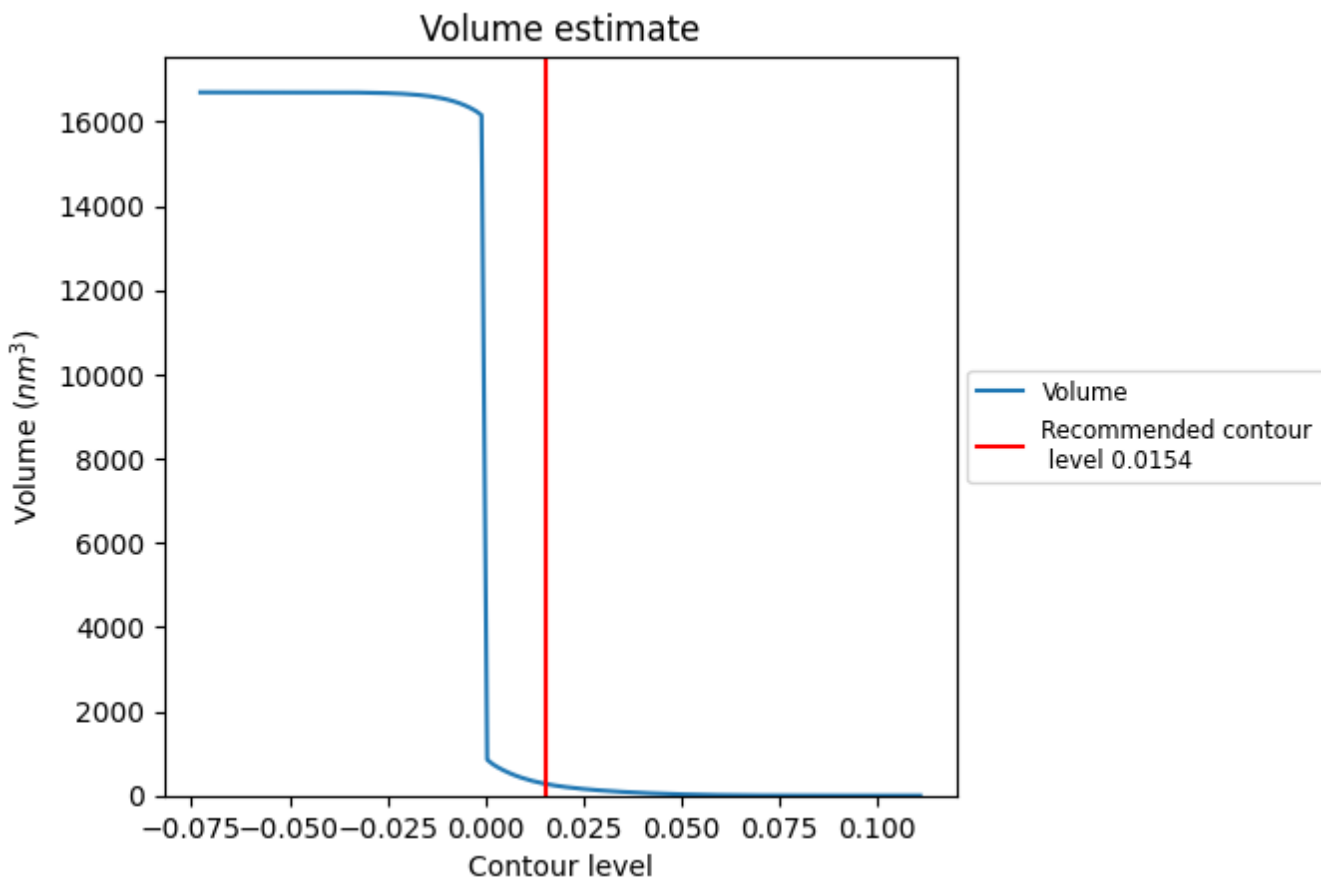
The volume at the recommended contour level is 277 nm^3; this corresponds to an approximate mass of 250 kDa.

