



## Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 07:28 PM JST

PDB ID : 7BVF  
EMDB ID : EMD-30218  
Title : Cryo-EM structure of Mycobacterium tuberculosis arabinosyltransferase  
EmbA-EmbB-AcpM2 in complex with ethambutol  
Authors : Zhang, L.; Zhao, Y.; Gao, Y.; Wang, Q.; Li, J.; Besra, G.S.; Rao, Z.  
Deposited on : 2020-04-10  
Resolution : 2.97 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

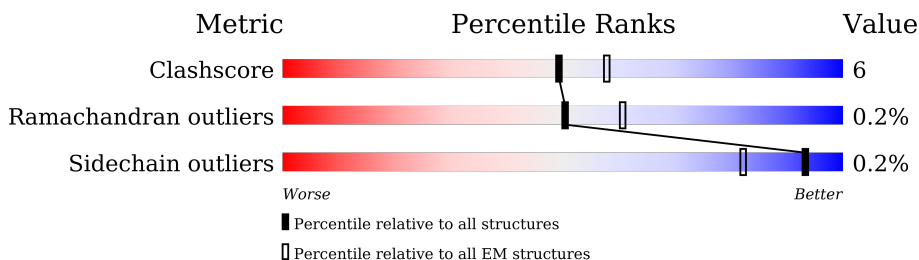
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.97 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	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  $\geq 3$ , 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  $\leq 5\%$ . 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	B	1116	 81% 13% 6%
2	A	1102	 86% 13% .
3	P	99	 63% 18% 19%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16933 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 Probable arabinosyltransferase B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	1054	7993	5189	1367	1403	34	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1099	HIS	-	expression tag	UNP P9WNL7
B	1100	LEU	-	expression tag	UNP P9WNL7
B	1101	GLY	-	expression tag	UNP P9WNL7
B	1102	GLY	-	expression tag	UNP P9WNL7
B	1103	ILE	-	expression tag	UNP P9WNL7
B	1104	LYS	-	expression tag	UNP P9WNL7
B	1105	ALA	-	expression tag	UNP P9WNL7
B	1106	PHE	-	expression tag	UNP P9WNL7
B	1107	HIS	-	expression tag	UNP P9WNL7
B	1108	HIS	-	expression tag	UNP P9WNL7
B	1109	HIS	-	expression tag	UNP P9WNL7
B	1110	HIS	-	expression tag	UNP P9WNL7
B	1111	HIS	-	expression tag	UNP P9WNL7
B	1112	HIS	-	expression tag	UNP P9WNL7
B	1113	HIS	-	expression tag	UNP P9WNL7
B	1114	HIS	-	expression tag	UNP P9WNL7
B	1115	HIS	-	expression tag	UNP P9WNL7
B	1116	HIS	-	expression tag	UNP P9WNL7

- Molecule 2 is a protein called Probable arabinosyltransferase A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	1087	8128	5254	1416	1438	20	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P9WNL9
A	-6	TYR	-	expression tag	UNP P9WNL9
A	-5	LYS	-	expression tag	UNP P9WNL9
A	-4	ASP	-	expression tag	UNP P9WNL9
A	-3	ASP	-	expression tag	UNP P9WNL9
A	-2	ASP	-	expression tag	UNP P9WNL9
A	-1	ASP	-	expression tag	UNP P9WNL9
A	0	LYS	-	expression tag	UNP P9WNL9
A	1	VAL	-	expression tag	UNP P9WNL9

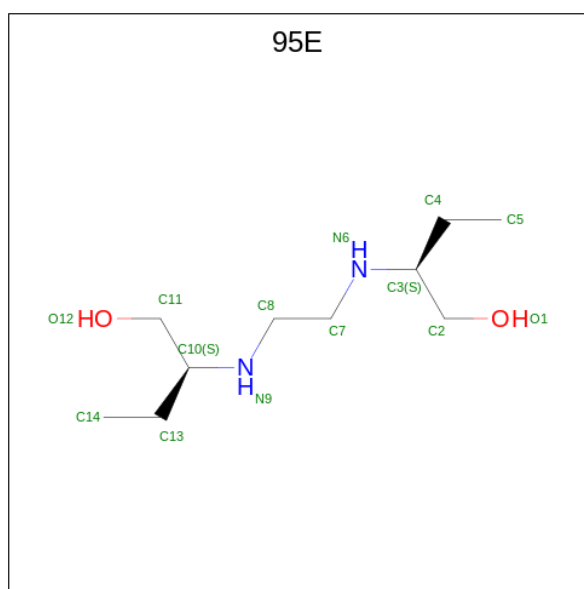
- Molecule 3 is a protein called Meromycolate extension acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	80	Total	C	N	O	S	0	0
			607	382	90	134	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

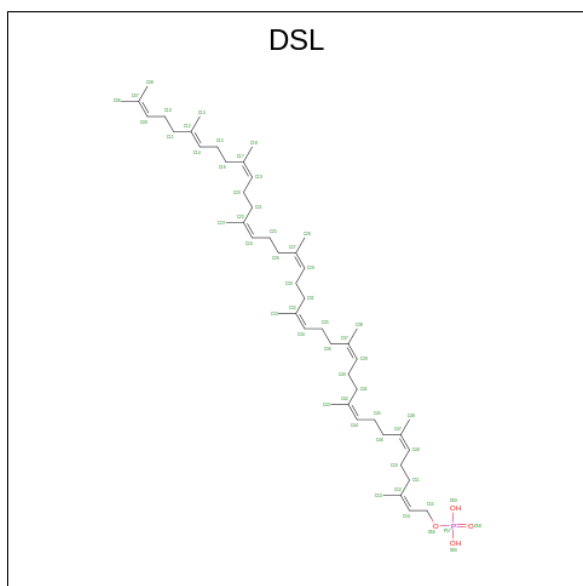
Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Ca	0
			1	1	

- Molecule 5 is Ethambutol (three-letter code: 95E) (formula:  $C_{10}H_{24}N_2O_2$ ) (labeled as "Ligand of Interest" by depositor).



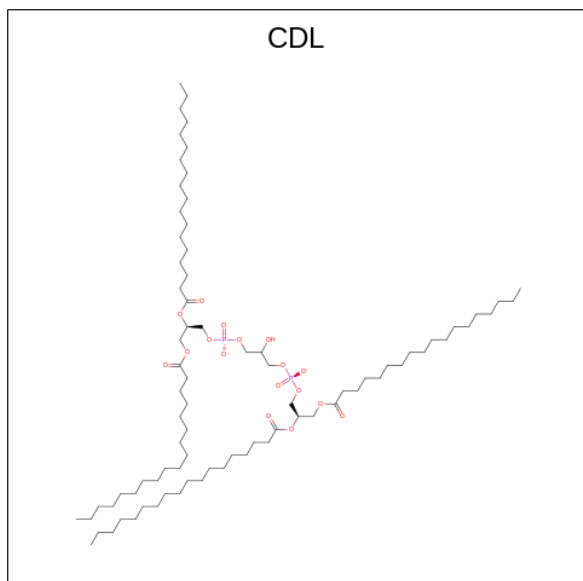
Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			14	10	2	2	

- Molecule 6 is MONO-TRANS, OCTA-CIS DECAPRENYL-PHOSPHATE (three-letter code: DSL) (formula:  $C_{50}H_{83}O_4P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	O	P	0
			46	41	4	1	

- Molecule 7 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ) (labeled as "Ligand of Interest" by depositor).

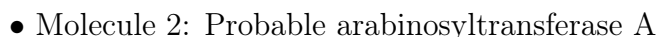


Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	O	P	0
			66	47	17	2	
7	A	1	Total	C	O	P	0
			78	59	17	2	



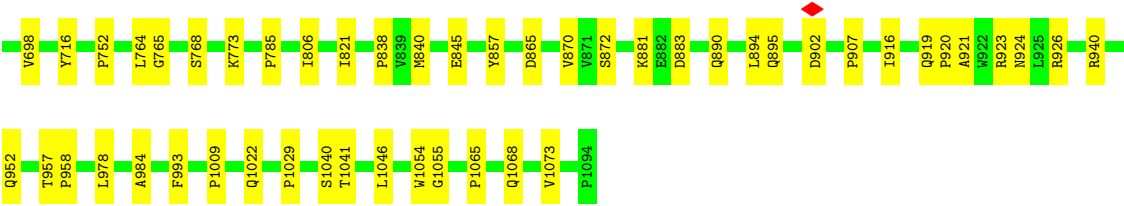
- Molecule 1: Probable arabinosyltransferase B

Response	Percentage
Yes, it is a crisis	81%
No, it is not a crisis	13%
I don't know	6%



86% 13%





● Molecule 3: Meromycolate extension acyl carrier protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	521803	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50, 50, 50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.011	Depositor
Minimum map value	-1.808	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.069	Depositor
Recommended contour level	0.25	Depositor
Map size ( $\text{\AA}$ )	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.82, 0.82, 0.82	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DSL, CDL, 95E

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	B	0.33	1/8219 (0.0%)	0.52	3/11270 (0.0%)
2	A	0.33	1/8340 (0.0%)	0.52	1/11428 (0.0%)
3	P	0.26	0/612	0.47	0/832
All	All	0.33	2/17171 (0.0%)	0.52	4/23530 (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	B	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	43	ILE	C-O	-5.78	1.12	1.23
1	B	731	PRO	C-O	-5.68	1.11	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	PRO	N-CA-C	7.76	132.28	112.10
2	A	49	SER	N-CA-CB	6.12	119.68	110.50
1	B	59	PRO	N-CA-CB	-5.70	96.33	102.60
1	B	60	GLN	N-CA-CB	5.69	120.85	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	328	ASP	Peptide
1	B	58	TRP	Peptide
1	B	730	TYR	Peptide

## 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	B	7993	0	8110	92	0
2	A	8128	0	8294	89	0
3	P	607	0	600	10	0
4	B	1	0	0	0	0
5	B	14	0	0	1	0
6	B	46	0	64	15	0
7	A	78	0	103	3	0
7	B	66	0	79	9	0
All	All	16933	0	17250	210	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 6.

