



Full wwPDB EM Validation Report ⓘ

Nov 16, 2022 – 07:29 PM JST

PDB ID : 7BVG
EMDB ID : EMD-30219
Title : Cryo-EM structure of Mycobacterium smegmatis arabinosyltransferase EmbA-EmbB-AcpM2 in complex with di-arabinose.
Authors : Zhang, L.; Zhao, Y.; Gao, Y.; Wang, Q.; Li, J.; Besra, G.S.; Rao, Z.
Deposited on : 2020-04-10
Resolution : 3.10 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

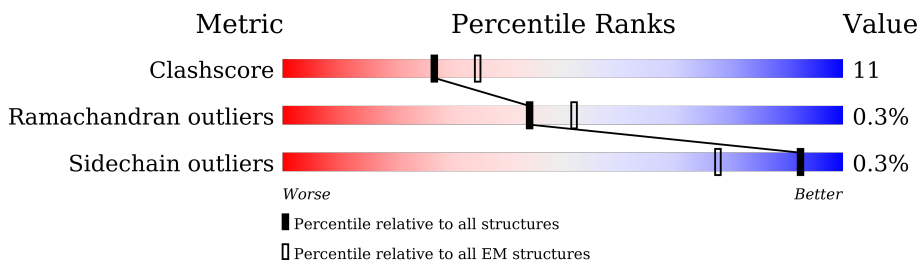
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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 $\leq 5\%$. 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	A	1088	 77% 21% ..
2	B	1100	 76% 20% .
3	P	99	 75% 19% 6%
4	C	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	PNS	B	1202	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17231 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 indolylacetylinsitol 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 indolylacetylinsitol 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.

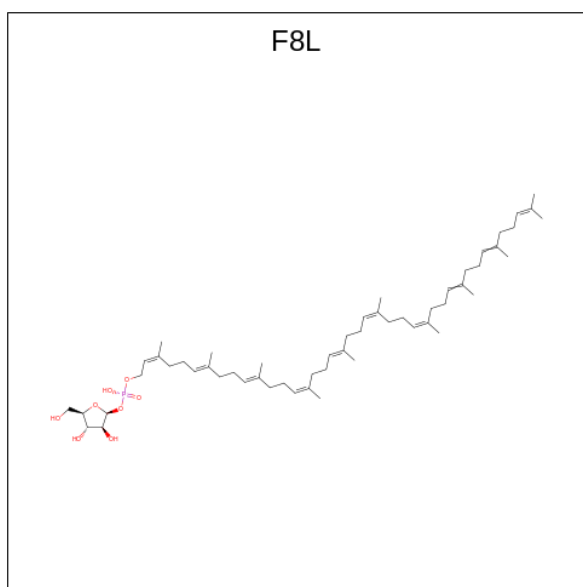
Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	93	Total	C	N	O	S	0	0
			706	441	108	156	1		

- Molecule 4 is an oligosaccharide called alpha-D-arabinofuranose-(1-5)-alpha-D-arabinofuranose.



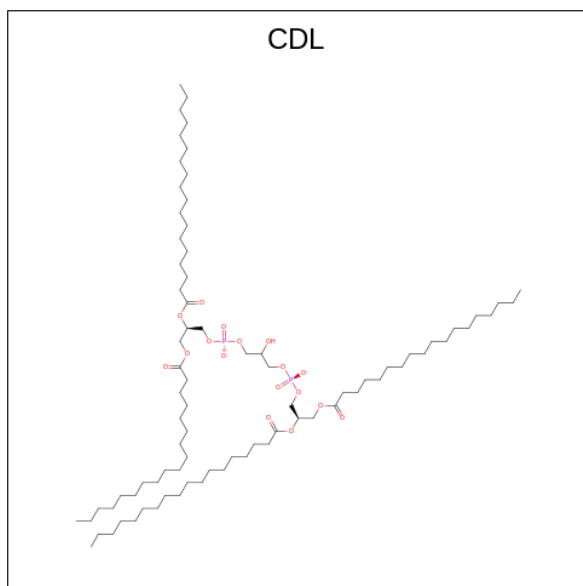
Mol	Chain	Residues	Atoms			AltConf	Trace
4	C	2	Total	C	O	0	0
			19	10	9		

- Molecule 5 is [(2Z,6E,10E,14Z,18E,22Z,26Z)-3,7,11,15,19,23,27,31,35,39-decamethyltetracont-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: C₅₅H₉₁O₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O	P	0
			39	30	8	1	

- Molecule 6 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

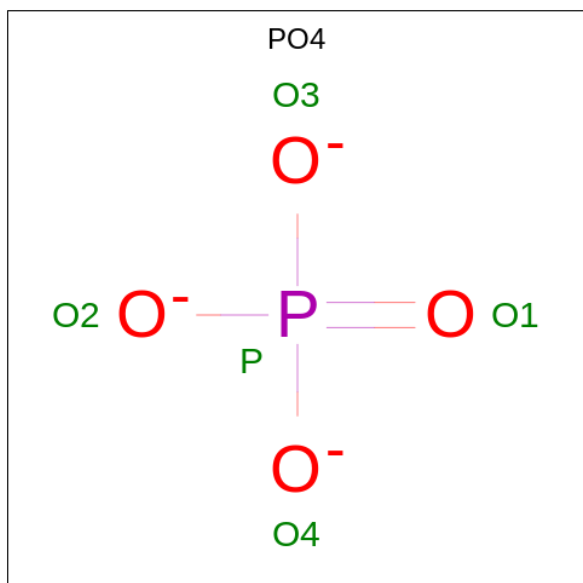


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	O	P	0
			86	67	17	2	
6	B	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

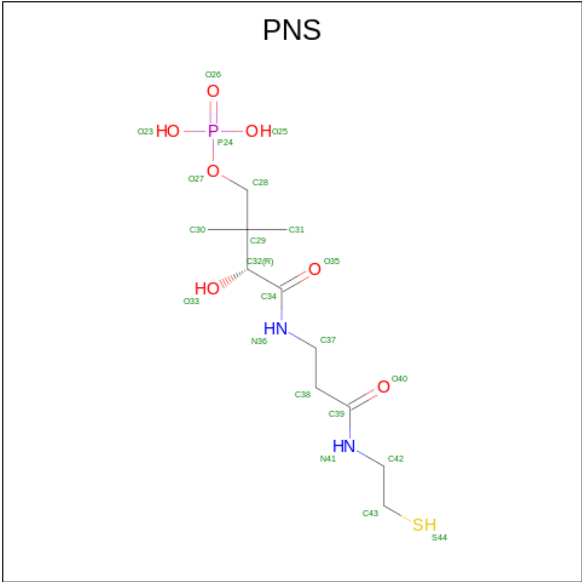
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	
7	B	1	Total	Ca	0
			1	1	

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 9 is 4'-PHOSPHOPANTETHEINE (three-letter code: PNS) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).

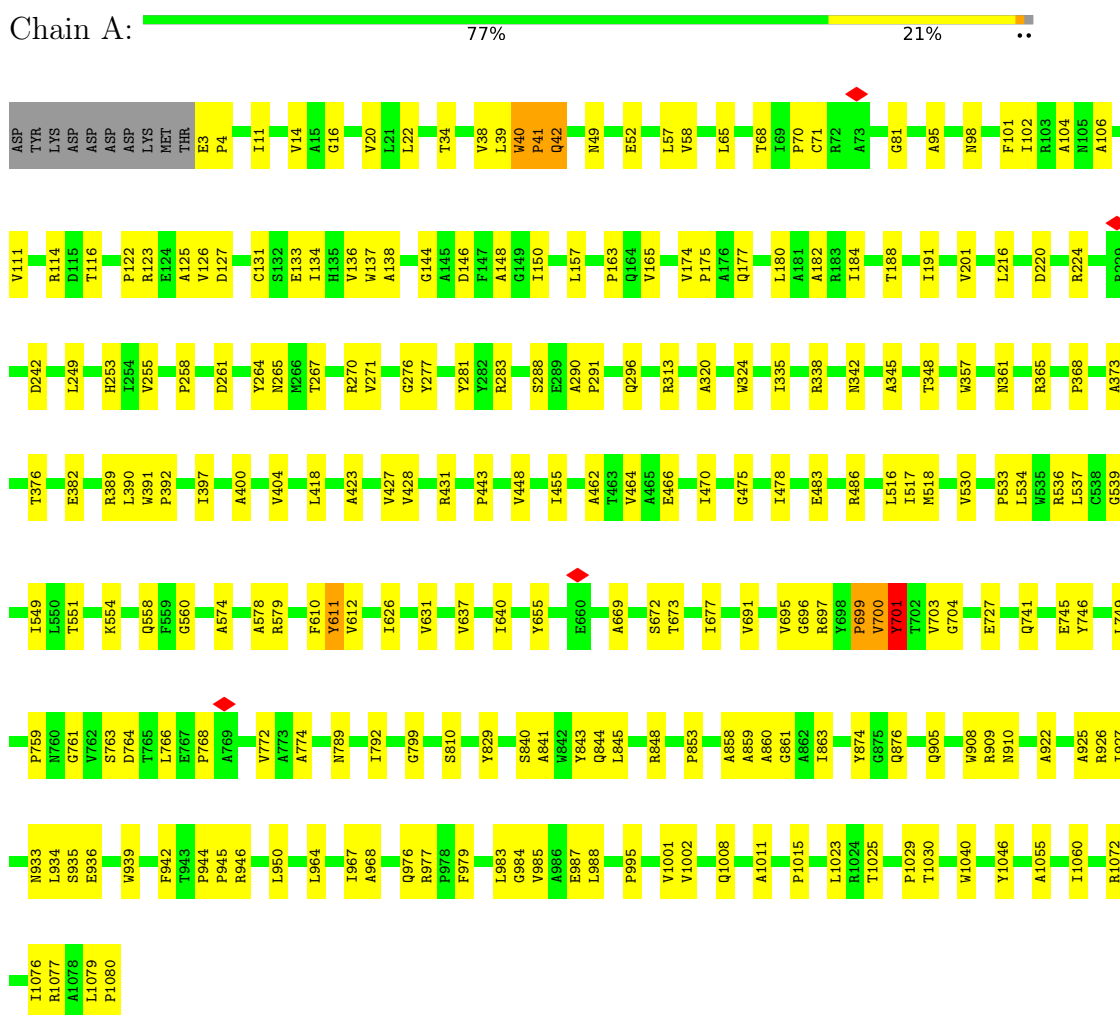


Mol	Chain	Residues	Atoms						AltConf
9	B	1	Total	C	N	O	P	S	0
			22	11	2	7	1	1	

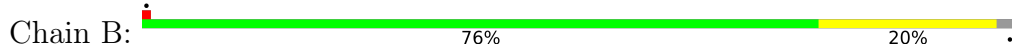
3 Residue-property plots

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

- Molecule 1: Integral membrane indolylacetyltransferase EmbA



- Molecule 2: Integral membrane indolylacetyltransferase EmbB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	209894	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.203	Depositor
Minimum map value	-1.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BXY, PNS, PO4, CA, F8L, 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	0/8365	0.48	1/11466 (0.0%)
2	B	0.28	0/8315	0.48	1/11393 (0.0%)
3	P	0.24	0/712	0.43	0/967
All	All	0.28	0/17392	0.48	2/23826 (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	2
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	701	TYR	CB-CA-C	-7.93	94.54	110.40
2	B	716	THR	N-CA-CB	6.54	122.72	110.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	TRP	Peptide
2	B	58	TRP	Peptide
2	B	910	THR	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	A	8147	0	8211	155	0
2	B	8105	0	8168	193	0
3	P	706	0	694	18	0
4	C	19	0	16	1	0
5	A	39	0	0	1	0
6	A	86	0	122	16	0
6	B	100	0	156	12	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	5	0	0	0	0
9	B	22	0	20	42	0
All	All	17231	0	17387	377	0

