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)

Dec 10, 2022 – 09:45 am GMT

PDB ID	:	5FMG
EMDB ID	:	EMD-3231
Title	:	Structure and function based design of Plasmodium-selective proteasome inhibitors
Authors	:	Li, H.; O'Donoghue, A.J.; van der Linden, W.A.; Xie, S.C.; Yoo, E.; Foe, I.T.; Tilley, L.; Craik, C.S.; da Fonseca, P.C.A.; Bogyo, M.
Deposited on	:	2015-11-04
Resolution	:	3.60 Å(reported)
Based on initial model	:	1IRU

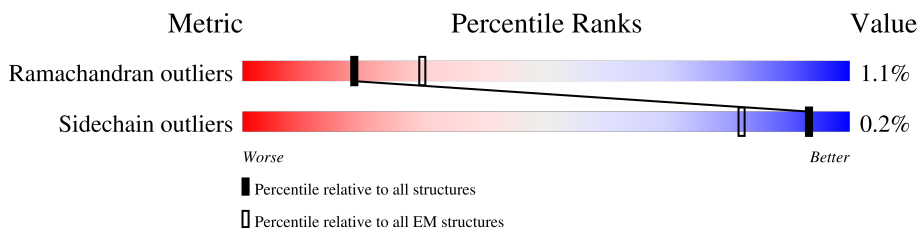The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, 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 3.60 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	Percentile Ranks	Value
Ramachandran outliers		1.1%
Sidechain outliers		0.2%

Worse   *Better*

▊ Percentile relative to all structures

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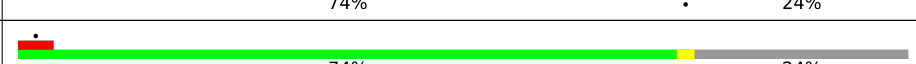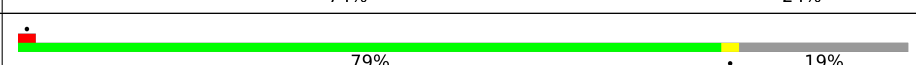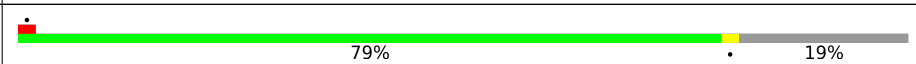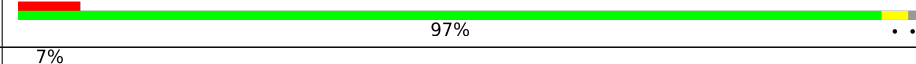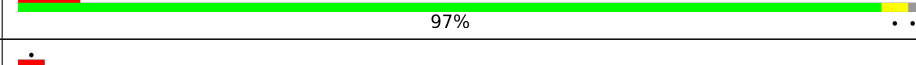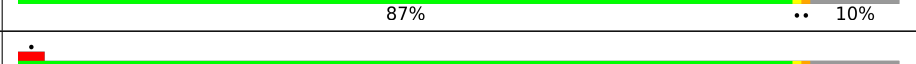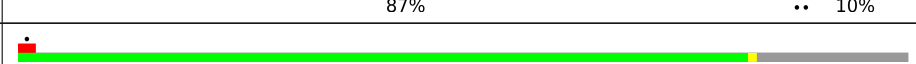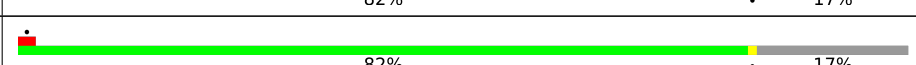
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	83% 16%
1	O	260	83% 16%
2	B	235	5% 89% • 10%
2	P	235	89% • 10%
3	C	246	88% • 11%
3	Q	246	88% • 11%
4	D	241	6% 88% • 11%
4	R	241	6% 88% • 11%
5	E	256	83% • 15%

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
5	S	256	83% · 15%
6	F	254	85% · 14%
6	T	254	85% · 14%
7	G	252	87% 13%
7	U	252	87% 13%
8	H	252	74% · 24%
8	V	252	74% · 24%
9	I	229	79% · 19%
9	W	229	79% · 19%
10	J	218	5% 87% · 12%
10	X	218	87% · 12%
11	K	195	7% 97% ··
11	Y	195	7% 97% ··
12	L	211	87% ·· 10%
12	Z	211	87% ·· 10%
13	M	240	82% · 17%
13	a	240	82% · 17%
14	N	265	70% 29%
14	b	265	70% 29%

2   Entry composition ⓘ

There are 15 unique types of molecules in this entry. The entry contains 39334 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, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		
1	O	219	Total	C	N	O	S	0	0
			1440	907	251	274	8		

- Molecule 2 is a protein called PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		
2	P	212	Total	C	N	O	S	0	0
			1381	895	232	250	4		

- Molecule 3 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		
3	Q	220	Total	C	N	O	S	0	0
			1527	984	251	289	3		

- Molecule 4 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		
4	R	215	Total	C	N	O	S	0	0
			1409	904	241	259	5		

- Molecule 5 is a protein called PROTEASOME SUBUNIT ALPHA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		
5	S	217	Total	C	N	O	S	0	0
			1440	914	241	277	8		

- Molecule 6 is a protein called PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		
6	T	219	Total	C	N	O	S	0	0
			1492	956	244	287	5		

- Molecule 7 is a protein called PROTEASOME COMPONENT C8, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		
7	U	219	Total	C	N	O	S	0	0
			1542	988	265	281	8		

- Molecule 8 is a protein called PROTEASOME, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		
8	V	191	Total	C	N	O	S	0	0
			1316	832	224	253	7		

- Molecule 9 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		
9	W	186	Total	C	N	O	S	0	0
			1241	774	218	236	13		

- Molecule 10 is a protein called BETA3 PROTEASOME SUBUNIT, PUTATIVE.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	191	Total	C	N	O	S	0	0
			1273	803	215	243	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	191	Total 1273	C 803	N 215	O 243	S 12	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	MET	-	initiating methionine	UNP Q8I261
J	2	GLY	-	expression tag	UNP Q8I261
J	3	SER	-	expression tag	UNP Q8I261
J	4	ILE	-	expression tag	UNP Q8I261
J	5	TYR	-	expression tag	UNP Q8I261
J	6	ASN	-	expression tag	UNP Q8I261
J	7	TYR	-	expression tag	UNP Q8I261
J	8	ASN	-	expression tag	UNP Q8I261
J	9	GLY	-	expression tag	UNP Q8I261
J	10	GLY	-	expression tag	UNP Q8I261
J	11	CYS	-	expression tag	UNP Q8I261
J	12	VAL	-	expression tag	UNP Q8I261
J	13	LEU	-	expression tag	UNP Q8I261
J	14	GLY	-	expression tag	UNP Q8I261
X	1	MET	-	initiating methionine	UNP Q8I261
X	2	GLY	-	expression tag	UNP Q8I261
X	3	SER	-	expression tag	UNP Q8I261
X	4	ILE	-	expression tag	UNP Q8I261
X	5	TYR	-	expression tag	UNP Q8I261
X	6	ASN	-	expression tag	UNP Q8I261
X	7	TYR	-	expression tag	UNP Q8I261
X	8	ASN	-	expression tag	UNP Q8I261
X	9	GLY	-	expression tag	UNP Q8I261
X	10	GLY	-	expression tag	UNP Q8I261
X	11	CYS	-	expression tag	UNP Q8I261
X	12	VAL	-	expression tag	UNP Q8I261
X	13	LEU	-	expression tag	UNP Q8I261
X	14	GLY	-	expression tag	UNP Q8I261

