WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 12:28 PM JST

PDB ID	:	8XCJ
EMDB ID	:	EMD-38245
Title	:	Open State of central tail fiber of bacteriophage lambda upon binding to LamB (gpJ713-LamB complex)
Authors	:	Ge, X.F.; Wang, J.W.
Deposited on	:	2023-12-09
Resolution	:	2.98 Å(reported)

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

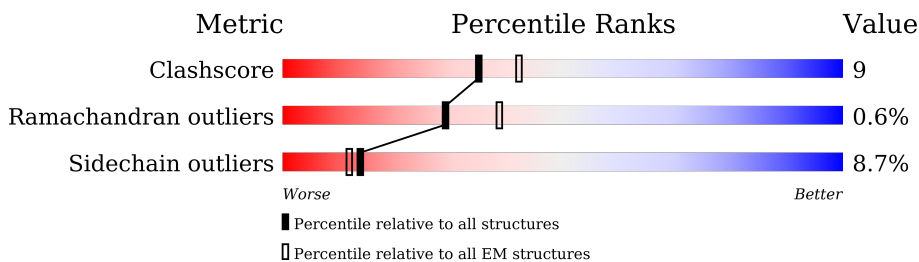|		
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.98 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
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		8.7%

Worse   *Better*

▮ Percentile relative to all structures
❘ Percentile relative to all EM structures

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	422	77% · 22% ·
1	B	422	74% · 23% ·
1	C	422	76% · 22% ·
2	F	420	7% · 73% · 24% ·
2	J	420	6% · 71% · 26% ·
2	Z	420	7% · 70% · 27% ·

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 19809 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 Maltoporin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	422	Total	C	N	O	S	0	0
			3360	2118	572	656	14		
1	B	422	Total	C	N	O	S	0	0
			3360	2118	572	656	14		
1	C	422	Total	C	N	O	S	0	0
			3360	2118	572	656	14		

- Molecule 2 is a protein called Tip attachment protein J.

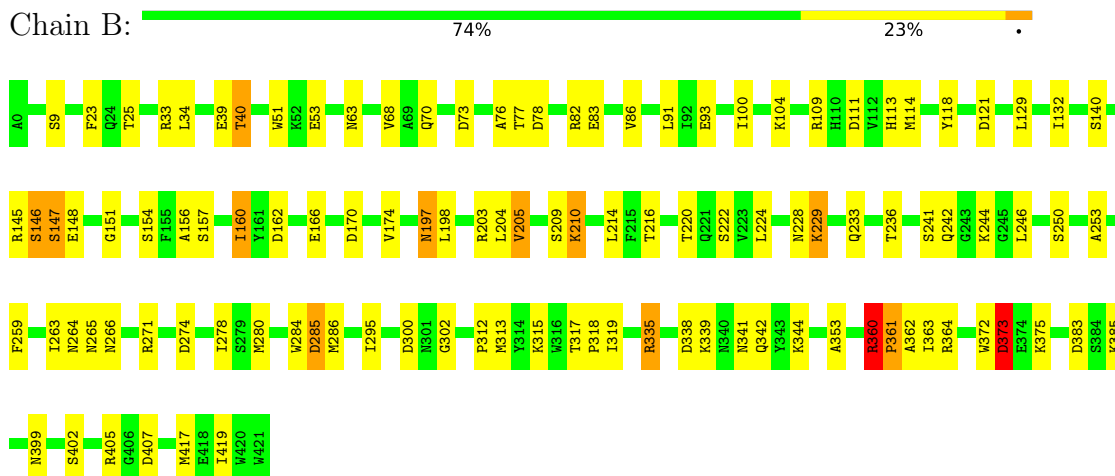| Mol	Chain	Residues	Atoms					AltConf	Trace
2	Z	420	Total	C	N	O	S	0	0
			3243	2058	550	625	10		
2	J	420	Total	C	N	O	S	0	0
			3243	2058	550	625	10		
2	F	420	Total	C	N	O	S	0	0
			3243	2058	550	625	10		

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.
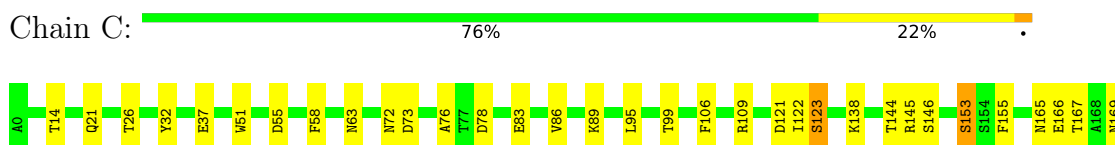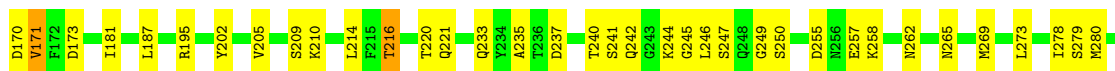
- Molecule 1: Maltoporin
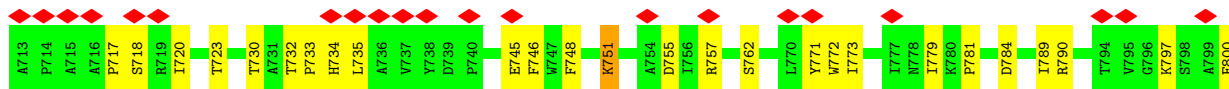
Chain A:

- Molecule 1: Maltoporin

Chain B:

- Molecule 1: Maltoporin

Chain C:

D170 V171 F172 D173 I181 L187 R195 Y202 V205 S209 K210 L214 F215 T216 T220 Q221 Q233 Y234 A235 T236 D237 T240 S241 Q242 G243 K244 G245 L246 S247 Q248 G249 S250 D255 N256 E257 K258 N262 N265 M269 L273 I278 S279 M280

W284 Y288 M291 I295 D300 T303 T307 M313 T317 P318 I319 M320 D329 R335 N340 T346 Q350 W351 Q352 A353 S359 R360 P361 A362 I363 D379 Y380 D383 S384 N387 N399 M417 E418 I419 W420 W421
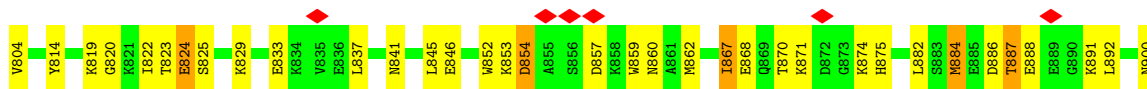
• Molecule 2: Tip attachment protein J

Chain Z:

A713 P714 A715 A716 P717 S718 R719 I720 T723 T730 A731 T732 P733 H734 L735 A736 V737 Y738 D739 P740 E745 F746 W747 F748 K751 A754 D755 I756 R757 S762 L770 Y771 W772 I773 I777 N778 I779 K780 P781 D784 I789 R790 T794 V795 G796 K797 S798 A799 F800

V801 V804 D810 Y814 F818 K819 G820 K821 E824 L827 G828 K829 E830 L831 L832 E833 K834 L837 N841 R844 L845 E851 W852 K853 D854 A855 S856 D857 E858 W859 N860 A861 M862 K866 I867 E868 K871 D872 G873 K874 H875 Y876 S883 M884 E885 E888

L892 S893 Q894 F895 L896 R901 I902 I905 T913 P914 M915 D927 L930 L933 P936 T939 S940 G941 P944 F947 P951 K954 L955 T956 N969 L973 I978 C982 T987 L988 R989 K992 G995 V998 K999 R1009 E1010 S1011

D1014 W1015 T1021 T1025 D1026 F1030 V1035 R1046 S1049 T1052 Y1058 V1061 Y1069 A1073 V1077 Q1078 V1079 F1080 S1081 R1082 G1089 T1100 S1101 T1102 R1103 H1104 S1105 A1106 D1107 P1110 Y1111 V1117 M1120 V1121 I1122 K1123 K1124 L1127 V1132
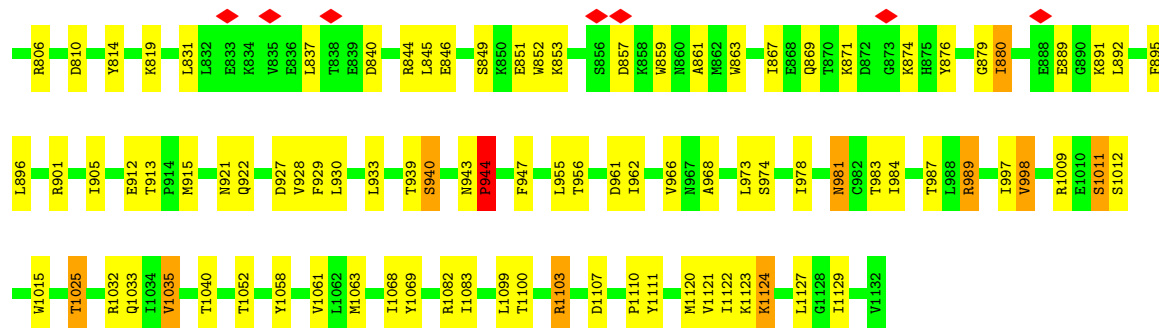
• Molecule 2: Tip attachment protein J

Chain J:

A713 P714 A715 A716 R719 I720 E721 L722 Q728 T732 P733 H734 L735 A736 V737 Y738 D739 P740 T741 V742 Q743 F744 E745 F746 Q752 I753 A754 D755 I756 R757 Y765 L766 G767 L770 Y771 W772 I773 P781 Y786 I789 N793 T794 V795 G796 K797 S798 A799 F800 A803

V804 Y814 K819 G820 K821 I822 T823 E824 S825 K829 E833 K834 V835 E836 L837 N841 L845 E846 W852 K853 D854 A855 S856 D857 E858 W859 N860 A861 M862 I867 E868 Q869 T870 K871 D872 G873 K874 H875 L882 S883 M884 E885 D886 T887 E888 E889 G890 K891 L892 N900

R901 I905 D906 N911 P914 V917 N921 Q922 D927 V928 F929 L930 K931 R932 L933 T939 S940 G941 G942 N943 P944 F947 S948 L949 T950 P951 D952 G953 K954 L955 T956 N959 N969 L973 S974 I978 C982 T983 R989 D996 I997 V998 R1009 E1010

S1011 S1012 W1015 T1019 T1023 V1024 T1025 Q1033 I1034 V1035 R1042 K1045 R1051 V1061 Y1069 F1080 S1081 R1082 I1083 L1099 R1103 P1110 Y1111 V1117 V1121 I1122 K1123 K1124 V1132

• Molecule 2: Tip attachment protein J

Chain F:

A713 P714 A715 A716 P717 S718 R719 I720 E721 T732 P733 H734 L735 A736 V737 Y738 D739 F744 E745 F746 S749 E750 K751 A754 D755 I756 R757 E760 T763 L766 L770 Y771 W772 S776 P781 D784 F787 Y788 I789 R790 N793 T794 V795 G796 K797 S798 A799