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

All (377) 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)
2:B:253:ARG:O	9:B:1202:PNS:N36	1.60	1.33
2:B:251:MET:HG3	9:B:1202:PNS:C37	1.56	1.32
2:B:252:HIS:HB2	9:B:1202:PNS:C30	1.61	1.29
2:B:251:MET:HG3	9:B:1202:PNS:H371	1.22	1.19
4:C:1:BCY:O4	4:C:1:BCY:C1	1.65	1.19
2:B:252:HIS:CB	9:B:1202:PNS:H301	1.72	1.18
2:B:253:ARG:HB2	9:B:1202:PNS:H32	1.18	1.15
9:B:1202:PNS:O25	3:P:41:SER:CB	1.96	1.13
2:B:314:ASP:CB	2:B:315:PRO:HD3	1.83	1.06
1:A:518:MET:HE3	6:A:1102:CDL:H791	1.38	1.05
2:B:253:ARG:HE	9:B:1202:PNS:H282	1.19	1.03
2:B:253:ARG:CB	9:B:1202:PNS:H32	1.87	1.03
2:B:253:ARG:N	9:B:1202:PNS:C30	2.25	0.99
2:B:314:ASP:HB2	2:B:315:PRO:HD3	1.41	0.99
2:B:611:ARG:HB3	2:B:687:THR:HG21	1.43	0.99
9:B:1202:PNS:O25	3:P:41:SER:OG	1.81	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1202:PNS:P24	3:P:41:SER:OG	2.22	0.97
2:B:253:ARG:H	9:B:1202:PNS:H303	1.29	0.96
2:B:252:HIS:CB	9:B:1202:PNS:C30	2.35	0.95
2:B:251:MET:HG3	9:B:1202:PNS:H372	1.50	0.93
2:B:253:ARG:N	9:B:1202:PNS:H302	1.84	0.92
2:B:252:HIS:N	9:B:1202:PNS:H303	1.84	0.91
2:B:251:MET:CG	9:B:1202:PNS:C37	2.47	0.91
2:B:314:ASP:HB2	2:B:315:PRO:CD	2.02	0.90
2:B:252:HIS:CA	9:B:1202:PNS:C30	2.52	0.88
2:B:609:ARG:HH21	6:B:1203:CDL:H542	1.37	0.88
2:B:252:HIS:H	9:B:1202:PNS:H303	1.40	0.87
2:B:252:HIS:HB2	9:B:1202:PNS:H301	0.88	0.87
2:B:253:ARG:N	9:B:1202:PNS:H303	1.90	0.87
2:B:314:ASP:CB	2:B:315:PRO:CD	2.49	0.86
2:B:253:ARG:HB2	9:B:1202:PNS:C32	2.04	0.85
9:B:1202:PNS:O23	3:P:41:SER:OG	1.94	0.85
1:A:281:TYR:OH	1:A:979:PHE:CE1	2.30	0.84
2:B:314:ASP:HB3	2:B:315:PRO:HD3	1.58	0.84
1:A:696:GLY:O	1:A:697:ARG:HB3	1.76	0.82
2:B:253:ARG:H	9:B:1202:PNS:C30	1.87	0.81
2:B:687:THR:O	2:B:687:THR:HG22	1.80	0.81
1:A:699:PRO:O	1:A:701:TYR:N	2.14	0.81
2:B:253:ARG:NE	9:B:1202:PNS:H282	1.96	0.80
9:B:1202:PNS:O25	3:P:41:SER:HB3	1.79	0.79
1:A:483:GLU:HG3	1:A:549:ILE:HG12	1.64	0.79
2:B:314:ASP:OD1	2:B:491:ALA:CB	2.32	0.78
2:B:314:ASP:OD1	2:B:491:ALA:HB3	1.85	0.76
2:B:609:ARG:NH2	6:B:1203:CDL:H542	2.02	0.75
2:B:251:MET:CG	9:B:1202:PNS:H372	2.14	0.75
2:B:546:ARG:NH2	2:B:604:VAL:O	2.20	0.74
2:B:251:MET:CG	9:B:1202:PNS:H371	2.12	0.74
6:A:1102:CDL:H252	6:A:1102:CDL:H212	1.69	0.73
2:B:57:ASN:OD1	2:B:57:ASN:N	2.17	0.73
2:B:405:ILE:HD11	2:B:441:LEU:HD23	1.71	0.73
1:A:106:ALA:HA	1:A:123:ARG:HH11	1.53	0.73
2:B:252:HIS:N	9:B:1202:PNS:C30	2.52	0.72
2:B:314:ASP:OD2	2:B:491:ALA:HB3	1.89	0.72
6:A:1102:CDL:H331	6:A:1102:CDL:H752	1.70	0.72
2:B:314:ASP:CG	2:B:491:ALA:HB3	2.10	0.72
2:B:252:HIS:H	9:B:1202:PNS:C30	2.02	0.72
2:B:784:ARG:NH2	2:B:796:TRP:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:507:GLU:HG3	2:B:572:MET:HG2	1.71	0.71
2:B:640:ALA:HB3	2:B:643:ASN:HB3	1.73	0.71
2:B:291:GLN:HA	2:B:291:GLN:NE2	2.07	0.70
1:A:71:CYS:HB2	1:A:134:ILE:HD11	1.74	0.68
1:A:749:LEU:HD11	1:A:944:PRO:HD3	1.74	0.68
2:B:252:HIS:C	9:B:1202:PNS:C30	2.61	0.68
1:A:290:ALA:HB1	1:A:464:VAL:HG22	1.75	0.68
1:A:910:ASN:OD1	1:A:946:ARG:NH2	2.26	0.67
2:B:494:ILE:HG12	2:B:1080:ILE:HD11	1.76	0.67
1:A:123:ARG:HA	1:A:126:VAL:HG12	1.76	0.67
2:B:739:VAL:HG23	2:B:1035:THR:HG22	1.76	0.67
2:B:36:LEU:HA	2:B:39:VAL:HG22	1.76	0.66
1:A:42:GLN:O	1:A:42:GLN:HG3	1.97	0.65
1:A:224:ARG:HD3	1:A:389:ARG:HD3	1.80	0.65
2:B:60:GLN:HA	2:B:60:GLN:OE1	1.97	0.64
2:B:252:HIS:CA	9:B:1202:PNS:H303	2.23	0.64
2:B:317:GLY:O	2:B:321:ASN:ND2	2.30	0.64
2:B:252:HIS:C	9:B:1202:PNS:H302	2.17	0.64
2:B:607:SER:OG	2:B:610:ASN:ND2	2.30	0.64
3:P:65:ALA:O	3:P:68:ARG:NH2	2.27	0.64
6:A:1102:CDL:H212	6:A:1102:CDL:C25	2.27	0.64
2:B:253:ARG:O	9:B:1202:PNS:C37	2.45	0.64
2:B:294:ARG:NH2	2:B:981:GLN:O	2.27	0.64
2:B:251:MET:SD	9:B:1202:PNS:H372	2.38	0.63
2:B:454:ARG:NH1	3:P:53:ASP:OD2	2.32	0.63
2:B:713:GLN:NE2	2:B:1040:ASP:OD1	2.31	0.63
1:A:174:VAL:HB	1:A:177:GLN:HE21	1.64	0.62
2:B:58:TRP:CE3	2:B:192:VAL:HG11	2.35	0.62
1:A:361:ASN:HB3	1:A:368:PRO:HG3	1.82	0.62
1:A:462:ALA:HB1	1:A:1072:ARG:HB2	1.81	0.61
1:A:518:MET:HE1	6:A:1102:CDL:H771	1.83	0.60
6:B:1203:CDL:H662	6:B:1203:CDL:H451	1.82	0.60
2:B:333:SER:O	2:B:337:ARG:NH1	2.33	0.60
1:A:637:VAL:HA	1:A:640:ILE:HG12	1.84	0.60
2:B:58:TRP:CH2	2:B:194:THR:HB	2.36	0.60
2:B:1080:ILE:HG22	2:B:1081:ARG:HG3	1.83	0.60
6:B:1203:CDL:H531	6:B:1203:CDL:OB7	2.02	0.60
1:A:382:GLU:OE1	1:A:536:ARG:NH1	2.35	0.59
2:B:831:THR:OG1	2:B:832:GLU:OE1	2.20	0.59
2:B:119:THR:HG22	2:B:120:GLU:H	1.67	0.59
1:A:860:ALA:HB2	1:A:908:TRP:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ILE:HA	2:B:292:MET:HG2	1.85	0.59
1:A:68:THR:OG1	1:A:133:GLU:OE1	2.20	0.59
1:A:861:GLY:O	1:A:909:ARG:NH2	2.36	0.58
2:B:252:HIS:HB2	9:B:1202:PNS:H302	1.77	0.58
2:B:357:PRO:HA	2:B:364:ALA:HB2	1.84	0.58
1:A:98:ASN:HA	1:A:114:ARG:HD2	1.84	0.58
1:A:478:ILE:HD11	1:A:554:LYS:HB2	1.85	0.58
1:A:853:PRO:HD2	1:A:950:LEU:HD12	1.84	0.58
2:B:288:TYR:HD2	2:B:288:TYR:O	1.85	0.58
2:B:107:ARG:NH1	2:B:789:GLN:O	2.37	0.58
2:B:219:THR:HG22	2:B:220:ALA:H	1.68	0.58
2:B:867:THR:HB	2:B:881:GLN:HE22	1.67	0.58
2:B:61:GLN:NE2	2:B:1061:GLU:OE2	2.37	0.57
2:B:147:ARG:NH2	2:B:149:GLU:OE2	2.37	0.57
2:B:716:THR:HG21	2:B:1040:ASP:HB2	1.86	0.57
1:A:65:LEU:HD12	1:A:184:ILE:HG12	1.85	0.57
1:A:611:TYR:CD2	1:A:612:VAL:HG23	2.40	0.57
1:A:863:ILE:HA	1:A:876:GLN:H	1.69	0.57
2:B:373:ALA:HB2	2:B:594:ALA:HB2	1.85	0.57
2:B:636:SER:OG	2:B:719:ASN:ND2	2.38	0.57
1:A:774:ALA:HB3	1:A:789:ASN:HB3	1.85	0.57
1:A:673:THR:HG22	1:A:677:ILE:HG13	1.87	0.56
2:B:251:MET:HG3	9:B:1202:PNS:N36	2.17	0.56
6:A:1102:CDL:H711	2:B:558:TRP:CE3	2.40	0.56
1:A:516:LEU:HD21	1:A:534:LEU:HD11	1.86	0.56
1:A:242:ASP:OD1	1:A:324:TRP:NE1	2.39	0.56
2:B:673:HIS:CE1	6:B:1203:CDL:OA7	2.58	0.56
1:A:70:PRO:HD3	1:A:180:LEU:HA	1.88	0.55
1:A:517:ILE:HD13	6:B:1203:CDL:H721	1.88	0.55
1:A:291:PRO:HA	1:A:455:ILE:HG23	1.89	0.55
1:A:1008:GLN:HB3	1:A:1015:PRO:HD2	1.88	0.55
2:B:389:ARG:NH2	2:B:391:GLU:OE2	2.37	0.55
1:A:102:ILE:HD11	1:A:136:VAL:HG21	1.89	0.55
1:A:772:VAL:HG11	1:A:1001:VAL:HG21	1.89	0.55
2:B:55:THR:HG22	2:B:57:ASN:OD1	2.07	0.54
2:B:372:ALA:HB2	2:B:692:PRO:HG3	1.89	0.54
2:B:714:TYR:C	2:B:714:TYR:CD2	2.80	0.54
1:A:518:MET:CE	6:A:1102:CDL:H771	2.37	0.54
6:A:1102:CDL:H112	6:A:1102:CDL:HA62	1.89	0.54
2:B:892:PRO:HG2	2:B:895:THR:HB	1.90	0.54
2:B:169:GLY:O	2:B:170:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:N	1:A:39:LEU:HD12	2.22	0.54
1:A:49:ASN:HA	1:A:175:PRO:HA	1.90	0.54
2:B:304:ASN:ND2	2:B:313:GLU:OE2	2.41	0.54
2:B:334:ILE:HG13	2:B:334:ILE:O	2.08	0.54
2:B:41:SER:OG	2:B:473:THR:O	2.21	0.54
1:A:258:PRO:HD3	1:A:703:VAL:HG21	1.90	0.54
1:A:283:ARG:HH21	1:A:475:GLY:HA2	1.72	0.54
1:A:1025:THR:HG22	1:A:1046:TYR:HE1	1.72	0.54
2:B:259:TRP:NE1	2:B:354:GLU:OE2	2.40	0.54
1:A:669:ALA:O	1:A:673:THR:OG1	2.26	0.53
2:B:830:SER:O	2:B:834:GLN:NE2	2.42	0.53
2:B:919:PRO:HG2	2:B:922:GLU:HG2	1.90	0.53
1:A:390:LEU:HD11	1:A:428:VAL:HG22	1.90	0.53
1:A:626:ILE:HG12	1:A:631:VAL:HG22	1.91	0.53
2:B:498:ILE:HD11	2:B:1080:ILE:HG23	1.90	0.53
6:A:1102:CDL:C25	6:A:1102:CDL:C21	2.85	0.53
2:B:412:GLY:O	2:B:455:ARG:NH1	2.42	0.53
1:A:391:TRP:CG	1:A:392:PRO:HD3	2.43	0.53
2:B:530:VAL:HG21	2:B:625:CYS:SG	2.49	0.53
1:A:39:LEU:N	1:A:39:LEU:CD1	2.71	0.53
1:A:265:ASN:OD1	1:A:296:GLN:NE2	2.42	0.53
2:B:750:PRO:HG2	2:B:760:PRO:HB2	1.90	0.53
1:A:373:ALA:HA	1:A:376:THR:HG22	1.90	0.53
1:A:1001:VAL:HG23	1:A:1002:VAL:HG13	1.91	0.52
2:B:282:ASN:HB3	2:B:286:ASP:OD2	2.09	0.52
1:A:1030:THR:HG1	1:A:1040:TRP:HE1	1.57	0.52
2:B:278:VAL:O	2:B:723:ASN:ND2	2.39	0.52
1:A:486:ARG:NH1	1:A:558:GLN:OE1	2.43	0.52
1:A:1011:ALA:O	1:A:1080:PRO:HG2	2.10	0.52
2:B:301:TYR:HD2	2:B:312:PRO:HB3	1.75	0.52
2:B:687:THR:O	2:B:687:THR:CG2	2.53	0.52
2:B:904:PRO:HB3	2:B:918:TYR:CZ	2.45	0.52
2:B:906:ASP:OD1	2:B:914:ARG:NE	2.40	0.52
1:A:126:VAL:HG23	1:A:131:CYS:SG	2.50	0.51
1:A:165:VAL:HG11	1:A:184:ILE:HD13	1.92	0.51
1:A:335:ILE:HD11	1:A:537:LEU:HD22	1.93	0.51
1:A:338:ARG:HH21	1:A:579:ARG:HH22	1.58	0.51
1:A:191:ILE:HG23	1:A:276:GLY:HA3	1.92	0.51
2:B:252:HIS:NE2	3:P:61:ASP:OD2	2.35	0.51
1:A:242:ASP:HA	1:A:324:TRP:HE1	1.74	0.51
2:B:58:TRP:HH2	2:B:194:THR:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:GLU:HG3	2:B:153:ASN:HB3	1.91	0.51
2:B:824:PRO:HD2	2:B:949:PRO:HG3	1.93	0.51
2:B:253:ARG:HB2	9:B:1202:PNS:H302	1.93	0.51
1:A:22:LEU:HD12	1:A:201:VAL:HG13	1.92	0.51
2:B:275:ILE:O	2:B:279:ILE:HG12	2.11	0.51
1:A:122:PRO:HG2	1:A:125:ALA:HB3	1.92	0.50
1:A:71:CYS:SG	1:A:126:VAL:HG22	2.52	0.50
1:A:220:ASP:OD1	1:A:431:ARG:NH1	2.44	0.50
1:A:551:THR:O	1:A:554:LYS:NZ	2.44	0.50
2:B:292:MET:O	2:B:302:MET:HE3	2.10	0.50
1:A:1077:ARG:NH1	1:A:1079:LEU:O	2.44	0.50
1:A:277:TYR:HD2	1:A:288:SER:HB3	1.75	0.50
6:A:1102:CDL:OB9	6:A:1102:CDL:H732	2.11	0.50
