



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 08:54 AM UTC

PDB ID : 8K9Q / pdb_00008k9q
EMDB ID : EMD-36995
Title : Cryo-EM structure of the GPI inositol-deacylase (PGAP1/Bst1) from *Chaetomium thermophilum*
Authors : Hong, J.; Li, T.; Qu, Q.; Li, D.
Deposited on : 2023-08-01
Resolution : 2.84 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

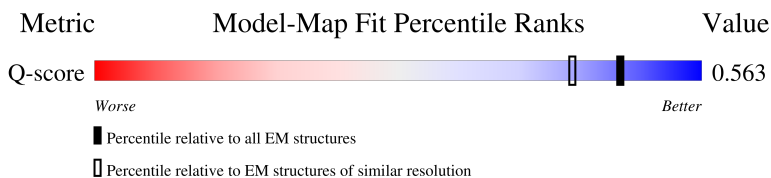
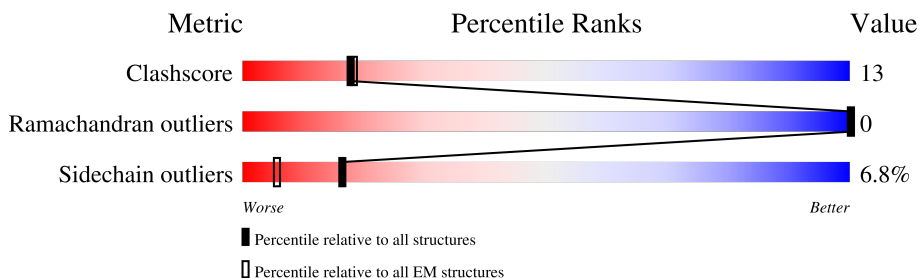
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

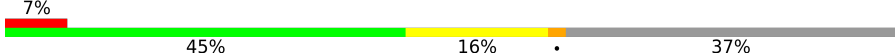
The reported resolution of this entry is 2.84 Å.

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	11884 (2.34 - 3.34)

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	1469	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7549 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.

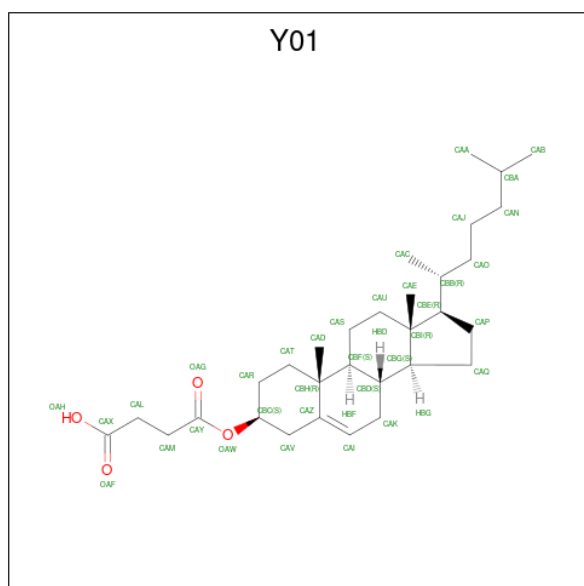
- Molecule 1 is a protein called GPI inositol-deacylase, fused thermostable green fluorescent protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	927	7340	4759	1238	1308	35	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP G0S652
A	0	GLY	-	expression tag	UNP G0S652
A	1	SER	-	expression tag	UNP G0S652

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (CCD ID: Y01) (formula: $C_{31}H_{50}O_4$).



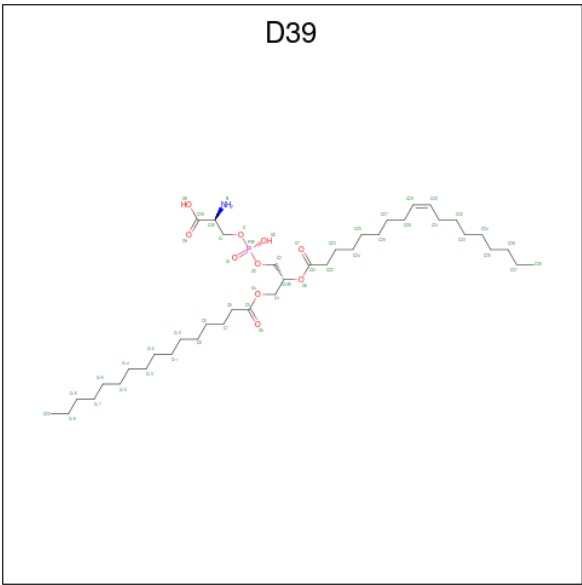
Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	C	O	0
			35	31	4	
2	A	1	Total	C	O	0
			35	31	4	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
2	A	1	35	31	4	0

