Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 07:22 PM JST

PDB ID	:	7BVC
EMDB ID	:	EMD-30216
Title	:	Cryo-EM structure of Mycobacterium smegmatis 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	:	2.90 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

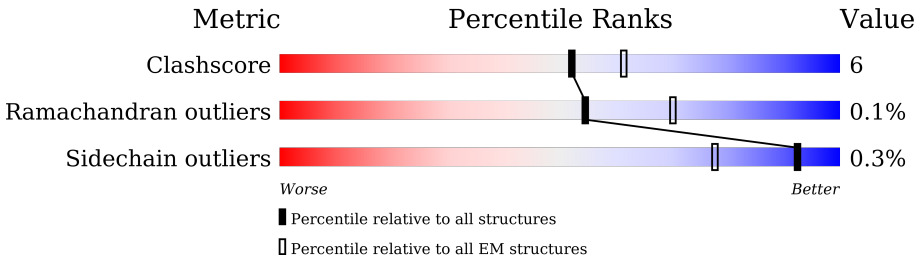
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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 >=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	1088	84% 15%
2	B	1100	85% 11%
3	P	99	85% 6% 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 17206 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 Integral membrane indolylacetylinositol arabinosyltransferase EmbA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1078	8147	5264	1408	1450	25	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP A0R613
A	-6	TYR	-	expression tag	UNP A0R613
A	-5	LYS	-	expression tag	UNP A0R613
A	-4	ASP	-	expression tag	UNP A0R613
A	-3	ASP	-	expression tag	UNP A0R613
A	-2	ASP	-	expression tag	UNP A0R613
A	-1	ASP	-	expression tag	UNP A0R613
A	0	LYS	-	expression tag	UNP A0R613

- Molecule 2 is a protein called Integral membrane indolylacetylinositol arabinosyltransferase EmbB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1063	8105	5212	1401	1459	33	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1083	HIS	-	expression tag	UNP I7GAQ2
B	1084	LEU	-	expression tag	UNP I7GAQ2
B	1085	GLY	-	expression tag	UNP I7GAQ2
B	1086	GLY	-	expression tag	UNP I7GAQ2
B	1087	ILE	-	expression tag	UNP I7GAQ2
B	1088	LYS	-	expression tag	UNP I7GAQ2
B	1089	ALA	-	expression tag	UNP I7GAQ2

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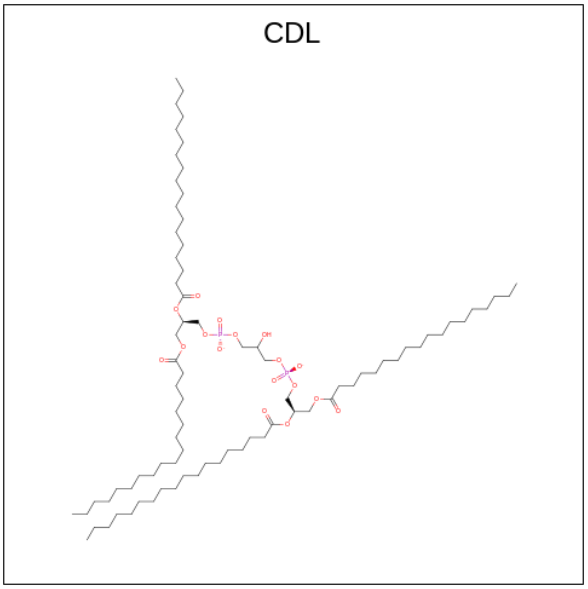
Chain	Residue	Modelled	Actual	Comment	Reference
B	1090	PHE	-	expression tag	UNP I7GAQ2
B	1091	HIS	-	expression tag	UNP I7GAQ2
B	1092	HIS	-	expression tag	UNP I7GAQ2
B	1093	HIS	-	expression tag	UNP I7GAQ2
B	1094	HIS	-	expression tag	UNP I7GAQ2
B	1095	HIS	-	expression tag	UNP I7GAQ2
B	1096	HIS	-	expression tag	UNP I7GAQ2
B	1097	HIS	-	expression tag	UNP I7GAQ2
B	1098	HIS	-	expression tag	UNP I7GAQ2
B	1099	HIS	-	expression tag	UNP I7GAQ2
B	1100	HIS	-	expression tag	UNP I7GAQ2

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

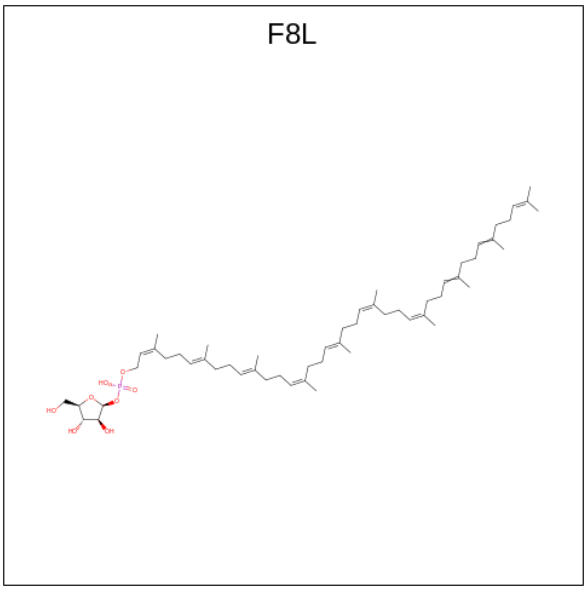
Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	90	Total	C	N	O	S	0	0
			673	422	101	149	1		

- Molecule 4 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
4	A	1	Total	C	O	P	0
			91	72	17	2	
4	B	1	Total	C	O	P	0
			98	79	17	2	

- Molecule 5 is [(2Z,6E,10E,14Z,18E,22Z,26Z)-3,7,11,15,19,23,27,31,35,39-decamethyltetracon ta-2,6,10,14,18,22,26,30,34,38-decaenyl] [(2S,3S,4S,5R)-5-(hydroxymethyl)-3,4-bis(oxidanyl) oxolan-2-yl] hydrogen phosphate (three-letter code: F8L) (formula: $C_{55}H_{91}O_8P$) (labeled as "Ligand of Interest" by depositor).

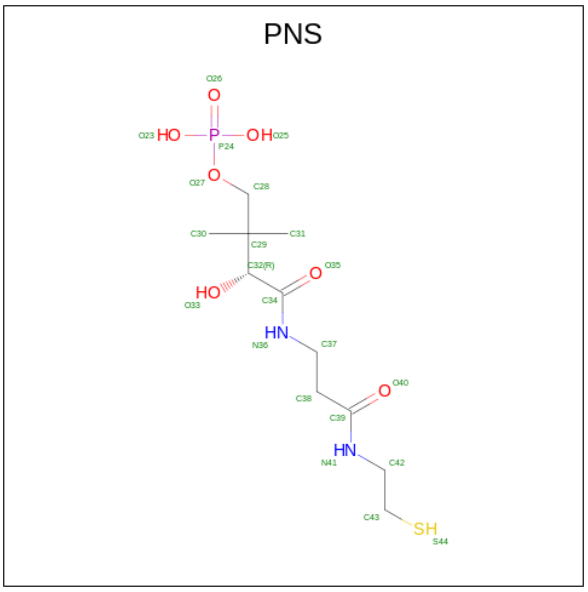


Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			49	40	8	1	

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

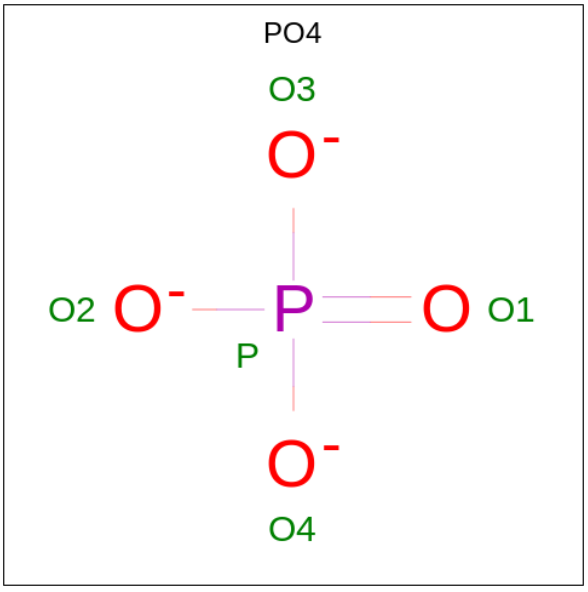
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Ca	0
			1	1	
6	B	1	Total	Ca	0
			1	1	

- Molecule 7 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: $C_{11}H_{23}N_2O_7PS$) (labeled as "Ligand of Interest" by depositor).



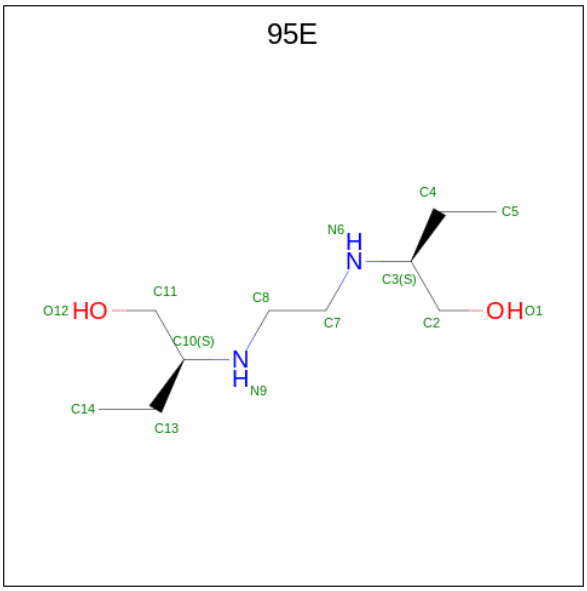
Mol	Chain	Residues	Atoms						AltConf
7	B	1	Total	C	N	O	P	S	0
			22	11	2	7	1	1	

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms				AltConf
8	B	1	Total	O	P		0
			5	4	1		

- Molecule 9 is Ethambutol (three-letter code: 95E) (formula: $C_{10}H_{24}N_2O_2$).



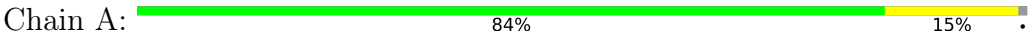
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	14	10	2	2	0

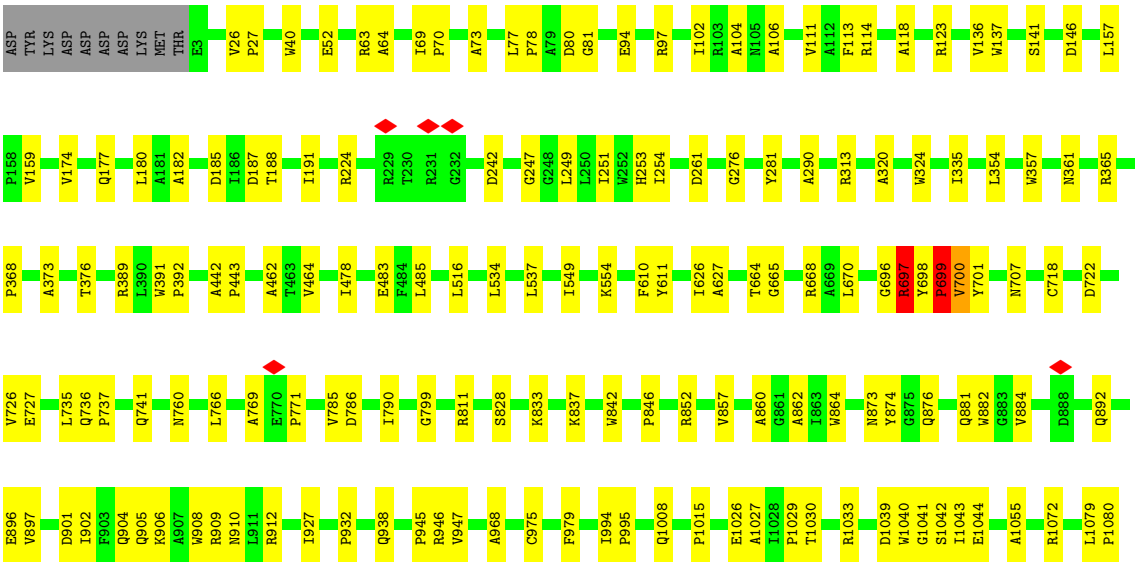
3 Residue-property plots (i)