2:B:771:PRO:HB3	2:B:808:ASN:HD22	1.77	0.50
1:A:859:ALA:HB3	1:A:909:ARG:HG3	1.94	0.50
2:B:367:ARG:HH11	2:B:371:TRP:HE1	1.60	0.49
1:A:977:ARG:NH2	1:A:987:GLU:OE2	2.42	0.49
1:A:281:TYR:OH	1:A:979:PHE:CD1	2.64	0.49
1:A:342:ASN:HB3	1:A:345:ALA:HB3	1.95	0.49
2:B:120:GLU:HG2	2:B:121:THR:HG23	1.93	0.49
2:B:410:THR:HG23	3:P:46:GLU:HB2	1.94	0.49
6:B:1203:CDL:H412	6:B:1203:CDL:H601	1.94	0.49
2:B:761:LEU:HD13	2:B:949:PRO:HD3	1.94	0.49
1:A:249:LEU:HD21	1:A:320:ALA:HB1	1.95	0.49
1:A:253:HIS:O	1:A:313:ARG:NH1	2.46	0.49
1:A:277:TYR:CD2	1:A:288:SER:HB3	2.48	0.48
1:A:131:CYS:SG	1:A:150:ILE:HG12	2.53	0.48
1:A:418:LEU:HB3	6:B:1203:CDL:H152	1.95	0.48
2:B:56:LEU:C	2:B:57:ASN:OD1	2.52	0.48
1:A:216:LEU:HD22	1:A:443:PRO:HB2	1.95	0.48
1:A:470:ILE:HD11	1:A:1076:ILE:HG21	1.95	0.48
1:A:768:PRO:HG2	1:A:792:ILE:HD11	1.94	0.48
5:A:1101:F8L:C43	5:A:1101:F8L:C39	2.85	0.48
2:B:137:ARG:HA	2:B:140:VAL:HG12	1.95	0.48
1:A:65:LEU:HD22	1:A:163:PRO:HG2	1.96	0.48
1:A:933:ASN:OD1	1:A:934:LEU:N	2.46	0.48
2:B:768:GLY:HA3	2:B:837:SER:HB3	1.96	0.48
2:B:361:PRO:HB3	3:P:38:ASP:HB3	1.95	0.48
1:A:146:ASP:OD1	1:A:148:ALA:N	2.46	0.48
2:B:286:ASP:OD1	2:B:388:LEU:N	2.37	0.48
2:B:853:GLU:O	2:B:857:HIS:ND1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1202:PNS:P24	3:P:41:SER:HG	2.32	0.48
1:A:964:LEU:HD13	1:A:979:PHE:HE1	1.78	0.48
2:B:61:GLN:OE1	2:B:63:ARG:NH2	2.45	0.47
2:B:117:ASN:HB2	2:B:124:ASP:OD1	2.13	0.47
1:A:530:VAL:HG23	1:A:533:PRO:HD2	1.95	0.47
2:B:287:GLY:HA2	2:B:975:GLY:HA3	1.96	0.47
2:B:295:THR:HG22	2:B:985:LEU:HD23	1.96	0.47
1:A:40:TRP:HB3	1:A:182:ALA:HB3	1.95	0.47
1:A:611:TYR:CD1	1:A:611:TYR:C	2.86	0.47
2:B:287:GLY:O	2:B:291:GLN:HG2	2.14	0.47
3:P:67:LEU:HD13	3:P:73:VAL:HG22	1.96	0.47
1:A:11:ILE:HA	1:A:14:VAL:HG22	1.95	0.47
2:B:414:LEU:HD12	2:B:464:LEU:HD22	1.95	0.47
1:A:348:THR:HG21	1:A:574:ALA:HB3	1.97	0.47
2:B:497:ALA:HB1	2:B:1081:ARG:HH12	1.79	0.47
2:B:569:PHE:O	2:B:572:MET:HG3	2.15	0.47
2:B:244:ASP:OD2	2:B:414:LEU:N	2.46	0.47
1:A:518:MET:CE	6:A:1102:CDL:C77	2.93	0.46
1:A:858:ALA:O	1:A:942:PHE:HA	2.15	0.46
2:B:58:TRP:CE3	2:B:58:TRP:O	2.69	0.46
2:B:271:GLY:O	2:B:275:ILE:HG12	2.15	0.46
6:B:1203:CDL:H552	6:B:1203:CDL:H581	1.43	0.46
1:A:123:ARG:HG2	1:A:127:ASP:OD2	2.15	0.46
1:A:361:ASN:HD21	1:A:560:GLY:HA3	1.80	0.46
2:B:778:ILE:HD13	2:B:944:TRP:HH2	1.79	0.46
2:B:819:ASP:OD1	2:B:819:ASP:N	2.47	0.46
2:B:252:HIS:CB	9:B:1202:PNS:H302	2.39	0.46
2:B:152:SER:HB2	2:B:157:THR:HG23	1.96	0.46
2:B:758:LEU:HD22	2:B:771:PRO:HG3	1.97	0.46
1:A:761:GLY:O	1:A:829:TYR:HB3	2.15	0.46
1:A:38:VAL:C	1:A:39:LEU:HD12	2.36	0.46
1:A:397:ILE:HG21	1:A:448:VAL:HG22	1.97	0.46
1:A:848:ARG:HH21	1:A:922:ALA:HB3	1.80	0.46
2:B:244:ASP:OD2	2:B:415:THR:N	2.46	0.46
2:B:609:ARG:NH2	6:B:1203:CDL:C54	2.77	0.46
1:A:255:VAL:HG12	1:A:704:GLY:HA3	1.98	0.45
1:A:578:ALA:HB2	1:A:672:SER:HB3	1.98	0.45
2:B:869:THR:HG22	2:B:880:GLY:N	2.30	0.45
2:B:716:THR:HG23	2:B:717:TYR:N	2.32	0.45
1:A:58:VAL:HG22	1:A:984:GLY:O	2.16	0.45
2:B:750:PRO:HG3	2:B:844:TYR:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ALA:HB3	1:A:291:PRO:HD3	1.98	0.45
3:P:79:LYS:HA	3:P:82:GLU:OE2	2.16	0.45
1:A:116:THR:HB	1:A:157:LEU:HD21	1.96	0.45
1:A:927:ILE:HD11	1:A:945:PRO:HD3	1.99	0.45
1:A:968:ALA:HB3	1:A:995:PRO:HG3	1.98	0.45
1:A:102:ILE:HG23	1:A:111:VAL:HG22	1.99	0.45
1:A:935:SER:OG	1:A:936:GLU:OE1	2.34	0.45
9:B:1202:PNS:O27	9:B:1202:PNS:O33	2.35	0.45
3:P:90:ALA:HB1	3:P:94:LYS:HE2	1.99	0.45
1:A:763:SER:OG	1:A:764:ASP:N	2.50	0.45
1:A:16:GLY:O	1:A:20:VAL:HG23	2.17	0.45
6:A:1102:CDL:H711	2:B:558:TRP:HE3	1.81	0.45
2:B:161:PHE:HB2	2:B:176:GLN:HB3	1.99	0.45
1:A:52:GLU:O	1:A:1055:ALA:HA	2.17	0.44
2:B:261:THR:O	2:B:353:ARG:NH2	2.49	0.44
1:A:859:ALA:HB1	1:A:863:ILE:HD12	1.99	0.44
2:B:77:LEU:HD23	2:B:77:LEU:HA	1.85	0.44
1:A:264:TYR:HD1	1:A:967:ILE:HG23	1.83	0.44
1:A:400:ALA:O	1:A:404:VAL:HG23	2.17	0.44
6:A:1102:CDL:H802	6:A:1102:CDL:H832	1.71	0.44
2:B:242:ARG:O	2:B:242:ARG:NH1	2.51	0.44
2:B:58:TRP:O	2:B:58:TRP:CD2	2.70	0.44
1:A:57:LEU:HD23	1:A:985:VAL:HG12	2.00	0.44
1:A:759:PRO:HB2	1:A:810:SER:HB3	1.99	0.44
1:A:829:TYR:HB2	1:A:939:TRP:CD2	2.53	0.44
1:A:840:SER:OG	1:A:841:ALA:N	2.50	0.44
2:B:116:VAL:HG22	2:B:125:VAL:HG13	2.00	0.44
1:A:65:LEU:HB3	1:A:138:ALA:HB3	1.99	0.44
1:A:281:TYR:O	1:A:281:TYR:CG	2.70	0.44
2:B:288:TYR:C	2:B:288:TYR:CD2	2.91	0.44
2:B:751:LEU:HD23	2:B:752:PRO:HD3	2.00	0.44
1:A:281:TYR:O	1:A:281:TYR:CD2	2.71	0.44
1:A:700:VAL:O	1:A:701:TYR:HB2	2.17	0.44
1:A:983:LEU:HD13	1:A:1060:ILE:HG21	1.99	0.44
3:P:79:LYS:O	3:P:83:GLU:HG3	2.18	0.44
2:B:45:PRO:HG3	2:B:480:PHE:CD2	2.53	0.43
2:B:758:LEU:HB2	2:B:762:GLY:HA3	1.99	0.43
2:B:872:SER:HB3	2:B:906:ASP:O	2.17	0.43
1:A:518:MET:HE1	6:A:1102:CDL:C77	2.47	0.43
1:A:766:LEU:HD12	1:A:766:LEU:H	1.84	0.43
1:A:745:GLU:HG2	1:A:746:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:GLN:OE1	2:B:717:TYR:O	2.36	0.43
2:B:626:PHE:HZ	2:B:701:VAL:HG21	1.83	0.43
2:B:634:TYR:CZ	2:B:974:VAL:HG12	2.53	0.43
1:A:391:TRP:CD1	1:A:392:PRO:HD3	2.53	0.43
2:B:846:LEU:HG	2:B:847:PRO:HD2	2.00	0.43
2:B:909:PRO:O	2:B:914:ARG:HD3	2.18	0.43
1:A:466:GLU:OE1	1:A:1072:ARG:NH2	2.52	0.43
1:A:774:ALA:HB2	1:A:1002:VAL:HG11	2.00	0.43
2:B:156:GLY:HA3	2:B:181:PRO:HA	2.01	0.43
1:A:188:THR:HB	1:A:191:ILE:HD12	2.01	0.43
1:A:697:ARG:O	1:A:697:ARG:HG2	2.19	0.43
1:A:988:LEU:HD22	1:A:1023:LEU:HD11	2.01	0.42
1:A:34:THR:O	1:A:188:THR:OG1	2.28	0.42
1:A:844:GLN:NE2	1:A:845:LEU:O	2.51	0.42
2:B:107:ARG:HH11	2:B:788:PRO:HB2	1.84	0.42
2:B:307:ARG:HH11	2:B:499:GLY:HA2	1.83	0.42
2:B:367:ARG:HG3	2:B:371:TRP:HD1	1.85	0.42
2:B:540:LEU:HD22	2:B:565:PHE:CZ	2.55	0.42
3:P:28:THR:OG1	3:P:31:LYS:HG2	2.20	0.42
2:B:819:ASP:OD2	2:B:822:ARG:NE	2.35	0.42
1:A:261:ASP:OD1	1:A:365:ARG:NH1	2.52	0.42
1:A:478:ILE:HD11	1:A:554:LYS:HD2	2.02	0.42
2:B:210:ILE:HG13	2:B:1062:LEU:HD11	2.01	0.42
2:B:277:TYR:HE1	2:B:337:ARG:O	2.03	0.42
2:B:921:SER:OG	2:B:922:GLU:OE2	2.37	0.42
6:B:1203:CDL:H662	6:B:1203:CDL:H632	1.73	0.42
1:A:137:TRP:CZ2	1:A:144:GLY:HA3	2.55	0.42
2:B:536:LEU:HD11	2:B:565:PHE:CE2	2.55	0.42
1:A:335:ILE:O	1:A:530:VAL:HG22	2.20	0.42
1:A:741:GLN:NE2	1:A:841:ALA:O	2.46	0.42
6:A:1102:CDL:H171	6:A:1102:CDL:H201	1.59	0.42
2:B:394:ILE:HD11	2:B:431:GLN:HB2	2.02	0.41
1:A:81:GLY:HA3	1:A:104:ALA:HB3	2.02	0.41
1:A:320:ALA:HB2	1:A:357:TRP:CZ2	2.54	0.41
2:B:64:LEU:HD21	2:B:200:ALA:HA	2.02	0.41
2:B:448:ILE:O	2:B:452:VAL:HG23	2.20	0.41
2:B:33:ALA:HA	2:B:36:LEU:HG	2.02	0.41
1:A:267:THR:O	1:A:271:VAL:HG22	2.20	0.41
2:B:226:MET:SD	2:B:481:ALA:HA	2.59	0.41
2:B:484:THR:HG21	2:B:1071:GLY:HA2	2.02	0.41
1:A:840:SER:HB3	1:A:926:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:TYR:O	2:B:288:TYR:CD2	2.70	0.41
3:P:49:VAL:O	3:P:52:GLU:HG2	2.20	0.41
1:A:95:ALA:HB1	1:A:101:PHE:HZ	1.85	0.41
2:B:314:ASP:HB3	2:B:315:PRO:CD	2.32	0.41
2:B:792:THR:HB	2:B:796:TRP:CD1	2.56	0.41
1:A:270:ARG:NH2	1:A:976:GLN:O	2.42	0.41
2:B:285:ASP:HB2	2:B:389:ARG:HG2	2.02	0.41
2:B:338:LEU:N	2:B:339:PRO:HD2	2.36	0.41
1:A:539:GLY:HA3	6:B:1203:CDL:HA61	2.03	0.41
1:A:610:PHE:CG	1:A:611:TYR:N	2.89	0.41
1:A:727:GLU:HB3	1:A:1029:PRO:HG2	2.02	0.41
1:A:766:LEU:HB2	1:A:799:GLY:HA2	2.03	0.41
2:B:132:VAL:HG13	2:B:179:GLY:HA2	2.03	0.41
2:B:1014:ASP:OD1	2:B:1015:GLY:N	2.54	0.41
1:A:3:GLU:HA	1:A:4:PRO:HD3	1.93	0.41
1:A:261:ASP:HB2	1:A:365:ARG:HD3	2.02	0.41
1:A:874:TYR:OH	1:A:933:ASN:ND2	2.48	0.41
2:B:258:ARG:HD3	3:P:40:ASP:OD2	2.21	0.41
2:B:301:TYR:CD2	2:B:312:PRO:HB3	2.56	0.41
1:A:691:VAL:O	1:A:695:VAL:HG23	2.21	0.40
2:B:133:ALA:HB2	2:B:178:THR:HB	2.02	0.40
2:B:305:TYR:OH	2:B:984:MET:HB3	2.21	0.40
2:B:527:VAL:HG13	2:B:531:PHE:CD1	2.57	0.40
2:B:1030:ALA:HB2	2:B:1051:PHE:HE1	1.86	0.40
1:A:655:TYR:OH	2:B:449:LEU:HG	2.20	0.40
6:A:1102:CDL:H271	6:A:1102:CDL:H241	1.80	0.40
2:B:291:GLN:NE2	2:B:291:GLN:CA	2.72	0.40
2:B:849:ARG:HH12	2:B:927:ALA:C	2.25	0.40
1:A:423:ALA:O	1:A:427:VAL:HG13	2.22	0.40
1:A:843:TYR:N	1:A:925:ALA:O	2.54	0.40
1:A:905:GLN:O	1:A:909:ARG:NH1	2.35	0.40
2:B:21:LYS:HD2	2:B:21:LYS:HA	1.95	0.40
2:B:378:LEU:HD23	2:B:378:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1076/1088 (99%)	968 (90%)	104 (10%)	4 (0%)	34	69
2	B	1061/1100 (96%)	975 (92%)	83 (8%)	3 (0%)	41	73
3	P	91/99 (92%)	87 (96%)	4 (4%)	0	100	100
All	All	2228/2287 (97%)	2030 (91%)	191 (9%)	7 (0%)	44	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	PRO
1	A	700	VAL
1	A	701	TYR
2	B	314	ASP
2	B	716	THR
1	A	699	PRO
2	B	59	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	831/841 (99%)	828 (100%)	3 (0%)	91	96
2	B	849/878 (97%)	846 (100%)	3 (0%)	91	96
3	P	77/81 (95%)	77 (100%)	0	100	100
All	All	1757/1800 (98%)	1751 (100%)	6 (0%)	92	96