- Molecule 3 is (2 {S})-2-azanyl-3-[[[(2 {R})-3-hexadecanoyloxy-2-[({Z})-octadec-9-enoyl]oxypropoxy]-oxidanyl-phosphoryl]oxy-propanoic acid (CCD ID: D39) (formula: C₄₀H₇₆NO₁₀P).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	52	40	1	10	1	0
3	A	1	52	40	1	10	1	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	407921	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 ($e^-/\text{\AA}^2$)	60.0	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.725	Depositor
Minimum map value	-2.930	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.173	Depositor
Recommended contour level	0.743	Depositor
Map size (Å)	232.96, 232.96, 232.96	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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: D39, Y01

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	1.10	19/7530 (0.3%)	1.39	36/10269 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	813	TYR	C-O	-8.49	1.14	1.24
1	A	742	GLN	C-O	-7.64	1.14	1.24
1	A	748	TYR	C-O	-7.43	1.14	1.23
1	A	765	GLY	C-O	-7.42	1.16	1.24
1	A	812	LEU	C-O	-7.25	1.15	1.24
1	A	281	HIS	C-O	-6.68	1.16	1.24
1	A	819	VAL	C-O	-6.60	1.16	1.24
1	A	824	PRO	C-O	-6.40	1.15	1.24
1	A	811	LYS	C-O	-6.05	1.16	1.24
1	A	820	PHE	C-O	-5.76	1.16	1.24
1	A	247	TYR	C-O	-5.75	1.17	1.24
1	A	815	ARG	C-O	-5.74	1.16	1.24
1	A	763	LEU	C-O	-5.65	1.16	1.23
1	A	236	GLN	C-O	-5.64	1.16	1.24
1	A	768	PRO	C-O	-5.50	1.16	1.24
1	A	743	TYR	C-O	-5.35	1.17	1.23
1	A	861	PRO	C-O	-5.19	1.17	1.24
1	A	844	SER	CA-CB	-5.11	1.46	1.53
1	A	764	HIS	C-O	-5.06	1.16	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1125	GLY	CA-C-N	-8.95	111.78	122.35
1	A	1125	GLY	C-N-CA	-8.95	111.78	122.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	508	ILE	N-CA-C	-7.47	105.92	113.47
1	A	252	LEU	N-CA-C	7.21	119.22	111.36
1	A	813	TYR	CA-C-O	-7.10	113.03	120.55
1	A	993	MET	N-CA-C	7.03	121.37	111.52
1	A	314	ASP	N-CA-C	-7.01	104.73	113.28
1	A	511	ASP	N-CA-C	-6.57	104.12	111.28
1	A	659	LYS	N-CA-C	-6.27	104.21	113.61
1	A	244	ALA	N-CA-C	-6.25	104.36	112.23
1	A	234	TYR	N-CA-C	-6.10	105.80	113.18
1	A	427	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	824	PRO	CB-CA-C	-6.02	102.83	111.62
1	A	1135	PHE	N-CA-C	-5.98	105.64	113.12
1	A	738	PRO	N-CA-CB	-5.95	98.02	103.31
1	A	223	PRO	N-CA-C	5.94	119.77	110.80
1	A	470	SER	N-CA-C	-5.85	101.38	110.10
1	A	300	LEU	N-CA-C	-5.83	105.27	112.38
1	A	768	PRO	N-CA-C	5.82	124.46	112.47
1	A	698	LEU	N-CA-C	-5.69	102.61	109.72
1	A	184	PRO	N-CA-C	5.69	121.04	111.32
1	A	463	ILE	N-CA-C	-5.68	107.59	113.10
1	A	636	PRO	CB-CA-C	5.63	117.79	110.92
1	A	820	PHE	CA-CB-CG	-5.51	108.29	113.80
1	A	191	ASP	N-CA-C	-5.37	105.43	111.28
1	A	273	PHE	N-CA-C	-5.34	105.21	112.26
1	A	757	ARG	N-CA-C	-5.30	99.50	110.80
1	A	304	LEU	N-CA-C	-5.29	106.50	113.17
1	A	426	GLY	N-CA-C	5.25	117.21	110.96
1	A	1092	PRO	N-CA-CB	-5.18	98.70	103.31
1	A	168	VAL	N-CA-C	-5.15	107.39	113.42
1	A	213	ILE	N-CA-C	-5.07	108.56	113.53
1	A	348	ASN	N-CA-C	-5.06	107.05	113.43
1	A	167	SER	N-CA-C	-5.06	107.14	113.72
1	A	330	GLY	N-CA-C	-5.06	108.39	114.66
1	A	305	ASP	CB-CA-C	-5.03	104.12	109.85