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	621549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.061	Depositor
Minimum map value	-2.229	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	386.712, 386.712, 386.712	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	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	0.33	1/3454 (0.0%)	0.53	0/4683
1	B	0.31	0/3454	0.53	1/4683 (0.0%)
1	C	0.32	1/3454 (0.0%)	0.52	0/4683
2	F	0.29	1/3313 (0.0%)	0.58	3/4503 (0.1%)
2	J	0.27	0/3313	0.58	1/4503 (0.0%)
2	Z	0.28	0/3313	0.59	3/4503 (0.1%)
All	All	0.30	3/20301 (0.0%)	0.56	8/27558 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	SER	CA-CB	-7.39	1.41	1.52
1	C	359	SER	CA-CB	-5.97	1.44	1.52
2	F	940	SER	CA-CB	-5.52	1.44	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Z	944	PRO	N-CA-CB	-10.50	90.70	103.30
2	J	944	PRO	N-CA-CB	-9.84	91.50	103.30
2	F	944	PRO	N-CA-CB	-9.76	91.58	103.30
1	B	373	ASP	CB-CG-OD2	5.46	123.21	118.30
2	F	944	PRO	CA-N-CD	-5.45	103.87	111.50
2	Z	927	ASP	CB-CG-OD1	5.42	123.18	118.30
2	F	943	ASN	CB-CA-C	5.14	120.68	110.40
2	Z	944	PRO	CA-N-CD	-5.05	104.43	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3360	0	3086	53	0
1	B	3360	0	3086	68	0
1	C	3360	0	3086	53	0
2	F	3243	0	3206	70	0
2	J	3243	0	3206	79	0
2	Z	3243	0	3206	85	0
All	All	19809	0	18876	337	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 9.