All (210) 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)
6:B:1403:DSL:H49	6:B:1403:DSL:H431	1.42	1.00
1:B:506:THR:HG23	6:B:1403:DSL:H412	1.45	0.98
6:B:1403:DSL:H49	6:B:1403:DSL:C43	1.97	0.93
1:B:728:ARG:O	1:B:729:GLN:CB	2.26	0.82
6:B:1403:DSL:H431	6:B:1403:DSL:C49	2.09	0.82
2:A:105:LEU:HD12	2:A:117:ALA:O	1.84	0.78
1:B:728:ARG:O	1:B:729:GLN:HB2	1.82	0.78
2:A:872:SER:O	2:A:957:THR:HG22	1.84	0.77
2:A:376:ASN:HB3	2:A:383:PRO:HG3	1.68	0.76
2:A:890:GLN:HE21	2:A:952:GLN:HE21	1.34	0.74
1:B:662:LYS:HA	1:B:667:THR:HA	1.69	0.73
2:A:872:SER:HB2	2:A:957:THR:HG21	1.70	0.73
1:B:128:ARG:NH2	1:B:182:ARG:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:ILE:HD11	1:B:455:LEU:HD23	1.72	0.72
2:A:119:ARG:NH2	2:A:167:LYS:O	2.21	0.72
2:A:821:ILE:HD11	2:A:838:PRO:HD3	1.73	0.71
2:A:295:ARG:HH11	2:A:490:GLY:HA2	1.58	0.68
2:A:537:ARG:C	2:A:538:ARG:HG2	2.13	0.68
1:B:180:ASN:ND2	1:B:1097:GLY:O	2.27	0.67
2:A:957:THR:OG1	2:A:958:PRO:HD2	1.94	0.67
1:B:85:CYS:SG	1:B:89:ARG:NH2	2.68	0.66
1:B:592:TRP:CD1	6:B:1403:DSL:O60	2.50	0.64
1:B:80:THR:HG23	1:B:151:THR:HG22	1.80	0.64
1:B:174:SER:OG	1:B:175:GLY:N	2.29	0.64
2:A:566:THR:O	2:A:569:LYS:NZ	2.31	0.64
1:B:166:ASP:N	1:B:170:ALA:O	2.29	0.63
3:P:32:SER:HA	3:P:69:THR:HA	1.81	0.63
1:B:60:GLN:HA	1:B:60:GLN:OE1	1.99	0.62
2:A:469:VAL:O	2:A:472:ARG:NH1	2.33	0.62
7:B:1404:CDL:OB7	7:B:1404:CDL:HB32	2.00	0.61
2:A:364:ALA:HB2	2:A:586:ALA:HB2	1.83	0.61
3:P:29:PRO:HA	3:P:70:VAL:HG13	1.83	0.61
2:A:507:VAL:HG22	2:A:508:GLU:H	1.65	0.60
2:A:81:THR:HG21	2:A:179:VAL:HG11	1.84	0.59
1:B:973:SER:HB3	1:B:976:GLU:HG3	1.84	0.59
1:B:522:ASN:ND2	2:A:506:THR:O	2.36	0.59
1:B:522:ASN:ND2	2:A:506:THR:OG1	2.36	0.58
1:B:420:GLU:OE1	1:B:573:ARG:NH1	2.32	0.58
3:P:4:THR:HB	3:P:78:GLN:HE22	1.67	0.58
1:B:164:LEU:HB2	1:B:172:LEU:HD12	1.86	0.58
2:A:359:VAL:HG11	2:A:688:THR:HG22	1.86	0.58
2:A:890:GLN:NE2	2:A:952:GLN:HE21	2.01	0.57
6:B:1403:DSL:H283	6:B:1403:DSL:C24	2.34	0.57
2:A:254:ASP:OD1	2:A:336:TRP:NE1	2.35	0.57
1:B:956:THR:HG22	1:B:958:GLU:H	1.69	0.57
2:A:919:GLN:HB3	2:A:920:PRO:HD3	1.87	0.56
1:B:111:LEU:HD12	1:B:112:GLN:H	1.70	0.56
7:B:1404:CDL:OA7	7:B:1404:CDL:HA61	2.05	0.56
1:B:322:TRP:HZ2	1:B:513:GLY:HA3	1.70	0.55
1:B:117:VAL:HG23	1:B:124:ASP:OD1	2.07	0.55
2:A:269:ALA:H	2:A:377:ASN:HD22	1.54	0.55
3:P:28:THR:H	3:P:31:LYS:HE3	1.72	0.55
1:B:347:SER:O	1:B:351:ARG:NH2	2.39	0.55
1:B:860:SER:OG	1:B:861:ALA:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:LEU:HD11	2:A:89:VAL:HG22	1.88	0.55
1:B:97:VAL:HG22	1:B:117:VAL:HG12	1.88	0.54
6:B:1403:DSL:C24	6:B:1403:DSL:C28	2.86	0.54
3:P:4:THR:HA	3:P:8:ILE:HG13	1.88	0.54
1:B:730:TYR:C	1:B:730:TYR:CD2	2.81	0.54
1:B:45:PRO:HB3	1:B:494:PHE:CG	2.43	0.54
2:A:537:ARG:O	2:A:538:ARG:CG	2.56	0.53
2:A:785:PRO:HG3	2:A:806:ILE:HD11	1.89	0.53
1:B:512:ILE:HD11	1:B:1096:ILE:HB	1.90	0.52
1:B:844:LEU:HD11	1:B:929:TRP:HH2	1.74	0.52
1:B:867:LYS:HG3	1:B:868:PRO:HD2	1.91	0.52
2:A:921:ALA:O	2:A:923:ARG:NH1	2.43	0.52
1:B:321:ARG:O	1:B:1035:GLY:N	2.39	0.52
1:B:1046:ALA:HB2	1:B:1067:PHE:CE1	2.45	0.52
7:B:1404:CDL:HA61	7:B:1404:CDL:H321	1.92	0.52
2:A:105:LEU:CD1	2:A:117:ALA:O	2.56	0.52
1:B:89:ARG:NH1	1:B:142:SER:O	2.42	0.52
1:B:480:SER:HB2	1:B:481:PRO:HD3	1.92	0.52
2:A:118:PHE:O	2:A:120:ASP:N	2.43	0.51
2:A:354:LEU:HD22	2:A:544:LEU:HD12	1.92	0.51
2:A:605:LEU:HA	2:A:608:THR:HG22	1.92	0.51
1:B:300:ASP:HB3	1:B:992:LEU:HD22	1.91	0.51
2:A:648:SER:O	2:A:652:THR:HG23	2.10	0.51
1:B:229:THR:HG21	1:B:488:VAL:HG21	1.92	0.51
1:B:933:ARG:HD2	1:B:1057:TRP:O	2.11	0.51
2:A:537:ARG:O	2:A:538:ARG:O	2.28	0.50
2:A:537:ARG:C	2:A:538:ARG:CG	2.78	0.50
1:B:318:ASN:HD22	1:B:322:TRP:HE3	1.59	0.50
1:B:373:LEU:HB2	1:B:377:VAL:HG21	1.91	0.50
7:B:1404:CDL:H321	7:B:1404:CDL:CA6	2.41	0.50
1:B:111:LEU:O	1:B:112:GLN:HG2	2.12	0.50
3:P:60:PRO:HG2	3:P:63:ASP:HB2	1.94	0.50
1:B:699:ILE:HA	1:B:702:LEU:HG	1.94	0.50
2:A:1040:SER:OG	2:A:1041:THR:N	2.45	0.49
1:B:168:SER:OG	1:B:169:GLY:N	2.44	0.49
1:B:412:SER:HA	1:B:451:ALA:HB2	1.94	0.49
2:A:50:THR:HG22	2:A:54:ASN:O	2.12	0.49
1:B:640:TRP:HE1	1:B:714:MET:HE1	1.78	0.49
1:B:295:ALA:O	1:B:400:ASN:ND2	2.37	0.49
2:A:46:PRO:HB3	2:A:55:ILE:CG2	2.42	0.49
2:A:688:THR:N	2:A:689:PRO:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:GLN:NE2	1:B:1056:ASP:OD2	2.45	0.48
2:A:598:HIS:HB2	2:A:674:THR:HG23	1.94	0.48
6:B:1403:DSL:H533	6:B:1403:DSL:H501	1.59	0.48
2:A:353:GLY:HA3	2:A:590:PHE:CE1	2.47	0.48
1:B:366:SER:OG	1:B:367:ARG:NH1	2.46	0.48
1:B:309:VAL:HG12	1:B:1001:LEU:HD23	1.95	0.48
1:B:800:GLU:OE1	1:B:835:TYR:OH	2.22	0.48
2:A:9:SER:O	2:A:9:SER:OG	2.32	0.48
2:A:110:ASN:ND2	2:A:111:GLN:O	2.47	0.48
2:A:214:VAL:HG11	2:A:465:LEU:HD22	1.96	0.48
2:A:498:ASP:N	2:A:498:ASP:OD1	2.45	0.47
2:A:916:ILE:HD13	2:A:926:ARG:HH12	1.78	0.47
2:A:1065:PRO:HD2	2:A:1068:GLN:HE21	1.79	0.47
2:A:110:ASN:O	2:A:128:ARG:NH2	2.44	0.47
2:A:211:VAL:HG12	2:A:465:LEU:HD11	1.97	0.47
2:A:894:LEU:HA	2:A:940:ARG:O	2.14	0.47
1:B:127:ASP:O	1:B:129:ASN:N	2.47	0.47
1:B:124:ASP:OD1	1:B:124:ASP:N	2.48	0.47
1:B:445:GLN:HG3	1:B:446:PRO:HD2	1.97	0.47
1:B:878:THR:O	1:B:964:THR:OG1	2.32	0.47
7:B:1404:CDL:HA31	7:B:1404:CDL:OA9	2.15	0.47
1:B:126:THR:HG22	1:B:127:ASP:H	1.80	0.47
1:B:827:ASN:ND2	1:B:844:LEU:O	2.48	0.47
2:A:107:VAL:HG13	2:A:116:VAL:HG22	1.97	0.47
1:B:109:ALA:O	1:B:113:ALA:HB3	2.15	0.47
2:A:354:LEU:HD12	2:A:354:LEU:HA	1.74	0.47
2:A:919:GLN:O	2:A:923:ARG:NH1	2.48	0.46
1:B:920:ASP:HB3	1:B:932:LEU:CD2	2.45	0.46
2:A:430:ALA:O	2:A:434:THR:HG23	2.15	0.46
1:B:320:PHE:O	1:B:1035:GLY:HA2	2.16	0.46
2:A:1046:LEU:HB2	2:A:1054:TRP:CD1	2.51	0.46
2:A:99:ASP:OD1	2:A:102:LYS:NZ	2.49	0.46
2:A:587:VAL:O	2:A:591:THR:HG23	2.16	0.46
6:B:1403:DSL:H552	6:B:1403:DSL:H511	1.57	0.46
2:A:122:VAL:HG11	2:A:125:VAL:HG23	1.98	0.46
1:B:588:THR:O	1:B:591:LYS:NZ	2.47	0.46
2:A:752:PRO:HA	2:A:857:TYR:HA	1.98	0.45
2:A:865:ASP:OD1	2:A:865:ASP:N	2.46	0.45
1:B:269:ILE:HD12	1:B:270:PRO:HD2	1.97	0.45
2:A:88:LEU:HD11	2:A:91:SER:HB2	1.97	0.45
3:P:41:SER:O	3:P:45:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:GLN:OE1	1:B:501:THR:HG21	2.17	0.45
1:B:592:TRP:NE1	6:B:1403:DSL:O60	2.50	0.45
1:B:329:PRO:HG3	1:B:502:VAL:HG13	1.98	0.45
2:A:136:CYS:SG	2:A:137:SER:N	2.90	0.45
2:A:412:ILE:O	2:A:416:THR:HG23	2.17	0.45
2:A:493:ILE:HD13	2:A:500:LEU:HD11	1.98	0.45
7:A:1101:CDL:OB7	7:A:1101:CDL:H532	2.17	0.45
2:A:537:ARG:HG2	2:A:538:ARG:HG2	1.99	0.45
2:A:1022:GLN:HB3	2:A:1029:PRO:HD2	1.97	0.45
2:A:773:LYS:NZ	2:A:845:GLU:OE2	2.42	0.45
1:B:549:CYS:HA	1:B:552:THR:HG22	1.98	0.44
2:A:768:SER:O	2:A:768:SER:OG	2.28	0.44
1:B:901:GLU:HB2	1:B:914:GLY:O	2.17	0.44
2:A:627:VAL:HG11	2:A:716:TYR:HE2	1.83	0.44
7:A:1101:CDL:H751	7:A:1101:CDL:H721	1.65	0.44
1:B:322:TRP:O	1:B:324:GLY:N	2.49	0.44
1:B:460:ARG:NH2	2:A:669:ASP:OD1	2.48	0.44
7:B:1404:CDL:CA3	7:B:1404:CDL:HA22	2.48	0.44
1:B:424:ARG:HD2	1:B:425:TYR:CZ	2.52	0.44
1:B:506:THR:HG23	6:B:1403:DSL:C41	2.31	0.44
1:B:562:ARG:CZ	1:B:568:ARG:HH21	2.31	0.44
1:B:123:VAL:HG21	1:B:140:VAL:HG21	2.00	0.44
2:A:978:LEU:HD13	2:A:993:PHE:HE1	1.82	0.44
1:B:1025:THR:O	1:B:1029:GLU:HG2	2.18	0.44
7:A:1101:CDL:OA7	7:A:1101:CDL:HA31	2.17	0.44
7:B:1404:CDL:H602	7:B:1404:CDL:H572	1.64	0.43
2:A:222:ALA:O	2:A:226:ARG:HG2	2.18	0.43
1:B:101:THR:CG2	1:B:185:ILE:HA	2.47	0.43
2:A:881:LYS:O	2:A:883:ASP:N	2.52	0.43
2:A:1073:VAL:HG12	2:A:1073:VAL:O	2.19	0.43
1:B:900:LEU:HA	1:B:947:ARG:O	2.19	0.43
1:B:1086:SER:OG	1:B:1087:GLY:N	2.51	0.43
1:B:158:PHE:HD1	1:B:175:GLY:HA2	1.84	0.43
1:B:386:ALA:HB2	1:B:708:PRO:HG3	2.00	0.43
1:B:874:LEU:HD12	1:B:933:ARG:HB2	2.00	0.43
2:A:679:ASN:OD1	2:A:680:ARG:N	2.49	0.43
2:A:872:SER:HB2	2:A:957:THR:CG2	2.44	0.43
2:A:870:VAL:HG13	2:A:924:ASN:HB3	2.01	0.43
1:B:118:VAL:HG13	1:B:123:VAL:HG22	2.00	0.43
2:A:1009:PRO:C	2:A:1055:GLY:HA2	2.39	0.43
1:B:900:LEU:HD23	1:B:900:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:275:GLY:HA3	2:A:984:ALA:HB3	2.00	0.42
1:B:208:THR:O	1:B:208:THR:OG1	2.37	0.42
2:A:78:ALA:O	2:A:81:THR:HG22	2.20	0.42
1:B:983:PRO:HB2	1:B:1010:PRO:HA	2.01	0.42
1:B:893:THR:O	1:B:893:THR:OG1	2.34	0.42
2:A:202:LEU:C	2:A:204:LYS:H	2.22	0.42
2:A:178:LYS:HB2	2:A:178:LYS:HE2	1.80	0.42
2:A:236:TRP:CD1	2:A:237:LEU:HD13	2.55	0.42
6:B:1403:DSL:H202	6:B:1403:DSL:H233	1.79	0.42
1:B:442:LEU:HD23	6:B:1403:DSL:H211	2.02	0.42
3:P:2:ALA:HA	3:P:7:GLU:HG2	2.00	0.42
1:B:299:ASP:OD2	5:B:1402:95E:C2	2.68	0.41
6:B:1403:DSL:H431	6:B:1403:DSL:H452	1.30	0.41
2:A:302:ALA:HB1	2:A:479:VAL:HG22	2.02	0.41
7:B:1404:CDL:H552	7:B:1404:CDL:H581	1.83	0.41
1:B:150:VAL:HG12	1:B:150:VAL:O	2.21	0.41
6:B:1403:DSL:H312	6:B:1403:DSL:H382	2.01	0.41
2:A:902:ASP:N	2:A:902:ASP:OD1	2.53	0.41
1:B:473:VAL:HG23	1:B:473:VAL:O	2.20	0.41
7:B:1404:CDL:CA3	7:B:1404:CDL:CA7	2.98	0.41
2:A:765:GLY:HA2	2:A:840:MET:SD	2.61	0.41
3:P:52:GLU:HG2	3:P:57:VAL:O	2.21	0.41
1:B:273:TRP:HZ2	1:B:368:GLU:OE2	2.04	0.41
2:A:764:LEU:HD22	2:A:958:PRO:HD3	2.03	0.41
1:B:642:THR:OG1	1:B:643:THR:N	2.53	0.40
1:B:896:GLN:HB2	1:B:961:ILE:HD11	2.02	0.40
2:A:321:GLY:O	2:A:325:ARG:NH1	2.54	0.40
1:B:158:PHE:CD1	1:B:175:GLY:HA2	2.56	0.40
2:A:694:ALA:O	2:A:698:VAL:HG23	2.22	0.40
1:B:470:HIS:CD2	1:B:475:THR:HB	2.56	0.40
2:A:276:TYR:HD2	2:A:277:LEU:HD12	1.86	0.40
3:P:40:ASP:OD2	3:P:40:ASP:N	2.46	0.40
2:A:895:GLN:NE2	2:A:907:PRO:HB2	2.36	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	B	1050/1116 (94%)	912 (87%)	136 (13%)	2 (0%)	47	80
2	A	1085/1102 (98%)	944 (87%)	139 (13%)	2 (0%)	47	80
3	P	78/99 (79%)	71 (91%)	7 (9%)	0	100	100
All	All	2213/2317 (96%)	1927 (87%)	282 (13%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	59	PRO
1	B	60	GLN
2	A	49	SER
2	A	538	ARG

