Full wwPDB EM Validation Report ⓘ

Jan 27, 2025 – 05:44 PM EST

PDB ID	:	9C39
EMDB ID	:	EMD-45162
Title	:	Bacteriophage Sf14 neck C6 reconstruction
Authors	:	Subramanian, S.; Kerns, H.R.; Braverman, S.G.; Doore, S.M.
Deposited on	:	2024-05-31
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:

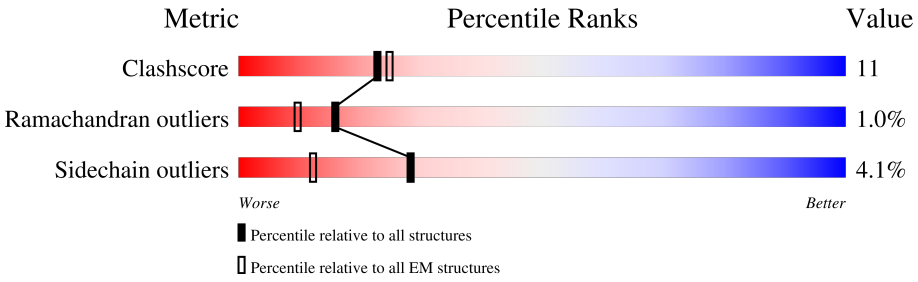
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	488	14% 60% 23% • 14%
1	B	488	13% 60% 25% • 14%
2	C	149	• 63% 23% • 13%
2	D	149	• 60% 26% • 13%
3	E	133	• 79% 19% •
4	F	199	• 75% 21% • •
5	G	148	• 77% 18% • •
6	H	450	• 77% 19% • •

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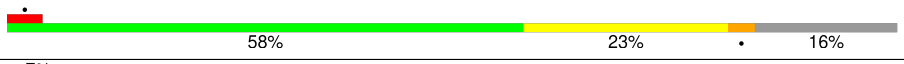
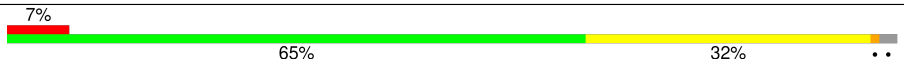
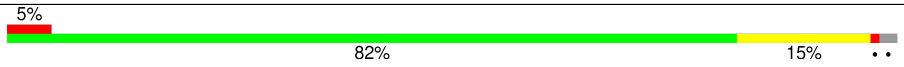
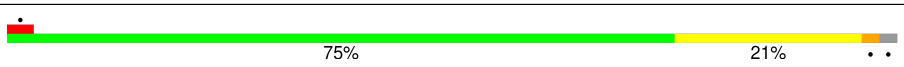
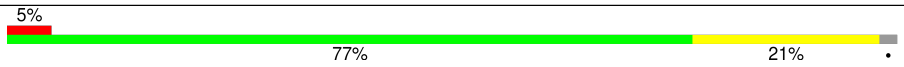
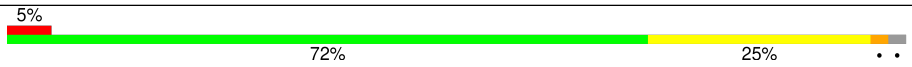
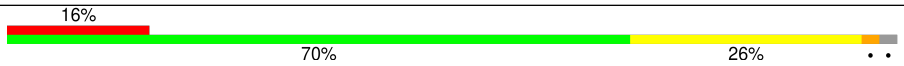
Mol	Chain	Length	Quality of chain
7	I	166	
7	J	166	
8	K	110	
8	L	110	
8	M	110	
8	N	110	
8	O	110	
8	P	110	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22110 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 Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	421	Total	C	N	O	S	0	0
			3202	2044	531	610	17		
1	B	421	Total	C	N	O	S	0	0
			3175	2031	527	600	17		

- Molecule 2 is a protein called Phage protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	130	Total	C	N	O	S	0	0
			1018	639	178	198	3		
2	D	129	Total	C	N	O	S	0	0
			1011	639	175	194	3		

- Molecule 3 is a protein called Head-closure protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	130	Total	C	N	O	S	0	0
			1035	651	187	193	4		

- Molecule 4 is a protein called gp119.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	195	Total	C	N	O	S	0	0
			1525	964	258	299	4		

- Molecule 5 is a protein called gp40.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	142	Total	C	N	O	S	0	0
			1087	682	179	221	5		

- Molecule 6 is a protein called Putative structural protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	442	Total	C	N	O	S	0	0
			3212	2032	558	617	5		

- Molecule 7 is a protein called gp127.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	156	Total	C	N	O	S	0	0
			1153	733	206	209	5		
7	J	139	Total	C	N	O	S	0	0
			1016	641	179	191	5		

- Molecule 8 is a protein called Phage protein.

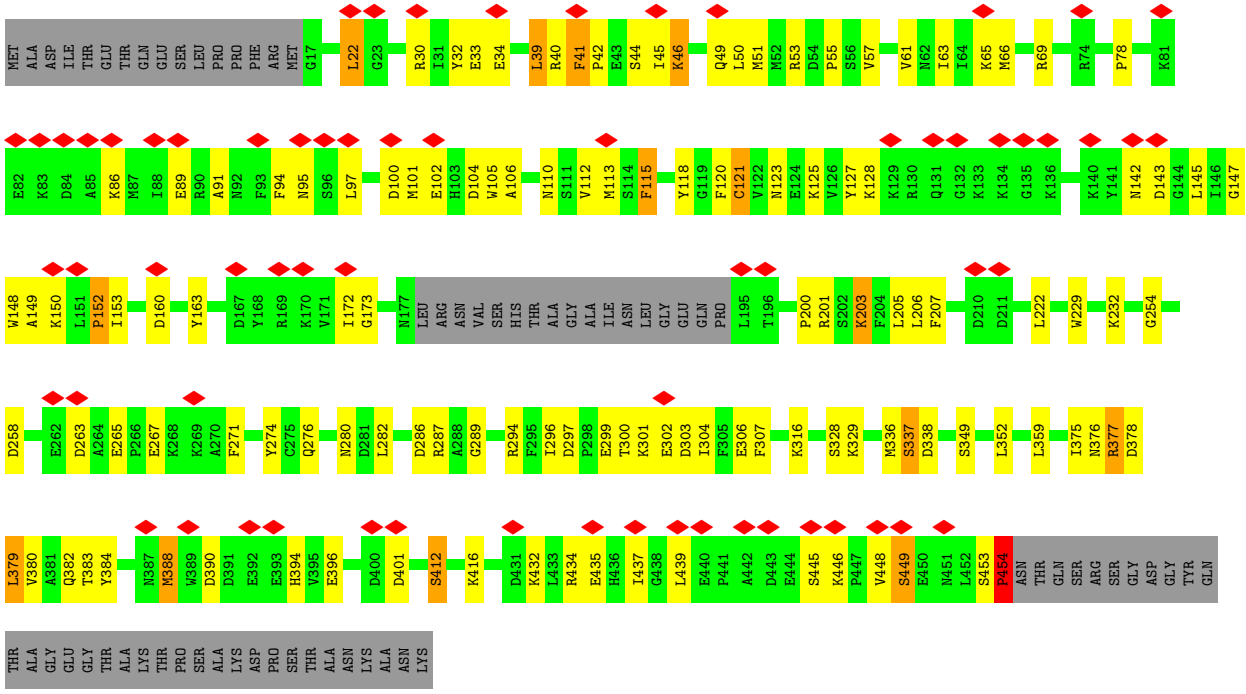
Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	108	Total	C	N	O	S	0	0
			797	506	127	163	1		
8	L	108	Total	C	N	O	S	0	0
			790	503	126	160	1		
8	M	108	Total	C	N	O	S	0	0
			782	499	127	155	1		
8	N	108	Total	C	N	O	S	0	0
			789	502	127	159	1		
8	O	108	Total	C	N	O	S	0	0
			770	492	125	152	1		
8	P	108	Total	C	N	O	S	0	0
			748	473	125	149	1		

3 Residue-property plots (i)

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

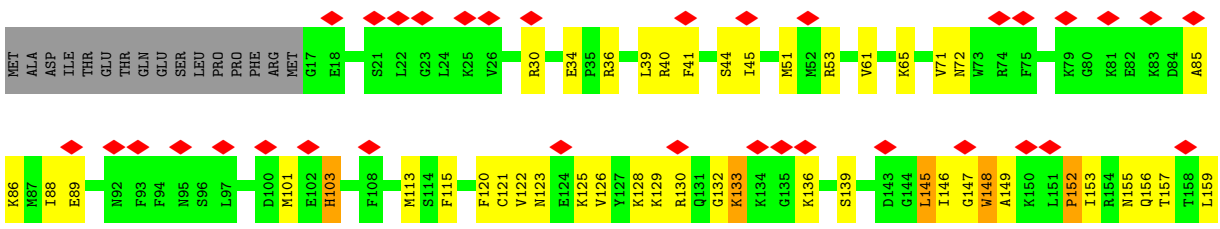
• Molecule 1: Portal protein

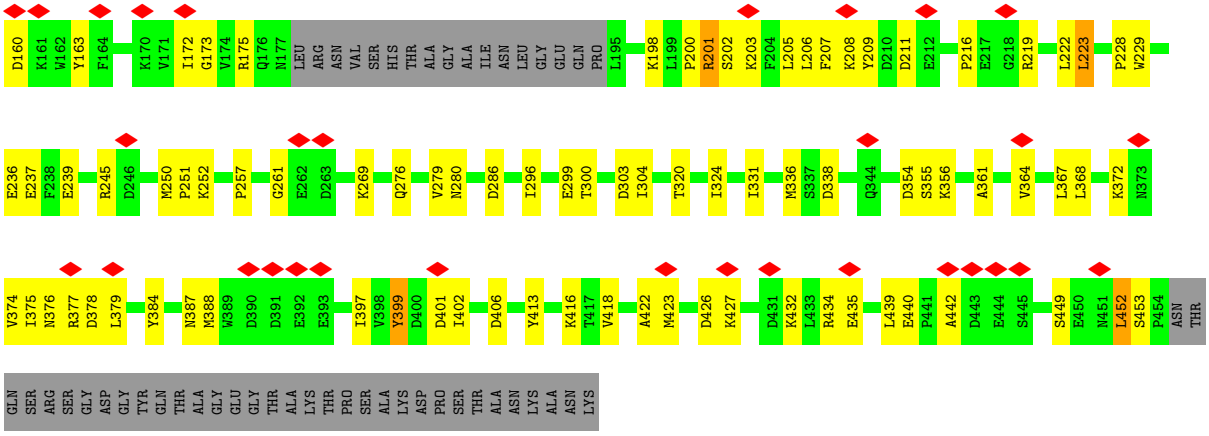
Chain A:



• Molecule 1: Portal protein

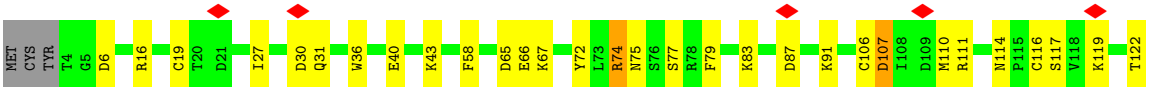
Chain B:

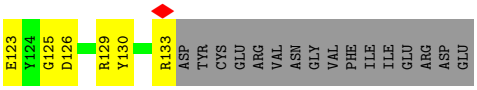




• Molecule 2: Phage protein

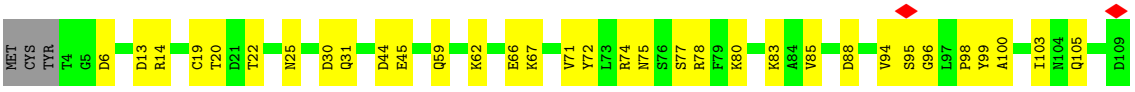
Chain C:

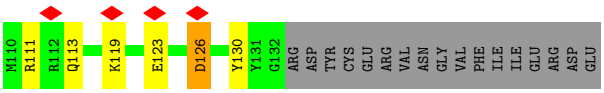




• Molecule 2: Phage protein

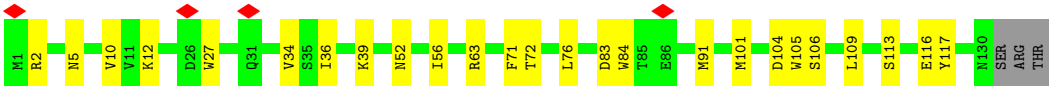
Chain D:





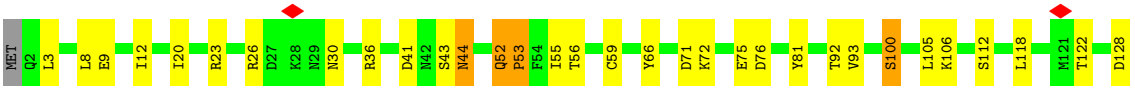
• Molecule 3: Head-closure protein

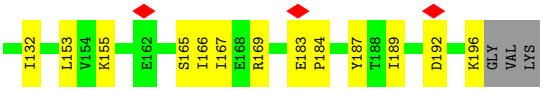
Chain E:



• Molecule 4: gp119

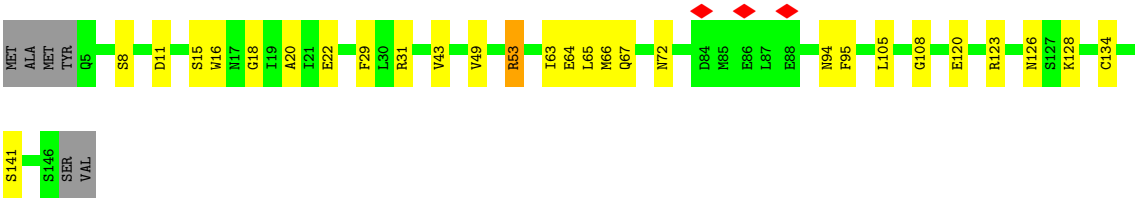
Chain F:





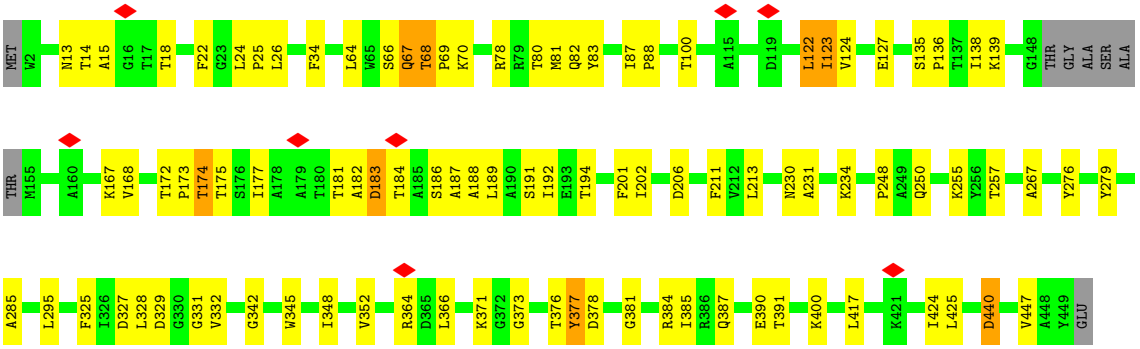
• Molecule 5: gp40

Chain G:



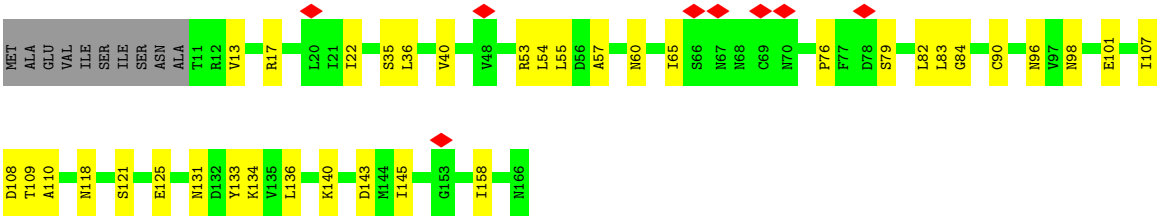
• Molecule 6: Putative structural protein

Chain H:



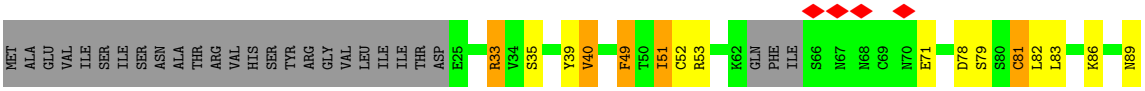
• Molecule 7: gp127

Chain I:



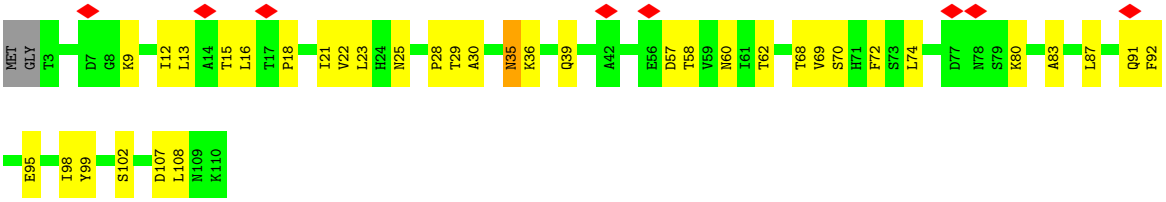
• Molecule 7: gp127

Chain J:



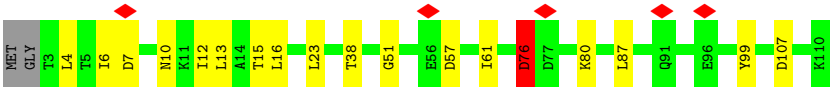
• Molecule 8: Phage protein

Chain K:



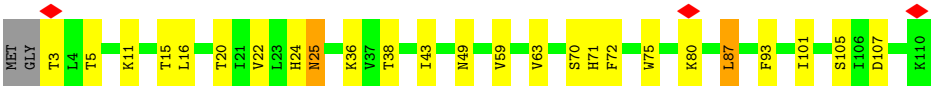
• Molecule 8: Phage protein

Chain L:



• Molecule 8: Phage protein

Chain M:

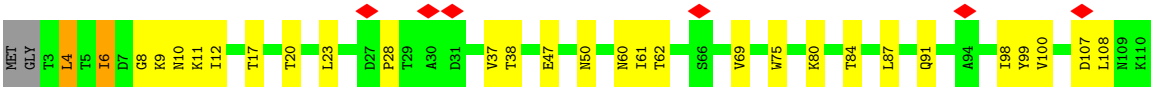


• Molecule 8: Phage protein

Chain N:

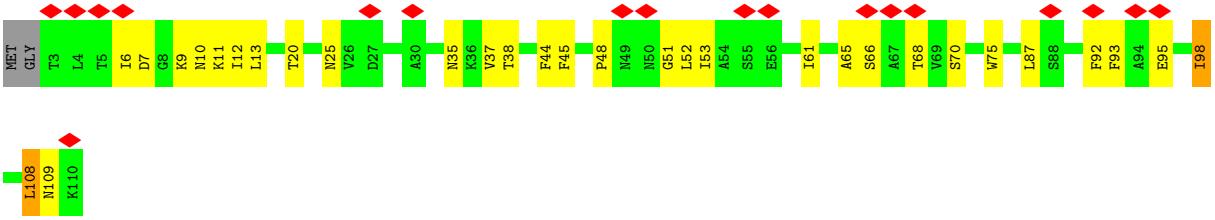
• Molecule 8: Phage protein

Chain O:



• Molecule 8: Phage protein

Chain P:


MET
GLY
T3
L4
T5
I6
D7
G8
K9
N10
K11
I12
L13
T20
N25
V26
D27
A30
N35
K36
V37
T38
F44
F45
P48
N49
N50
G51
L52
I53
A54
S55
E56
I61
A65
S66
A67
T68
V69
S70
W75
L87
S88
F92
F93
A94
E95
I98
L108
N109
K110

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	37006	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 ($e^-/Å^2$)	33	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.203	Depositor
Minimum map value	-0.529	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.242	Depositor
Map size (Å)	489.59998, 489.59998, 489.59998	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.816, 0.816, 0.816	Depositor