All (337) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ASN:HB3	1:B:83:GLU:HB3	1.57	0.84
1:C:360:ARG:O	1:C:361:PRO:C	2.15	0.84
1:A:360:ARG:O	1:A:361:PRO:C	2.16	0.82
1:B:360:ARG:O	1:B:361:PRO:C	2.21	0.78
2:Z:939:THR:HG22	2:Z:941:GLY:H	1.50	0.75
1:A:342:GLN:OE1	1:A:405:ARG:NH2	2.22	0.72
2:Z:1103:ARG:HB3	2:Z:1110:PRO:HD3	1.72	0.72
1:B:93:GLU:OE2	1:B:93:GLU:N	2.19	0.71
1:A:269:MET:HG3	1:A:295:ILE:HG12	1.71	0.71
2:Z:861:ALA:HB3	2:J:867:ILE:HD13	1.73	0.70
2:J:939:THR:HG22	2:J:941:GLY:H	1.55	0.70
1:B:40:THR:HG22	1:B:70:GLN:HB3	1.74	0.69
1:C:241:SER:HB3	1:C:265:ASN:HD22	1.57	0.69
1:B:361:PRO:HD3	1:B:419:ILE:HG13	1.74	0.69
1:B:253:ALA:HB2	1:B:263:ILE:HD13	1.76	0.68
2:F:853:LYS:HD3	2:F:857:ASP:HA	1.73	0.68
1:B:242:GLN:HE21	1:B:244:LYS:HB2	1.58	0.68
1:C:269:MET:HG3	1:C:295:ILE:HG12	1.77	0.67
1:C:379:ASP:OD1	1:C:387:ASN:ND2	2.27	0.67
2:Z:930:LEU:HD22	2:J:933:LEU:HD11	1.76	0.67
1:A:379:ASP:OD1	1:A:387:ASN:ND2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:NH1	1:A:170:ASP:OD1	2.28	0.66
1:B:285:ASP:OD1	1:B:315:LYS:NZ	2.27	0.66
1:A:198:LEU:HD11	1:A:204:LEU:HG	1.78	0.66
2:J:722:LEU:HD11	2:J:803:ALA:HB1	1.77	0.66
2:Z:858:LYS:HE2	2:J:871:LYS:HD2	1.77	0.66
1:A:296:ASN:OD1	1:A:334:GLN:NE2	2.29	0.66
2:Z:914:PRO:HD3	2:F:819:LYS:HB2	1.77	0.65
1:B:241:SER:OG	1:B:265:ASN:ND2	2.26	0.64
1:B:78:ASP:HB3	1:C:76:ALA:HB1	1.80	0.64
2:Z:755:ASP:OD2	2:Z:757:ARG:NH2	2.31	0.64
1:C:165:ASN:HD22	1:C:202:TYR:HE2	1.44	0.64
1:A:317:THR:HG22	1:A:319:ILE:H	1.63	0.63
2:F:962:ILE:HD12	2:F:966:VAL:HG22	1.78	0.63
1:A:361:PRO:HD3	1:A:419:ILE:HG13	1.81	0.62
2:J:746:PHE:HD2	2:J:772:TRP:HB2	1.64	0.62
1:A:14:THR:OG1	1:A:19:GLU:O	2.14	0.62
2:Z:859:TRP:HE1	2:J:841:ASN:HB3	1.63	0.62
2:J:735:LEU:HD11	2:J:744:PHE:HZ	1.64	0.62
2:J:854:ASP:OD2	2:J:860:ASN:ND2	2.33	0.62
1:B:170:ASP:OD2	1:B:197:ASN:ND2	2.29	0.62
2:Z:884:MET:HE3	2:J:867:ILE:HD11	1.81	0.61
1:C:14:THR:HG21	1:C:21:GLN:HG3	1.82	0.60
1:A:399:ASN:HB2	2:J:1011:SER:HA	1.83	0.60
2:Z:720:ILE:HG12	2:Z:789:ILE:HG21	1.82	0.60
2:J:1080:PHE:HE1	2:J:1082:ARG:HE	1.49	0.60
2:F:760:GLU:OE2	2:F:790:ARG:NH1	2.35	0.59
1:A:242:GLN:HE21	1:A:244:LYS:HD2	1.66	0.59
2:F:746:PHE:HD2	2:F:772:TRP:HB2	1.67	0.59
1:C:360:ARG:O	1:C:362:ALA:N	2.35	0.59
1:B:145:ARG:NH2	1:B:170:ASP:OD1	2.34	0.59
1:B:162:ASP:OD1	2:Z:1058:TYR:OH	2.17	0.59
1:B:233:GLN:OE1	1:B:271:ARG:NH1	2.35	0.59
1:C:361:PRO:HD3	1:C:419:ILE:HG13	1.83	0.59
1:A:360:ARG:O	1:A:362:ALA:N	2.35	0.58
2:Z:732:THR:HG22	2:Z:771:TYR:HB2	1.84	0.58
1:A:32:TYR:HB2	1:A:344:LYS:HD3	1.85	0.58
2:Z:861:ALA:HB1	2:J:845:LEU:HD12	1.84	0.58
2:J:853:LYS:HE3	2:J:857:ASP:HA	1.85	0.58
1:C:106:PHE:HA	1:C:123:SER:HB3	1.85	0.58
2:J:943:ASN:O	2:J:944:PRO:C	2.41	0.58
1:B:383:ASP:OD2	2:F:1111:TYR:OH	2.14	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:745:GLU:HB2	2:Z:790:ARG:HG2	1.86	0.57
2:Z:831:LEU:HA	2:Z:866:LYS:HD3	1.84	0.57
1:A:340:ASN:HB2	1:A:374:GLU:HA	1.87	0.57
2:Z:837:LEU:HD11	2:Z:844:ARG:HB3	1.87	0.57
2:F:732:THR:HG22	2:F:771:TYR:HB2	1.86	0.57
2:F:733:PRO:HD3	2:F:746:PHE:HZ	1.68	0.57
2:Z:876:TYR:HD2	2:F:891:LYS:HB2	1.69	0.57
2:J:772:TRP:HE3	2:J:773:ILE:H	1.53	0.56
2:J:930:LEU:HD22	2:F:933:LEU:HD11	1.86	0.56
2:Z:859:TRP:NE1	2:J:841:ASN:O	2.38	0.56
1:B:241:SER:HG	1:B:265:ASN:HD22	1.52	0.56
1:C:106:PHE:HB3	1:C:109:ARG:HD2	1.86	0.56
1:B:295:ILE:O	1:B:302:GLY:HA3	2.05	0.56
1:C:399:ASN:HB2	2:Z:1011:SER:HA	1.87	0.56
1:C:121:ASP:OD1	1:C:123:SER:OG	2.22	0.56
1:B:91:LEU:HD12	1:B:100:ILE:HD11	1.88	0.56
2:Z:1061:VAL:HB	2:Z:1069:TYR:HB3	1.88	0.55
1:B:280:MET:O	1:B:284:TRP:HB2	2.07	0.55
1:A:255:ASP:OD2	1:A:384:SER:OG	2.24	0.55
1:C:146:SER:HB3	1:C:246:LEU:HD13	1.87	0.55
2:F:849:SER:HB3	2:F:863:TRP:HD1	1.72	0.55
1:C:350:GLN:NE2	1:C:352:GLN:OE1	2.35	0.55
2:Z:819:LYS:HB2	2:J:914:PRO:HD3	1.89	0.55
1:C:255:ASP:OD2	1:C:384:SER:OG	2.21	0.55
2:Z:1107:ASP:OD1	2:Z:1107:ASP:N	2.38	0.55
2:J:752:GLN:HB2	2:J:786:TYR:CZ	2.42	0.55
2:J:1024:VAL:HG22	2:F:1129:ILE:HG22	1.89	0.55
1:B:342:GLN:HG3	1:B:372:TRP:HB3	1.89	0.55
1:C:278:ILE:HG12	1:C:288:TYR:HE1	1.70	0.55
2:J:996:ASP:HB3	2:J:1123:LYS:HD2	1.88	0.55
1:B:228:ASN:ND2	1:B:274:ASP:OD1	2.40	0.54
2:F:784:ASP:OD1	2:F:784:ASP:N	2.39	0.54
1:A:280:MET:HG2	1:A:284:TRP:HB2	1.88	0.54
2:J:732:THR:HG22	2:J:771:TYR:HB2	1.89	0.54
2:J:859:TRP:O	2:J:891:LYS:NZ	2.40	0.54
2:F:981:ASN:OD1	2:F:981:ASN:N	2.39	0.54
1:B:34:LEU:O	1:B:344:LYS:NZ	2.41	0.54
2:Z:876:TYR:CD2	2:F:891:LYS:HB2	2.43	0.54
1:A:26:THR:OG1	1:A:340:ASN:ND2	2.41	0.54
2:J:891:LYS:HB2	2:F:876:TYR:HD2	1.73	0.53
2:Z:781:PRO:HG3	2:Z:814:TYR:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:HG	1:B:132:ILE:HD11	1.90	0.53
1:B:156:ALA:HA	1:B:203:ARG:HD2	1.91	0.53
1:C:307:THR:OG1	1:C:329:ASP:OD1	2.24	0.53
2:J:823:THR:OG1	2:F:912:GLU:OE1	2.24	0.53
2:Z:896:LEU:HD11	2:J:905:ILE:HD12	1.91	0.53
1:B:220:THR:OG1	1:B:229:LYS:NZ	2.41	0.53
2:J:982:CYS:HB3	2:F:984:ILE:HD13	1.91	0.53
2:J:1035:VAL:HG12	2:J:1083:ILE:HG12	1.90	0.53
2:Z:902:ILE:HG23	2:F:895:PHE:HD2	1.73	0.53
1:C:242:GLN:OE1	1:C:246:LEU:HB2	2.08	0.52
1:C:153:SER:OG	1:C:155:PHE:O	2.27	0.52
2:Z:810:ASP:OD1	2:Z:810:ASP:N	2.38	0.52
2:Z:746:PHE:CD2	2:Z:772:TRP:HB2	2.45	0.52
2:F:749:SER:HB2	2:F:763:THR:HG22	1.92	0.52
2:J:973:LEU:O	2:F:978:ILE:HA	2.10	0.51
2:F:1103:ARG:HB3	2:F:1110:PRO:HD3	1.91	0.51
1:A:27:GLY:HA3	1:A:331:VAL:HG11	1.93	0.51
1:B:360:ARG:O	1:B:362:ALA:N	2.42	0.51
2:F:947:PHE:HA	2:F:956:THR:O	2.10	0.51
1:A:383:ASP:HB2	1:A:386:VAL:HG22	1.92	0.51
1:B:317:THR:HG22	1:B:319:ILE:H	1.75	0.51
2:Z:781:PRO:HB2	2:F:929:PHE:CZ	2.46	0.51
1:A:91:LEU:HD12	1:A:100:ILE:HD11	1.92	0.51
2:J:954:LYS:HE3	2:F:961:ASP:OD2	2.11	0.50
2:Z:723:THR:OG1	2:Z:730:THR:HB	2.11	0.50
2:Z:733:PRO:HB3	2:Z:789:ILE:HD11	1.92	0.50
2:F:998:VAL:HA	2:F:1121:VAL:O	2.11	0.50
1:B:204:LEU:HD12	1:B:210:LYS:HG2	1.93	0.50
2:Z:927:ASP:HB2	2:J:932:ARG:HB3	1.92	0.50
2:F:721:GLU:OE2	2:F:732:THR:OG1	2.28	0.50
1:C:317:THR:HG22	1:C:320:MET:H	1.76	0.50
1:C:380:TYR:O	2:Z:1046:ARG:NH2	2.34	0.50
1:A:76:ALA:HB1	1:C:78:ASP:HB3	1.93	0.50
2:Z:989:ARG:HD2	2:F:983:THR:HG23	1.93	0.50
1:A:45:LYS:HG2	1:A:63:ASN:HD22	1.77	0.50
2:Z:884:MET:HB3	2:J:867:ILE:HD11	1.94	0.50
2:Z:915:MET:HB2	2:F:921:ASN:HA	1.93	0.50
2:J:868:GLU:HB3	2:J:875:HIS:CE1	2.47	0.50
2:J:882:LEU:HD22	2:F:880:ILE:HG22	1.93	0.50
1:A:371:LYS:HD2	1:A:409:ASP:HB3	1.94	0.49
2:Z:954:LYS:HD2	2:J:959:ASN:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:952:ASP:OD1	2:J:952:ASP:N	2.26	0.49
1:B:63:ASN:HD22	1:B:82:ARG:HB2	1.75	0.49
2:F:745:GLU:HB2	2:F:790:ARG:HG2	1.94	0.49
2:Z:883:SER:OG	2:Z:885:GLU:OE2	2.27	0.49
2:F:1033:GLN:HG3	2:F:1124:LYS:HD2	1.95	0.49
1:C:181:ILE:HD11	1:C:187:LEU:HD22	1.93	0.49
2:F:744:PHE:HD2	2:F:770:LEU:HA	1.78	0.49
1:A:214:LEU:HD12	1:A:235:ALA:HB2	1.94	0.49
1:A:383:ASP:OD1	2:J:1111:TYR:OH	2.30	0.49
1:A:335:ARG:NH1	1:A:393:ALA:O	2.43	0.49
1:A:350:GLN:HB3	1:A:364:ARG:HG2	1.94	0.49
2:Z:913:THR:HA	2:F:819:LYS:HB2	1.95	0.49
1:C:280:MET:O	1:C:284:TRP:HB2	2.12	0.49
2:J:1033:GLN:HG3	2:J:1124:LYS:HD2	1.94	0.49
1:C:169:ASN:HD21	1:C:249:GLY:H	1.61	0.48
1:C:214:LEU:HD12	1:C:235:ALA:HB2	1.94	0.48
2:Z:845:LEU:HD23	2:F:861:ALA:HB1	1.95	0.48
1:B:23:PHE:HB3	1:B:405:ARG:HH22	1.77	0.48
1:B:148:GLU:OE1	1:B:250:SER:OG	2.25	0.48
2:Z:833:GLU:OE2	2:Z:833:GLU:N	2.46	0.48
1:C:317:THR:HG22	1:C:319:ILE:H	1.78	0.48
1:A:181:ILE:HD11	1:A:219:HIS:HD2	1.77	0.48
1:B:86:VAL:HG12	1:C:363:ILE:HD11	1.95	0.48
2:Z:1049:SER:O	2:Z:1049:SER:OG	2.27	0.48
1:C:216:THR:HB	1:C:233:GLN:HE21	1.79	0.48
2:Z:894:GLN:OE1	2:J:901:ARG:NE	2.46	0.48
1:B:353:ALA:HB3	1:B:361:PRO:HG2	1.96	0.48
1:B:399:ASN:HB2	2:F:1011:SER:HA	1.96	0.48
2:J:720:ILE:HG12	2:J:789:ILE:HG12	1.96	0.48
1:B:335:ARG:HE	1:B:335:ARG:HB3	1.49	0.48
1:A:332:GLU:HB2	1:A:339:LYS:HG2	1.96	0.47
2:Z:827:LEU:HB3	2:Z:831:LEU:HD13	1.95	0.47
1:A:319:ILE:HD11	1:C:51:TRP:CH2	2.50	0.47
2:Z:987:THR:O	2:F:981:ASN:HA	2.15	0.47
2:J:781:PRO:HG3	2:J:814:TYR:CZ	2.50	0.47
2:J:1103:ARG:HB3	2:J:1110:PRO:HD3	1.95	0.47
2:Z:1015:TRP:CE2	2:Z:1110:PRO:HG2	2.50	0.47
1:C:26:THR:HB	1:C:340:ASN:HD22	1.79	0.47
2:Z:772:TRP:HE3	2:Z:773:ILE:H	1.63	0.47
1:B:33:ARG:HD2	1:B:113:HIS:O	2.15	0.47
1:B:111:ASP:HB3	1:B:118:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LYS:NZ	1:C:72:ASN:O	2.48	0.47
2:Z:717:PRO:HA	2:Z:735:LEU:HD13	1.97	0.47
2:Z:827:LEU:HD11	2:Z:883:SER:OG	2.15	0.47
2:J:746:PHE:CD2	2:J:772:TRP:HB2	2.46	0.47
2:F:831:LEU:HD22	2:F:879:GLY:HA3	1.97	0.46
1:A:233:GLN:OE1	1:A:271:ARG:NH1	2.47	0.46
1:A:363:ILE:HD11	1:C:86:VAL:HG12	1.97	0.46
2:F:998:VAL:HG22	2:F:1122:ILE:HA	1.97	0.46
1:A:82:ARG:NH2	1:B:73:ASP:OD2	2.47	0.46
1:A:325:GLU:HB3	1:A:346:THR:HG23	1.98	0.46
2:F:781:PRO:HG3	2:F:814:TYR:CZ	2.51	0.46
1:C:144:THR:HB	1:C:171:VAL:HG12	1.98	0.46
2:J:950:THR:OG1	2:J:954:LYS:HB3	2.16	0.46
1:A:353:ALA:HB3	1:A:361:PRO:HG2	1.98	0.46
2:Z:856:SER:O	2:Z:856:SER:OG	2.33	0.46
2:J:822:ILE:HD13	2:F:905:ILE:HD11	1.97	0.46
1:B:160:ILE:HD12	1:B:205:VAL:HG21	1.98	0.46
2:Z:1058:TYR:HB2	2:Z:1100:THR:HG23	1.98	0.46
1:B:40:THR:HG23	1:B:68:VAL:HG23	1.97	0.46
1:C:383:ASP:OD2	2:Z:1111:TYR:OH	2.30	0.46
2:Z:748:PHE:CZ	2:Z:779:ILE:HD11	2.51	0.46
1:A:295:ILE:O	1:A:302:GLY:HA3	2.15	0.45
1:B:68:VAL:HG12	1:B:77:THR:HG21	1.99	0.45
2:Z:973:LEU:HD23	2:F:968:ALA:HB3	1.99	0.45
2:J:733:PRO:HD3	2:J:746:PHE:HZ	1.81	0.45
1:C:63:ASN:HB3	1:C:83:GLU:HB2	1.97	0.45
1:B:264:ASN:ND2	1:B:266:ASN:OD1	2.42	0.45
1:B:286:MET:HG3	1:B:312:PRO:HB3	1.97	0.45
2:Z:784:ASP:OD1	2:Z:784:ASP:N	2.46	0.45
2:F:1061:VAL:HB	2:F:1069:TYR:HB3	1.98	0.45
1:B:242:GLN:OE1	1:B:246:LEU:HB2	2.17	0.45
2:Z:872:ASP:HB3	2:Z:874:LYS:NZ	2.32	0.45
1:C:216:THR:HB	1:C:233:GLN:HG2	1.98	0.45
2:Z:930:LEU:HD23	2:Z:933:LEU:HB2	1.99	0.45
2:Z:940:SER:HB2	2:Z:947:PHE:CE2	2.52	0.45
2:Z:1127:LEU:HD12	2:Z:1127:LEU:HA	1.82	0.45
2:J:929:PHE:CZ	2:F:781:PRO:HB2	2.52	0.45
1:C:122:ILE:O	1:C:144:THR:HG21	2.17	0.45
2:Z:1073:ALA:HB2	2:Z:1078:GLN:HG3	1.99	0.45
2:Z:746:PHE:HD2	2:Z:772:TRP:HB2	1.82	0.44
2:Z:1009:ARG:HB2	2:Z:1014:ASP:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:936:PRO:HB2	2:Z:951:PRO:HG3	1.99	0.44
2:J:867:ILE:O	2:J:867:ILE:HG13	2.17	0.44
2:Z:999:LYS:HB2	2:Z:1121:VAL:HB	1.99	0.44
2:J:753:ILE:HD13	2:J:755:ASP:O	2.17	0.44
2:F:849:SER:HB3	2:F:863:TRP:CD1	2.51	0.44
1:A:40:THR:HB	1:A:68:VAL:HG23	1.99	0.44
1:A:162:ASP:OD1	2:F:1058:TYR:OH	2.24	0.44
2:Z:969:ASN:O	2:J:974:SER:HB2	2.17	0.44
2:J:884:MET:SD	2:F:869:GLN:HG3	2.58	0.44
1:B:360:ARG:HA	1:B:360:ARG:HD3	1.20	0.44
1:A:86:VAL:HG12	1:B:363:ILE:HD11	1.99	0.44
1:A:164:THR:HG22	1:A:254:PHE:HE1	1.82	0.44
1:A:78:ASP:HB3	1:B:76:ALA:HB1	1.99	0.43
1:B:51:TRP:CH2	1:C:319:ILE:HD11	2.53	0.43
1:B:147:SER:OG	1:B:166:GLU:OE2	2.29	0.43
2:Z:841:ASN:HB3	2:F:859:TRP:HE1	1.83	0.43
1:A:111:ASP:HB3	1:A:118:TYR:CD1	2.52	0.43
2:J:833:GLU:HG2	2:J:833:GLU:O	2.18	0.43
2:Z:818:PHE:CG	2:J:917:VAL:HG11	2.53	0.43
2:Z:1026:ASP:OD2	2:Z:1089:GLY:N	2.52	0.43
2:F:1082:ARG:HG3	2:F:1083:ILE:N	2.34	0.43
1:C:167:THR:HG21	1:C:250:SER:HB3	1.98	0.43
2:J:887:THR:OG1	2:J:888:GLU:N	2.52	0.43
2:J:921:ASN:HA	2:F:915:MET:HB2	2.00	0.43
1:B:40:THR:CG2	1:B:70:GLN:HB3	2.44	0.43
1:B:210:LYS:HD2	1:B:210:LYS:O	2.19	0.43
1:C:145:ARG:NH2	1:C:170:ASP:OD1	2.39	0.43
1:C:360:ARG:HA	1:C:360:ARG:HD3	1.27	0.43
2:Z:978:ILE:HA	2:F:973:LEU:O	2.18	0.43
2:F:874:LYS:HG3	2:F:876:TYR:CE1	2.54	0.43
1:B:9:SER:HB2	1:B:40:THR:HB	2.00	0.43
2:Z:998:VAL:HG22	2:Z:1122:ILE:HG22	1.99	0.43
2:J:825:SER:O	2:J:829:LYS:HD2	2.19	0.43
1:A:129:LEU:HG	1:A:132:ILE:HD11	2.01	0.43
1:B:146:SER:OG	1:B:147:SER:N	2.52	0.43
1:B:198:LEU:HD11	1:B:204:LEU:HG	2.00	0.43
1:B:338:ASP:HB3	1:B:375:LYS:HB2	2.00	0.43
2:F:763:THR:HG21	2:F:788:TYR:CD2	2.54	0.43
2:Z:1035:VAL:HG23	2:Z:1120:MET:HB2	2.00	0.42
2:J:845:LEU:HG	2:J:867:ILE:HG22	2.01	0.42
2:J:947:PHE:HA	2:J:956:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TYR:CE2	1:A:309:GLY:HA3	2.54	0.42
2:J:871:LYS:O	2:J:874:LYS:HG2	2.18	0.42
1:C:32:TYR:OH	1:C:307:THR:HG23	2.19	0.42
1:C:255:ASP:OD1	1:C:257:GLU:N	2.51	0.42
2:Z:746:PHE:CD1	2:Z:789:ILE:HG13	2.54	0.42
2:F:871:LYS:O	2:F:874:LYS:HG2	2.19	0.42
1:A:242:GLN:OE1	1:A:246:LEU:HB2	2.18	0.42
1:C:242:GLN:NE2	1:C:244:LYS:HB2	2.35	0.42
1:A:122:ILE:O	1:A:144:THR:HG21	2.19	0.42
2:F:1063:MET:HB3	2:F:1068:ILE:HG21	2.02	0.42
1:C:353:ALA:HB3	1:C:361:PRO:HG2	2.01	0.42
2:Z:955:LEU:HD22	2:J:955:LEU:HD21	2.01	0.42
2:F:790:ARG:NH1	2:F:797:LYS:HD2	2.35	0.42
2:F:1011:SER:HB3	2:F:1012:SER:H	1.68	0.42
2:F:1015:TRP:CE2	2:F:1110:PRO:HG2	2.54	0.42
1:B:242:GLN:NE2	1:B:244:LYS:HB2	2.30	0.42
2:J:765:TYR:CE1	2:J:767:GLY:HA2	2.54	0.42
1:A:64:VAL:HG22	1:A:81:PHE:HD1	1.83	0.42
2:Z:827:LEU:HD12	2:Z:827:LEU:H	1.85	0.42
2:Z:905:ILE:HD12	2:F:896:LEU:HD11	2.02	0.42
2:F:997:ILE:O	2:F:998:VAL:HB	2.20	0.42
2:F:1025:THR:O	2:F:1032:ARG:NH2	2.51	0.42
2:J:886:ASP:HB2	2:J:891:LYS:HZ2	1.85	0.42
2:J:983:THR:HG23	2:F:989:ARG:HG2	2.02	0.42
2:J:1061:VAL:HB	2:J:1069:TYR:HB3	2.02	0.42
1:B:51:TRP:CZ2	1:B:53:GLU:HG3	2.54	0.42
2:Z:927:ASP:OD1	2:F:922:GLN:HG2	2.20	0.42
2:J:922:GLN:HA	2:F:927:ASP:O	2.19	0.42
1:A:106:PHE:HA	1:A:123:SER:HB3	2.02	0.41
1:A:242:GLN:HE21	1:A:244:LYS:HB2	1.85	0.41
2:J:819:LYS:HB2	2:F:913:THR:HA	2.02	0.41
2:J:820:GLY:O	2:J:824:GLU:HG2	2.19	0.41
2:J:930:LEU:HD12	2:J:930:LEU:HA	1.93	0.41
2:F:845:LEU:HD23	2:F:867:ILE:HG12	2.01	0.41
2:Z:1080:PHE:HE1	2:Z:1082:ARG:HE	1.68	0.41
2:J:969:ASN:O	2:F:974:SER:HB2	2.20	0.41
1:C:171:VAL:HG21	1:C:245:GLY:O	2.20	0.41
1:C:273:LEU:HB2	1:C:291:MET:HE2	2.02	0.41
2:F:1035:VAL:HG22	2:F:1120:MET:HB2	2.01	0.41
1:A:360:ARG:HD3	1:A:360:ARG:HA	1.27	0.41
2:Z:995:GLY:HA2	2:Z:1030:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:TRP:CG	1:B:353:ALA:HB1	2.56	0.41
1:A:258:LYS:HB3	1:A:258:LYS:HE3	1.92	0.41
2:Z:830:GLU:O	2:Z:834:LYS:HD3	2.21	0.41
2:Z:871:LYS:O	2:Z:874:LYS:HG2	2.20	0.41
2:F:766:LEU:HD22	2:F:787:PHE:HE2	1.86	0.41
1:B:383:ASP:OD1	1:B:385:LYS:HB2	2.20	0.41
1:C:51:TRP:HB3	1:C:58:PHE:HB2	2.03	0.41
2:Z:947:PHE:HA	2:Z:956:THR:O	2.21	0.41
1:B:341:ASN:OD1	1:B:341:ASN:N	2.54	0.41
1:B:373:ASP:HA	1:B:407:ASP:HA	2.02	0.41
1:C:237:ASP:O	1:C:240:THR:OG1	2.32	0.41
1:C:300:ASP:O	1:C:335:ARG:HB3	2.21	0.41
1:B:151:GLY:HA3	1:B:250:SER:HB2	2.03	0.41
2:J:1015:TRP:CE2	2:J:1110:PRO:HG2	2.56	0.41
1:B:93:GLU:H	1:B:93:GLU:CD	2.17	0.40
2:J:746:PHE:CD1	2:J:789:ILE:HG22	2.56	0.40
2:J:906:ASP:O	2:J:911:ASN:HB3	2.22	0.40
1:B:82:ARG:NH2	1:C:73:ASP:OD2	2.39	0.40
1:B:224:LEU:HB2	1:B:278:ILE:HD12	2.03	0.40
2:Z:893:SER:OG	2:J:900:ASN:OD1	2.37	0.40
1:B:118:TYR:O	1:B:244:LYS:HG2	2.21	0.40
1:B:259:PHE:CE2	1:B:385:LYS:HE2	2.56	0.40
2:Z:751:LYS:HE2	2:Z:751:LYS:HB2	1.87	0.40
2:J:742:VAL:HG12	2:J:793:ASN:HB3	2.02	0.40
2:J:927:ASP:OD2	2:J:927:ASP:C	2.60	0.40
2:J:928:VAL:HG11	2:F:930:LEU:HD11	2.03	0.40
2:Z:821:LYS:HA	2:Z:821:LYS:HD3	1.84	0.40
2:Z:973:LEU:O	2:J:978:ILE:HA	2.22	0.40
2:J:1045:LYS:HB3	2:J:1045:LYS:HE2	1.91	0.40