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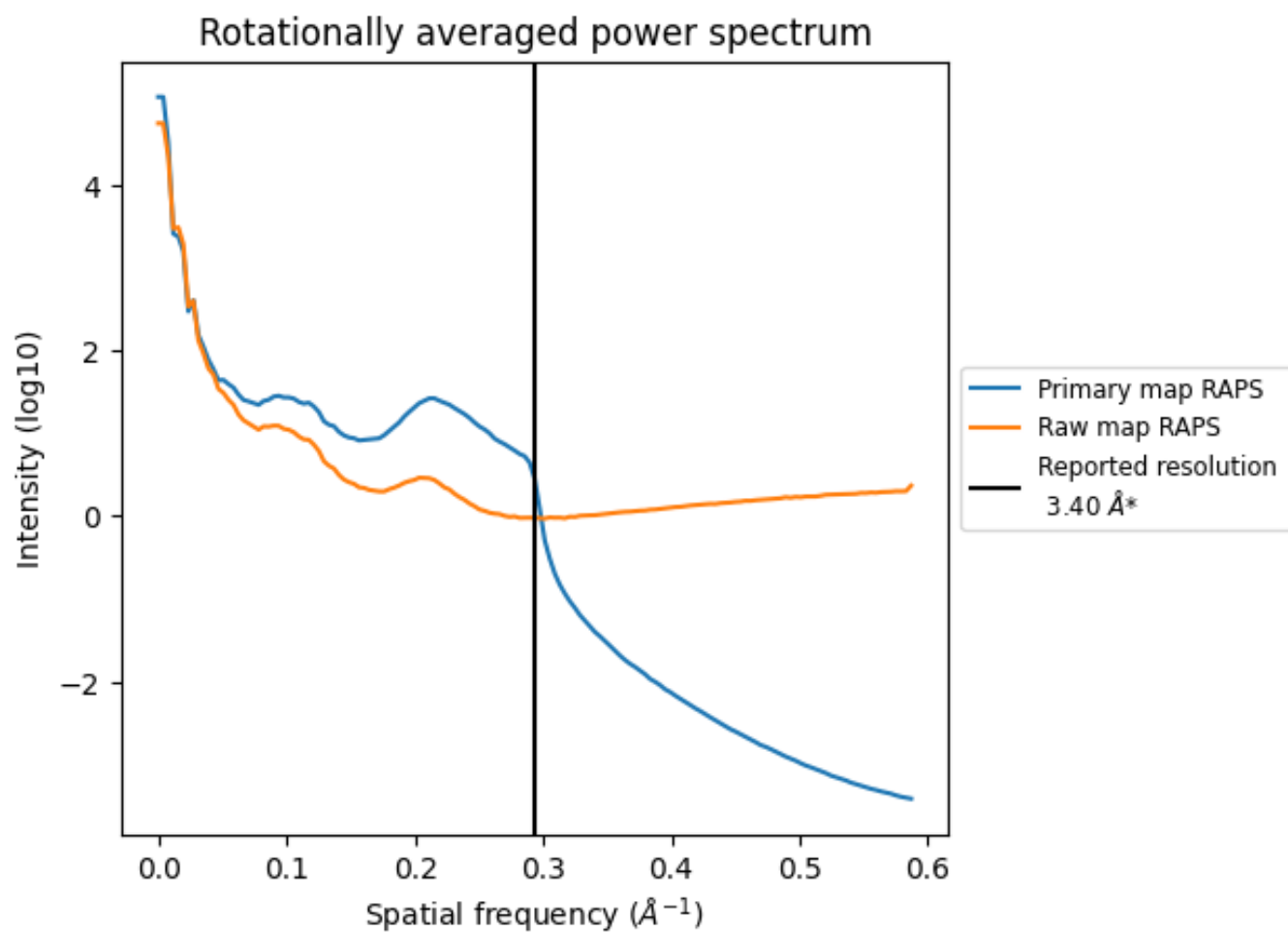
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation (i)

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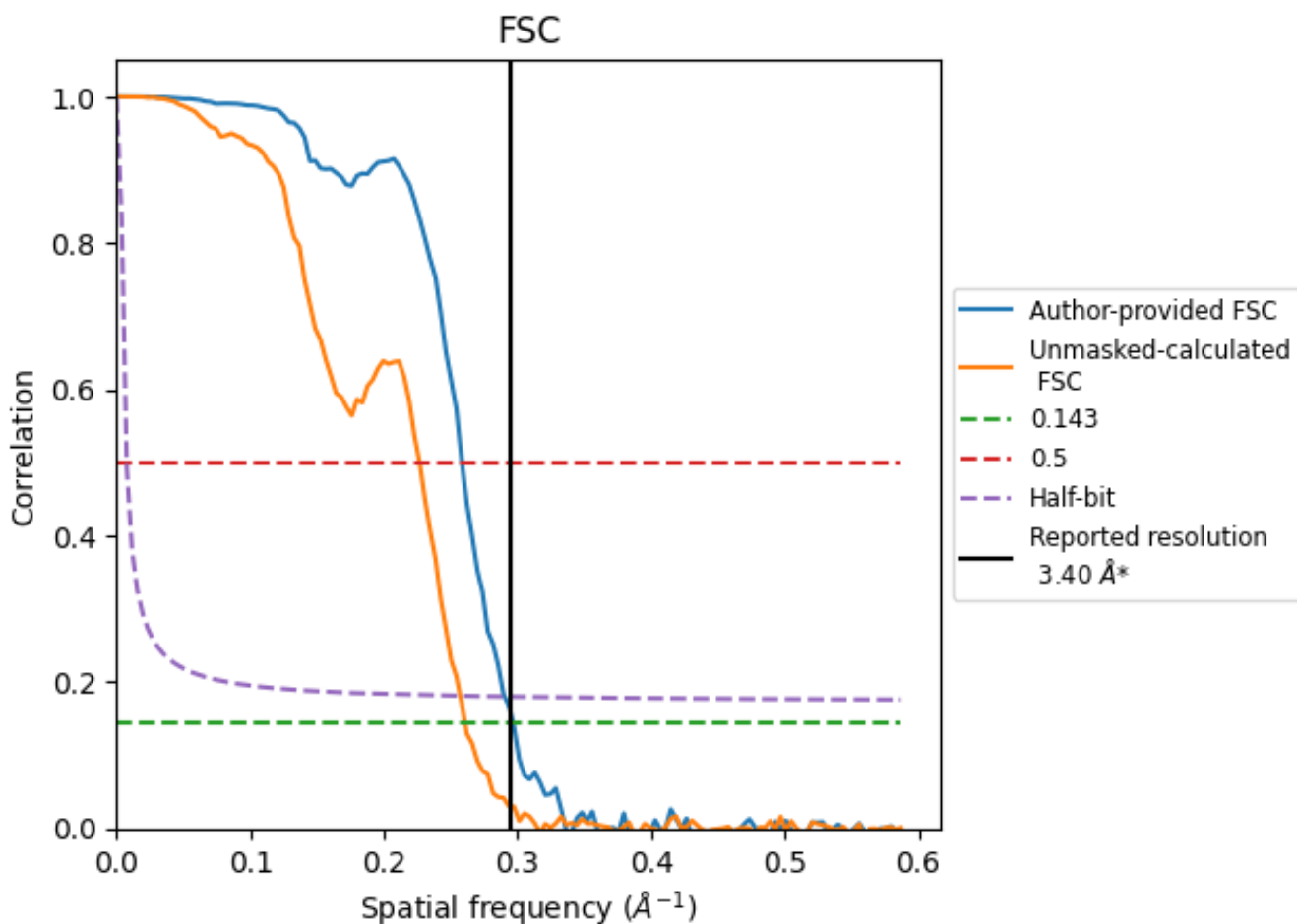
*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.37	3.87	3.44
