Full wwPDB EM Validation Report (i)

Oct 5, 2026 – 08:37 PM EDT

PDB ID	:	12XL / pdb_000012xl
EMDB ID	:	EMD-76832
Title	:	Candida albicans Chitin synthase 1 (CaChs1) intermediate state (DA-2), bound to UDP and diynyl arylamine (DA, aka RO-09-3143)
Authors	:	Ren, Z.; Lee, S.Y.
Deposited on	:	2026-04-21
Resolution	:	3.02 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 (i) 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 (i)) were used in the production of this report:

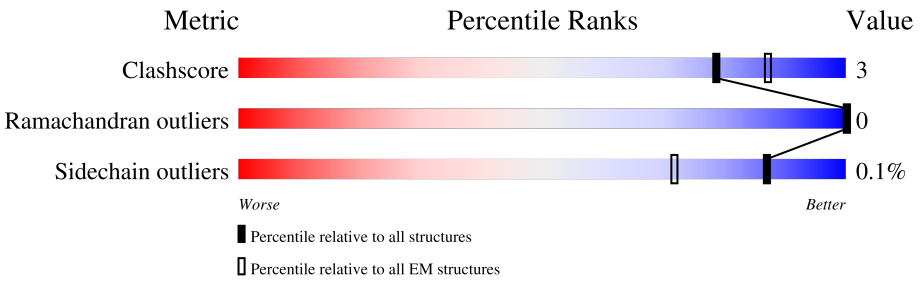
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

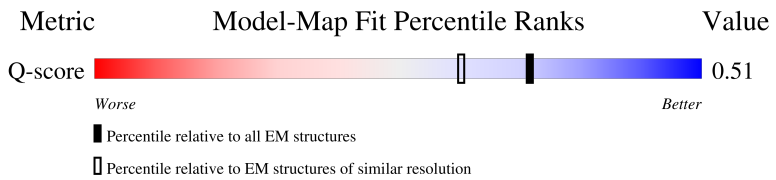
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.02 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13913 (2.52 - 3.52)

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	1058	65% • 31%
1	B	1058	65% • 31%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22308 atoms, of which 10837 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 Chitin synthase.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	727	10849	3640	5258	927	999	25	0	0
1	B	730	10918	3659	5295	934	1005	25	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1027	SER	-	expression tag	UNP G1UA94
A	1028	ASN	-	expression tag	UNP G1UA94
A	1029	SER	-	expression tag	UNP G1UA94
A	1030	LEU	-	expression tag	UNP G1UA94
A	1031	GLU	-	expression tag	UNP G1UA94
A	1032	VAL	-	expression tag	UNP G1UA94
A	1033	LEU	-	expression tag	UNP G1UA94
A	1034	PHE	-	expression tag	UNP G1UA94
A	1035	GLN	-	expression tag	UNP G1UA94
A	1036	GLY	-	expression tag	UNP G1UA94
A	1037	PRO	-	expression tag	UNP G1UA94
A	1038	ALA	-	expression tag	UNP G1UA94
A	1039	ALA	-	expression tag	UNP G1UA94
A	1040	ASP	-	expression tag	UNP G1UA94
A	1041	TYR	-	expression tag	UNP G1UA94
A	1042	LYS	-	expression tag	UNP G1UA94
A	1043	ASP	-	expression tag	UNP G1UA94
A	1044	ASP	-	expression tag	UNP G1UA94
A	1045	ASP	-	expression tag	UNP G1UA94
A	1046	ASP	-	expression tag	UNP G1UA94
A	1047	LYS	-	expression tag	UNP G1UA94
A	1048	ALA	-	expression tag	UNP G1UA94
A	1049	HIS	-	expression tag	UNP G1UA94
A	1050	HIS	-	expression tag	UNP G1UA94
A	1051	HIS	-	expression tag	UNP G1UA94
A	1052	HIS	-	expression tag	UNP G1UA94

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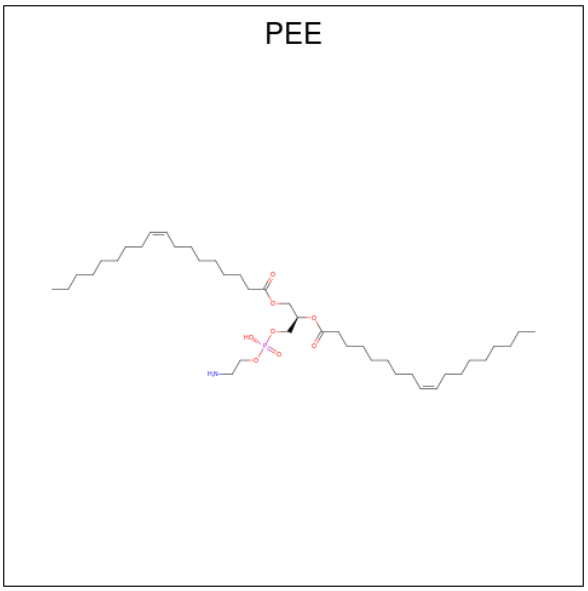
Chain	Residue	Modelled	Actual	Comment	Reference
A	1053	HIS	-	expression tag	UNP G1UA94
A	1054	HIS	-	expression tag	UNP G1UA94
A	1055	HIS	-	expression tag	UNP G1UA94
A	1056	HIS	-	expression tag	UNP G1UA94
A	1057	HIS	-	expression tag	UNP G1UA94
A	1058	HIS	-	expression tag	UNP G1UA94
B	1027	SER	-	expression tag	UNP G1UA94
B	1028	ASN	-	expression tag	UNP G1UA94
B	1029	SER	-	expression tag	UNP G1UA94
B	1030	LEU	-	expression tag	UNP G1UA94
B	1031	GLU	-	expression tag	UNP G1UA94
B	1032	VAL	-	expression tag	UNP G1UA94
B	1033	LEU	-	expression tag	UNP G1UA94
B	1034	PHE	-	expression tag	UNP G1UA94
B	1035	GLN	-	expression tag	UNP G1UA94
B	1036	GLY	-	expression tag	UNP G1UA94
B	1037	PRO	-	expression tag	UNP G1UA94
B	1038	ALA	-	expression tag	UNP G1UA94
B	1039	ALA	-	expression tag	UNP G1UA94
B	1040	ASP	-	expression tag	UNP G1UA94
B	1041	TYR	-	expression tag	UNP G1UA94
B	1042	LYS	-	expression tag	UNP G1UA94
B	1043	ASP	-	expression tag	UNP G1UA94
B	1044	ASP	-	expression tag	UNP G1UA94
B	1045	ASP	-	expression tag	UNP G1UA94
B	1046	ASP	-	expression tag	UNP G1UA94
B	1047	LYS	-	expression tag	UNP G1UA94
B	1048	ALA	-	expression tag	UNP G1UA94
B	1049	HIS	-	expression tag	UNP G1UA94
B	1050	HIS	-	expression tag	UNP G1UA94
B	1051	HIS	-	expression tag	UNP G1UA94
B	1052	HIS	-	expression tag	UNP G1UA94
B	1053	HIS	-	expression tag	UNP G1UA94
B	1054	HIS	-	expression tag	UNP G1UA94
B	1055	HIS	-	expression tag	UNP G1UA94
B	1056	HIS	-	expression tag	UNP G1UA94
B	1057	HIS	-	expression tag	UNP G1UA94
B	1058	HIS	-	expression tag	UNP G1UA94

- Molecule 2 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

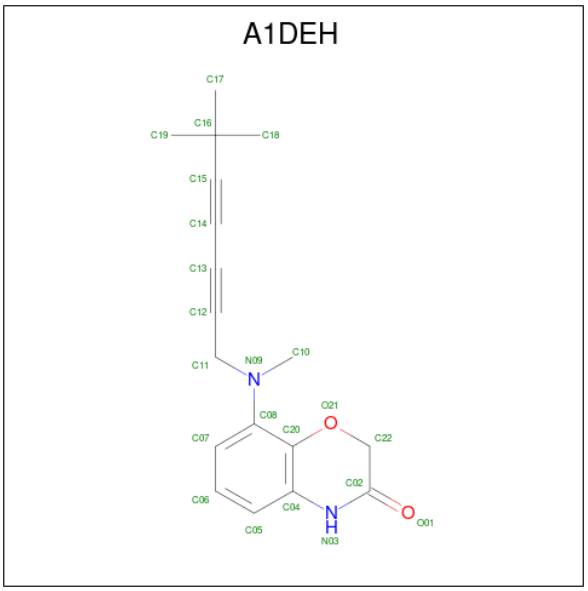


Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
2	A	1	59	18	31	1	8	1	0
			Total	C	H	N	O	P	
2	A	1	128	41	77	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	68	21	37	1	8	1	0
			Total	C	H	N	O	P	
2	B	1	128	41	77	1	8	1	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

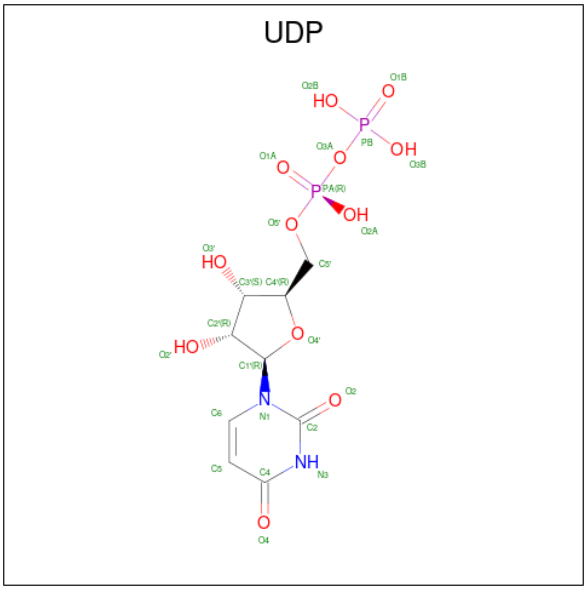
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
3	A	1	1	1	0
			Total	Mg	
3	B	1	1	1	0

- Molecule 4 is 8-[(6,6-dimethylhepta-2,4-diyn-1-yl)(methyl)amino]-2H-1,4-benzoxazin-3(4H)-one (CCD ID: A1DEH) (formula: $C_{18}H_{20}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			42	18	20	2	2	
4	B	1	Total	C	H	N	O	0
			42	18	20	2	2	

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).



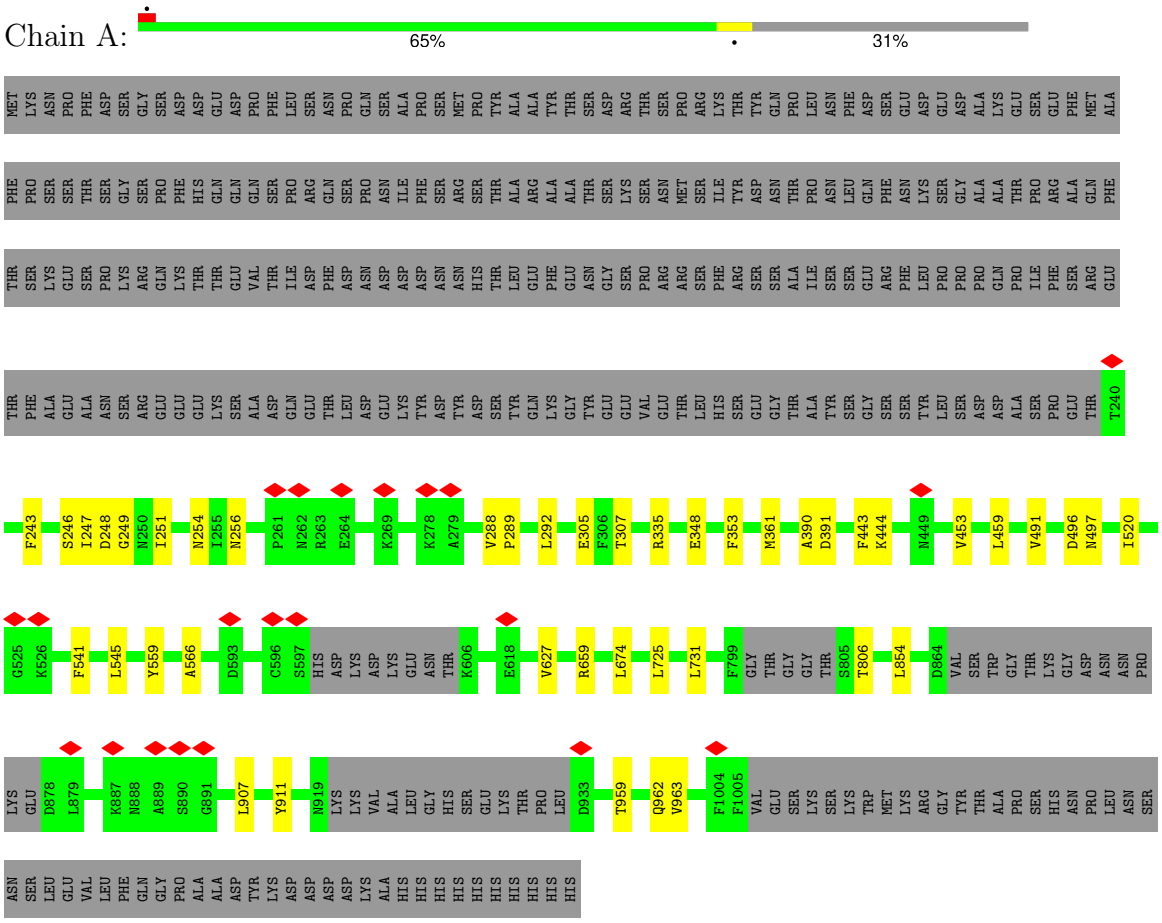
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	
5	B	1	Total	C	H	N	O	P	0
			36	9	11	2	12	2	

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.