There are no symmetry-related clashes.

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	420/422 (100%)	406 (97%)	12 (3%)	2 (0%)	29	66
1	B	420/422 (100%)	400 (95%)	18 (4%)	2 (0%)	29	66
1	C	420/422 (100%)	408 (97%)	10 (2%)	2 (0%)	29	66
2	F	418/420 (100%)	402 (96%)	12 (3%)	4 (1%)	15	50
2	J	418/420 (100%)	403 (96%)	12 (3%)	3 (1%)	22	58
2	Z	418/420 (100%)	397 (95%)	18 (4%)	3 (1%)	22	58
All	All	2514/2526 (100%)	2416 (96%)	82 (3%)	16 (1%)	29	61

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ARG
1	A	361	PRO
1	B	360	ARG
1	B	361	PRO
1	C	360	ARG
1	C	361	PRO
2	Z	944	PRO
2	J	944	PRO
2	F	944	PRO
2	Z	1124	LYS
2	J	1124	LYS
2	F	837	LEU
2	F	1124	LYS
2	J	837	LEU
2	F	998	VAL
2	Z	837	LEU

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	342/342 (100%)	322 (94%)	20 (6%)	20	53
1	B	342/342 (100%)	309 (90%)	33 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	342/342 (100%)	312 (91%)	30 (9%)	10	34
2	F	349/349 (100%)	315 (90%)	34 (10%)	8	29
2	J	349/349 (100%)	318 (91%)	31 (9%)	9	33
2	Z	349/349 (100%)	316 (90%)	33 (10%)	8	30
All	All	2073/2073 (100%)	1892 (91%)	181 (9%)	14	35

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ARG
1	A	36	ASN
1	A	39	GLU
1	A	55	ASP
1	A	56	LYS
1	A	89	LYS
1	A	205	VAL
1	A	209	SER
1	A	210	LYS
1	A	247	SER
1	A	269	MET
1	A	280	MET
1	A	307	THR
1	A	315	LYS
1	A	329	ASP
1	A	346	THR
1	A	356	SER
1	A	360	ARG
1	A	381	ASN
1	A	417	MET
1	B	25	THR
1	B	39	GLU
1	B	40	THR
1	B	109	ARG
1	B	114	MET
1	B	121	ASP
1	B	140	SER
1	B	146	SER
1	B	147	SER
1	B	154	SER
1	B	157	SER
1	B	160	ILE