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

Mol	Chain	Res	Type
1	A	41	PRO
1	A	42	GLN
1	A	611	TYR
2	B	57	ASN
2	B	288	TYR
2	B	1079	ARG

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	361	ASN
1	A	482	GLN
1	A	650	HIS
1	A	736	GLN
1	A	972	ASN
1	A	1008	GLN
2	B	291	GLN
2	B	393	GLN
2	B	502	GLN
2	B	508	ASN
2	B	610	ASN
2	B	653	GLN
2	B	673	HIS
2	B	719	ASN
2	B	834	GLN
2	B	881	GLN
2	B	941	GLN
2	B	959	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

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	BXY	C	1	4	10,10,10	9.81	5 (50%)	13,14,14	1.80	3 (23%)
4	BXY	C	2	4	9,9,10	7.62	6 (66%)	10,12,14	2.25	2 (20%)

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	BXY	C	1	4	-	2/2/18/18	0/1/1/1
4	BXY	C	2	4	-	2/2/15/18	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	BXY	C1-C2	-22.94	1.25	1.52
4	C	2	BXY	C2-C3	-19.33	1.22	1.53
4	C	1	BXY	O4-C1	18.59	1.65	1.43
4	C	2	BXY	O4-C4	-9.53	1.28	1.44
4	C	1	BXY	C3-C4	-6.69	1.35	1.53
4	C	2	BXY	C3-C4	5.62	1.67	1.53
4	C	1	BXY	C2-C3	5.38	1.68	1.53
4	C	2	BXY	O4-C1	3.21	1.50	1.43
4	C	1	BXY	O4-C4	3.08	1.51	1.45
4	C	2	BXY	C1-C2	2.61	1.56	1.51
4	C	2	BXY	O2-C2	2.55	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2	BXY	O4-C1-C2	-5.58	95.20	105.99
4	C	1	BXY	C2-C3-C4	3.50	109.44	102.64
4	C	1	BXY	C1-C2-C3	3.18	106.28	102.30
4	C	1	BXY	O3-C3-C2	-2.83	102.67	111.82
4	C	2	BXY	O2-C2-C1	-2.52	103.45	110.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

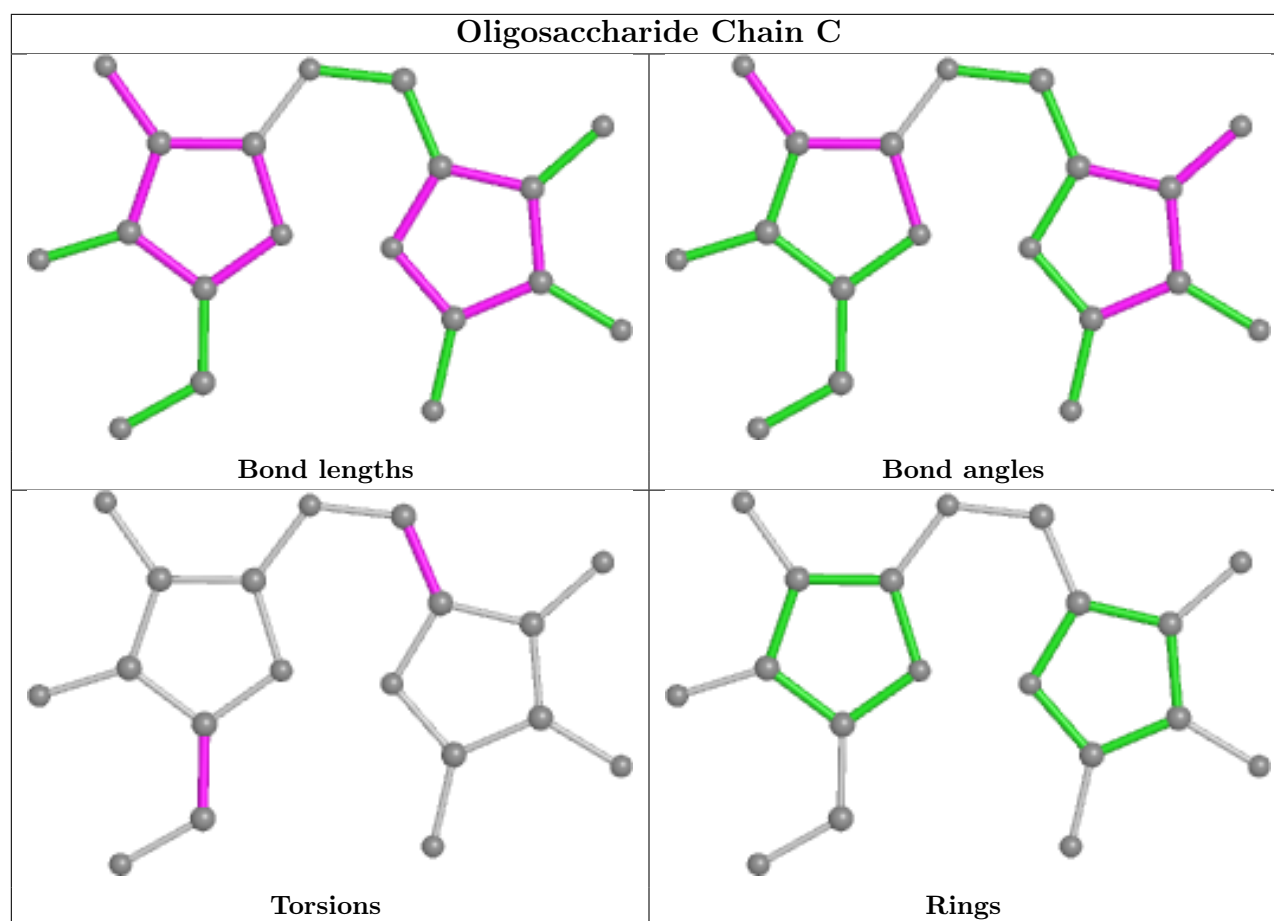
Mol	Chain	Res	Type	Atoms
4	C	1	BXY	O4-C4-C5-O5
4	C	1	BXY	C3-C4-C5-O5
4	C	2	BXY	C3-C4-C5-O5
4	C	2	BXY	O4-C4-C5-O5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	BXY	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 oligosaccharide.



5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	$\# Z > 2$
5	F8L	A	1101	-	38,39,64	3.53	7 (18%)	49,51,81	2.81	19 (38%)
6	CDL	A	1102	-	85,85,99	1.01	6 (7%)	91,97,111	1.27	9 (9%)
8	PO4	B	1201	-	4,4,4	0.92	0	6,6,6	0.43	0
6	CDL	B	1203	-	99,99,99	1.00	8 (8%)	105,111,111	1.49	13 (12%)
9	PNS	B	1202	-	17,21,21	2.12	4 (23%)	26,29,29	1.21	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
5	F8L	A	1101	-	-	10/37/54/84	0/1/1/1
9	PNS	B	1202	-	-	12/27/27/27	-
6	CDL	A	1102	-	-	51/96/96/110	-
6	CDL	B	1203	-	-	60/110/110/110	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1101	F8L	C55-C57	-16.37	1.32	1.52
5	A	1101	F8L	O56-C55	10.24	1.60	1.41
5	A	1101	F8L	C59-C61	-7.05	1.35	1.53
9	B	1202	PNS	C34-N36	5.52	1.45	1.33
9	B	1202	PNS	C39-N41	5.37	1.45	1.33
6	A	1102	CDL	OB8-CB7	4.23	1.45	1.33
6	A	1102	CDL	OB6-CB5	4.13	1.46	1.34
6	A	1102	CDL	OA8-CA7	3.99	1.45	1.33
6	B	1203	CDL	OA6-CA5	3.49	1.44	1.34
6	B	1203	CDL	OA8-CA7	3.24	1.42	1.33
6	B	1203	CDL	OB6-CB5	3.16	1.43	1.34
6	B	1203	CDL	OB6-CB4	-3.11	1.38	1.46
5	A	1101	F8L	C59-C57	2.93	1.61	1.53
6	B	1203	CDL	OB8-CB7	2.91	1.41	1.33
5	A	1101	F8L	O56-C61	2.84	1.51	1.45
6	A	1102	CDL	OA6-CA5	2.57	1.41	1.34
6	A	1102	CDL	OA6-CA4	-2.51	1.40	1.46
6	A	1102	CDL	OB6-CB4	-2.47	1.40	1.46
6	B	1203	CDL	OA8-CA6	-2.47	1.39	1.45
9	B	1202	PNS	O35-C34	-2.21	1.19	1.23
9	B	1202	PNS	O40-C39	-2.13	1.18	1.23
6	B	1203	CDL	PB2-OB4	-2.11	1.45	1.55
5	A	1101	F8L	P52-O54	2.10	1.66	1.60
6	B	1203	CDL	OB8-CB6	-2.05	1.40	1.45
5	A	1101	F8L	O51-C50	-2.04	1.40	1.43

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	F8L	C45-C44-C42	-7.30	110.08	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1101	F8L	C40-C39-C37	-6.86	111.14	127.66
5	A	1101	F8L	C50-C49-C47	-6.82	114.24	126.04
5	A	1101	F8L	C35-C34-C32	-6.52	111.95	127.66
5	A	1101	F8L	C48-C47-C46	6.01	125.39	115.27
6	B	1203	CDL	OA6-CA5-C11	5.61	123.60	111.50
6	A	1102	CDL	OB6-CB5-C51	5.06	122.40	111.50
5	A	1101	F8L	O56-C55-O54	-4.81	99.63	109.18
6	B	1203	CDL	OB8-CB7-C71	4.45	125.88	111.91
6	B	1203	CDL	OB6-CB5-C51	4.06	120.25	111.50
6	A	1102	CDL	OA6-CA5-C11	4.03	120.19	111.50
6	A	1102	CDL	OB8-CB7-C71	3.98	124.41	111.91
5	A	1101	F8L	C33-C32-C34	-3.80	113.92	123.68
5	A	1101	F8L	C46-C47-C49	-3.54	113.94	121.12
6	B	1203	CDL	CA4-OA6-CA5	-3.54	109.07	117.79
5	A	1101	F8L	C33-C32-C31	3.47	121.12	115.27
9	B	1202	PNS	C37-C38-C39	3.45	118.10	112.36
6	B	1203	CDL	OB8-CB7-OB9	-3.38	115.07	123.59
6	A	1102	CDL	OA6-CA5-OA7	-3.22	115.93	123.70
6	A	1102	CDL	OA8-CA7-C31	3.14	121.76	111.91
5	A	1101	F8L	C36-C35-C34	-3.11	101.66	111.88
5	A	1101	F8L	O54-C55-C57	3.06	111.91	106.72
5	A	1101	F8L	C40-C41-C42	-2.68	104.16	112.98
5	A	1101	F8L	C35-C36-C37	-2.66	104.22	112.98
6	B	1203	CDL	OB8-CB6-CB4	2.56	115.88	108.43
6	B	1203	CDL	OA6-CA5-OA7	-2.55	117.54	123.70
5	A	1101	F8L	C30-C29-C27	-2.53	119.10	127.75
5	A	1101	F8L	O63-C62-C61	-2.53	102.62	111.29
5	A	1101	F8L	C45-C46-C47	-2.51	104.70	112.98
6	A	1102	CDL	CA4-OA6-CA5	-2.47	111.71	117.79
5	A	1101	F8L	C28-C27-C26	2.36	119.81	114.60
6	A	1102	CDL	OB8-CB7-OB9	-2.31	117.75	123.59
6	B	1203	CDL	C52-C51-CB5	-2.31	105.21	113.62
5	A	1101	F8L	C31-C30-C29	-2.29	104.37	111.88
6	B	1203	CDL	C55-C54-C53	-2.26	102.96	114.42
6	B	1203	CDL	C37-C36-C35	-2.25	103.00	114.42
6	A	1102	CDL	OA8-CA7-OA9	-2.24	117.94	123.59
6	A	1102	CDL	OB4-PB2-OB3	2.22	123.22	112.24
6	B	1203	CDL	CB6-CB4-CB3	-2.21	106.55	111.79
9	B	1202	PNS	C38-C39-N41	2.14	120.02	116.42
5	A	1101	F8L	C46-C45-C44	2.13	118.88	111.88
6	B	1203	CDL	OA8-CA7-OA9	-2.10	118.30	123.59
6	B	1203	CDL	OA8-CA7-C31	2.09	118.46	111.91

There are no chirality outliers.