5 Model quality

5.1 Standard geometry

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	0.30	0/3272	0.52	2/4439 (0.0%)
1	B	0.32	0/3246	0.54	1/4408 (0.0%)
2	C	0.28	0/1034	0.57	1/1394 (0.1%)
2	D	0.27	0/1028	0.52	0/1386
3	E	0.27	0/1055	0.53	0/1429
4	F	0.26	0/1552	0.50	1/2114 (0.0%)
5	G	0.27	0/1106	0.51	0/1505
6	H	0.27	0/3268	0.49	0/4460
7	I	0.28	0/1170	0.52	0/1584
7	J	0.33	0/1029	0.57	0/1394
8	K	0.28	0/813	0.50	0/1119
8	L	0.27	0/806	0.57	2/1110 (0.2%)
8	M	0.27	0/798	0.51	0/1100
8	N	0.27	0/805	0.55	1/1109 (0.1%)
8	O	0.31	0/786	0.52	0/1086
8	P	0.37	0/763	0.50	0/1056
All	All	0.29	0/22531	0.52	8/30693 (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
4	F	0	1
5	G	0	1
7	J	0	3
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	107	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	22	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	286	ASP	CB-CG-OD1	5.32	123.09	118.30
8	L	107	ASP	CB-CG-OD1	5.29	123.06	118.30
8	L	76	ASP	CB-CG-OD1	5.22	123.00	118.30
8	N	57	ASP	CB-CG-OD1	5.17	122.95	118.30
4	F	128	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	454	PRO	N-CA-CB	-5.14	96.95	102.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	ARG	Sidechain
4	F	52	GLN	Peptide
5	G	123	ARG	Sidechain
7	J	33	ARG	Sidechain
7	J	90	CYS	Peptide
7	J	91	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3202	0	3000	99	0
1	B	3175	0	2959	97	0
2	C	1018	0	997	27	0
2	D	1011	0	996	35	0
3	E	1035	0	997	17	0
4	F	1525	0	1507	30	0
5	G	1087	0	1062	21	0
6	H	3212	0	3060	61	0
7	I	1153	0	1114	25	0
7	J	1016	0	946	23	0
8	K	797	0	784	28	0
8	L	790	0	776	14	0
8	M	782	0	770	20	0
8	N	789	0	776	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	O	770	0	743	23	0
8	P	748	0	689	22	0
All	All	22110	0	21176	474	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (474) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:48:PRO:HB3	8:P:53:ILE:HG12	1.47	0.95
1:B:129:LYS:HA	1:B:146:ILE:HD12	1.52	0.90
1:B:101:MET:SD	1:B:103:HIS:CE1	2.68	0.86
1:B:101:MET:SD	1:B:103:HIS:HE1	2.03	0.80
1:B:101:MET:CE	1:B:103:HIS:CE1	2.67	0.77
2:C:65:ASP:OD2	2:D:74:ARG:NH1	2.18	0.75
5:G:20:ALA:HB2	6:H:384:ARG:HD3	1.68	0.73
7:I:17:ARG:NH2	8:O:91:GLN:OE1	2.21	0.73
1:A:143:ASP:HB3	1:A:145:LEU:HD23	1.71	0.71
1:B:434:ARG:NH1	1:B:440:GLU:O	2.21	0.71
5:G:94:ASN:HD22	6:H:390:GLU:HG2	1.56	0.71
8:K:39:GLN:N	8:K:39:GLN:OE1	2.22	0.70
1:A:65:LYS:O	1:A:69:ARG:HG3	1.91	0.70
1:B:354:ASP:OD1	1:B:355:SER:N	2.25	0.69
4:F:118:LEU:O	4:F:122:THR:OG1	2.10	0.68
1:B:101:MET:CE	1:B:103:HIS:HE1	2.06	0.68
1:B:280:ASN:ND2	2:D:99:TYR:OH	2.26	0.68
6:H:82:GLN:HB2	6:H:181:THR:HG22	1.76	0.68
8:K:16:LEU:HD21	8:L:12:ILE:HD11	1.76	0.67
6:H:174:THR:HG23	6:H:175:THR:H	1.59	0.67
7:J:98:ASN:O	7:J:100:VAL:N	2.27	0.67
6:H:182:ALA:HB1	6:H:188:ALA:HB2	1.77	0.67
7:J:89:ASN:HB3	7:J:95:VAL:HB	1.76	0.67
4:F:72:LYS:NZ	6:H:378:ASP:OD2	2.28	0.67
1:A:53:ARG:HH21	1:B:36:ARG:HG3	1.60	0.67
4:F:55:ILE:HG12	4:F:93:VAL:HG22	1.77	0.66
1:A:282:LEU:O	1:B:245:ARG:NH1	2.28	0.66
8:L:12:ILE:HG22	8:L:13:LEU:HD23	1.76	0.66
8:N:107:ASP:OD1	8:N:109:ASN:N	2.27	0.66
2:C:74:ARG:HD3	2:C:74:ARG:H	1.61	0.66
6:H:13:ASN:OD1	6:H:14:THR:N	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLY:HA2	2:D:96:GLY:HA3	1.78	0.65
6:H:122:LEU:O	6:H:124:VAL:N	2.29	0.65
8:O:37:VAL:HG23	8:O:38:THR:HG23	1.78	0.65
1:B:354:ASP:OD1	1:B:356:LYS:N	2.29	0.65
7:J:97:VAL:O	7:J:119:LYS:NZ	2.25	0.65
1:B:53:ARG:HH22	2:C:130:TYR:HA	1.62	0.65
6:H:80:THR:OG1	6:H:181:THR:OG1	2.13	0.65
1:A:439:LEU:HD21	1:B:432:LYS:HD2	1.79	0.65
8:M:22:VAL:HG11	8:M:36:LYS:HD3	1.79	0.64
1:A:286:ASP:OD1	1:A:287:ARG:HG3	1.98	0.64
7:J:115:MET:HG2	7:J:126:TYR:HB2	1.78	0.64
8:K:80:LYS:HE2	8:L:7:ASP:HB3	1.78	0.64
4:F:189:ILE:HD11	6:H:352:VAL:HG13	1.79	0.64
7:J:89:ASN:N	7:J:93:LYS:O	2.30	0.64
2:C:87:ASP:HA	2:C:91:LYS:HB3	1.80	0.63
8:K:23:LEU:HD13	8:K:69:VAL:HG11	1.80	0.63
1:B:163:TYR:O	1:B:201:ARG:NH2	2.32	0.63
2:D:30:ASP:OD1	2:D:31:GLN:N	2.32	0.63
1:A:69:ARG:HH21	1:A:110:ASN:HD21	1.47	0.62
6:H:14:THR:HG22	6:H:15:ALA:H	1.63	0.62
1:B:303:ASP:OD1	1:B:304:ILE:N	2.32	0.62
8:P:12:ILE:HG23	8:P:13:LEU:HD22	1.81	0.62
8:P:25:ASN:O	8:P:70:SER:OG	2.16	0.62
8:M:11:LYS:NZ	8:N:76:ASP:OD2	2.32	0.62
7:I:76:PRO:O	7:I:79:SER:OG	2.18	0.61
1:B:145:LEU:HD22	1:B:387:ASN:HD21	1.64	0.61
5:G:43:VAL:HG22	5:G:49:VAL:HG22	1.82	0.61
1:A:106:ALA:O	1:A:110:ASN:ND2	2.29	0.61
1:A:148:TRP:HE1	1:A:383:THR:HG1	1.48	0.61
2:C:67:LYS:HB2	2:C:72:TYR:HD1	1.65	0.61
8:K:60:ASN:HB3	8:K:98:ILE:HD11	1.81	0.61
2:C:123:GLU:OE1	2:C:123:GLU:N	2.34	0.60
2:C:66:GLU:HG2	3:E:2:ARG:HH11	1.66	0.60
3:E:36:ILE:HD11	7:I:65:ILE:HD12	1.83	0.60
5:G:8:SER:OG	5:G:11:ASP:OD2	2.15	0.60
6:H:80:THR:HG1	6:H:181:THR:HG1	1.49	0.60
8:K:13:LEU:HD21	8:K:108:LEU:HD13	1.83	0.60
1:A:301:LYS:HD3	1:B:300:THR:HA	1.83	0.60
1:A:276:GLN:OE1	2:C:111:ARG:NH2	2.34	0.60
1:B:128:LYS:N	1:B:147:GLY:O	2.35	0.60
1:B:276:GLN:OE1	2:D:111:ARG:NH2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:81:MET:HE3	6:H:81:MET:HA	1.84	0.59
8:K:74:LEU:HD23	8:K:83:ALA:HB3	1.84	0.59
2:C:30:ASP:OD1	2:C:31:GLN:N	2.35	0.59
1:A:127:TYR:OH	1:A:382:GLN:HG2	2.03	0.59
6:H:183:ASP:H	6:H:187:ALA:HB3	1.68	0.59
3:E:27:TRP:HD1	4:F:41:ASP:HB2	1.68	0.59
7:I:54:LEU:HD13	7:I:84:GLY:HA3	1.84	0.58
4:F:166:ILE:HG22	6:H:376:THR:HA	1.85	0.58
1:A:453:SER:O	1:A:454:PRO:C	2.42	0.58
1:B:236:GLU:HG3	1:B:324:ILE:HD12	1.85	0.58
8:K:15:THR:HG21	8:L:15:THR:HG21	1.84	0.58
1:A:45:ILE:HG22	1:A:118:TYR:HE2	1.68	0.58
8:K:16:LEU:HB3	8:K:18:PRO:HD3	1.86	0.58
8:P:6:ILE:HD12	8:P:9:LYS:HB2	1.86	0.58
4:F:75:GLU:HG3	4:F:76:ASP:H	1.69	0.58
7:J:40:VAL:HG21	8:K:91:GLN:HE21	1.68	0.57
1:A:265:GLU:OE2	1:A:265:GLU:N	2.24	0.57
1:B:372:LYS:NZ	1:B:397:ILE:O	2.35	0.57
2:D:66:GLU:HB3	3:E:109:LEU:HD13	1.86	0.57
1:A:45:ILE:HG13	1:A:46:LYS:H	1.70	0.57
4:F:71:ASP:HA	5:G:22:GLU:HG3	1.85	0.57
1:A:51:MET:HG2	1:A:229:TRP:CD2	2.39	0.57
1:A:376:ASN:HD21	1:A:396:GLU:HB3	1.70	0.57
1:B:211:ASP:OD1	1:B:211:ASP:N	2.38	0.57
8:O:10:ASN:C	8:O:12:ILE:H	2.08	0.57
1:A:55:PRO:HG3	1:B:228:PRO:HG3	1.86	0.56
4:F:43:SER:OG	4:F:44:ASN:OD1	2.20	0.56
1:B:155:ASN:OD1	1:B:156:GLN:N	2.38	0.56
5:G:120:GLU:HG2	5:G:126:ASN:HD22	1.70	0.56
6:H:184:THR:O	6:H:186:SER:N	2.37	0.56
1:A:30:ARG:NH2	1:A:160:ASP:OD1	2.38	0.56
1:A:66:MET:SD	1:B:336:MET:HE1	2.45	0.56
7:J:78:ASP:O	7:J:133:TYR:HE2	1.87	0.56
4:F:196:LYS:HD3	4:F:196:LYS:N	2.18	0.56
8:O:87:LEU:HD12	8:O:87:LEU:H	1.70	0.56
1:A:338:ASP:OD1	1:A:338:ASP:N	2.33	0.56
2:D:25:ASN:OD1	3:E:5:ASN:ND2	2.29	0.56
1:A:102:GLU:HB2	1:B:377:ARG:HH21	1.71	0.56
7:I:96:ASN:OD1	7:I:98:ASN:ND2	2.39	0.56
8:M:15:THR:HG21	8:N:15:THR:HG21	1.87	0.56
2:D:22:THR:O	2:D:22:THR:OG1	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:345:TRP:HB2	6:H:348:ILE:HD12	1.88	0.56
8:K:58:THR:HG22	8:K:102:SER:HA	1.87	0.56
1:B:101:MET:HE1	1:B:152:PRO:HG2	1.87	0.55
1:B:122:VAL:HG21	1:B:159:LEU:HD21	1.87	0.55
1:A:102:GLU:OE1	1:B:377:ARG:NH2	2.39	0.55
2:D:99:TYR:OH	2:D:111:ARG:NH1	2.39	0.55
4:F:12:ILE:HD11	4:F:153:LEU:HD11	1.88	0.55
8:P:9:LYS:HZ3	8:P:108:LEU:HD12	1.72	0.55
2:C:67:LYS:HB3	2:D:72:TYR:HB3	1.88	0.55
8:K:12:ILE:HG23	8:L:12:ILE:HD12	1.87	0.55
1:A:45:ILE:HG13	1:A:46:LYS:N	2.22	0.55
1:B:71:VAL:HG21	1:B:368:LEU:HD11	1.89	0.55
3:E:76:LEU:HB2	3:E:117:TYR:CE2	2.42	0.55
7:J:86:LYS:HD2	7:J:94:ARG:NH1	2.21	0.55
1:B:219:ARG:HG3	1:B:223:LEU:HD12	1.90	0.54
1:A:125:LYS:HG2	1:A:379:LEU:HD12	1.89	0.54
1:A:352:LEU:HB2	1:A:401:ASP:OD1	2.07	0.54
1:A:445:SER:OG	1:A:446:LYS:NZ	2.40	0.54
8:P:20:THR:HB	8:P:75:TRP:HB2	1.88	0.54
8:O:20:THR:HB	8:O:75:TRP:HB2	1.89	0.54
8:N:22:VAL:HG11	8:N:36:LYS:HG3	1.88	0.54
8:O:9:LYS:HA	8:O:12:ILE:HD12	1.89	0.54
6:H:87:ILE:HD12	6:H:88:PRO:HD2	1.88	0.54
1:B:65:LYS:HD2	1:B:113:MET:HB3	1.90	0.54
2:C:107:ASP:HA	2:C:110:MET:HE2	1.90	0.54
6:H:34:PHE:O	6:H:78:ARG:NH2	2.41	0.53
8:M:80:LYS:NZ	8:N:7:ASP:O	2.41	0.53
1:A:449:SER:H	1:B:427:LYS:NZ	2.06	0.53
5:G:72:ASN:ND2	5:G:128:LYS:HE2	2.23	0.53
8:P:9:LYS:HZ2	8:P:51:GLY:HA3	1.73	0.53
5:G:29:PHE:HA	5:G:64:GLU:HB2	1.89	0.53
1:B:30:ARG:NH1	1:B:160:ASP:OD1	2.35	0.53
1:B:200:PRO:HD2	1:B:203:LYS:HB2	1.91	0.53
8:M:3:THR:O	8:N:84:THR:OG1	2.26	0.53
5:G:63:ILE:HD11	5:G:95:PHE:CZ	2.44	0.53
1:A:289:GLY:HA3	1:B:279:VAL:HG13	1.91	0.52
8:P:37:VAL:HG23	8:P:38:THR:HG23	1.91	0.52
1:A:263:ASP:N	1:A:263:ASP:OD1	2.42	0.52
8:N:17:THR:O	8:N:17:THR:OG1	2.24	0.52
1:A:125:LYS:NZ	1:A:378:ASP:OD1	2.34	0.52
7:I:83:LEU:O	7:I:125:GLU:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:325:PHE:HE2	6:H:327:ASP:HB2	1.75	0.52
8:N:23:LEU:HD12	8:N:61:ILE:HG21	1.91	0.52
1:A:274:TYR:HD2	2:D:98:PRO:HG2	1.75	0.52
1:B:156:GLN:N	1:B:156:GLN:OE1	2.42	0.52
7:I:107:ILE:HB	7:I:110:ALA:HB3	1.92	0.52
1:A:336:MET:HE3	1:A:359:LEU:HB3	1.91	0.51
1:A:271:PHE:CD1	2:D:98:PRO:HD3	2.46	0.51
4:F:9:GLU:OE1	4:F:36:ARG:NH1	2.41	0.51
3:E:104:ASP:OD1	3:E:106:SER:OG	2.16	0.51
1:A:97:LEU:HA	1:A:100:ASP:HB2	1.93	0.51
6:H:364:ARG:HG2	6:H:364:ARG:HH11	1.76	0.51
8:K:39:GLN:HE22	8:K:62:THR:HB	1.74	0.51
1:A:437:ILE:HD11	1:B:413:TYR:CD2	2.46	0.51
1:A:453:SER:HB2	1:A:454:PRO:HD2	1.93	0.51
1:B:374:VAL:O	1:B:378:ASP:HB2	2.11	0.51
1:B:401:ASP:OD1	1:B:402:ILE:N	2.44	0.51
7:I:53:ARG:HH21	7:I:76:PRO:HD3	1.75	0.51
8:L:10:ASN:OD1	8:L:51:GLY:N	2.35	0.51
8:O:8:GLY:O	8:O:9:LYS:C	2.49	0.51
1:B:148:TRP:CZ2	1:B:379:LEU:HD21	2.46	0.50
5:G:18:GLY:N	6:H:387:GLN:OE1	2.42	0.50
6:H:189:LEU:HA	6:H:192:ILE:HG22	1.94	0.50
1:B:239:GLU:HB2	1:B:320:THR:HG21	1.92	0.50
7:I:35:SER:OG	8:M:105:SER:OG	2.30	0.50
8:P:10:ASN:OD1	8:P:11:LYS:N	2.45	0.50
1:A:40:ARG:O	1:A:44:SER:N	2.41	0.50
8:M:87:LEU:HD12	8:M:87:LEU:H	1.77	0.50
4:F:23:ARG:NH2	4:F:100:SER:OG	2.31	0.50
8:M:5:THR:HG22	8:N:84:THR:HG23	1.93	0.50
1:A:22:LEU:O	1:A:22:LEU:HD12	2.11	0.49
1:A:120:PHE:HA	1:A:207:PHE:O	2.12	0.49
8:P:87:LEU:HD12	8:P:87:LEU:H	1.78	0.49
6:H:213:LEU:HD11	6:H:250:GLN:HB3	1.94	0.49
2:D:74:ARG:NH2	2:D:77:SER:OG	2.37	0.49
7:J:81:CYS:SG	7:J:82:LEU:N	2.84	0.49
1:B:296:ILE:HD13	1:B:303:ASP:HB2	1.94	0.49
3:E:39:LYS:O	3:E:72:THR:OG1	2.29	0.49
8:N:107:ASP:OD1	8:N:108:LEU:N	2.46	0.49
1:A:448:VAL:HA	1:B:427:LYS:NZ	2.28	0.49
1:A:51:MET:CE	1:A:222:LEU:HB3	2.43	0.49
8:K:12:ILE:HD11	8:L:16:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:31:ARG:HH22	5:G:64:GLU:HG3	1.78	0.48
8:O:4:LEU:HB2	8:O:9:LYS:HD3	1.95	0.48
1:A:300:THR:O	1:A:302:GLU:HG2	2.14	0.48
1:B:228:PRO:HB2	1:B:331:ILE:HG12	1.94	0.48
1:B:237:GLU:OE1	2:C:125:GLY:N	2.46	0.48
1:B:406:ASP:OD1	1:B:406:ASP:N	2.47	0.48
3:E:56:ILE:HD12	3:E:63:ARG:HH21	1.77	0.48
7:I:101:GLU:N	7:I:101:GLU:OE2	2.41	0.48
1:A:45:ILE:O	1:A:49:GLN:HG2	2.14	0.48
1:A:388:MET:O	1:A:390:ASP:N	2.47	0.48
1:A:91:ALA:O	1:A:95:ASN:ND2	2.47	0.48
8:O:107:ASP:OD1	8:O:108:LEU:N	2.47	0.48
8:P:68:THR:HG23	8:P:92:PHE:HB2	1.94	0.48
1:A:337:SER:O	1:A:337:SER:OG	2.30	0.48
2:D:6:ASP:OD2	7:I:140:LYS:HA	2.13	0.48
5:G:105:LEU:HD13	5:G:141:SER:HA	1.96	0.48
1:A:46:LYS:HB2	1:A:46:LYS:HE2	1.50	0.48
1:A:115:PHE:CE2	1:A:207:PHE:HB3	2.49	0.48
8:L:57:ASP:OD1	8:L:57:ASP:N	2.47	0.48
1:A:30:ARG:HB2	1:A:32:TYR:HE1	1.79	0.47
8:O:10:ASN:O	8:O:12:ILE:N	2.47	0.47
1:A:432:LYS:O	1:A:435:GLU:HG3	2.14	0.47
8:K:70:SER:O	8:K:70:SER:OG	2.31	0.47
8:N:24:HIS:N	8:N:71:HIS:O	2.39	0.47
8:N:61:ILE:HB	8:N:99:TYR:HB3	1.95	0.47
8:O:9:LYS:CA	8:O:12:ILE:HD12	2.44	0.47
1:B:299:GLU:O	1:B:300:THR:OG1	2.31	0.47
2:D:119:LYS:O	2:D:119:LYS:HG3	2.14	0.47
1:B:132:GLY:O	1:B:133:LYS:C	2.53	0.47
3:E:105:TRP:NE1	3:E:116:GLU:OE2	2.48	0.47
7:I:131:ASN:O	7:I:134:LYS:HG2	2.15	0.47