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: Integral membrane indolylacetylinositol arabinosyltransferase EmbA

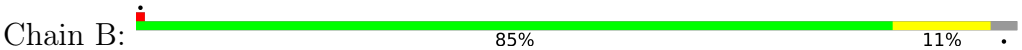
Chain A:

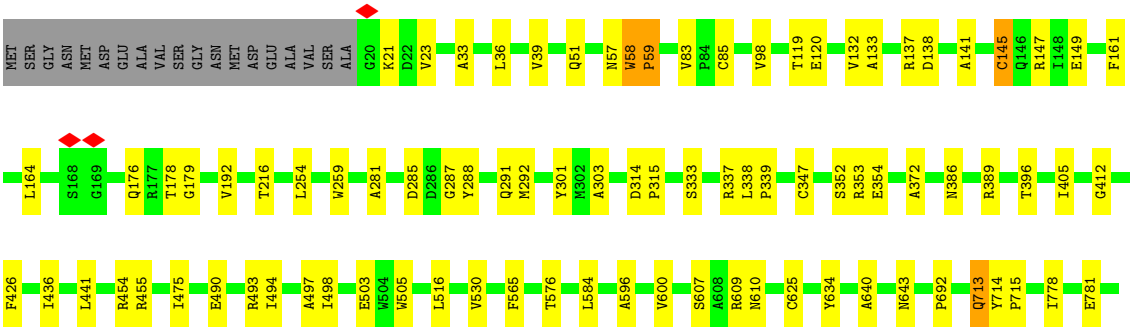


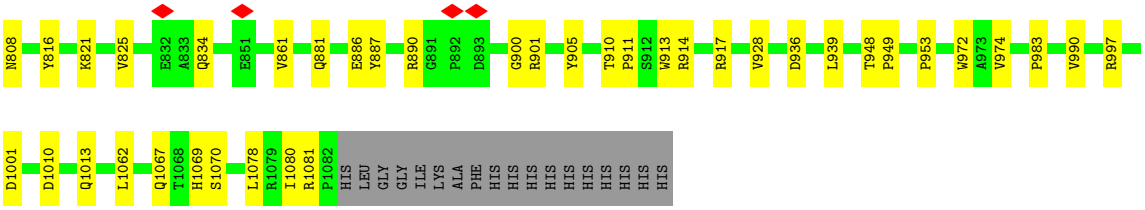


• Molecule 2: Integral membrane indolylacetylinositol arabinosyltransferase EmbB

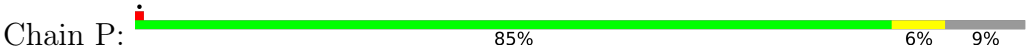
Chain B:

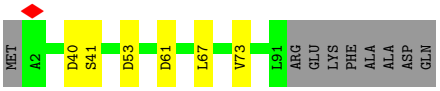






• Molecule 3: Meromycolate extension acyl carrier protein





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	227206	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; The CTF correction was done by patch CTF correction.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.055	Depositor
Minimum map value	-1.648	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PO4, F8L, CA, PNS, 95E, CDL

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	0.28	1/8365 (0.0%)	0.46	1/11466 (0.0%)
2	B	0.29	1/8315 (0.0%)	0.47	2/11393 (0.0%)
3	P	0.24	0/679	0.43	0/925
All	All	0.29	2/17359 (0.0%)	0.47	3/23784 (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
2	B	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	PRO	C-O	-5.61	1.12	1.23
2	B	715	PRO	C-O	-5.55	1.12	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	713	GLN	CB-CG-CD	-8.07	90.61	111.60
2	B	59	PRO	N-CA-CB	-6.69	95.24	102.60
1	A	697	ARG	CG-CD-NE	-5.12	101.04	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	698	TYR	Peptide
2	B	58	TRP	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	8147	0	8211	101	0
2	B	8105	0	8168	82	0
3	P	673	0	658	5	0
4	A	91	0	132	6	0
4	B	98	0	149	8	0
5	A	49	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	22	0	21	1	0
8	B	5	0	0	1	0
9	B	14	0	0	0	0
All	All	17206	0	17339	196	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 (196) 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:A:696:GLY:O	1:A:697:ARG:HB3	1.63	0.96
1:A:700:VAL:HG12	1:A:701:TYR:H	1.41	0.83
2:B:890:ARG:HG3	2:B:928:VAL:HG21	1.61	0.82
2:B:609:ARG:NH2	4:B:1204:CDL:H522	1.98	0.77
1:A:40:TRP:HB3	1:A:182:ALA:HB3	1.67	0.75
2:B:640:ALA:HB3	2:B:643:ASN:HB3	1.68	0.73
1:A:361:ASN:HB3	1:A:368:PRO:HG3	1.69	0.72
4:B:1204:CDL:OA6	4:B:1204:CDL:H312	1.90	0.71
2:B:405:ILE:HD11	2:B:441:LEU:HD23	1.74	0.70
2:B:314:ASP:HB2	2:B:315:PRO:HD3	1.74	0.70
1:A:700:VAL:CG1	1:A:701:TYR:H	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:808:ASN:ND2	2:B:825:VAL:O	2.27	0.68
2:B:494:ILE:HG12	2:B:1080:ILE:HD11	1.74	0.68
1:A:902:ILE:HG23	1:A:912:ARG:HH12	1.58	0.66
1:A:700:VAL:HG12	1:A:701:TYR:N	2.11	0.65
1:A:876:GLN:HE21	1:A:938:GLN:HE21	1.43	0.65
2:B:145:CYS:SG	2:B:164:LEU:HD13	2.38	0.64
1:A:81:GLY:HA3	1:A:104:ALA:HB3	1.80	0.64
2:B:972:TRP:HD1	2:B:1013:GLN:HE21	1.44	0.64
2:B:905:TYR:HB2	2:B:917:ARG:HB2	1.80	0.63
2:B:1080:ILE:HG22	2:B:1081:ARG:HG3	1.80	0.63
1:A:760:ASN:HD21	1:A:811:ARG:H	1.45	0.63
2:B:36:LEU:HA	2:B:39:VAL:HG22	1.82	0.62
1:A:290:ALA:HB1	1:A:464:VAL:HG22	1.82	0.61
1:A:727:GLU:HB3	1:A:1029:PRO:HG2	1.82	0.61
1:A:80:ASP:HA	1:A:106:ALA:HB2	1.82	0.60
2:B:85:CYS:CB	2:B:145:CYS:HB3	2.31	0.60
1:A:626:ILE:HG13	1:A:627:ALA:H	1.65	0.60
2:B:161:PHE:HB2	2:B:176:GLN:HB3	1.84	0.60
2:B:886:GLU:OE2	2:B:901:ARG:NH2	2.35	0.60
2:B:1067:GLN:OE1	2:B:1069:HIS:NE2	2.35	0.60
1:A:1008:GLN:HB3	1:A:1015:PRO:HD2	1.84	0.59
2:B:412:GLY:O	2:B:455:ARG:NH1	2.35	0.59
1:A:741:GLN:HE22	1:A:842:TRP:HD1	1.50	0.59
2:B:607:SER:OG	2:B:610:ASN:ND2	2.36	0.58
1:A:73:ALA:HB1	1:A:174:VAL:HG11	1.84	0.58
2:B:119:THR:O	2:B:137:ARG:NH1	2.36	0.58
1:A:862:ALA:O	1:A:876:GLN:N	2.37	0.58
2:B:119:THR:HG22	2:B:120:GLU:H	1.69	0.58
1:A:478:ILE:HD11	1:A:554:LYS:HB2	1.88	0.56
1:A:881:GLN:HG2	1:A:896:GLU:HG2	1.86	0.56
1:A:902:ILE:HB	1:A:1039:ASP:HB2	1.85	0.56
2:B:288:TYR:HD1	2:B:972:TRP:HB2	1.69	0.56
4:A:1101:CDL:OB7	4:A:1101:CDL:HB31	2.03	0.56
2:B:498:ILE:HD11	2:B:1080:ILE:HG23	1.88	0.56
2:B:990:VAL:HG21	2:B:1062:LEU:HD21	1.88	0.56
2:B:333:SER:O	2:B:337:ARG:NH1	2.40	0.55
1:A:106:ALA:HA	1:A:123:ARG:HH11	1.72	0.55
1:A:261:ASP:OD2	1:A:365:ARG:NH1	2.39	0.55
1:A:828:SER:OG	1:A:828:SER:O	2.25	0.54
2:B:609:ARG:HH22	4:B:1204:CDL:H522	1.72	0.54
2:B:57:ASN:N	2:B:57:ASN:OD1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:HIS:O	1:A:313:ARG:NH1	2.42	0.53
2:B:910:THR:O	2:B:914:ARG:NH1	2.41	0.53
3:P:40:ASP:N	3:P:40:ASP:OD1	2.41	0.53
1:A:254:ILE:O	1:A:707:ASN:ND2	2.37	0.53
1:A:864:TRP:HE3	1:A:874:TYR:O	1.91	0.53
1:A:249:LEU:HD21	1:A:320:ALA:HB1	1.91	0.53
1:A:462:ALA:HB1	1:A:1072:ARG:HB2	1.90	0.53
1:A:1026:GLU:HG2	1:A:1027:ALA:H	1.74	0.52
1:A:174:VAL:HB	1:A:177:GLN:HE22	1.74	0.52
2:B:21:LYS:HG3	2:B:23:VAL:HG12	1.91	0.52
2:B:133:ALA:HB2	2:B:178:THR:HB	1.91	0.52
2:B:576:THR:OG1	8:B:1202:PO4:O1	2.21	0.52
1:A:696:GLY:O	1:A:697:ARG:CB	2.37	0.52
2:B:352:SER:OG	2:B:353:ARG:NH1	2.42	0.52
1:A:281:TYR:OH	1:A:979:PHE:O	2.26	0.52
2:B:147:ARG:NH2	2:B:149:GLU:OE2	2.44	0.51
1:A:483:GLU:HG3	1:A:549:ILE:HG12	1.92	0.51
1:A:905:GLN:O	1:A:909:ARG:NH1	2.41	0.51
2:B:288:TYR:CD1	2:B:972:TRP:HB2	2.45	0.51
1:A:335:ILE:HD11	1:A:537:LEU:HD22	1.93	0.51
1:A:876:GLN:HE21	1:A:938:GLN:NE2	2.08	0.51
2:B:454:ARG:NH1	3:P:53:ASP:OD2	2.43	0.51
2:B:490:GLU:OE1	2:B:493:ARG:NH2	2.34	0.50
1:A:77:LEU:HB3	1:A:81:GLY:HA2	1.92	0.50
1:A:224:ARG:HD3	1:A:389:ARG:HD3	1.94	0.50
4:A:1101:CDL:OB9	4:A:1101:CDL:H732	2.11	0.50
2:B:609:ARG:HH21	4:B:1204:CDL:H522	1.74	0.50
1:A:242:ASP:HA	1:A:324:TRP:HE1	1.76	0.50
1:A:860:ALA:HB2	1:A:908:TRP:HA	1.94	0.50
1:A:242:ASP:OD1	1:A:324:TRP:NE1	2.45	0.49
1:A:1040:TRP:CG	1:A:1041:GLY:N	2.79	0.49
2:B:288:TYR:O	2:B:292:MET:HG3	2.12	0.49
2:B:503:GLU:HG3	2:B:505:TRP:CZ2	2.48	0.49
1:A:726:VAL:HA	1:A:1030:THR:HG22	1.94	0.49
1:A:735:LEU:HD12	1:A:945:PRO:HG2	1.95	0.49
1:A:873:ASN:ND2	1:A:904:GLN:OE1	2.46	0.48
2:B:133:ALA:HB1	2:B:161:PHE:HE1	1.78	0.48
2:B:997:ARG:NH1	2:B:1010:ASP:OD1	2.43	0.48
2:B:948:THR:OG1	2:B:949:PRO:HD2	2.13	0.48
1:A:70:PRO:HD3	1:A:180:LEU:HA	1.95	0.48
1:A:766:LEU:HD12	1:A:799:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:503:GLU:HG3	2:B:505:TRP:CE2	2.48	0.47
2:B:291:GLN:NE2	2:B:983:PRO:HB3	2.29	0.47
1:A:927:ILE:HD11	1:A:945:PRO:HD3	1.97	0.47
2:B:314:ASP:HB2	2:B:315:PRO:CD	2.41	0.47
2:B:530:VAL:HG21	2:B:625:CYS:SG	2.55	0.47
2:B:138:ASP:HA	2:B:141:ALA:HB3	1.96	0.47
1:A:52:GLU:HB2	1:A:1055:ALA:HB2	1.95	0.47
1:A:485:LEU:HD21	1:A:785:VAL:HG11	1.95	0.47
1:A:665:GLY:HA2	1:A:668:ARG:HH21	1.79	0.47
1:A:722:ASP:O	1:A:1033:ARG:NH1	2.47	0.47
1:A:864:TRP:N	1:A:876:GLN:O	2.23	0.47
1:A:391:TRP:CG	1:A:392:PRO:HD3	2.50	0.47
1:A:846:PRO:HG3	1:A:947:VAL:HG21	1.96	0.47
1:A:769:ALA:HB2	1:A:906:LYS:HE2	1.96	0.46
2:B:1070:SER:O	2:B:1070:SER:OG	2.25	0.46
4:B:1204:CDL:H231	4:B:1204:CDL:H473	1.96	0.46
1:A:118:ALA:HB2	1:A:157:LEU:HD21	1.96	0.46
1:A:882:TRP:HE1	1:A:897:VAL:HG21	1.80	0.46
2:B:132:VAL:HG13	2:B:179:GLY:HA2	1.97	0.46
4:A:1101:CDL:H832	4:A:1101:CDL:H862	1.67	0.46
2:B:254:LEU:H	2:B:254:LEU:HD23	1.81	0.46
2:B:861:VAL:HG12	2:B:953:PRO:HD3	1.98	0.46
1:A:106:ALA:HA	1:A:123:ARG:HD3	1.97	0.46
1:A:191:ILE:HG23	1:A:276:GLY:HA3	1.96	0.46
1:A:884:VAL:H	1:A:892:GLN:HB3	1.80	0.45
2:B:51:GLN:HB2	2:B:216:THR:HG22	1.97	0.45
4:A:1101:CDL:H722	4:A:1101:CDL:H751	1.36	0.45
2:B:436:ILE:HG21	2:B:584:LEU:HD13	1.98	0.45
1:A:700:VAL:CG1	1:A:701:TYR:N	2.68	0.45
1:A:373:ALA:HA	1:A:376:THR:HG22	1.99	0.45
4:A:1101:CDL:H392	4:A:1101:CDL:H361	1.61	0.45
2:B:1001:ASP:N	2:B:1001:ASP:OD1	2.49	0.45
1:A:736:GLN:NE2	1:A:737:PRO:O	2.50	0.45
2:B:497:ALA:O	2:B:1081:ARG:NH1	2.50	0.45
4:A:1101:CDL:H741	2:B:565:PHE:CD2	2.51	0.45
2:B:33:ALA:HA	2:B:36:LEU:HG	1.98	0.45
2:B:301:TYR:CZ	2:B:303:ALA:HB2	2.52	0.45
1:A:852:ARG:NH2	1:A:947:VAL:HG23	2.32	0.44
1:A:1079:LEU:N	1:A:1080:PRO:HD3	2.32	0.44
2:B:910:THR:HB	2:B:911:PRO:HD3	1.99	0.44
2:B:372:ALA:HB2	2:B:692:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1204:CDL:H531	4:B:1204:CDL:OB7	2.17	0.44
2:B:287:GLY:O	2:B:291:GLN:HG2	2.18	0.44
2:B:85:CYS:HG	2:B:145:CYS:CB	2.31	0.44
2:B:778:ILE:HG22	2:B:913:TRP:CD1	2.54	0.43
1:A:664:THR:O	1:A:668:ARG:NE	2.51	0.43
2:B:781:GLU:OE2	2:B:816:TYR:OH	2.24	0.43
1:A:141:SER:HA	1:A:159:VAL:HG11	2.00	0.43
2:B:285:ASP:HB2	2:B:389:ARG:HD3	2.01	0.43
1:A:354:LEU:HD23	1:A:354:LEU:HA	1.93	0.43
2:B:83:VAL:HG11	2:B:98:VAL:HG11	2.00	0.43
3:P:61:ASP:N	3:P:61:ASP:OD1	2.52	0.43
3:P:67:LEU:HD13	3:P:73:VAL:HG22	2.00	0.43
1:A:852:ARG:HH21	1:A:947:VAL:HG23	1.84	0.42
2:B:834:GLN:HG3	2:B:939:LEU:O	2.19	0.42
1:A:102:ILE:HG23	1:A:111:VAL:HG22	2.01	0.42
1:A:771:PRO:HB2	1:A:790:ILE:HG23	2.01	0.42
1:A:94:GLU:HB2	1:A:97:ARG:HB3	2.01	0.42
2:B:58:TRP:CD2	2:B:192:VAL:HG11	2.55	0.42
1:A:516:LEU:HD21	1:A:534:LEU:HD11	2.00	0.42
1:A:766:LEU:HB2	1:A:799:GLY:HA2	2.02	0.42
2:B:887:TYR:CZ	2:B:900:GLY:HA3	2.55	0.42
2:B:881:GLN:HG3	2:B:936:ASP:OD1	2.19	0.42
7:B:1201:PNS:P24	3:P:41:SER:HG	2.43	0.42
1:A:718:CYS:SG	1:A:975:CYS:HB2	2.60	0.42
1:A:994:ILE:O	1:A:1041:GLY:HA3	2.20	0.42
1:A:188:THR:O	1:A:188:THR:OG1	2.38	0.42
1:A:26:VAL:N	1:A:27:PRO:HD2	2.35	0.42
2:B:338:LEU:N	2:B:339:PRO:HD2	2.35	0.42
2:B:426:PHE:HA	2:B:475:ILE:HD12	2.02	0.42
1:A:857:VAL:O	1:A:910:ASN:HA	2.20	0.41
2:B:281:ALA:O	2:B:386:ASN:ND2	2.53	0.41
2:B:494:ILE:HD11	2:B:1078:LEU:HD12	2.01	0.41
1:A:136:VAL:HG12	1:A:136:VAL:O	2.21	0.41
2:B:436:ILE:HD13	2:B:584:LEU:HB3	2.00	0.41
1:A:69:ILE:HG22	1:A:70:PRO:O	2.20	0.41
1:A:735:LEU:HG	1:A:946:ARG:HA	2.01	0.41
1:A:876:GLN:OE1	1:A:932:PRO:HD2	2.20	0.41
1:A:901:ASP:OD1	1:A:901:ASP:N	2.53	0.41
2:B:634:TYR:CZ	2:B:974:VAL:HG12	2.55	0.41
4:B:1204:CDL:H832	4:B:1204:CDL:H802	1.79	0.41
1:A:64:ALA:HB3	1:A:185:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:PRO:C	1:A:80:ASP:H	2.24	0.41
1:A:786:ASP:OD1	2:B:516:LEU:HD22	2.21	0.41
1:A:188:THR:HB	1:A:191:ILE:HD12	2.02	0.41
1:A:247:GLY:O	1:A:251:ILE:HG23	2.21	0.41
1:A:610:PHE:CG	1:A:611:TYR:N	2.87	0.41
2:B:85:CYS:SG	2:B:145:CYS:HB3	2.61	0.41
2:B:259:TRP:NE1	2:B:354:GLU:OE2	2.43	0.41
2:B:347:CYS:SG	2:B:396:THR:OG1	2.64	0.41
1:A:320:ALA:HB2	1:A:357:TRP:CZ2	2.57	0.40
1:A:442:ALA:HB3	1:A:443:PRO:HD3	2.02	0.40
1:A:670:LEU:HD23	1:A:670:LEU:H	1.86	0.40
1:A:994:ILE:HD11	1:A:1044:GLU:HG3	2.02	0.40
1:A:63:ARG:NH1	1:A:187:ASP:OD1	2.54	0.40
4:B:1204:CDL:OB7	4:B:1204:CDL:C53	2.69	0.40
1:A:137:TRP:HZ3	1:A:146:ASP:HB3	1.86	0.40
1:A:968:ALA:HB3	1:A:995:PRO:HG3	2.04	0.40
1:A:1042:SER:OG	1:A:1043:ILE:N	2.55	0.40
2:B:596:ALA:O	2:B:600:VAL:HG22	2.21	0.40
2:B:821:LYS:HA	2:B:821:LYS:HD3	1.89	0.40
1:A:113:PHE:O	1:A:114:ARG:C	2.60	0.40
2:B:714:TYR:CD2	2:B:714:TYR:C	2.95	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	1076/1088 (99%)	967 (90%)	107 (10%)	2 (0%)	47 78
2	B	1061/1100 (96%)	991 (93%)	69 (6%)	1 (0%)	51 82
3	P	88/99 (89%)	81 (92%)	7 (8%)	0	100 100
All	All	2225/2287 (97%)	2039 (92%)	183 (8%)	3 (0%)	54 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	PRO
1	A	699	PRO
1	A	700	VAL