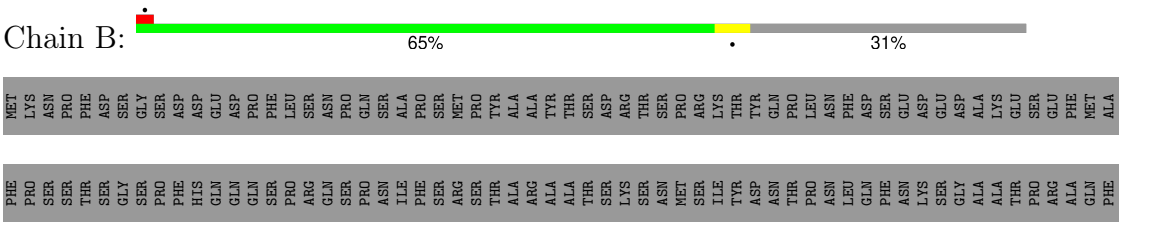
- Molecule 1: Chitin synthase

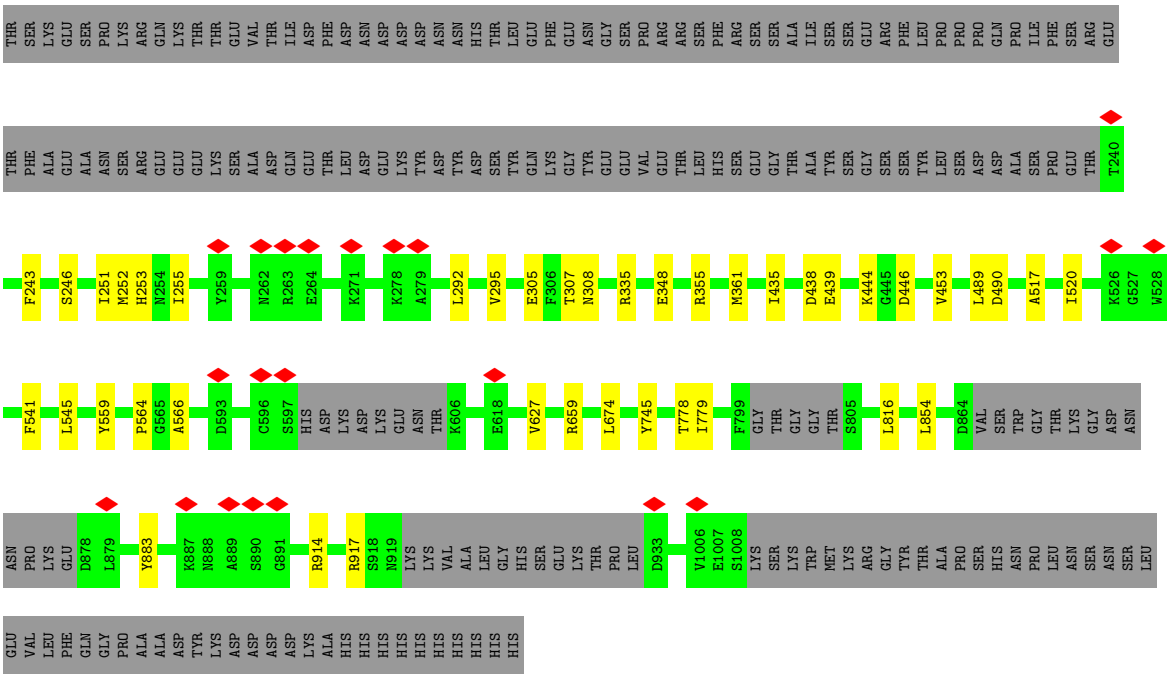
Chain A:



- Molecule 1: Chitin synthase

Chain B:




THR SER LYS GLU SER PRO LYS ARG GLN LYS THR THR GLU VAL THR ILE ASP PHE ASP ASN ASP ASP ASP ASN ASN HIS THR LEU GLU PHE GLU ASN GLY SER PRO ARG ARG SER PHE ARG SER SER ALA ILE SER SER GLU ARG PHE LEU PRO PRO PRO GLN PRO ILE PHE SER ARG GLU
THR PHE ALA GLU ALA ASN SER ARG GLU GLU GLU LYS SER ALA ASP GLN GLU THR LEU ASP GLU LYS TYR ASP TYR ASP SER TYR GLN LYS GLY TYR GLU GLU VAL GLU THR LEU HIS SER GLU GLY THR ALA TYR SER GLY SER SER TYR LEU SER ASP ASP ALA SER PRO GLU THR T240
F243 S246 I251 M252 H253 N254 I255 Y259 N262 R263 E264 K271 K278 A279 L292 V295 E305 F306 T307 N308 R335 E348 R355 M361 I435 D438 E439 K444 G445 D446 V453 L489 D490 A517 I520 K526 G527 W528
F541 L545 Y559 P564 G565 A566 D593 C596 S597 HIS ASP LYS ASP LYS GLU ASN THR K606 E618 V627 R659 L674 Y745 T778 I779 F799 GLY THR GLY GLY THR S805 L816 L854 D864 VAL SER TRP GLY THR LYS GLY ASP ASN
ASN PRO LYS GLU D878 L879 Y883 K887 N888 A889 S890 G891 R914 R917 S918 N919 LYS LYS VAL ALA LEU GLY HIS SER GLU LYS THR PRO LEU D933 V1006 E1007 S1008 LYS SER LYS TRP MET LYS ARG GLY TYR THR ALA PRO SER HIS ASN PRO LEU ASN SER ASN SER LEU
GLU VAL LEU PHE GLN GLY PRO ALA ALA ASP TYR LYS ASP ASP ASP ASP LYS ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66809	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.380	Depositor
Minimum map value	-0.873	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	297.6, 297.6, 297.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.93, 0.93, 0.93	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1DEH, MG, UDP, PEE

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	0.12	0/5724	0.24	0/7794
1	B	0.14	0/5756	0.26	0/7835
All	All	0.13	0/11480	0.25	0/15629

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5591	5258	5342	34	0
1	B	5623	5295	5391	34	0
2	A	79	108	112	0	0
2	B	82	114	118	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	22	20	0	0	0
4	B	22	20	0	0	0
5	A	25	11	10	1	0
5	B	25	11	10	1	0
All	All	11471	10837	10983	63	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 3.

All (63) 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:305:GLU:OE2	1:A:335:ARG:NH2	2.27	0.67
1:A:288:VAL:CG1	1:A:292:LEU:HD23	2.27	0.65
1:A:348:GLU:OE1	1:A:348:GLU:N	2.30	0.65
1:A:243:PHE:HZ	1:A:361:MET:HE2	1.63	0.63
1:A:496:ASP:OD1	1:A:497:ASN:N	2.32	0.61
1:B:305:GLU:OE2	1:B:335:ARG:NH2	2.34	0.60
1:B:246:SER:HA	1:B:444:LYS:HA	1.86	0.57
1:A:907:LEU:O	1:B:255:ILE:HD11	2.05	0.56
1:B:438:ASP:OD1	1:B:439:GLU:N	2.38	0.56
1:B:251:ILE:HG12	1:B:295:VAL:HG21	1.88	0.55
1:A:248:ASP:OD1	1:A:249:GLY:N	2.39	0.55
1:A:247:ILE:N	1:A:443:PHE:O	2.38	0.55
1:A:911:TYR:HB2	1:B:255:ILE:HD12	1.89	0.53
1:A:248:ASP:OD2	1:B:917:ARG:NH1	2.42	0.53
1:A:243:PHE:CZ	1:A:361:MET:HE2	2.42	0.53
1:A:725:LEU:HD22	1:A:731:LEU:HD11	1.91	0.52
1:B:243:PHE:CZ	1:B:361:MET:HE2	2.45	0.52
1:B:251:ILE:CG1	1:B:295:VAL:HG21	2.39	0.52
1:B:361:MET:HE3	1:B:453:VAL:CG2	2.40	0.52
1:B:559:TYR:HD1	1:B:627:VAL:HG21	1.75	0.51
1:A:559:TYR:HD1	1:A:627:VAL:HG21	1.75	0.50
1:B:489:LEU:HD23	1:B:490:ASP:N	2.27	0.49
1:B:779:ILE:HG12	2:B:1101:PEE:H65	1.94	0.49
1:A:725:LEU:CD2	1:A:731:LEU:HD11	2.42	0.49
1:B:674:LEU:C	1:B:674:LEU:HD23	2.37	0.49
1:A:659:ARG:HB2	1:A:854:LEU:HD22	1.96	0.48
1:A:674:LEU:C	1:A:674:LEU:HD23	2.38	0.48
1:B:348:GLU:N	1:B:348:GLU:OE1	2.47	0.48
1:A:251:ILE:O	1:A:254:ASN:ND2	2.47	0.47
1:B:490:ASP:OD1	5:B:1105:UDP:O3'	2.27	0.47
1:A:959:THR:O	1:A:963:VAL:HG23	2.15	0.47
1:B:361:MET:HE3	1:B:453:VAL:HG22	1.95	0.47
1:A:361:MET:HE3	1:A:453:VAL:CG2	2.46	0.46
1:B:292:LEU:HD11	1:B:435:ILE:HD12	1.98	0.45
1:A:353:PHE:HA	1:A:491:VAL:HG23	1.99	0.45
1:B:816:LEU:HD13	2:B:1104:PEE:H31	1.97	0.45
1:B:355:ARG:HG2	1:B:439:GLU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:HG13	1:A:292:LEU:HD23	1.99	0.45
1:B:659:ARG:HB2	1:B:854:LEU:HD22	1.98	0.45
1:A:806:THR:O	1:A:806:THR:HG22	2.17	0.44
1:B:243:PHE:HA	1:B:446:ASP:HB3	1.99	0.44
1:B:243:PHE:HZ	1:B:361:MET:HE2	1.81	0.44
1:A:962:GLN:OE1	1:B:745:TYR:OH	2.33	0.44
1:A:725:LEU:HD22	1:A:731:LEU:CD1	2.48	0.43
1:B:816:LEU:HD13	2:B:1104:PEE:C20	2.48	0.43
1:A:256:ASN:HA	1:B:914:ARG:HH12	1.82	0.43
1:A:288:VAL:HG23	1:A:307:THR:C	2.44	0.43
1:B:778:THR:HG21	2:B:1101:PEE:H57	2.01	0.43
1:A:559:TYR:CD1	1:A:627:VAL:HG21	2.53	0.43
1:B:559:TYR:CD1	1:B:627:VAL:HG21	2.53	0.42
1:A:391:ASP:OD2	5:A:1105:UDP:N3	2.51	0.42
1:B:517:ALA:HB1	1:B:564:PRO:HD2	2.01	0.42
1:A:348:GLU:HG2	1:A:491:VAL:HG13	2.01	0.42
1:A:541:PHE:CE2	1:A:545:LEU:HD11	2.55	0.42
1:B:520:ILE:HD12	1:B:566:ALA:HB3	2.01	0.42
1:A:520:ILE:CD1	1:A:566:ALA:HB3	2.51	0.41
1:B:307:THR:HG23	1:B:308:ASN:OD1	2.21	0.41
1:B:541:PHE:CE2	1:B:545:LEU:HD11	2.56	0.41
1:B:520:ILE:CD1	1:B:566:ALA:HB3	2.50	0.41
1:A:246:SER:HA	1:A:444:LYS:HA	2.03	0.40
1:B:252:MET:O	1:B:253:HIS:C	2.63	0.40
1:A:288:VAL:HG13	1:A:289:PRO:HD2	2.03	0.40
1:A:390:ALA:HB3	1:A:459:LEU:HD12	2.03	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	717/1058 (68%)	700 (98%)	17 (2%)	0	100	100
1	B	720/1058 (68%)	702 (98%)	18 (2%)	0	100	100
All	All	1437/2116 (68%)	1402 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	558/931 (60%)	558 (100%)	0	100	100
1	B	564/931 (61%)	563 (100%)	1 (0%)	87	91
All	All	1122/1862 (60%)	1121 (100%)	1 (0%)	87	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	883	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	425	ASN
1	A	502	ASN
1	A	578	HIS
1	A	694	HIS
1	B	371	HIS
1	B	694	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	A1DEH	A	1103	-	22,23,23	2.63	7 (31%)	26,32,32	1.09	1 (3%)
4	A1DEH	B	1103	-	22,23,23	2.64	7 (31%)	26,32,32	1.07	1 (3%)
5	UDP	A	1105	-	25,26,26	3.82	14 (56%)	38,40,40	1.54	5 (13%)
2	PEE	B	1104	-	50,50,50	1.12	3 (6%)	53,55,55	1.00	2 (3%)
2	PEE	A	1104	-	50,50,50	1.13	3 (6%)	53,55,55	1.00	2 (3%)
2	PEE	B	1101	-	30,30,50	1.27	3 (10%)	33,35,55	1.19	2 (6%)
2	PEE	A	1101	-	27,27,50	1.32	3 (11%)	30,32,55	1.12	2 (6%)
5	UDP	B	1105	-	25,26,26	3.82	14 (56%)	38,40,40	1.62	7 (18%)