- Molecule 11 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	194	Total 1452	C 932	N 240	O 273	S 7	0	0
11	Y	194	Total 1452	C 932	N 240	O 273	S 7	0	0

- Molecule 12 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	189	Total 1355	C 870	N 223	O 256	S 6	0	0
12	Z	189	Total 1355	C 870	N 223	O 256	S 6	0	0

- Molecule 13 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	199	Total 1413	C 908	N 236	O 263	S 6	0	0
13	a	199	Total 1413	C 908	N 236	O 263	S 6	0	0

- Molecule 14 is a protein called PROTEASOME SUBUNIT BETA TYPE.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	187	Total 1337	C 852	N 233	O 249	S 3	0	0
14	b	187	Total 1337	C 852	N 233	O 249	S 3	0	0

- Molecule 15 is (2S)-N-[(E,2S)-1-(1H-indol-3-yl)-4-methylsulfonyl-but-3-en-2-yl]-2-[[(2S)-3-(1 H-indol-3-yl)-2-(2-morpholin-4-ylethanoylamino)propanoyl]amino]-4-methyl-pentanamide (three-letter code: 7F1) (formula: $C_{36}H_{46}N_6O_6S$).
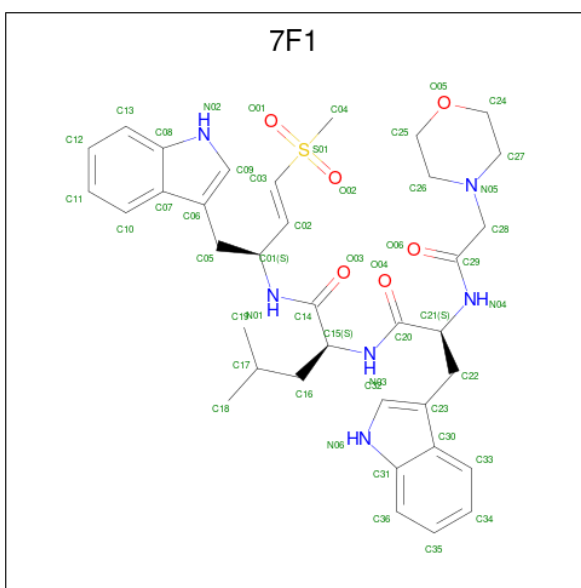
Mol	Chain	Residues	Atoms					AltConf
15	I	1	Total	C	N	O	S	0
			49	36	6	6	1	
15	W	1	Total	C	N	O	S	0
			49	36	6	6	1	

3   Residue-property plots ⓘ

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

• Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE

Chain A:

• Molecule 1: PROTEASOME SUBUNIT ALPHA, PUTATIVE

Chain O:

• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE

Chain B:

• Molecule 2: PROTEASOME SUBUNIT ALPHA TYPE 2, PUTATIVE

Chain P:

- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

Chain C:

- Molecule 3: PROTEASOME SUBUNIT ALPHA TYPE

Chain Q:

- Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE

Chain D:

- Molecule 4: PROTEASOME SUBUNIT ALPHA TYPE

Chain R:

- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE

Chain E:

- Molecule 5: PROTEASOME SUBUNIT ALPHA TYPE

Chain S:

- Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

Chain F:

85%   14%

MET TYR ARG ASN LEU TYR D7 A28 I53 S54 E61 G129 N139 G150 A162 C181 S182 K195 CYS SER LEU SER SER GLU SER LEU THR ILE SER N208 P219 S224 M237 ASP ALA GLU GLN GLU GLN VAL GLU GLU ASN VAL GLN ASN GLU

ALA ASN GLU

• Molecule 6: PROTEOSOME SUBUNIT ALPHA TYPE 1, PUTATIVE

Chain T:

85%   14%

MET TYR ARG ASN LEU TYR D7 A28 I53 S54 E61 G129 N139 G150 A162 C181 S182 K195 CYS SER LEU SER SER GLU SER LEU THR ILE SER N208 P219 S224 M237 ASP ALA GLU GLN GLU GLN VAL GLU GLU ASN VAL GLN ASN GLU

ALA ASN GLU

• Molecule 7: PROTEASOME COMPONENT C8, PUTATIVE

Chain G:

87%   13%

MET ALA GLY LEU SER ALA GLY Y8 N54 MET ASP LYS ASN LYS M60 K63 Y66 K146 N157 G158 A159 Y184 K198 L201 THR SER ASP ASP HIS MET ASN LYS ASN LEU GLN ASN L215 H233 A244 VAL GLU TYR ILE GLU LYS LEU ASN

• Molecule 7: PROTEASOME COMPONENT C8, PUTATIVE

Chain U:

87%   13%

MET ALA GLY LEU SER ALA GLY Y8 N54 MET ASP LYS ASN LYS M60 K63 Y66 K146 N157 G158 A159 Y184 K198 L201 THR SER ASP ASP HIS MET ASN LYS ASN LEU GLN ASN L215 H233 A244 VAL GLU TYR ILE GLU LYS LEU ASN

• Molecule 8: PROTEASOME, PUTATIVE

Chain H:

74%   24%

T1 D17 G23 K72 D89 GLU GLU ILE ASP ILE ASP SER ILE ASN TYR LEU ASP TYR ASN ASN ASN ASP ASN ASN LEU VAL THR LYS ASN LYS TYR PHE TYR GLU ASP LYS PHE ASN ASP TYR ASN PRO LEU VAL GLU ASN VAL ALA HIS ILE THR LYS LYS ILE ILE

TYR THR ASN ASN ASN F146 F153 K176 H177 S182 G183 S184 S223 I233 S236 F237 N245 T246 Q247 MET ASN PHE GLN TYR

• Molecule 8: PROTEASOME, PUTATIVE

Chain V:

74%   24%

• Molecule 9: PROTEASOME SUBUNIT BETA TYPE

Chain I:

• Molecule 9: PROTEASOME SUBUNIT BETA TYPE

Chain W:

• Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE

Chain J:

• Molecule 10: BETA3 PROTEASOME SUBUNIT, PUTATIVE

Chain X:

• Molecule 11: PROTEASOME SUBUNIT BETA TYPE

Chain K:

• Molecule 11: PROTEASOME SUBUNIT BETA TYPE

Chain Y:

7%

97%

MET D2 F12 I25 I26 K27 L28 T34 Q71 T74 R94 R95 N96 K109 Y134 E155 L172 N177 D185 N186 V195

• Molecule 12: PROTEASOME SUBUNIT BETA TYPE

Chain L:

87%

10%

T1 L4 G23 Q29 N30 V31 E32 K33 I37 N71 E72 Y90 LYS GLY TYR GLY LEU C96 T107 D144 N182 F194 ASP LEU HIS TYR HIS TYR THR ASN PRO GLU GLN LYS ASP GLN TYR VAL MET

• Molecule 12: PROTEASOME SUBUNIT BETA TYPE

Chain Z:

87%

10%

T1 L4 G23 Q29 N30 V31 E32 K33 I37 N71 E72 Y90 LYS GLY TYR GLY LEU C96 T107 D144 N182 F194 ASP LEU HIS TYR HIS TYR THR ASN PRO GLU GLN LYS ASP GLN TYR VAL MET

• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

Chain M:

82%

17%

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 LYS ARG TRP TYR P32 L51 L59 Y64 T75 E143 ASN ASN K146 Q186 LEU ILE LYS ASN T191 F201 D218 T234 L235 D236

LEU LYS GLN ASP

• Molecule 13: PROTEASOME SUBUNIT BETA TYPE

Chain a:

82%

17%

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 LYS ARG TRP TYR P32 L51 L59 Y64 T75 E143 ASN ASN K146 Q186 LEU ILE LYS ASN T191 F201 D218 T234 L235 D236