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	831/841 (99%)	827 (100%)	4 (0%)	88 96
2	B	849/878 (97%)	847 (100%)	2 (0%)	93 98
3	P	73/81 (90%)	73 (100%)	0	100 100
All	All	1753/1800 (97%)	1747 (100%)	6 (0%)	92 98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	697	ARG
1	A	699	PRO
1	A	833	LYS
1	A	837	LYS
2	B	145	CYS
2	B	713	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	HIS
1	A	177	GLN
1	A	301	HIS
1	A	361	ASN
1	A	482	GLN
1	A	741	GLN
1	A	760	ASN

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Mol	Chain	Res	Type
1	A	832	ASN
1	A	873	ASN
1	A	938	GLN
1	A	960	GLN
2	B	291	GLN
2	B	393	GLN
2	B	610	ASN
2	B	653	GLN
2	B	719	ASN
2	B	875	ASN
2	B	956	GLN
2	B	959	GLN
2	B	1013	GLN

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

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	CDL	A	1101	-	90,90,99	1.14	7 (7%)	96,102,111	1.71	11 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	PO4	B	1202	-	4,4,4	0.95	0	6,6,6	0.47	0
4	CDL	B	1204	-	97,97,99	1.29	13 (13%)	103,109,111	1.79	16 (15%)
9	95E	B	1203	-	13,13,13	0.62	0	10,14,14	1.38	1 (10%)
5	F8L	A	1102	-	48,49,64	3.31	14 (29%)	61,63,81	2.51	17 (27%)
7	PNS	B	1201	-	17,21,21	2.09	4 (23%)	26,29,29	1.20	2 (7%)