All (133) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1101	F8L	C40-C41-C42-C43
5	A	1101	F8L	C40-C41-C42-C44
6	A	1102	CDL	C11-CA5-OA6-CA4
6	A	1102	CDL	CB2-OB2-PB2-OB4
6	A	1102	CDL	CB2-OB2-PB2-OB5
6	A	1102	CDL	OB7-CB5-OB6-CB4
6	B	1203	CDL	CA3-OA5-PA1-OA4
6	B	1203	CDL	C11-CA5-OA6-CA4
6	B	1203	CDL	CB2-OB2-PB2-OB3
6	B	1203	CDL	CB3-OB5-PB2-OB3
6	B	1203	CDL	OB6-CB4-CB6-OB8
6	B	1203	CDL	OB9-CB7-OB8-CB6
6	B	1203	CDL	C71-CB7-OB8-CB6
9	B	1202	PNS	C28-O27-P24-O23
9	B	1202	PNS	C28-O27-P24-O25
9	B	1202	PNS	C28-O27-P24-O26
9	B	1202	PNS	C28-C29-C32-O33
9	B	1202	PNS	C28-C29-C32-C34
9	B	1202	PNS	C31-C29-C32-O33
9	B	1202	PNS	C31-C29-C32-C34
9	B	1202	PNS	N36-C37-C38-C39
9	B	1202	PNS	N41-C42-C43-S44
6	B	1203	CDL	OA9-CA7-OA8-CA6
6	A	1102	CDL	OA7-CA5-OA6-CA4
6	B	1203	CDL	OA7-CA5-OA6-CA4
6	B	1203	CDL	C31-CA7-OA8-CA6
6	A	1102	CDL	C51-CB5-OB6-CB4
9	B	1202	PNS	C38-C37-N36-C34
6	B	1203	CDL	C20-C21-C22-C23
6	B	1203	CDL	O1-C1-CB2-OB2
6	A	1102	CDL	C71-CB7-OB8-CB6
6	A	1102	CDL	C80-C81-C82-C83
6	A	1102	CDL	C22-C23-C24-C25
6	A	1102	CDL	C17-C18-C19-C20
6	A	1102	CDL	OB9-CB7-OB8-CB6
5	A	1101	F8L	C29-C30-C31-C32
5	A	1101	F8L	C34-C35-C36-C37
6	B	1203	CDL	C63-C64-C65-C66
6	B	1203	CDL	C43-C44-C45-C46
6	B	1203	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
6	B	1203	CDL	CA5-C11-C12-C13
6	A	1102	CDL	CB5-C51-C52-C53
5	A	1101	F8L	C50-O51-P52-O54
6	B	1203	CDL	CA3-OA5-PA1-OA2
6	B	1203	CDL	C81-C82-C83-C84
6	B	1203	CDL	C22-C23-C24-C25
6	A	1102	CDL	O1-C1-CB2-OB2
6	A	1102	CDL	C16-C17-C18-C19
6	A	1102	CDL	C34-C35-C36-C37
6	B	1203	CDL	C14-C15-C16-C17
6	B	1203	CDL	C23-C24-C25-C26
6	B	1203	CDL	C37-C38-C39-C40
6	A	1102	CDL	C82-C83-C84-C85
6	A	1102	CDL	C12-C13-C14-C15
6	A	1102	CDL	C13-C14-C15-C16
6	A	1102	CDL	C24-C25-C26-C27
6	A	1102	CDL	C72-C73-C74-C75
6	A	1102	CDL	C36-C37-C38-C39
6	B	1203	CDL	C11-C12-C13-C14
6	A	1102	CDL	C37-C38-C39-C40
6	B	1203	CDL	CB7-C71-C72-C73
6	B	1203	CDL	C38-C39-C40-C41
5	A	1101	F8L	C45-C46-C47-C49
6	B	1203	CDL	CB3-OB5-PB2-OB2
6	A	1102	CDL	C35-C36-C37-C38
6	A	1102	CDL	C77-C78-C79-C80
6	B	1203	CDL	C77-C78-C79-C80
6	B	1203	CDL	CB3-CB4-CB6-OB8
6	B	1203	CDL	C76-C77-C78-C79
5	A	1101	F8L	C45-C46-C47-C48
6	B	1203	CDL	C59-C60-C61-C62
6	B	1203	CDL	C84-C85-C86-C87
9	B	1202	PNS	C30-C29-C32-O33
6	A	1102	CDL	C39-C40-C41-C42
6	B	1203	CDL	C56-C57-C58-C59
6	A	1102	CDL	OB5-CB3-CB4-OB6
6	B	1203	CDL	C24-C25-C26-C27
6	B	1203	CDL	C82-C83-C84-C85
6	B	1203	CDL	CA2-C1-CB2-OB2
6	B	1203	CDL	C33-C34-C35-C36
6	B	1203	CDL	C15-C16-C17-C18
6	B	1203	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
6	A	1102	CDL	C32-C33-C34-C35
6	A	1102	CDL	C19-C20-C21-C22
6	A	1102	CDL	C74-C75-C76-C77
6	B	1203	CDL	C17-C18-C19-C20
6	B	1203	CDL	CB2-OB2-PB2-OB5
6	B	1203	CDL	C42-C43-C44-C45
6	A	1102	CDL	C14-C15-C16-C17
5	A	1101	F8L	C50-O51-P52-O53
6	B	1203	CDL	CA3-OA5-PA1-OA3
6	B	1203	CDL	CB3-OB5-PB2-OB4
6	A	1102	CDL	OB5-CB3-CB4-CB6
6	B	1203	CDL	OB5-CB3-CB4-CB6
6	B	1203	CDL	OB5-CB3-CB4-OB6
6	B	1203	CDL	C32-C33-C34-C35
6	A	1102	CDL	CA5-C11-C12-C13
6	B	1203	CDL	C41-C42-C43-C44
6	B	1203	CDL	C71-C72-C73-C74
6	A	1102	CDL	CA3-CA4-OA6-CA5
6	A	1102	CDL	C83-C84-C85-C86
6	A	1102	CDL	CA2-OA2-PA1-OA5
6	A	1102	CDL	CA3-OA5-PA1-OA2
6	A	1102	CDL	CB3-OB5-PB2-OB2
6	B	1203	CDL	CA2-OA2-PA1-OA5
6	B	1203	CDL	C79-C80-C81-C82
6	B	1203	CDL	C39-C40-C41-C42
6	A	1102	CDL	C23-C24-C25-C26
6	A	1102	CDL	CA2-C1-CB2-OB2
6	B	1203	CDL	O1-C1-CA2-OA2
6	B	1203	CDL	C83-C84-C85-C86
6	B	1203	CDL	C55-C56-C57-C58
6	A	1102	CDL	C73-C74-C75-C76
6	B	1203	CDL	C80-C81-C82-C83
6	B	1203	CDL	C35-C36-C37-C38
6	A	1102	CDL	OA9-CA7-OA8-CA6
6	A	1102	CDL	C31-CA7-OA8-CA6
6	A	1102	CDL	C81-C82-C83-C84
6	A	1102	CDL	C75-C76-C77-C78
6	A	1102	CDL	C11-C12-C13-C14
5	A	1101	F8L	C30-C31-C32-C33
9	B	1202	PNS	C30-C29-C32-C34
6	A	1102	CDL	OB6-CB4-CB6-OB8
6	B	1203	CDL	C72-C73-C74-C75

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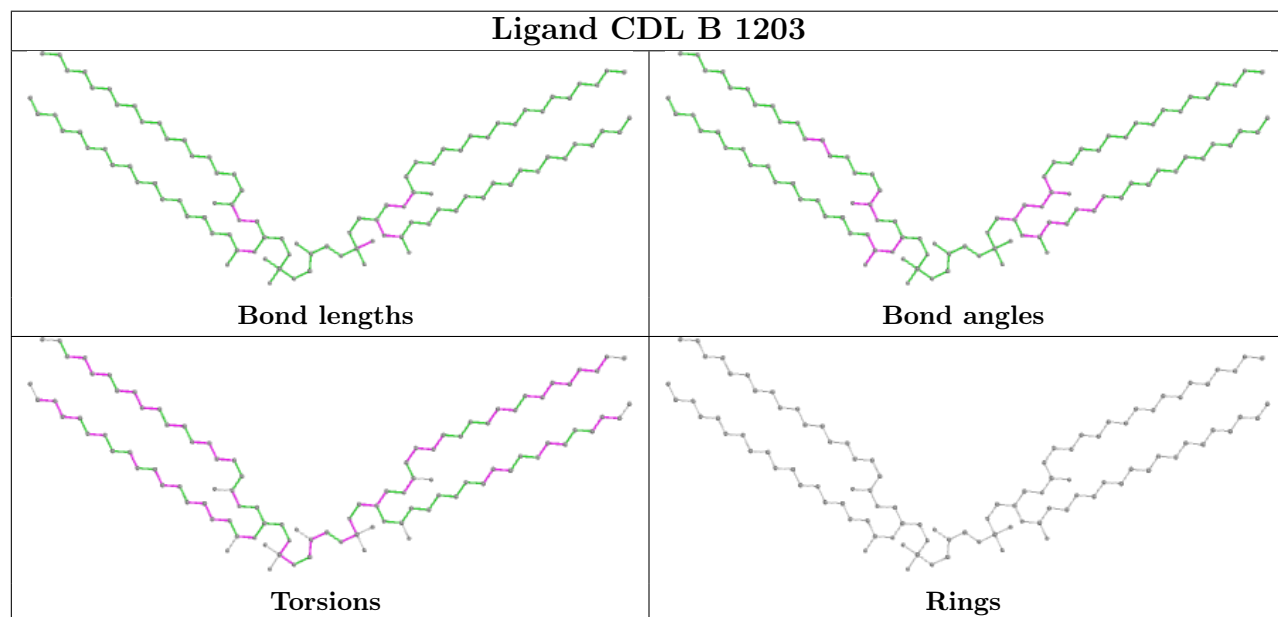
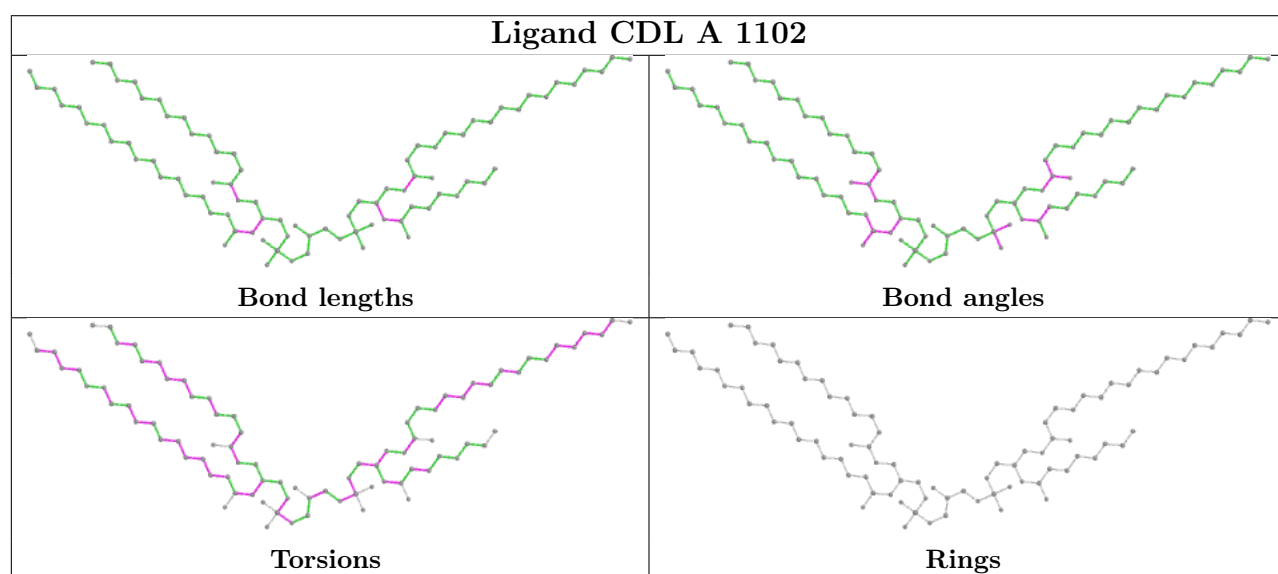
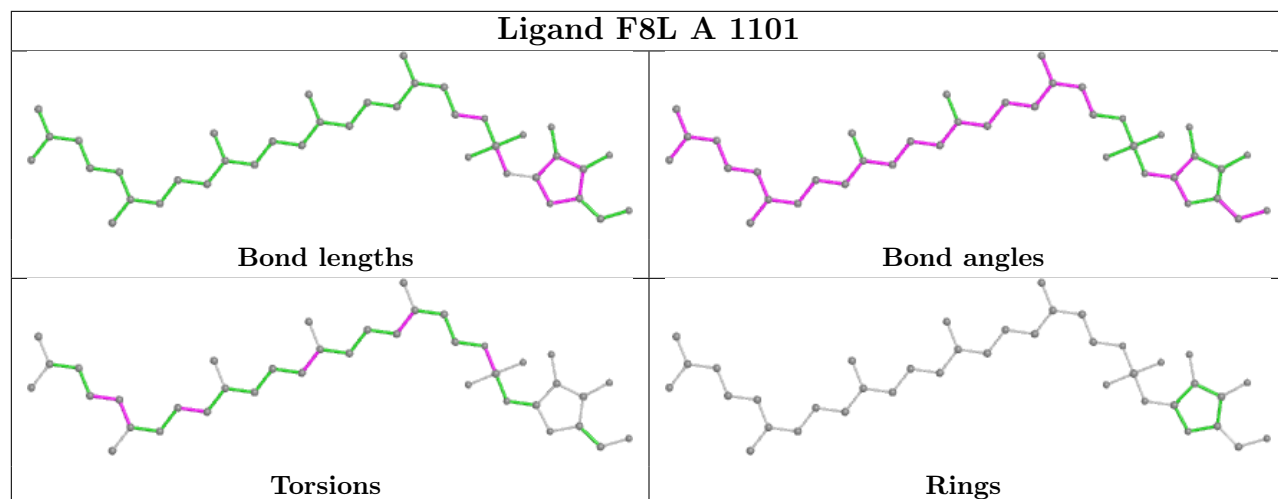
Mol	Chain	Res	Type	Atoms
6	B	1203	CDL	C12-C13-C14-C15
5	A	1101	F8L	C50-O51-P52-O64
6	A	1102	CDL	CA2-OA2-PA1-OA3
6	A	1102	CDL	CA3-OA5-PA1-OA3
6	B	1203	CDL	CA2-OA2-PA1-OA3
6	A	1102	CDL	C32-C31-CA7-OA8
6	B	1203	CDL	C64-C65-C66-C67
6	A	1102	CDL	C84-C85-C86-C87
6	A	1102	CDL	C32-C31-CA7-OA9