LEU LYS GLN ASP

• Molecule 14: PROTEASOME SUBUNIT BETA TYPE

Chain N:

70%

29%

MET THR LEU GLY PRO V6 K18 S33 N75 L76 SER GLU LYS LYS ARG LYS GLU ASP D84 N104 ARG ILE ASP P108 I118 ASN SER GLN LYS TYR ASP ASN ASN ASP ASN VAL LEU LEU TYR THR ASN LYS ASN ASP ASP GLU GLN ASN GLU TYR LYS ASN ASN GLU

GLU TYR LYS GLU ILE HIS LYS ASP D158 E201 D217 E238 I241 LEU PRO CYS VAL LEU ASN SER ALA ASP TYR VAL TYR PRO SER THR LEU LEU PRO PRO ALA GLY CYS MET TRP

• Molecule 14: PROTEASOME SUBUNIT BETA TYPE

Chain b:

70% 29%

4   Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	97720	Depositor
Resolution determination method	Not provided	
CTF correction method	FULL RECORDED IMAGE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/Å^2)$	4.8	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	15.982	Depositor
Minimum map value	-10.651	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.0	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7F1

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	0.49	0/1455	0.60	0/1988
1	O	0.49	0/1455	0.60	0/1988
2	B	0.50	0/1400	0.62	0/1921
2	P	0.50	0/1400	0.62	0/1921
3	C	0.52	0/1554	0.64	1/2131 (0.0%)
3	Q	0.52	0/1554	0.64	1/2131 (0.0%)
4	D	0.49	0/1427	0.59	0/1964
4	R	0.49	0/1427	0.59	0/1964
5	E	0.49	0/1457	0.60	0/1997
5	S	0.49	0/1457	0.60	0/1997
6	F	0.49	0/1519	0.58	0/2082
6	T	0.49	0/1519	0.58	0/2082
7	G	0.51	0/1571	0.61	0/2150
7	U	0.51	0/1571	0.61	0/2150
8	H	0.57	0/1332	0.63	0/1814
8	V	0.57	0/1332	0.63	0/1814
9	I	0.69	1/1257 (0.1%)	0.71	1/1721 (0.1%)
9	W	0.69	1/1257 (0.1%)	0.71	1/1721 (0.1%)
10	J	0.53	0/1283	0.66	0/1751
10	X	0.53	0/1283	0.66	0/1751
11	K	0.56	0/1482	0.68	1/2017 (0.0%)
11	Y	0.56	0/1482	0.68	1/2017 (0.0%)
12	L	0.54	0/1378	0.71	4/1866 (0.2%)
12	Z	0.54	0/1378	0.71	4/1866 (0.2%)
13	M	0.54	0/1434	0.65	0/1956
13	a	0.54	0/1434	0.65	0/1956
14	N	0.53	0/1355	0.64	0/1844
14	b	0.53	0/1355	0.64	0/1844
All	All	0.53	2/39808 (0.0%)	0.64	14/54404 (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
1	A	0	1
1	O	0	1
11	K	0	1
11	Y	0	1
12	L	0	2
12	Z	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	THR	C-N	15.29	1.69	1.34
9	W	1	THR	C-N	15.29	1.69	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	1	THR	O-C-N	-13.05	101.81	122.70
9	W	1	THR	O-C-N	-13.05	101.81	122.70
12	L	32	GLU	O-C-N	-6.86	111.73	122.70
12	Z	32	GLU	O-C-N	-6.86	111.73	122.70
12	L	33	LYS	CA-C-N	-5.63	104.82	117.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	THR	Peptide
11	K	12	PHE	Peptide
12	L	32	GLU	Mainchain
12	L	33	LYS	Mainchain
1	O	236	THR	Peptide

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	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	17	57
1	O	211/260 (81%)	202 (96%)	7 (3%)	2 (1%)	17	57
2	B	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	29	68
2	P	206/235 (88%)	200 (97%)	5 (2%)	1 (0%)	29	68
3	C	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	17	57
3	Q	216/246 (88%)	202 (94%)	12 (6%)	2 (1%)	17	57
4	D	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	15	55
4	R	209/241 (87%)	200 (96%)	7 (3%)	2 (1%)	15	55
5	E	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	8	42
5	S	213/256 (83%)	201 (94%)	8 (4%)	4 (2%)	8	42
6	F	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	11	48
6	T	215/254 (85%)	196 (91%)	16 (7%)	3 (1%)	11	48
7	G	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	29	68
7	U	213/252 (84%)	200 (94%)	12 (6%)	1 (0%)	29	68
8	H	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	9	46
8	V	187/252 (74%)	170 (91%)	14 (8%)	3 (2%)	9	46
9	I	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	6	39
9	W	182/229 (80%)	164 (90%)	14 (8%)	4 (2%)	6	39
10	J	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	14	53
10	X	187/218 (86%)	178 (95%)	7 (4%)	2 (1%)	14	53
11	K	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	9	46
11	Y	192/195 (98%)	181 (94%)	8 (4%)	3 (2%)	9	46
12	L	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	14	53
12	Z	185/211 (88%)	174 (94%)	9 (5%)	2 (1%)	14	53
13	M	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	15	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a	193/240 (80%)	176 (91%)	15 (8%)	2 (1%)	15	55
14	N	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
14	b	179/265 (68%)	171 (96%)	8 (4%)	0	100	100
All	All	5576/6708 (83%)	5230 (94%)	284 (5%)	62 (1%)	18	53

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	38	SER
5	E	151	ASN
9	I	24	PRO
9	I	188	PRO
13	M	64	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	118/231 (51%)	118 (100%)	0	100	100
1	O	118/231 (51%)	118 (100%)	0	100	100
2	B	111/205 (54%)	110 (99%)	1 (1%)	78	90
2	P	111/205 (54%)	110 (99%)	1 (1%)	78	90
3	C	129/213 (61%)	129 (100%)	0	100	100
3	Q	129/213 (61%)	129 (100%)	0	100	100
4	D	107/207 (52%)	107 (100%)	0	100	100
4	R	107/207 (52%)	107 (100%)	0	100	100
5	E	126/223 (56%)	126 (100%)	0	100	100
5	S	126/223 (56%)	126 (100%)	0	100	100
6	F	127/227 (56%)	127 (100%)	0	100	100
6	T	127/227 (56%)	127 (100%)	0	100	100
7	G	140/229 (61%)	140 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	140/229 (61%)	140 (100%)	0	100	100
8	H	118/231 (51%)	117 (99%)	1 (1%)	81	91
8	V	118/231 (51%)	117 (99%)	1 (1%)	81	91
9	I	117/194 (60%)	117 (100%)	0	100	100
9	W	117/194 (60%)	117 (100%)	0	100	100
10	J	118/191 (62%)	118 (100%)	0	100	100
10	X	118/191 (62%)	118 (100%)	0	100	100
11	K	138/174 (79%)	138 (100%)	0	100	100
11	Y	138/174 (79%)	138 (100%)	0	100	100
12	L	127/176 (72%)	127 (100%)	0	100	100
12	Z	127/176 (72%)	127 (100%)	0	100	100
13	M	139/216 (64%)	138 (99%)	1 (1%)	84	93
13	a	139/216 (64%)	138 (99%)	1 (1%)	84	93
14	N	122/239 (51%)	121 (99%)	1 (1%)	81	91
14	b	122/239 (51%)	121 (99%)	1 (1%)	81	91
All	All	3474/5912 (59%)	3466 (100%)	8 (0%)	93	98

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	b	75	ASN
13	a	234	THR
2	P	163	VAL
14	N	75	ASN
8	V	89	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
7	U	130	HIS
11	Y	132	HIS
8	V	194	GLN
9	W	114	HIS
12	Z	106	HIS