8:P:9:LYS:NZ	8:P:109:ASN:HD21	2.12	0.47
1:A:303:ASP:OD1	1:A:304:ILE:N	2.48	0.47
1:A:86:LYS:O	1:A:89:GLU:HG3	2.14	0.47
4:F:183:GLU:HB3	4:F:184:PRO:HD3	1.97	0.47
5:G:63:ILE:HD11	5:G:95:PHE:HZ	1.79	0.47
7:J:40:VAL:HG22	8:K:99:TYR:CE1	2.50	0.47
8:K:21:ILE:HD12	8:K:22:VAL:H	1.79	0.47
8:P:61:ILE:O	8:P:98:ILE:HA	2.15	0.47
1:A:101:MET:HG3	1:A:149:ALA:HA	1.96	0.47
1:B:361:ALA:O	1:B:364:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:91:GLN:OE1	8:N:91:GLN:HA	2.15	0.47
6:H:387:GLN:NE2	6:H:391:THR:OG1	2.48	0.47
8:K:25:ASN:ND2	8:K:35:ASN:HB3	2.30	0.47
1:A:113:MET:HA	1:A:113:MET:HE2	1.96	0.46
1:A:254:GLY:N	1:A:306:GLU:O	2.45	0.46
1:B:51:MET:HE2	1:B:222:LEU:HB3	1.96	0.46
1:B:202:SER:O	1:B:202:SER:OG	2.32	0.46
6:H:376:THR:O	6:H:381:GLY:HA3	2.14	0.46
8:L:23:LEU:HD11	8:L:61:ILE:HD13	1.96	0.46
2:C:67:LYS:HG3	2:C:72:TYR:HB2	1.97	0.46
2:C:119:LYS:NZ	2:C:133:ARG:HE	2.13	0.46
2:D:75:ASN:HA	2:D:78:ARG:HD2	1.96	0.46
8:K:22:VAL:HG21	8:K:36:LYS:HE2	1.98	0.46
8:M:16:LEU:HD13	8:N:12:ILE:HD12	1.98	0.46
1:B:86:LYS:O	1:B:89:GLU:HG3	2.15	0.46
6:H:18:THR:OG1	6:H:70:LYS:O	2.24	0.46
6:H:83:TYR:CE2	6:H:167:LYS:HA	2.51	0.46
7:I:55:LEU:N	7:I:84:GLY:O	2.45	0.46
1:A:128:LYS:O	1:A:147:GLY:N	2.47	0.46
2:D:126:ASP:OD1	2:D:126:ASP:N	2.49	0.46
8:O:61:ILE:HG13	8:O:99:TYR:HB3	1.98	0.46
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.77	0.46
8:P:108:LEU:HD22	8:P:108:LEU:HA	1.80	0.46
1:B:155:ASN:OD1	1:B:157:THR:HG22	2.15	0.46
8:K:28:PRO:O	8:K:30:ALA:N	2.49	0.46
1:A:33:GLU:HA	1:A:33:GLU:OE2	2.16	0.46
1:A:294:ARG:NH2	1:A:296:ILE:HD11	2.31	0.46
8:M:38:THR:HG22	8:M:63:VAL:HG22	1.98	0.46
1:A:294:ARG:NH1	1:B:303:ASP:O	2.38	0.46
6:H:136:PRO:HA	6:H:139:LYS:HD2	1.97	0.46
7:I:22:ILE:HD11	8:N:93:PHE:HE1	1.81	0.46
8:O:28:PRO:HG3	8:O:84:THR:HB	1.98	0.46
1:A:51:MET:HE2	1:A:222:LEU:HB3	1.98	0.46
8:K:12:ILE:HG22	8:K:13:LEU:HD22	1.98	0.46
8:K:83:ALA:HA	8:L:4:LEU:HA	1.97	0.46
8:N:79:SER:O	8:N:80:LYS:HD3	2.16	0.46
7:I:40:VAL:HG12	8:M:93:PHE:CE1	2.52	0.45
6:H:123:ILE:O	6:H:127:GLU:N	2.35	0.45
6:H:231:ALA:HB2	6:H:267:ALA:HB3	1.99	0.45
1:B:452:LEU:H	1:B:452:LEU:HG	1.45	0.45
6:H:26:LEU:HD23	6:H:202:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:328:LEU:HG	6:H:331:GLY:HA2	1.98	0.45
7:J:49:PHE:O	7:J:49:PHE:CG	2.69	0.45
8:M:70:SER:OG	8:M:71:HIS:ND1	2.49	0.45
8:O:80:LYS:NZ	8:P:7:ASP:OD2	2.45	0.45
2:C:36:TRP:CH2	2:D:14:ARG:HD3	2.52	0.45
2:C:6:ASP:OD2	7:J:140:LYS:HA	2.17	0.45
1:B:51:MET:HG2	1:B:229:TRP:CD2	2.52	0.45
3:E:63:ARG:HE	3:E:63:ARG:HB3	1.65	0.45
6:H:417:LEU:HD23	6:H:417:LEU:HA	1.83	0.45
7:J:107:ILE:HG22	7:J:110:ALA:HB3	1.99	0.45
4:F:52:GLN:HB3	4:F:53:PRO:CD	2.47	0.45
6:H:230:ASN:HD22	6:H:248:PRO:HD3	1.82	0.45
8:L:23:LEU:HD13	8:L:38:THR:HG21	1.99	0.45
1:A:112:VAL:O	1:A:115:PHE:HB2	2.17	0.44
1:B:34:GLU:HG2	1:B:39:LEU:HB2	1.98	0.44
8:L:76:ASP:OD2	8:L:80:LYS:NZ	2.35	0.44
4:F:106:LYS:HD2	4:F:132:ILE:HD11	1.99	0.44
4:F:165:SER:O	6:H:377:TYR:HB2	2.17	0.44
7:I:57:ALA:HB1	7:I:158:ILE:HG22	1.99	0.44
1:A:271:PHE:HD1	2:D:98:PRO:HD3	1.82	0.44
1:A:307:PHE:O	1:B:252:LYS:NZ	2.51	0.44
2:C:67:LYS:O	2:D:71:VAL:HA	2.17	0.44
6:H:68:THR:OG1	6:H:69:PRO:HD3	2.17	0.44
1:A:434:ARG:HG2	1:A:439:LEU:HB2	2.00	0.44
1:B:163:TYR:N	1:B:173:GLY:O	2.51	0.44
6:H:373:GLY:O	6:H:384:ARG:NH2	2.46	0.44
7:I:17:ARG:NH1	8:O:99:TYR:OH	2.51	0.44
7:J:52:CYS:HB3	7:J:53:ARG:NH1	2.32	0.44
8:O:17:THR:O	8:O:17:THR:OG1	2.23	0.44
8:P:9:LYS:HZ3	8:P:109:ASN:HD21	1.66	0.44
1:A:127:TYR:OH	1:A:382:GLN:CG	2.65	0.44
1:B:40:ARG:O	1:B:44:SER:N	2.26	0.44
2:D:67:LYS:HB2	2:D:72:TYR:CD1	2.52	0.44
6:H:440:ASP:OD1	6:H:440:ASP:N	2.51	0.44
1:A:163:TYR:N	1:A:173:GLY:O	2.50	0.44
1:B:372:LYS:O	1:B:375:ILE:HB	2.18	0.44
6:H:25:PRO:HG3	6:H:64:LEU:HD11	1.99	0.44
6:H:135:SER:HB3	6:H:138:ILE:HB	2.00	0.44
1:B:418:VAL:HG12	1:B:423:MET:HB2	2.00	0.44
3:E:27:TRP:CD1	4:F:41:ASP:HB2	2.50	0.44
6:H:191:SER:O	6:H:194:THR:OG1	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:255:LYS:HA	6:H:255:LYS:HD2	1.81	0.44
7:J:86:LYS:HD2	7:J:94:ARG:HH11	1.81	0.44
1:A:104:ASP:OD1	1:A:105:TRP:N	2.50	0.44
2:C:58:PHE:HB3	2:D:20:THR:HG21	2.00	0.44
2:C:110:MET:HE2	2:C:110:MET:HB2	1.86	0.44
2:D:80:LYS:HE2	2:D:80:LYS:HA	1.99	0.44
7:I:82:LEU:HD21	7:I:125:GLU:HG2	2.00	0.44
1:B:368:LEU:HB3	1:B:399:TYR:CD2	2.52	0.44
2:C:117:SER:O	2:D:105:GLN:HB2	2.17	0.44
8:M:20:THR:OG1	8:M:75:TRP:HB2	2.18	0.44
8:M:24:HIS:CE1	8:M:36:LYS:HG2	2.53	0.44
1:A:127:TYR:HA	1:A:147:GLY:O	2.18	0.43
1:A:434:ARG:HH22	1:B:426:ASP:HB3	1.83	0.43
2:C:16:ARG:NH1	2:C:27:ILE:HD11	2.33	0.43
8:M:59:VAL:HB	8:M:101:ILE:HB	2.00	0.43
1:B:113:MET:HA	1:B:113:MET:CE	2.47	0.43
1:B:205:LEU:HD23	1:B:378:ASP:HB3	2.00	0.43
1:B:434:ARG:CZ	1:B:442:ALA:HB2	2.48	0.43
1:A:297:ASP:OD1	1:A:299:GLU:N	2.51	0.43
1:A:375:ILE:O	1:A:380:VAL:HG23	2.18	0.43
1:B:61:VAL:O	1:B:65:LYS:HG3	2.17	0.43
4:F:72:LYS:HD3	4:F:81:TYR:CE2	2.53	0.43
8:K:68:THR:HB	8:K:92:PHE:HD1	1.84	0.43
1:A:50:LEU:HA	1:A:53:ARG:HH11	1.83	0.43
1:B:257:PRO:HB3	2:D:94:VAL:HG12	2.00	0.43
1:B:261:GLY:HA3	2:D:95:SER:OG	2.18	0.43
5:G:63:ILE:HG22	5:G:65:LEU:HG	1.99	0.43
1:A:78:PRO:HG3	1:A:396:GLU:OE1	2.18	0.43
3:E:12:LYS:HA	3:E:34:VAL:O	2.19	0.43
4:F:56:THR:HB	4:F:92:THR:HG23	2.00	0.43
5:G:95:PHE:HB3	5:G:108:GLY:HA3	2.00	0.43
7:I:36:LEU:HD13	8:M:72:PHE:CD2	2.53	0.43
8:P:65:ALA:HA	8:P:95:GLU:O	2.17	0.43
1:B:129:LYS:O	1:B:130:ARG:C	2.57	0.43
7:J:129:SER:OG	7:J:132:ASP:OD2	2.33	0.43
1:A:41:PHE:N	1:A:42:PRO:HD2	2.33	0.43
1:B:101:MET:HE1	1:B:103:HIS:HE1	1.82	0.43
6:H:100:THR:O	6:H:168:VAL:HA	2.18	0.43
7:J:106:THR:HG23	7:J:106:THR:O	2.18	0.43
8:N:61:ILE:HG22	8:N:63:VAL:HG23	2.01	0.43
8:P:45:PHE:CD1	8:P:53:ILE:HG22	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:10:VAL:HG23	3:E:91:MET:HG3	2.01	0.43
5:G:67:GLN:OE1	5:G:126:ASN:N	2.49	0.43
2:C:83:LYS:NZ	2:D:88:ASP:OD2	2.35	0.43
6:H:66:SER:OG	6:H:67:GLN:N	2.52	0.43
6:H:279:TYR:HB2	6:H:295:LEU:HD21	2.00	0.43
8:M:43:ILE:HD13	8:M:59:VAL:HG21	2.00	0.43
1:A:57:VAL:O	1:A:61:VAL:HG13	2.19	0.42
1:A:123:ASN:HB3	1:A:152:PRO:HA	2.00	0.42
1:B:121:CYS:SG	1:B:123:ASN:ND2	2.91	0.42
2:D:74:ARG:HH22	2:D:77:SER:HG	1.63	0.42
4:F:187:TYR:CE1	6:H:352:VAL:HG11	2.54	0.42
5:G:94:ASN:ND2	6:H:390:GLU:HG2	2.30	0.42
8:O:12:ILE:HG22	8:P:12:ILE:HD11	2.00	0.42
1:A:102:GLU:HG2	1:A:150:LYS:H	1.83	0.42
1:B:45:ILE:HD13	1:B:157:THR:HA	2.01	0.42
3:E:76:LEU:N	3:E:117:TYR:OH	2.52	0.42
8:L:87:LEU:HD13	8:L:99:TYR:CZ	2.54	0.42
8:O:6:ILE:HD12	8:O:50:ASN:HA	2.00	0.42
1:B:209:TYR:HE1	1:B:367:LEU:HD11	1.83	0.42
4:F:23:ARG:HH22	4:F:100:SER:HG	1.58	0.42
8:K:12:ILE:HD13	8:K:12:ILE:HA	1.84	0.42
8:K:87:LEU:HD12	8:K:87:LEU:HA	1.91	0.42
8:O:60:ASN:OD1	8:O:100:VAL:HG23	2.19	0.42
6:H:25:PRO:HA	6:H:201:PHE:HB2	2.02	0.42
7:I:145:ILE:HD12	7:I:145:ILE:N	2.34	0.42
8:K:39:GLN:H	8:K:39:GLN:CD	2.22	0.42
1:A:63:ILE:O	1:A:66:MET:HB3	2.19	0.42
2:C:36:TRP:O	2:C:40:GLU:HG2	2.19	0.42
4:F:169:ARG:HH21	4:F:192:ASP:CG	2.22	0.42
7:J:96:ASN:HA	7:J:122:ASN:OD1	2.18	0.42
1:A:294:ARG:HD3	1:B:304:ILE:O	2.20	0.42
1:A:437:ILE:HD11	1:B:413:TYR:HD2	1.84	0.42
7:J:82:LEU:HD11	7:J:125:GLU:HB2	2.01	0.42
8:P:20:THR:O	8:P:75:TRP:N	2.50	0.42
1:A:34:GLU:HG2	1:A:39:LEU:HB2	2.01	0.42
1:A:205:LEU:HD23	1:A:378:ASP:HB3	2.01	0.42
1:A:232:LYS:NZ	1:A:328:SER:OG	2.33	0.42
6:H:172:THR:HG23	6:H:173:PRO:HD3	2.02	0.42
7:I:60:ASN:HB3	7:I:90:CYS:HA	2.02	0.42
8:P:52:LEU:HD12	8:P:52:LEU:HA	1.85	0.42
1:B:34:GLU:HG3	1:B:36:ARG:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:LEU:HD13	4:F:155:LYS:HD3	2.01	0.42
5:G:16:TRP:HB2	5:G:95:PHE:CD2	2.55	0.42
7:I:108:ASP:OD1	7:I:109:THR:HG23	2.19	0.42
8:O:23:LEU:HD13	8:O:69:VAL:HB	2.02	0.42
1:A:316:LYS:HD2	1:A:316:LYS:HA	1.83	0.42
1:B:126:VAL:HB	1:B:149:ALA:O	2.20	0.42
2:C:43:LYS:HB3	2:C:43:LYS:HE2	1.85	0.42
7:I:79:SER:HB3	7:J:157:THR:H	1.84	0.42
7:I:118:ASN:OD1	7:I:121:SER:N	2.52	0.42
1:A:267:GLU:OE1	2:D:94:VAL:HG23	2.20	0.41
1:B:129:LYS:HA	1:B:146:ILE:CD1	2.36	0.41
4:F:66:TYR:HA	5:G:66:MET:HE1	2.02	0.41
8:P:66:SER:N	8:P:93:PHE:O	2.54	0.41
1:A:51:MET:HG2	1:A:229:TRP:CE3	2.56	0.41
1:A:453:SER:CB	1:A:454:PRO:HD2	2.49	0.41
8:O:62:THR:HA	8:O:98:ILE:HD13	2.02	0.41
1:A:55:PRO:CG	1:B:228:PRO:HG3	2.49	0.41
1:B:172:ILE:N	1:B:201:ARG:HE	2.19	0.41
2:D:14:ARG:NE	2:D:45:GLU:OE1	2.52	0.41
1:B:250:MET:HA	1:B:251:PRO:HD3	1.95	0.41
1:A:286:ASP:OD2	2:D:123:GLU:HA	2.19	0.41
2:C:114:ASN:OD1	2:C:116:CYS:N	2.53	0.41
7:I:79:SER:H	7:I:133:TYR:HE2	1.68	0.41
8:L:6:ILE:O	8:L:10:ASN:ND2	2.54	0.41
1:A:172:ILE:C	1:A:201:ARG:HG3	2.41	0.41
1:B:223:LEU:HD23	1:B:223:LEU:HA	1.87	0.41
3:E:71:PHE:CD1	3:E:116:GLU:HG2	2.56	0.41
3:E:109:LEU:O	3:E:113:SER:OG	2.39	0.41
4:F:169:ARG:HD3	6:H:424:ILE:HD11	2.01	0.41
6:H:206:ASP:HB3	6:H:211:PHE:CD2	2.56	0.41
7:J:51:ILE:CB	7:J:82:LEU:HB3	2.51	0.41
1:A:163:TYR:O	1:A:201:ARG:NH2	2.48	0.41
1:A:299:GLU:O	1:A:300:THR:OG1	2.35	0.41
1:A:446:LYS:HE3	1:A:446:LYS:HB3	1.94	0.41
1:B:175:ARG:HA	1:B:198:LYS:HA	2.01	0.41
1:B:200:PRO:HD2	1:B:203:LYS:CB	2.51	0.41
1:B:452:LEU:HD12	1:B:453:SER:H	1.85	0.41
1:A:412:SER:HA	1:B:416:LYS:NZ	2.36	0.41
1:B:101:MET:HE2	1:B:103:HIS:CE1	2.52	0.41
2:D:59:GLN:HE21	2:D:59:GLN:HB3	1.65	0.41
5:G:72:ASN:HD22	5:G:128:LYS:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:366:LEU:HD22	6:H:384:ARG:HH21	1.85	0.41
1:A:121:CYS:SG	1:A:123:ASN:ND2	2.94	0.41
1:B:40:ARG:N	1:B:44:SER:HB3	2.36	0.41
1:B:208:LYS:NZ	1:B:216:PRO:HA	2.35	0.41
7:J:83:LEU:O	7:J:125:GLU:HA	2.20	0.41
8:K:95:GLU:N	8:K:95:GLU:OE2	2.54	0.41
8:M:63:VAL:HG11	8:M:93:PHE:HD2	1.86	0.41
8:O:10:ASN:C	8:O:12:ILE:N	2.73	0.41
2:C:79:PHE:CZ	2:D:85:VAL:HG23	2.56	0.41
7:J:140:LYS:HB3	7:J:142:TYR:CE2	2.56	0.41
1:A:200:PRO:HD2	1:A:203:LYS:HB3	2.03	0.40
2:D:62:LYS:HB2	2:D:62:LYS:HE2	1.82	0.40
4:F:8:LEU:HD12	4:F:8:LEU:HA	1.91	0.40
6:H:22:PHE:HB3	6:H:285:ALA:HB2	2.03	0.40
6:H:234:LYS:HB3	6:H:234:LYS:HE2	1.78	0.40
6:H:257:THR:HG22	6:H:342:GLY:HA3	2.03	0.40
4:F:20:ILE:HG21	4:F:105:LEU:HD22	2.03	0.40
4:F:167:ILE:HD12	6:H:425:LEU:HB2	2.02	0.40
1:B:85:ALA:O	1:B:88:ILE:HG22	2.21	0.40
1:B:269:LYS:HE3	1:B:269:LYS:HB2	1.83	0.40
6:H:24:LEU:HD23	6:H:24:LEU:HA	1.81	0.40
8:M:25:ASN:OD1	8:M:25:ASN:N	2.55	0.40
2:C:125:GLY:O	2:C:129:ARG:NH1	2.54	0.40
4:F:26:ARG:HB3	4:F:30:ASN:HA	2.02	0.40
6:H:385:ILE:HD13	6:H:425:LEU:HD23	2.04	0.40
8:K:9:LYS:O	8:K:13:LEU:HD23	2.22	0.40
1:B:101:MET:HE1	1:B:103:HIS:CE1	2.52	0.40
1:B:120:PHE:HA	1:B:207:PHE:O	2.22	0.40
2:D:100:ALA:HB3	2:D:103:ILE:HD13	2.02	0.40
5:G:53:ARG:H	5:G:53:ARG:HD3	1.86	0.40
6:H:192:ILE:HD12	6:H:192:ILE:HA	1.91	0.40
6:H:206:ASP:OD2	8:O:47:GLU:HG2	2.21	0.40
8:M:25:ASN:O	8:M:70:SER:OG	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	417/488 (86%)	373 (89%)	40 (10%)	4 (1%)	13 39
1	B	417/488 (86%)	371 (89%)	40 (10%)	6 (1%)	9 31
2	C	128/149 (86%)	122 (95%)	5 (4%)	1 (1%)	16 44
2	D	127/149 (85%)	116 (91%)	11 (9%)	0	100 100
3	E	128/133 (96%)	120 (94%)	7 (6%)	1 (1%)	16 44
4	F	193/199 (97%)	172 (89%)	20 (10%)	1 (0%)	25 54
5	G	140/148 (95%)	127 (91%)	13 (9%)	0	100 100
6	H	438/450 (97%)	380 (87%)	49 (11%)	9 (2%)	5 24
7	I	154/166 (93%)	140 (91%)	13 (8%)	1 (1%)	22 50
7	J	135/166 (81%)	114 (84%)	17 (13%)	4 (3%)	3 19
8	K	106/110 (96%)	98 (92%)	7 (7%)	1 (1%)	14 41
8	L	106/110 (96%)	100 (94%)	6 (6%)	0	100 100
8	M	106/110 (96%)	101 (95%)	5 (5%)	0	100 100
8	N	106/110 (96%)	99 (93%)	7 (7%)	0	100 100
8	O	106/110 (96%)	97 (92%)	8 (8%)	1 (1%)	14 41
8	P	106/110 (96%)	96 (91%)	9 (8%)	1 (1%)	14 41
All	All	2913/3196 (91%)	2626 (90%)	257 (9%)	30 (1%)	16 39