### 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	B	836/887 (94%)	833 (100%)	3 (0%)	91	97
2	A	831/845 (98%)	831 (100%)	0	100	100
3	P	68/81 (84%)	68 (100%)	0	100	100
All	All	1735/1813 (96%)	1732 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	57	ASP
1	B	59	PRO
1	B	697	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	129	ASN
1	B	241	GLN
1	B	296	ASN
1	B	522	ASN
1	B	784	ASN
1	B	791	ASN
2	A	111	GLN
2	A	265	HIS
2	A	377	ASN
2	A	441	GLN
2	A	598	HIS
2	A	800	ASN
2	A	890	GLN
2	A	990	GLN
2	A	1004	GLN
3	P	5	GLN
3	P	78	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	DSL	B	1403	-	45,45,54	1.04	4 (8%)	54,55,66	2.35	17 (31%)
5	95E	B	1402	-	13,13,13	1.19	2 (15%)	10,14,14	1.99	4 (40%)
7	CDL	A	1101	-	77,77,99	1.29	9 (11%)	83,89,111	1.51	9 (10%)
7	CDL	B	1404	-	65,65,99	1.14	7 (10%)	71,77,111	1.43	10 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DSL	B	1403	-	-	15/51/51/61	-
5	95E	B	1402	-	-	5/15/15/15	-
7	CDL	A	1101	-	-	40/88/88/110	-
7	CDL	B	1404	-	-	34/76/76/110	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1404	CDL	OA6-CA5	4.62	1.47	1.34
7	A	1101	CDL	OA8-CA7	4.20	1.45	1.33
7	A	1101	CDL	OB8-CB7	3.69	1.44	1.33
7	A	1101	CDL	OA6-CA5	3.41	1.43	1.34
7	B	1404	CDL	OB8-CB7	3.18	1.42	1.33
7	A	1101	CDL	OB6-CB4	-3.09	1.38	1.46
7	B	1404	CDL	OB6-CB4	-2.88	1.39	1.46
5	B	1402	95E	C3-N6	-2.88	1.40	1.48
7	A	1101	CDL	PB2-OB4	-2.87	1.41	1.55
7	B	1404	CDL	OB6-CB5	2.86	1.42	1.34
6	B	1403	DSL	O56-C55	-2.85	1.39	1.43
7	A	1101	CDL	OB7-CB5	-2.62	1.14	1.22
7	B	1404	CDL	OA8-CA7	2.60	1.40	1.33
7	A	1101	CDL	OB6-CB5	2.48	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1101	CDL	PB2-OB3	-2.27	1.42	1.50
7	B	1404	CDL	OB8-CB6	-2.25	1.40	1.45
6	B	1403	DSL	P57-O60	-2.23	1.46	1.54
7	B	1404	CDL	OA8-CA6	-2.20	1.40	1.45
7	A	1101	CDL	PB2-OB2	-2.16	1.50	1.59
6	B	1403	DSL	P57-O59	-2.05	1.46	1.54
5	B	1402	95E	C10-N9	-2.02	1.43	1.48
6	B	1403	DSL	C25-C24	2.00	1.56	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1101	CDL	OB6-CB5-C51	6.99	126.56	111.50
6	B	1403	DSL	C45-C44-C42	-6.73	111.44	127.66
6	B	1403	DSL	O60-P57-O56	6.11	122.99	106.73
7	B	1404	CDL	OA6-CA5-C11	5.72	123.83	111.50
6	B	1403	DSL	C40-C39-C37	-4.89	115.89	127.66
6	B	1403	DSL	O60-P57-O58	-4.57	92.78	110.68
6	B	1403	DSL	C55-C54-C52	-4.52	118.22	126.04
7	A	1101	CDL	OA6-CA5-C11	4.42	121.03	111.50
7	B	1404	CDL	OB6-CB5-C51	4.32	120.81	111.50
7	B	1404	CDL	OB8-CB7-C71	4.31	122.68	111.38
7	A	1101	CDL	OB6-CB5-OB7	-4.09	113.83	123.70
6	B	1403	DSL	C38-C37-C36	3.94	121.90	115.27
6	B	1403	DSL	C50-C51-C52	-3.57	101.25	112.98
6	B	1403	DSL	O59-P57-O56	3.49	116.01	106.73
5	B	1402	95E	C7-N6-C3	-3.46	107.35	114.14
6	B	1403	DSL	C46-C47-C49	-3.41	114.21	121.12
6	B	1403	DSL	C38-C37-C39	-3.17	115.55	123.68
6	B	1403	DSL	C48-C47-C46	3.12	120.52	115.27
7	A	1101	CDL	OA8-CA6-CA4	3.08	117.40	108.43
5	B	1402	95E	C14-C13-C10	-3.05	100.96	113.86
7	A	1101	CDL	OA8-CA7-C31	3.03	121.41	111.91
6	B	1403	DSL	C35-C34-C32	-2.97	120.52	127.66
5	B	1402	95E	O12-C11-C10	-2.91	104.44	111.95
7	A	1101	CDL	CA6-OA8-CA7	2.79	127.46	117.12
7	A	1101	CDL	CA4-OA6-CA5	2.69	124.40	117.79
6	B	1403	DSL	C45-C46-C47	-2.61	104.39	112.98
7	B	1404	CDL	OA8-CA7-C31	2.61	120.08	111.91
6	B	1403	DSL	C28-C27-C26	2.59	119.62	115.27
5	B	1402	95E	C4-C3-C2	2.46	115.67	111.72
7	B	1404	CDL	OB6-CB5-OB7	-2.42	117.86	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1101	CDL	OB8-CB7-C71	2.33	119.20	111.91
6	B	1403	DSL	C18-C17-C19	-2.32	117.72	123.68
7	B	1404	CDL	OA8-CA7-OA9	-2.23	117.95	123.59
7	A	1101	CDL	C13-C12-C11	-2.20	105.28	113.19
7	B	1404	CDL	OA7-CA5-C11	-2.12	115.47	123.73
6	B	1403	DSL	C28-C27-C29	-2.11	118.27	123.68
6	B	1403	DSL	C21-C20-C19	-2.11	104.96	111.88
7	B	1404	CDL	OB8-CB7-OB9	-2.08	118.35	123.59
7	B	1404	CDL	CA4-OA6-CA5	2.04	122.81	117.79
7	B	1404	CDL	CB4-OB6-CB5	-2.01	112.84	117.79