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	7340	0	7394	195	0
2	A	105	0	147	19	0
3	A	104	0	0	0	0
All	All	7549	0	7541	202	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 13.

All (202) 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:271:VAL:HG11	1:A:292:LEU:HD21	1.19	1.13
1:A:689:LEU:HD13	1:A:694:ILE:HG13	1.32	1.09
1:A:689:LEU:HD13	1:A:694:ILE:CG1	1.86	1.06
1:A:174:PRO:HB2	1:A:627:PHE:HZ	1.19	1.03
1:A:689:LEU:CD1	1:A:694:ILE:HG13	1.87	1.02
1:A:271:VAL:HG11	1:A:292:LEU:CD2	1.97	0.94
1:A:707:GLU:HG3	1:A:786:GLN:HG2	1.58	0.86
1:A:157:ILE:HD11	1:A:928:VAL:HG23	1.55	0.86
2:A:1503:Y01:HAE2	2:A:1503:Y01:HAC1	1.57	0.86
1:A:518:ALA:HB3	1:A:521:GLU:HG3	1.58	0.85
1:A:174:PRO:HB2	1:A:627:PHE:CZ	2.10	0.84
1:A:282:GLY:HA3	1:A:367:GLN:HB2	1.60	0.82
1:A:903:LEU:HD21	1:A:1123:VAL:HG22	1.63	0.80
1:A:518:ALA:HB3	1:A:521:GLU:CG	2.11	0.80
1:A:576:VAL:O	1:A:604:LEU:HD12	1.81	0.80
1:A:528:LEU:HD13	1:A:569:LEU:HD11	1.65	0.79
1:A:225:LEU:HD21	1:A:292:LEU:HD22	1.67	0.77
1:A:1060:VAL:HG12	1:A:1060:VAL:O	1.84	0.76
1:A:538:LEU:HD12	1:A:655:ALA:HB2	1.66	0.76
1:A:228:PRO:HD2	1:A:271:VAL:HG22	1.68	0.76
1:A:817:ARG:NE	2:A:1501:Y01:HAD3	2.01	0.75
1:A:689:LEU:HD13	1:A:694:ILE:CD1	2.16	0.74
1:A:277:ILE:CG2	1:A:280:PHE:HD2	2.01	0.74
1:A:568:LYS:C	1:A:569:LEU:HD12	2.12	0.73
1:A:1021:LEU:HD12	1:A:1026:ASN:ND2	2.04	0.72
1:A:278:THR:HG23	1:A:285:LEU:HB2	1.73	0.71
1:A:216:ASP:OD2	1:A:218:LYS:HB2	1.91	0.71
1:A:228:PRO:HD2	1:A:271:VAL:CG2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:727:LEU:O	1:A:727:LEU:HG	1.90	0.69
2:A:1503:Y01:CAN	2:A:1503:Y01:HAC3	2.23	0.69
1:A:168:VAL:HG23	1:A:169:THR:HG23	1.73	0.68
1:A:157:ILE:HD11	1:A:928:VAL:CG2	2.22	0.67
1:A:777:GLU:CD	1:A:778:PRO:HD2	2.19	0.67
1:A:724:ILE:CD1	1:A:740:VAL:HG21	2.25	0.67
1:A:727:LEU:HD23	1:A:738:PRO:HG3	1.76	0.66
1:A:1032:TYR:HB2	1:A:1090:MET:HE1	1.77	0.66
1:A:315:LEU:HD22	1:A:466:VAL:HG13	1.77	0.66
1:A:817:ARG:O	2:A:1501:Y01:CAE	2.44	0.65
1:A:987:LEU:HA	1:A:990:VAL:HG22	1.78	0.65
1:A:727:LEU:CD2	1:A:738:PRO:HG3	2.27	0.65
1:A:990:VAL:HA	1:A:994:ILE:HD11	1.78	0.64
1:A:990:VAL:HG21	1:A:1079:ILE:CD1	2.27	0.64
1:A:768:PRO:CD	1:A:815:ARG:HG2	2.27	0.64
1:A:1009:GLY:HA3	2:A:1503:Y01:HAD2	1.80	0.63
1:A:817:ARG:O	2:A:1501:Y01:HAE1	1.97	0.63
1:A:516:ILE:HG12	1:A:538:LEU:HD23	1.81	0.63
1:A:746:GLU:OE2	1:A:773:PRO:HB3	1.99	0.63