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO
1	A	388	MET
1	B	152	PRO
2	C	106	CYS
4	F	53	PRO
6	H	67	GLN

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Mol	Chain	Res	Type
6	H	122	LEU
6	H	123	ILE
6	H	177	ILE
7	J	40	VAL
8	K	29	THR
1	A	379	LEU
1	B	388	MET
6	H	174	THR
6	H	329	ASP
6	H	447	VAL
7	I	13	VAL
7	J	79	SER
8	O	11	LYS
8	P	98	ILE
1	B	133	LYS
1	B	136	LYS
1	B	153	ILE
1	B	422	ALA
6	H	68	THR
7	J	99	SER
1	A	153	ILE
6	H	371	LYS
3	E	101	MET
7	J	51	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	321/424 (76%)	301 (94%)	20 (6%)	15	40
1	B	314/424 (74%)	295 (94%)	19 (6%)	15	40
2	C	107/130 (82%)	101 (94%)	6 (6%)	17	43
2	D	106/130 (82%)	99 (93%)	7 (7%)	14	39
3	E	109/121 (90%)	106 (97%)	3 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	F	168/176 (96%)	164 (98%)	4 (2%)	44 66
5	G	121/127 (95%)	118 (98%)	3 (2%)	42 65
6	H	307/368 (83%)	301 (98%)	6 (2%)	50 70
7	I	117/150 (78%)	115 (98%)	2 (2%)	56 74
7	J	100/150 (67%)	91 (91%)	9 (9%)	8 27
8	K	92/95 (97%)	88 (96%)	4 (4%)	25 50
8	L	90/95 (95%)	89 (99%)	1 (1%)	70 81
8	M	88/95 (93%)	84 (96%)	4 (4%)	23 50
8	N	90/95 (95%)	89 (99%)	1 (1%)	70 81
8	O	84/95 (88%)	82 (98%)	2 (2%)	44 66
8	P	76/95 (80%)	73 (96%)	3 (4%)	27 53
All	All	2290/2770 (83%)	2196 (96%)	94 (4%)	28 51

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	41	PHE
1	A	46	LYS
1	A	94	PHE
1	A	115	PHE
1	A	121	CYS
1	A	142	ASN
1	A	203	LYS
1	A	258	ASP
1	A	280	ASN
1	A	329	LYS
1	A	337	SER
1	A	349	SER
1	A	377	ARG
1	A	384	TYR
1	A	394	HIS
1	A	412	SER
1	A	416	LYS
1	A	449	SER
1	A	454	PRO
1	B	41	PHE
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	103	HIS
1	B	115	PHE
1	B	125	LYS
1	B	139	SER
1	B	145	LEU
1	B	148	TRP
1	B	201	ARG
1	B	206	LEU
1	B	223	LEU
1	B	338	ASP
1	B	376	ASN
1	B	384	TYR
1	B	399	TYR
1	B	435	GLU
1	B	439	LEU
1	B	449	SER
1	B	452	LEU
2	C	19	CYS
2	C	74	ARG
2	C	75	ASN
2	C	77	SER
2	C	122	THR
2	C	126	ASP
2	D	13	ASP
2	D	19	CYS
2	D	44	ASP
2	D	83	LYS
2	D	113	GLN
2	D	126	ASP
2	D	130	TYR
3	E	52	ASN
3	E	83	ASP
3	E	84	TRP
4	F	44	ASN
4	F	59	CYS
4	F	100	SER
4	F	112	SER
5	G	15	SER
5	G	53	ARG
5	G	134	CYS
6	H	183	ASP
6	H	276	TYR

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Mol	Chain	Res	Type
6	H	332	VAL
6	H	377	TYR
6	H	400	LYS
6	H	440	ASP
7	I	136	LEU
7	I	143	ASP
7	J	33	ARG
7	J	35	SER
7	J	39	TYR
7	J	49	PHE
7	J	71	GLU
7	J	81	CYS
7	J	108	ASP
7	J	150	ASP
7	J	152	SER
8	K	35	ASN
8	K	57	ASP
8	K	72	PHE
8	K	107	ASP
8	L	76	ASP
8	M	25	ASN
8	M	49	ASN
8	M	87	LEU
8	M	107	ASP
8	N	92	PHE
8	O	4	LEU
8	O	6	ILE
8	P	35	ASN
8	P	44	PHE
8	P	108	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	GLN
1	B	103	HIS
1	B	387	ASN
8	P	109	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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

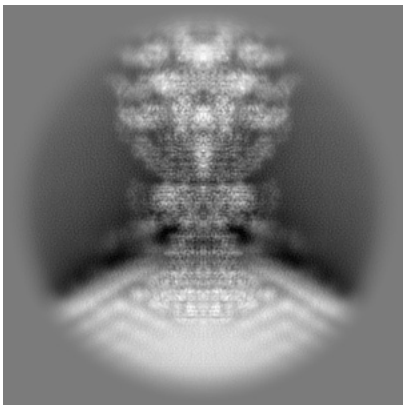
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-45162. These allow visual inspection of the internal detail of the map and identification of artifacts.