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1402	95E	C2-C3-C4-C5
5	B	1402	95E	N6-C3-C4-C5
6	B	1403	DSL	C15-C16-C17-C18
6	B	1403	DSL	C15-C16-C17-C19
6	B	1403	DSL	C20-C21-C22-C23
6	B	1403	DSL	C34-C35-C36-C37
6	B	1403	DSL	C55-O56-P57-O58
6	B	1403	DSL	C55-O56-P57-O59
7	B	1404	CDL	O1-C1-CB2-OB2
7	B	1404	CDL	CA2-C1-CB2-OB2
7	B	1404	CDL	CA3-OA5-PA1-OA4
7	A	1101	CDL	CA2-OA2-PA1-OA3
7	A	1101	CDL	CA2-OA2-PA1-OA4
7	A	1101	CDL	CA2-OA2-PA1-OA5
7	A	1101	CDL	CA3-OA5-PA1-OA4
7	A	1101	CDL	C51-CB5-OB6-CB4
7	B	1404	CDL	OA9-CA7-OA8-CA6
7	A	1101	CDL	OA9-CA7-OA8-CA6
7	B	1404	CDL	C31-CA7-OA8-CA6
7	A	1101	CDL	C31-CA7-OA8-CA6
6	B	1403	DSL	C20-C21-C22-C24
7	B	1404	CDL	OB7-CB5-OB6-CB4
7	A	1101	CDL	OB7-CB5-OB6-CB4
7	B	1404	CDL	C11-CA5-OA6-CA4
7	B	1404	CDL	C51-CB5-OB6-CB4
7	B	1404	CDL	C57-C58-C59-C60
6	B	1403	DSL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
6	B	1403	DSL	C49-C50-C51-C52
5	B	1402	95E	N6-C7-C8-N9
7	B	1404	CDL	OA7-CA5-OA6-CA4
7	B	1404	CDL	C55-C56-C57-C58
7	A	1101	CDL	CA7-C31-C32-C33
7	B	1404	CDL	CA2-OA2-PA1-OA5
7	A	1101	CDL	CA3-OA5-PA1-OA2
7	A	1101	CDL	CB2-OB2-PB2-OB5
6	B	1403	DSL	C30-C31-C32-C33
7	B	1404	CDL	C31-C32-C33-C34
7	B	1404	CDL	CA6-CA4-OA6-CA5
7	A	1101	CDL	CB6-CB4-OB6-CB5
7	A	1101	CDL	C11-C12-C13-C14
7	A	1101	CDL	C72-C73-C74-C75
7	B	1404	CDL	C54-C55-C56-C57
7	A	1101	CDL	C71-C72-C73-C74
7	A	1101	CDL	C52-C53-C54-C55
7	A	1101	CDL	C60-C61-C62-C63
6	B	1403	DSL	C39-C40-C41-C42
7	A	1101	CDL	C12-C13-C14-C15
5	B	1402	95E	C7-C8-N9-C10
7	B	1404	CDL	C53-C54-C55-C56
7	B	1404	CDL	C34-C35-C36-C37
7	A	1101	CDL	C14-C15-C16-C17
7	A	1101	CDL	C78-C79-C80-C81
7	A	1101	CDL	C80-C81-C82-C83
7	A	1101	CDL	C33-C34-C35-C36
7	B	1404	CDL	C33-C34-C35-C36
6	B	1403	DSL	C45-C46-C47-C48
7	A	1101	CDL	CA3-CA4-OA6-CA5
7	A	1101	CDL	OA5-CA3-CA4-OA6
7	B	1404	CDL	C32-C31-CA7-OA8
7	A	1101	CDL	OA6-CA4-CA6-OA8
7	A	1101	CDL	C53-C54-C55-C56
6	B	1403	DSL	C45-C46-C47-C49
7	A	1101	CDL	C11-CA5-OA6-CA4
7	A	1101	CDL	C54-C55-C56-C57
7	B	1404	CDL	C51-C52-C53-C54
7	A	1101	CDL	C59-C60-C61-C62
7	A	1101	CDL	CA3-CA4-CA6-OA8
6	B	1403	DSL	C30-C31-C32-C34
7	B	1404	CDL	C59-C60-C61-C62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
7	B	1404	CDL	OB6-CB4-CB6-OB8
7	A	1101	CDL	OA7-CA5-OA6-CA4
5	B	1402	95E	C11-C10-N9-C8
7	B	1404	CDL	CB6-CB4-OB6-CB5
7	B	1404	CDL	CA3-CA4-CA6-OA8
7	B	1404	CDL	CB3-CB4-CB6-OB8
7	A	1101	CDL	CB2-OB2-PB2-OB3
7	B	1404	CDL	C12-C13-C14-C15
7	A	1101	CDL	OA5-CA3-CA4-CA6
7	B	1404	CDL	C35-C36-C37-C38
7	A	1101	CDL	CA5-C11-C12-C13
7	B	1404	CDL	OA6-CA4-CA6-OA8
7	B	1404	CDL	C58-C59-C60-C61
7	B	1404	CDL	C61-C62-C63-C64
7	A	1101	CDL	OB9-CB7-OB8-CB6
7	A	1101	CDL	C79-C80-C81-C82
7	B	1404	CDL	C32-C31-CA7-OA9
7	A	1101	CDL	C1-CB2-OB2-PB2
7	A	1101	CDL	C77-C78-C79-C80
7	B	1404	CDL	C62-C63-C64-C65
7	A	1101	CDL	C71-CB7-OB8-CB6
7	A	1101	CDL	CB2-C1-CA2-OA2
7	B	1404	CDL	CA2-OA2-PA1-OA3
7	B	1404	CDL	CA3-OA5-PA1-OA3
6	B	1403	DSL	C19-C20-C21-C22

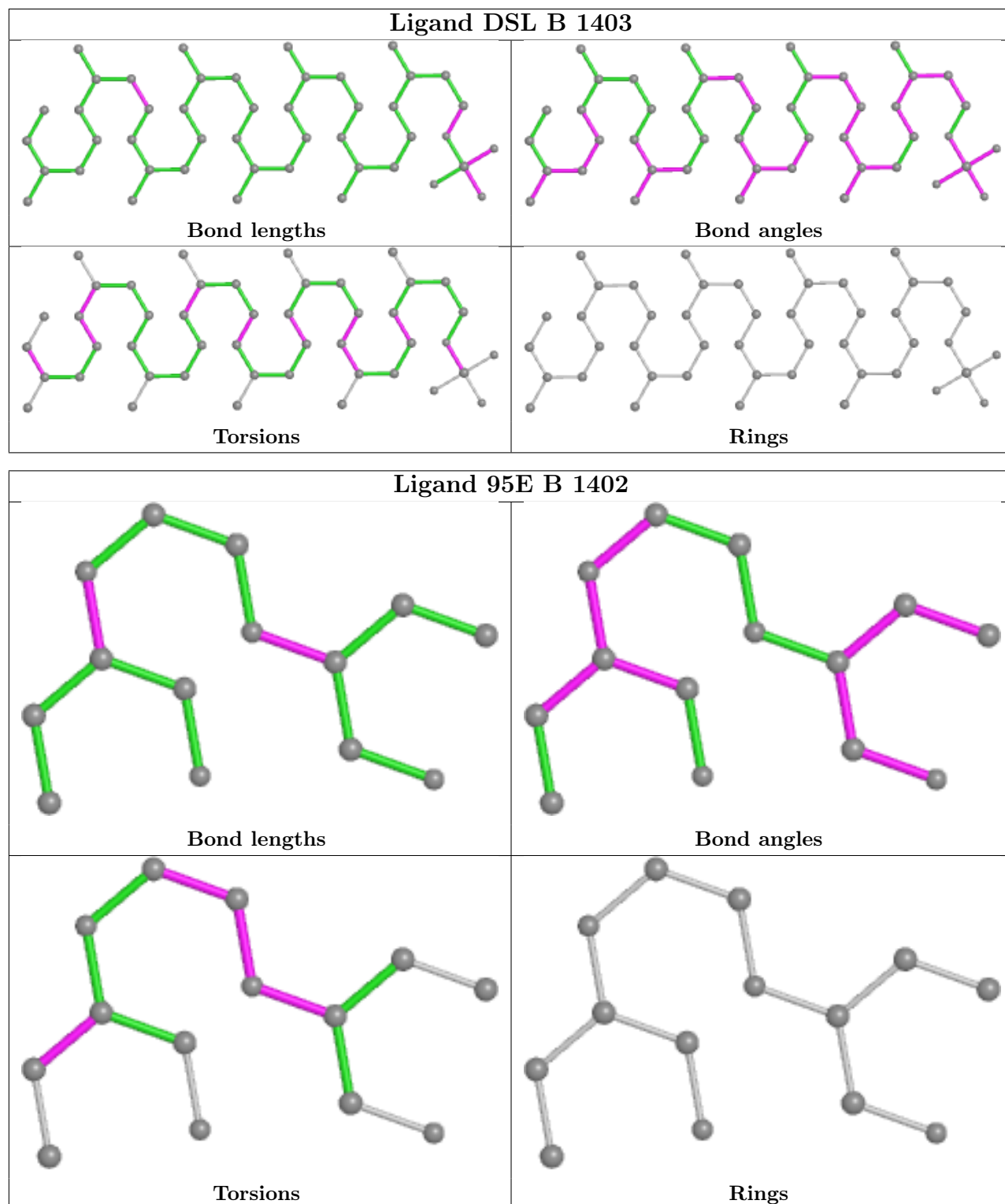
There are no ring outliers.