Unmasked-calculated*	3.83	4.41	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 3.83 differs from the reported value 3.4 by more than 10 %

9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-10462 and PDB model 6TCZ. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay (i)
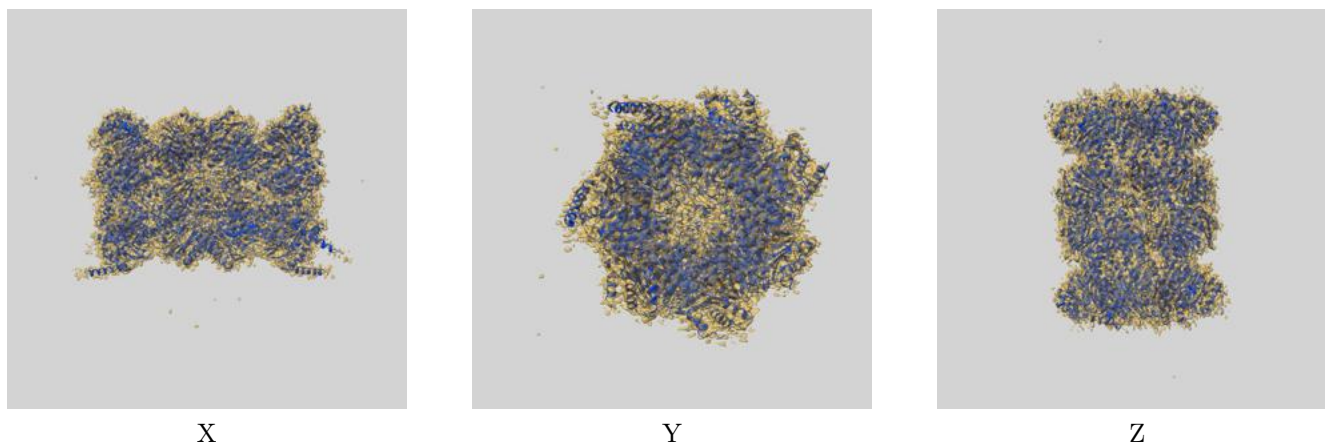
| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.0154 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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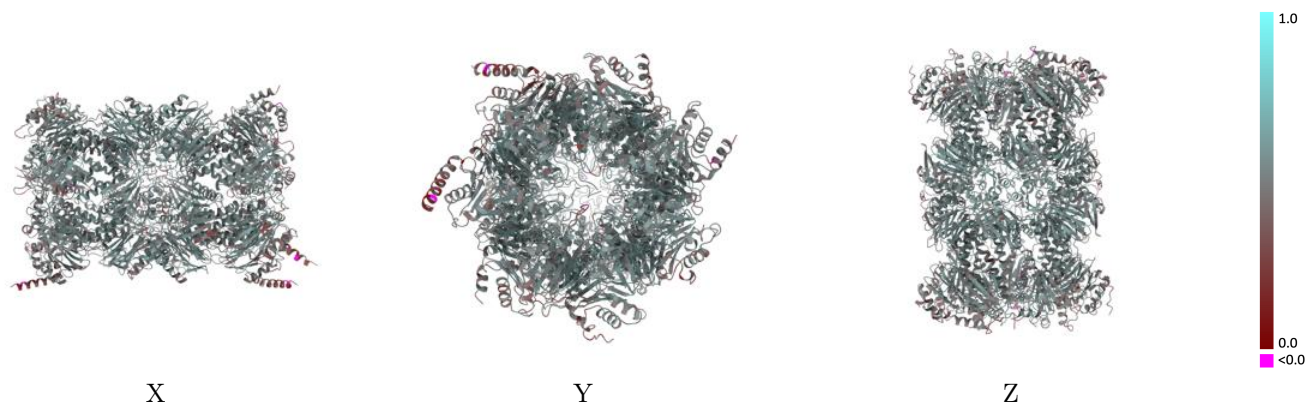
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model ⓘ

X   Y   Z
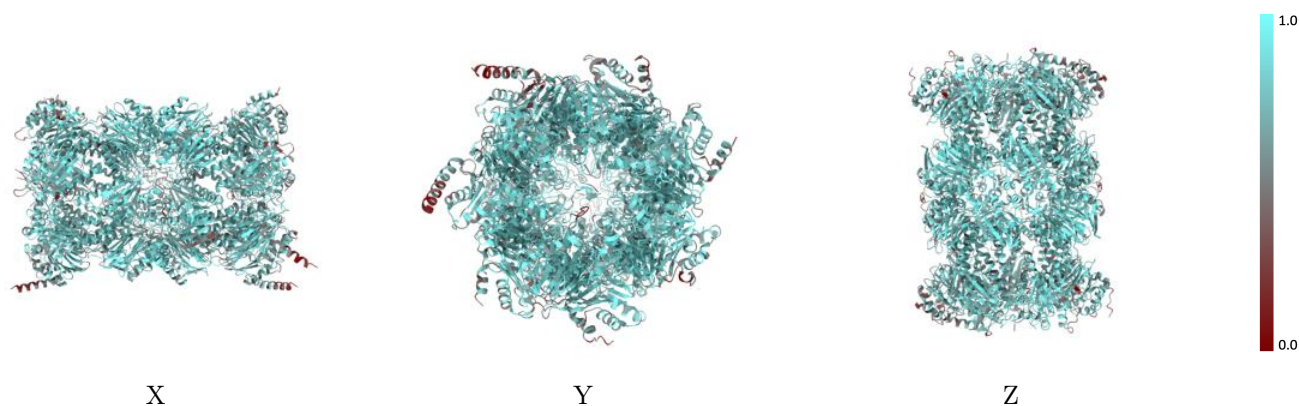
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0154).

