Full wwPDB EM Validation Report ⓘ

Feb 12, 2024 – 03:33 pm GMT

PDB ID	:	8CG5
EMDB ID	:	EMD-16631
Title	:	The ACP crosslinked to the KS of the cercosporin fungal non-reducing polyketide synthase (NR-PKS) CTB1 (SAT-KS:ACP-MAT)
Authors	:	Munoz-Hernandez, H.; Tittes, Y.U.; Maier, T.
Deposited on	:	2023-02-03
Resolution	:	2.70 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:

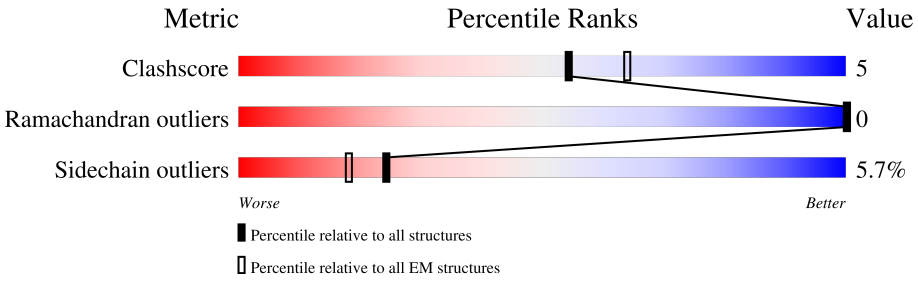
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1304	85% 13%
1	B	1304	84% 14%
2	C	88	9% 58% 24% 5% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 39732 atoms, of which 19716 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 Non-reducing polyketide synthase CTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1282	Total	C	H	N	O	S	0	0
			19248	6080	9554	1722	1850	42		
1	B	1282	Total	C	H	N	O	S	0	0
			19249	6080	9555	1722	1850	42		

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	ALA	CYS	engineered mutation	UNP Q6DQW3
A	321	ALA	THR	engineered mutation	UNP Q6DQW3
A	1010	ALA	SER	engineered mutation	UNP Q6DQW3
A	1294	ALA	-	expression tag	UNP Q6DQW3
A	1295	ALA	-	expression tag	UNP Q6DQW3
A	1296	ALA	-	expression tag	UNP Q6DQW3
A	1297	LEU	-	expression tag	UNP Q6DQW3
A	1298	GLU	-	expression tag	UNP Q6DQW3
A	1299	HIS	-	expression tag	UNP Q6DQW3
A	1300	HIS	-	expression tag	UNP Q6DQW3
A	1301	HIS	-	expression tag	UNP Q6DQW3
A	1302	HIS	-	expression tag	UNP Q6DQW3
A	1303	HIS	-	expression tag	UNP Q6DQW3
A	1304	HIS	-	expression tag	UNP Q6DQW3
B	119	ALA	CYS	engineered mutation	UNP Q6DQW3
B	321	ALA	THR	engineered mutation	UNP Q6DQW3
B	1010	ALA	SER	engineered mutation	UNP Q6DQW3
B	1294	ALA	-	expression tag	UNP Q6DQW3
B	1295	ALA	-	expression tag	UNP Q6DQW3
B	1296	ALA	-	expression tag	UNP Q6DQW3
B	1297	LEU	-	expression tag	UNP Q6DQW3
B	1298	GLU	-	expression tag	UNP Q6DQW3
B	1299	HIS	-	expression tag	UNP Q6DQW3
B	1300	HIS	-	expression tag	UNP Q6DQW3
B	1301	HIS	-	expression tag	UNP Q6DQW3
B	1302	HIS	-	expression tag	UNP Q6DQW3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1303	HIS	-	expression tag	UNP Q6DQW3
B	1304	HIS	-	expression tag	UNP Q6DQW3

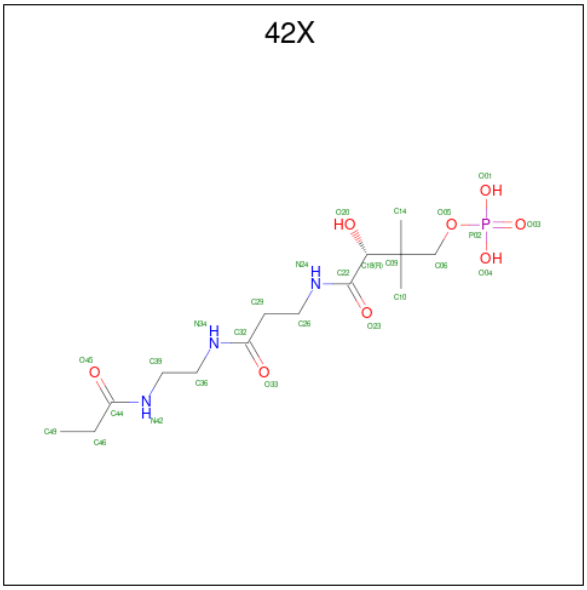
- Molecule 2 is a protein called Acyl carrier protein (ACP) of Non-reducing polyketide synthase CTB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	76	Total	C	H	N	O	S	0	0
			1185	376	582	98	127	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	GLY	-	expression tag	UNP Q6DQW3
C	2	SER	-	expression tag	UNP Q6DQW3
C	3	HIS	-	expression tag	UNP Q6DQW3
C	4	MET	-	expression tag	UNP Q6DQW3

- Molecule 3 is N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-N-[2-(propanoylamino)ethyl]-beta-alaninamide (three-letter code: 42X) (formula: $C_{14}H_{28}N_3O_8P$) (labeled as "Ligand of Interest" by depositor).



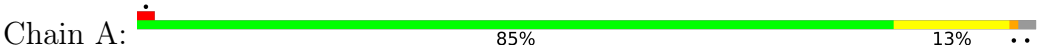
Mol	Chain	Residues	Atoms						AltConf
3	C	1	Total	C	H	N	O	P	0
			50	14	25	3	7	1	

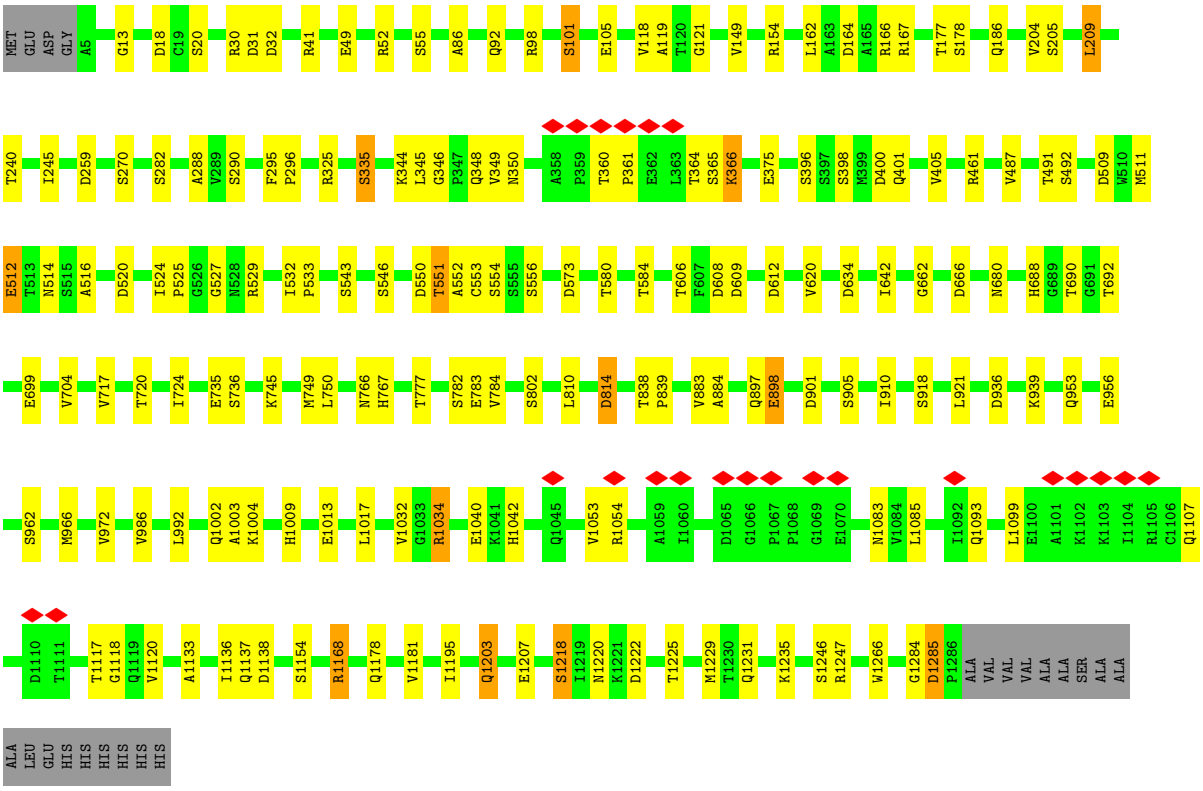
3 Residue-property plots (i)

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: Non-reducing polyketide synthase CTB1

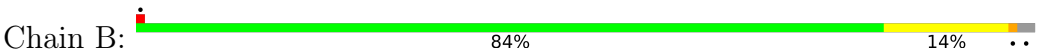
Chain A:

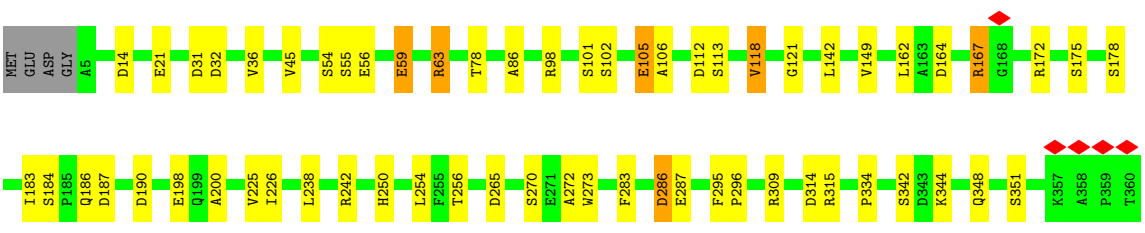


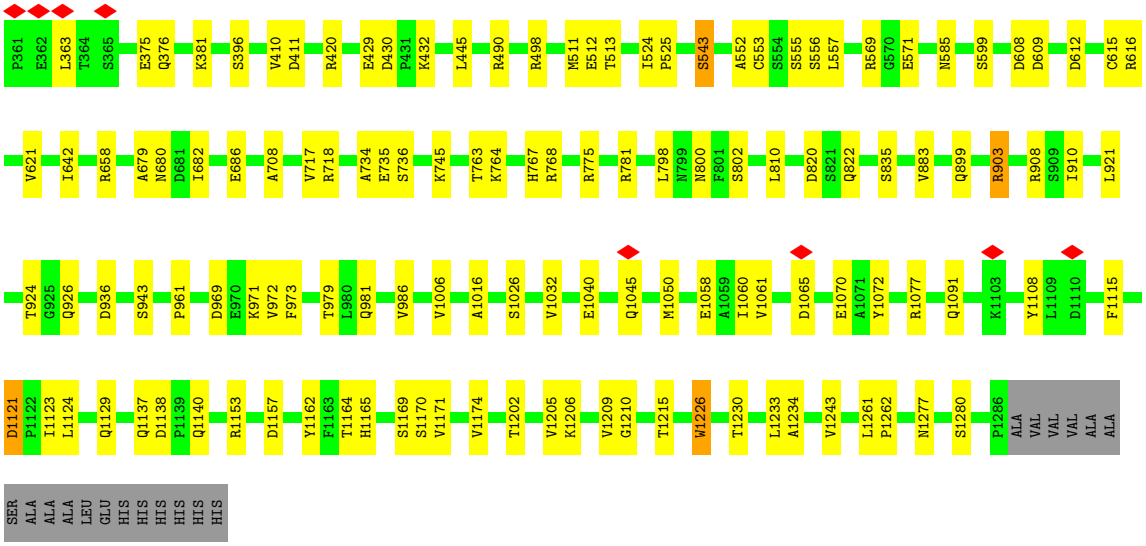


• Molecule 1: Non-reducing polyketide synthase CTB1

Chain B:

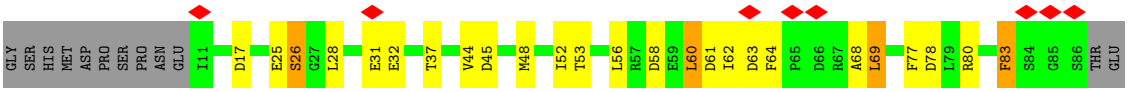






• Molecule 2: Acyl carrier protein (ACP) of Non-reducing polyketide synthase CTB1

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	255766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3300	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.535	Depositor
Minimum map value	-0.284	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.055	Depositor
Map size (Å)	314.88, 314.88, 314.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 42X

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	0.26	0/9909	0.51	0/13504
1	B	0.27	0/9909	0.52	4/13504 (0.0%)
2	C	0.27	0/610	0.60	0/823
All	All	0.27	0/20428	0.52	4/27831 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	334	PRO	CA-N-CD	-7.10	101.56	111.50
1	B	961	PRO	CA-N-CD	-6.46	102.46	111.50
1	B	334	PRO	N-CD-CG	-5.47	95.00	103.20
1	B	961	PRO	N-CD-CG	-5.07	95.59	103.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9694	9554	9591	103	0
1	B	9694	9555	9592	108	0
2	C	603	582	582	15	0
3	C	25	25	26	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20016	19716	19791	215	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 5.