4 monomers are involved in 28 short contacts:

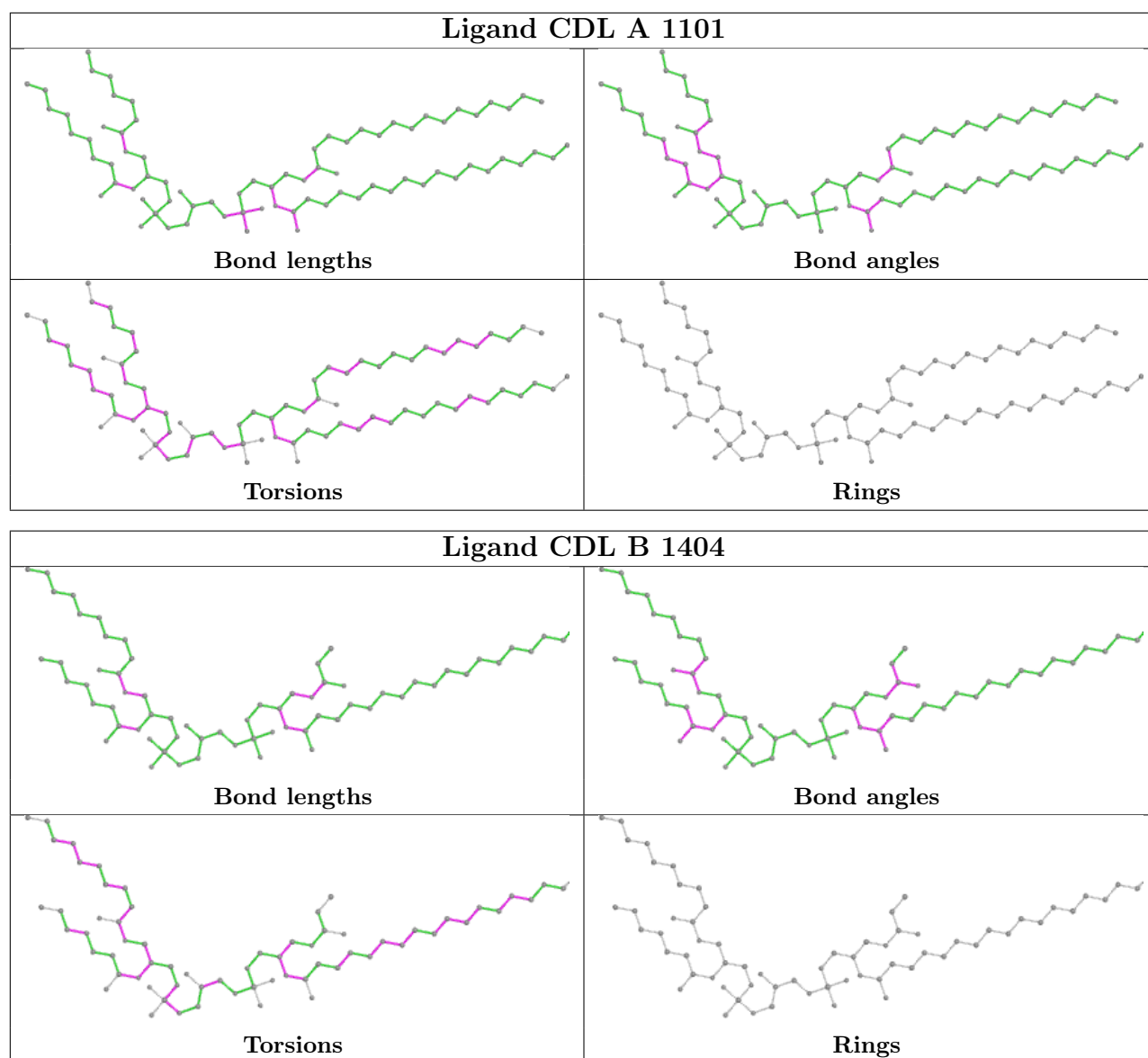
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1403	DSL	15	0
5	B	1402	95E	1	0
7	A	1101	CDL	3	0
7	B	1404	CDL	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

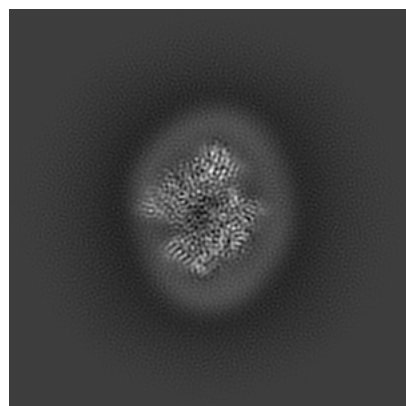
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30218. These allow visual inspection of the internal detail of the map and identification of artifacts.

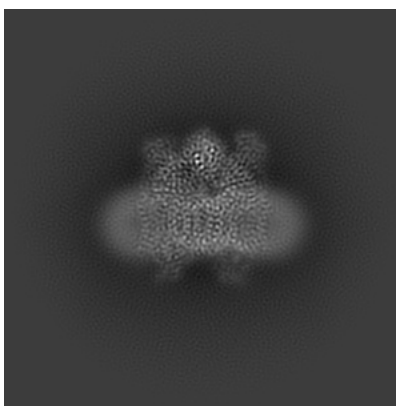
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

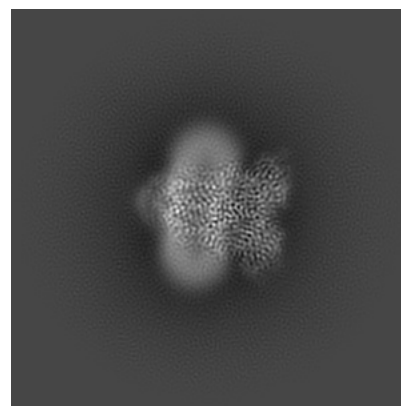
#### 6.1.1 Primary map



X

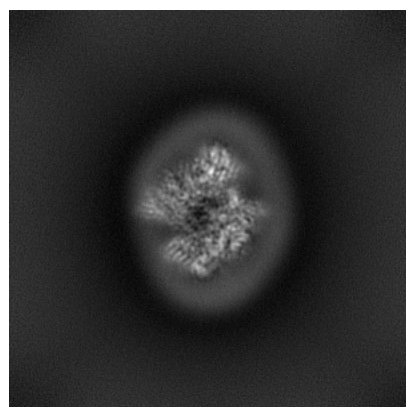


Y

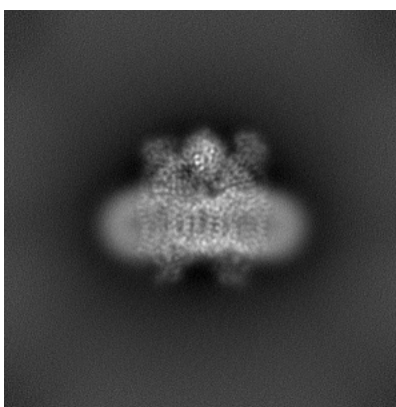


Z

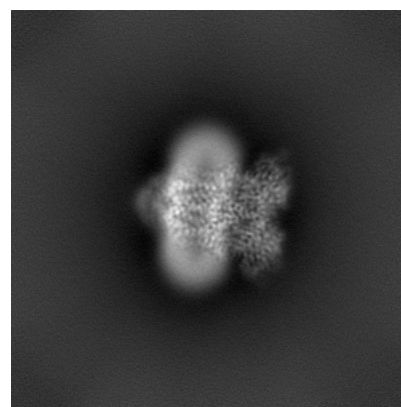
#### 6.1.2 Raw map



X



Y

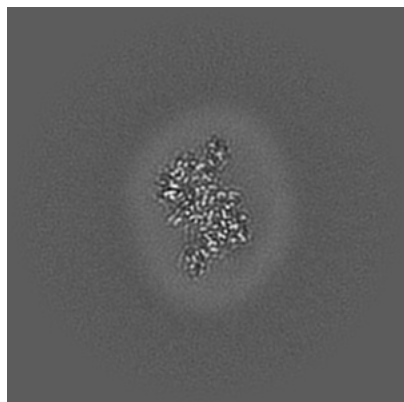


Z

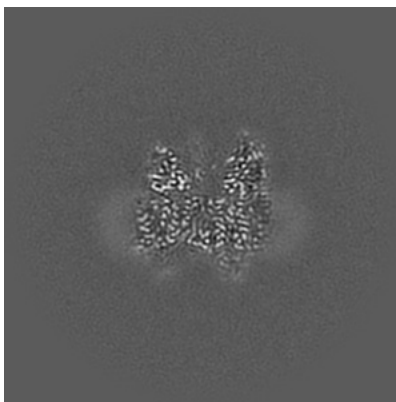
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