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Mol	Chain	Res	Type
1	B	174	VAL
1	B	197	ASN
1	B	205	VAL
1	B	209	SER
1	B	210	LYS
1	B	214	LEU
1	B	216	THR
1	B	222	SER
1	B	229	LYS
1	B	236	THR
1	B	285	ASP
1	B	300	ASP
1	B	313	MET
1	B	318	PRO
1	B	335	ARG
1	B	339	LYS
1	B	360	ARG
1	B	364	ARG
1	B	373	ASP
1	B	402	SER
1	B	417	MET
1	C	37	GLU
1	C	55	ASP
1	C	89	LYS
1	C	95	LEU
1	C	99	THR
1	C	123	SER
1	C	138	LYS
1	C	153	SER
1	C	166	GLU
1	C	171	VAL
1	C	173	ASP
1	C	195	ARG
1	C	205	VAL
1	C	209	SER
1	C	210	LYS
1	C	216	THR
1	C	220	THR
1	C	221	GLN
1	C	247	SER
1	C	258	LYS
1	C	262	ASN

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Mol	Chain	Res	Type
1	C	279	SER
1	C	300	ASP
1	C	303	THR
1	C	307	THR
1	C	313	MET
1	C	317	THR
1	C	346	THR
1	C	360	ARG
1	C	417	MET
2	Z	718	SER
2	Z	734	HIS
2	Z	751	LYS
2	Z	762	SER
2	Z	797	LYS
2	Z	800	PHE
2	Z	804	VAL
2	Z	829	LYS
2	Z	844	ARG
2	Z	845	LEU
2	Z	851	GLU
2	Z	852	TRP
2	Z	853	LYS
2	Z	862	MET
2	Z	868	GLU
2	Z	892	LEU
2	Z	901	ARG
2	Z	944	PRO
2	Z	982	CYS
2	Z	989	ARG
2	Z	992	LYS
2	Z	1009	ARG
2	Z	1021	THR
2	Z	1025	THR
2	Z	1030	PHE
2	Z	1049	SER
2	Z	1052	THR
2	Z	1077	VAL
2	Z	1100	THR
2	Z	1102	THR
2	Z	1103	ARG
2	Z	1105	SER
2	Z	1117	VAL

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Mol	Chain	Res	Type
2	J	728	GLN
2	J	772	TRP
2	J	797	LYS
2	J	800	PHE
2	J	804	VAL
2	J	824	GLU
2	J	846	GLU
2	J	852	TRP
2	J	854	ASP
2	J	862	MET
2	J	867	ILE
2	J	870	THR
2	J	884	MET
2	J	887	THR
2	J	892	LEU
2	J	944	PRO
2	J	948	SER
2	J	952	ASP
2	J	989	ARG
2	J	998	VAL
2	J	1009	ARG
2	J	1012	SER
2	J	1019	THR
2	J	1023	THR
2	J	1025	THR
2	J	1042	ARG
2	J	1051	ARG
2	J	1099	LEU
2	J	1103	ARG
2	J	1117	VAL
2	J	1121	VAL
2	F	751	LYS
2	F	776	SER
2	F	784	ASP
2	F	806	ARG
2	F	810	ASP
2	F	840	ASP
2	F	844	ARG
2	F	846	GLU
2	F	851	GLU
2	F	852	TRP
2	F	880	ILE

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Mol	Chain	Res	Type
2	F	889	GLU
2	F	892	LEU
2	F	901	ARG
2	F	928	VAL
2	F	939	THR
2	F	940	SER
2	F	944	PRO
2	F	955	LEU
2	F	981	ASN
2	F	987	THR
2	F	989	ARG
2	F	1009	ARG
2	F	1011	SER
2	F	1025	THR
2	F	1035	VAL
2	F	1040	THR
2	F	1052	THR
2	F	1099	LEU
2	F	1100	THR
2	F	1103	ARG
2	F	1107	ASP
2	F	1123	LYS
2	F	1127	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	GLN
1	A	340	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

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-38245. 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 ⓘ
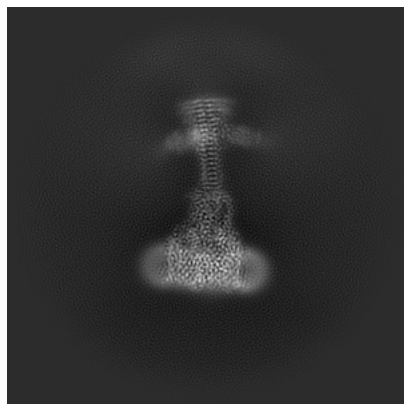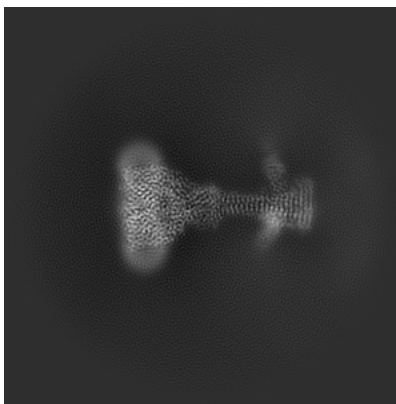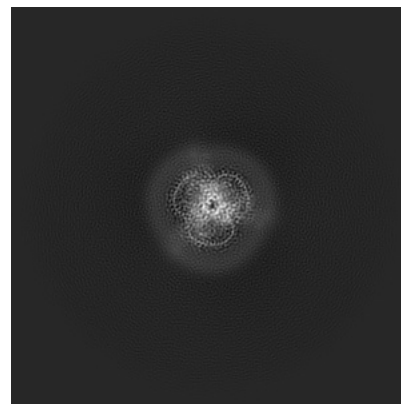
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

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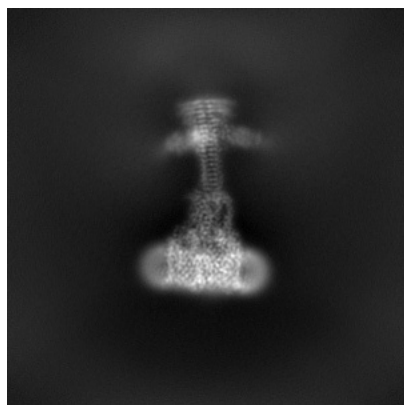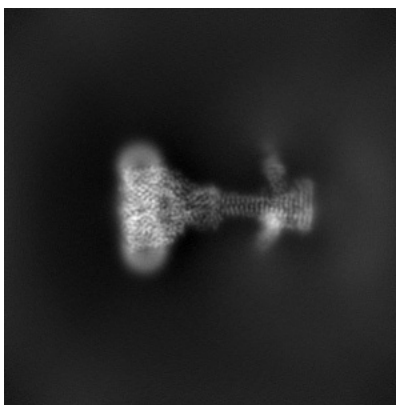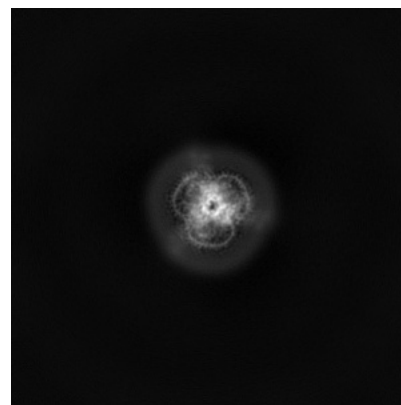
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
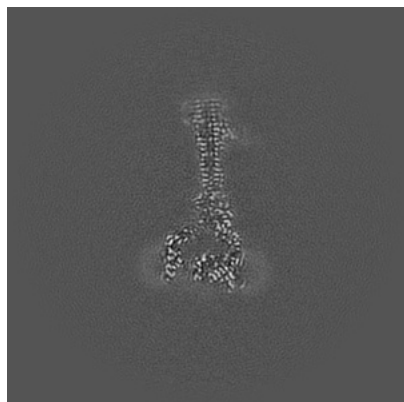
6.2.1 Primary map
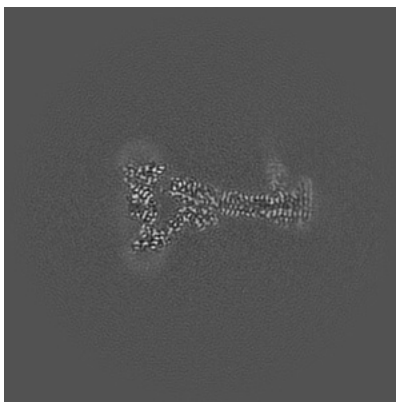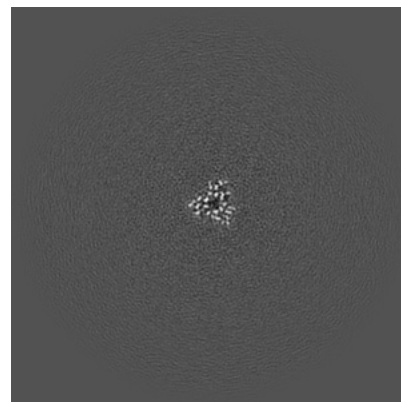
X Index: 180	Y Index: 180	Z Index: 180

6.2.2 Raw map
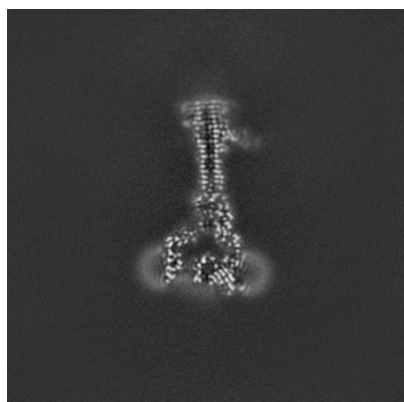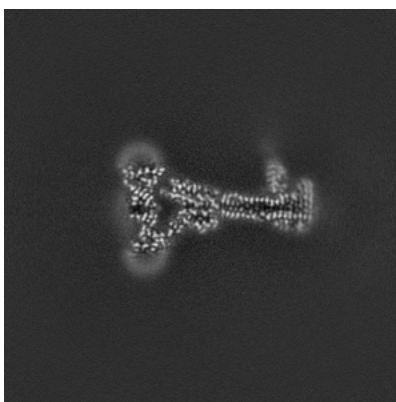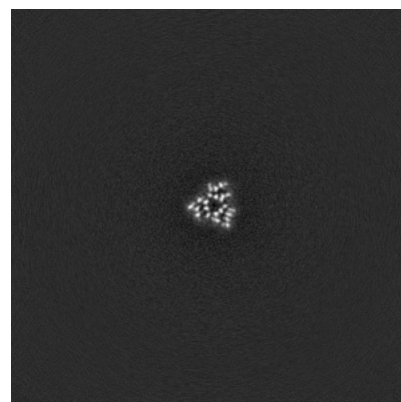
X Index: 180	Y Index: 180	Z Index: 180