All (215) 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:167:ARG:NH1	1:B:1138:ASP:O	2.06	0.89
1:A:186:GLN:OE1	1:A:186:GLN:N	2.10	0.85
1:B:971:LYS:O	1:B:971:LYS:NZ	2.09	0.85
1:B:21:GLU:N	1:B:21:GLU:OE1	2.09	0.84
1:B:186:GLN:N	1:B:186:GLN:OE1	2.11	0.83
1:A:166:ARG:NH2	1:B:1137:GLN:OE1	2.14	0.80
1:B:552:ALA:O	1:B:555:SER:OG	1.99	0.80
1:A:529:ARG:NH2	1:A:550:ASP:OD2	2.16	0.79
1:B:608:ASP:OD1	1:B:609:ASP:N	2.18	0.76
1:A:398:SER:OG	1:A:400:ASP:OD1	2.02	0.75
1:B:820:ASP:O	1:B:822:GLN:NE2	2.20	0.74
1:A:1284:GLY:O	1:B:1277:ASN:ND2	2.20	0.74
1:A:1247:ARG:NH2	1:B:59:GLU:OE1	2.21	0.72
1:B:162:LEU:HD11	1:B:254:LEU:HD21	1.72	0.71
1:B:708:ALA:O	1:B:775:ARG:NH1	2.23	0.71
1:B:32:ASP:OD2	1:B:101:SER:OG	2.13	0.67
1:A:910:ILE:HD12	1:A:910:ILE:O	1.93	0.67
2:C:56:LEU:HD11	2:C:83:PHE:HZ	1.60	0.66
1:A:1054:ARG:NH1	1:A:1107:GLN:OE1	2.29	0.65
1:A:1120:VAL:O	1:A:1120:VAL:HG22	1.96	0.65
1:B:250:HIS:ND1	1:B:309:ARG:O	2.28	0.65
1:A:167:ARG:NE	1:B:1140:GLN:OE1	2.30	0.65
1:B:1121:ASP:HA	1:B:1124:LEU:HD23	1.79	0.65
1:B:556:SER:OG	1:B:736:SER:O	2.14	0.64
1:B:910:ILE:HD12	1:B:910:ILE:O	1.98	0.64
1:A:608:ASP:OD1	1:A:609:ASP:N	2.31	0.64
1:B:225:VAL:HG23	1:B:226:ILE:HD12	1.78	0.64
1:A:897:GLN:NE2	1:A:901:ASP:OD1	2.34	0.61
1:A:556:SER:OG	1:A:736:SER:O	2.19	0.61
1:B:936:ASP:OD1	1:B:936:ASP:N	2.33	0.60
1:A:41:ARG:NH2	1:B:376:GLN:O	2.34	0.60
1:B:118:VAL:O	1:B:121:GLY:N	2.33	0.60
1:A:514:ASN:OD1	1:A:584:THR:HG21	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HE3	1:B:344:LYS:HA	1.84	0.60
1:B:430:ASP:OD2	1:B:432:LYS:NZ	2.36	0.59
1:A:986:VAL:HG21	1:A:1032:VAL:HG21	1.84	0.59
1:A:18:ASP:OD1	1:A:20:SER:OG	2.20	0.59
1:A:400:ASP:OD1	1:A:400:ASP:N	2.36	0.58
1:B:1205:VAL:O	1:B:1209:VAL:HG12	2.03	0.58
1:B:1006:VAL:CG1	1:B:1016:ALA:HB1	2.35	0.57
1:A:1034:ARG:HE	1:A:1034:ARG:HA	1.70	0.57
1:A:580:THR:HG22	1:A:620:VAL:HG13	1.85	0.57
1:A:401:GLN:O	1:A:405:VAL:HG13	2.04	0.57
1:B:420:ARG:NH2	1:B:445:LEU:O	2.38	0.56
1:A:162:LEU:HD21	1:A:204:VAL:HG12	1.86	0.56
1:B:734:ALA:O	1:B:735:GLU:HG2	2.06	0.56
1:A:543:SER:O	1:A:543:SER:OG	2.20	0.55
1:B:1226:TRP:O	1:B:1230:THR:OG1	2.22	0.55
1:B:543:SER:O	1:B:543:SER:OG	2.20	0.55
1:A:1117:THR:O	1:A:1168:ARG:NH1	2.40	0.55
1:A:1178:GLN:HE21	1:A:1178:GLN:HA	1.72	0.55
1:B:348:GLN:O	1:B:351:SER:OG	2.25	0.55
1:A:750:LEU:HD22	1:A:814:ASP:OD1	2.07	0.55
1:B:14:ASP:N	1:B:14:ASP:OD1	2.41	0.54
1:B:45:VAL:HG21	1:B:142:LEU:HD12	1.88	0.54
1:A:118:VAL:HG12	1:A:119:ALA:H	1.71	0.54
1:B:513:THR:OG1	1:B:585:ASN:OD1	2.25	0.54
1:A:584:THR:HG22	1:A:584:THR:O	2.07	0.54
1:A:1203:GLN:O	1:A:1207:GLU:HG3	2.07	0.54
1:A:1002:GLN:HA	1:A:1002:GLN:OE1	2.08	0.53
2:C:26:SER:HA	2:C:48:MET:HE1	1.88	0.53
1:B:498:ARG:NH2	1:B:571:GLU:O	2.41	0.53
1:B:164:ASP:OD1	1:B:164:ASP:N	2.40	0.53
1:A:1285:ASP:OD1	1:A:1285:ASP:N	2.41	0.53
1:B:552:ALA:CB	1:B:802:SER:OG	2.57	0.53
1:B:926:GLN:HG2	1:B:926:GLN:O	2.08	0.53
2:C:53:THR:HG21	2:C:68:ALA:HA	1.91	0.53
1:A:690:THR:HG23	1:A:692:THR:HG23	1.89	0.53
1:A:921:LEU:HD23	1:A:1003:ALA:CB	2.40	0.52
1:A:177:THR:HG22	1:A:245:ILE:HB	1.91	0.52
1:A:282:SER:N	1:A:288:ALA:O	2.40	0.52
1:A:205:SER:O	1:A:205:SER:OG	2.28	0.52
1:A:1195:ILE:HG22	1:A:1195:ILE:O	2.09	0.52
1:A:325:ARG:HB3	1:A:325:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:ILE:HD12	1:B:910:ILE:C	2.31	0.51
1:A:491:THR:HG21	1:A:634:ASP:OD1	2.09	0.51
1:A:956:GLU:OE1	1:A:956:GLU:HA	2.10	0.51
2:C:31:GLU:OE2	2:C:31:GLU:O	2.28	0.51
2:C:56:LEU:HD21	2:C:83:PHE:CZ	2.46	0.51
1:A:552:ALA:HB1	1:A:802:SER:OG	2.11	0.51
1:B:86:ALA:HB2	1:B:149:VAL:HG22	1.93	0.51
1:A:724:ILE:HD12	1:A:777:THR:CG2	2.41	0.50
1:A:724:ILE:HD12	1:A:777:THR:HG21	1.93	0.50
1:A:745:LYS:O	1:A:749:MET:HG3	2.10	0.50
1:A:86:ALA:HB2	1:A:149:VAL:HG22	1.91	0.50
1:B:286:ASP:OD2	1:B:287:GLU:N	2.45	0.50
1:B:642:ILE:HG23	1:B:810:LEU:CD1	2.41	0.50
1:A:936:ASP:OD1	1:A:936:ASP:N	2.45	0.50
1:A:361:PRO:O	1:A:364:THR:OG1	2.29	0.50
1:A:939:LYS:HB3	1:A:939:LYS:NZ	2.27	0.49
1:A:491:THR:HG22	1:A:492:SER:N	2.28	0.49
2:C:56:LEU:HD11	2:C:83:PHE:CZ	2.46	0.49
1:B:679:ALA:O	1:B:718:ARG:NH2	2.45	0.49
1:B:969:ASP:C	1:B:969:ASP:OD1	2.50	0.49
1:B:283:PHE:O	1:B:315:ARG:NH1	2.46	0.48
1:B:273:TRP:HB3	1:B:296:PRO:HD3	1.95	0.48
1:A:118:VAL:HG12	1:A:119:ALA:N	2.29	0.48
1:B:183:ILE:HD11	1:B:238:LEU:CD1	2.44	0.48
1:A:366:LYS:NZ	1:B:272:ALA:HB2	2.28	0.48
1:B:616:ARG:NH2	1:B:735:GLU:OE2	2.42	0.48
1:B:682:ILE:O	1:B:718:ARG:NH2	2.43	0.48
1:A:511:MET:O	1:A:516:ALA:HB2	2.13	0.47
1:A:1120:VAL:O	1:A:1120:VAL:CG2	2.61	0.47
1:A:1231:GLN:O	1:A:1235:LYS:HD2	2.14	0.47
1:A:13:GLY:O	1:A:92:GLN:NE2	2.45	0.47
1:A:553:CYS:HA	1:A:735:GLU:O	2.15	0.47
1:A:966:MET:SD	1:A:972:VAL:HG23	2.54	0.47
2:C:44:VAL:HG23	2:C:44:VAL:O	2.15	0.47
1:B:1202:THR:HG21	1:B:1215:THR:HB	1.96	0.47
1:A:32:ASP:CG	1:A:101:SER:HG	2.18	0.47
1:B:183:ILE:HD11	1:B:238:LEU:HD11	1.97	0.47
2:C:58:ASP:OD2	2:C:58:ASP:C	2.52	0.47
3:C:2000:42X:N24	3:C:2000:42X:H2	2.30	0.47
2:C:26:SER:HB3	2:C:28:LEU:HG	1.96	0.47
1:A:1178:GLN:HA	1:A:1178:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:NE	1:A:259:ASP:OD1	2.41	0.46
1:B:1077:ARG:O	1:B:1174:VAL:HG13	2.14	0.46
1:A:1203:GLN:HA	1:A:1203:GLN:OE1	2.14	0.46
1:A:1053:VAL:HG11	1:A:1099:LEU:HD21	1.98	0.46
1:B:553:CYS:HA	1:B:735:GLU:O	2.15	0.46
1:B:1045:GLN:N	1:B:1045:GLN:OE1	2.49	0.46
1:B:686:GLU:OE2	1:B:745:LYS:NZ	2.32	0.46
1:B:768:ARG:HG2	1:B:768:ARG:HH11	1.80	0.46
1:A:838:THR:HG22	1:A:839:PRO:HD2	1.99	0.45
1:A:898:GLU:C	1:A:898:GLU:OE1	2.55	0.45
1:B:32:ASP:OD2	1:B:102:SER:OG	2.34	0.45
1:A:360:THR:HG23	1:A:360:THR:O	2.17	0.45
1:A:346:GLY:O	1:A:350:ASN:ND2	2.50	0.45
1:B:314:ASP:OD1	1:B:314:ASP:C	2.54	0.45
1:B:883:VAL:HG11	1:B:1234:ALA:HB1	1.98	0.45
1:A:295:PHE:HB3	1:A:296:PRO:HD3	1.98	0.45
1:B:112:ASP:OD2	1:B:112:ASP:C	2.55	0.45
1:B:1124:LEU:HD12	1:B:1164:THR:HB	1.98	0.45
1:B:78:THR:O	1:B:78:THR:HG22	2.17	0.45
1:A:688:HIS:N	1:A:699:GLU:OE2	2.48	0.44
1:B:1165:HIS:CD2	1:B:1169:SER:HB2	2.52	0.44
2:C:32:GLU:O	2:C:37:THR:OG1	2.33	0.44
1:A:1117:THR:OG1	1:A:1118:GLY:N	2.49	0.44
1:A:366:LYS:HZ1	1:B:272:ALA:HB2	1.83	0.44
1:A:584:THR:O	1:A:584:THR:CG2	2.66	0.44
1:A:953:GLN:OE1	1:B:256:THR:OG1	2.35	0.44
1:A:512:GLU:HG3	1:B:512:GLU:HG2	1.99	0.44
1:A:1137:GLN:OE1	1:B:167:ARG:NH2	2.37	0.44
1:A:662:GLY:O	1:A:666:ASP:OD1	2.36	0.43
1:A:335:SER:O	1:A:335:SER:OG	2.28	0.43
1:A:1136:ILE:HG22	1:A:1137:GLN:N	2.33	0.43
1:B:986:VAL:HG21	1:B:1032:VAL:HG21	2.00	0.43
1:A:209:LEU:H	1:A:209:LEU:HD23	1.83	0.43
1:B:273:TRP:HB3	1:B:295:PHE:HB3	2.00	0.43
1:A:992:LEU:HD21	1:A:1218:SER:OG	2.18	0.43
1:B:1006:VAL:HG11	1:B:1016:ALA:HB1	2.00	0.43
1:B:105:GLU:OE1	1:B:106:ALA:N	2.50	0.43
1:B:1209:VAL:HG13	1:B:1210:GLY:N	2.33	0.43
1:A:365:SER:O	1:A:365:SER:OG	2.35	0.43
1:B:411:ASP:OD1	1:B:411:ASP:O	2.37	0.43
1:B:524:ILE:HB	1:B:525:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1206:LYS:HE3	1:B:1215:THR:HG21	2.01	0.43
1:B:429:GLU:HA	1:B:429:GLU:OE1	2.19	0.43
1:A:921:LEU:N	1:A:921:LEU:HD22	2.34	0.43
1:B:187:ASP:HA	1:B:190:ASP:OD2	2.18	0.43
1:B:768:ARG:HG2	1:B:768:ARG:NH1	2.33	0.43
1:B:45:VAL:CG2	1:B:142:LEU:HD12	2.49	0.43
1:B:1121:ASP:OD1	1:B:1121:ASP:N	2.50	0.43
1:A:345:LEU:O	1:A:349:VAL:HG23	2.19	0.42
1:A:511:MET:HG3	1:A:527:GLY:HA3	2.01	0.42
2:C:62:ILE:HG22	2:C:63:ASP:H	1.85	0.42
1:B:1202:THR:CG2	1:B:1215:THR:HB	2.50	0.42
1:A:580:THR:CG2	1:A:620:VAL:HG13	2.49	0.42
1:B:557:LEU:HD22	1:B:800:ASN:HB2	2.02	0.42
1:B:1233:LEU:HD12	1:B:1243:VAL:HG11	2.01	0.42
2:C:69:LEU:N	2:C:69:LEU:HD23	2.35	0.42
2:C:44:VAL:O	2:C:44:VAL:CG2	2.67	0.42
1:B:1070:GLU:O	1:B:1091:GLN:NE2	2.53	0.41
1:B:1123:ILE:O	1:B:1123:ILE:HD12	2.19	0.41
1:B:1209:VAL:HG13	1:B:1210:GLY:H	1.84	0.41
1:A:344:LYS:O	1:A:348:GLN:HG2	2.20	0.41
1:A:1013:GLU:O	1:A:1017:LEU:HG	2.20	0.41
1:A:554:SER:O	1:A:554:SER:OG	2.29	0.41
1:B:63:ARG:HH11	1:B:63:ARG:HG2	1.85	0.41
1:B:59:GLU:CA	1:B:59:GLU:OE2	2.69	0.41
1:B:658:ARG:HG2	1:B:658:ARG:HH11	1.86	0.41
1:B:1040:GLU:C	1:B:1040:GLU:OE2	2.59	0.41
1:B:642:ILE:HG23	1:B:810:LEU:HD11	2.03	0.41
1:B:971:LYS:O	1:B:971:LYS:CD	2.68	0.41
2:C:17:ASP:HB2	2:C:60:LEU:HD21	2.03	0.41
1:B:54:SER:OG	1:B:56:GLU:OE1	2.37	0.41
1:B:899:GLN:O	1:B:903:ARG:HG2	2.21	0.41
1:A:766:ASN:OD1	1:A:767:HIS:N	2.54	0.41
1:A:883:VAL:HG22	1:A:884:ALA:N	2.36	0.41
1:A:1040:GLU:OE2	1:A:1040:GLU:C	2.60	0.41
1:B:183:ILE:HG22	1:B:184:SER:O	2.21	0.41
1:B:1060:ILE:HG23	1:B:1061:VAL:N	2.34	0.41
1:B:1162:TYR:CD1	1:B:1162:TYR:C	2.94	0.41
2:C:25:GLU:CB	2:C:52:ILE:HD11	2.50	0.41
1:A:524:ILE:HB	1:A:525:PRO:HD3	2.02	0.41
1:B:686:GLU:HB2	1:B:798:LEU:HD12	2.02	0.41
1:A:118:VAL:O	1:A:121:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ASP:OD2	1:A:1225:THR:OG1	2.15	0.40
1:A:1009:HIS:O	1:A:1009:HIS:ND1	2.54	0.40
1:A:1178:GLN:O	1:A:1181:VAL:HG12	2.21	0.40
1:B:763:THR:HG23	1:B:764:LYS:N	2.35	0.40
1:A:551:THR:HG22	1:A:552:ALA:N	2.37	0.40
1:A:1133:ALA:HB2	1:B:200:ALA:O	2.21	0.40
1:B:31:ASP:OD1	1:B:31:ASP:C	2.60	0.40
1:B:1169:SER:OG	1:B:1170:SER:N	2.54	0.40
1:A:209:LEU:H	1:A:209:LEU:CD2	2.35	0.40
1:A:532:ILE:HB	1:A:533:PRO:HD3	2.04	0.40
1:A:642:ILE:HG23	1:A:810:LEU:CD1	2.51	0.40
1:A:1034:ARG:HA	1:A:1034:ARG:NE	2.34	0.40
1:A:1085:LEU:N	1:A:1085:LEU:HD23	2.37	0.40
1:B:32:ASP:O	1:B:36:VAL:HG23	2.21	0.40
1:B:286:ASP:OD2	1:B:286:ASP:C	2.60	0.40
1:B:612:ASP:N	1:B:612:ASP:OD1	2.54	0.40
1:B:972:VAL:O	1:B:972:VAL:HG22	2.21	0.40
1:B:1261:LEU:HB3	1:B:1262:PRO:HD2	2.04	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	1280/1304 (98%)	1243 (97%)	37 (3%)	0	100	100
1	B	1280/1304 (98%)	1251 (98%)	29 (2%)	0	100	100
2	C	74/88 (84%)	69 (93%)	5 (7%)	0	100	100
All	All	2634/2696 (98%)	2563 (97%)	71 (3%)	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	1031/1046 (99%)	975 (95%)	56 (5%)	22 47
1	B	1031/1046 (99%)	975 (95%)	56 (5%)	22 47
2	C	69/80 (86%)	59 (86%)	10 (14%)	3 8
All	All	2131/2172 (98%)	2009 (94%)	122 (6%)	24 44