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	7F1	I	300	9	50,53,53	3.45	18 (36%)	61,74,74	1.65	13 (21%)
15	7F1	W	300	9	50,53,53	3.45	18 (36%)	61,74,74	1.65	13 (21%)

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	7F1	I	300	9	-	16/39/50/50	0/5/5/5
15	7F1	W	300	9	-	16/39/50/50	0/5/5/5

The worst 5 of 36 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	I	300	7F1	C03-C02	14.75	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	300	7F1	C03-C02	14.75	1.55	1.31
15	I	300	7F1	C03-S01	7.26	1.84	1.75
15	W	300	7F1	C03-S01	7.26	1.84	1.75
15	I	300	7F1	C14-N01	7.13	1.49	1.34

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	I	300	7F1	C02-C03-S01	-5.01	109.64	122.06
15	W	300	7F1	C02-C03-S01	-5.01	109.64	122.06
15	I	300	7F1	C22-C23-C32	-3.80	123.28	127.97
15	W	300	7F1	C22-C23-C32	-3.80	123.28	127.97
15	I	300	7F1	C05-C06-C09	-3.68	123.42	127.97

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	I	300	7F1	N01-C01-C02-C03
15	I	300	7F1	C05-C01-C02-C03
15	I	300	7F1	C02-C03-S01-O01
15	I	300	7F1	C01-C02-C03-S01
15	W	300	7F1	N01-C01-C02-C03

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 7F1 I 300

Bond lengths

Bond angles

Torsions

Rings

Ligand 7F1 W 300

Bond lengths

Bond angles

Torsions

Rings
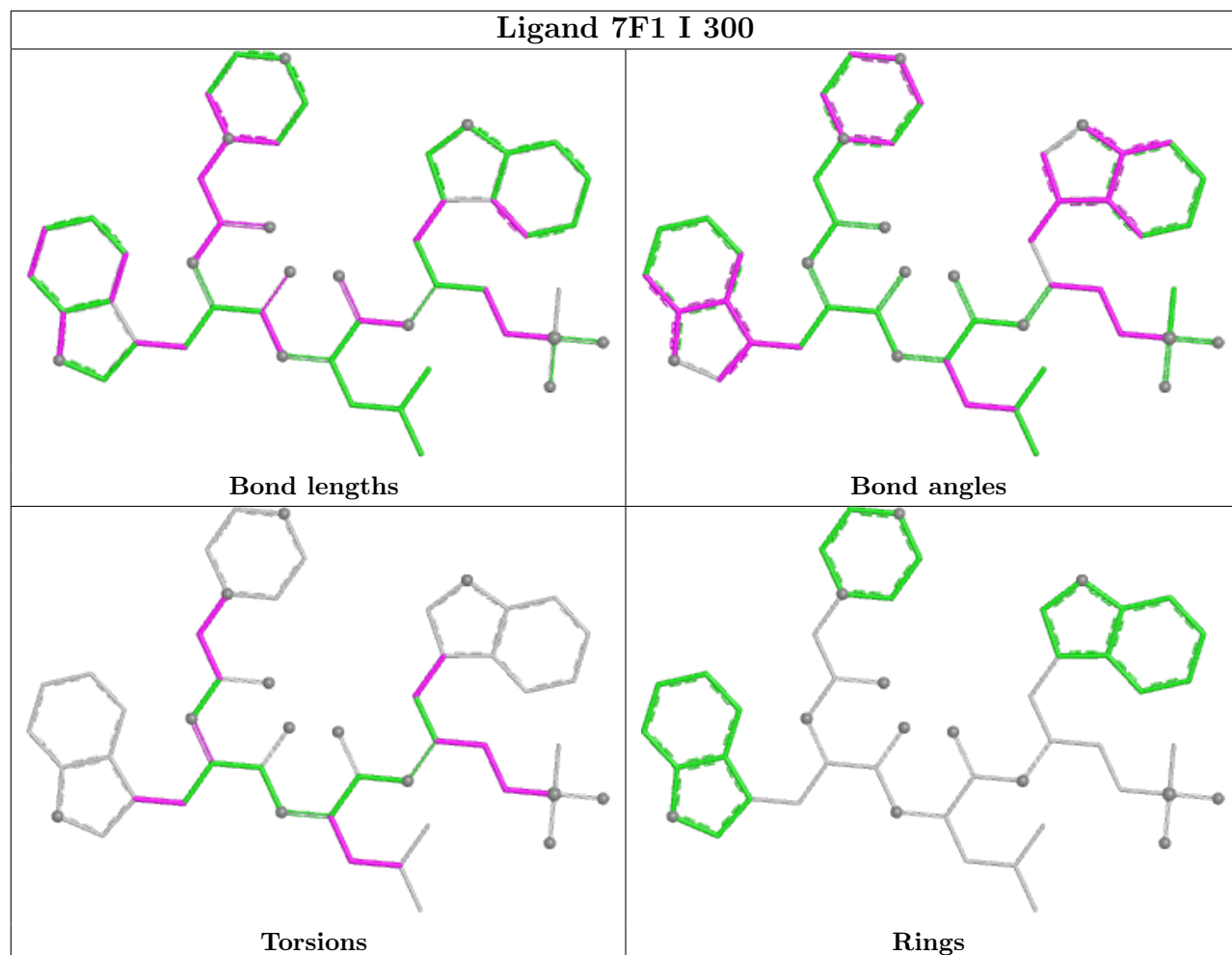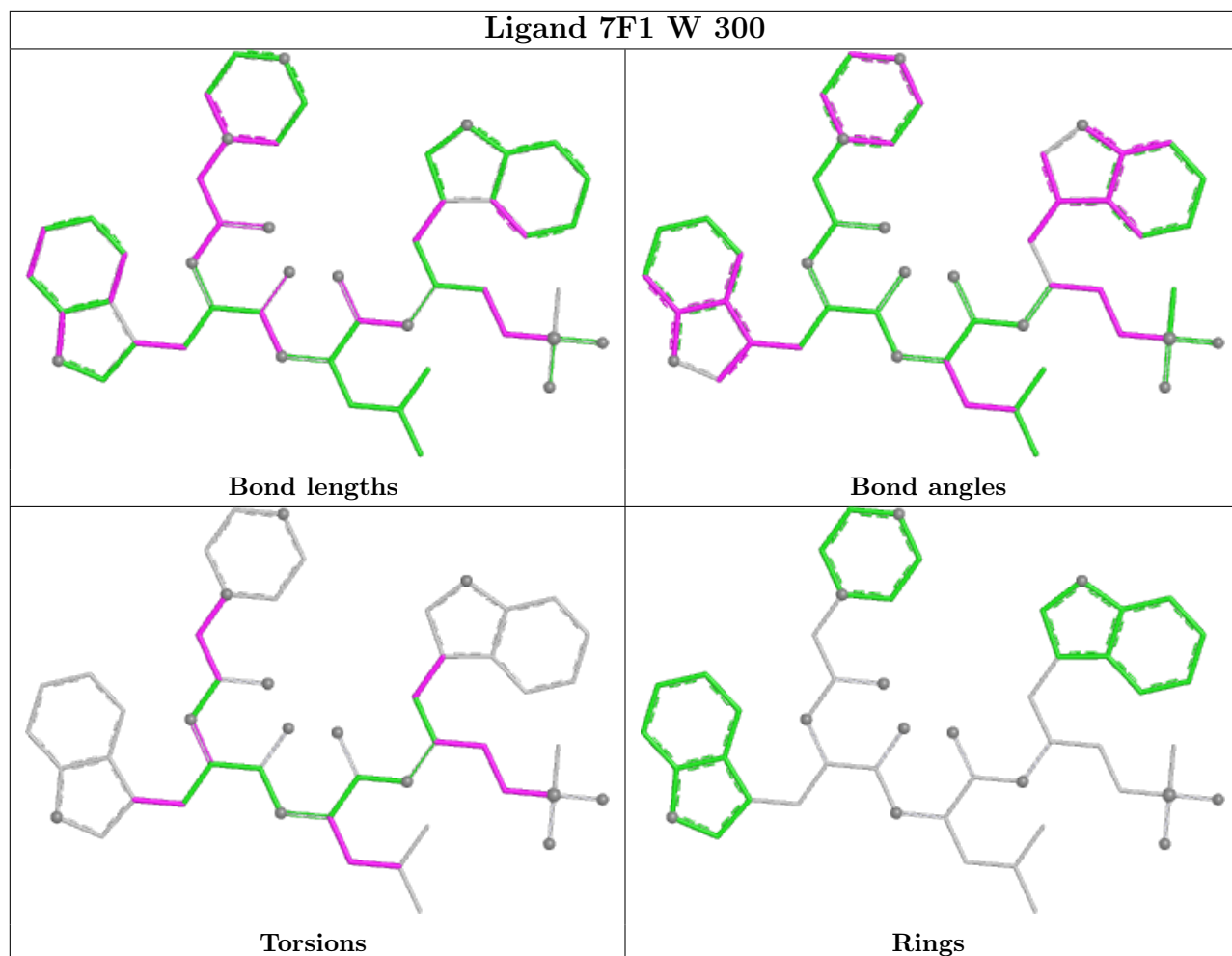
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	I	1
9	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	1:THR	C	2:THR	N	1.69
1	W	1:THR	C	2:THR	N	1.69