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

6.3　Largest variance slices ⓘ

6.3.1　Primary map
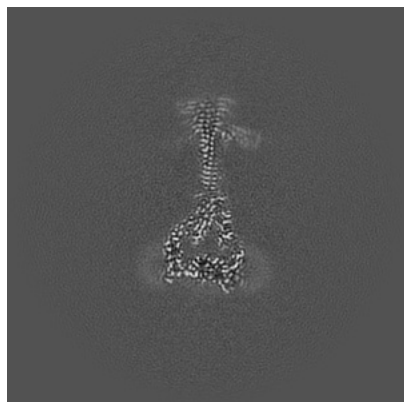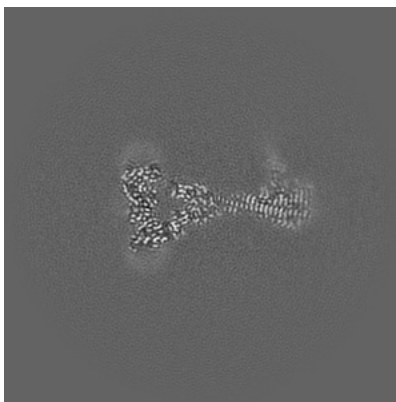
| X Index: 175 | Y Index: 175 | Z Index: 130 |
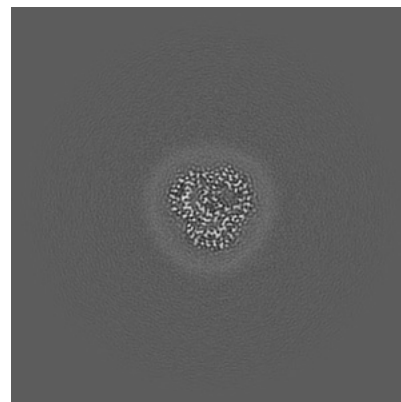
6.3.2　Raw map
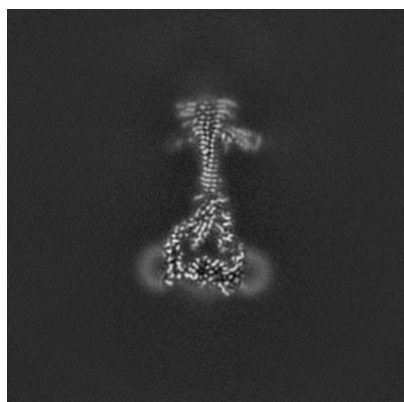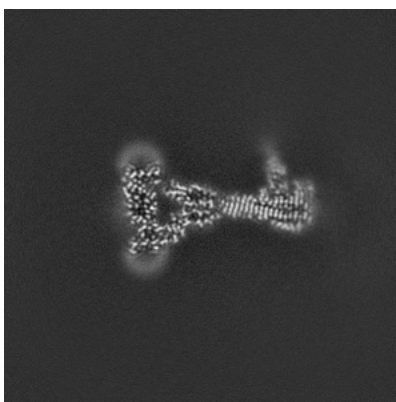
| X Index: 175 | Y Index: 176 | Z Index: 115 |
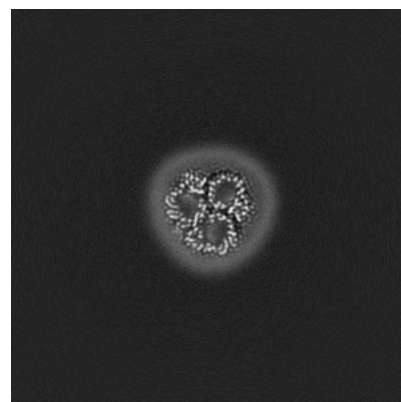
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map
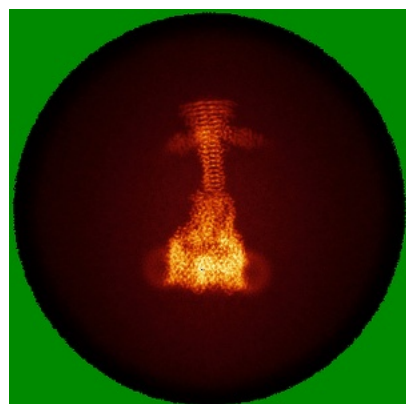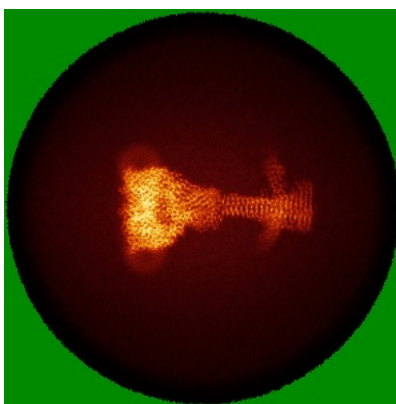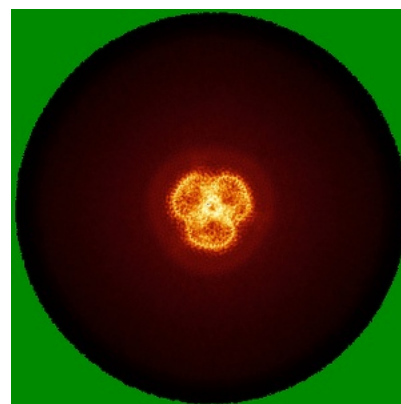
X   Y   Z

6.4.2 Raw map

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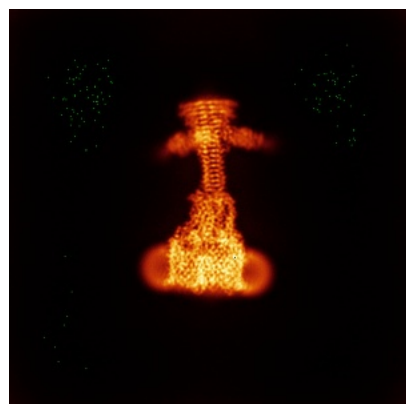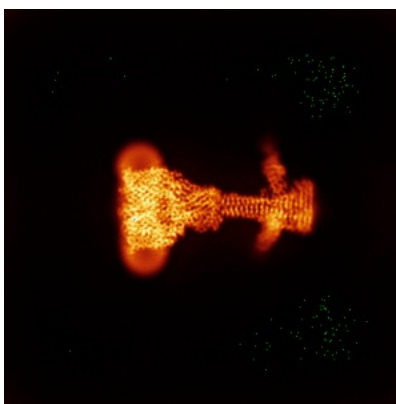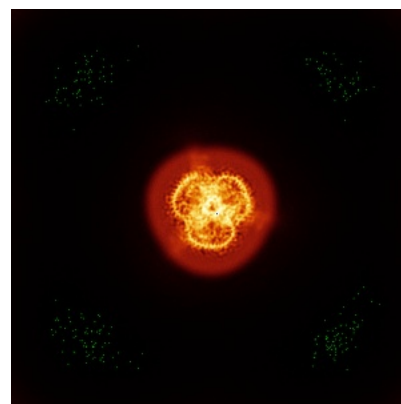
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

X	Y	Z
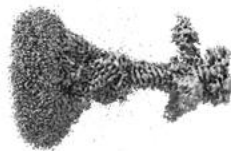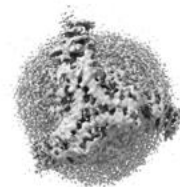
The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map
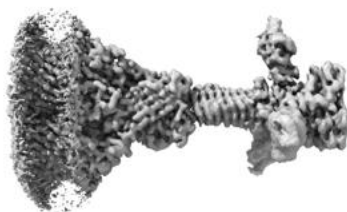
X	Y	Z