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	A1DEH	A	1103	-	-	4/12/22/22	0/2/2/2
4	A1DEH	B	1103	-	-	3/12/22/22	0/2/2/2
5	UDP	A	1105	-	-	3/16/32/32	0/2/2/2
2	PEE	B	1104	-	-	30/54/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEE	A	1104	-	-	29/54/54/54	-
2	PEE	B	1101	-	-	15/34/34/54	-
2	PEE	A	1101	-	-	14/31/31/54	-
5	UDP	B	1105	-	-	3/16/32/32	0/2/2/2

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1105	UDP	C3'-C4'	-7.43	1.34	1.53
5	B	1105	UDP	C3'-C4'	-7.25	1.34	1.53
4	B	1103	A1DEH	C14-C13	7.16	1.52	1.37
5	A	1105	UDP	O4'-C4'	7.15	1.60	1.45
5	B	1105	UDP	O4'-C4'	7.12	1.60	1.45
4	A	1103	A1DEH	C14-C13	7.05	1.52	1.37
5	A	1105	UDP	C2-N1	7.01	1.49	1.38
5	B	1105	UDP	C2-N1	6.96	1.49	1.38
5	B	1105	UDP	C2-N3	6.64	1.49	1.38
5	A	1105	UDP	C2-N3	6.62	1.49	1.38
5	B	1105	UDP	C6-C5	6.10	1.49	1.35
5	A	1105	UDP	C6-C5	6.10	1.49	1.35
4	B	1103	A1DEH	C02-N03	5.77	1.41	1.35
4	A	1103	A1DEH	C02-N03	5.66	1.41	1.35
4	A	1103	A1DEH	O21-C20	5.64	1.46	1.37
5	B	1105	UDP	PA-O3A	5.63	1.65	1.59
5	A	1105	UDP	PA-O3A	5.51	1.65	1.59
4	B	1103	A1DEH	O21-C20	5.51	1.45	1.37
5	B	1105	UDP	O4'-C1'	-5.38	1.29	1.42
5	A	1105	UDP	O4'-C1'	-5.24	1.29	1.42
5	A	1105	UDP	C4-N3	4.21	1.45	1.38
5	B	1105	UDP	C4-N3	4.19	1.45	1.38
5	B	1105	UDP	C6-N1	3.16	1.45	1.38
5	A	1105	UDP	C6-N1	3.11	1.45	1.38
4	B	1103	A1DEH	C04-N03	3.02	1.45	1.39
4	A	1103	A1DEH	C04-N03	2.93	1.44	1.39
5	A	1105	UDP	O4-C4	-2.79	1.19	1.24
2	B	1101	PEE	O3-C30	2.78	1.41	1.33
5	B	1105	UDP	O4-C4	-2.78	1.19	1.24
2	B	1104	PEE	O3-C30	2.77	1.41	1.33
2	A	1104	PEE	O3-C30	2.75	1.41	1.33
2	A	1101	PEE	O3-C30	2.74	1.41	1.33
5	B	1105	UDP	O2'-C2'	-2.71	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1105	UDP	O2'-C2'	-2.69	1.36	1.43
5	A	1105	UDP	O3'-C3'	2.68	1.49	1.43
5	B	1105	UDP	O3'-C3'	2.63	1.49	1.43
4	A	1103	A1DEH	C11-C12	2.62	1.53	1.47
5	B	1105	UDP	C5-C4	2.61	1.49	1.43
4	B	1103	A1DEH	C11-C12	2.56	1.53	1.47
5	A	1105	UDP	C5-C4	2.52	1.49	1.43
4	A	1103	A1DEH	C16-C15	2.43	1.53	1.48
2	B	1101	PEE	O2-C10	2.40	1.41	1.34
5	A	1105	UDP	O2-C2	-2.38	1.18	1.23
5	B	1105	UDP	O2-C2	-2.37	1.18	1.23
2	A	1104	PEE	O2-C10	2.36	1.40	1.34
2	B	1104	PEE	O2-C10	2.36	1.40	1.34
2	A	1101	PEE	O2-C10	2.33	1.40	1.34
4	B	1103	A1DEH	C16-C15	2.27	1.52	1.48
4	B	1103	A1DEH	O01-C02	-2.25	1.18	1.23
4	A	1103	A1DEH	O01-C02	-2.21	1.18	1.23
2	A	1101	PEE	O2-C2	-2.14	1.41	1.46
2	B	1101	PEE	O2-C2	-2.07	1.41	1.46
2	B	1104	PEE	O2-C2	-2.06	1.41	1.46
2	A	1104	PEE	O2-C2	-2.02	1.41	1.46

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1105	UDP	C4-N3-C2	-5.39	119.93	126.61
5	A	1105	UDP	C4-N3-C2	-5.23	120.12	126.61
2	B	1101	PEE	O2-C10-C11	3.93	119.99	111.48
5	B	1105	UDP	N3-C2-N1	3.92	120.00	114.89
2	A	1101	PEE	O2-C10-C11	3.83	119.76	111.48
4	A	1103	A1DEH	C04-N03-C02	-3.76	119.94	124.45
4	B	1103	A1DEH	C04-N03-C02	-3.75	119.97	124.45
5	A	1105	UDP	N3-C2-N1	3.71	119.72	114.89
5	A	1105	UDP	C5-C4-N3	3.70	119.98	114.80
5	B	1105	UDP	C5-C4-N3	3.69	119.96	114.80
2	B	1104	PEE	O2-C10-C11	3.57	119.20	111.48
2	A	1104	PEE	O2-C10-C11	3.55	119.17	111.48
5	B	1105	UDP	O4-C4-C5	-3.02	119.96	125.16
5	A	1105	UDP	O4-C4-C5	-3.02	119.96	125.16
2	B	1101	PEE	O3-C30-C31	2.71	120.08	111.83
2	A	1101	PEE	O3-C30-C31	2.68	119.29	111.15
2	B	1104	PEE	O3-C30-C31	2.67	119.99	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1104	PEE	O3-C30-C31	2.66	119.94	111.83
5	B	1105	UDP	O2-C2-N1	-2.30	119.81	122.80
5	A	1105	UDP	O2-C2-N1	-2.18	119.96	122.80
5	B	1105	UDP	C4'-O4'-C1'	-2.11	104.81	109.47
5	B	1105	UDP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	PEE	C1-O3P-P-O4P
2	A	1101	PEE	C4-O4P-P-O2P
2	A	1101	PEE	C4-O4P-P-O1P
2	A	1101	PEE	O4P-C4-C5-N
2	A	1104	PEE	C1-O3P-P-O2P
2	A	1104	PEE	C1-O3P-P-O4P
2	A	1104	PEE	C4-O4P-P-O3P
2	A	1104	PEE	C4-O4P-P-O2P
2	A	1104	PEE	C4-O4P-P-O1P
2	A	1104	PEE	O4P-C4-C5-N
2	B	1101	PEE	C11-C10-O2-C2
2	B	1101	PEE	O4P-C4-C5-N
2	B	1104	PEE	C1-O3P-P-O2P
2	B	1104	PEE	C4-O4P-P-O3P
2	B	1104	PEE	C4-O4P-P-O2P
2	B	1104	PEE	O4P-C4-C5-N
4	A	1103	A1DEH	C12-C13-C14-C15
4	A	1103	A1DEH	C20-C08-N09-C10
4	A	1103	A1DEH	C12-C11-N09-C10
4	B	1103	A1DEH	C20-C08-N09-C10
4	B	1103	A1DEH	C12-C11-N09-C10
5	B	1105	UDP	O4'-C4'-C5'-O5'
5	B	1105	UDP	PB-O3A-PA-O5'
2	B	1101	PEE	O4-C10-O2-C2
2	A	1104	PEE	C31-C30-O3-C3
2	B	1104	PEE	C31-C30-O3-C3
2	A	1104	PEE	O5-C30-O3-C3
2	B	1104	PEE	O5-C30-O3-C3
2	B	1101	PEE	C31-C30-O3-C3
2	B	1101	PEE	O5-C30-O3-C3
2	B	1104	PEE	C10-C11-C12-C13
2	A	1104	PEE	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
2	B	1104	PEE	C13-C14-C15-C16
2	A	1104	PEE	C13-C14-C15-C16
2	B	1104	PEE	C34-C35-C36-C37
2	A	1104	PEE	C34-C35-C36-C37
2	A	1104	PEE	C41-C42-C43-C44
5	B	1105	UDP	C3'-C4'-C5'-O5'
2	B	1104	PEE	C43-C44-C45-C46
2	A	1101	PEE	O2-C2-C3-O3
2	A	1104	PEE	C39-C40-C41-C42
2	B	1104	PEE	O2-C2-C3-O3
2	B	1104	PEE	C39-C40-C41-C42
2	B	1104	PEE	C41-C42-C43-C44
2	B	1104	PEE	C14-C15-C16-C17
2	A	1101	PEE	C1-C2-C3-O3
2	A	1101	PEE	C15-C16-C17-C18
2	B	1104	PEE	C31-C32-C33-C34
2	A	1104	PEE	C43-C44-C45-C46
2	A	1104	PEE	C31-C32-C33-C34
2	A	1104	PEE	C15-C16-C17-C18
2	B	1101	PEE	O3P-C1-C2-O2
2	B	1104	PEE	C12-C13-C14-C15
2	A	1104	PEE	O2-C2-C3-O3
2	B	1104	PEE	C15-C16-C17-C18
2	A	1101	PEE	C13-C14-C15-C16
2	B	1104	PEE	C24-C25-C26-C27
2	A	1104	PEE	C12-C13-C14-C15
2	A	1104	PEE	C24-C25-C26-C27
2	A	1104	PEE	C14-C15-C16-C17
2	B	1104	PEE	C1-C2-C3-O3
2	A	1104	PEE	O3-C30-C31-C32
2	B	1104	PEE	O3-C30-C31-C32
2	B	1101	PEE	O3P-C1-C2-C3
2	A	1104	PEE	C36-C37-C38-C39
2	B	1101	PEE	C33-C34-C35-C36
2	A	1101	PEE	C11-C12-C13-C14
2	A	1104	PEE	C1-C2-C3-O3
2	A	1101	PEE	C1-O3P-P-O2P
2	A	1101	PEE	C4-O4P-P-O3P
2	B	1101	PEE	C4-O4P-P-O3P
2	B	1101	PEE	C4-O4P-P-O2P
2	B	1101	PEE	C4-O4P-P-O1P
2	B	1104	PEE	C1-O3P-P-O1P

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Mol	Chain	Res	Type	Atoms
2	B	1104	PEE	C1-O3P-P-O4P
2	B	1104	PEE	C4-O4P-P-O1P
5	A	1105	UDP	C5'-O5'-PA-O1A
2	B	1101	PEE	C31-C32-C33-C34
2	A	1104	PEE	C16-C17-C18-C19
2	A	1104	PEE	C3-C2-O2-C10
2	B	1104	PEE	C3-C2-O2-C10
2	B	1104	PEE	C16-C17-C18-C19
2	B	1104	PEE	C35-C36-C37-C38
2	A	1101	PEE	O2-C10-C11-C12
2	B	1101	PEE	C11-C12-C13-C14
2	B	1104	PEE	C36-C37-C38-C39
2	A	1104	PEE	C40-C41-C42-C43
2	A	1104	PEE	C11-C12-C13-C14
2	B	1101	PEE	C32-C33-C34-C35
2	B	1104	PEE	C11-C12-C13-C14
2	B	1104	PEE	C21-C22-C23-C24
2	A	1101	PEE	C12-C13-C14-C15
5	A	1105	UDP	PB-O3A-PA-O5'
5	A	1105	UDP	O4'-C4'-C5'-O5'
2	B	1101	PEE	C36-C37-C38-C39
2	B	1104	PEE	C40-C41-C42-C43
2	A	1104	PEE	C21-C22-C23-C24
4	A	1103	A1DEH	C07-C08-N09-C10
4	B	1103	A1DEH	C07-C08-N09-C10
2	A	1101	PEE	C16-C17-C18-C19
2	A	1104	PEE	O5-C30-C31-C32

There are no ring outliers.