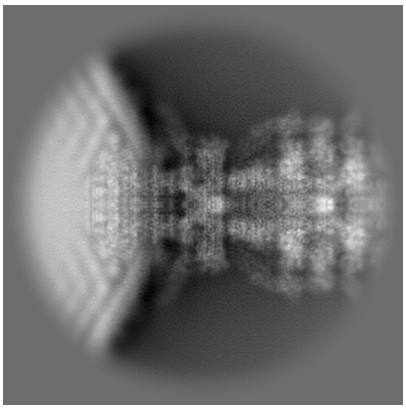
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

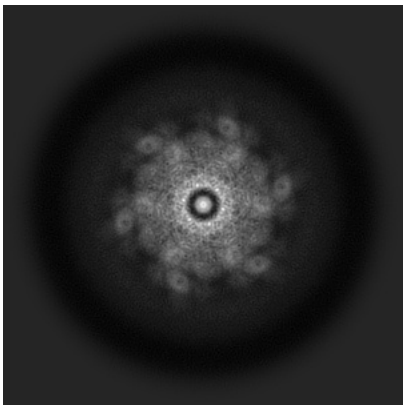
6.1.1 Primary map



X

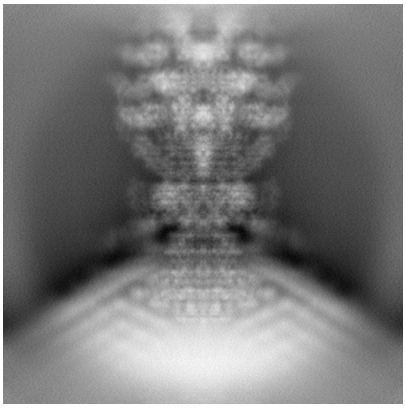


Y

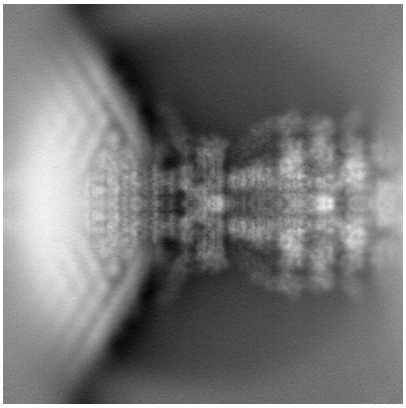


Z

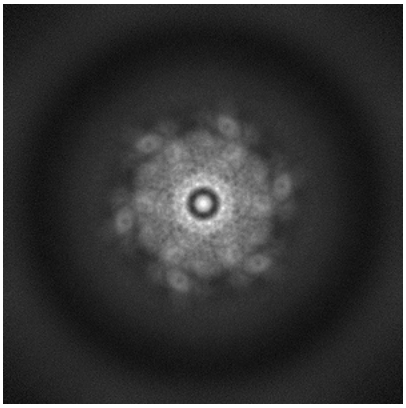
6.1.2 Raw map



X



Y

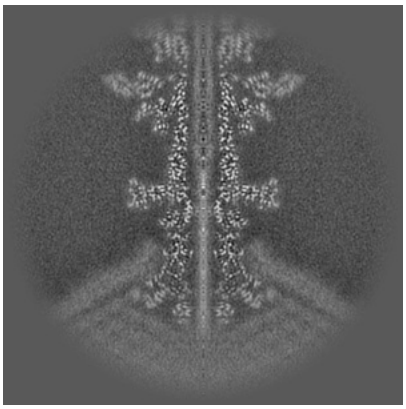


Z

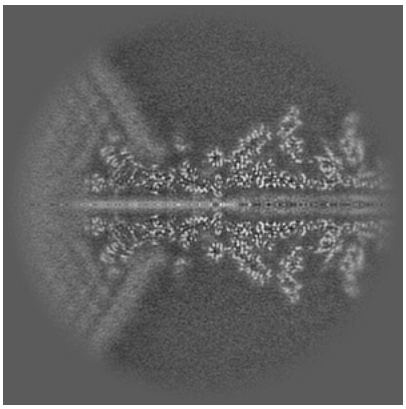
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

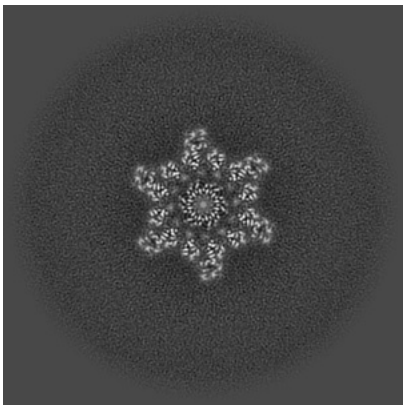
6.2.1 Primary map



X Index: 300

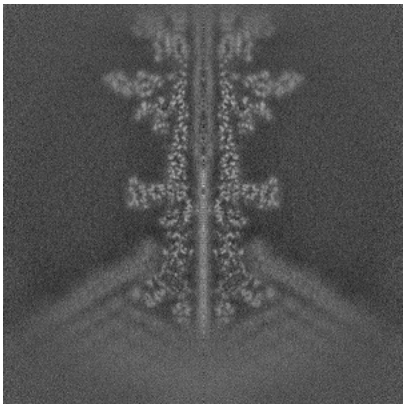


Y Index: 300

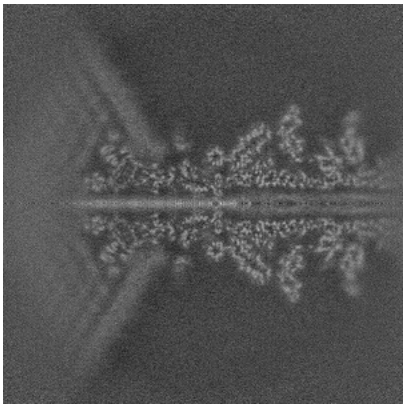


Z Index: 300

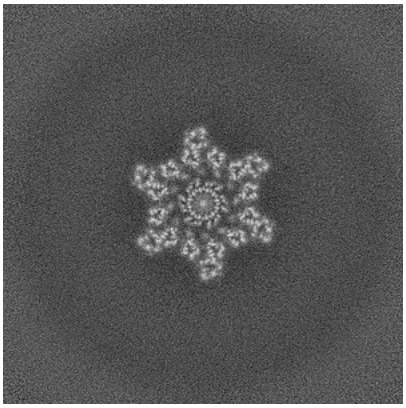
6.2.2 Raw map



X Index: 300



Y Index: 300

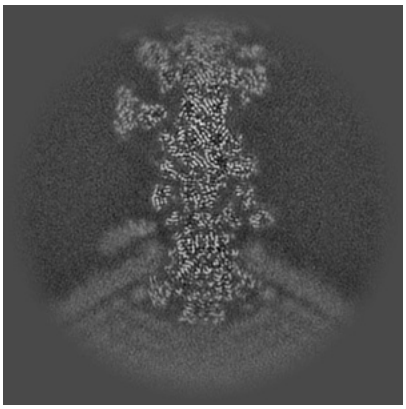


Z Index: 300

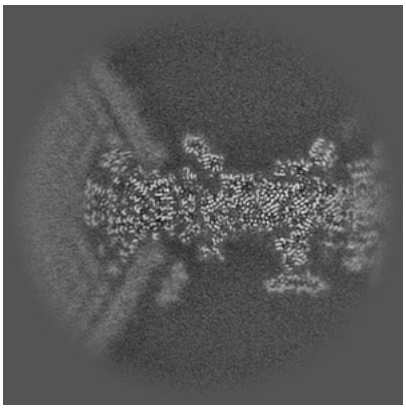
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

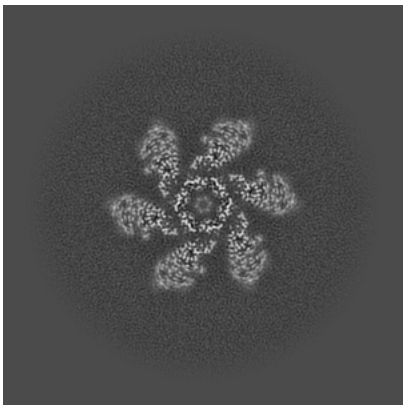
6.3.1 Primary map



X Index: 271

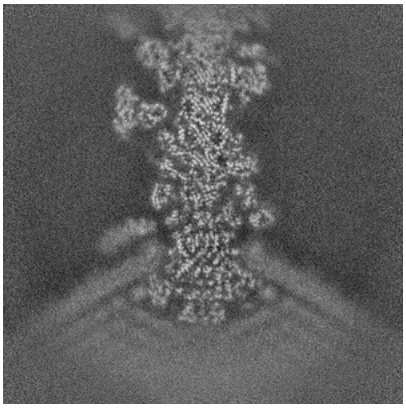


Y Index: 271

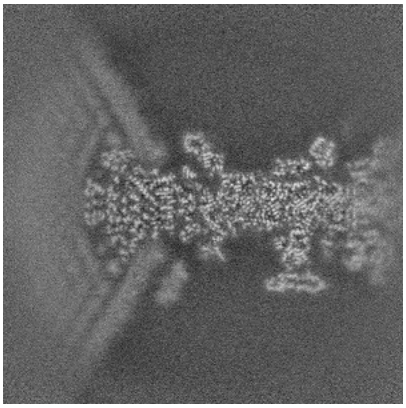


Z Index: 429

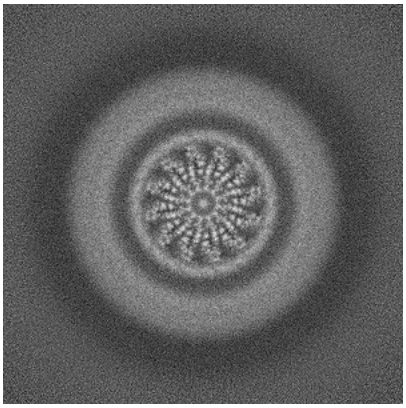
6.3.2 Raw map



X Index: 271



Y Index: 270

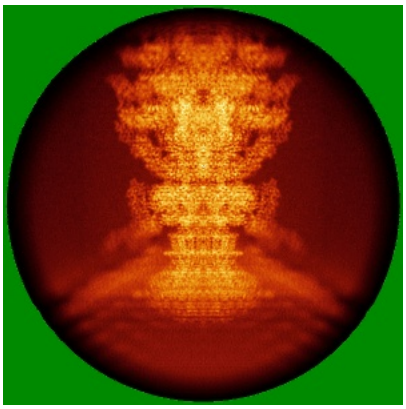


Z Index: 169

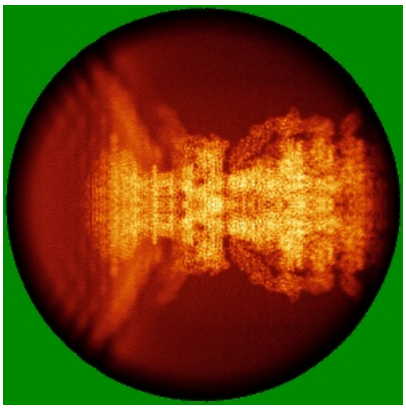
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

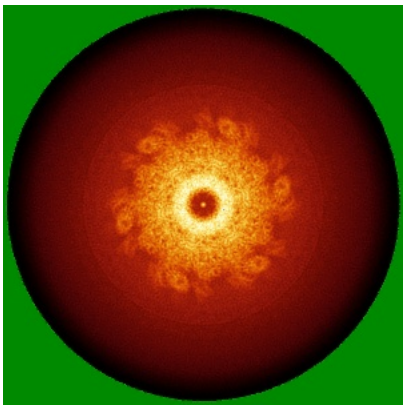
6.4.1 Primary map



X

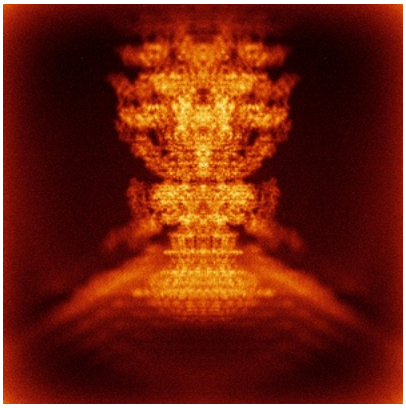


Y

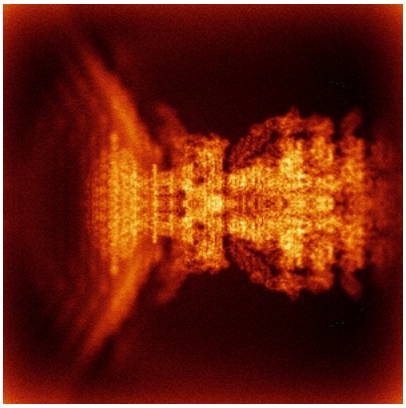


Z

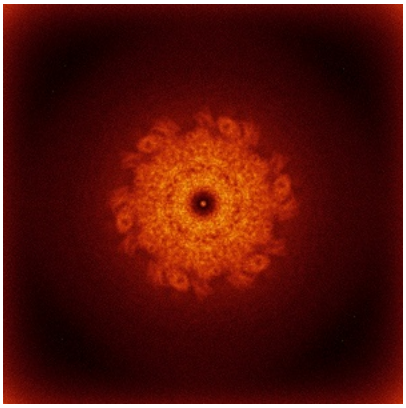
6.4.2 Raw map



X



Y

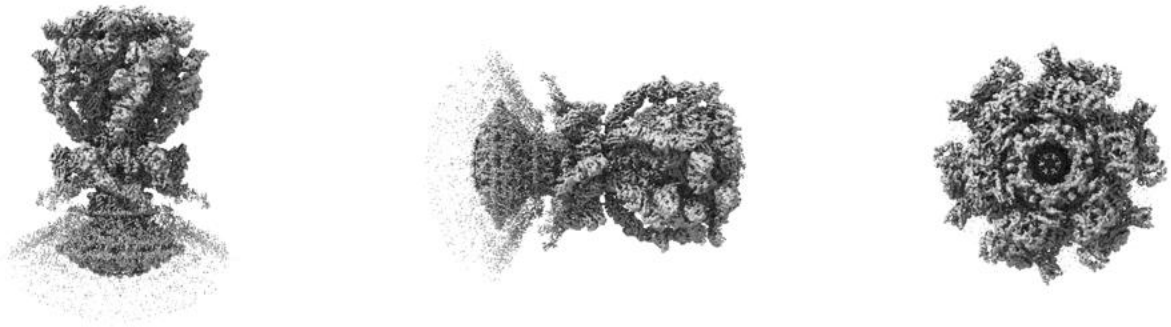


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

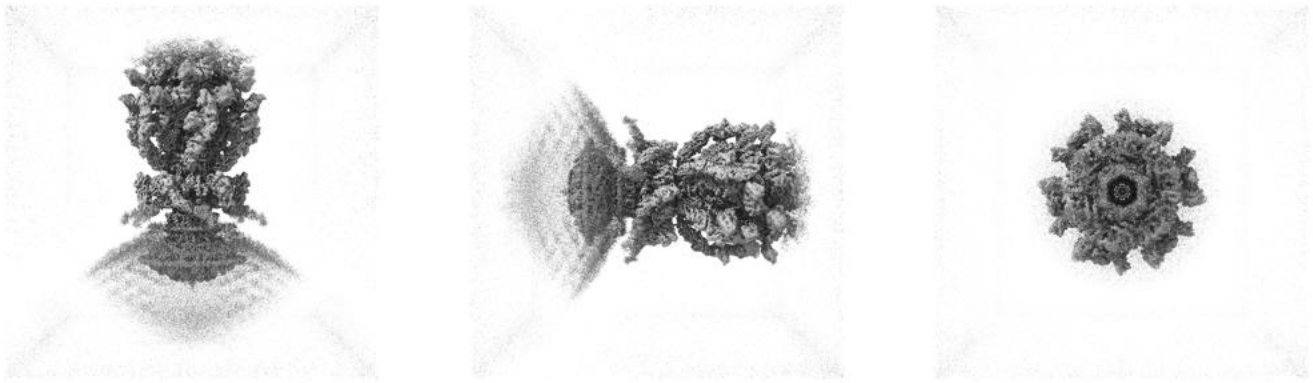
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.242. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