1:A:222:VAL:HG13	1:A:471:GLN:HB3	1.82	0.62
1:A:817:ARG:CD	2:A:1501:Y01:HAD3	2.30	0.62
1:A:1009:GLY:HA2	2:A:1503:Y01:HAT2	1.82	0.61
1:A:336:MET:HE2	1:A:347:ILE:HD11	1.82	0.61
1:A:1000:TYR:HB2	1:A:1075:ILE:HD11	1.82	0.61
1:A:1091:ILE:HD12	1:A:1143:LEU:HD22	1.82	0.61
1:A:525:LEU:O	1:A:667:PHE:HA	2.01	0.61
2:A:1503:Y01:HAC3	2:A:1503:Y01:HAN2	1.82	0.60
1:A:308:VAL:HG12	1:A:308:VAL:O	2.02	0.60
1:A:716:SER:OG	1:A:815:ARG:NH2	2.34	0.60
1:A:768:PRO:HD2	1:A:815:ARG:HG2	1.84	0.59
1:A:1094:THR:HB	1:A:1106:LEU:HD23	1.83	0.59
1:A:550:LYS:HE2	1:A:672:PHE:HB3	1.83	0.59
1:A:724:ILE:HD12	1:A:740:VAL:HG21	1.85	0.59
1:A:689:LEU:HD13	1:A:694:ILE:HD11	1.84	0.59
1:A:817:ARG:NE	2:A:1501:Y01:CAD	2.66	0.59
1:A:836:PHE:HE1	1:A:1091:ILE:HD13	1.66	0.59
1:A:417:ILE:HD12	1:A:421:VAL:HG21	1.84	0.58
1:A:725:SER:OG	1:A:797:ILE:HG13	2.02	0.58
1:A:271:VAL:CG1	1:A:292:LEU:HD21	2.13	0.58
1:A:694:ILE:HD13	1:A:710:ILE:HD12	1.84	0.58
1:A:674:ASP:HB3	1:A:677:ASN:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:LEU:O	1:A:464:VAL:HG13	2.03	0.58
1:A:517:THR:HG22	1:A:518:ALA:N	2.19	0.57
1:A:572:MET:HG2	1:A:608:ASN:HA	1.87	0.57
1:A:417:ILE:HG13	1:A:421:VAL:CG2	2.35	0.56
1:A:820:PHE:HE2	1:A:921:ILE:HG22	1.69	0.56
1:A:835:GLN:NE2	1:A:846:ILE:O	2.37	0.56
1:A:1021:LEU:CD1	1:A:1026:ASN:ND2	2.68	0.56
1:A:278:THR:CG2	1:A:285:LEU:HB2	2.35	0.56
1:A:517:THR:HG22	1:A:518:ALA:H	1.71	0.56
1:A:817:ARG:HD2	2:A:1501:Y01:HAD3	1.88	0.56
1:A:332:VAL:O	1:A:336:MET:HG3	2.05	0.55
1:A:856:LEU:HD11	1:A:923:VAL:HG11	1.88	0.55
1:A:417:ILE:HG13	1:A:421:VAL:HG22	1.89	0.55
1:A:222:VAL:HG22	1:A:471:GLN:HG2	1.89	0.54
1:A:277:ILE:HG21	1:A:280:PHE:HD2	1.73	0.54
1:A:266:LEU:HD21	1:A:464:VAL:HG11	1.88	0.54
1:A:430:PHE:CG	1:A:749:GLU:HG3	2.42	0.54
2:A:1503:Y01:CAN	2:A:1503:Y01:CAC	2.86	0.54
1:A:774:MET:O	1:A:774:MET:HG2	2.08	0.54
1:A:176:GLY:HA3	1:A:627:PHE:CD1	2.43	0.54
1:A:554:LEU:HD12	1:A:670:ALA:HB2	1.89	0.54
1:A:518:ALA:HB3	1:A:521:GLU:HG2	1.86	0.53
1:A:824:PRO:O	1:A:828:VAL:HG23	2.07	0.53
1:A:230:ASN:HD21	1:A:277:ILE:HG23	1.73	0.53
1:A:411:PRO:HD3	1:A:817:ARG:NH2	2.24	0.53
1:A:990:VAL:HG21	1:A:1079:ILE:HD12	1.90	0.53
1:A:563:PRO:HD3	1:A:608:ASN:HD22	1.73	0.53
1:A:689:LEU:CD1	1:A:694:ILE:CD1	2.86	0.53
1:A:362:VAL:HG13	1:A:364:PHE:H	1.74	0.52
1:A:570:GLU:HB2	1:A:659:LYS:HE3	1.91	0.52
1:A:699:PRO:O	1:A:702:ARG:HB3	2.09	0.52