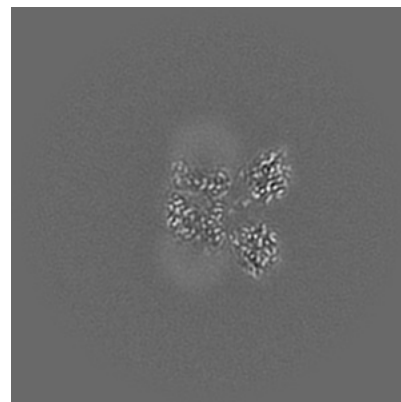
### 6.2.1 Primary map



X Index: 192

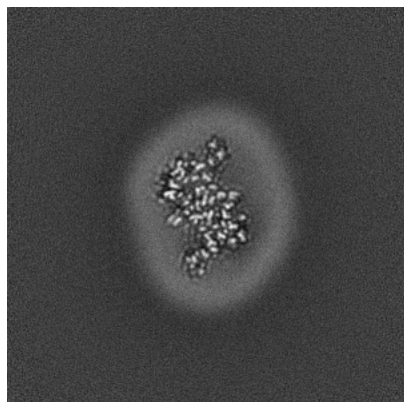


Y Index: 192

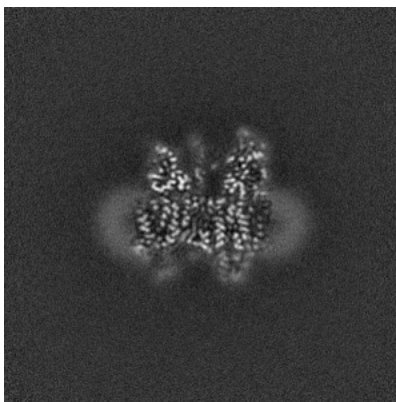


Z Index: 192

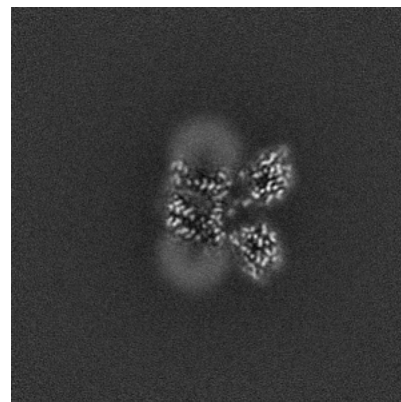
### 6.2.2 Raw map



X Index: 192



Y Index: 192

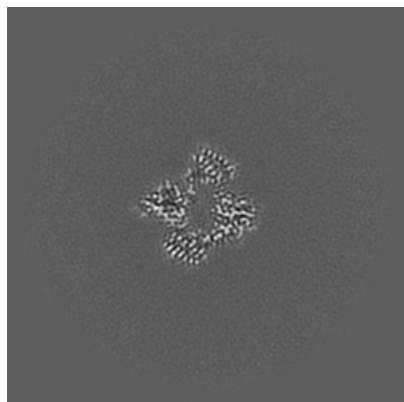


Z Index: 192

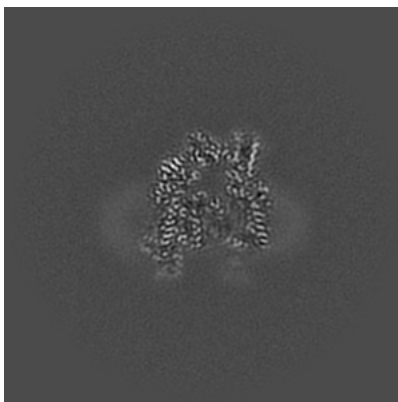
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

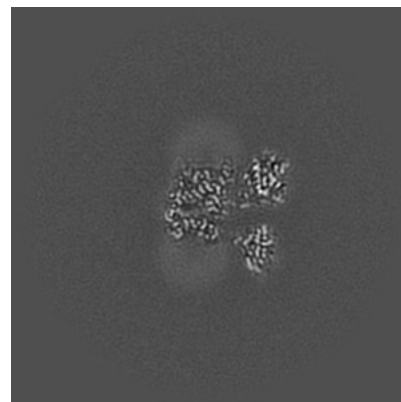
### 6.3.1 Primary map



X Index: 237

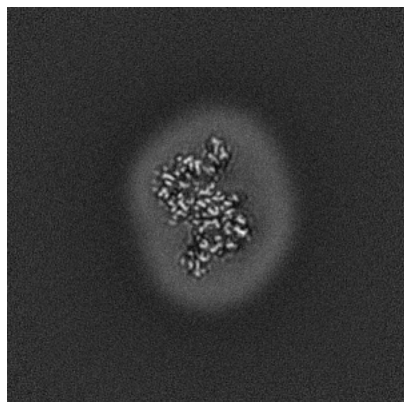


Y Index: 204

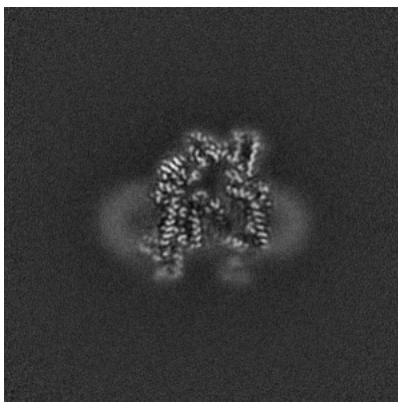


Z Index: 185

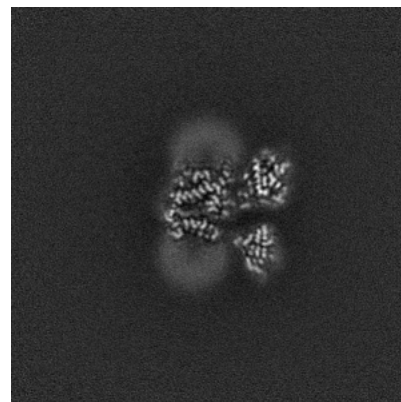
### 6.3.2 Raw map



X Index: 196



Y Index: 204

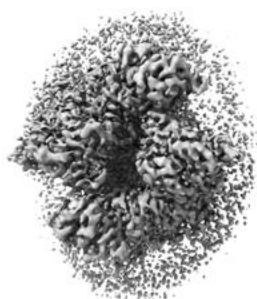


Z Index: 185

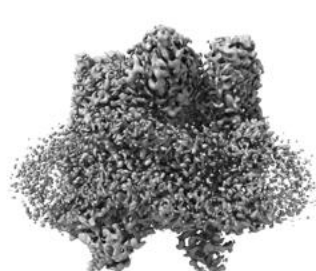
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

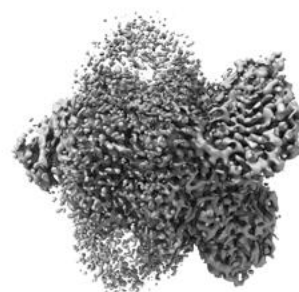
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

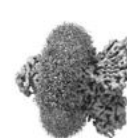
### 6.4.2 Raw map



X



Y



Z

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

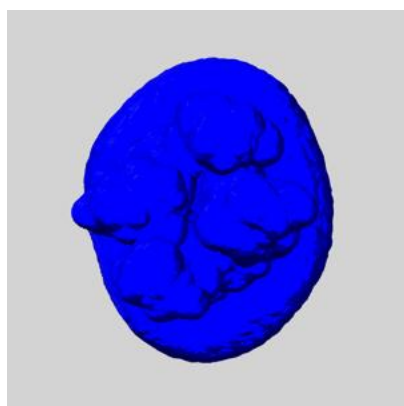
## 6.5 Mask visualisation [i](#)

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

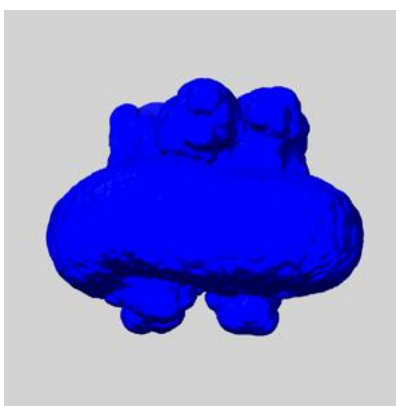
A mask typically either:

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

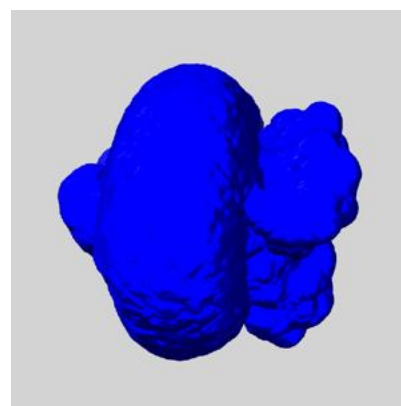
### 6.5.1 emd\_30218\_msk\_1.map [i](#)