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
4	CDL	A	1101	-	-	57/101/101/110	-
4	CDL	B	1204	-	-	60/108/108/110	-
9	95E	B	1203	-	-	3/15/15/15	-
5	F8L	A	1102	-	-	17/49/66/84	0/1/1/1
7	PNS	B	1201	-	-	10/27/27/27	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1102	F8L	C55-C57	-15.58	1.33	1.52
5	A	1102	F8L	O56-C55	10.27	1.60	1.41
5	A	1102	F8L	C59-C61	-6.23	1.37	1.53
7	B	1201	PNS	C34-N36	5.32	1.45	1.33
7	B	1201	PNS	C39-N41	5.30	1.45	1.33
4	A	1101	CDL	OA6-CA5	4.91	1.48	1.34
4	B	1204	CDL	OB8-CB6	-4.15	1.35	1.45
4	B	1204	CDL	OA8-CA7	4.02	1.45	1.33
4	A	1101	CDL	OB6-CB5	3.96	1.45	1.34
5	A	1102	F8L	O56-C61	3.83	1.53	1.45
5	A	1102	F8L	C59-C57	3.76	1.63	1.53
4	A	1101	CDL	OA8-CA7	3.64	1.44	1.33
4	B	1204	CDL	OA6-CA5	3.62	1.44	1.34
4	B	1204	CDL	OB6-CB5	3.38	1.43	1.34
4	A	1101	CDL	OB8-CB6	-3.20	1.37	1.45
4	B	1204	CDL	PB2-OB4	-2.81	1.42	1.55
4	A	1101	CDL	OB6-CB4	-2.80	1.39	1.46
5	A	1102	F8L	C26-C27	2.70	1.56	1.51
4	A	1101	CDL	OB8-CB7	2.62	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1204	CDL	OA6-CA4	-2.53	1.40	1.46
4	B	1204	CDL	PA1-OA3	-2.49	1.42	1.50
5	A	1102	F8L	C31-C32	2.49	1.56	1.51
5	A	1102	F8L	C41-C42	2.44	1.56	1.51
5	A	1102	F8L	C21-C22	2.40	1.56	1.51
5	A	1102	F8L	C36-C37	2.37	1.56	1.51
4	B	1204	CDL	PA1-OA4	-2.34	1.44	1.55
5	A	1102	F8L	P52-O54	2.32	1.66	1.60
5	A	1102	F8L	C16-C17	2.32	1.56	1.50
7	B	1201	PNS	O35-C34	-2.29	1.18	1.23
4	B	1204	CDL	OB5-CB3	-2.28	1.36	1.44
4	A	1101	CDL	OB9-CB7	-2.27	1.15	1.22
5	A	1102	F8L	C50-C49	2.26	1.55	1.49
7	B	1201	PNS	O40-C39	-2.19	1.18	1.23
5	A	1102	F8L	C46-C47	2.16	1.55	1.51
4	B	1204	CDL	OB8-CB7	2.13	1.39	1.33
4	B	1204	CDL	C71-CB7	-2.12	1.44	1.50
4	B	1204	CDL	OB9-CB7	-2.10	1.16	1.22
4	B	1204	CDL	PB2-OB3	-2.09	1.43	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1204	CDL	CB6-CB4-CB3	-8.81	90.95	111.79
5	A	1102	F8L	C50-C49-C47	-7.42	113.21	126.04
4	A	1101	CDL	OA6-CA5-C11	6.73	126.01	111.50
4	B	1204	CDL	OA6-CA5-C11	6.44	125.39	111.50
5	A	1102	F8L	C35-C34-C32	-6.37	112.31	127.66
5	A	1102	F8L	C30-C29-C27	-6.28	112.55	127.66
4	A	1101	CDL	OB6-CB5-C51	6.23	124.94	111.50
5	A	1102	F8L	C40-C39-C37	-6.19	112.75	127.66
5	A	1102	F8L	C45-C44-C42	-6.19	112.76	127.66
5	A	1102	F8L	C25-C24-C22	-6.12	112.94	127.66
4	A	1101	CDL	CA6-CA4-CA3	-5.71	98.29	111.79
4	B	1204	CDL	OB6-CB5-C51	4.87	121.99	111.50
5	A	1102	F8L	C55-C57-C59	4.69	108.24	102.30
5	A	1102	F8L	C20-C19-C17	-4.58	112.08	127.75
4	A	1101	CDL	OB8-CB7-C71	4.42	125.77	111.91
4	A	1101	CDL	OA8-CA7-C31	4.27	125.32	111.91
4	A	1101	CDL	OA8-CA7-OA9	-3.71	114.22	123.59
4	A	1101	CDL	OB8-CB7-OB9	-3.55	114.63	123.59
4	A	1101	CDL	OB6-CB5-OB7	-3.40	115.48	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1204	CDL	OA8-CA7-C31	3.35	122.41	111.91
4	A	1101	CDL	CB6-CB4-CB3	-3.31	103.95	111.79
5	A	1102	F8L	C48-C47-C46	2.81	120.00	115.27
4	B	1204	CDL	OA8-CA6-CA4	2.80	116.58	108.43
4	B	1204	CDL	OB8-CB7-C71	2.74	120.51	111.91
5	A	1102	F8L	C28-C27-C26	2.74	119.88	115.27
7	B	1201	PNS	C37-C38-C39	2.72	116.89	112.36
5	A	1102	F8L	C57-C59-C61	2.67	107.83	102.64
5	A	1102	F8L	C33-C32-C31	2.58	119.61	115.27
5	A	1102	F8L	C23-C22-C21	2.54	119.55	115.27
5	A	1102	F8L	C38-C37-C36	2.53	119.52	115.27
4	A	1101	CDL	CA4-OA6-CA5	2.45	123.83	117.79
4	B	1204	CDL	C73-C72-C71	-2.44	104.41	113.19
9	B	1203	95E	C8-N9-C10	-2.44	109.36	114.14
4	B	1204	CDL	OB8-CB7-OB9	-2.39	117.55	123.59
4	A	1101	CDL	OA7-CA5-C11	-2.39	114.43	123.73
4	B	1204	CDL	OA2-PA1-OA3	-2.36	99.83	109.07
5	A	1102	F8L	C43-C42-C41	2.30	119.14	115.27
4	B	1204	CDL	CA6-OA8-CA7	2.30	125.63	117.12
4	B	1204	CDL	OA6-CA5-OA7	-2.29	118.16	123.70
4	B	1204	CDL	C76-C75-C74	-2.23	103.08	114.42
7	B	1201	PNS	C38-C39-N41	2.22	120.16	116.42
5	A	1102	F8L	O54-C55-C57	2.21	110.47	106.72
4	B	1204	CDL	C84-C83-C82	-2.19	103.30	114.42
5	A	1102	F8L	C18-C17-C16	2.18	119.43	114.60
4	B	1204	CDL	C78-C77-C76	-2.17	103.42	114.42
4	B	1204	CDL	OB6-CB5-OB7	-2.12	118.58	123.70
4	B	1204	CDL	C41-C40-C39	-2.11	103.73	114.42

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	CDL	CA3-OA5-PA1-OA2
4	A	1101	CDL	CA3-OA5-PA1-OA3
4	A	1101	CDL	CB2-OB2-PB2-OB3
4	A	1101	CDL	CB2-OB2-PB2-OB5
4	A	1101	CDL	CB3-OB5-PB2-OB2
4	A	1101	CDL	CB3-OB5-PB2-OB3
4	A	1101	CDL	CB3-OB5-PB2-OB4
4	B	1204	CDL	CA3-OA5-PA1-OA2
4	B	1204	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
4	B	1204	CDL	CA3-OA5-PA1-OA4
4	B	1204	CDL	C11-CA5-OA6-CA4
4	B	1204	CDL	CB2-OB2-PB2-OB3
4	B	1204	CDL	CB3-OB5-PB2-OB3
4	B	1204	CDL	OB9-CB7-OB8-CB6
4	B	1204	CDL	C71-CB7-OB8-CB6
5	A	1102	F8L	C25-C26-C27-C28
5	A	1102	F8L	C25-C26-C27-C29
5	A	1102	F8L	C39-C40-C41-C42
5	A	1102	F8L	C40-C41-C42-C43
5	A	1102	F8L	C40-C41-C42-C44
5	A	1102	F8L	C50-O51-P52-O64
7	B	1201	PNS	C28-O27-P24-O23
7	B	1201	PNS	C28-O27-P24-O25
7	B	1201	PNS	N41-C42-C43-S44
9	B	1203	95E	C11-C10-C13-C14
4	A	1101	CDL	OB9-CB7-OB8-CB6
4	A	1101	CDL	C71-CB7-OB8-CB6
4	B	1204	CDL	C31-CA7-OA8-CA6
4	B	1204	CDL	OA9-CA7-OA8-CA6
4	A	1101	CDL	OA7-CA5-OA6-CA4
4	B	1204	CDL	OA7-CA5-OA6-CA4
4	A	1101	CDL	C11-CA5-OA6-CA4
7	B	1201	PNS	C38-C39-N41-C42
9	B	1203	95E	N6-C7-C8-N9
4	A	1101	CDL	C36-C37-C38-C39
4	A	1101	CDL	C83-C84-C85-C86
5	A	1102	F8L	C45-C46-C47-C48
5	A	1102	F8L	C45-C46-C47-C49
7	B	1201	PNS	O40-C39-N41-C42
4	B	1204	CDL	C54-C55-C56-C57
4	B	1204	CDL	CA7-C31-C32-C33
4	A	1101	CDL	C15-C16-C17-C18
5	A	1102	F8L	C44-C45-C46-C47
4	A	1101	CDL	CA2-OA2-PA1-OA5
4	B	1204	CDL	CB3-OB5-PB2-OB2
5	A	1102	F8L	C50-O51-P52-O54
4	A	1101	CDL	C38-C39-C40-C41
4	A	1101	CDL	C18-C19-C20-C21
4	B	1204	CDL	C41-C42-C43-C44
4	A	1101	CDL	C37-C38-C39-C40
4	B	1204	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
4	A	1101	CDL	CA6-CA4-OA6-CA5
4	A	1101	CDL	C13-C14-C15-C16
4	B	1204	CDL	C19-C20-C21-C22
4	B	1204	CDL	C22-C23-C24-C25
4	B	1204	CDL	O1-C1-CB2-OB2
4	B	1204	CDL	C17-C18-C19-C20
4	A	1101	CDL	C74-C75-C76-C77
4	A	1101	CDL	C63-C64-C65-C66
4	B	1204	CDL	C58-C59-C60-C61
4	A	1101	CDL	C78-C79-C80-C81
4	B	1204	CDL	C40-C41-C42-C43
4	B	1204	CDL	C57-C58-C59-C60
5	A	1102	F8L	C34-C35-C36-C37
4	B	1204	CDL	C71-C72-C73-C74
4	A	1101	CDL	C62-C63-C64-C65
4	B	1204	CDL	C35-C36-C37-C38
4	A	1101	CDL	C56-C57-C58-C59
4	B	1204	CDL	CA5-C11-C12-C13
4	B	1204	CDL	C81-C82-C83-C84
4	B	1204	CDL	C74-C75-C76-C77
4	B	1204	CDL	C11-C12-C13-C14
4	B	1204	CDL	C84-C85-C86-C87
4	A	1101	CDL	C31-CA7-OA8-CA6
4	A	1101	CDL	C19-C20-C21-C22
4	A	1101	CDL	C35-C36-C37-C38
4	B	1204	CDL	C53-C54-C55-C56
7	B	1201	PNS	N36-C37-C38-C39
4	B	1204	CDL	C42-C43-C44-C45
4	A	1101	CDL	C51-CB5-OB6-CB4
4	A	1101	CDL	OA5-CA3-CA4-OA6
4	A	1101	CDL	C31-C32-C33-C34
4	A	1101	CDL	OB7-CB5-OB6-CB4
4	B	1204	CDL	OB5-CB3-CB4-CB6
4	A	1101	CDL	C16-C17-C18-C19
4	A	1101	CDL	CB3-CB4-CB6-OB8
4	B	1204	CDL	C36-C37-C38-C39
4	A	1101	CDL	C32-C33-C34-C35
9	B	1203	95E	N9-C10-C13-C14
7	B	1201	PNS	C28-O27-P24-O26
4	B	1204	CDL	C80-C81-C82-C83
4	A	1101	CDL	C72-C73-C74-C75
5	A	1102	F8L	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
5	A	1102	F8L	C35-C36-C37-C39
4	A	1101	CDL	OA9-CA7-OA8-CA6
4	B	1204	CDL	C23-C24-C25-C26
4	A	1101	CDL	C20-C21-C22-C23
4	A	1101	CDL	C75-C76-C77-C78
4	A	1101	CDL	OA5-CA3-CA4-CA6
5	A	1102	F8L	C29-C30-C31-C32
4	B	1204	CDL	C20-C21-C22-C23
4	A	1101	CDL	CA3-CA4-CA6-OA8
4	B	1204	CDL	C60-C61-C62-C63
4	B	1204	CDL	C37-C38-C39-C40
4	A	1101	CDL	C51-C52-C53-C54
4	A	1101	CDL	C58-C59-C60-C61
4	B	1204	CDL	C15-C16-C17-C18
4	B	1204	CDL	OB5-CB3-CB4-OB6
4	A	1101	CDL	C59-C60-C61-C62
4	B	1204	CDL	C24-C25-C26-C27
4	A	1101	CDL	OA6-CA4-CA6-OA8
4	B	1204	CDL	OA6-CA4-CA6-OA8
4	B	1204	CDL	C1-CB2-OB2-PB2
4	B	1204	CDL	C55-C56-C57-C58
4	A	1101	CDL	CB6-CB4-OB6-CB5
4	B	1204	CDL	C72-C73-C74-C75
4	A	1101	CDL	C79-C80-C81-C82
4	B	1204	CDL	CB2-OB2-PB2-OB5
4	A	1101	CDL	O1-C1-CA2-OA2
4	A	1101	CDL	CA2-OA2-PA1-OA3
4	A	1101	CDL	CA2-OA2-PA1-OA4
4	A	1101	CDL	CA3-OA5-PA1-OA4
4	B	1204	CDL	CB3-OB5-PB2-OB4
5	A	1102	F8L	C50-O51-P52-O53
4	B	1204	CDL	C77-C78-C79-C80
5	A	1102	F8L	C19-C20-C21-C22
4	B	1204	CDL	C34-C35-C36-C37
7	B	1201	PNS	O27-C28-C29-C32
4	B	1204	CDL	C21-C22-C23-C24
7	B	1201	PNS	O27-C28-C29-C31
4	B	1204	CDL	CA6-CA4-OA6-CA5
4	B	1204	CDL	C12-C13-C14-C15
4	A	1101	CDL	OB6-CB4-CB6-OB8
4	A	1101	CDL	C76-C77-C78-C79
4	A	1101	CDL	C52-C53-C54-C55