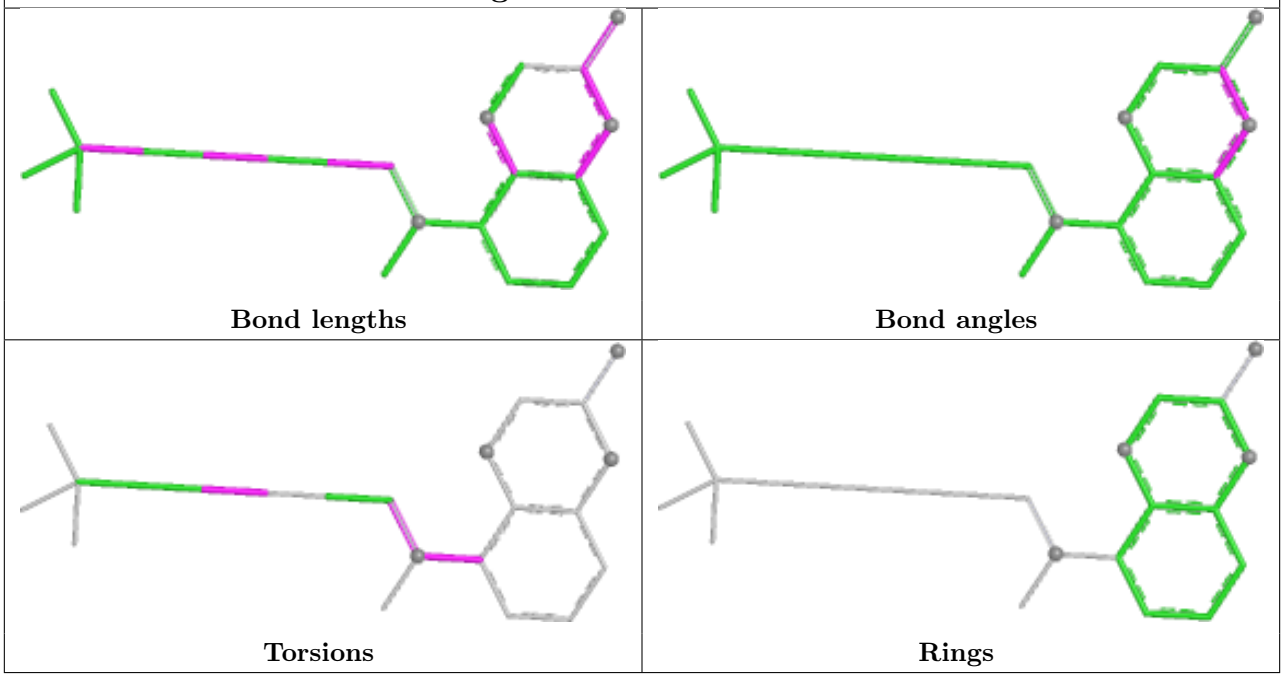
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1105	UDP	1	0
2	B	1104	PEE	2	0
2	B	1101	PEE	2	0
5	B	1105	UDP	1	0

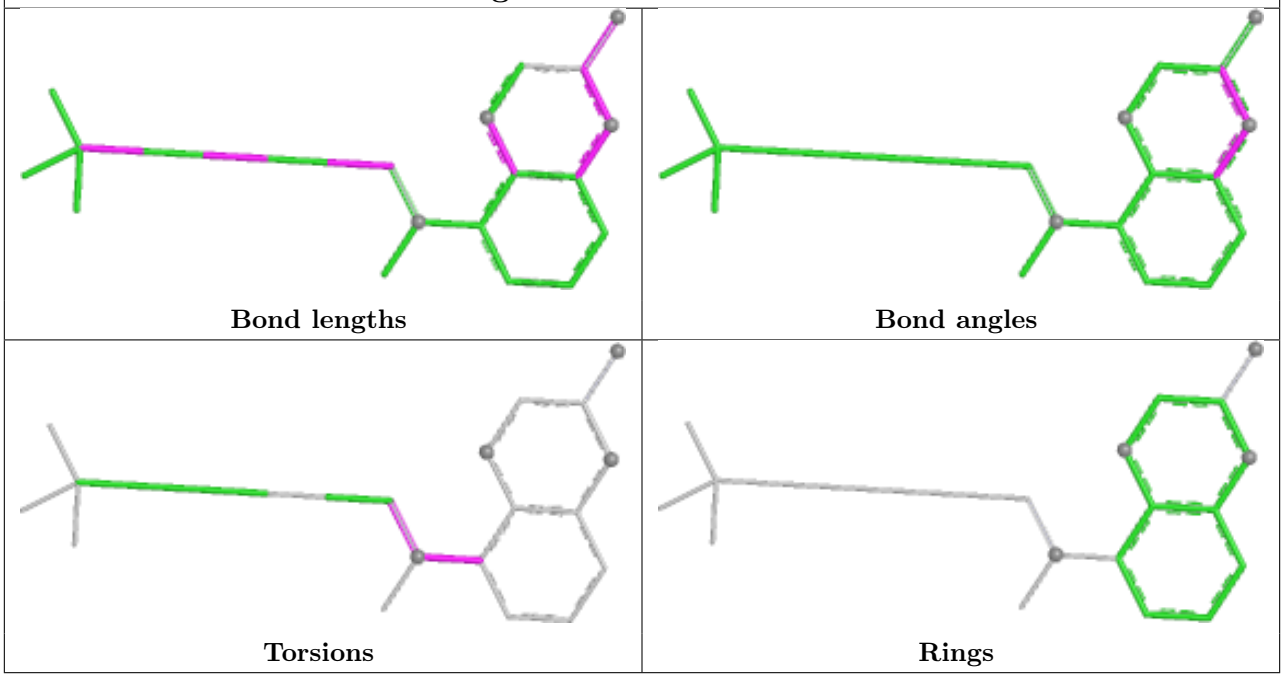
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