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	31	ASP
1	A	49	GLU
1	A	52	ARG
1	A	55	SER
1	A	98	ARG
1	A	101	SER
1	A	105	GLU
1	A	164	ASP
1	A	178	SER
1	A	209	LEU
1	A	240	THR
1	A	270	SER
1	A	290	SER
1	A	335	SER
1	A	366	LYS
1	A	375	GLU
1	A	396	SER
1	A	461	ARG
1	A	487	VAL
1	A	509	ASP
1	A	512	GLU
1	A	520	ASP
1	A	546	SER
1	A	551	THR
1	A	573	ASP

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Mol	Chain	Res	Type
1	A	606	THR
1	A	612	ASP
1	A	680	ASN
1	A	704	VAL
1	A	717	VAL
1	A	720	THR
1	A	782	SER
1	A	783	GLU
1	A	784	VAL
1	A	814	ASP
1	A	898	GLU
1	A	905	SER
1	A	918	SER
1	A	962	SER
1	A	1004	LYS
1	A	1034	ARG
1	A	1042	HIS
1	A	1083	ASN
1	A	1093	GLN
1	A	1138	ASP
1	A	1154	SER
1	A	1168	ARG
1	A	1203	GLN
1	A	1218	SER
1	A	1220	ASN
1	A	1222	ASP
1	A	1229	MET
1	A	1246	SER
1	A	1266	TRP
1	A	1285	ASP
1	B	55	SER
1	B	59	GLU
1	B	63	ARG
1	B	98	ARG
1	B	105	GLU
1	B	113	SER
1	B	118	VAL
1	B	167	ARG
1	B	172	ARG
1	B	175	SER
1	B	178	SER
1	B	198	GLU

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Mol	Chain	Res	Type
1	B	242	ARG
1	B	265	ASP
1	B	270	SER
1	B	286	ASP
1	B	342	SER
1	B	363	LEU
1	B	375	GLU
1	B	381	LYS
1	B	396	SER
1	B	410	VAL
1	B	490	ARG
1	B	511	MET
1	B	543	SER
1	B	569	ARG
1	B	599	SER
1	B	615	CYS
1	B	621	VAL
1	B	680	ASN
1	B	717	VAL
1	B	767	HIS
1	B	781	ARG
1	B	835	SER
1	B	903	ARG
1	B	908	ARG
1	B	921	LEU
1	B	924	THR
1	B	943	SER
1	B	973	PHE
1	B	979	THR
1	B	981	GLN
1	B	1026	SER
1	B	1050	MET
1	B	1058	GLU
1	B	1065	ASP
1	B	1072	TYR
1	B	1108	TYR
1	B	1115	PHE
1	B	1121	ASP
1	B	1129	GLN
1	B	1153	ARG
1	B	1157	ASP
1	B	1171	VAL

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Mol	Chain	Res	Type
1	B	1226	TRP
1	B	1280	SER
2	C	26	SER
2	C	45	ASP
2	C	60	LEU
2	C	61	ASP
2	C	64	PHE
2	C	69	LEU
2	C	77	PHE
2	C	78	ASP
2	C	80	ARG
2	C	83	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	ASN
1	A	508	ASN
1	A	897	GLN
1	A	1140	GLN
1	A	1178	GLN
1	A	1214	GLN
1	A	1277	ASN
1	B	15	GLN
1	B	92	GLN
1	B	348	GLN
1	B	632	GLN
1	B	680	ASN
1	B	856	HIS
1	B	1081	GLN
1	B	1178	GLN
1	B	1231	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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
3	42X	C	2000	1,2	18,24,25	2.46	6 (33%)	24,31,34	1.65	3 (12%)

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
3	42X	C	2000	1,2	-	16/29/31/32	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2000	42X	C22-N24	5.44	1.45	1.33
3	C	2000	42X	C44-N42	5.40	1.45	1.33
3	C	2000	42X	C32-N34	5.35	1.45	1.33
3	C	2000	42X	O23-C22	-2.28	1.18	1.23
3	C	2000	42X	O45-C44	-2.15	1.18	1.23
3	C	2000	42X	O33-C32	-2.15	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2000	42X	C46-C44-N42	4.60	120.65	115.79
3	C	2000	42X	C29-C32-N34	2.61	120.82	116.42
3	C	2000	42X	C18-C22-N24	2.53	121.62	116.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2000	42X	C14-C09-C18-O20
3	C	2000	42X	C14-C09-C18-C22
3	C	2000	42X	C10-C09-C18-C22
3	C	2000	42X	C06-C09-C18-O20
3	C	2000	42X	C06-C09-C18-C22
3	C	2000	42X	C09-C18-C22-O23
3	C	2000	42X	C09-C18-C22-N24
3	C	2000	42X	N24-C26-C29-C32
3	C	2000	42X	N34-C36-C39-N42
3	C	2000	42X	C10-C09-C18-O20
3	C	2000	42X	O20-C18-C22-N24
3	C	2000	42X	C29-C26-N24-C22
3	C	2000	42X	O05-C06-C09-C18
3	C	2000	42X	O05-C06-C09-C10
3	C	2000	42X	C26-C29-C32-O33
3	C	2000	42X	C26-C29-C32-N34

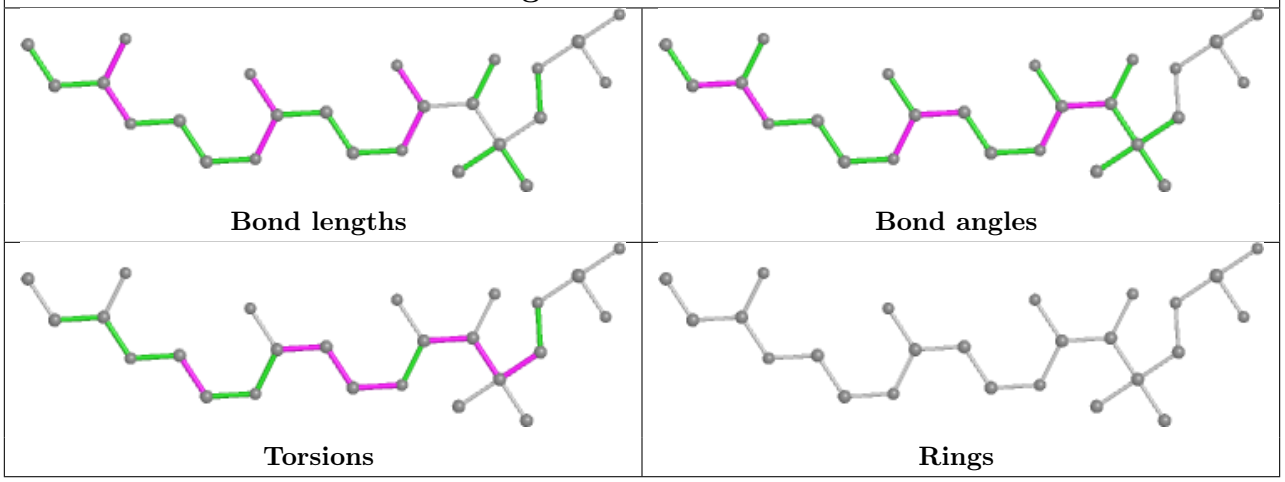
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2000	42X	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 42X C 2000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

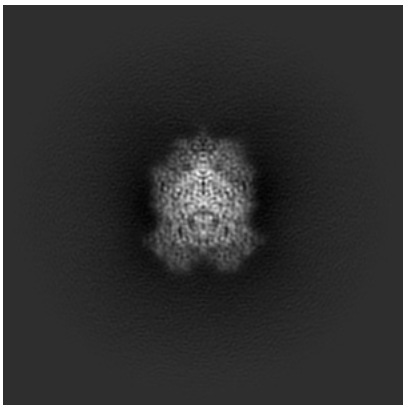
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16631. These allow visual inspection of the internal detail of the map and identification of artifacts.