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Mol	Chain	Res	Type	Atoms
4	A	1101	CDL	C73-C74-C75-C76
7	B	1201	PNS	O27-C28-C29-C30
4	B	1204	CDL	CA3-CA4-OA6-CA5
4	A	1101	CDL	C39-C40-C41-C42
4	B	1204	CDL	OB6-CB4-CB6-OB8
4	B	1204	CDL	CA2-C1-CB2-OB2
4	B	1204	CDL	C39-C40-C41-C42
4	B	1204	CDL	CA3-CA4-CA6-OA8
4	B	1204	CDL	C52-C53-C54-C55
5	A	1102	F8L	C57-C55-O54-P52
4	A	1101	CDL	C52-C51-CB5-OB6
4	B	1204	CDL	C38-C39-C40-C41

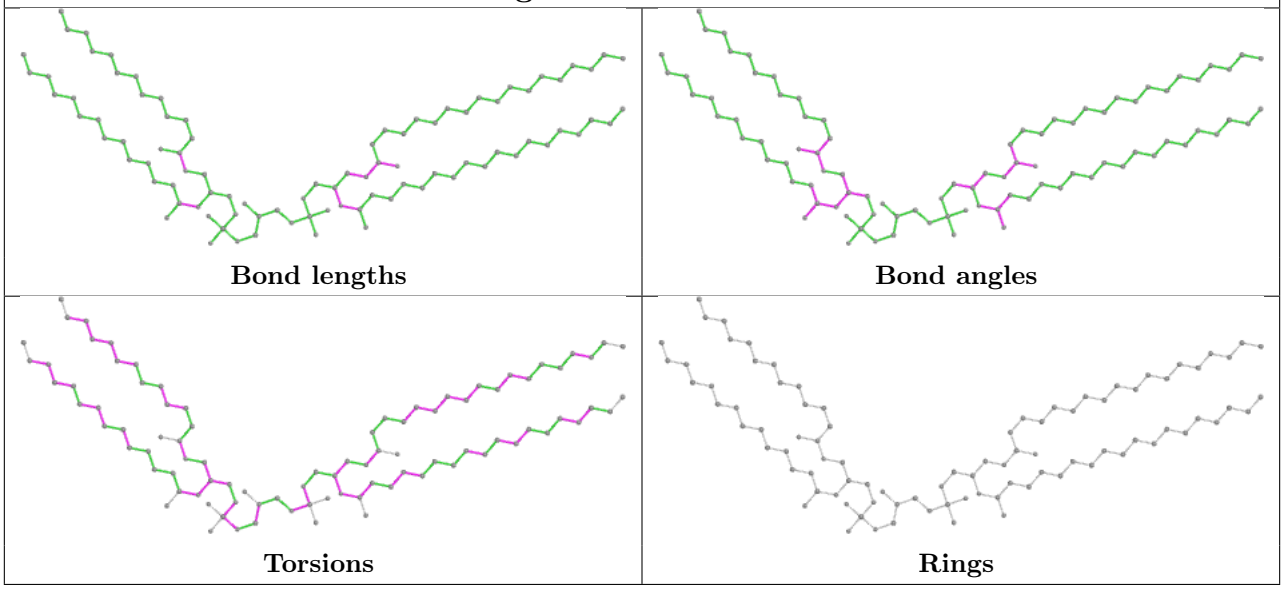
There are no ring outliers.

4 monomers are involved in 16 short contacts:

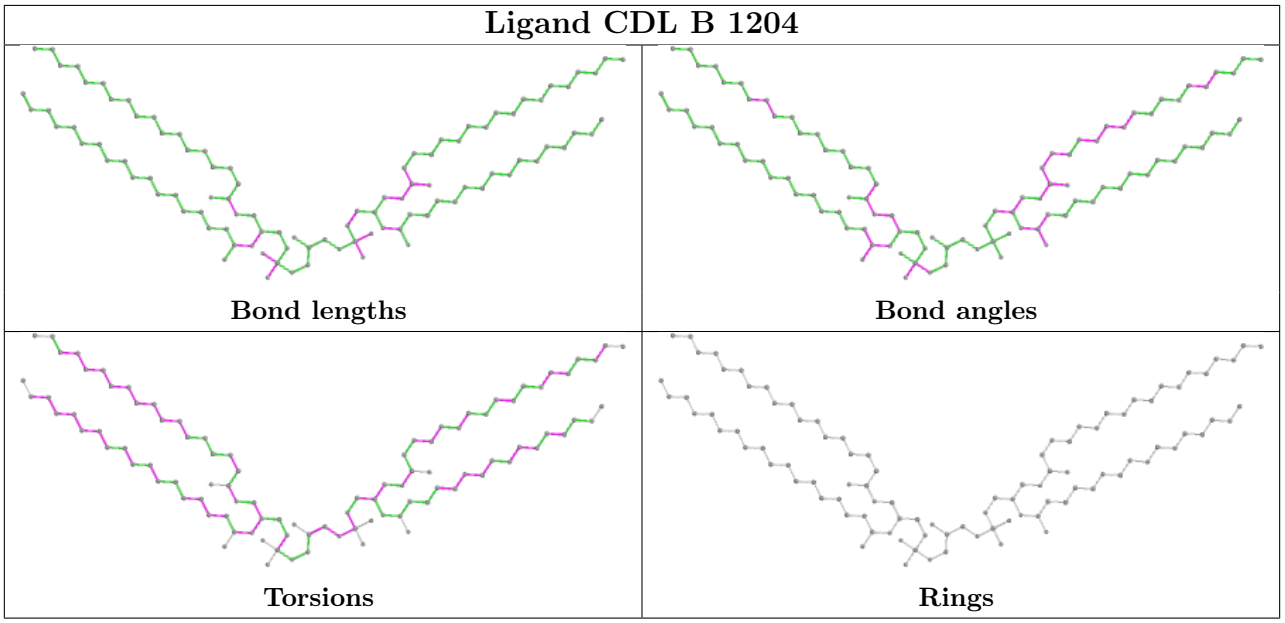
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	CDL	6	0
8	B	1202	PO4	1	0
4	B	1204	CDL	8	0
7	B	1201	PNS	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

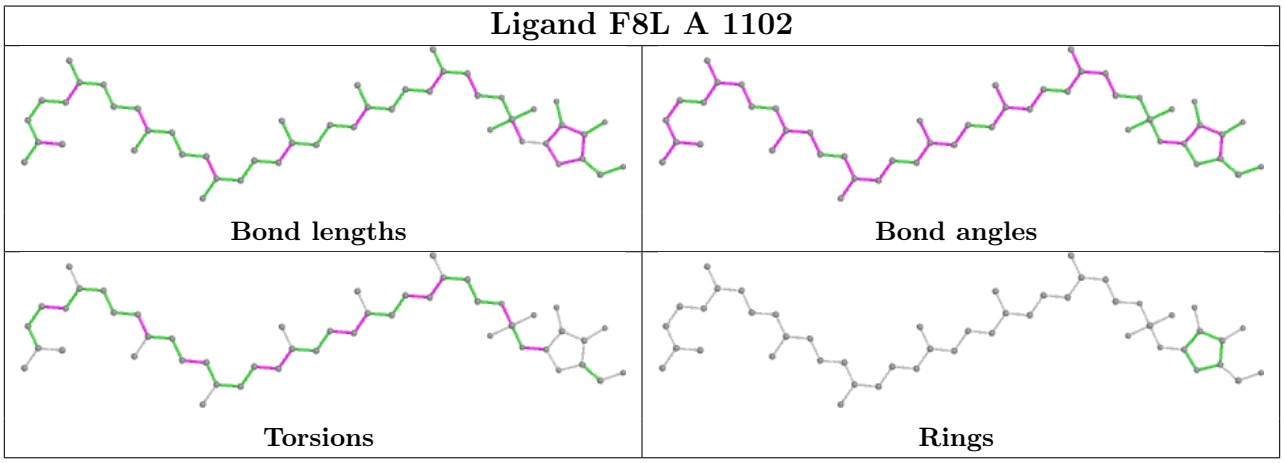
Ligand CDL A 1101



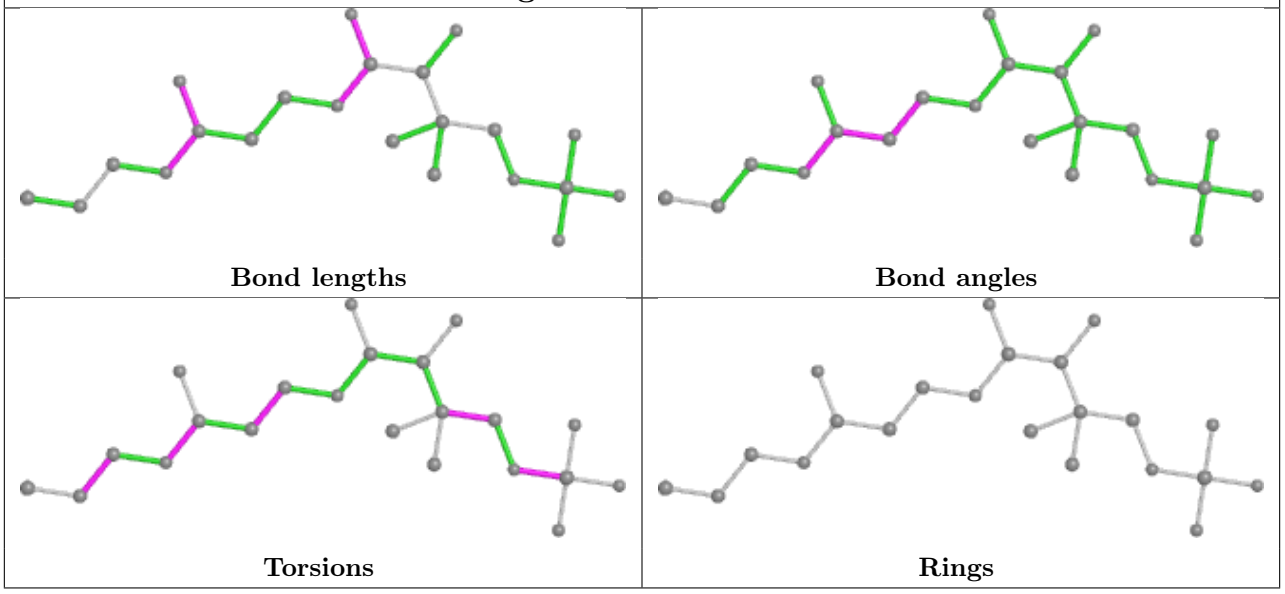
Ligand CDL B 1204



Ligand F8L A 1102



Ligand PNS B 1201



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.

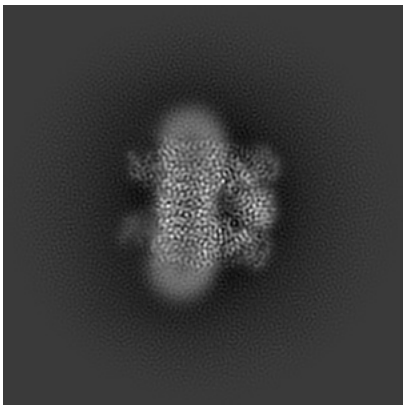
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-30216. These allow visual inspection of the internal detail of the map and identification of artifacts.