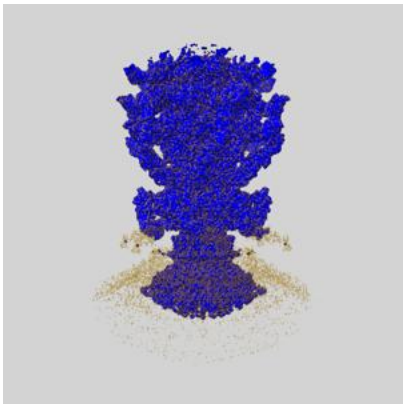
6.6 Mask visualisation (i)

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

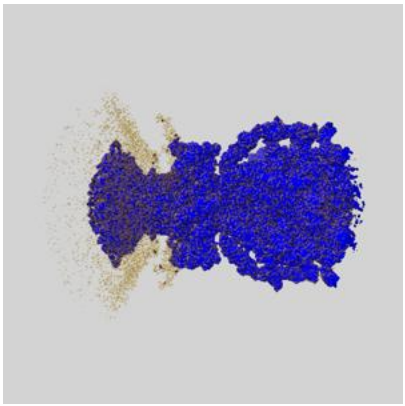
A mask typically either:

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

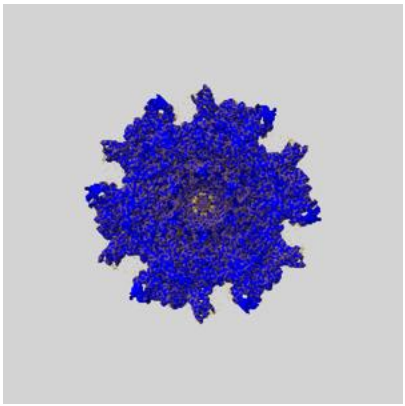
6.6.1 emd_45162_msk_1.map (i)



X



Y

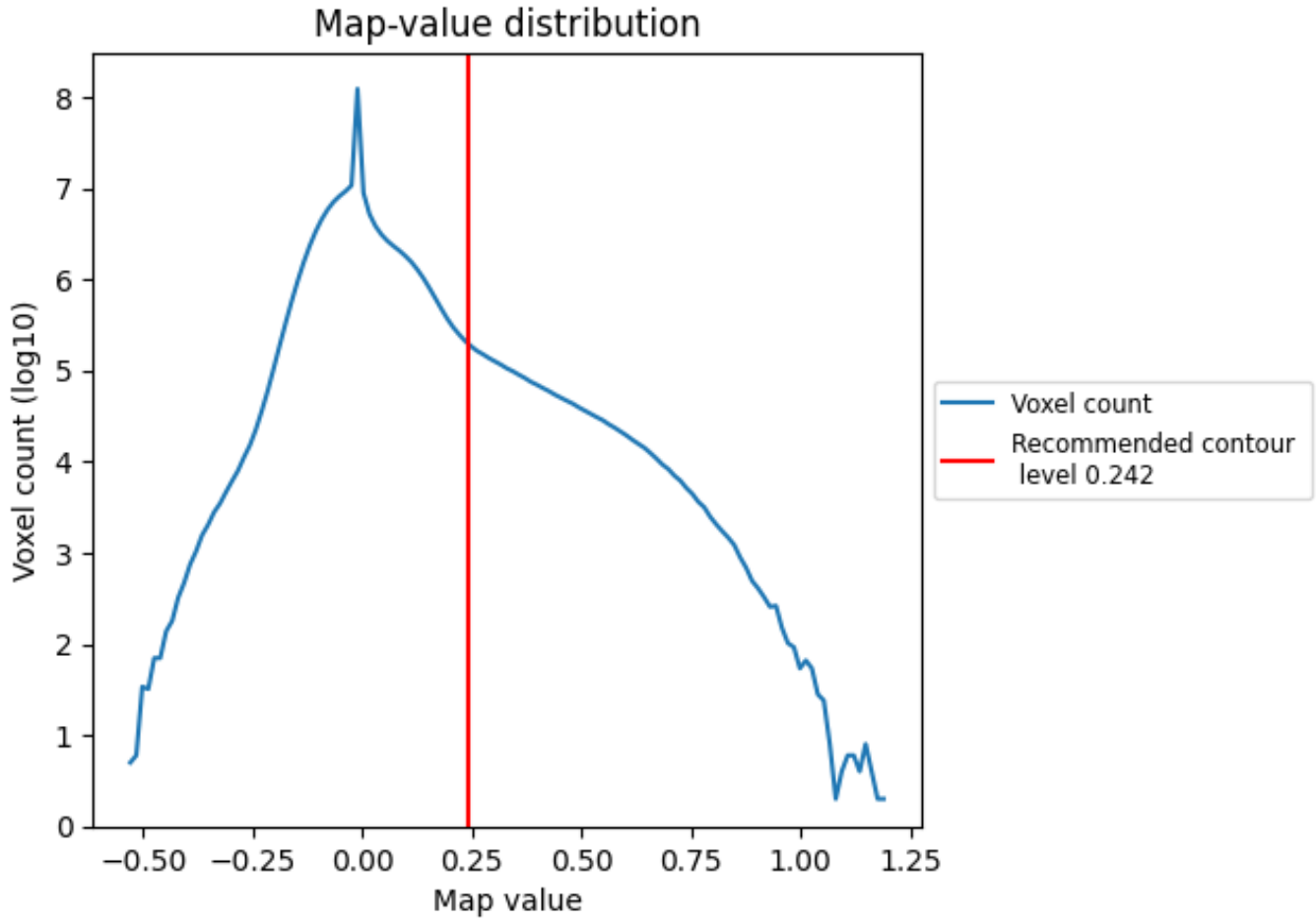


Z

7 Map analysis

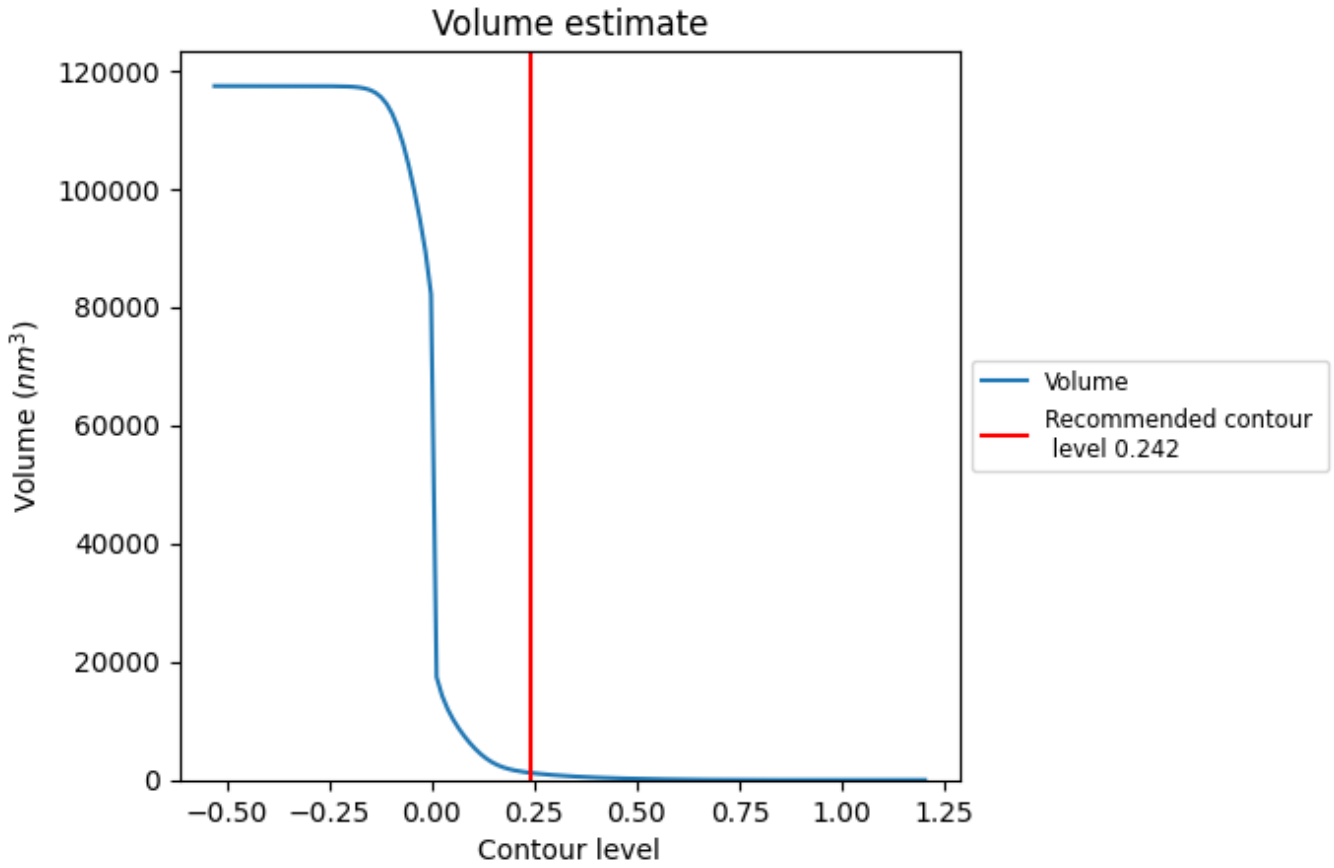
This section contains the results of statistical analysis of the map.

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.

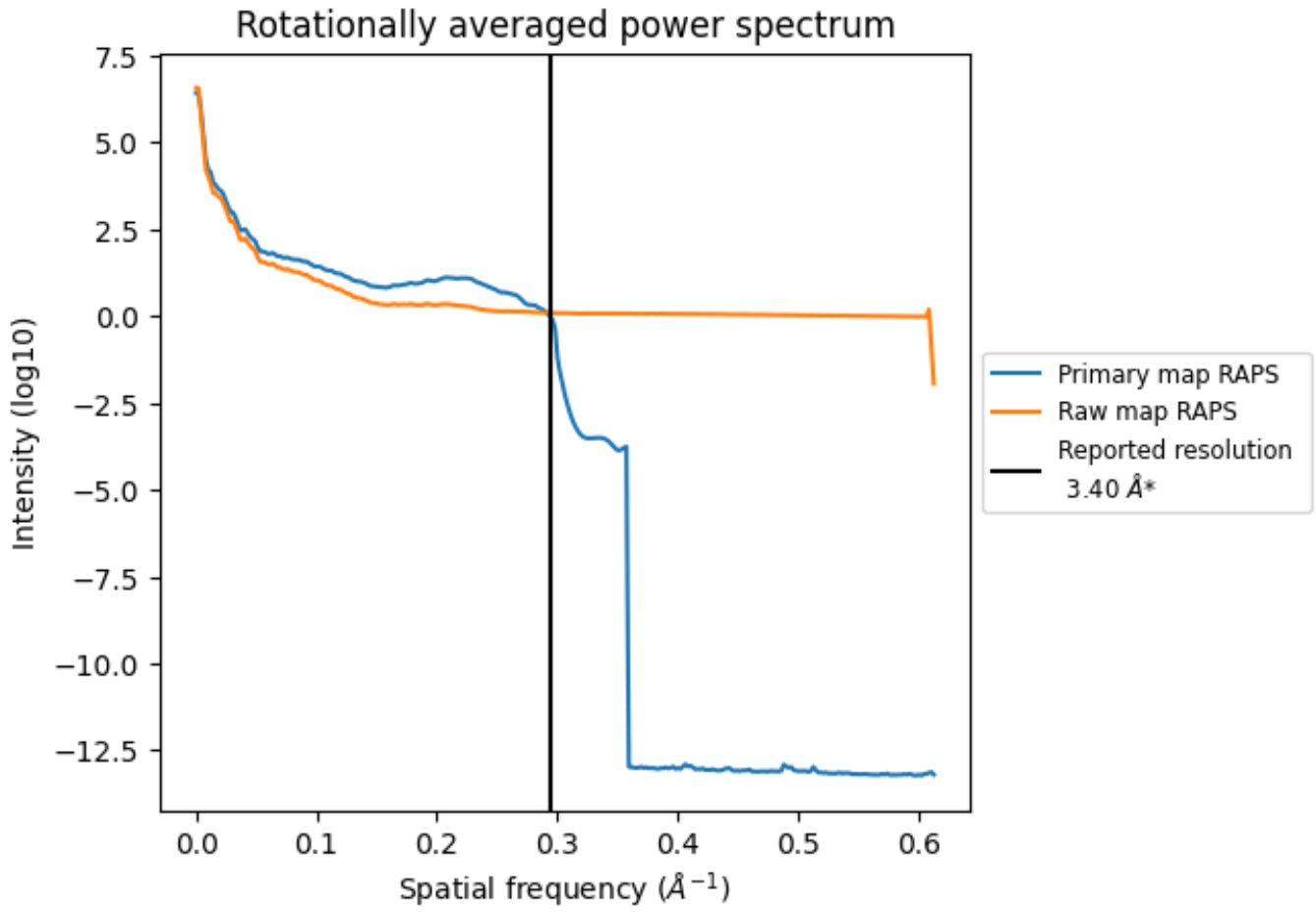
7.2 Volume estimate



The volume at the recommended contour level is 1189 nm^3; this corresponds to an approximate mass of 1074 kDa.