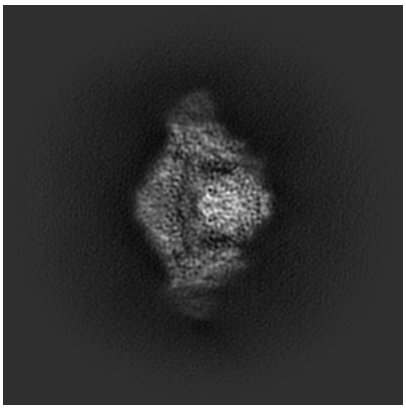
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

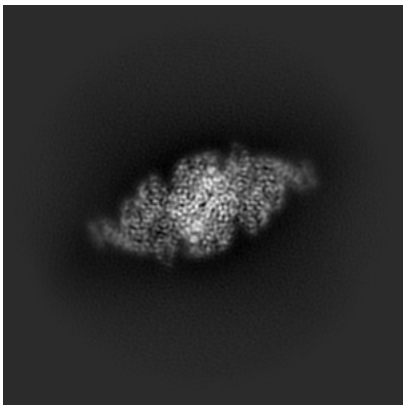
6.1.1 Primary map



X

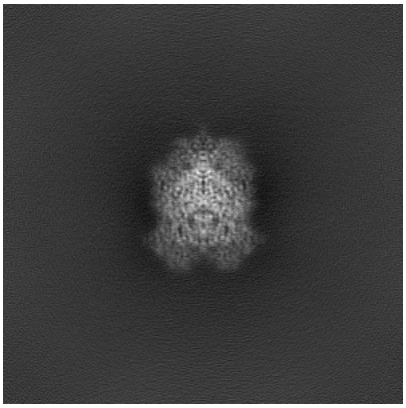


Y

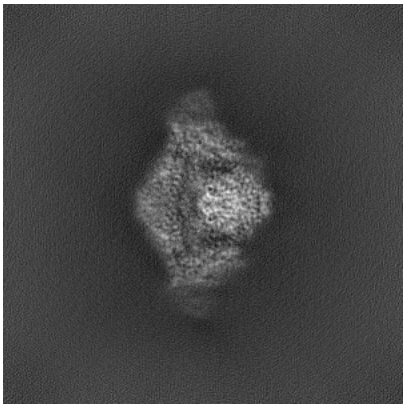


Z

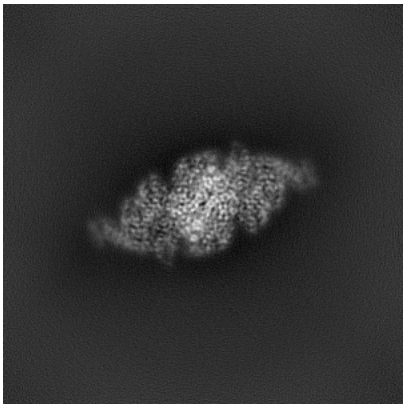
6.1.2 Raw map



X



Y

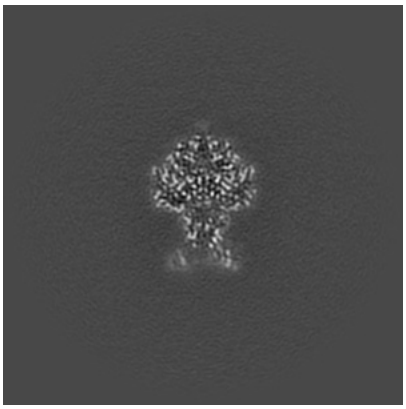


Z

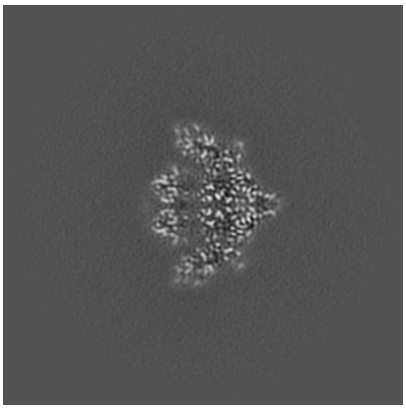
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

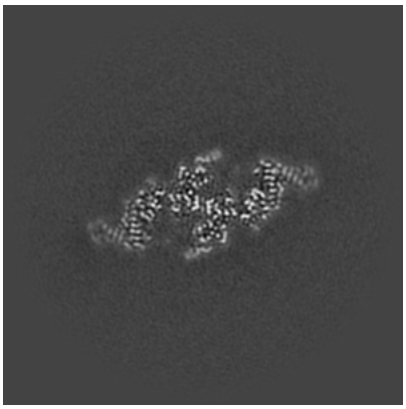
6.2.1 Primary map



X Index: 192

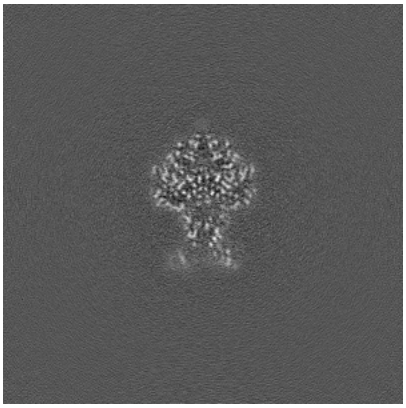


Y Index: 192

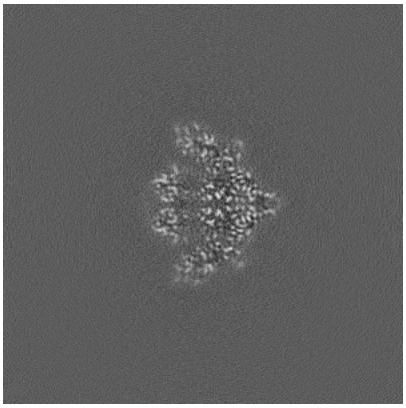


Z Index: 192

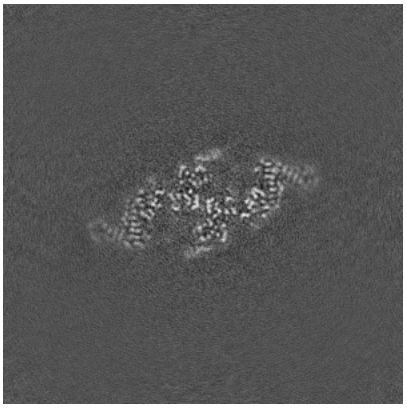
6.2.2 Raw map



X Index: 192



Y Index: 192

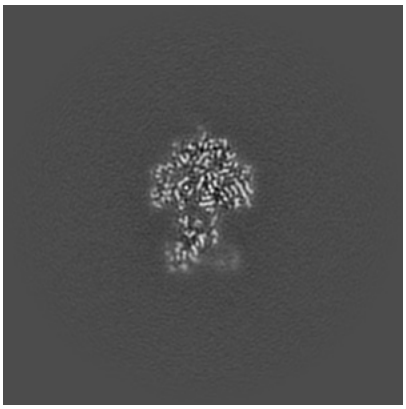


Z Index: 192

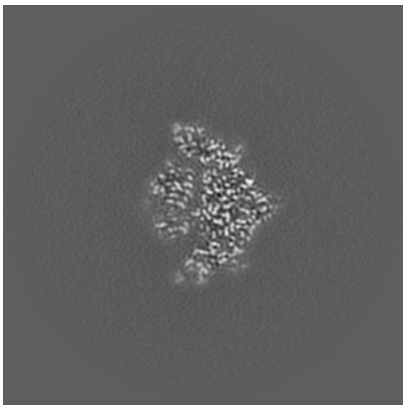
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