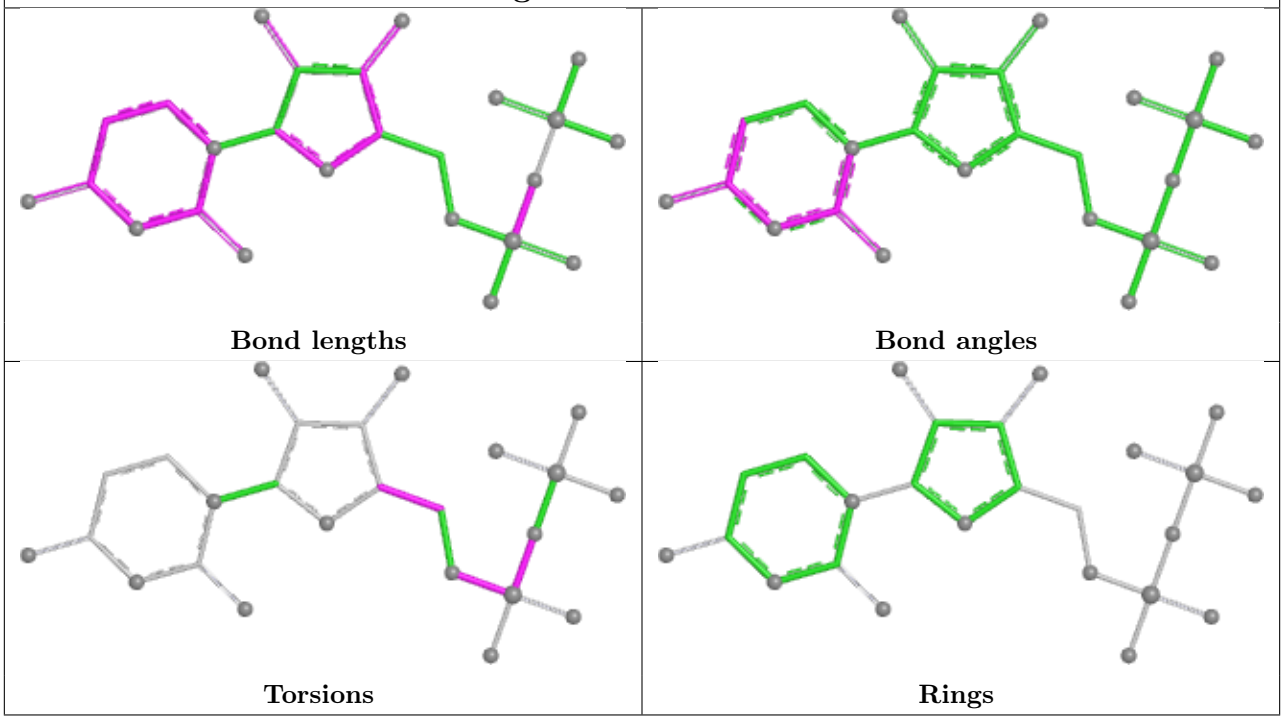
Ligand A1DEH A 1103



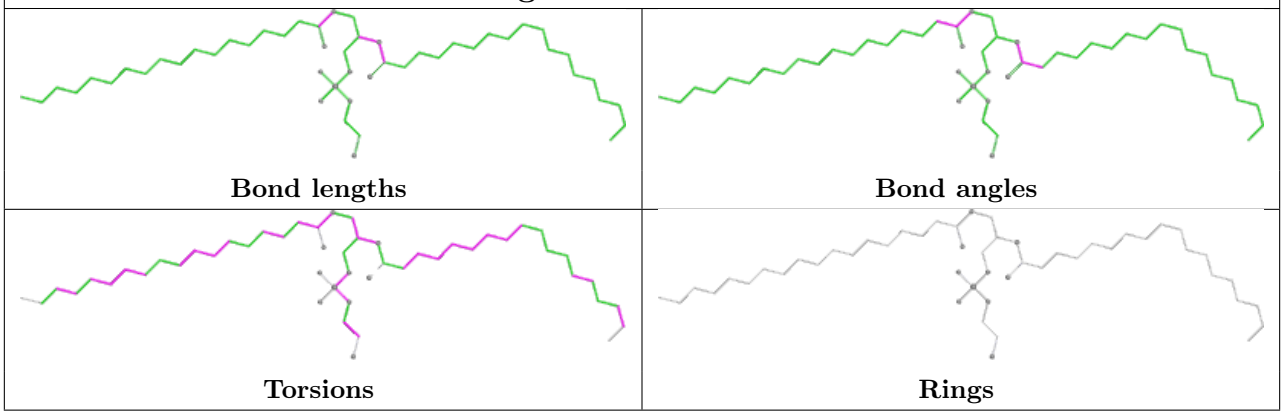
Ligand A1DEH B 1103



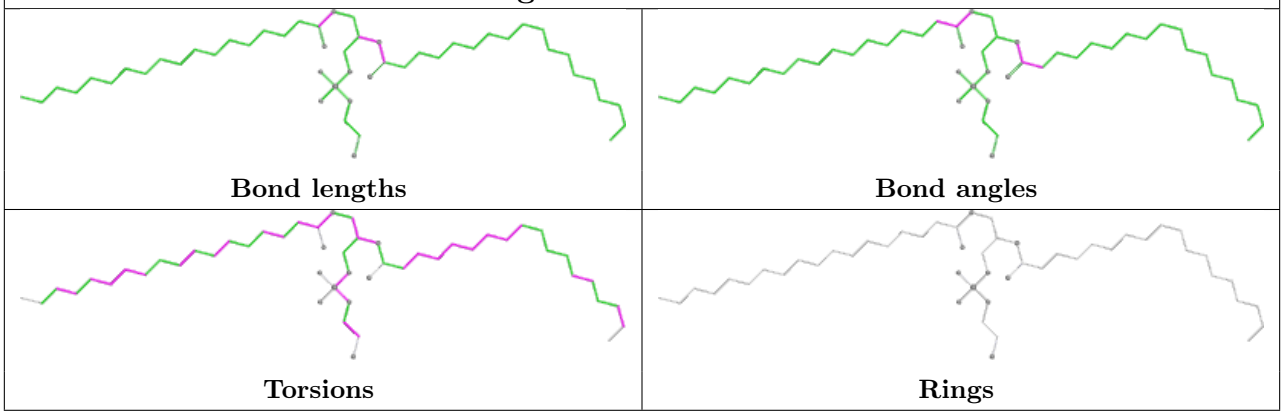
Ligand UDP A 1105



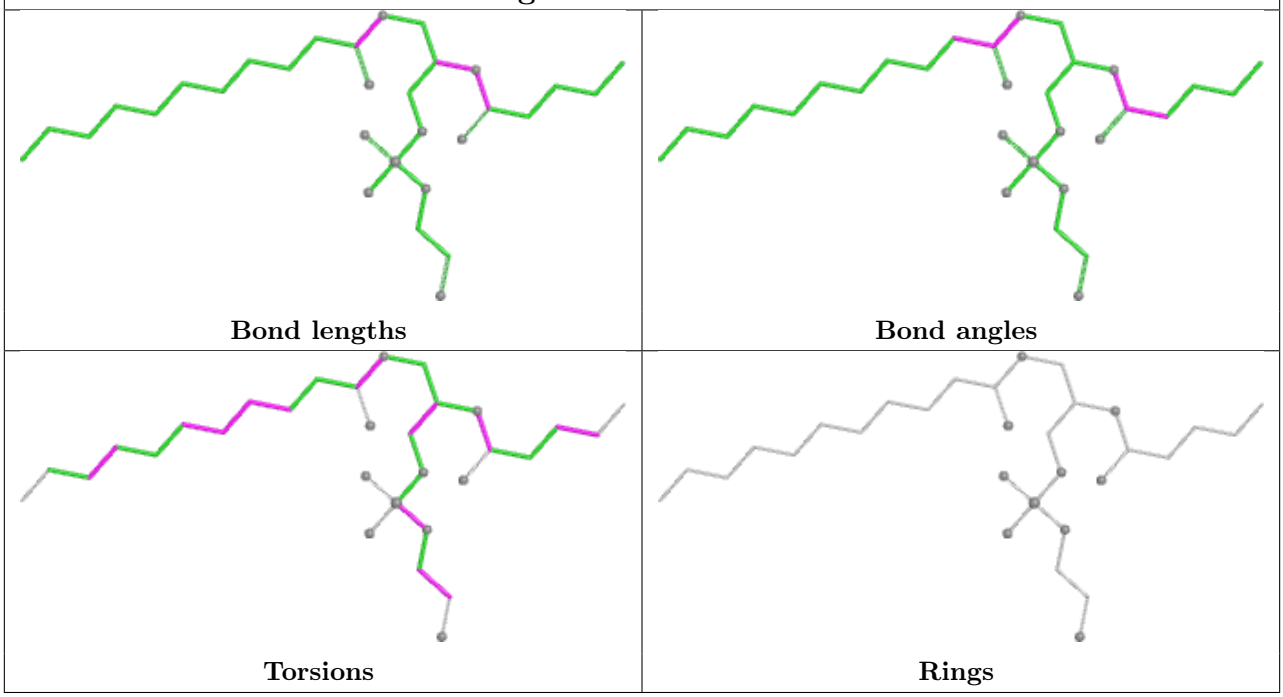
Ligand PEE B 1104



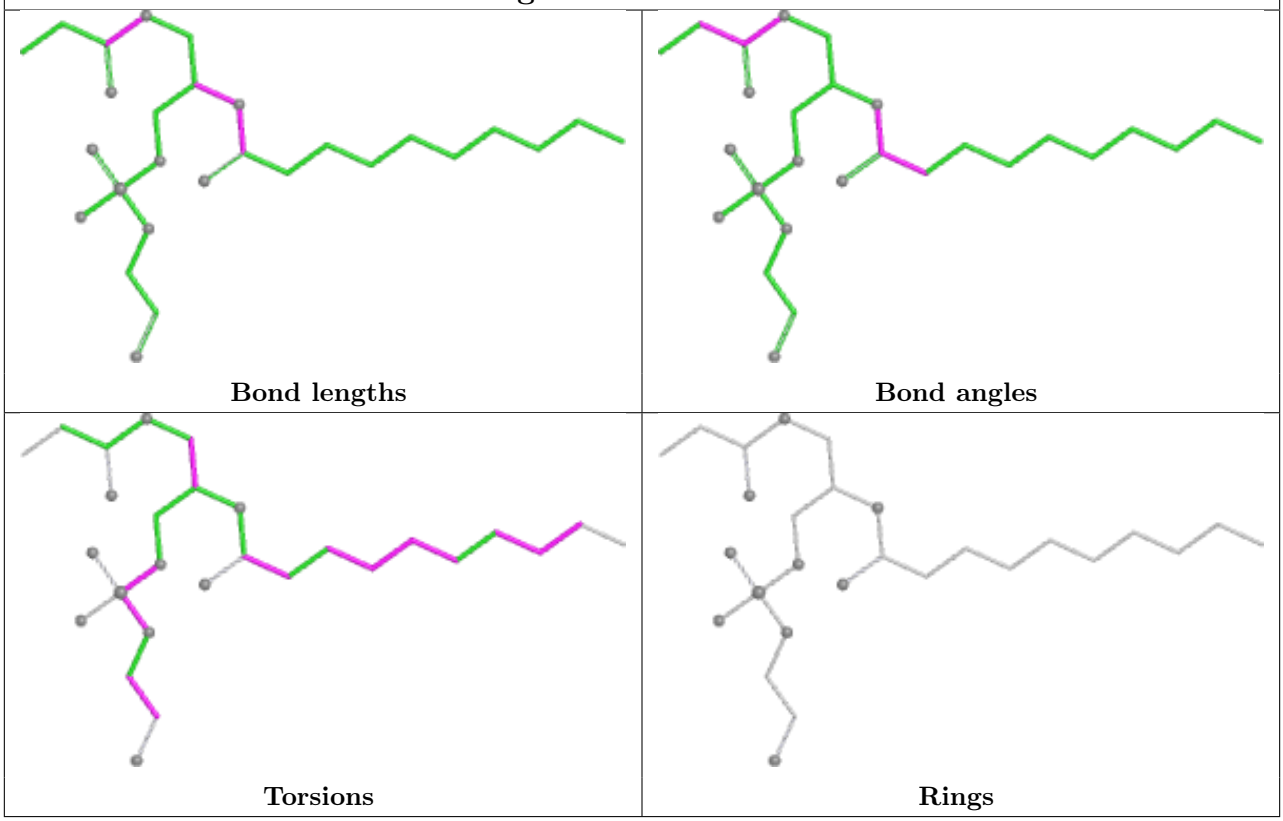
Ligand PEE A 1104

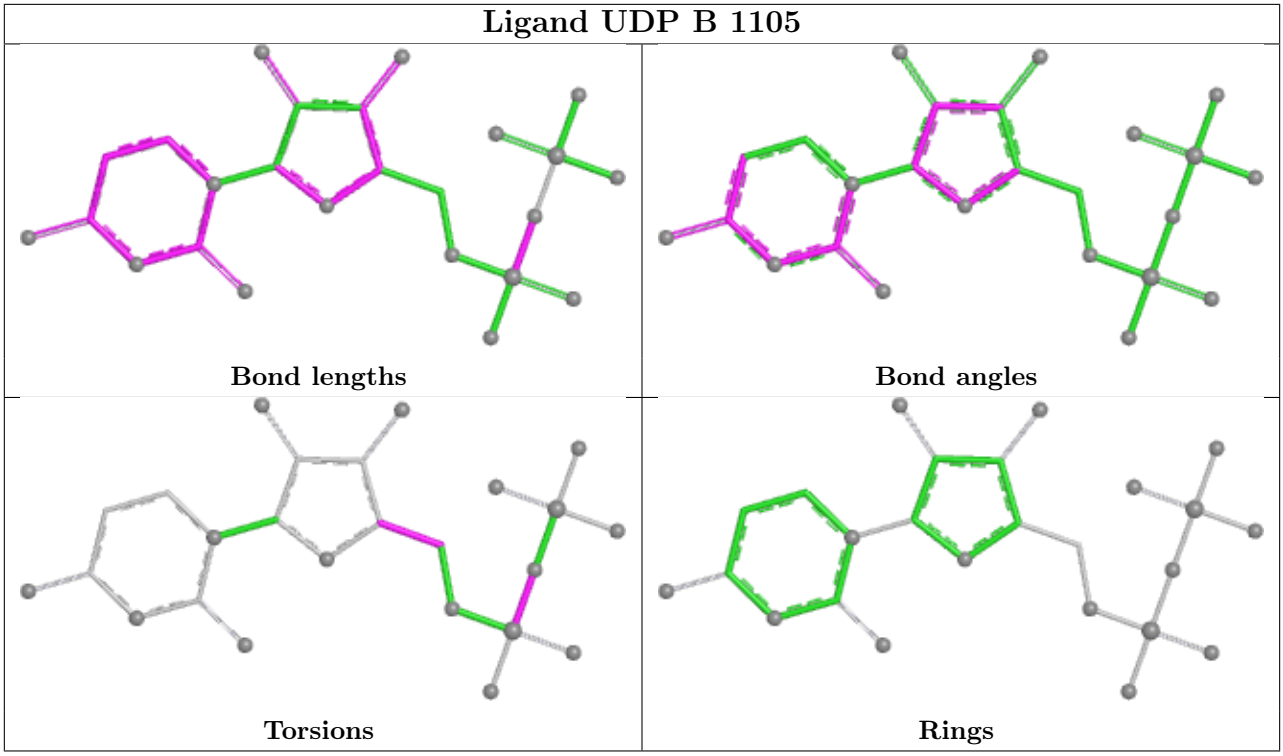


Ligand PEE B 1101



Ligand PEE A 1101





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.

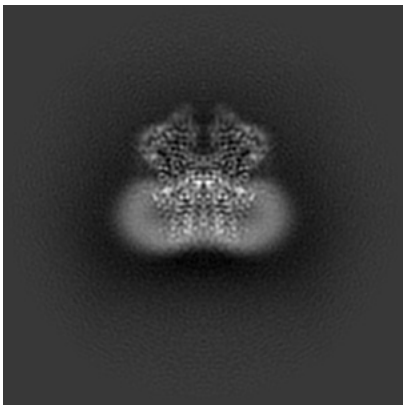
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-76832. These allow visual inspection of the internal detail of the map and identification of artifacts.

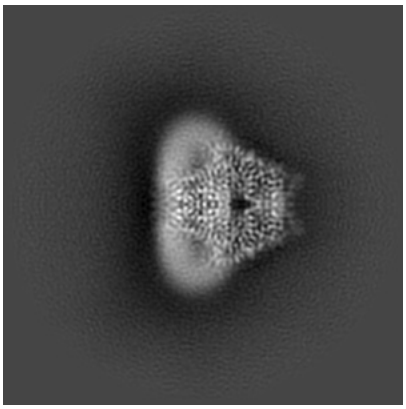
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