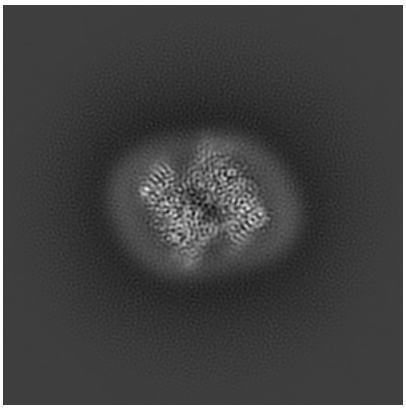
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

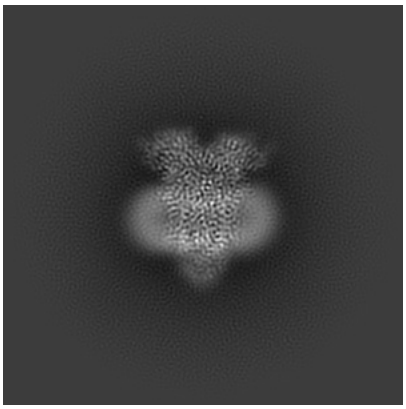
6.1.1 Primary map



X

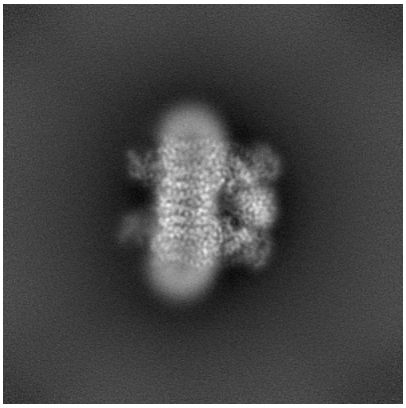


Y

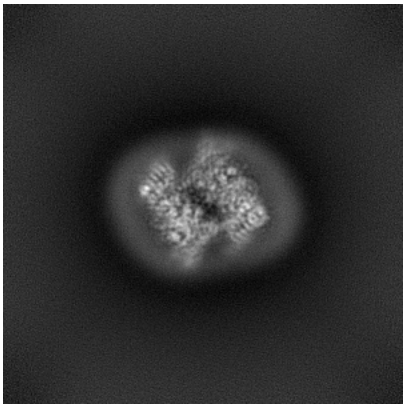


Z

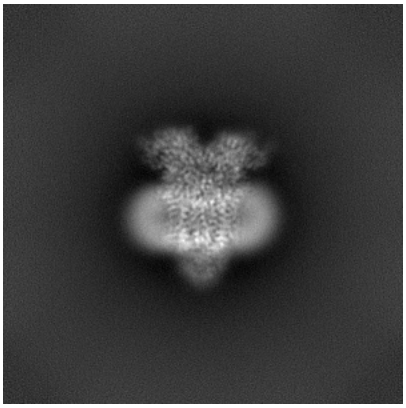
6.1.2 Raw map



X



Y

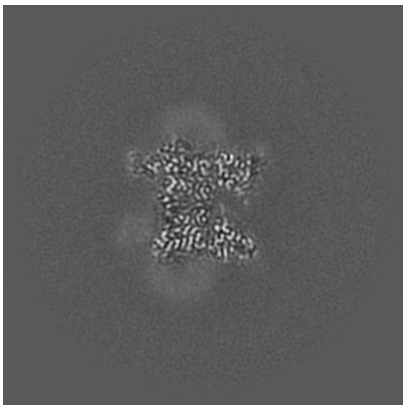


Z

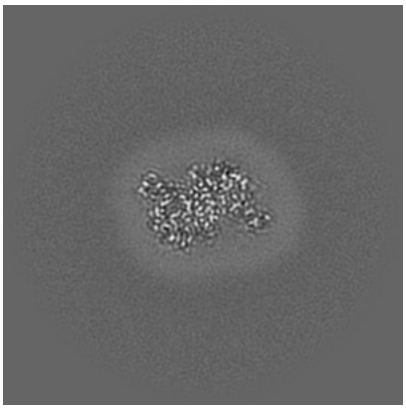
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

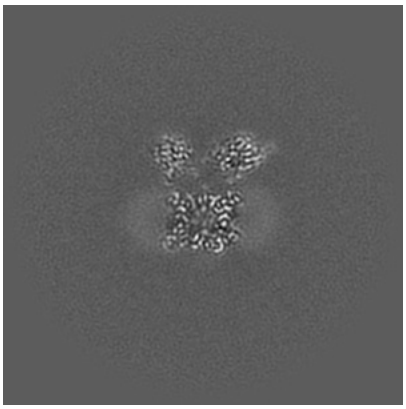
6.2.1 Primary map



X Index: 192

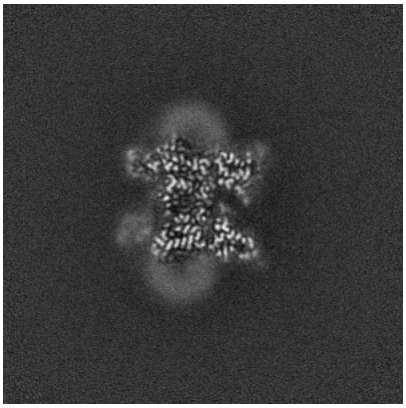


Y Index: 192

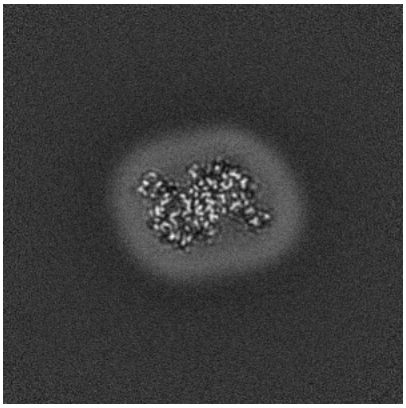


Z Index: 192

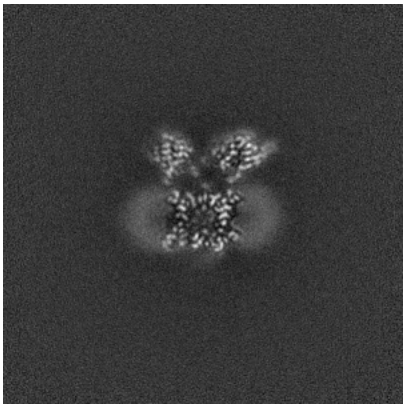
6.2.2 Raw map



X Index: 192



Y Index: 192

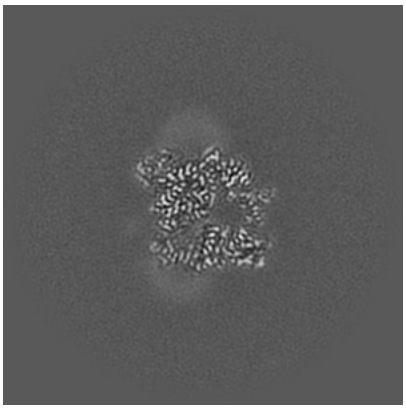


Z Index: 192

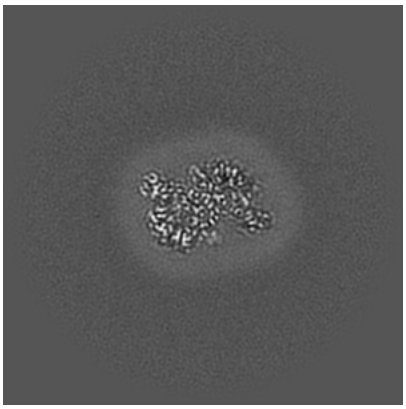
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

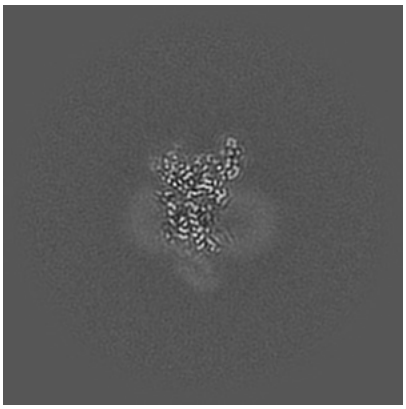
6.3.1 Primary map



X Index: 208

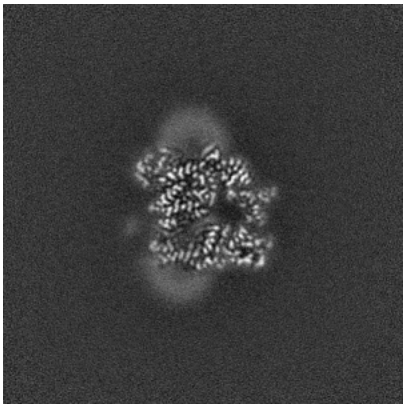


Y Index: 194

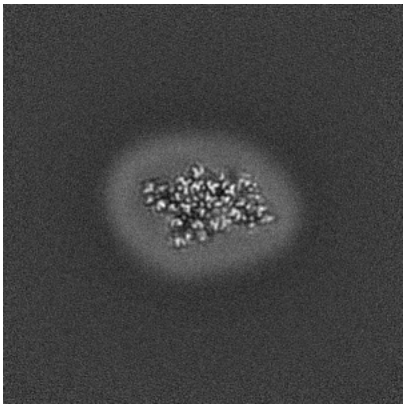


Z Index: 162

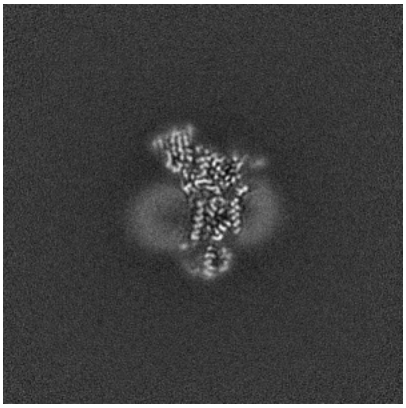
6.3.2 Raw map



X Index: 208



Y Index: 159

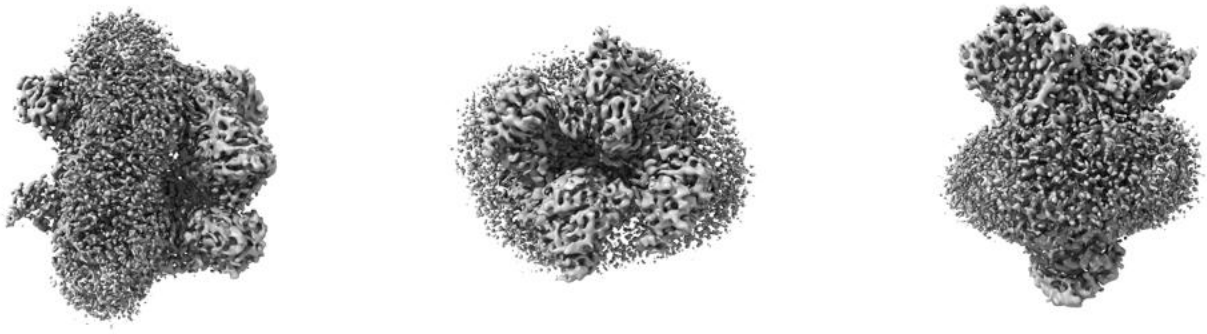


Z Index: 220

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.