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-3231. 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 ⓘ

6.1.1 Primary map

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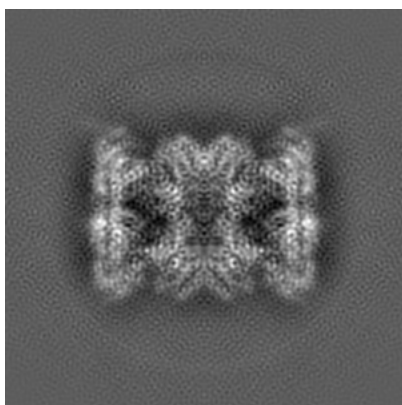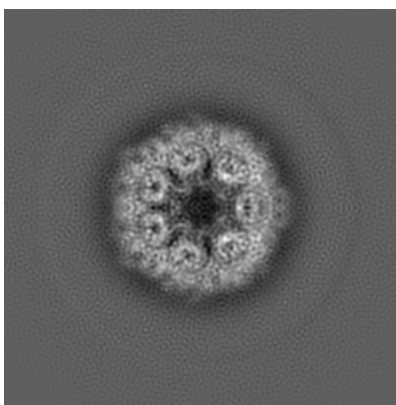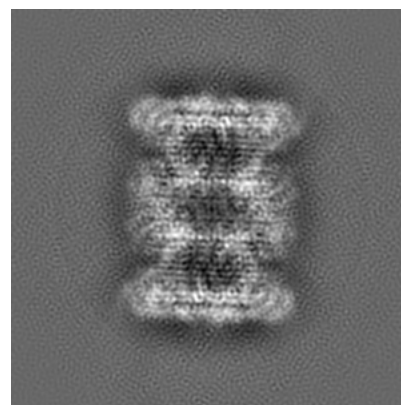
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
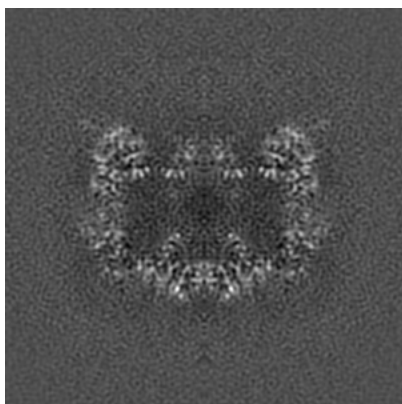
6.2.1 Primary map
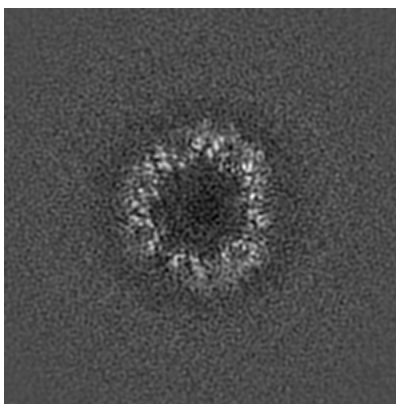
| X Index: 128 | Y Index: 128 | Z Index: 128 |
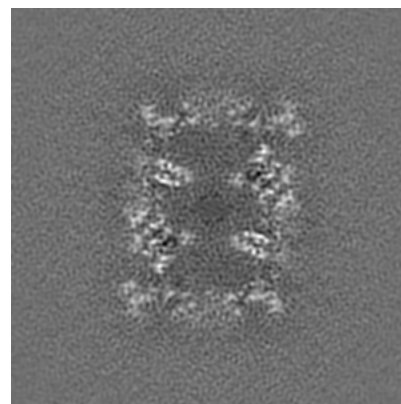
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
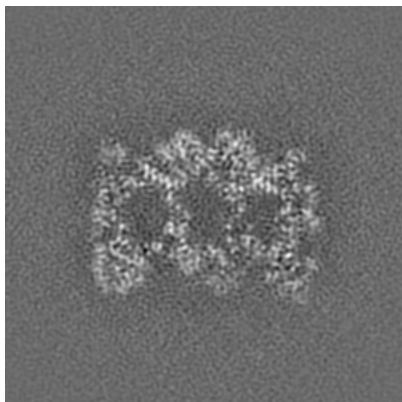
6.3.1 Primary map
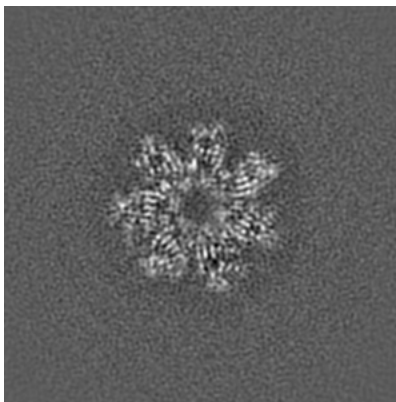
| X Index: 109 | Y Index: 145 | Z Index: 101 |
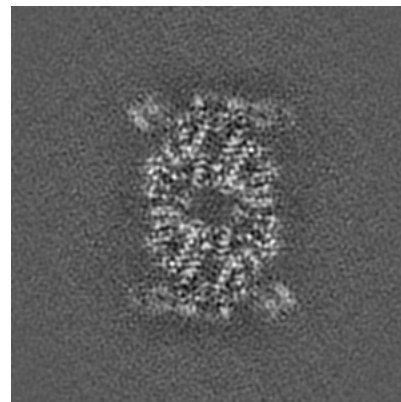
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map

| X | Y | Z |
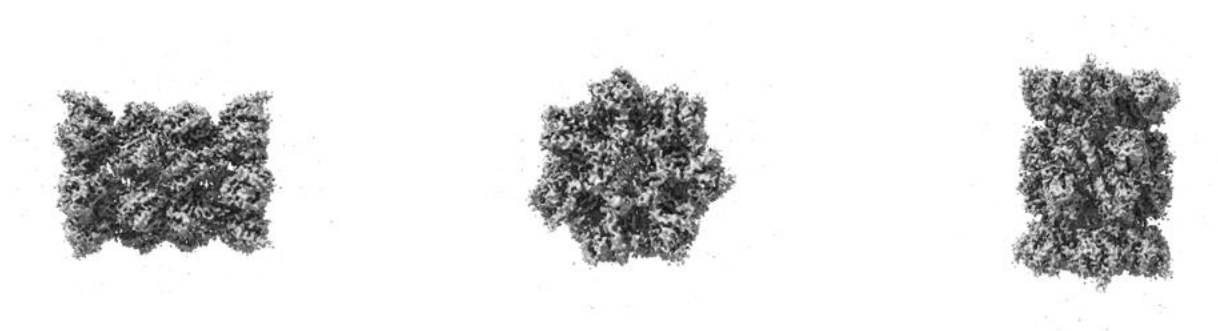
The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