1:A:311:ARG:HH12	1:A:317:ASP:HA	1.74	0.52
1:A:1080:LEU:O	1:A:1084:THR:HG23	2.10	0.51
1:A:777:GLU:HG2	1:A:780:ALA:HB3	1.93	0.51
1:A:408:THR:HG23	1:A:814:MET:HE1	1.92	0.51
1:A:219:VAL:HG22	1:A:308:VAL:O	2.10	0.51
1:A:429:VAL:CG2	1:A:433:THR:CG2	2.90	0.50
1:A:528:LEU:HD13	1:A:569:LEU:CD1	2.39	0.50
1:A:852:LEU:HD21	1:A:923:VAL:HG13	1.94	0.50
1:A:216:ASP:CG	1:A:218:LYS:HB2	2.37	0.49
1:A:696:LEU:HD23	1:A:708:VAL:HG21	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ARG:HH12	1:A:796:SER:HA	1.78	0.49
1:A:1021:LEU:CD1	1:A:1026:ASN:HD21	2.25	0.49
1:A:324:LEU:HD22	1:A:351:ILE:HB	1.95	0.49
1:A:777:GLU:HG2	1:A:780:ALA:O	2.13	0.49
1:A:817:ARG:O	2:A:1501:Y01:HAE3	2.13	0.49
1:A:248:PHE:HA	1:A:252:LEU:HB2	1.95	0.49
1:A:216:ASP:O	1:A:216:ASP:OD1	2.30	0.48
1:A:299:ILE:C	1:A:301:SER:N	2.71	0.48
1:A:720:TYR:HB3	1:A:802:THR:O	2.13	0.48
1:A:817:ARG:HE	2:A:1501:Y01:CAD	2.26	0.48
1:A:438:TRP:O	1:A:627:PHE:HD2	1.96	0.48
1:A:239:PRO:HG2	1:A:448:TRP:HA	1.96	0.48
1:A:282:GLY:HA2	1:A:368:ILE:HG12	1.95	0.48
1:A:1094:THR:HB	1:A:1106:LEU:CD2	2.43	0.47
1:A:1060:VAL:O	1:A:1060:VAL:CG1	2.54	0.47
1:A:429:VAL:HG23	1:A:433:THR:HG21	1.96	0.47
1:A:466:VAL:HA	1:A:471:GLN:HG3	1.96	0.47
1:A:554:LEU:HD22	1:A:641:LEU:HD12	1.96	0.47
1:A:903:LEU:CD2	1:A:1123:VAL:HG22	2.39	0.47
1:A:277:ILE:HG21	1:A:280:PHE:CD2	2.49	0.47
1:A:768:PRO:HG2	1:A:815:ARG:HG2	1.96	0.47
1:A:417:ILE:CD1	1:A:421:VAL:HG21	2.45	0.47
1:A:987:LEU:CA	1:A:990:VAL:HG22	2.45	0.47
1:A:1009:GLY:CA	2:A:1503:Y01:HAD2	2.42	0.47
1:A:568:LYS:O	1:A:569:LEU:HD12	2.15	0.47
1:A:277:ILE:HG22	1:A:280:PHE:HD2	1.77	0.47
1:A:763:LEU:HD22	1:A:783:LEU:HD22	1.96	0.46
1:A:817:ARG:HE	2:A:1501:Y01:HAD3	1.77	0.46
1:A:1050:THR:HG22	1:A:1050:THR:O	2.15	0.46
1:A:727:LEU:HD23	1:A:738:PRO:CG	2.45	0.46
1:A:163:VAL:HG12	1:A:813:TYR:HB2	1.96	0.46
1:A:431:THR:HG23	1:A:439:THR:O	2.14	0.46
1:A:675:HIS:ND1	1:A:675:HIS:C	2.72	0.46
1:A:450:ASP:O	1:A:454:LYS:HG3	2.15	0.46
1:A:786:GLN:HE21	1:A:786:GLN:HB3	1.52	0.45
1:A:820:PHE:CD1	1:A:820:PHE:N	2.84	0.45
1:A:825:LEU:HD23	1:A:825:LEU:HA	1.75	0.45
1:A:277:ILE:CG2	1:A:280:PHE:CD2	2.91	0.45
1:A:571:VAL:O	1:A:609:VAL:HG22	2.15	0.45
1:A:176:GLY:HA2	1:A:629:VAL:HG22	1.98	0.45
1:A:271:VAL:HG21	1:A:273:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LEU:HD21	1:A:668:VAL:CG2	2.47	0.45