X



Y

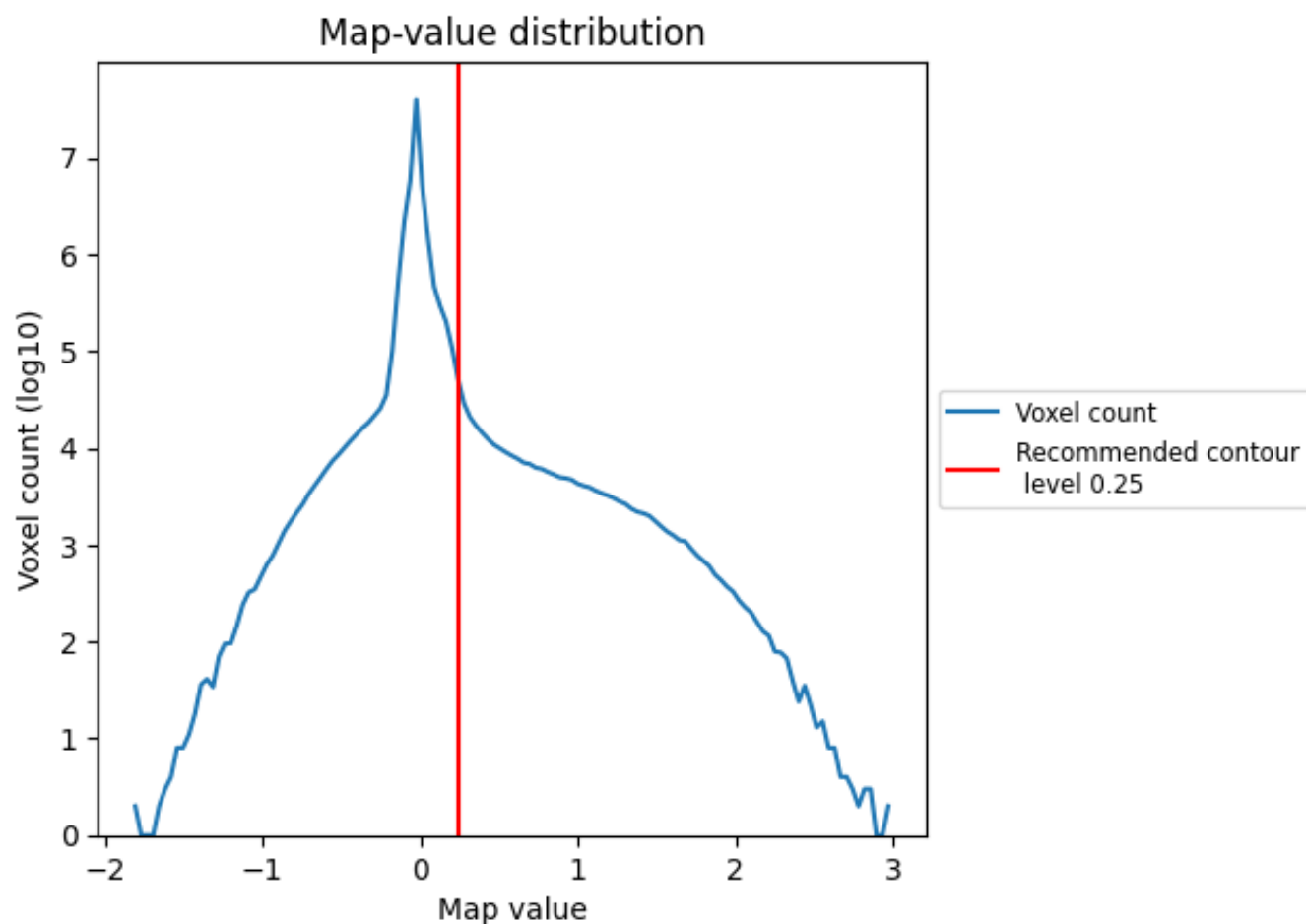


Z

## 7 Map analysis [i](#)

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

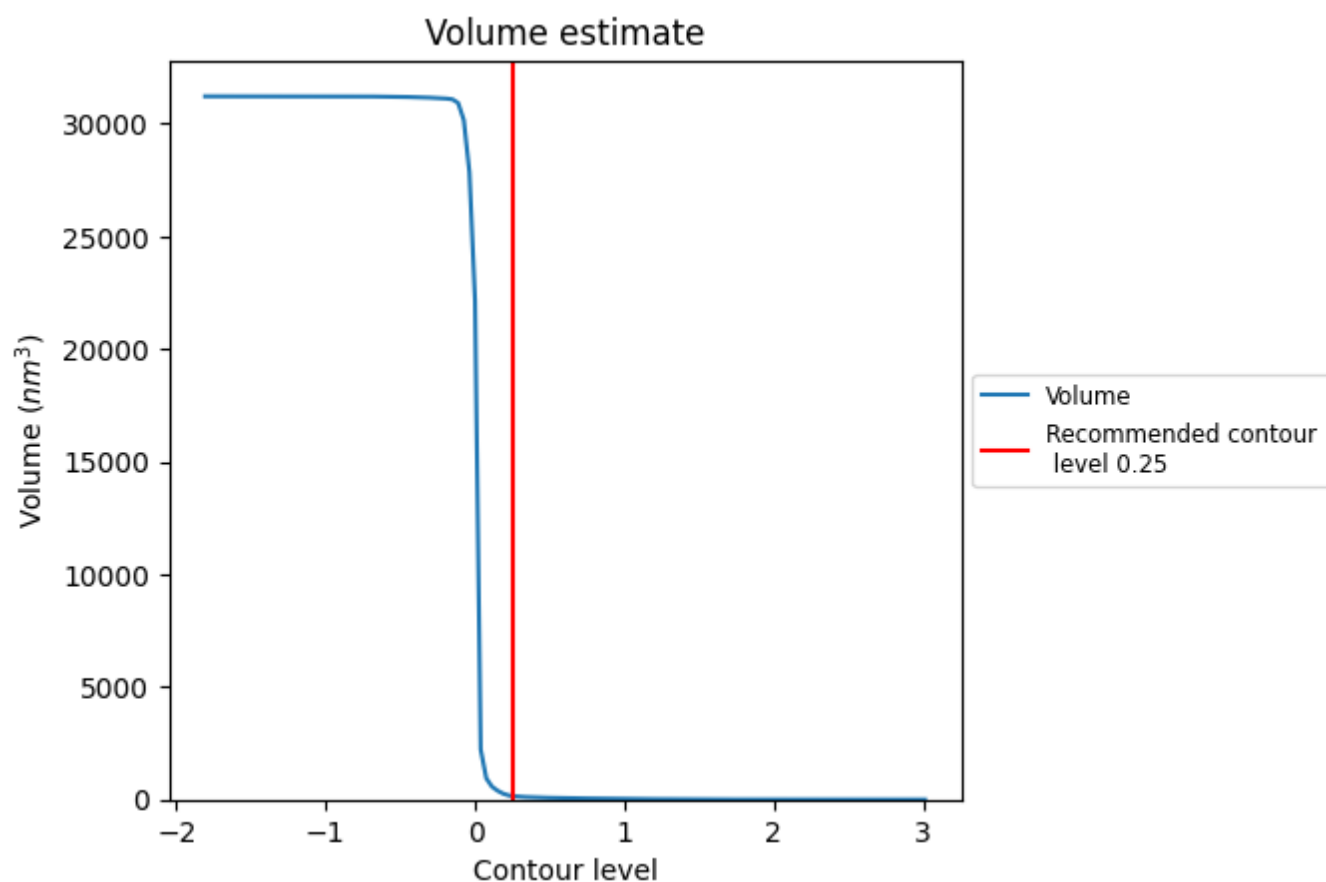
### 7.1 Map-value distribution [i](#)



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



## 7.2 Volume estimate [i](#)

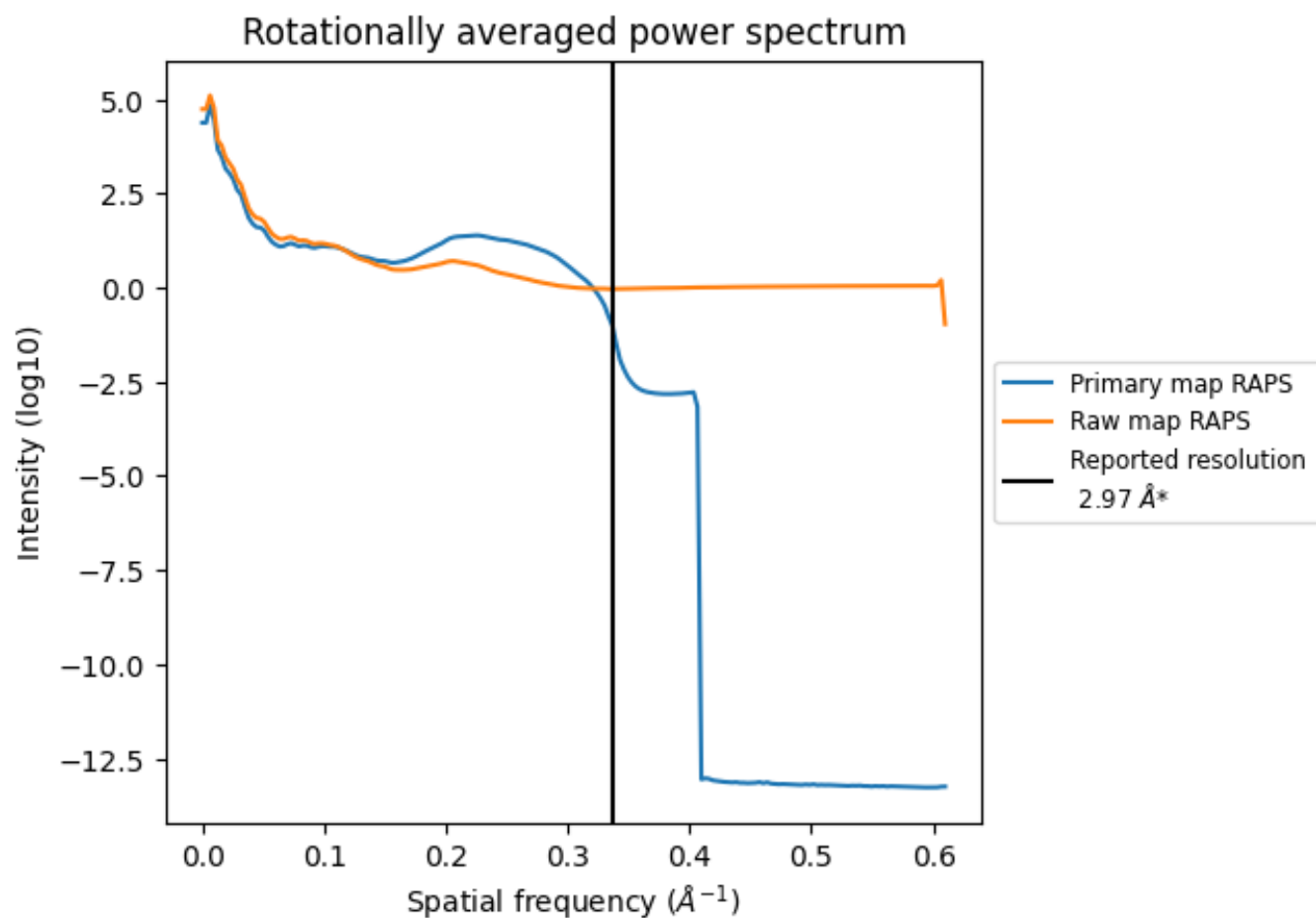


The volume at the recommended contour level is 157 nm<sup>3</sup>; this corresponds to an approximate mass of 142 kDa.

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 ⓘ

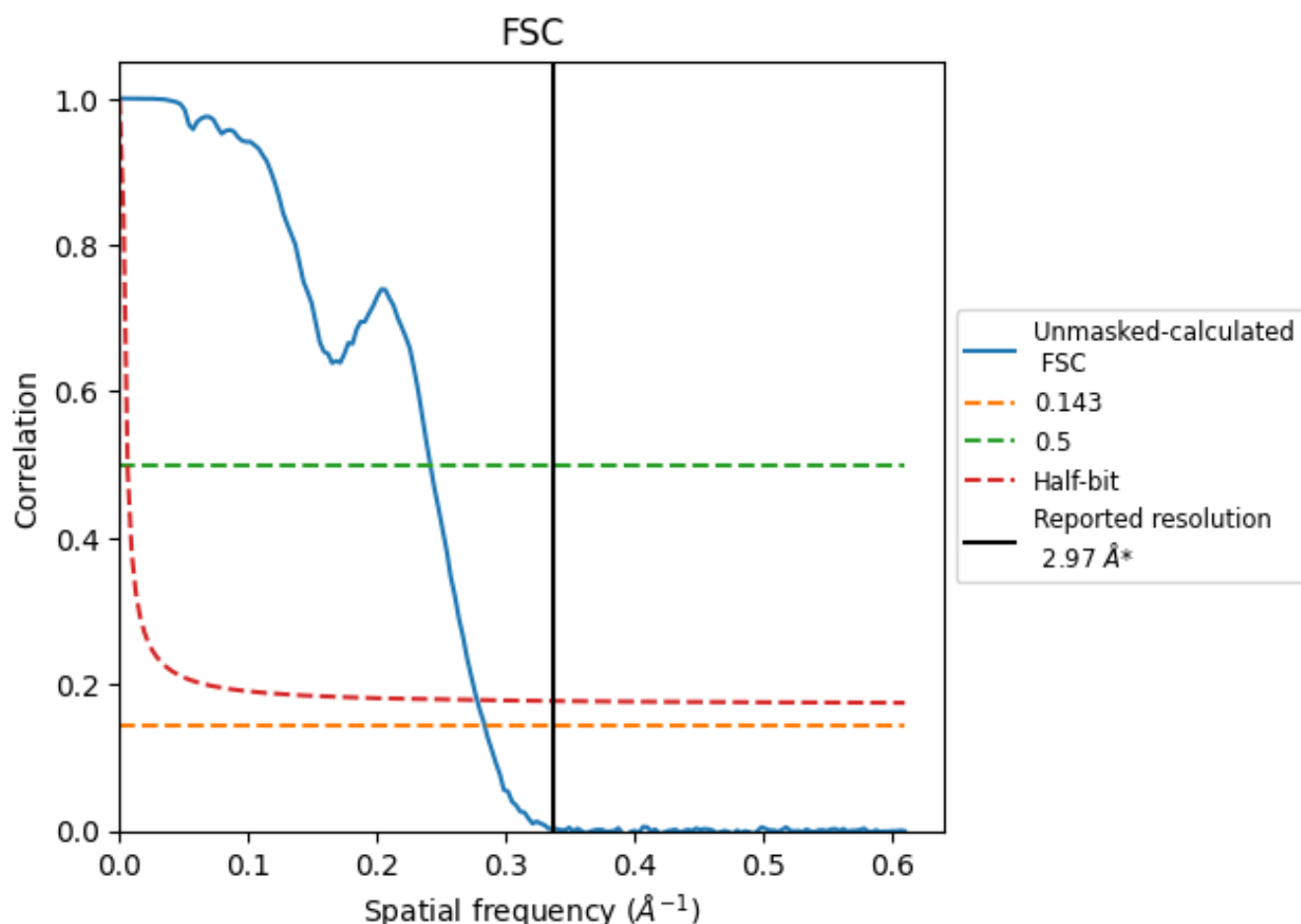


\*Reported resolution corresponds to spatial frequency of 0.337 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.337  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