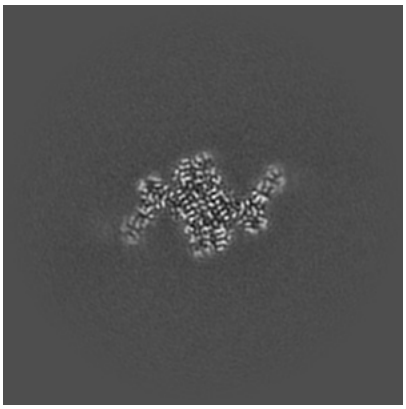
6.3.1 Primary map



X Index: 186

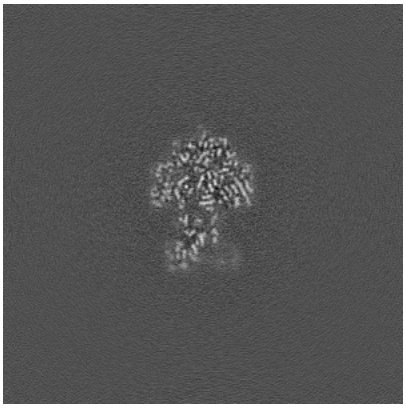


Y Index: 195

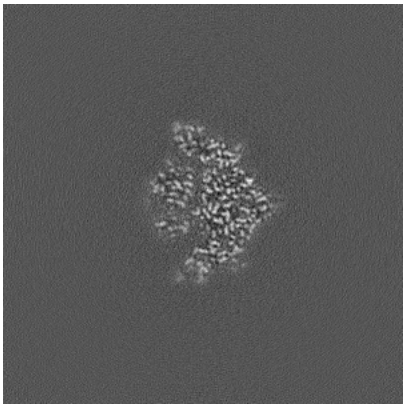


Z Index: 206

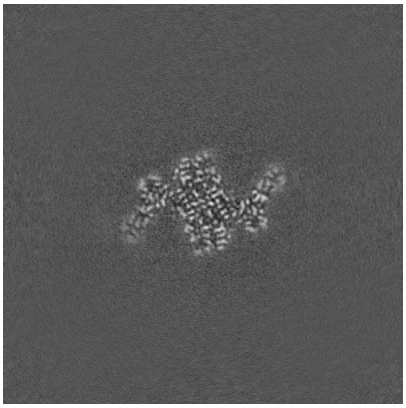
6.3.2 Raw map



X Index: 186



Y Index: 195

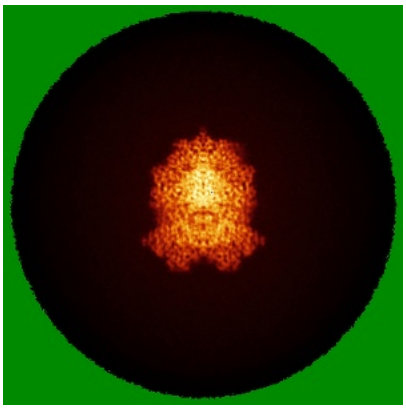


Z Index: 206

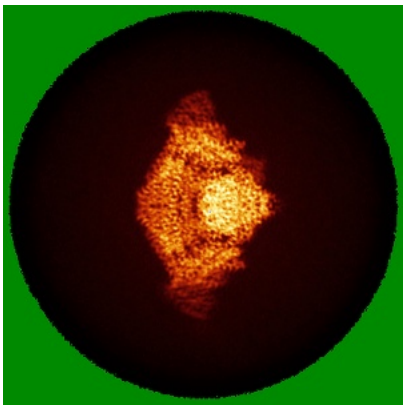
The images above show the largest variance slices of the map in three orthogonal directions.

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

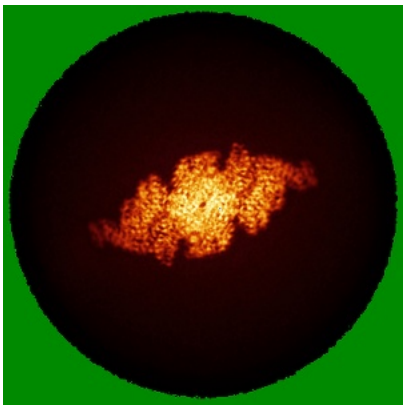
6.4.1 Primary map



X

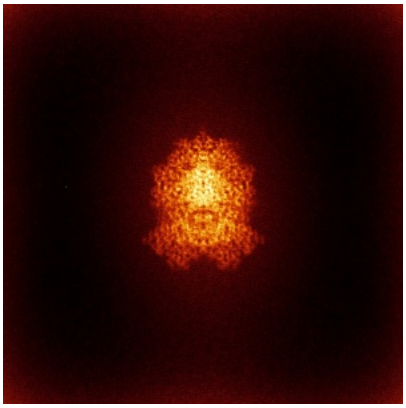


Y

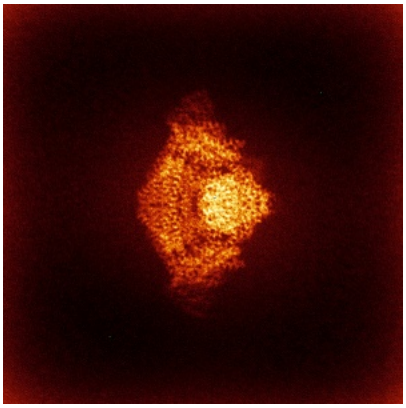


Z

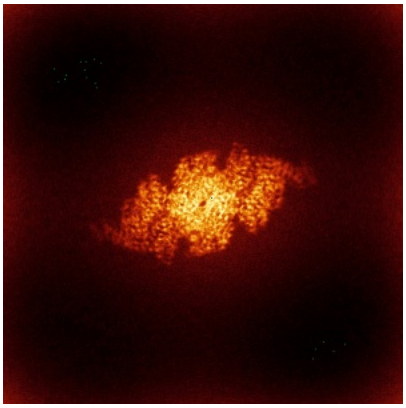
6.4.2 Raw map



X



Y

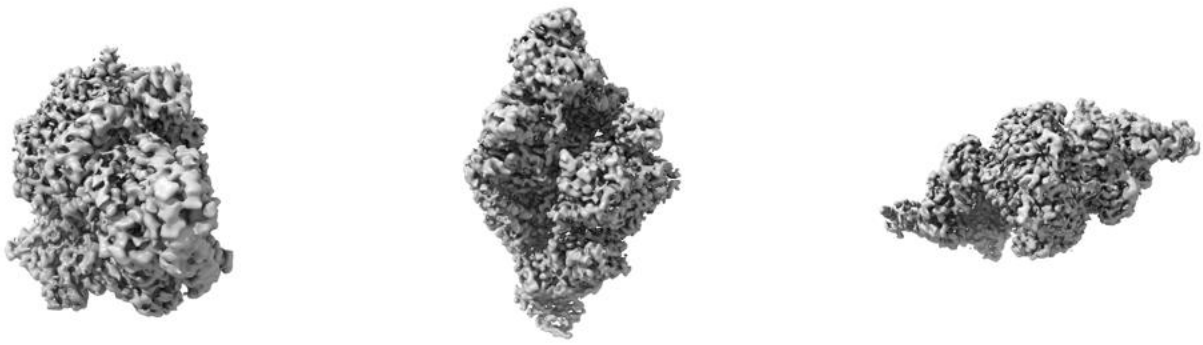


Z

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 0.055. 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.

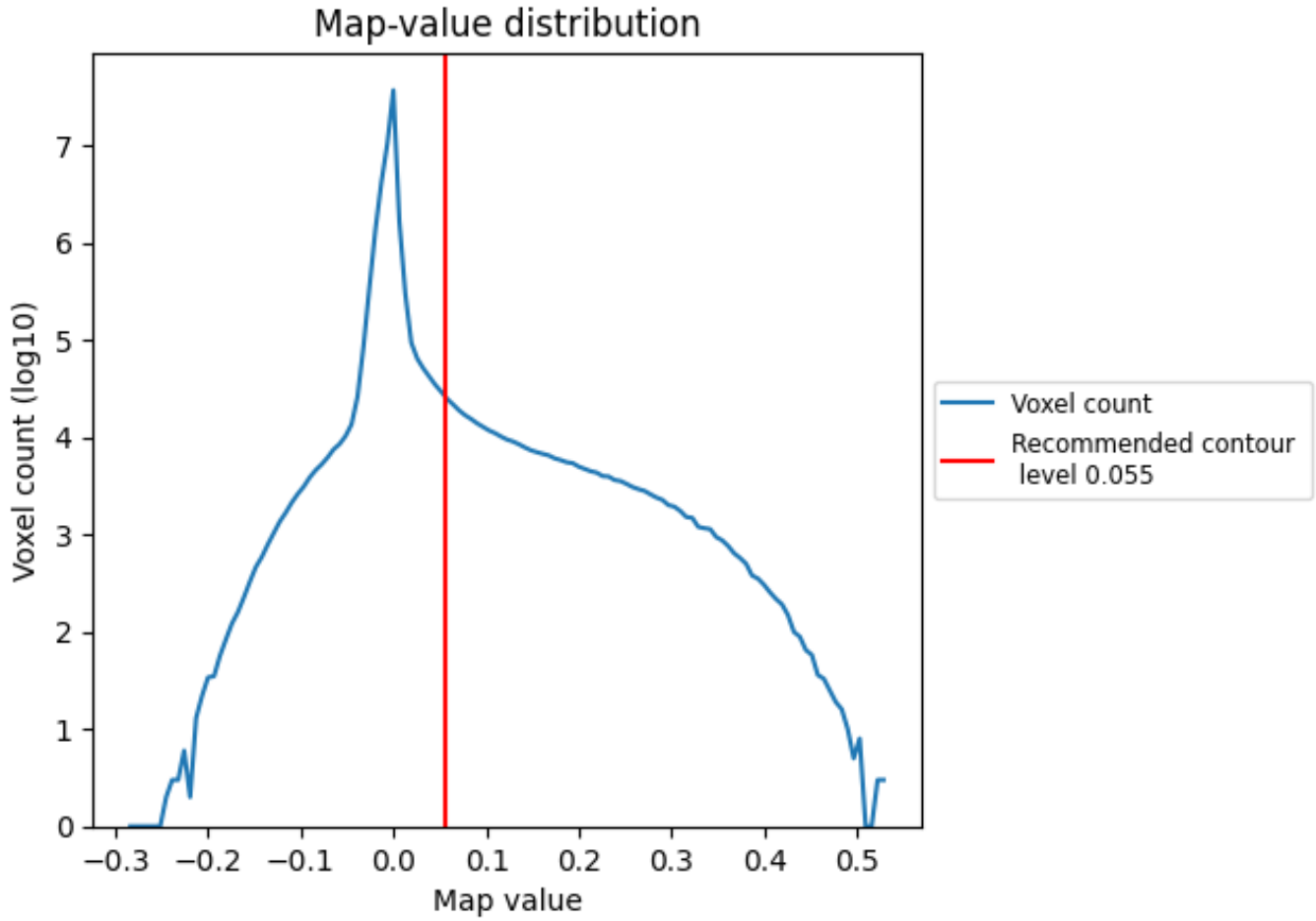
6.6 Mask visualisation (i)