1:A:538:LEU:CD1	1:A:655:ALA:HB2	2.40	0.44
1:A:185:SER:HB3	1:A:209:ARG:O	2.17	0.44
1:A:240:ILE:H	1:A:240:ILE:HG13	1.55	0.44
1:A:689:LEU:CD1	1:A:694:ILE:CG1	2.64	0.44
1:A:348:ASN:O	1:A:396:VAL:HA	2.16	0.44
1:A:630:ARG:HE	1:A:630:ARG:HB3	1.58	0.44
1:A:1058:LEU:HD12	1:A:1058:LEU:HA	1.78	0.44
2:A:1502:Y01:HAP1	2:A:1502:Y01:HAO2	1.42	0.43
1:A:768:PRO:CG	1:A:815:ARG:HG2	2.48	0.43
1:A:157:ILE:CD1	1:A:928:VAL:CG2	2.95	0.43
1:A:431:THR:OG1	1:A:441:MET:HE2	2.18	0.43
1:A:460:LEU:HA	1:A:463:ILE:HG12	2.00	0.43
1:A:556:THR:HG21	1:A:560:LEU:HD21	1.99	0.43
1:A:345:ASN:HD22	1:A:345:ASN:HA	1.64	0.43
1:A:724:ILE:CG2	1:A:797:ILE:HD11	2.49	0.43
1:A:768:PRO:HD2	1:A:815:ARG:CG	2.48	0.43
1:A:328:MET:HE3	1:A:328:MET:HB3	1.82	0.43
1:A:191:ASP:HB2	1:A:298:TYR:OH	2.19	0.43
1:A:302:LEU:HG	1:A:308:VAL:HG11	2.00	0.43
1:A:139:TRP:CG	1:A:1022:ARG:HH21	2.37	0.42
1:A:507:LEU:HD12	1:A:507:LEU:HA	1.69	0.42
1:A:684:ILE:HG13	1:A:688:ASN:HB2	2.01	0.42
1:A:553:THR:HG22	1:A:642:GLU:HG3	2.00	0.42
1:A:836:PHE:CE1	1:A:1091:ILE:HD13	2.51	0.42
1:A:569:LEU:CD2	1:A:668:VAL:CG2	2.97	0.42
1:A:864:LEU:HD11	1:A:919:GLY:HA3	2.01	0.42
1:A:372:TYR:O	1:A:376:ASN:HB2	2.20	0.42
1:A:774:MET:O	1:A:774:MET:CG	2.66	0.42
1:A:903:LEU:HD23	1:A:1123:VAL:HA	2.02	0.42
1:A:1079:ILE:HD13	1:A:1079:ILE:HA	1.98	0.42
2:A:1503:Y01:HAA2	2:A:1503:Y01:HAJ1	1.90	0.42
1:A:315:LEU:HD13	1:A:466:VAL:HG21	2.02	0.42
1:A:610:ALA:O	1:A:613:VAL:HG23	2.20	0.42
1:A:538:LEU:HG	1:A:653:PHE:HB3	2.01	0.42
1:A:714:LYS:O	1:A:765:GLY:HA3	2.20	0.42
1:A:944:ILE:HD13	1:A:944:ILE:HA	1.94	0.42
1:A:450:ASP:HA	1:A:453:ARG:HD3	2.01	0.42
1:A:1044:LEU:HD23	1:A:1044:LEU:HA	1.93	0.42
1:A:411:PRO:HD3	1:A:817:ARG:HH22	1.86	0.41
1:A:1011:LEU:HD21	1:A:1034:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ARG:HE	1:A:183:ARG:HB3	1.65	0.41
1:A:435:PRO:O	1:A:436:ASN:HB2	2.20	0.41
1:A:342:TYR:HE1	1:A:347:ILE:HD12	1.86	0.41
1:A:1076:MET:HE2	1:A:1076:MET:HB2	1.65	0.41
1:A:163:VAL:O	1:A:167:SER:HB3	2.21	0.41
1:A:702:ARG:HA	1:A:703:PRO:HD3	1.96	0.40
1:A:813:TYR:CD1	1:A:813:TYR:O	2.74	0.40
1:A:271:VAL:HG23	1:A:271:VAL:O	2.20	0.40
2:A:1502:Y01:HAE2	2:A:1502:Y01:HBB	1.90	0.40
1:A:508:ILE:O	1:A:508:ILE:HG22	2.21	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	915/1469 (62%)	897 (98%)	18 (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	819/1257 (65%)	763 (93%)	56 (7%)	14	31