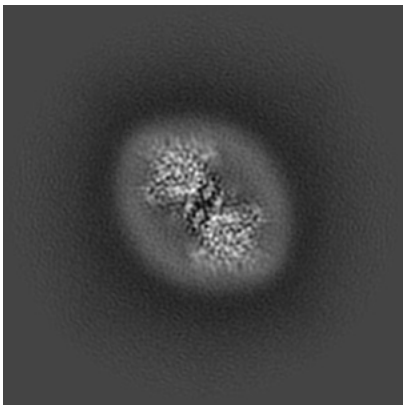
6.1.1 Primary map



X

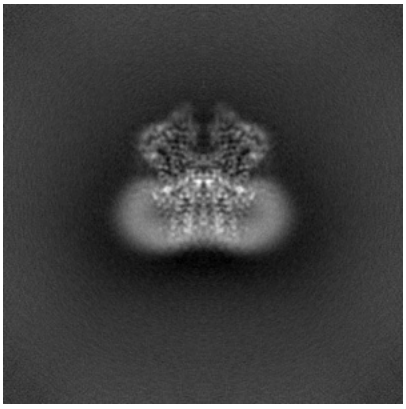


Y

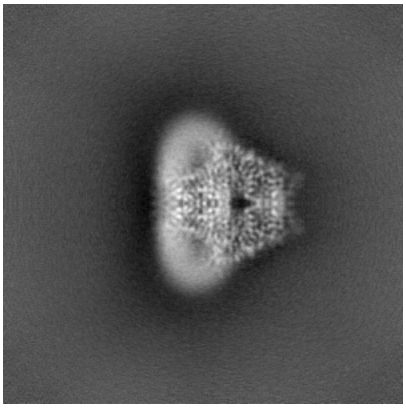


Z

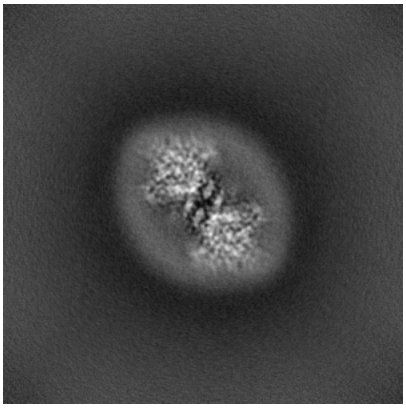
6.1.2 Raw map



X



Y

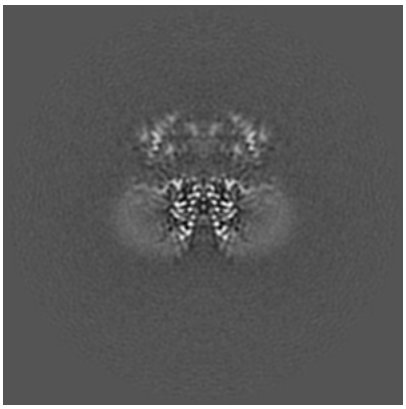


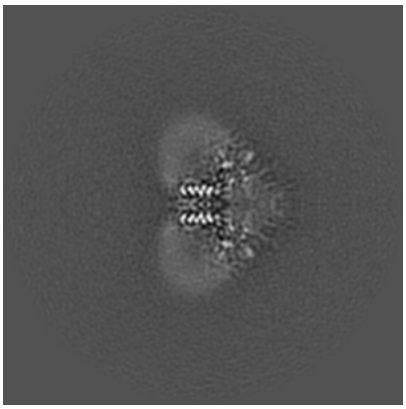
Z

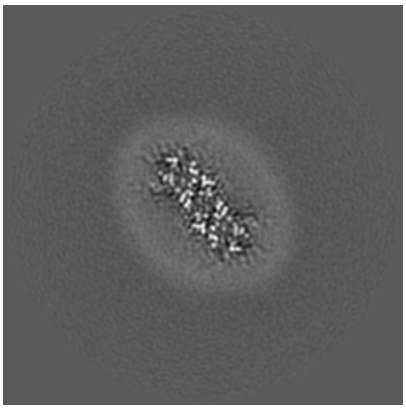
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

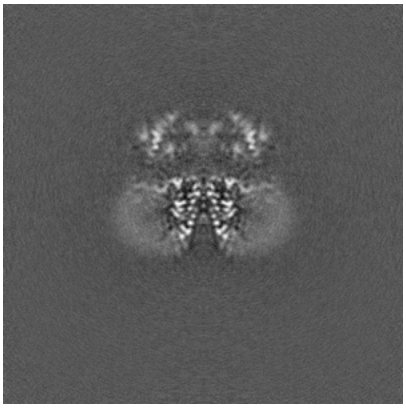
6.2.1 Primary map

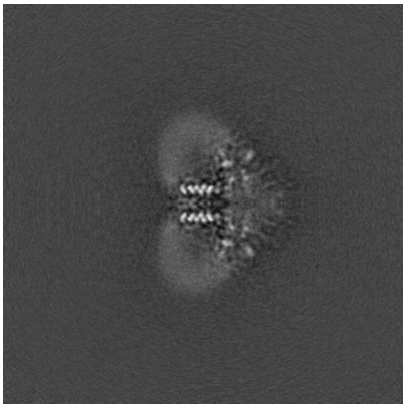

X Index: 160

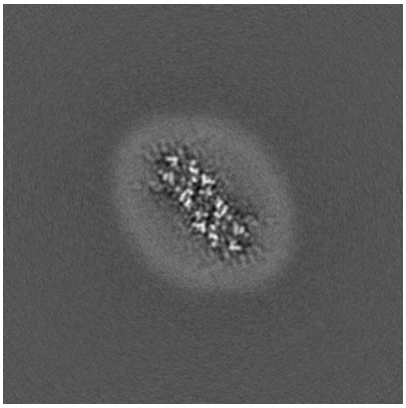

Y Index: 160


Z Index: 160

6.2.2 Raw map


X Index: 160

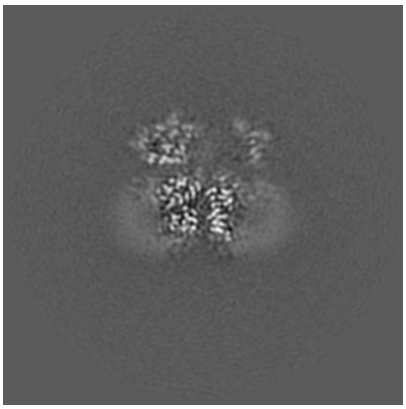

Y Index: 160

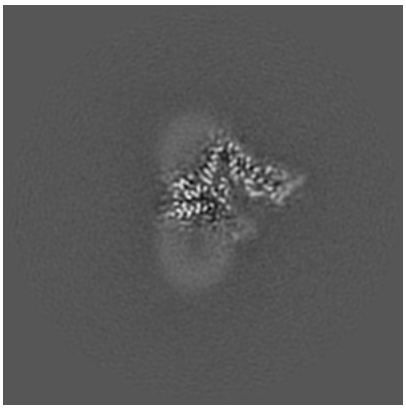

Z Index: 160

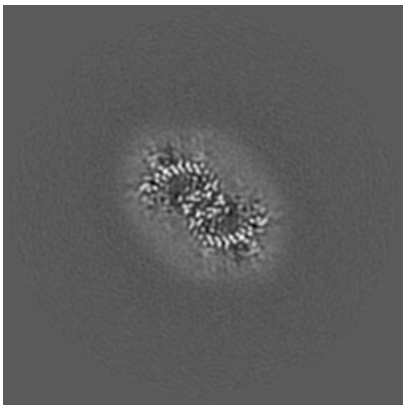
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

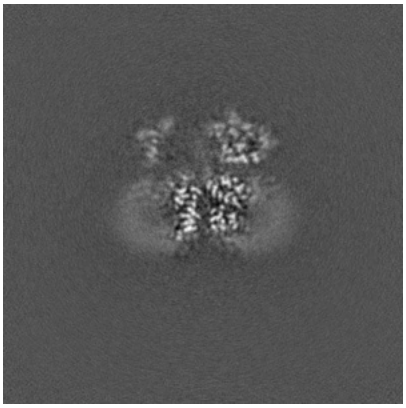
6.3.1 Primary map

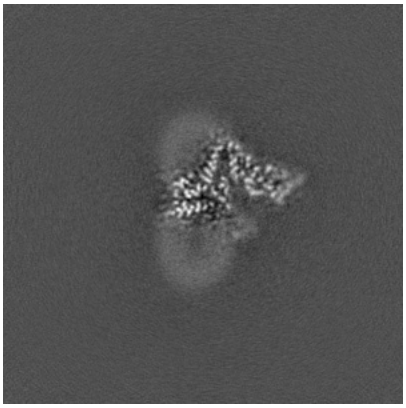

X Index: 165

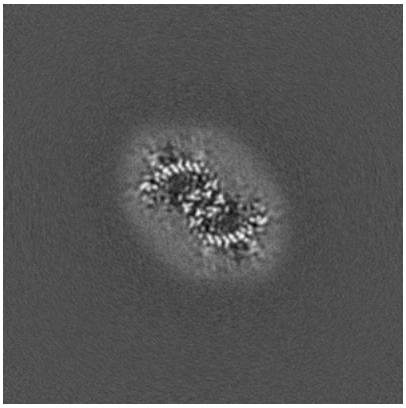

Y Index: 149


Z Index: 172

6.3.2 Raw map


X Index: 155

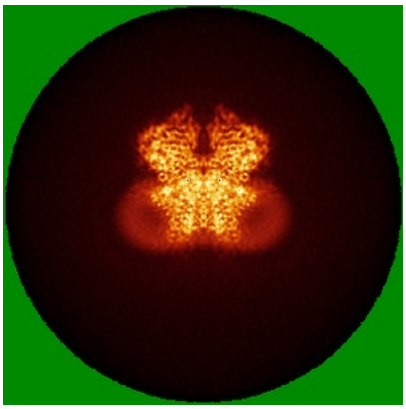

Y Index: 149

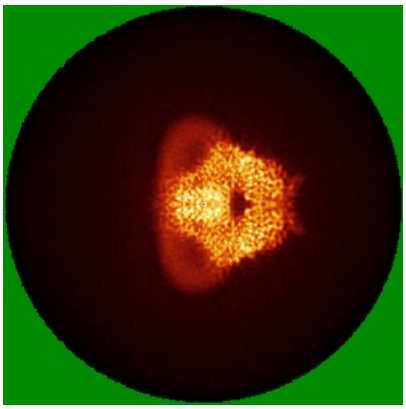

Z Index: 172

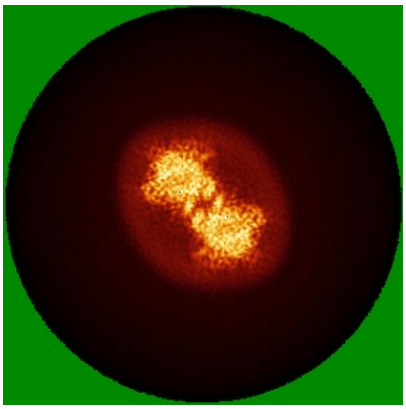
The images above show the largest variance slices of the map in three orthogonal directions.

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

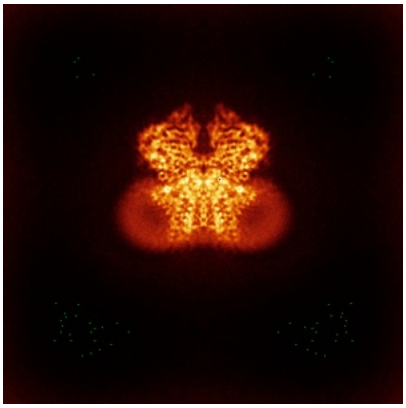
6.4.1 Primary map

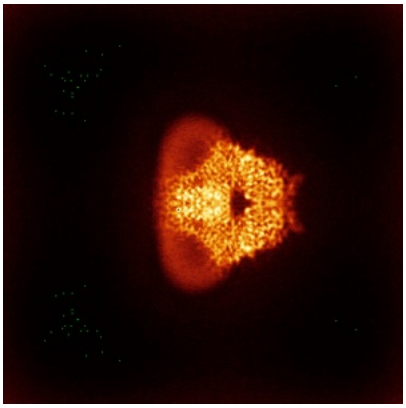

X

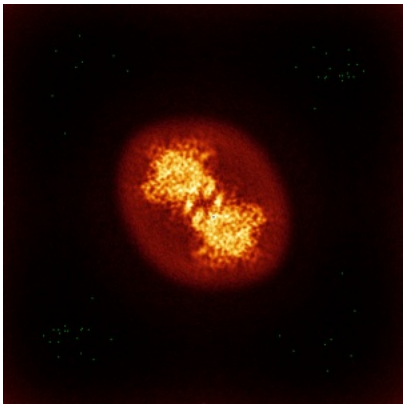

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

6.5.2 Raw map

X Y Z

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

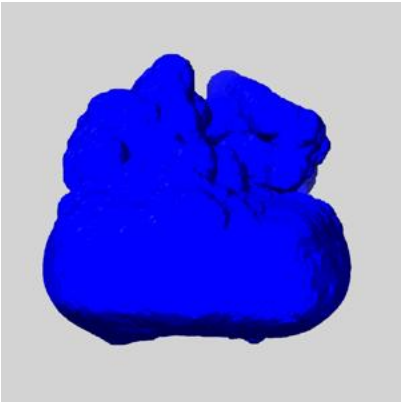
6.6 Mask visualisation (i)

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

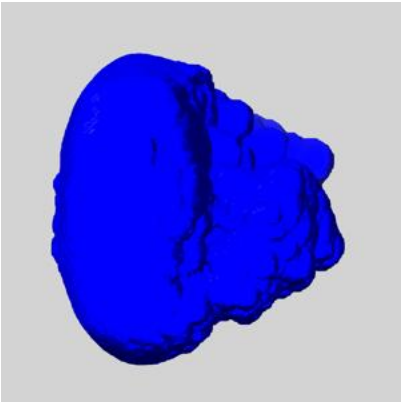
A mask typically either:

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

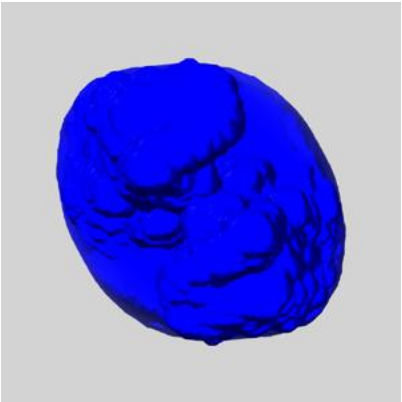
6.6.1 emd_76832_msk_1.map (i)



X



Y

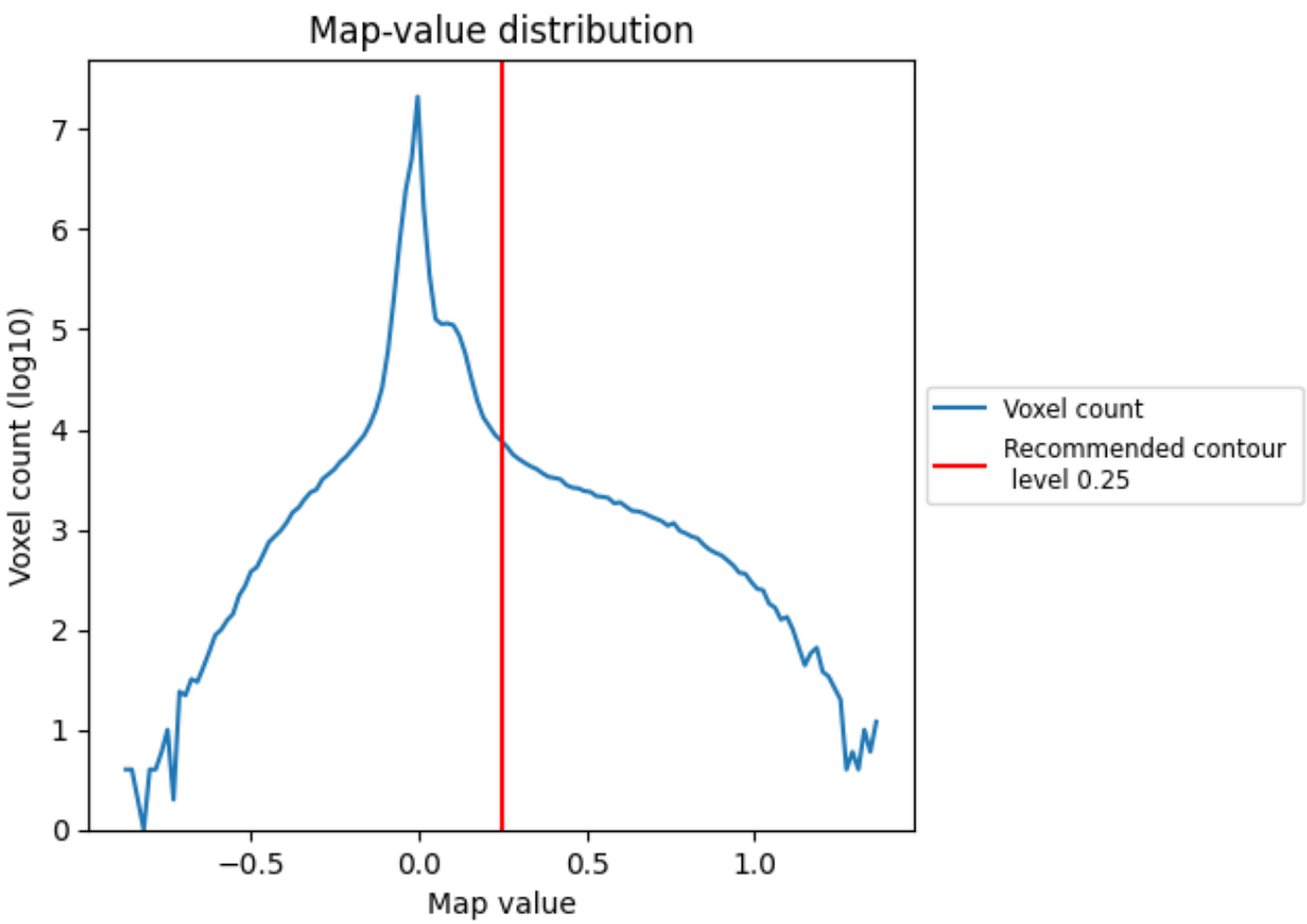


Z

7 Map analysis (i)

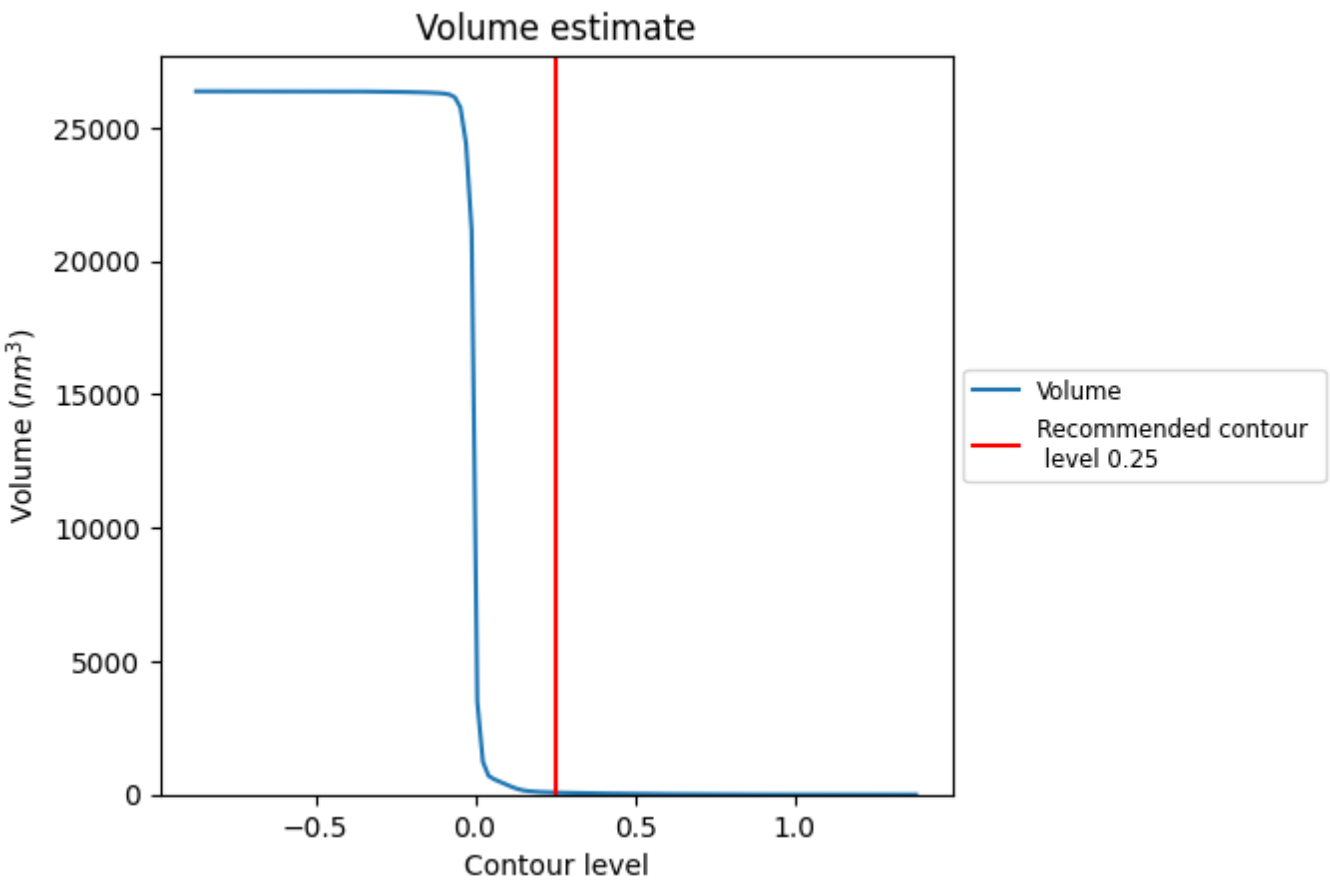
This section contains the results of statistical analysis of the map.

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.

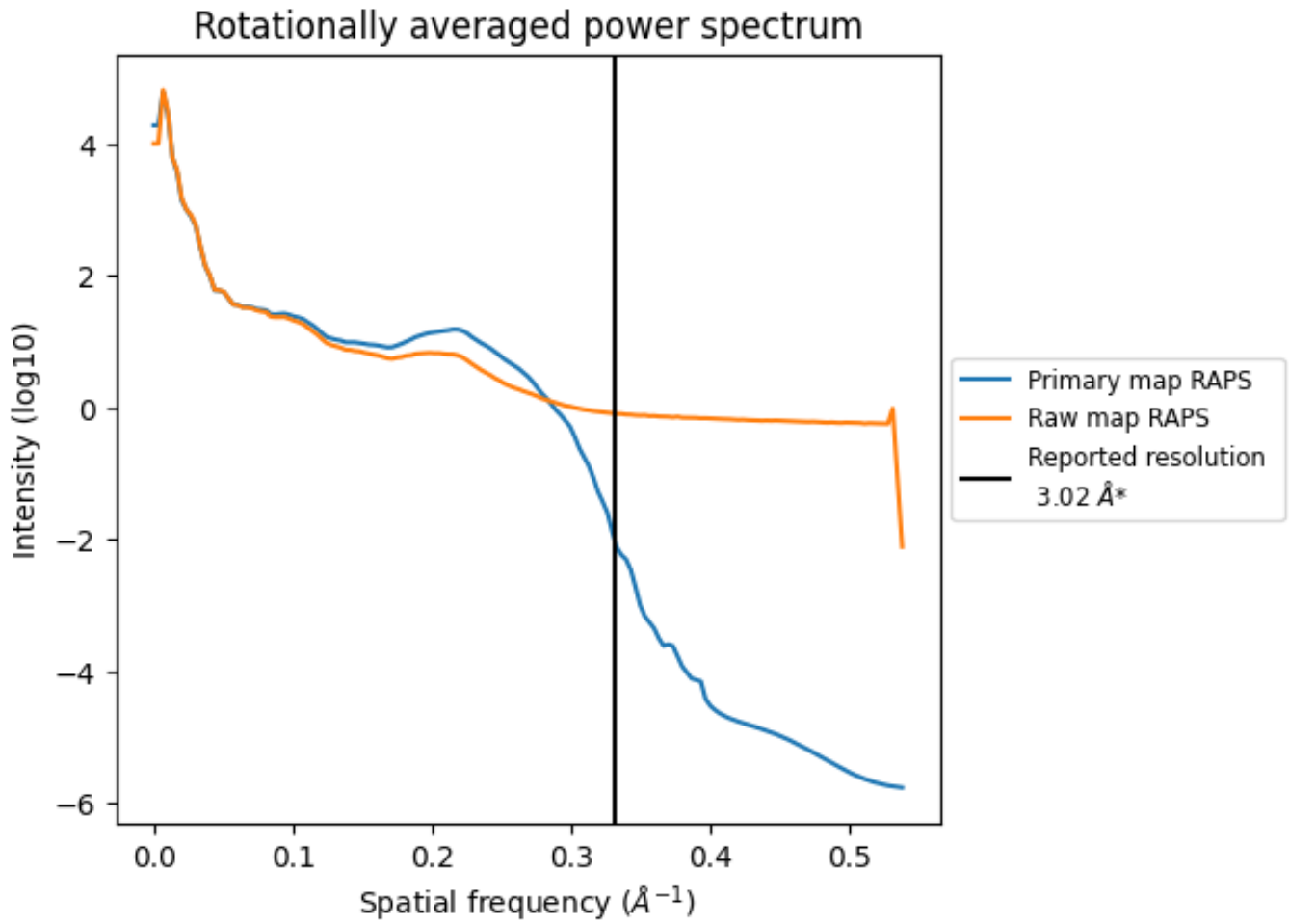
7.2 Volume estimate (i)



The volume at the recommended contour level is 75 nm^3; this corresponds to an approximate mass of 68 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)