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

7.3 Rotationally averaged power spectrum (i)

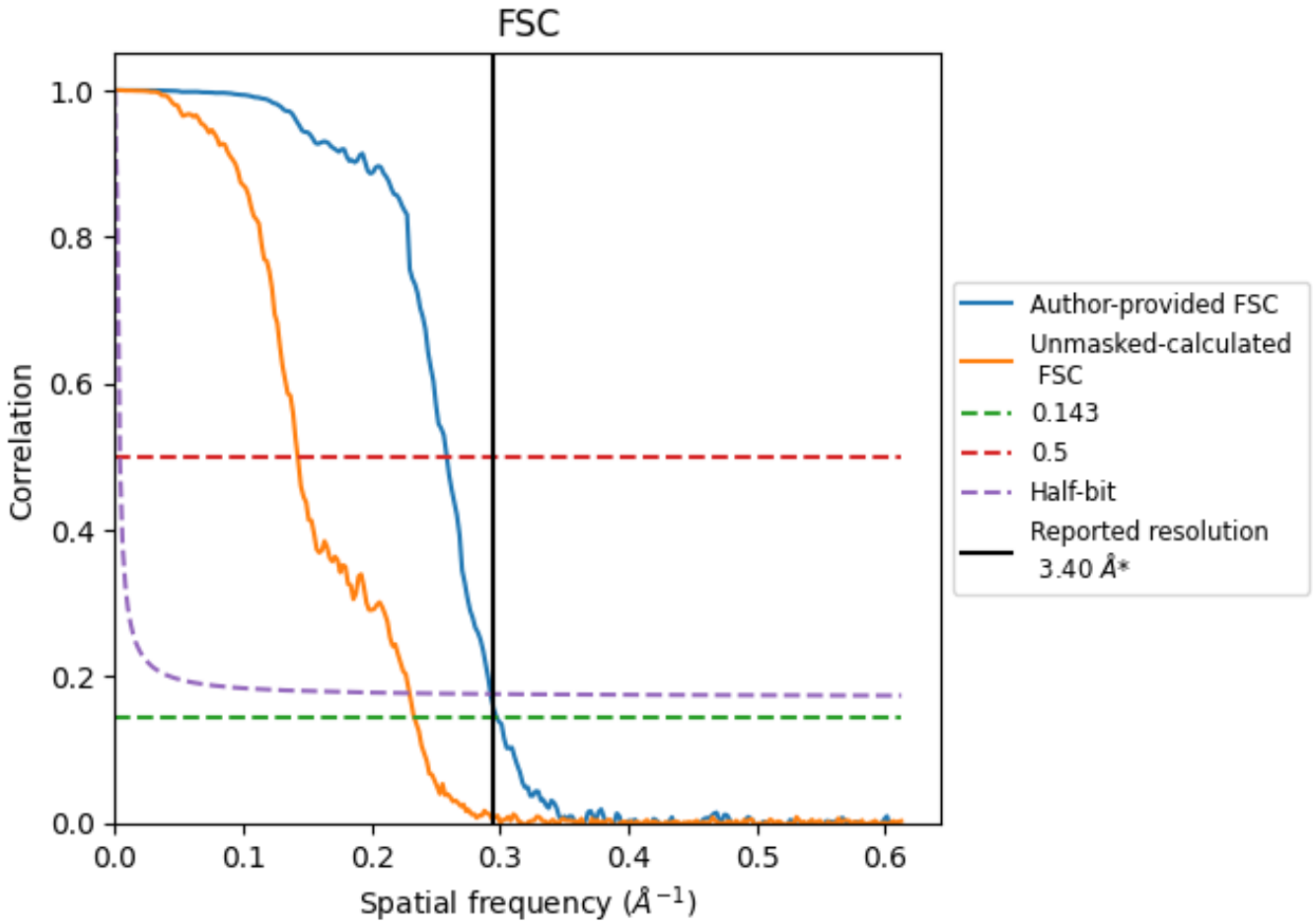


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

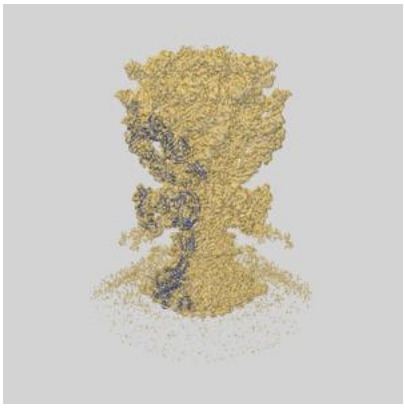
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.36	3.87	3.42
Unmasked-calculated*	4.28	7.02	4.36

*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 4.28 differs from the reported value 3.4 by more than 10 %

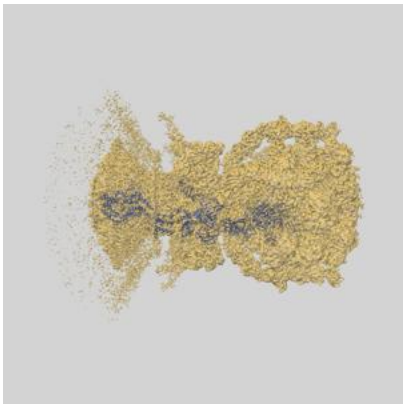
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-45162 and PDB model 9C39. Per-residue inclusion information can be found in section 3 on page 6.

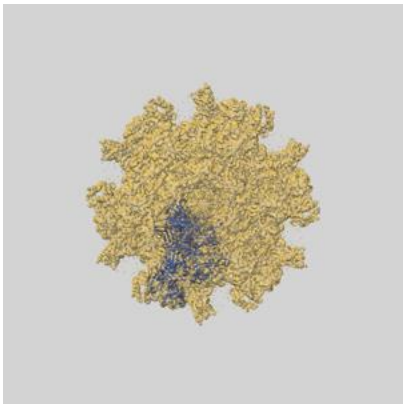
9.1 Map-model overlay



X



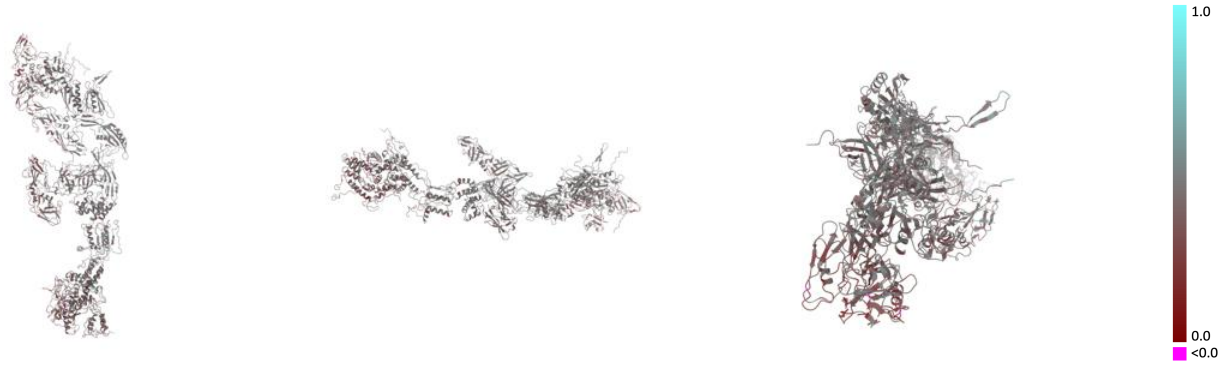
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.242 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

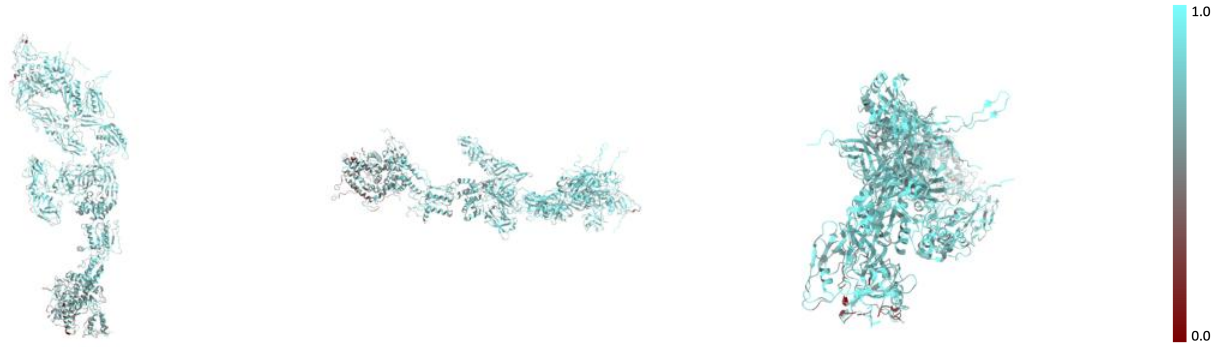
9.2 Q-score mapped to coordinate model (i)



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.

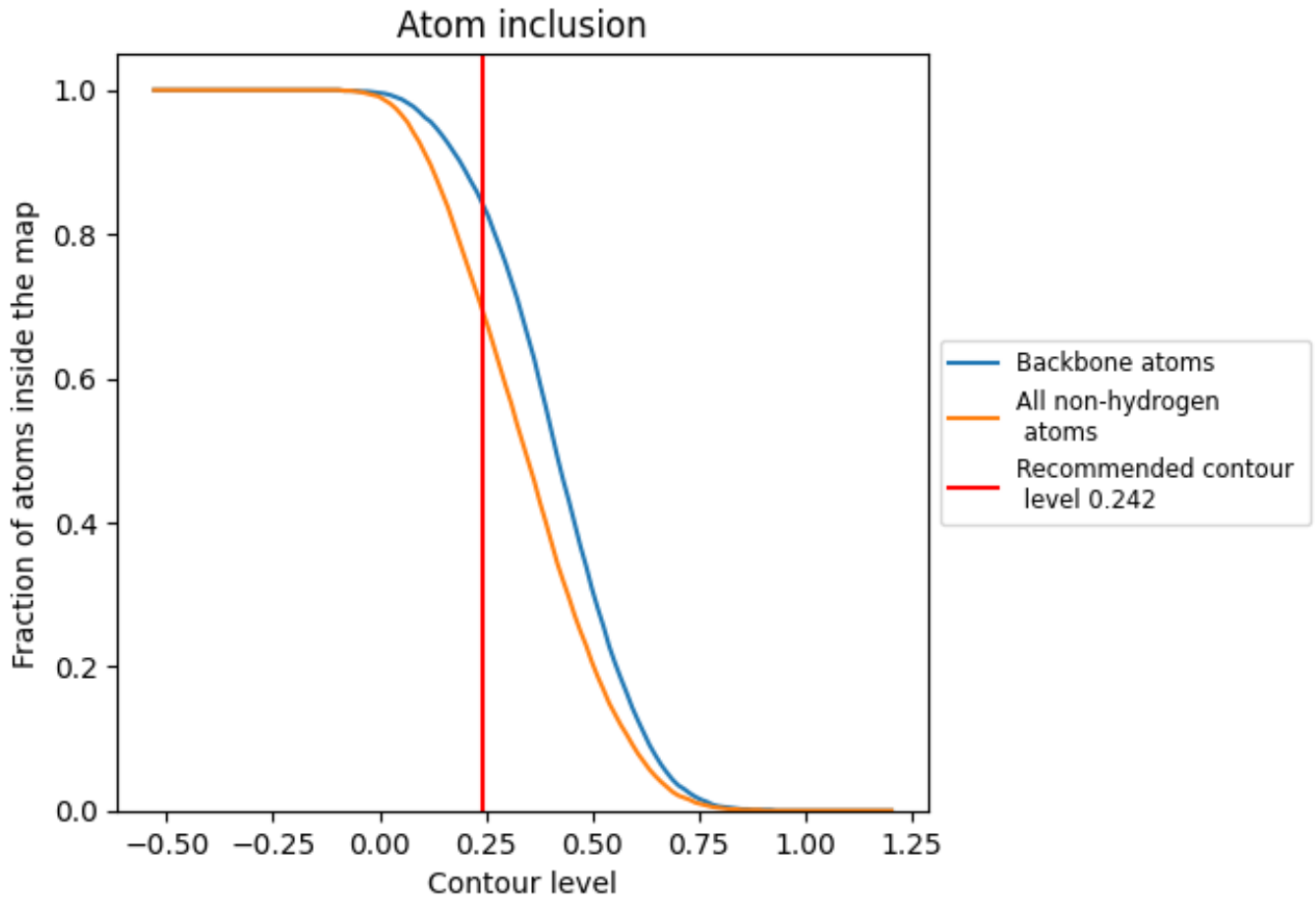
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.242).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 69% 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 (0.242) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6940	0.4160
A	0.6020	0.4080
B	0.5980	0.3910
C	0.6780	0.4410
D	0.6820	0.4360
E	0.7340	0.4560
F	0.7560	0.4510
G	0.7580	0.4520
H	0.7700	0.4220
I	0.7420	0.4190
J	0.7290	0.4380
K	0.7170	0.3960
L	0.7070	0.4110
M	0.7370	0.4220
N	0.7340	0.4120
O	0.7240	0.3700
P	0.6550	0.3350