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	TRP
1	A	154	LEU
1	A	183	ARG
1	A	190	SER
1	A	207	LEU
1	A	235	LYS
1	A	240	ILE
1	A	259	LEU
1	A	285	LEU
1	A	290	GLU
1	A	296	ILE
1	A	302	LEU
1	A	309	SER
1	A	310	GLU
1	A	311	ARG
1	A	312	ASP
1	A	327	SER
1	A	338	ILE
1	A	359	ARG
1	A	362	VAL
1	A	373	LYS
1	A	397	THR
1	A	409	VAL
1	A	444	GLN
1	A	449	CYS
1	A	457	ILE
1	A	471	GLN
1	A	472	THR
1	A	477	GLN
1	A	496	LYS
1	A	506	LEU
1	A	509	VAL
1	A	539	MET
1	A	561	ASP
1	A	621	ARG
1	A	629	VAL
1	A	690	LEU
1	A	710	ILE
1	A	750	SER
1	A	763	LEU
1	A	809	LEU
1	A	811	LYS

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Mol	Chain	Res	Type
1	A	814	MET
1	A	819	VAL
1	A	825	LEU
1	A	826	PHE
1	A	827	ILE
1	A	829	SER
1	A	832	LEU
1	A	915	ILE
1	A	927	THR
1	A	1001	LEU
1	A	1056	HIS
1	A	1075	ILE
1	A	1076	MET
1	A	1078	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	236	GLN
1	A	274	ASN
1	A	344	HIS
1	A	385	GLN
1	A	537	HIS
1	A	566	ASN
1	A	608	ASN
1	A	675	HIS
1	A	677	ASN
1	A	688	ASN
1	A	786	GLN
1	A	837	GLN
1	A	1007	GLN
1	A	1026	ASN
1	A	1047	ASN
1	A	1057	ASN
1	A	1069	HIS
1	A	1134	GLN