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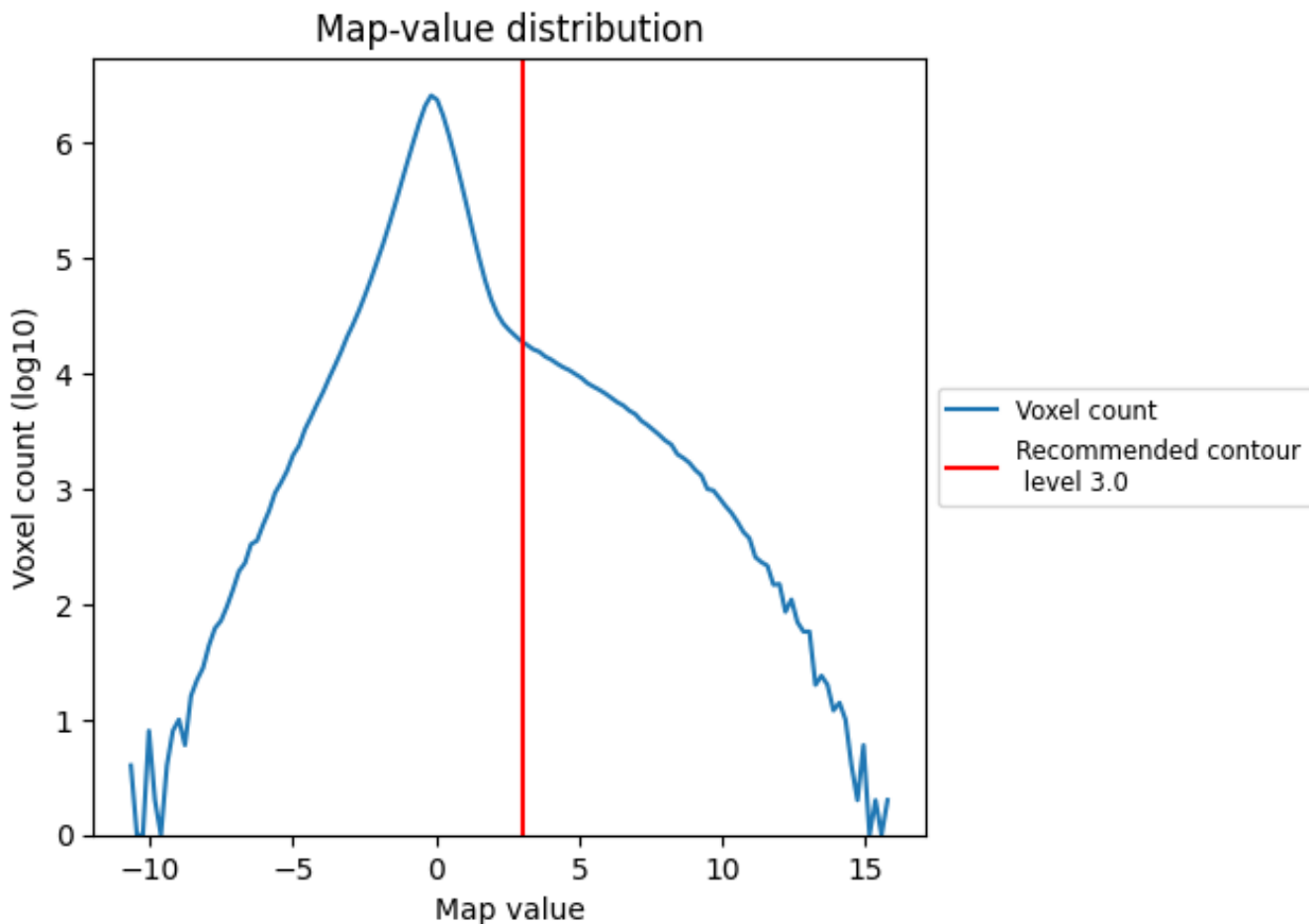
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate (i)
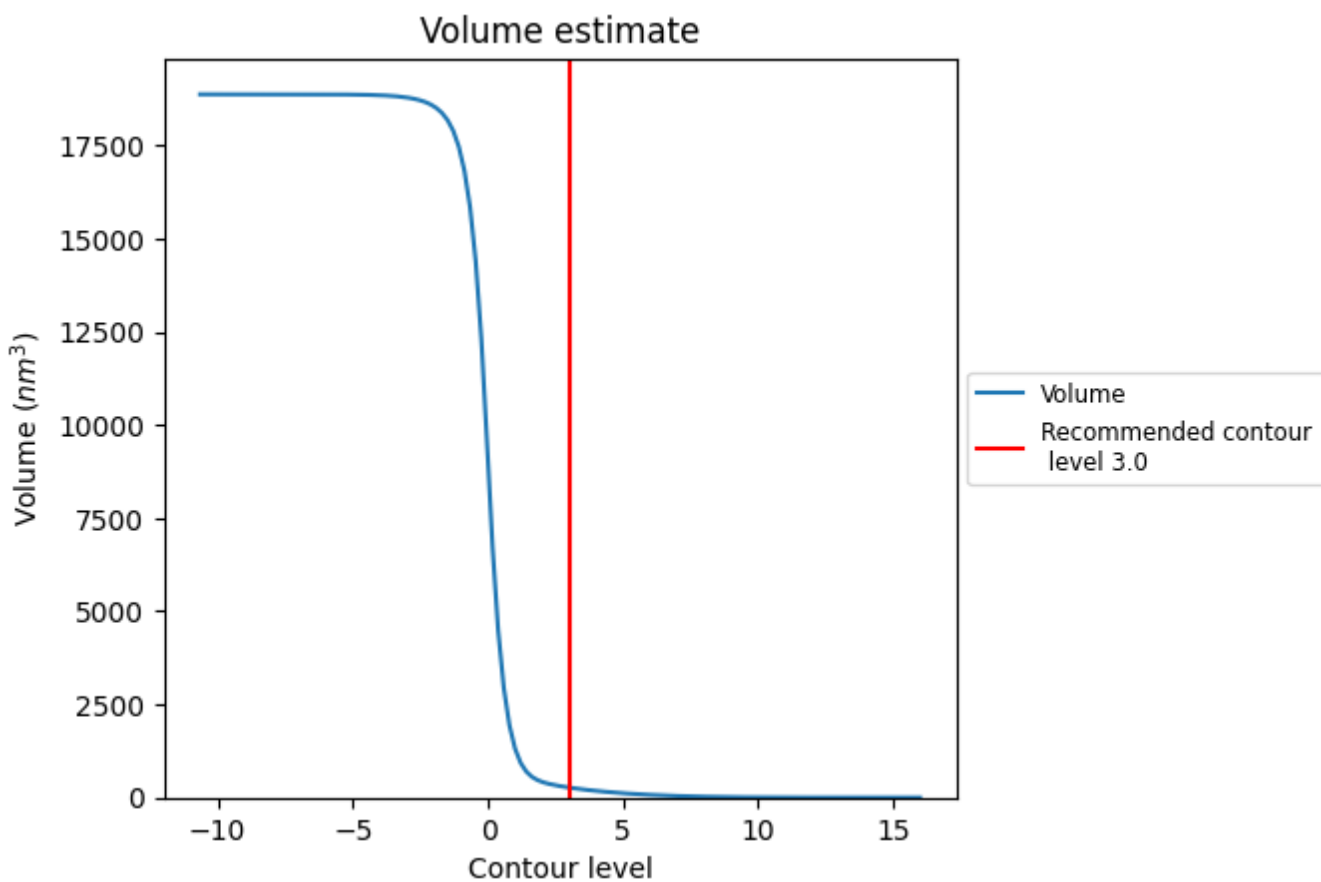
The volume at the recommended contour level is 268 nm^3; this corresponds to an approximate mass of 242 kDa.