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 ⓘ

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

7 Map analysis ⓘ

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

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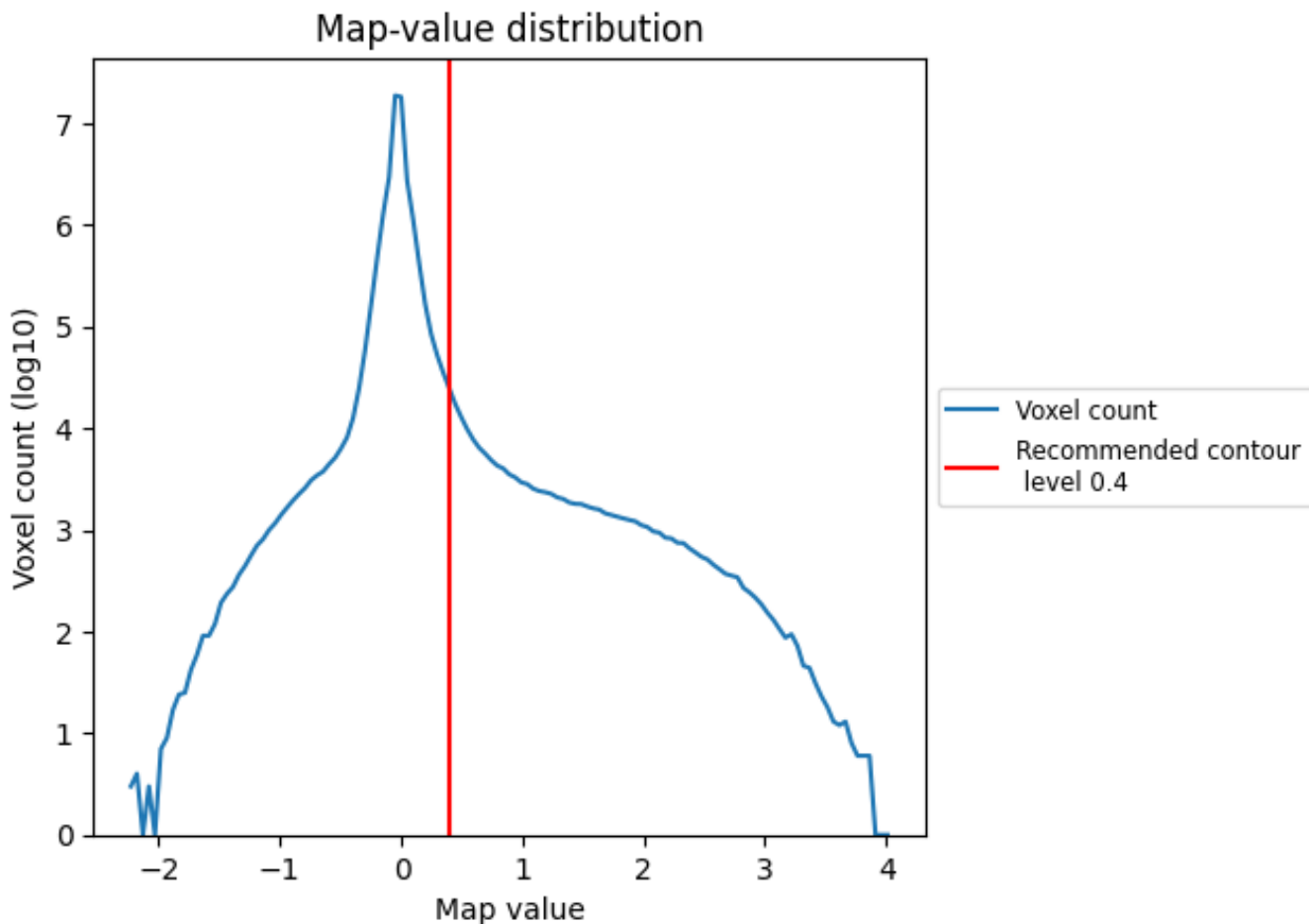
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate ⓘ
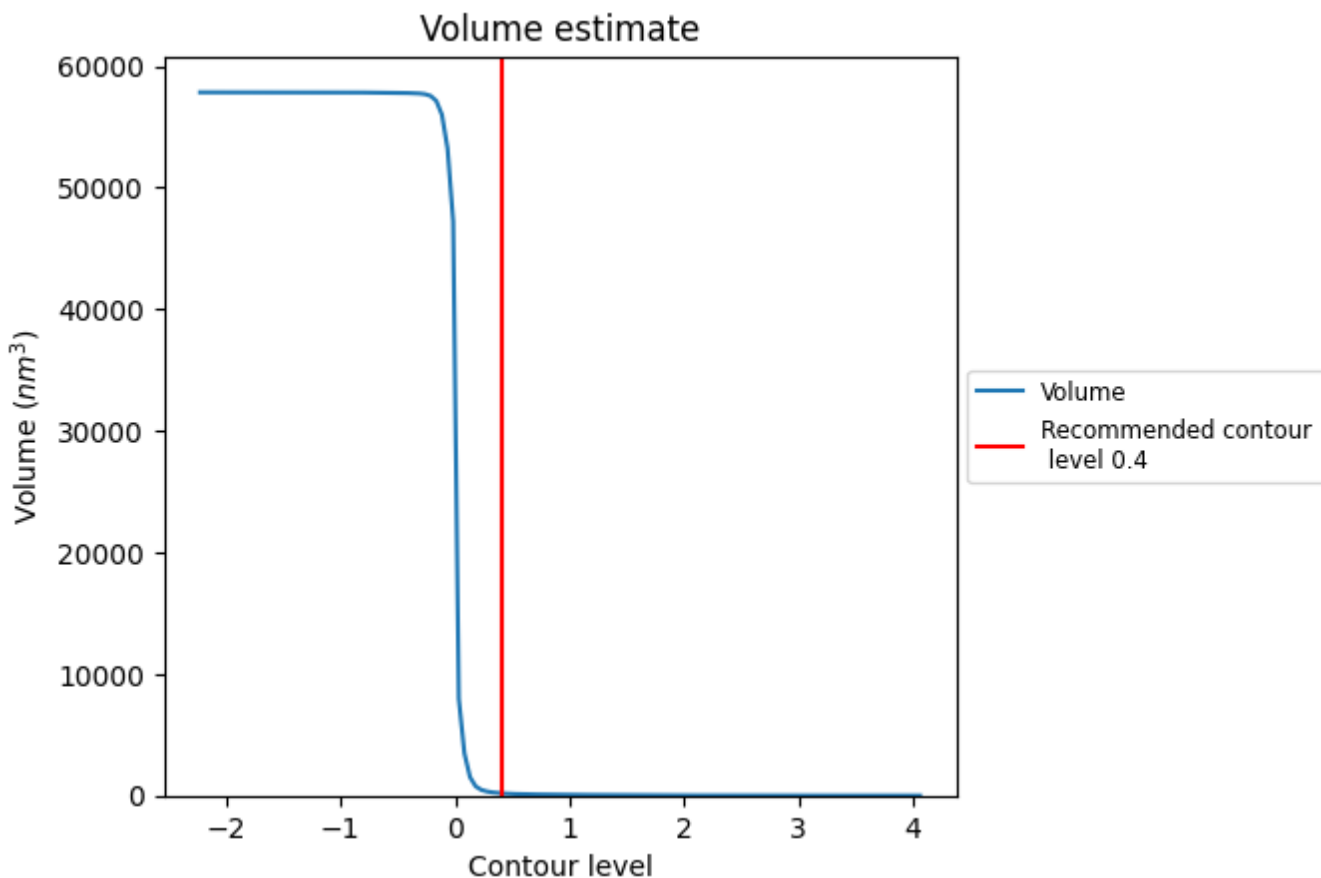
The volume at the recommended contour level is 192 nm^3; this corresponds to an approximate mass of 173 kDa.

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　ⓘ
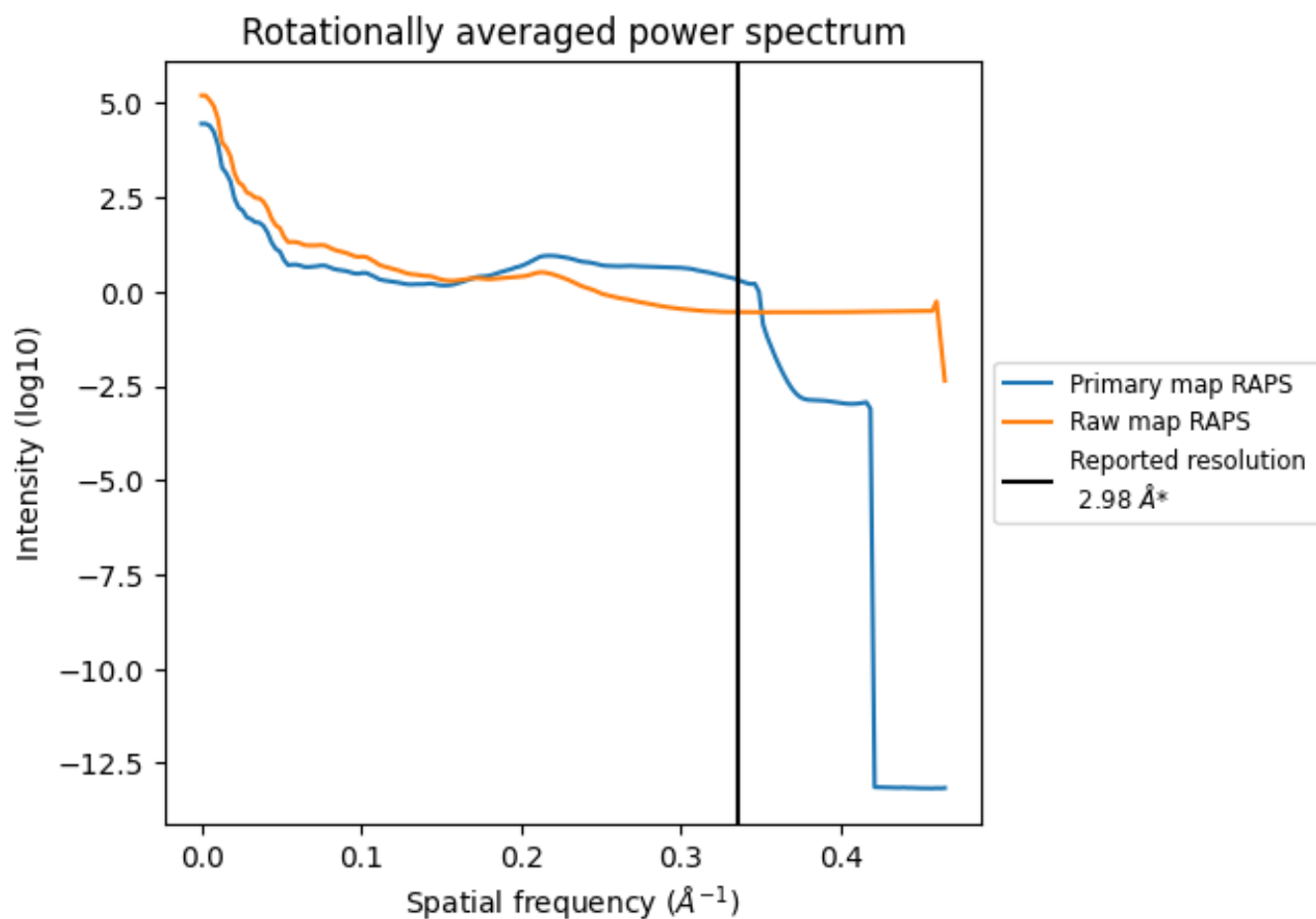
*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

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 ⓘ
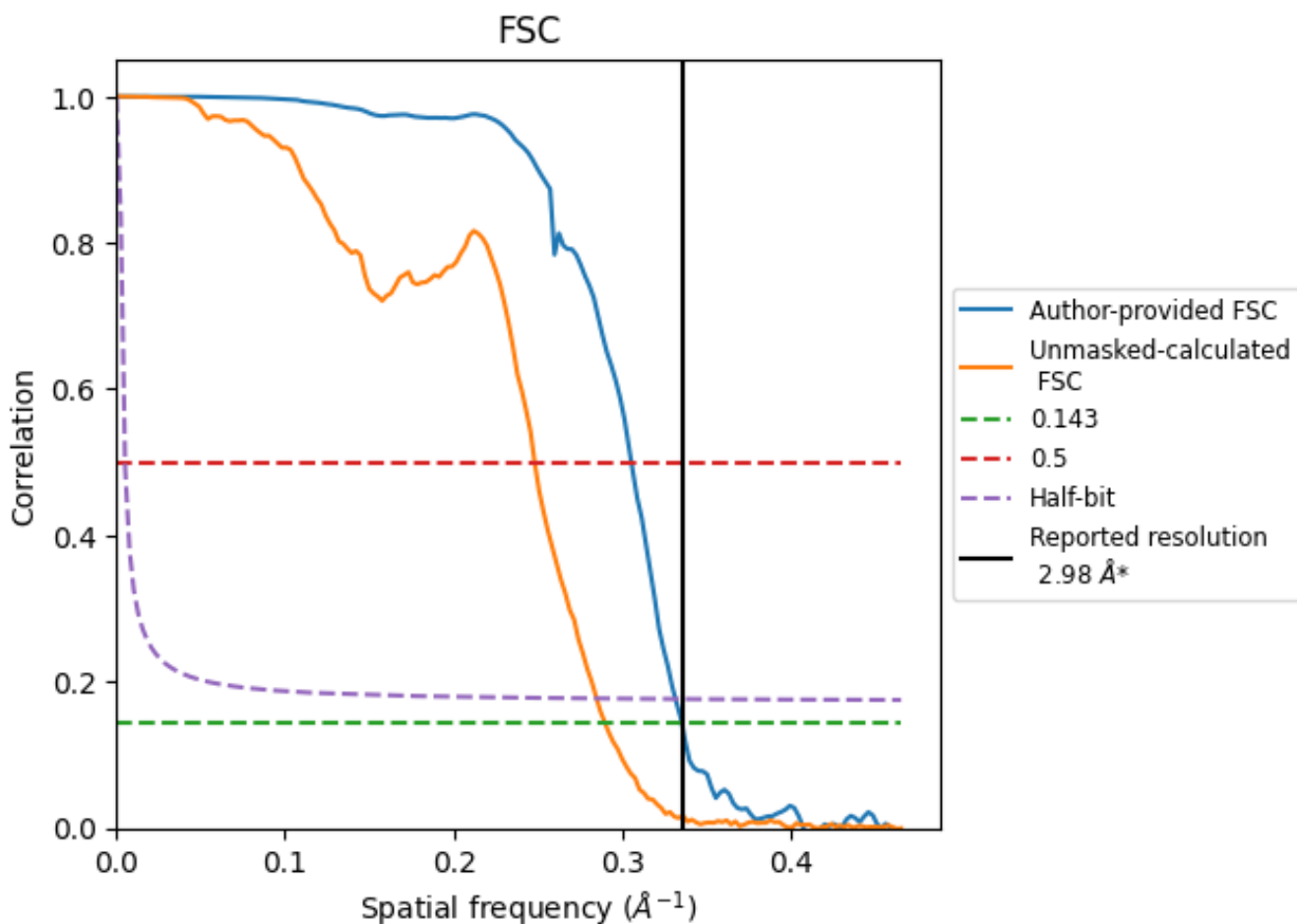
*Reported resolution corresponds to spatial frequency of 0.336 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.98	3.27	3.01
Unmasked-calculated*	3.45	4.03	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 2.98 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-38245 and PDB model 8XCJ. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay ⓘ