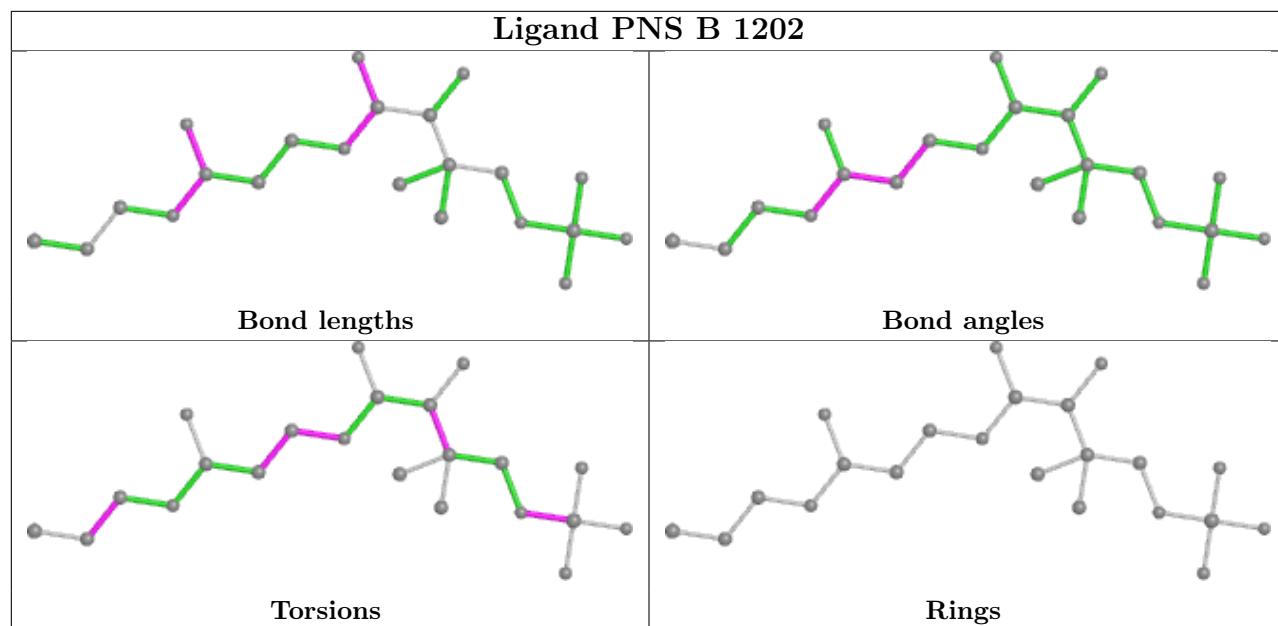
There are no ring outliers.

4 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1101	F8L	1	0
6	A	1102	CDL	16	0
6	B	1203	CDL	12	0
9	B	1202	PNS	42	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.

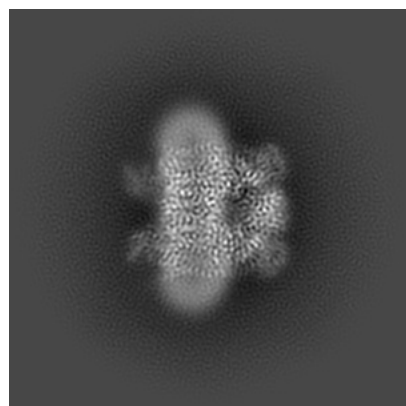
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30219. These allow visual inspection of the internal detail of the map and identification of artifacts.

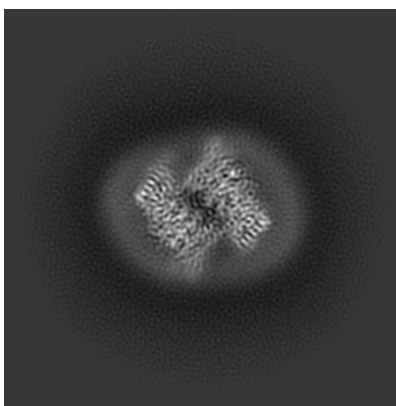
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

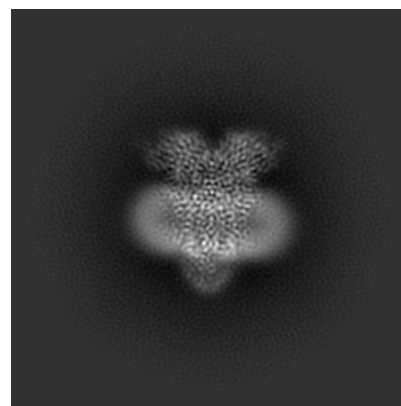
6.1.1 Primary map



X

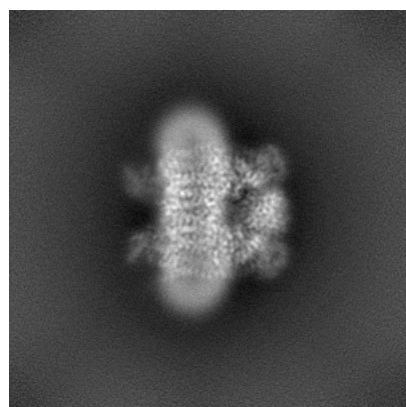


Y

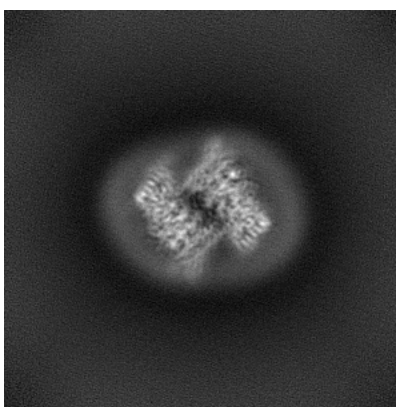


Z

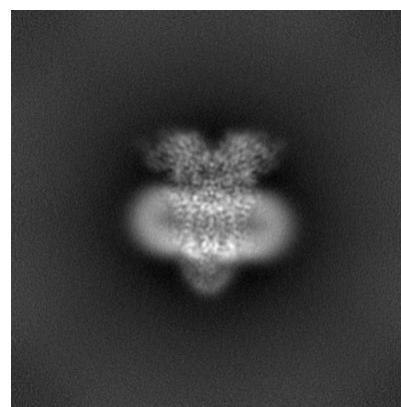
6.1.2 Raw map



X



Y

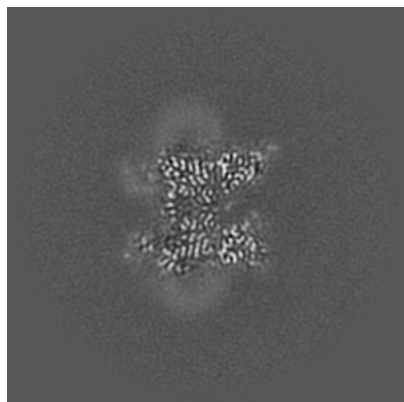


Z

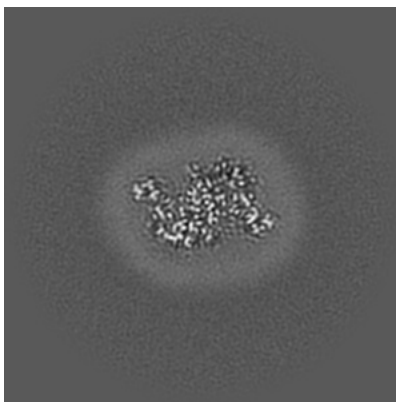
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

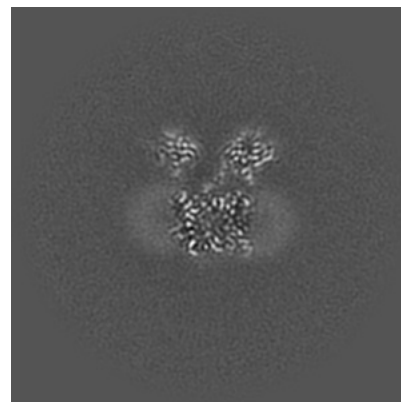
6.2.1 Primary map



X Index: 180

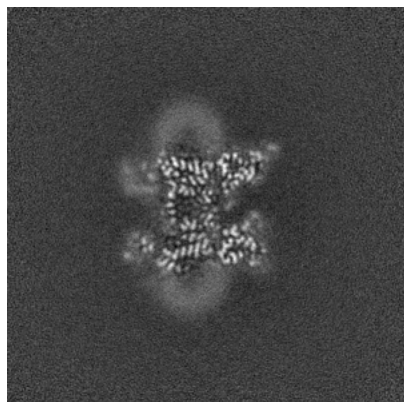


Y Index: 180

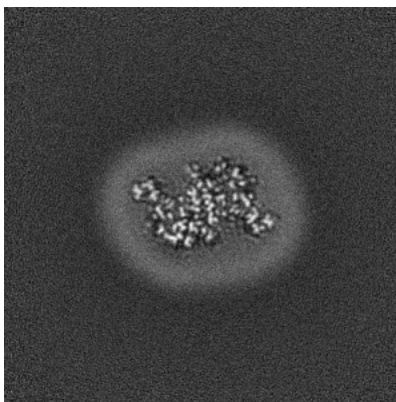


Z Index: 180

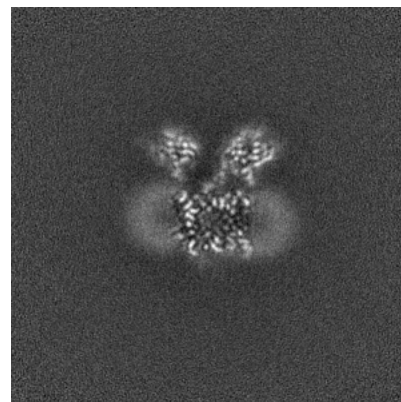
6.2.2 Raw map



X Index: 180



Y Index: 180

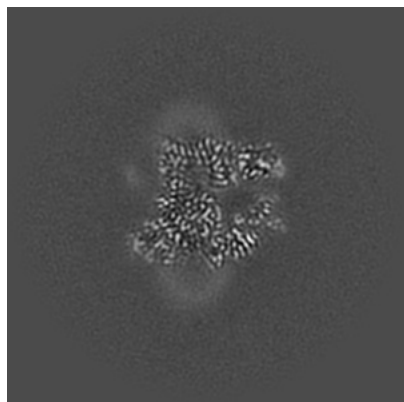


Z Index: 180

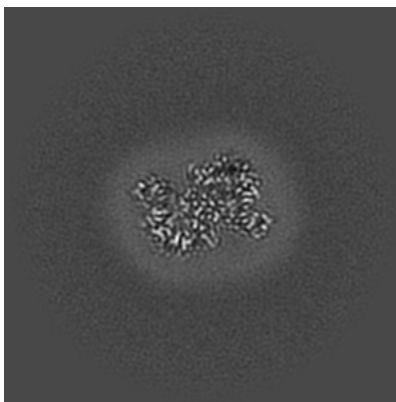
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

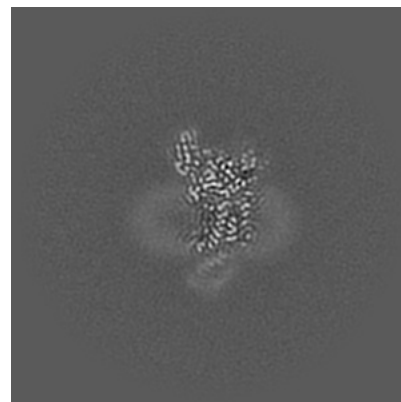
6.3.1 Primary map



X Index: 165

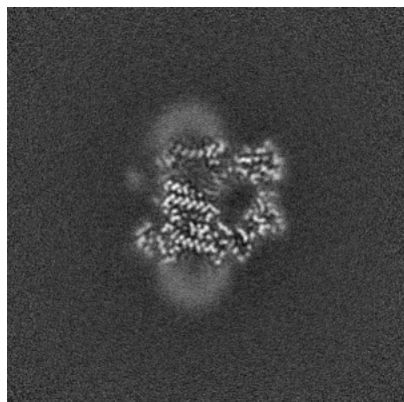


Y Index: 185

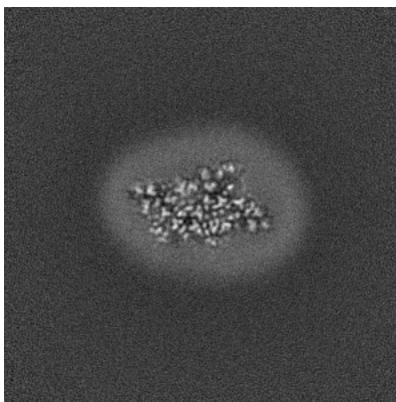


Z Index: 208

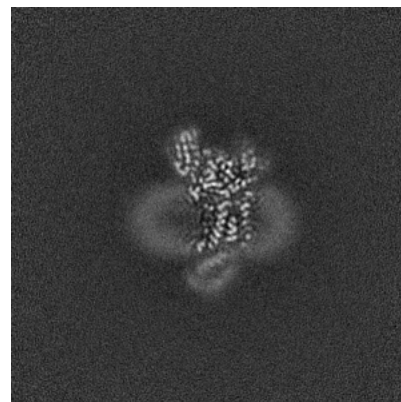
6.3.2 Raw map



X Index: 160



Y Index: 148

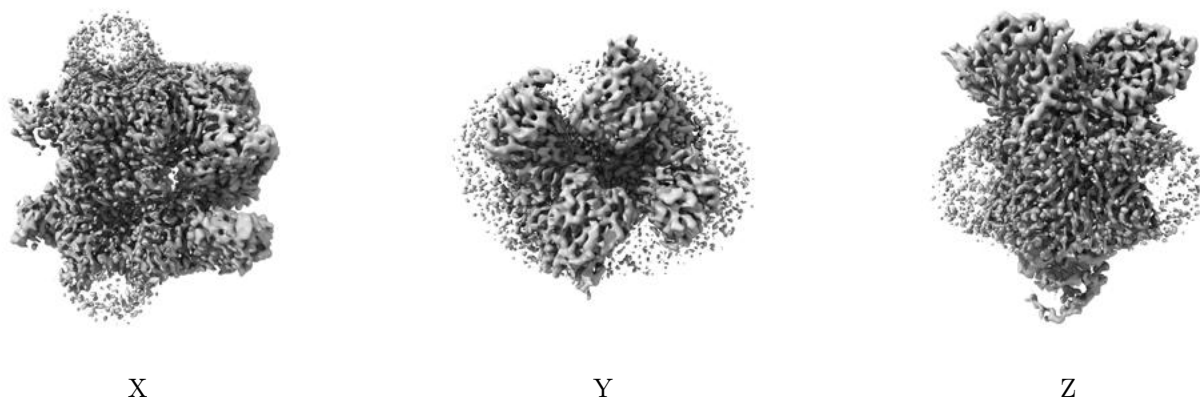


Z Index: 208

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

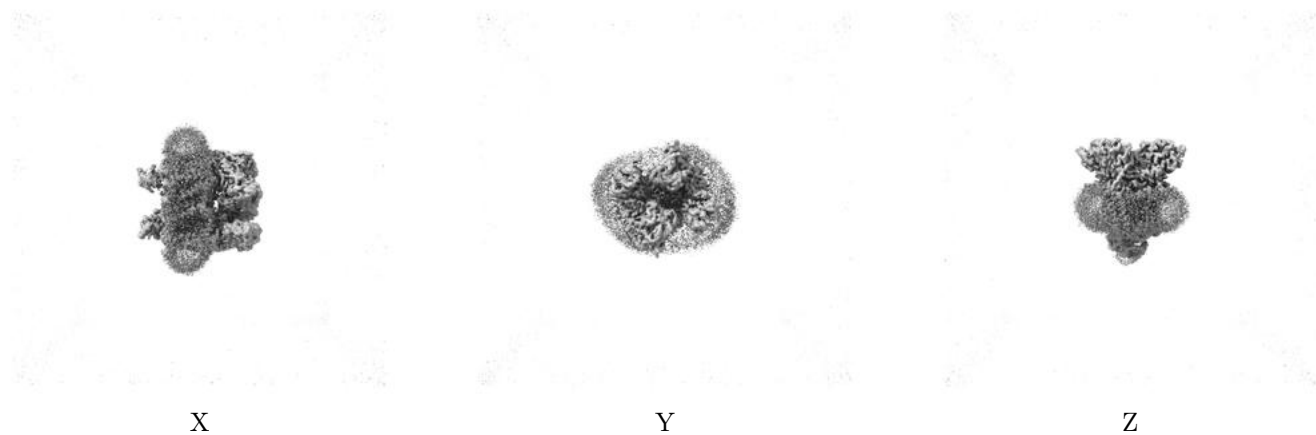
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



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



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.