9.4 Atom inclusion ⓘ
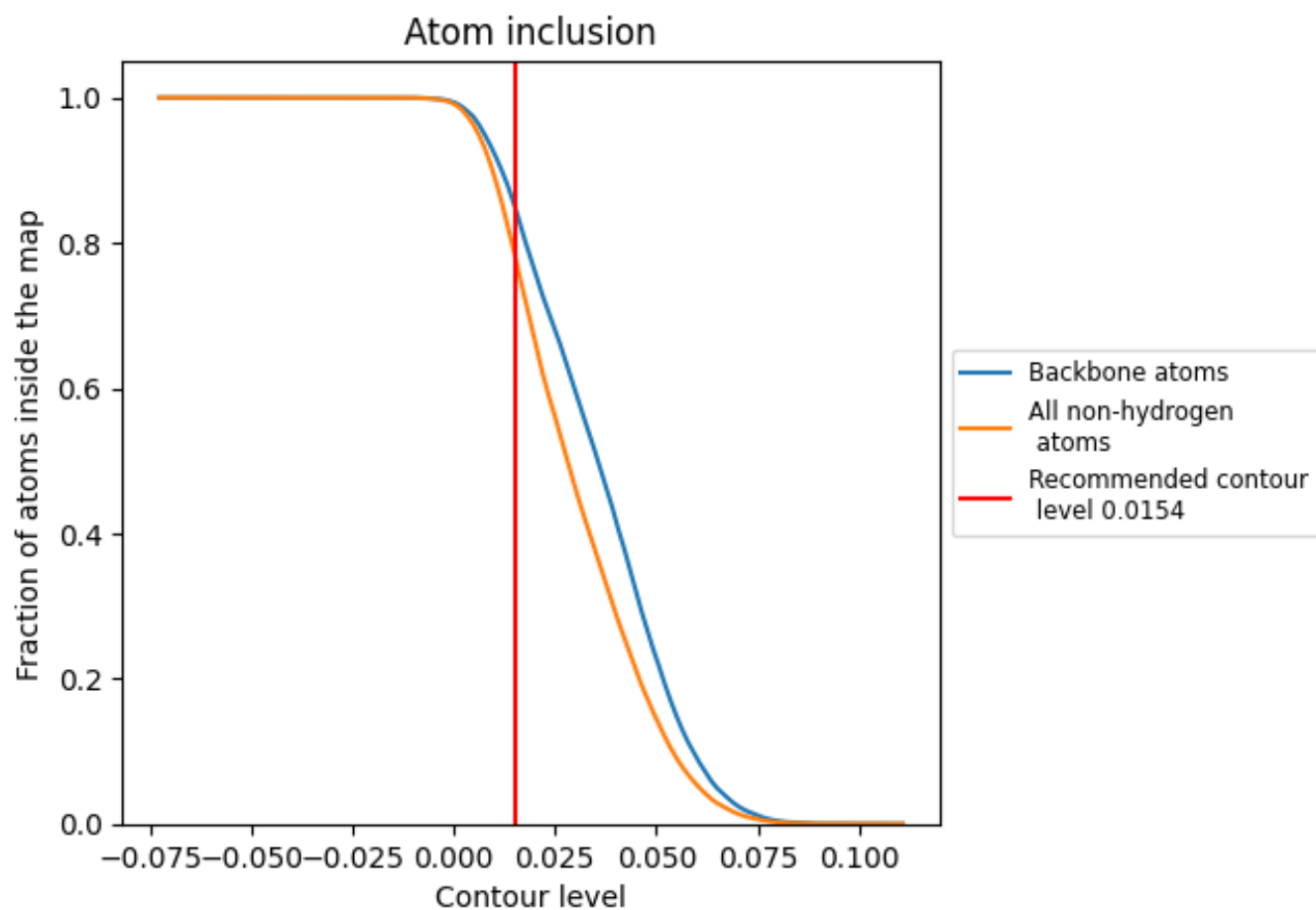
At the recommended contour level, 84% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0154) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7761	0.5140
A	0.7349	0.4980
B	0.7391	0.5050
C	0.7160	0.4910
D	0.7213	0.4820
E	0.7411	0.4920
F	0.7564	0.5090
G	0.7624	0.5040
H	0.8386	0.5470
I	0.7545	0.5100
J	0.8266	0.5330
K	0.8135	0.5310
L	0.8370	0.5410
M	0.8044	0.5320
N	0.8485	0.5440
a	0.7415	0.4980
b	0.7420	0.5040
c	0.7179	0.4900
d	0.7245	0.4830
e	0.7445	0.4900
f	0.7603	0.5070
g	0.7636	0.5040
h	0.8410	0.5460
i	0.7538	0.5080
j	0.8207	0.5340
k	0.8071	0.5300
l	0.8414	0.5390
m	0.8062	0.5320
n	0.8485	0.5470

1.0

0.0
<0.0