| X | Y | Z |
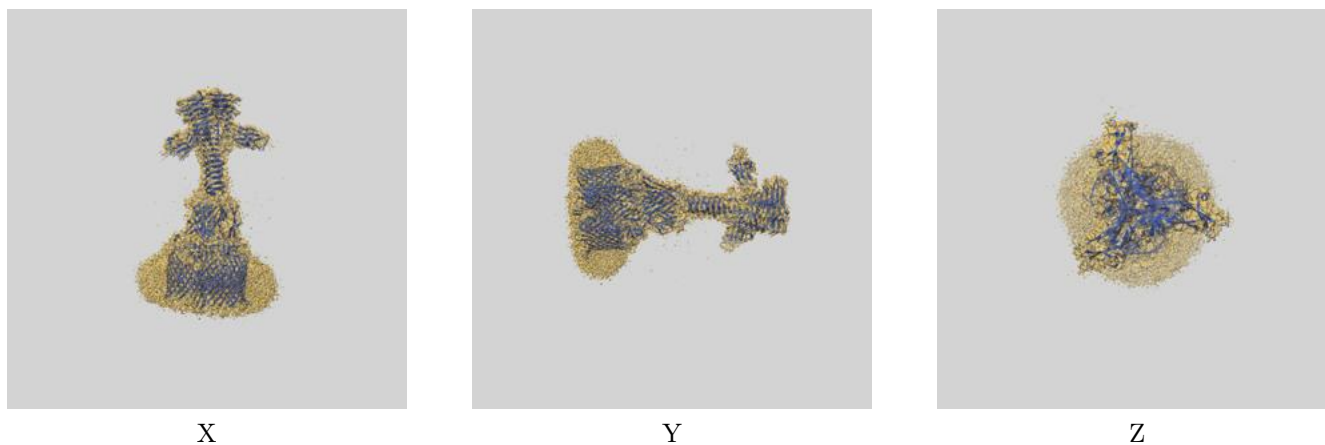
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2　Q-score mapped to coordinate model ⓘ
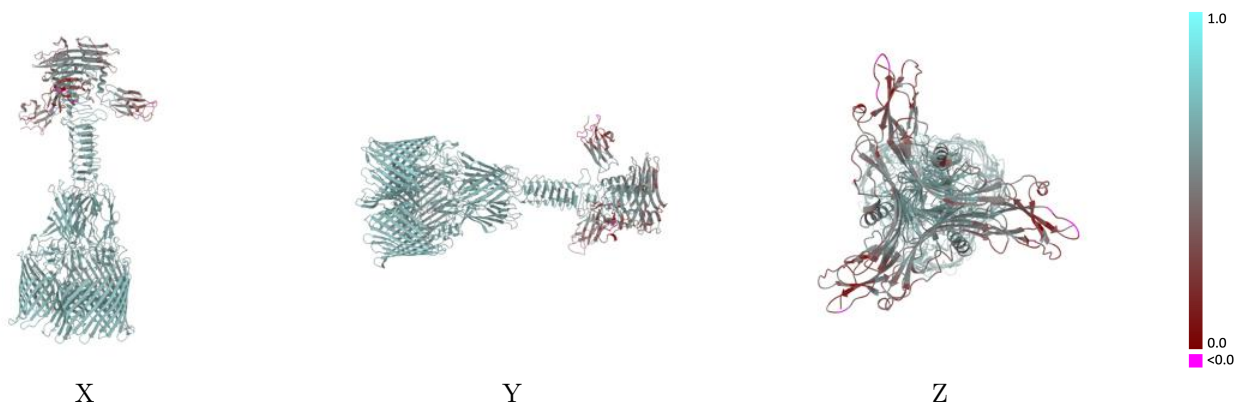
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 ⓘ
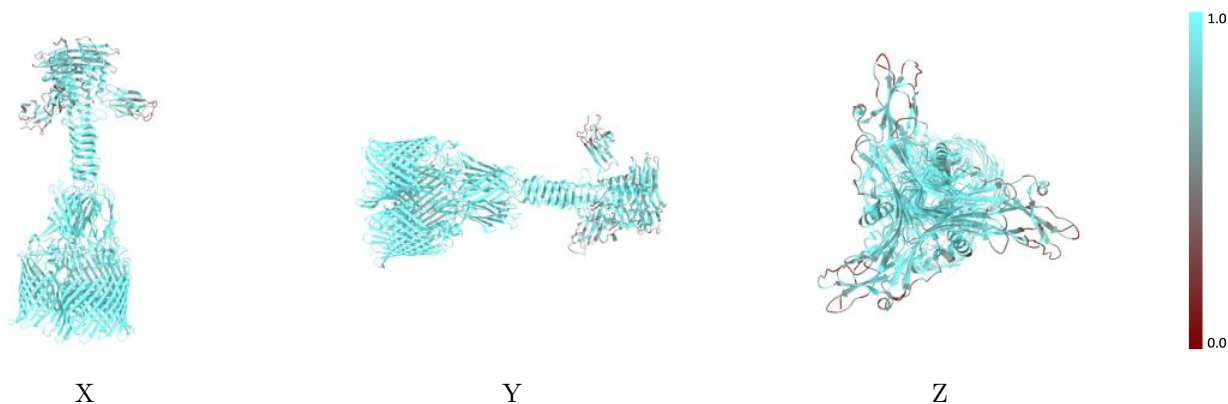
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

9.4 Atom inclusion ⓘ
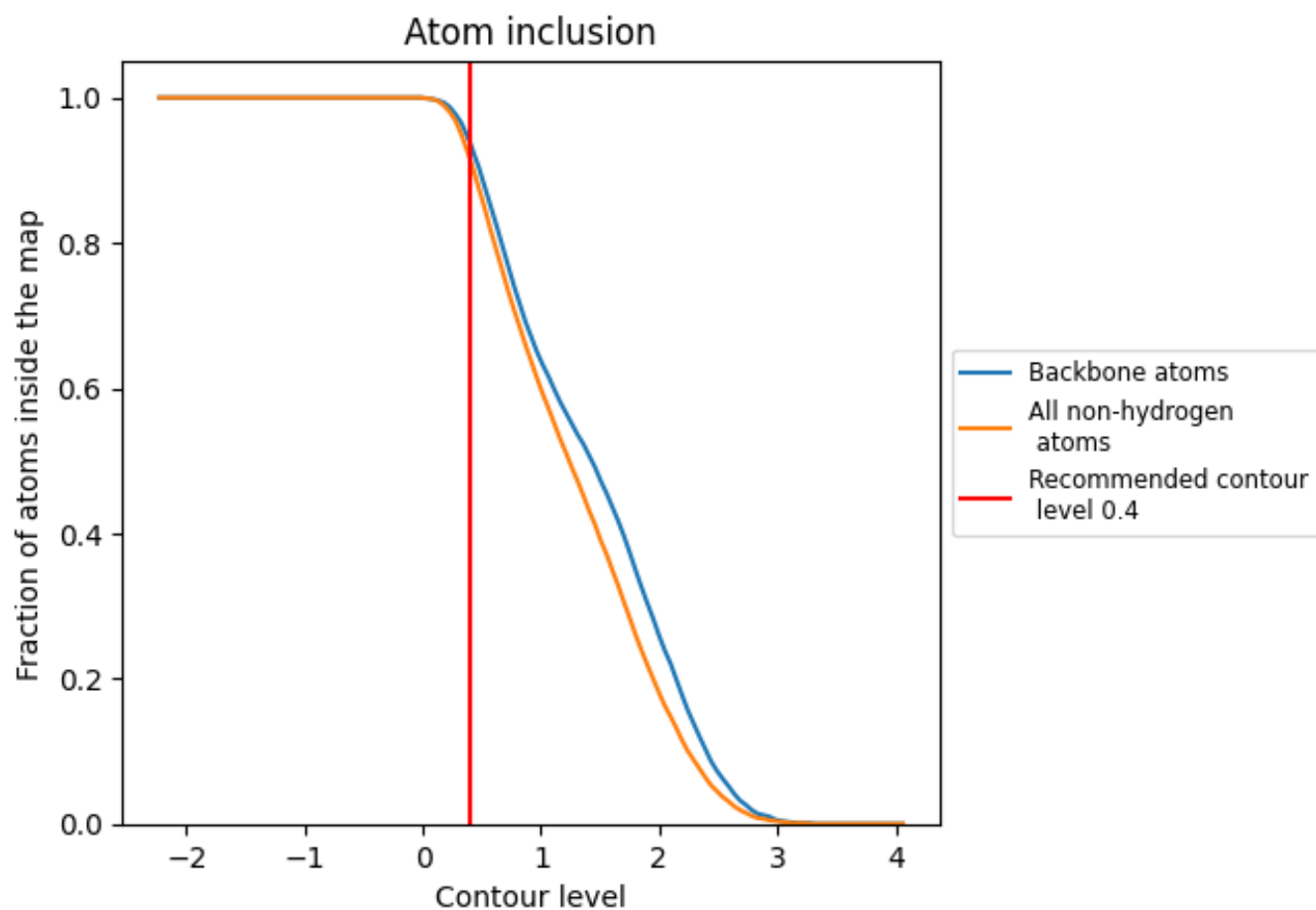
At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9150	0.5680
A	0.9820	0.6230
B	0.9820	0.6240
C	0.9800	0.6220
F	0.8470	0.5120
J	0.8530	0.5110
Z	0.8400	0.5120

1.0

0.0
<0.0