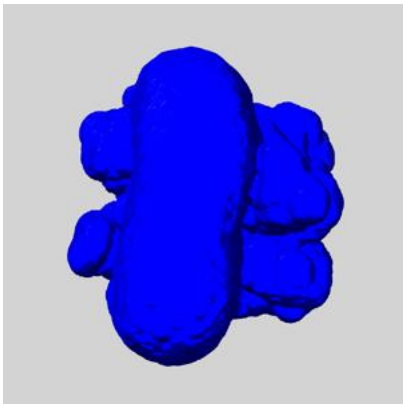
6.5 Mask visualisation (i)

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

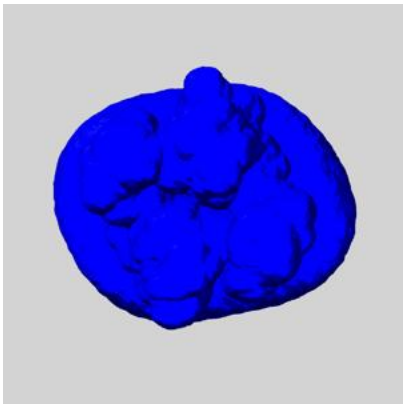
A mask typically either:

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

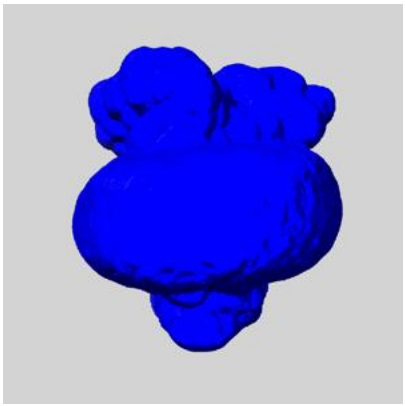
6.5.1 emd_30216_msk_1.map (i)



X



Y

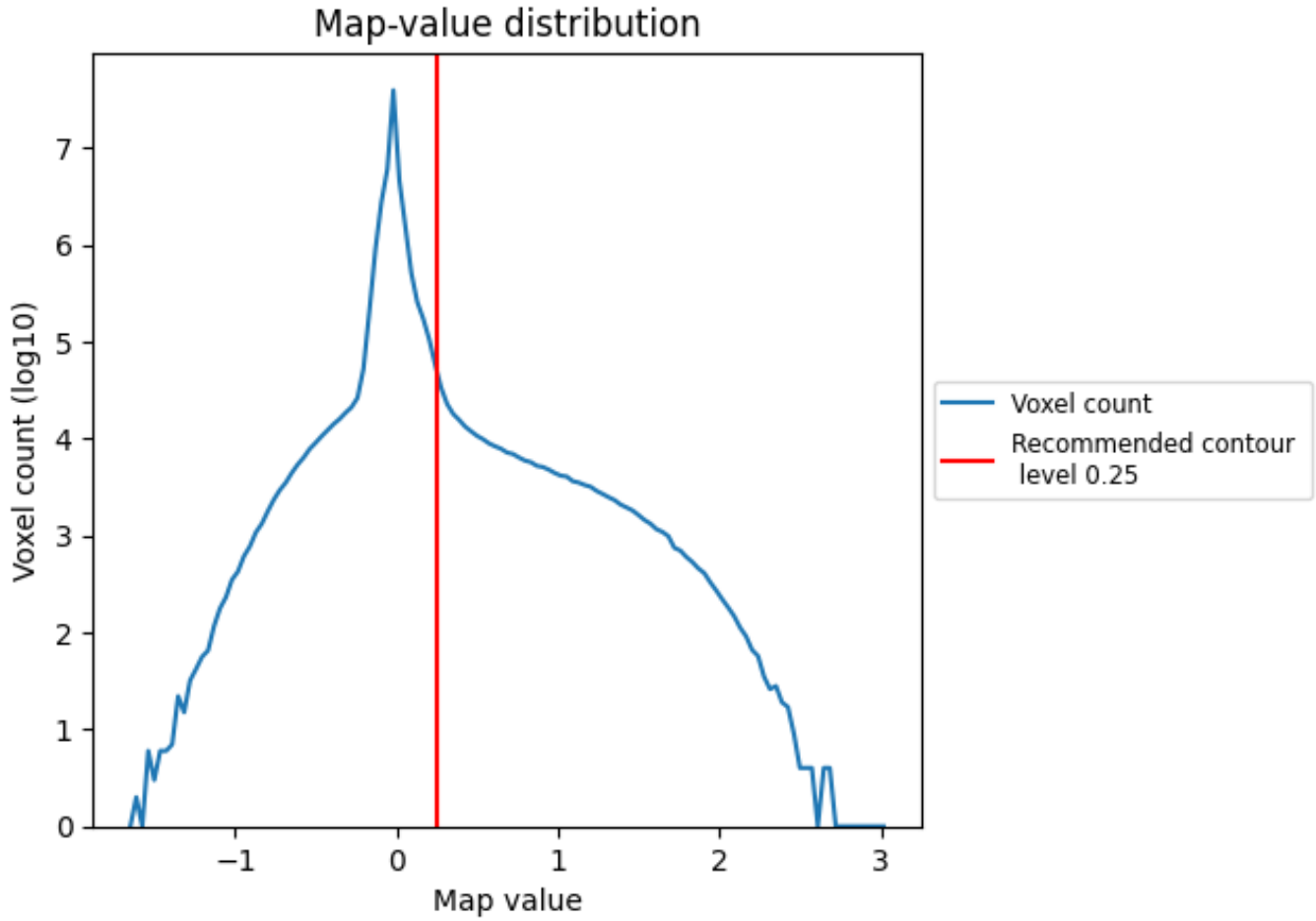


Z

7 Map analysis

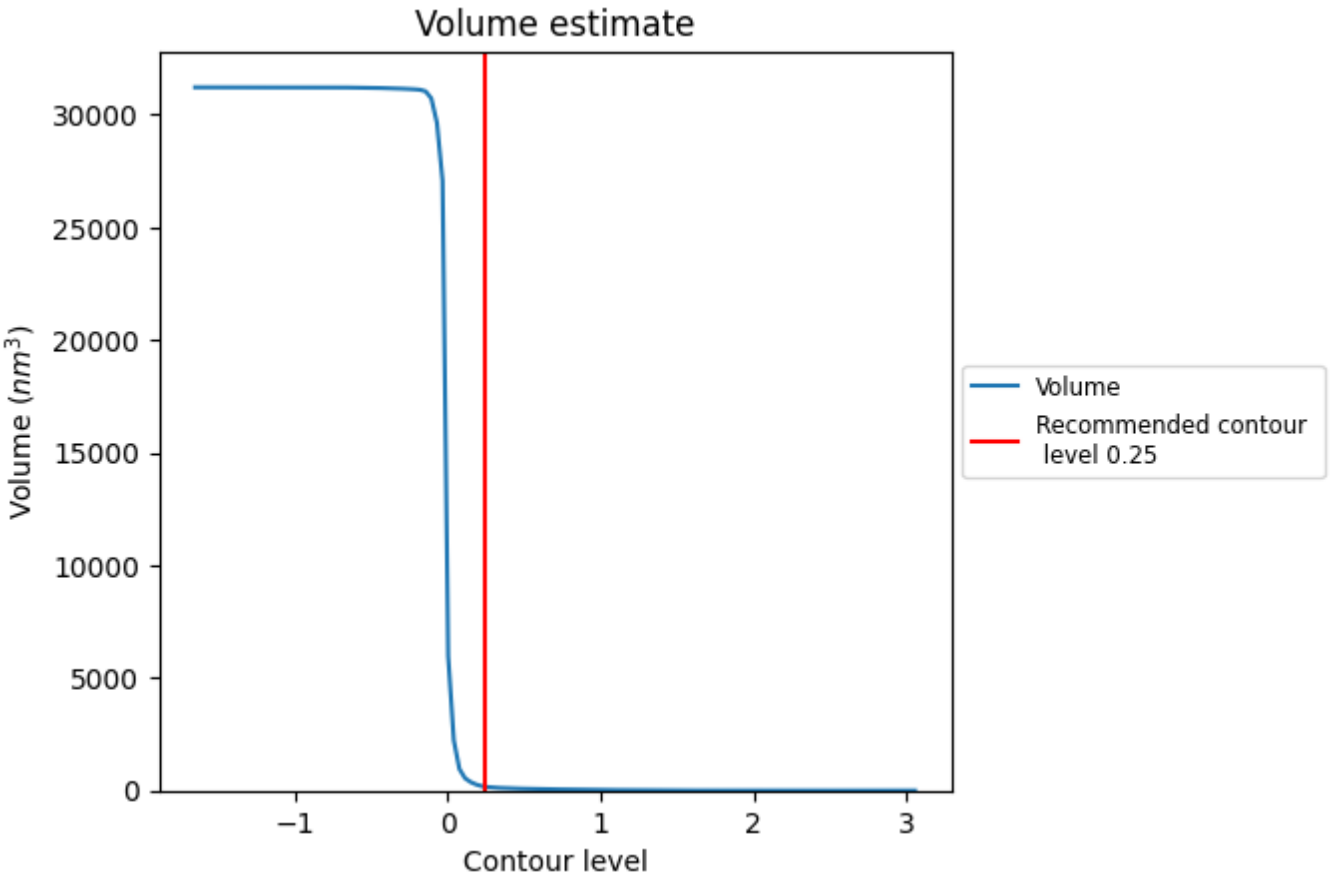
This section contains the results of statistical analysis of the map.

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.

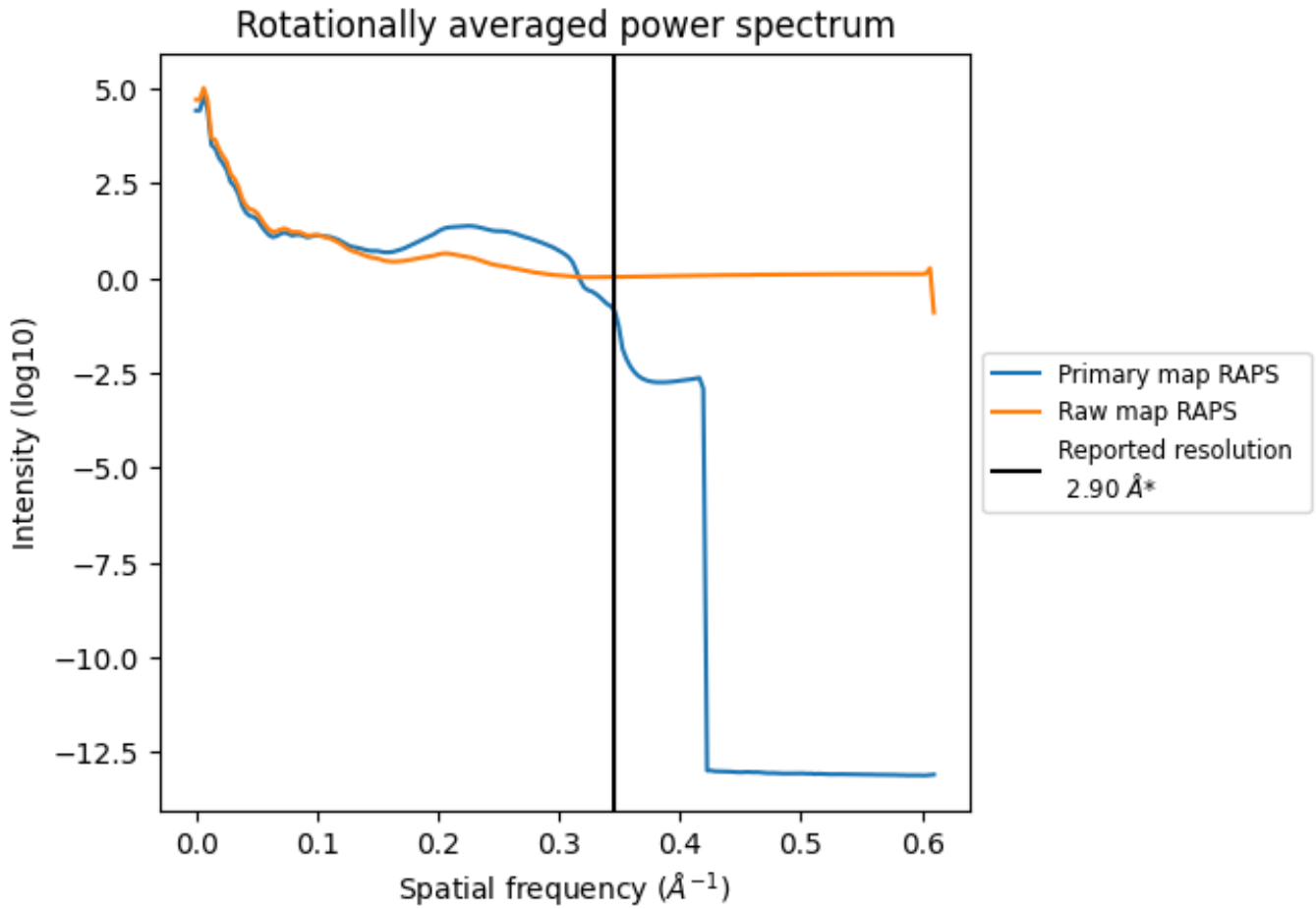
7.2 Volume estimate



The volume at the recommended contour level is 169 nm^3; this corresponds to an approximate mass of 152 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)