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

7 Map analysis

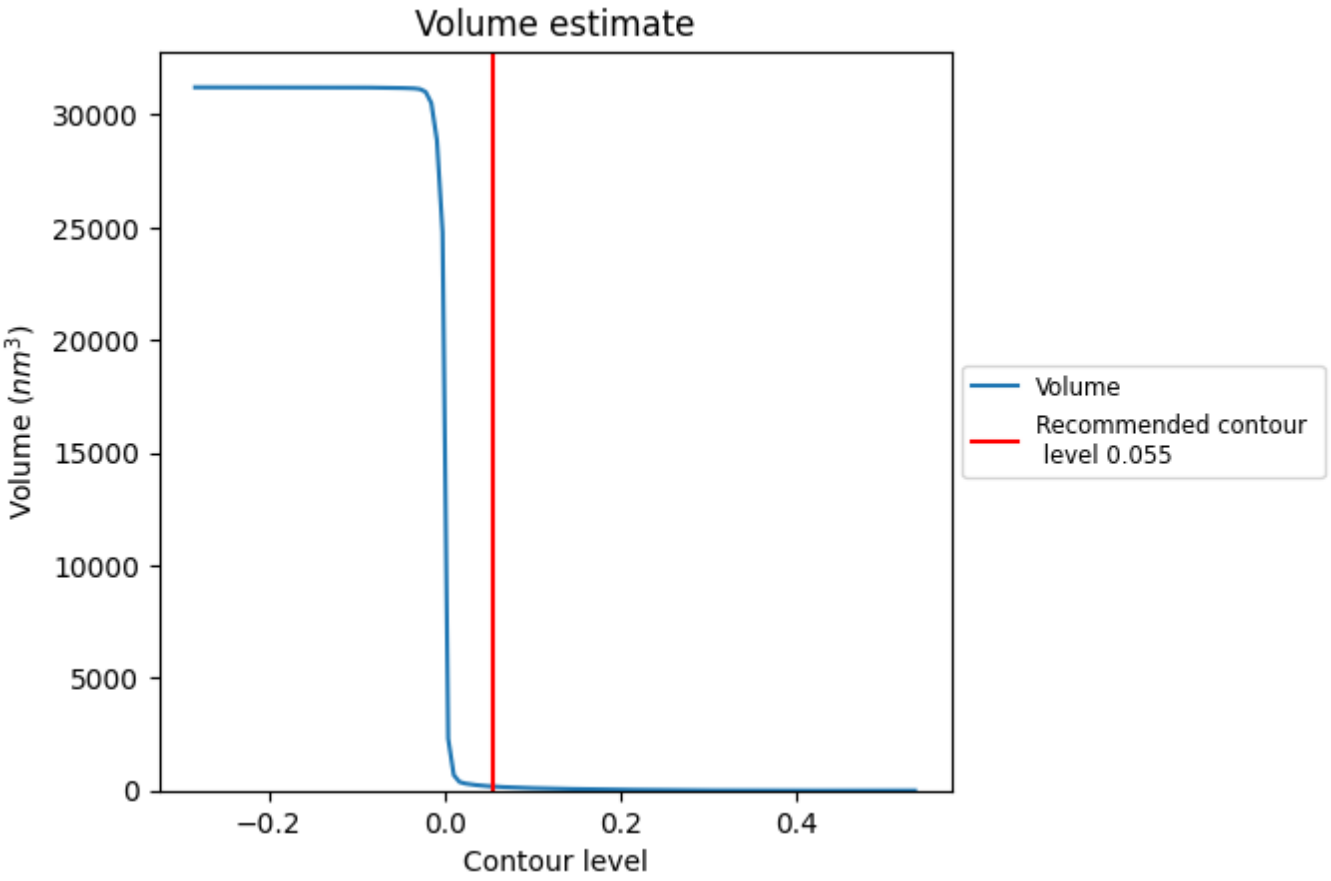
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

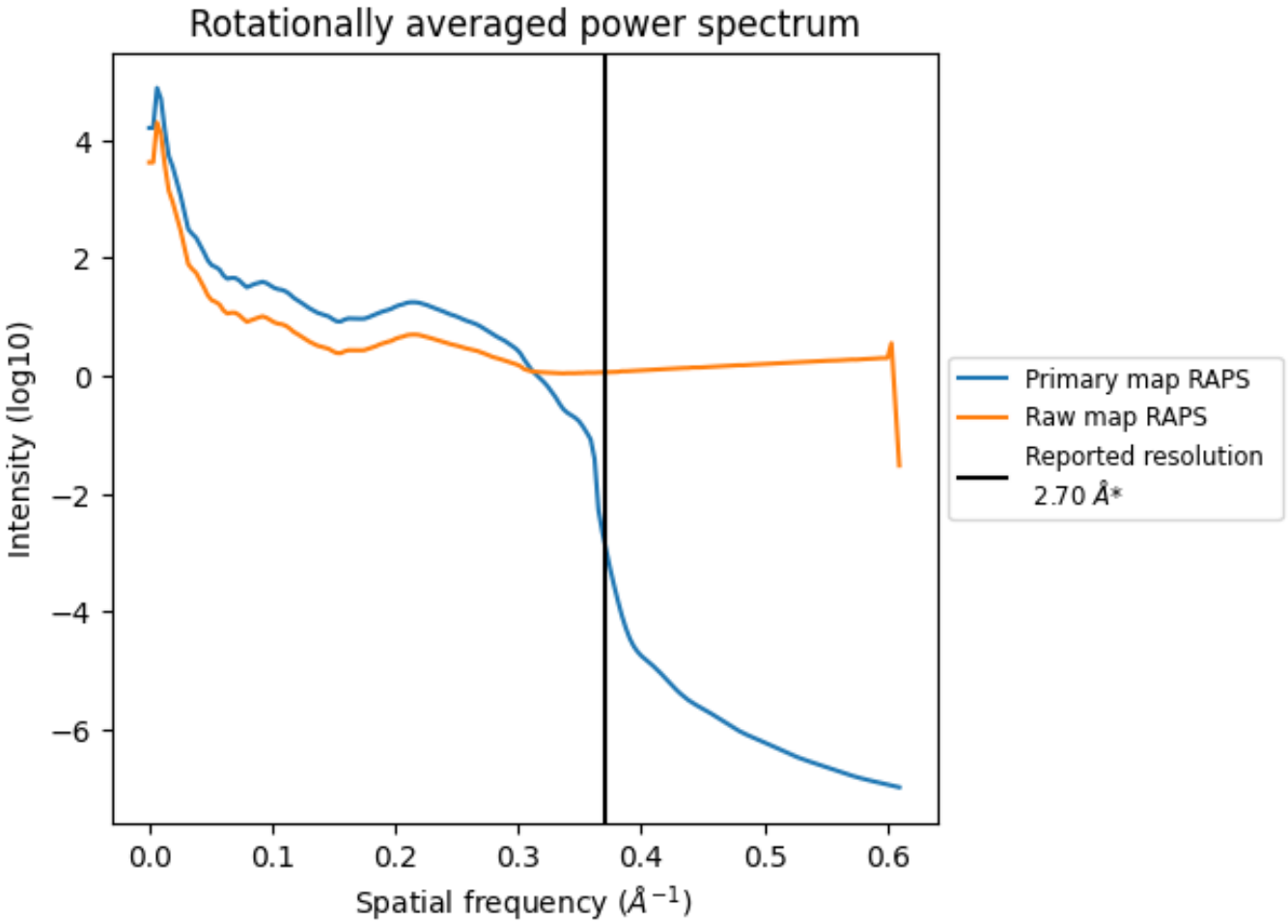
7.2 Volume estimate



The volume at the recommended contour level is 181 nm^3; this corresponds to an approximate mass of 163 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)