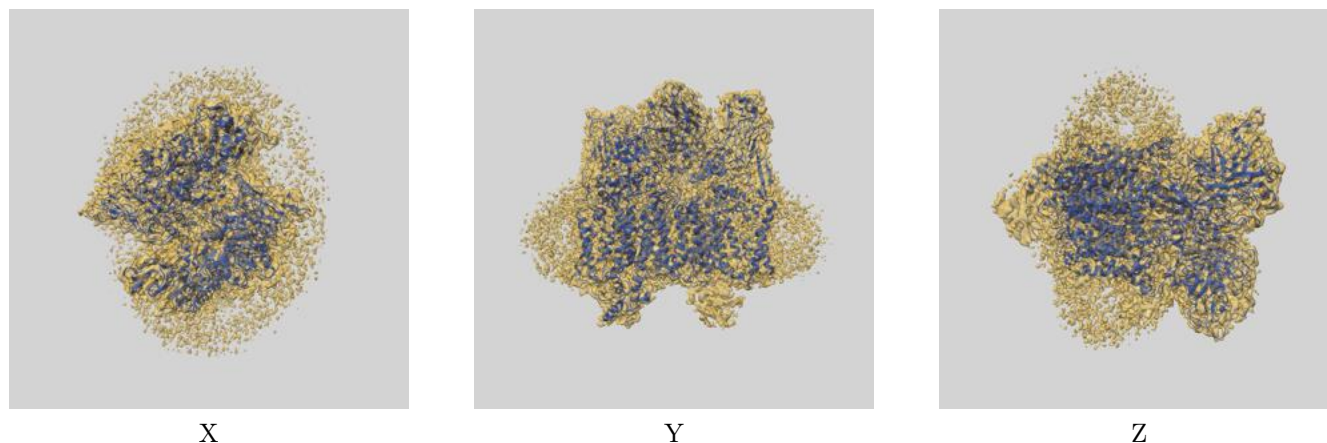
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.53	4.14	3.60

\*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 3.53 differs from the reported value 2.97 by more than 10 %

## 9 Map-model fit [i](#)

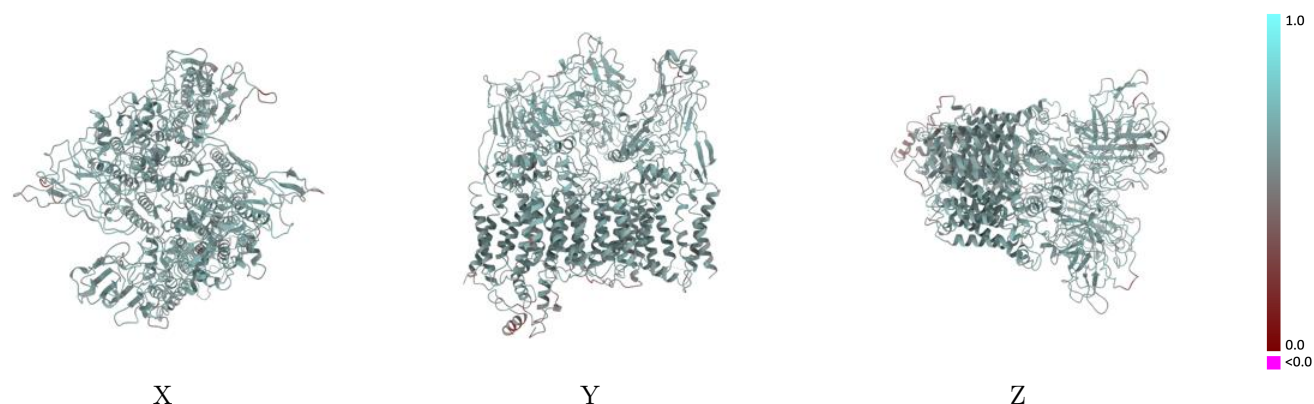
This section contains information regarding the fit between EMDB map EMD-30218 and PDB model 7BVF. Per-residue inclusion information can be found in section [3](#) on page [7](#).

### 9.1 Map-model overlay [i](#)



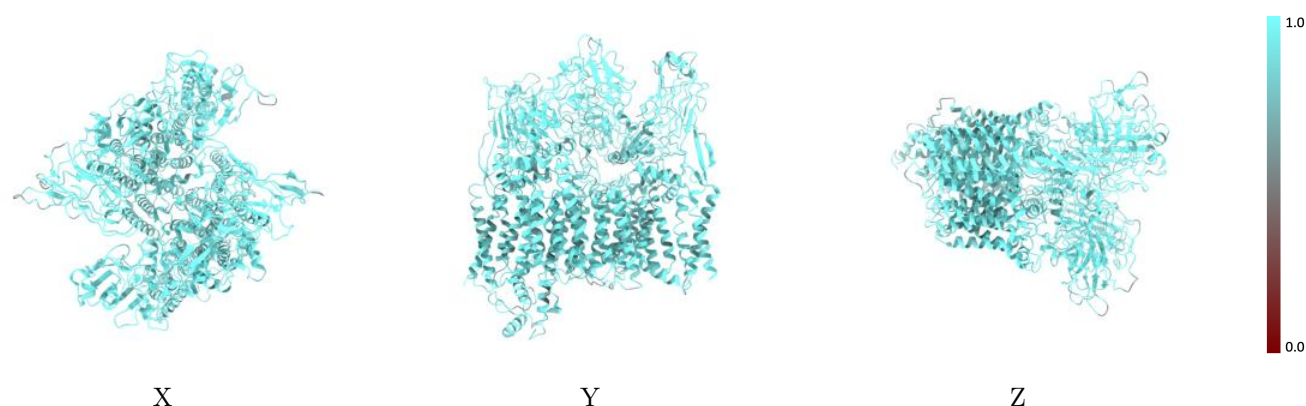
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



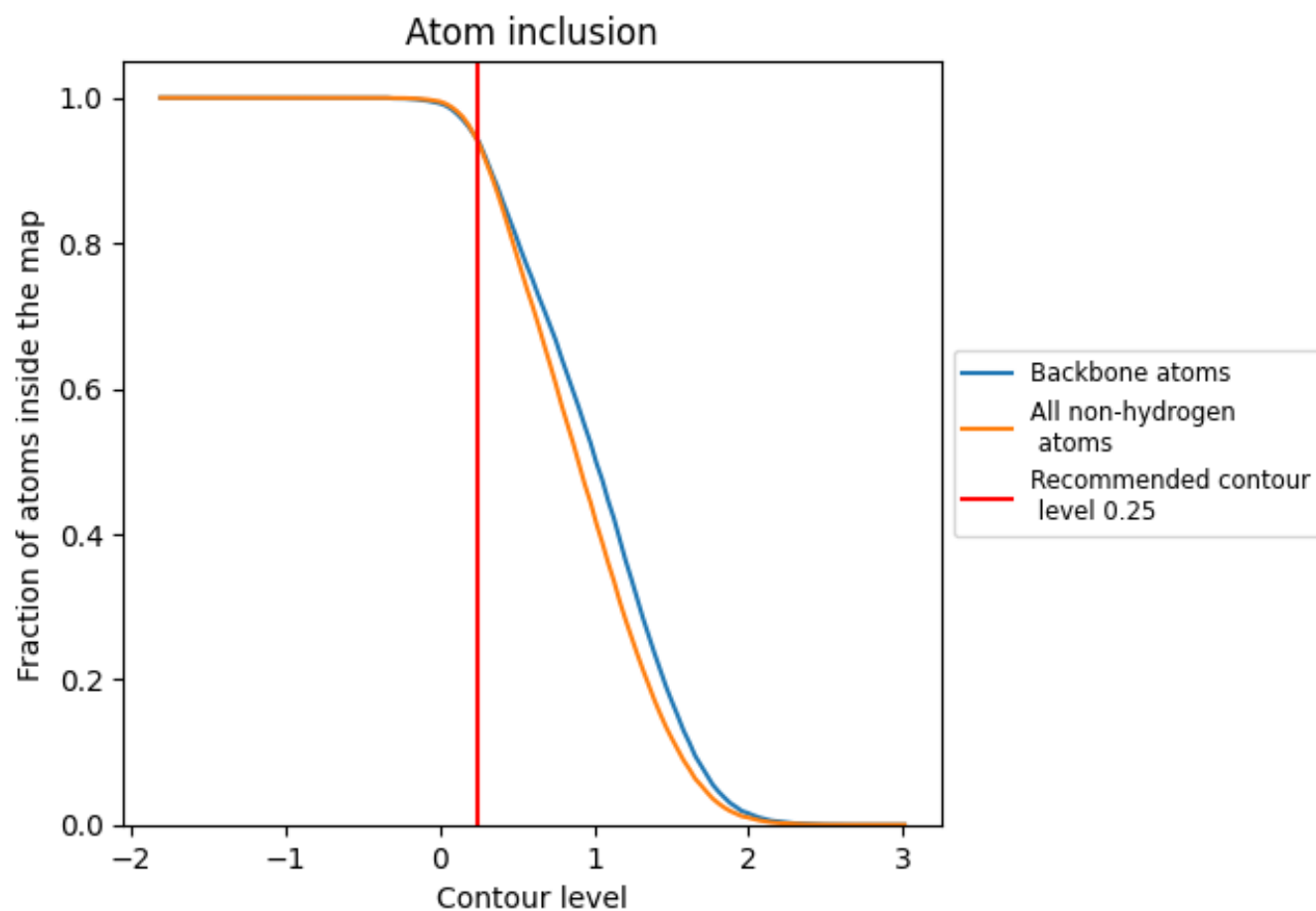
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.25).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9388	<div></div> 0.5800
A	<div></div> 0.9417	<div></div> 0.5830
B	<div></div> 0.9428	<div></div> 0.5850
P	<div></div> 0.8474	<div></div> 0.4890