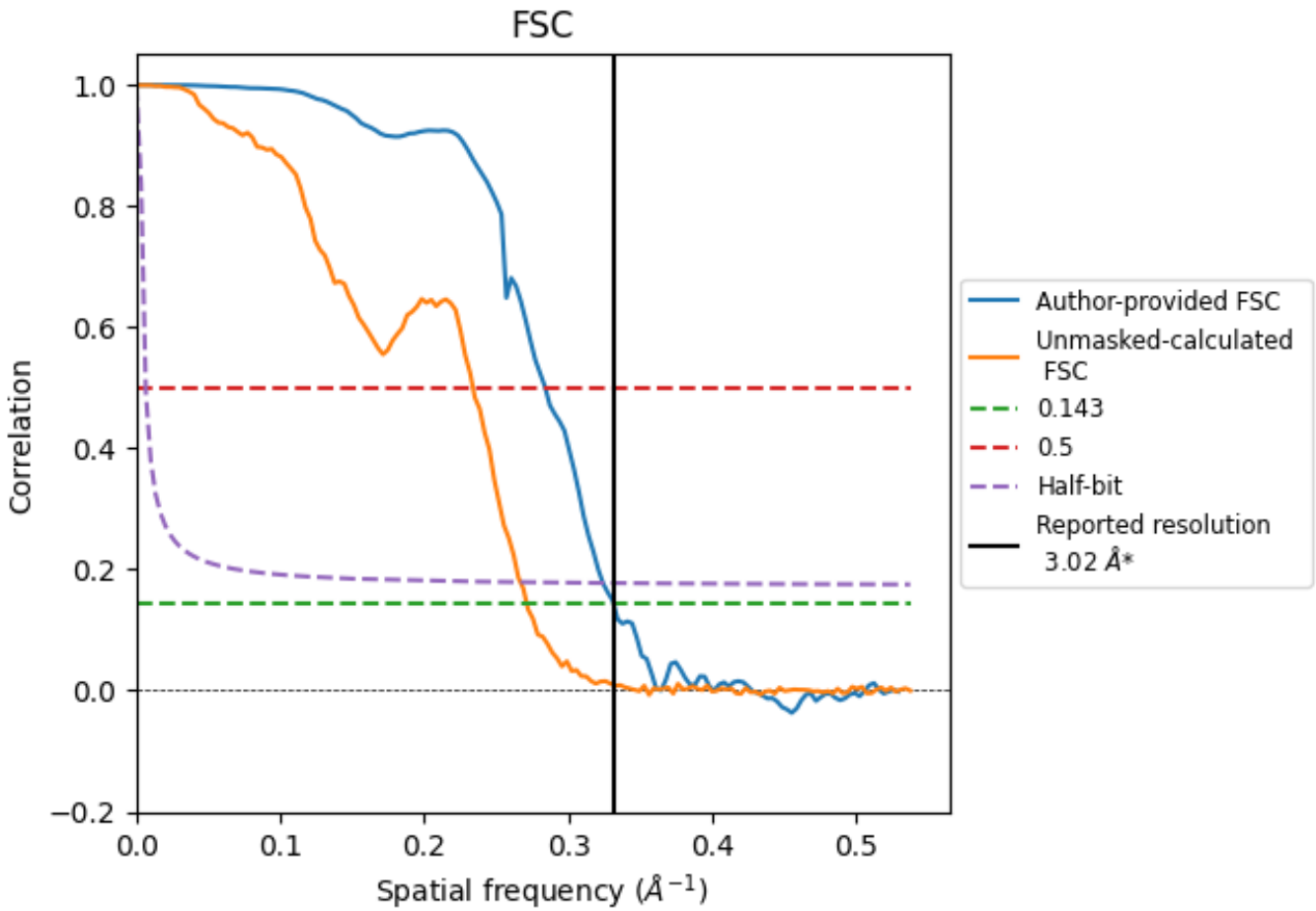


*Reported resolution corresponds to spatial frequency of 0.331 Å^{-1}

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 0.331 Å^{-1}

8.2 Resolution estimates (i)

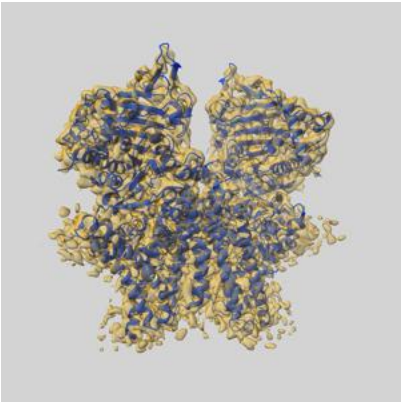
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.02	-	-
Author-provided FSC curve	3.02	3.52	3.09
Unmasked-calculated*	3.69	4.28	3.75

*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 3.69 differs from the reported value 3.02 by more than 10 %

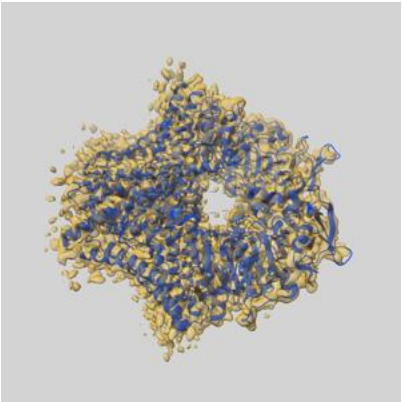
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-76832 and PDB model 12XL. Per-residue inclusion information can be found in section 3 on page 7.

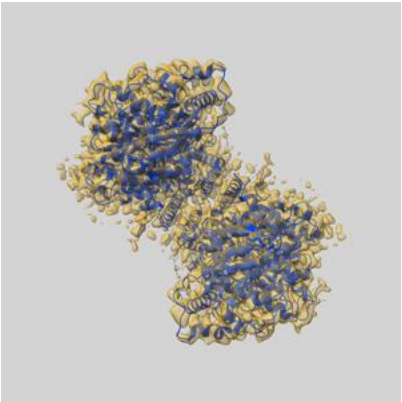
9.1 Map-model overlay (i)



X



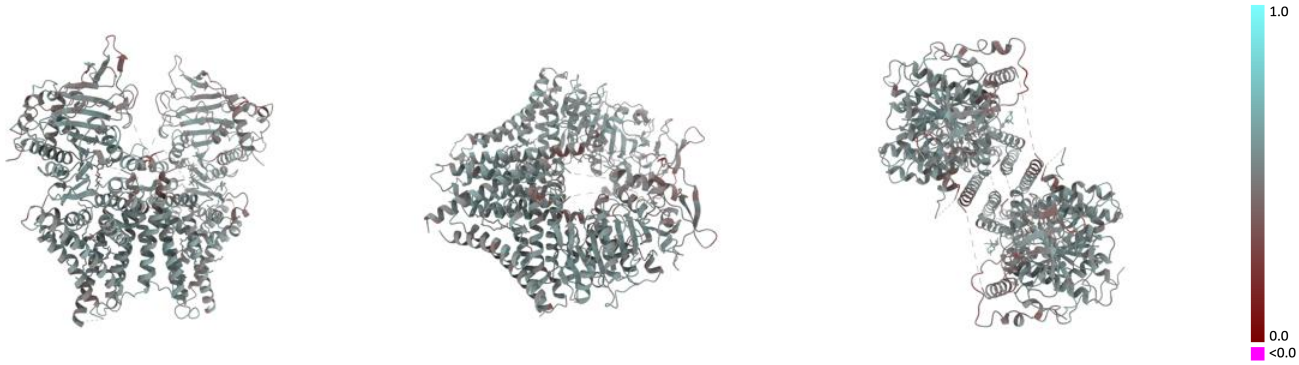
Y



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.

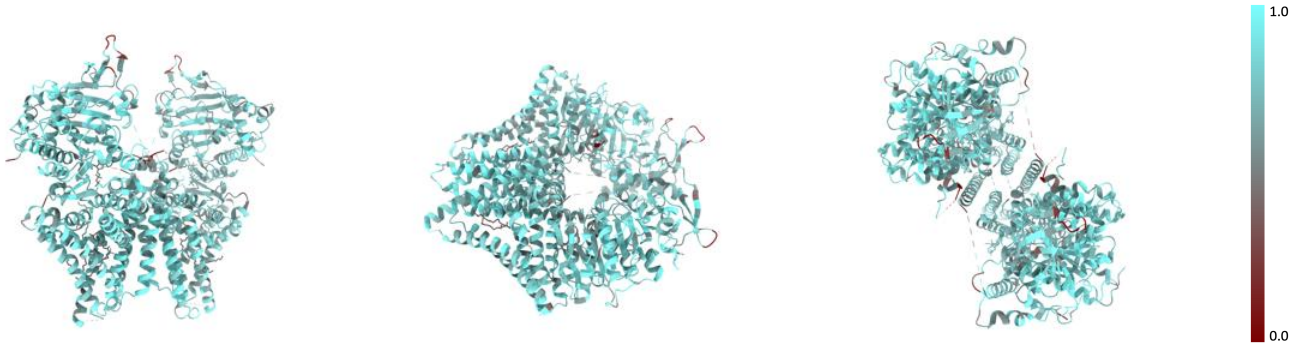
9.2 Q-score mapped to coordinate model (i)



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.

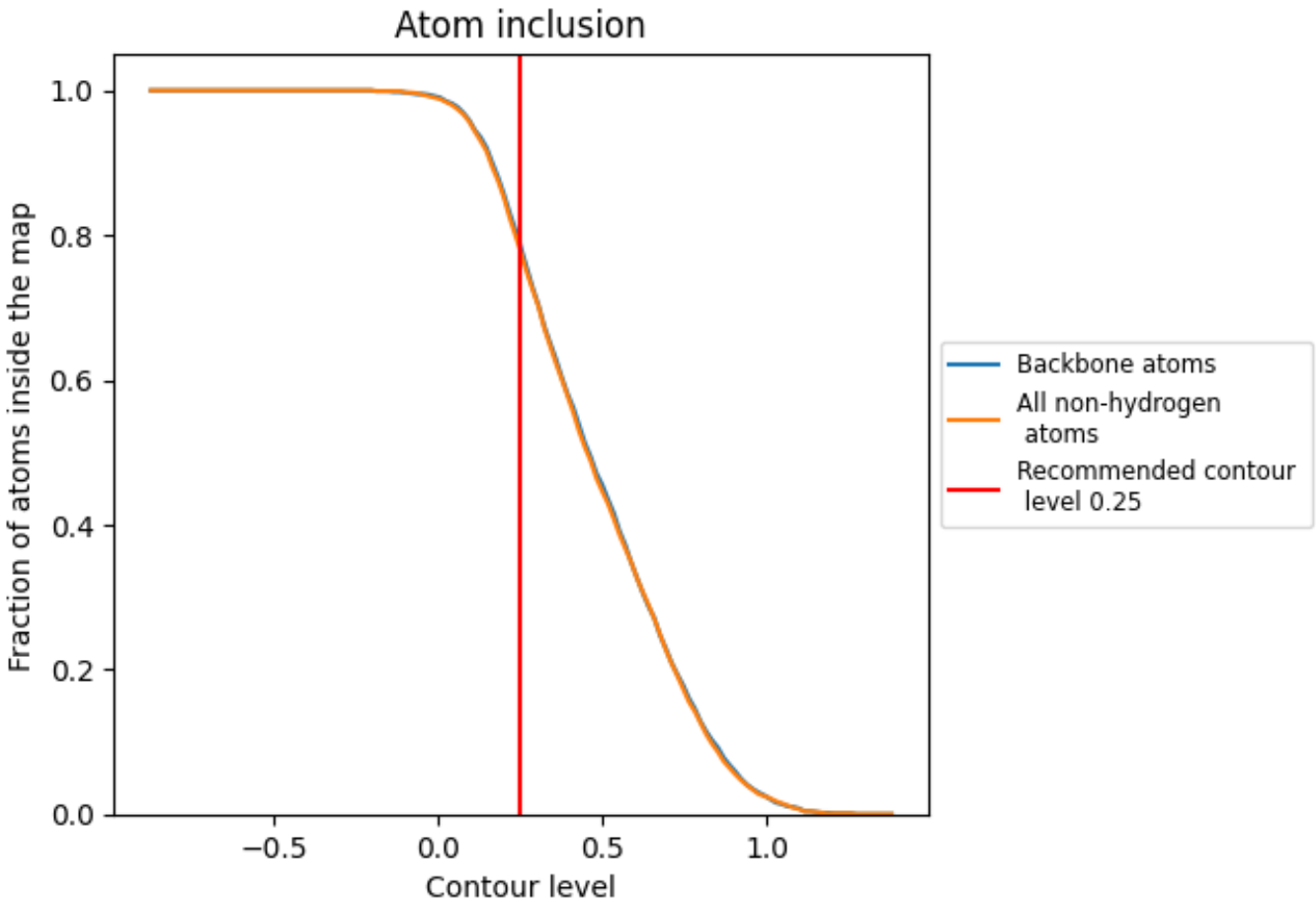
9.3 Atom inclusion mapped to coordinate model (i)



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, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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	0.7800	0.5100
A	0.7900	0.5100
B	0.7900	0.5100