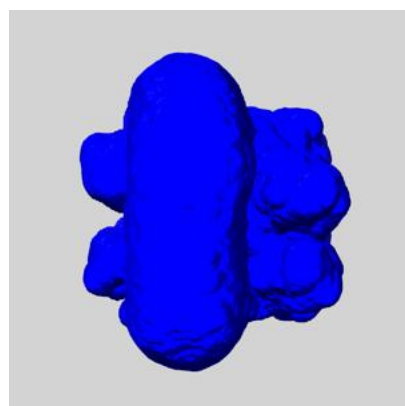
6.5 Mask visualisation [i](#)

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

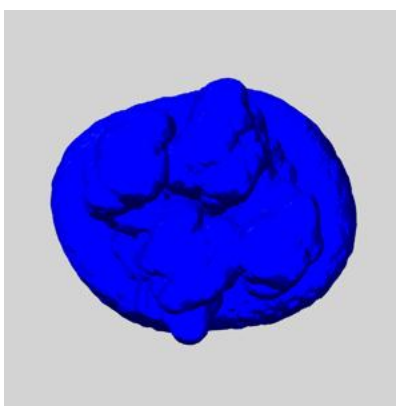
A mask typically either:

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

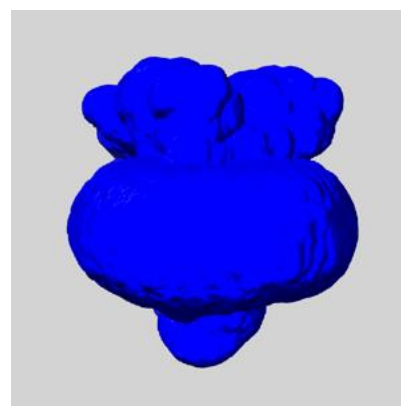
6.5.1 emd_30219_msk_1.map [i](#)



X



Y

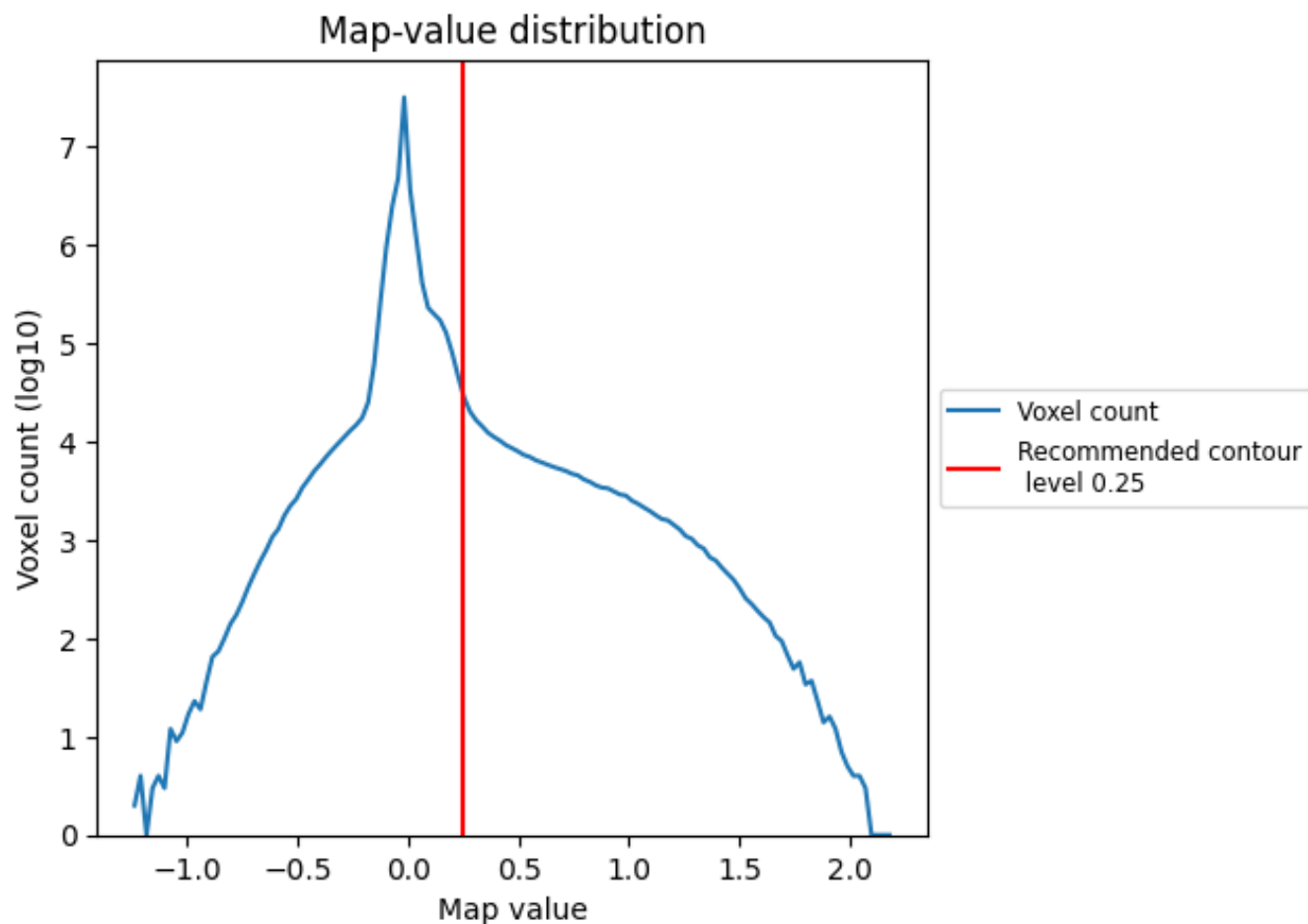


Z

7 Map analysis [i](#)

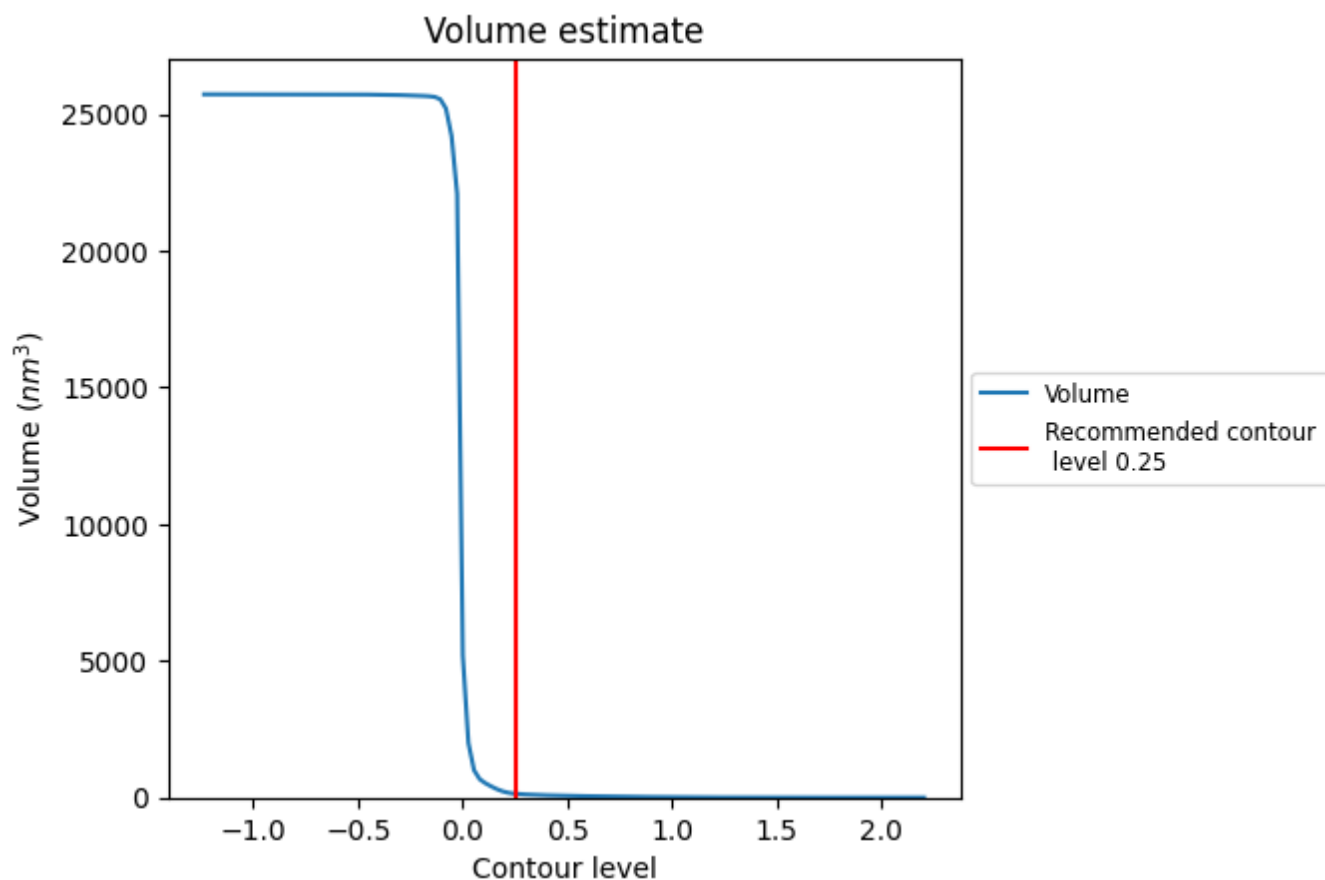
This section contains the results of statistical analysis of the map.

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.

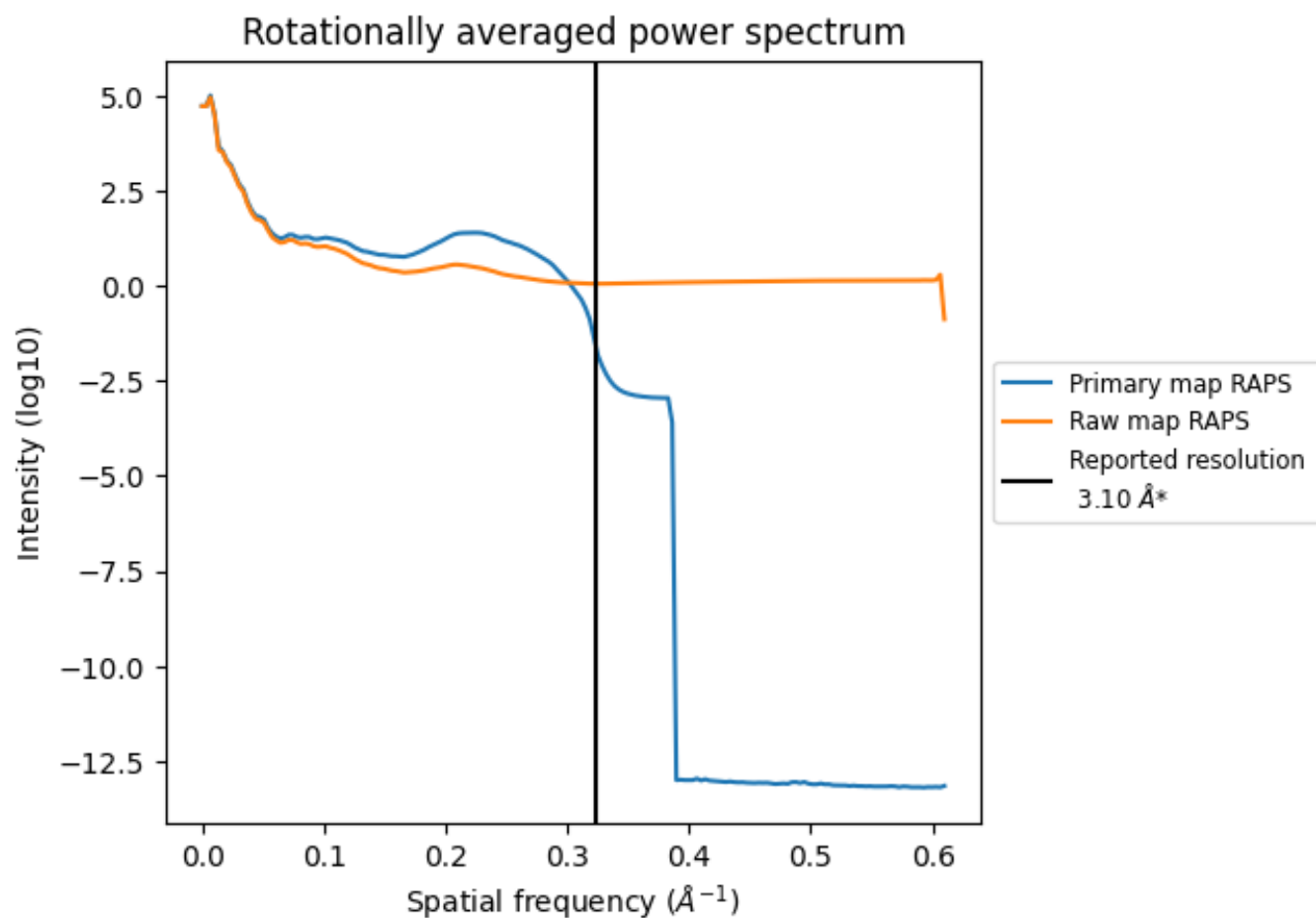
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm^3 ; this corresponds to an approximate mass of 128 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 ⓘ