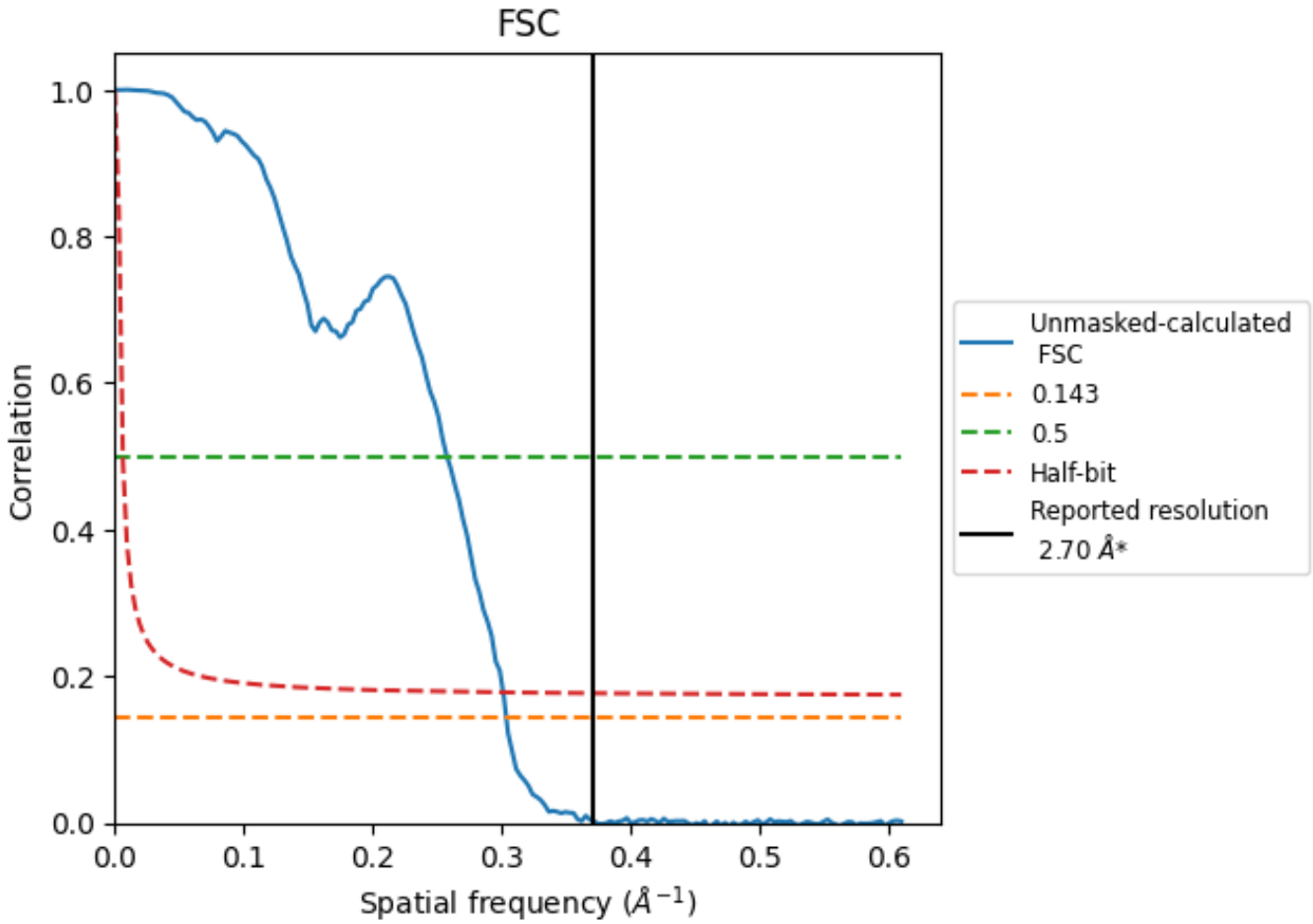


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

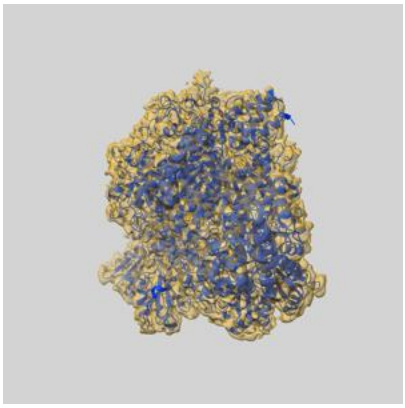
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.29	3.88	3.32

*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 3.29 differs from the reported value 2.7 by more than 10 %

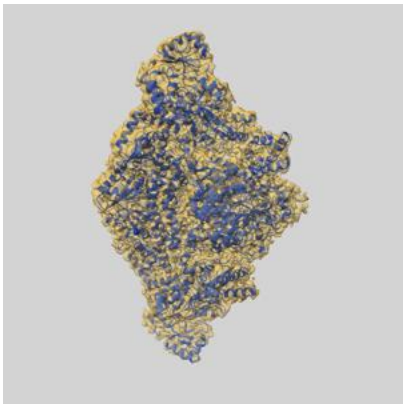
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16631 and PDB model 8CG5. Per-residue inclusion information can be found in section 3 on page 5.

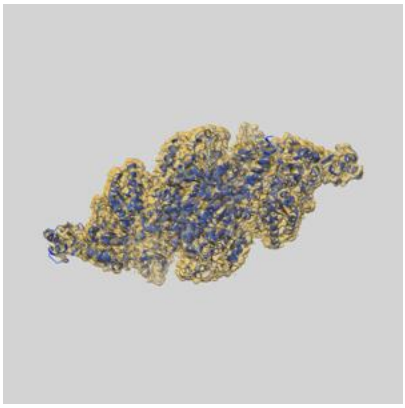
9.1 Map-model overlay



X



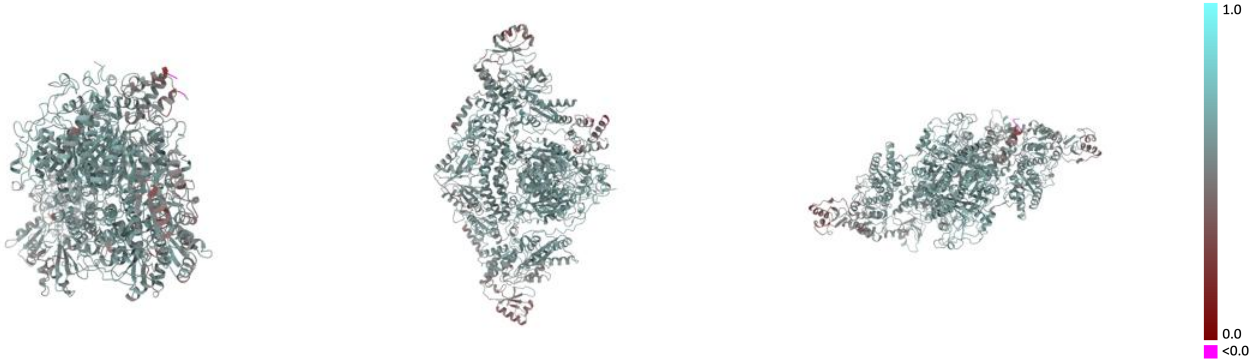
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.055 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.

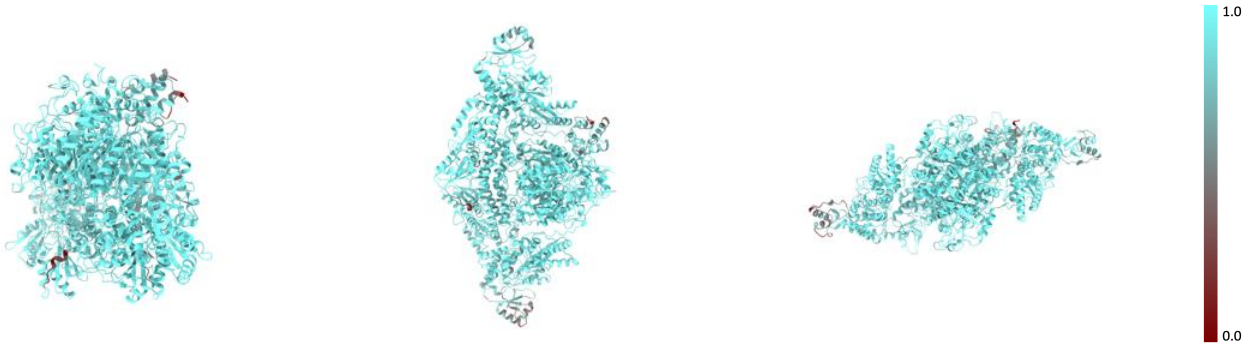
9.2 Q-score mapped to coordinate model (i)



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.

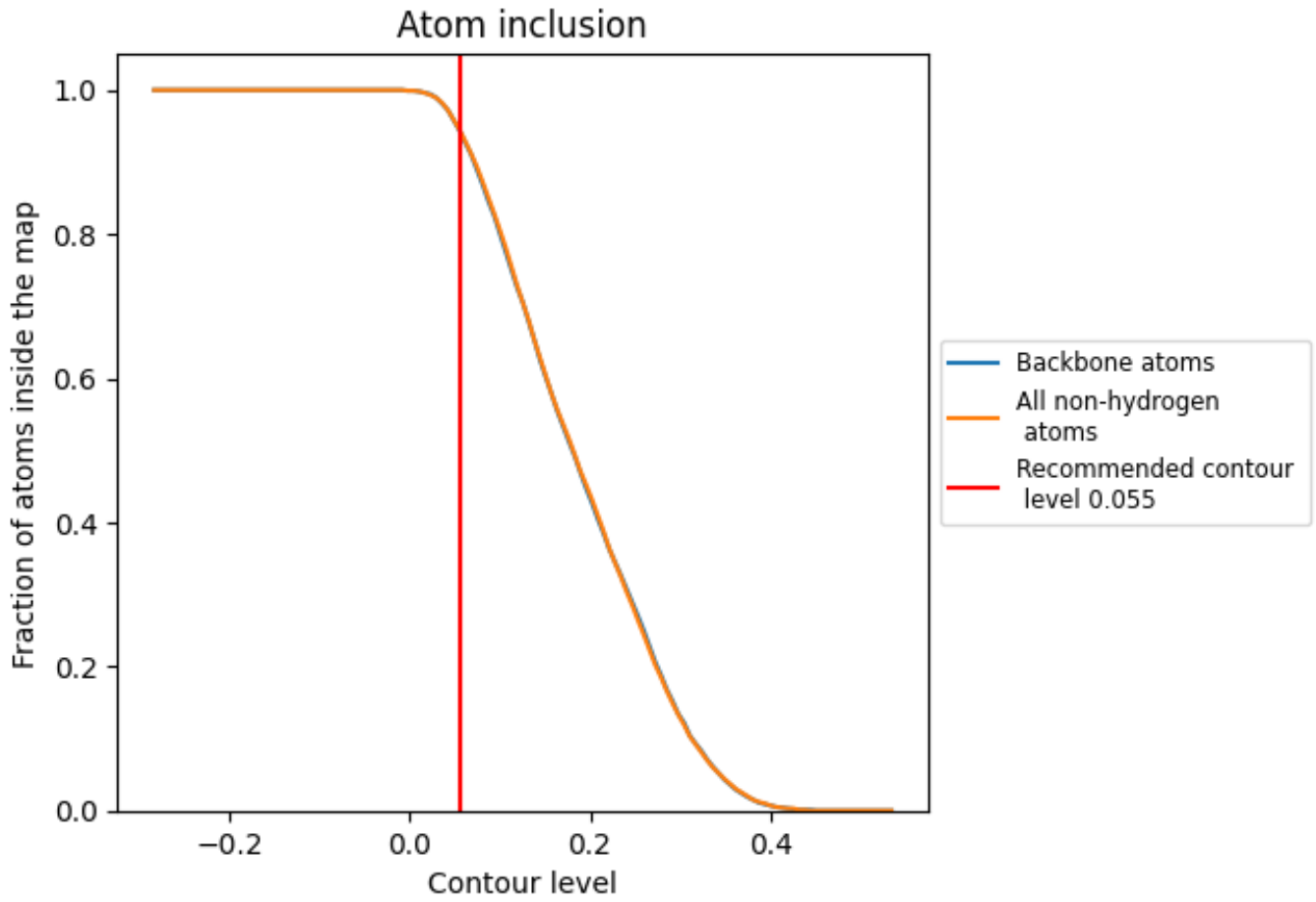
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.055).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9450	0.5620
A	0.9450	0.5630
B	0.9620	0.5690
C	0.7150	0.4420