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

7.3　Rotationally averaged power spectrum ⓘ
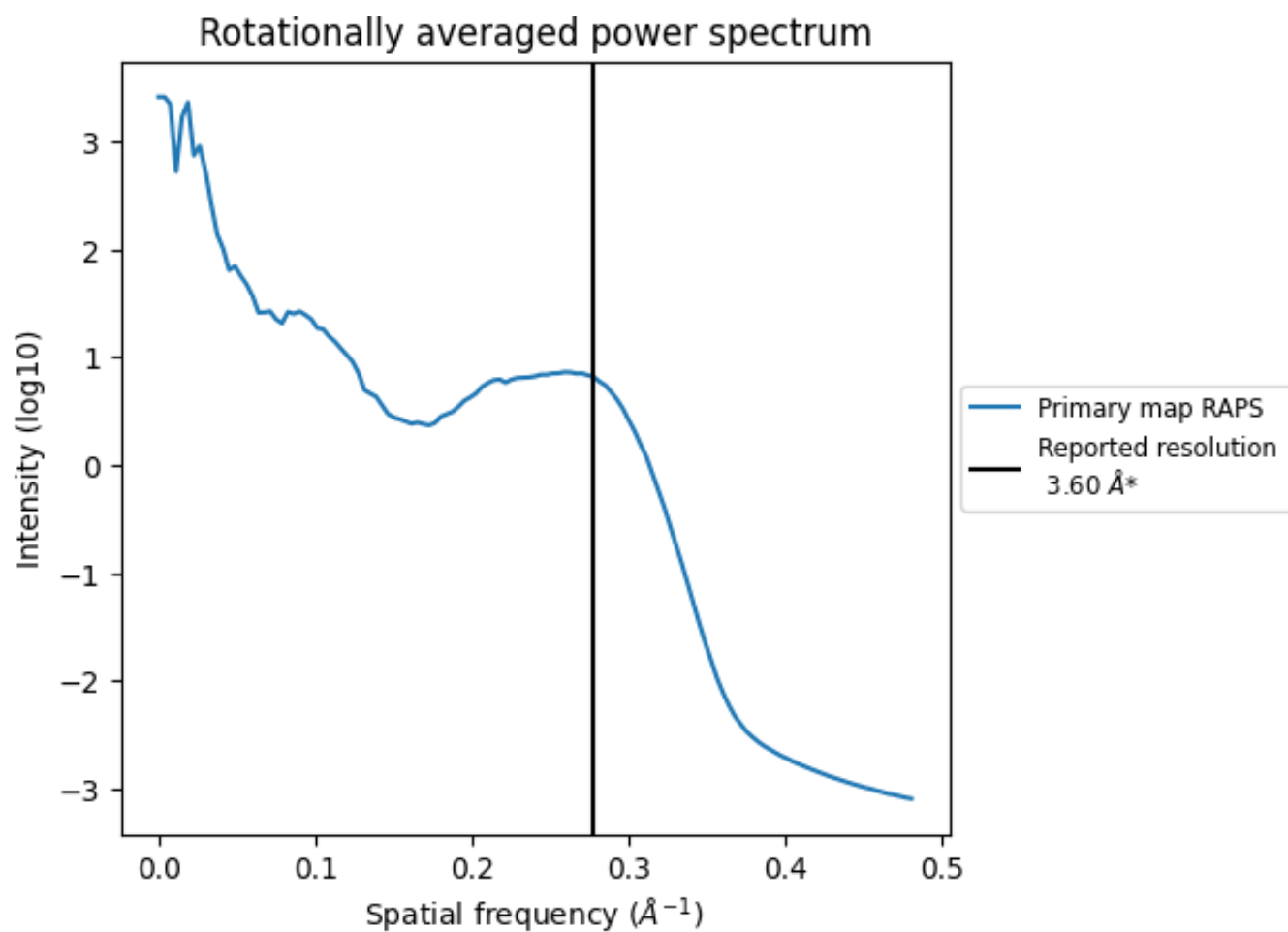
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-3231 and PDB model 5FMG. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay ⓘ