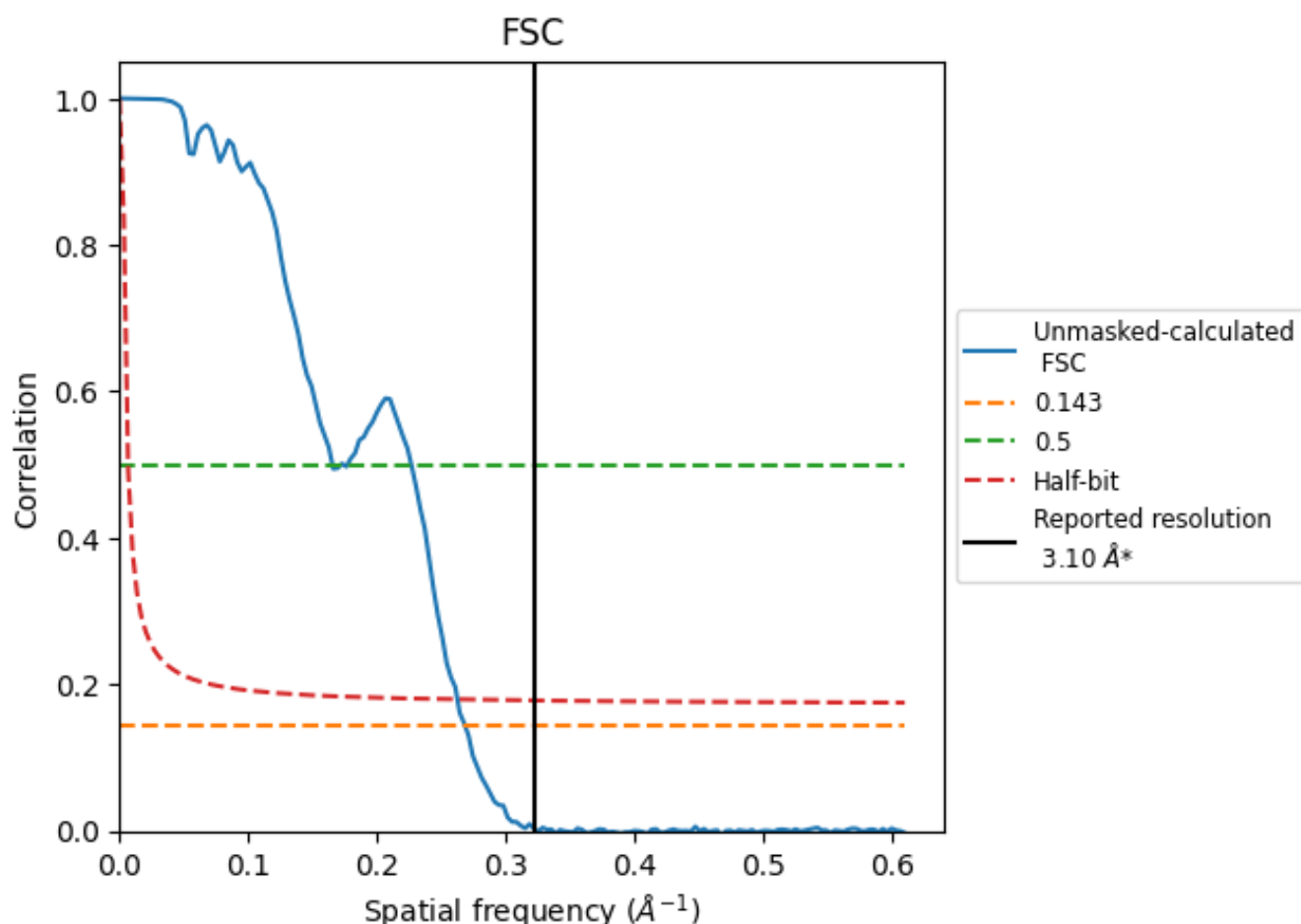


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

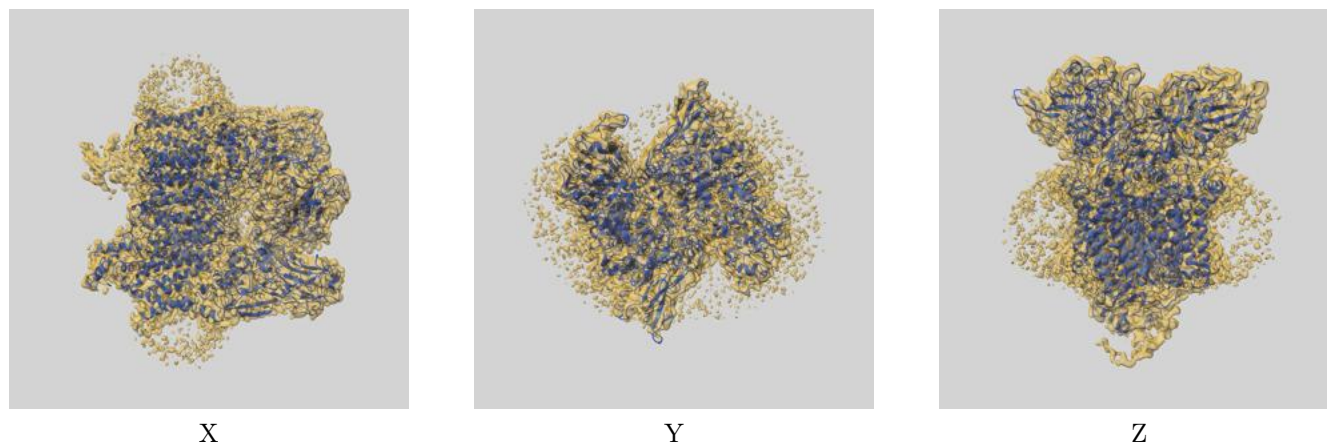
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.73	6.05	3.81

*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 3.73 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

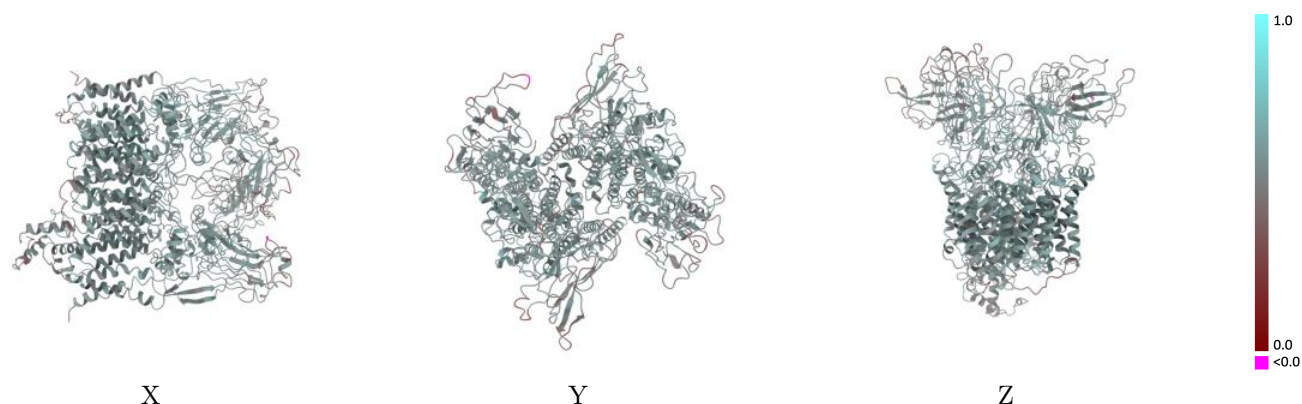
This section contains information regarding the fit between EMDB map EMD-30219 and PDB model 7BVG. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



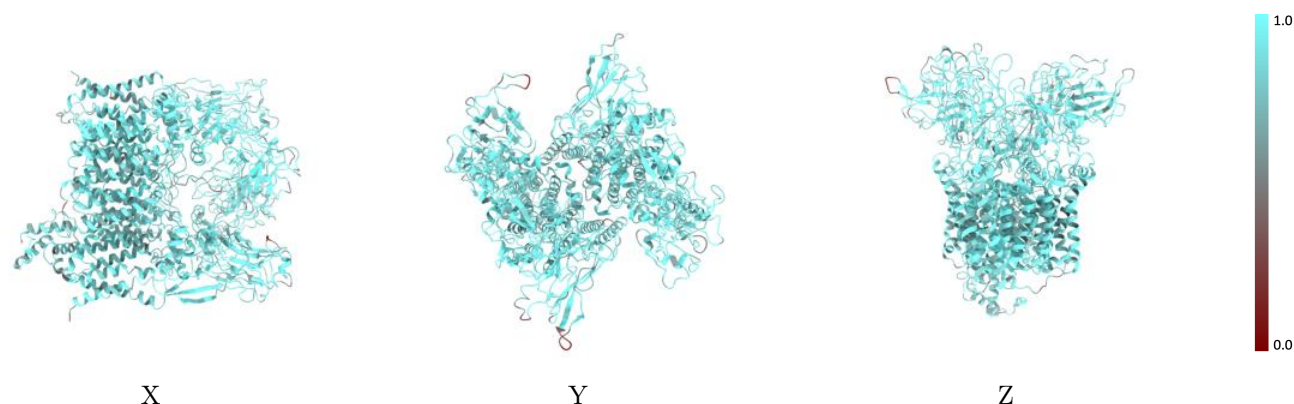
The images above show the 3D surface view of the map at the recommended contour level 0.25 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



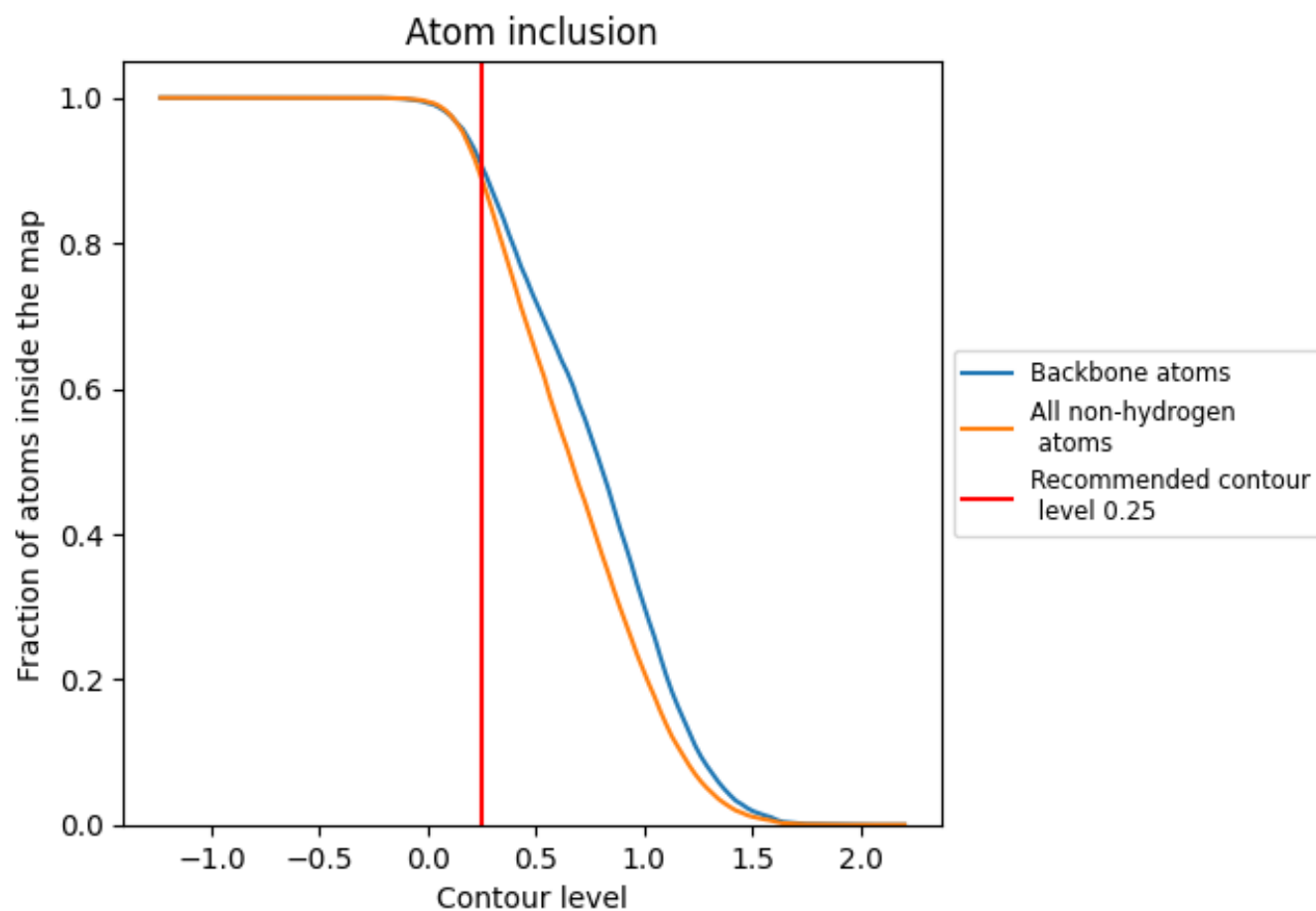
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 91% of all backbone atoms, 89% 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> 0.8887	<div></div> 0.5370
A	<div></div> 0.8956	<div></div> 0.5390
B	<div></div> 0.8894	<div></div> 0.5400
C	<div></div> 0.7895	<div></div> 0.6030
P	<div></div> 0.8029	<div></div> 0.4890