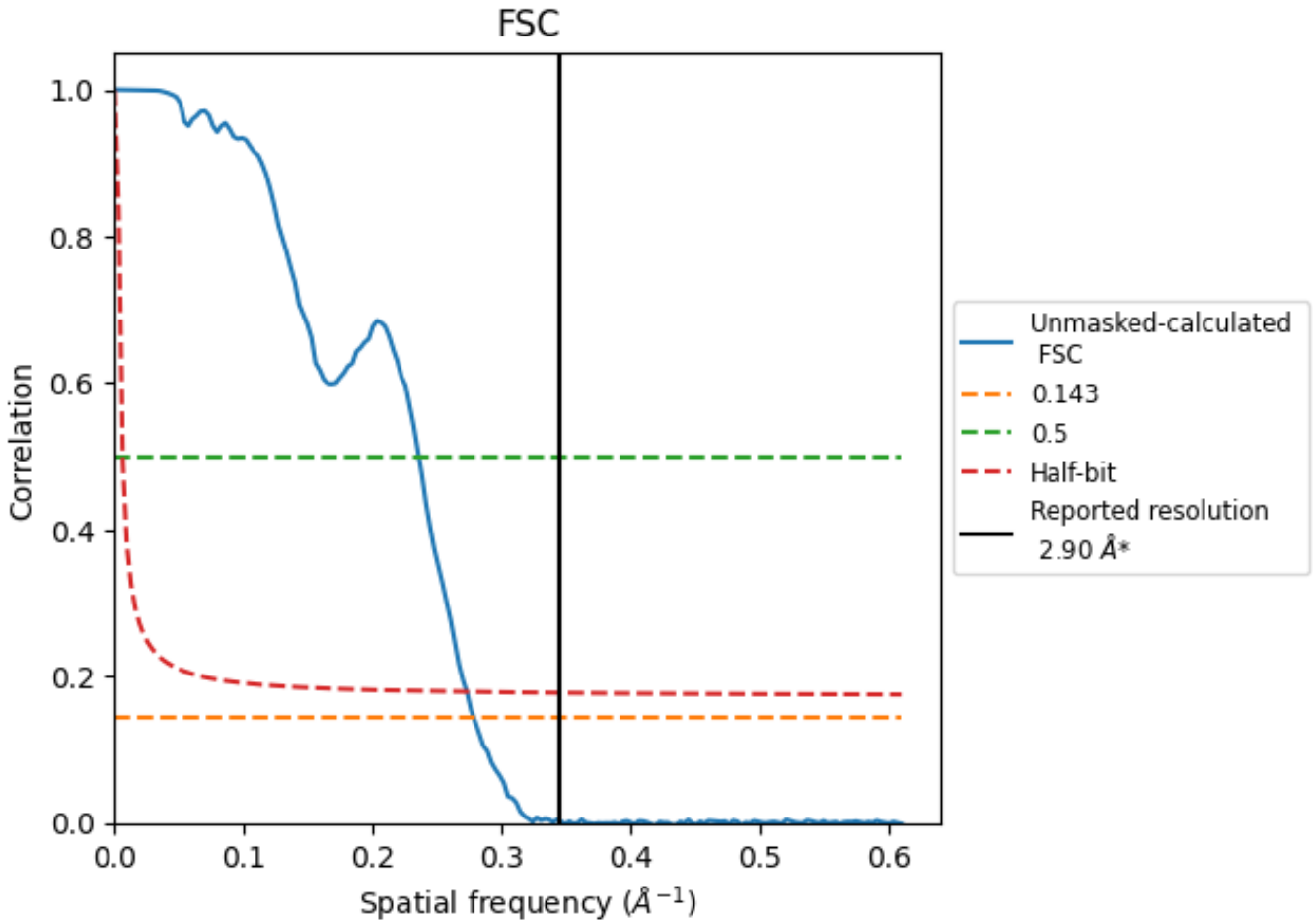


*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

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 0.345 Å^{-1}

8.2 Resolution estimates (i)

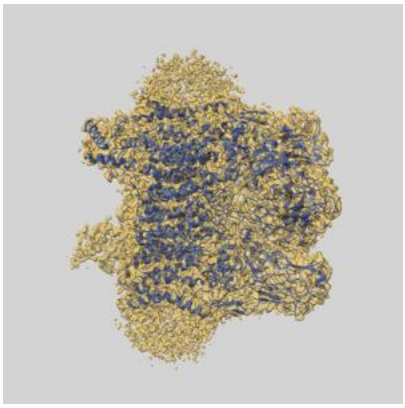
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.59	4.24	3.66

*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 3.59 differs from the reported value 2.9 by more than 10 %

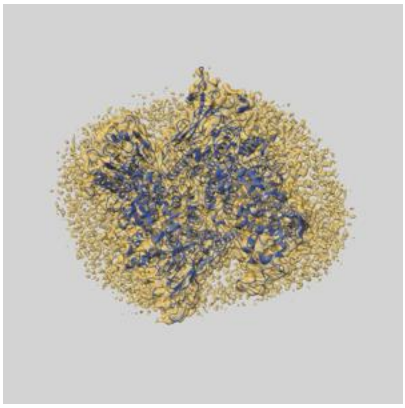
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-30216 and PDB model 7BVC. Per-residue inclusion information can be found in section 3 on page 8.

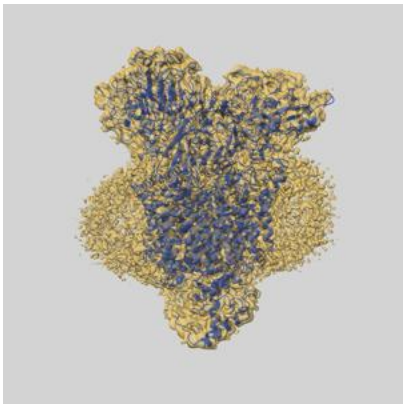
9.1 Map-model overlay



X



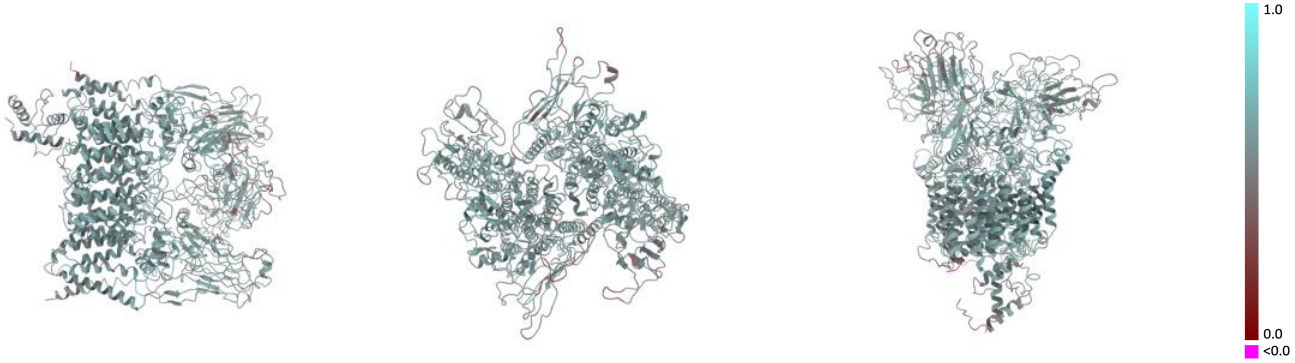
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

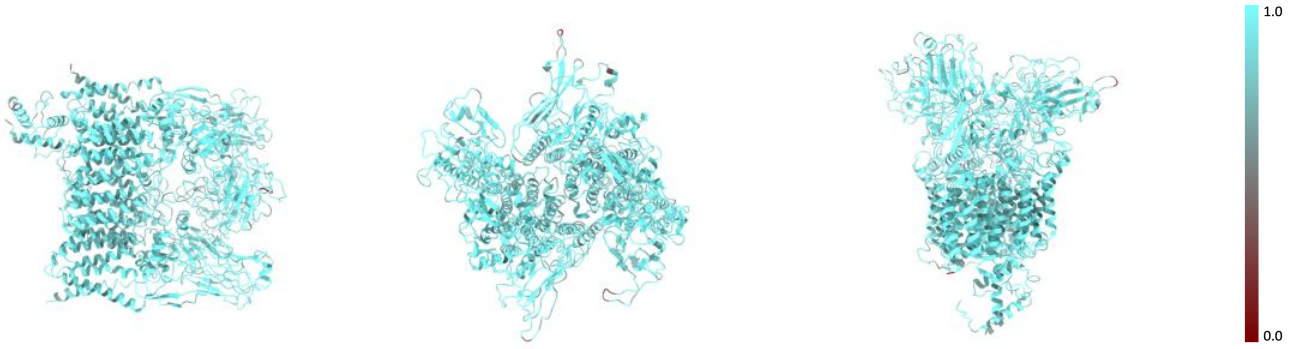
9.2 Q-score mapped to coordinate model (i)



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.

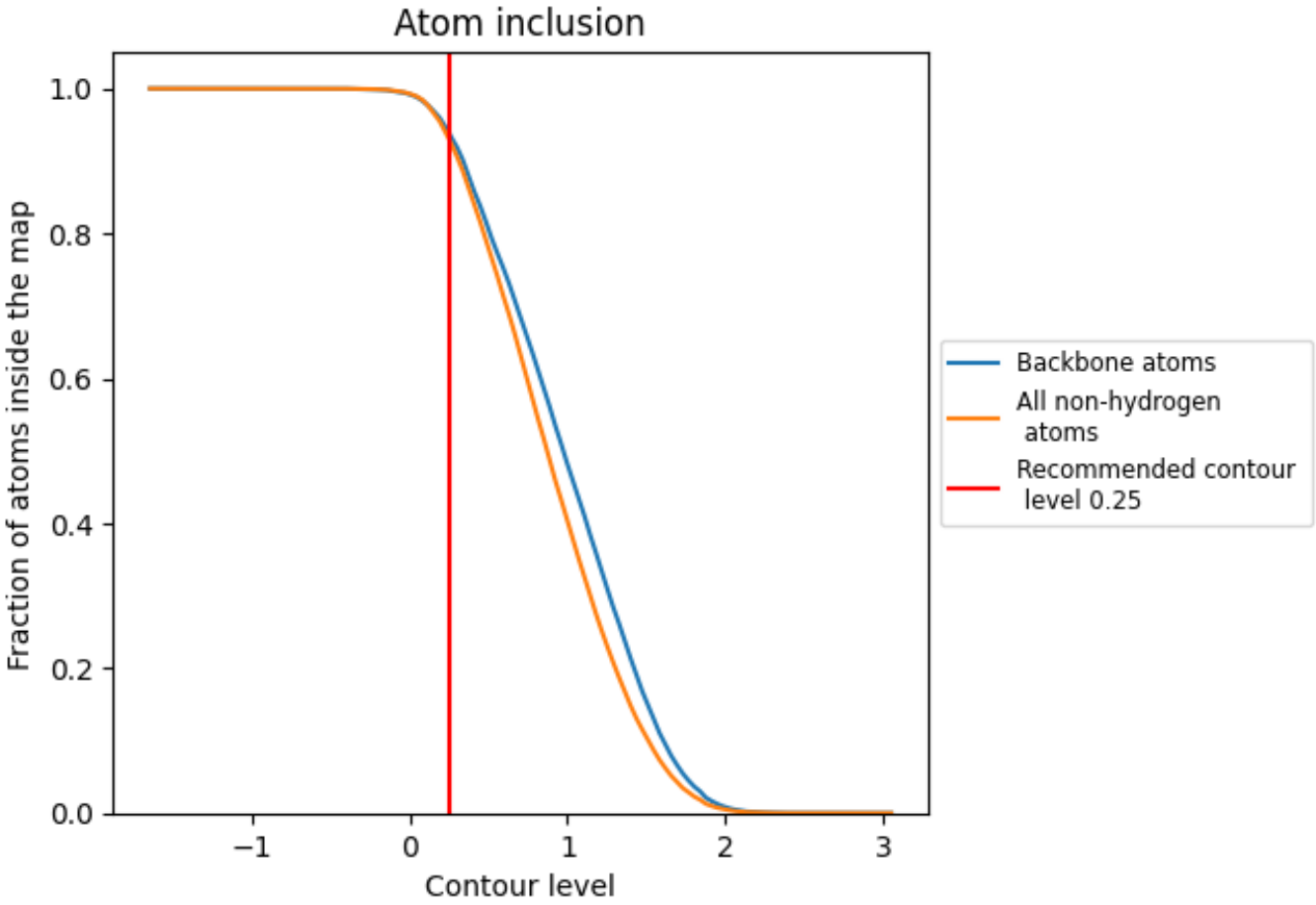
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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	0.9298	0.5640
A	0.9320	0.5610
B	0.9342	0.5720
P	0.8505	0.5140