X   Y   Z
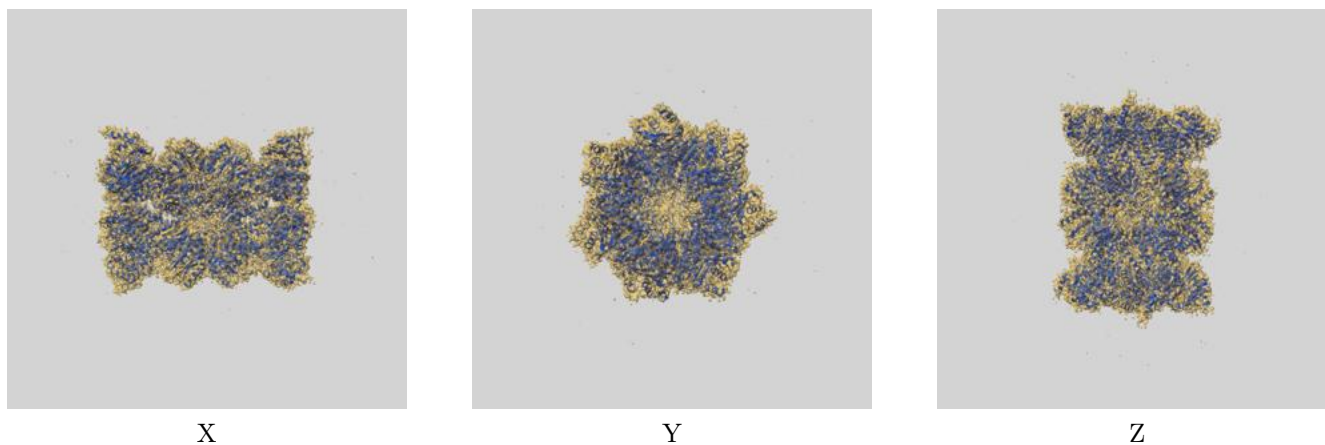
The images above show the 3D surface view of the map at the recommended contour level 3.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model   ⓘ
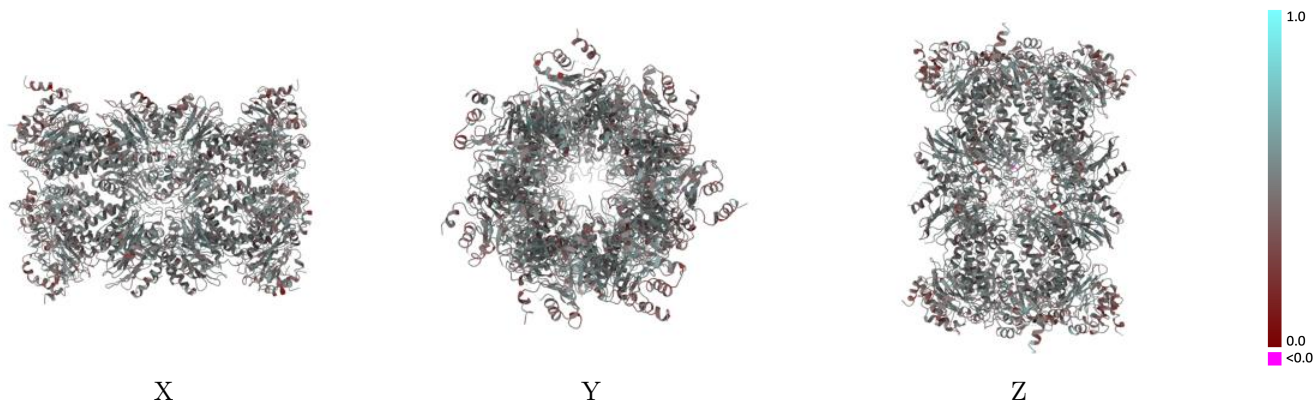
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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   ⓘ
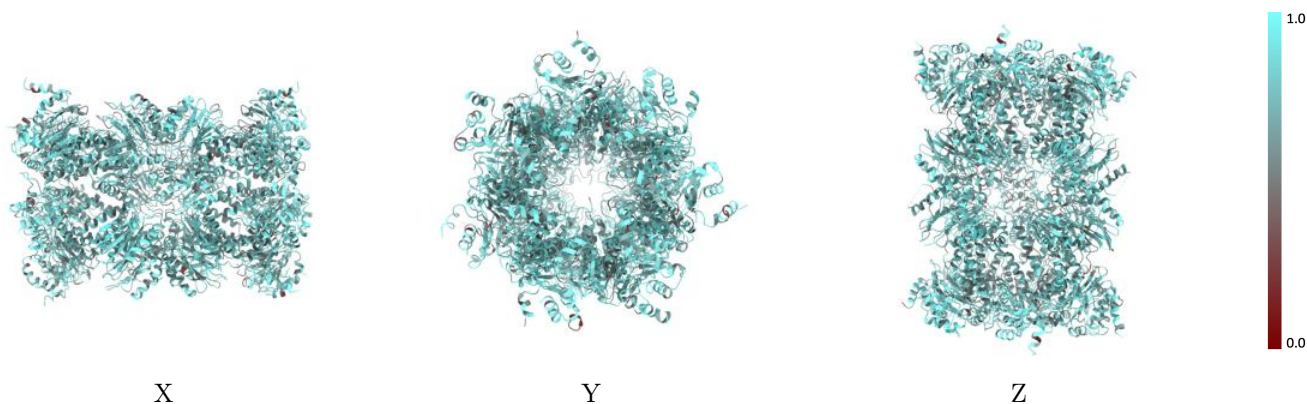
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.0).

9.4 Atom inclusion ⓘ
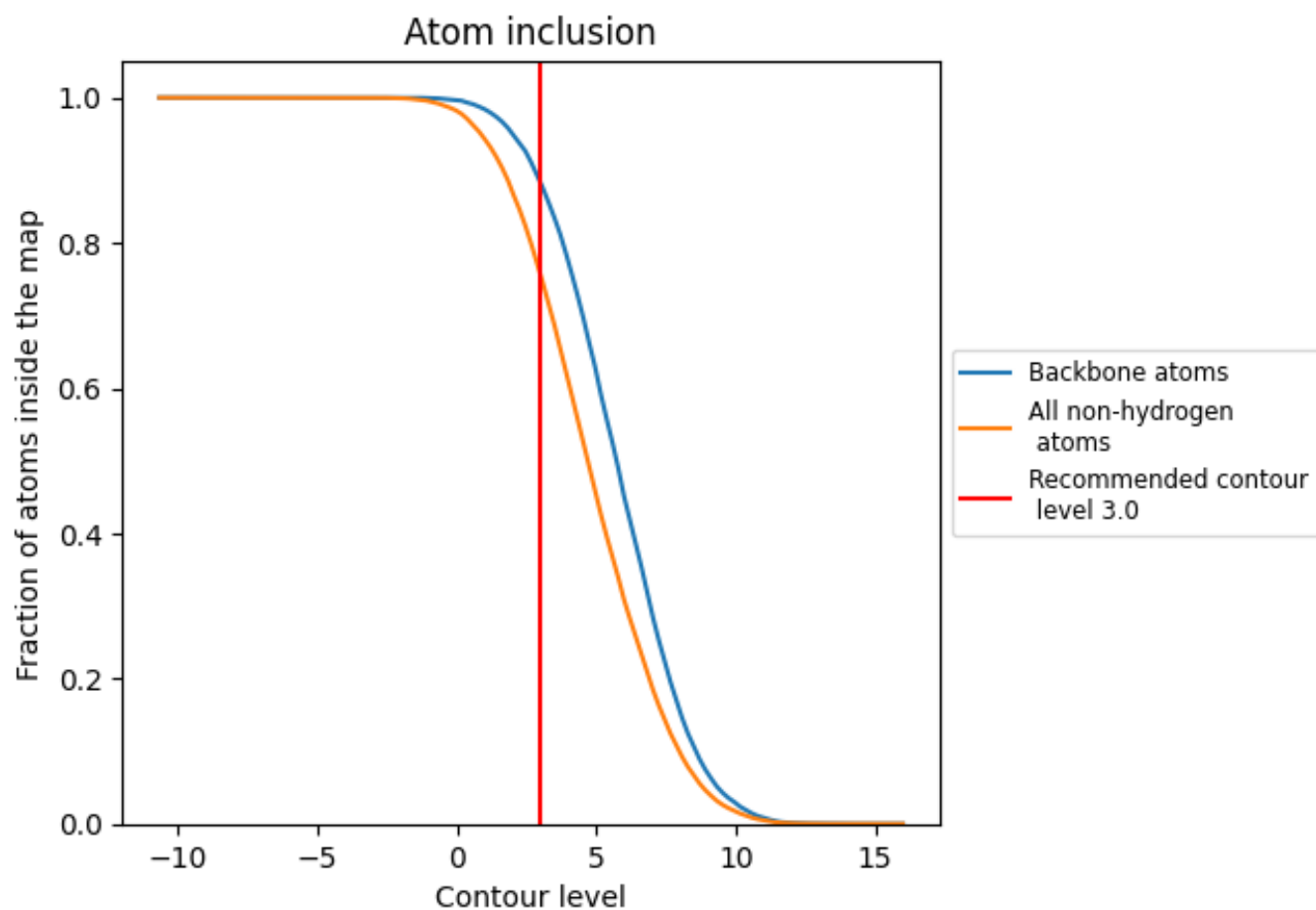
At the recommended contour level, 88% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7567	0.4700
A	0.7360	0.4620
B	0.7642	0.4720
C	0.7842	0.4600
D	0.7348	0.4640
E	0.7712	0.4570
F	0.7546	0.4710
G	0.7474	0.4590
H	0.7523	0.4790
I	0.7877	0.4880
J	0.7132	0.4780
K	0.7360	0.4600
L	0.7888	0.4720
M	0.7654	0.4800
N	0.7563	0.4840
O	0.7374	0.4610
P	0.7672	0.4720
Q	0.7882	0.4600
R	0.7362	0.4630
S	0.7740	0.4580
T	0.7512	0.4730
U	0.7487	0.4600
V	0.7569	0.4790
W	0.7814	0.4850
X	0.7100	0.4780
Y	0.7360	0.4590
Z	0.7896	0.4730
a	0.7626	0.4800
b	0.7540	0.4860

1.0

0.0
<0.0