5.3.3 RNA ⓘ

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](#)

5 ligands 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	$\# Z > 2$
2	Y01	A	1501	-	38,38,38	0.52	0	57,57,57	0.55	0
2	Y01	A	1502	-	38,38,38	0.58	0	57,57,57	1.27	6 (10%)
3	D39	A	1504	-	50,51,51	0.41	0	52,58,58	0.42	0
3	D39	A	1505	-	50,51,51	0.53	0	52,58,58	0.40	0
2	Y01	A	1503	-	38,38,38	0.45	0	57,57,57	0.44	0

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
2	Y01	A	1501	-	-	13/19/77/77	0/4/4/4
2	Y01	A	1502	-	-	13/19/77/77	0/4/4/4
3	D39	A	1504	-	-	26/57/57/57	-
3	D39	A	1505	-	-	38/57/57/57	-
2	Y01	A	1503	-	-	11/19/77/77	0/4/4/4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1502	Y01	CAQ-CBG-CBI	3.11	107.50	103.84
2	A	1502	Y01	CAU-CBI-CBG	-2.96	102.81	107.25
2	A	1502	Y01	CBG-CBI-CBE	2.95	103.48	100.10
2	A	1502	Y01	CAP-CAQ-CBG	-2.68	99.90	105.14
2	A	1502	Y01	CBF-CBD-CBG	-2.68	105.59	109.09
2	A	1502	Y01	CAE-CBI-CAU	-2.04	107.60	110.61

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	Y01	OAG-CAY-OAW-CBC
2	A	1502	Y01	CAO-CBB-CBE-CBI
2	A	1502	Y01	CAC-CBB-CBE-CBI
2	A	1503	Y01	CAM-CAY-OAW-CBC
3	A	1504	D39	C2-O3-P-O
3	A	1504	D39	C2-O3-P-O1
3	A	1504	D39	O6-C3-C4-O4
3	A	1504	D39	C22-C21-O6-C3
3	A	1504	D39	N-C-C1-O
3	A	1504	D39	C39-C-C1-O
3	A	1505	D39	C2-O3-P-O
3	A	1505	D39	C2-O3-P-O1
3	A	1505	D39	C2-O3-P-O2
3	A	1505	D39	N-C-C1-O
3	A	1505	D39	C39-C-C1-O
3	A	1505	D39	C1-C-C39-O8
3	A	1505	D39	C1-C-C39-O9
2	A	1502	Y01	CAV-CBC-OAW-CAY
2	A	1503	Y01	CAV-CBC-OAW-CAY
2	A	1502	Y01	CAC-CBB-CBE-CAP
2	A	1502	Y01	CAO-CBB-CBE-CAP
2	A	1503	Y01	OAG-CAY-OAW-CBC
3	A	1504	D39	O7-C21-O6-C3
2	A	1501	Y01	CAM-CAY-OAW-CBC
2	A	1503	Y01	CAJ-CAO-CBB-CAC
2	A	1503	Y01	CAC-CBB-CBE-CBI
3	A	1504	D39	C30-C31-C32-C33
3	A	1504	D39	C28-C29-C30-C31
2	A	1503	Y01	CAJ-CAO-CBB-CBE
2	A	1501	Y01	CAR-CBC-OAW-CAY
2	A	1503	Y01	CAO-CBB-CBE-CAP
2	A	1502	Y01	CAJ-CAO-CBB-CAC

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Mol	Chain	Res	Type	Atoms
2	A	1501	Y01	CAJ-CAO-CBB-CBE
2	A	1501	Y01	CAJ-CAO-CBB-CAC
3	A	1505	D39	C24-C25-C26-C27
2	A	1502	Y01	CAJ-CAO-CBB-CBE
2	A	1502	Y01	CAX-CAL-CAM-CAY
2	A	1502	Y01	OAG-CAY-OAW-CBC
3	A	1505	D39	C32-C33-C34-C35
2	A	1501	Y01	CAO-CAJ-CAN-CBA
2	A	1503	Y01	CAO-CAJ-CAN-CBA
2	A	1501	Y01	CAN-CAJ-CAO-CBB
2	A	1503	Y01	CAX-CAL-CAM-CAY
2	A	1502	Y01	CAM-CAY-OAW-CBC
2	A	1501	Y01	CAV-CBC-OAW-CAY
2	A	1501	Y01	CAX-CAL-CAM-CAY
3	A	1505	D39	C5-C6-C7-C8
2	A	1501	Y01	CAJ-CAN-CBA-CAA
3	A	1504	D39	C23-C24-C25-C26
2	A	1502	Y01	CAO-CAJ-CAN-CBA
3	A	1504	D39	C34-C35-C36-C37
2	A	1502	Y01	CAJ-CAN-CBA-CAA
3	A	1504	D39	C10-C11-C12-C13
2	A	1503	Y01	CAC-CBB-CBE-CAP
3	A	1505	D39	C22-C21-O6-C3
3	A	1504	D39	C17-C18-C19-C20
3	A	1505	D39	C33-C34-C35-C36
3	A	1505	D39	C25-C26-C27-C28
3	A	1504	D39	O3-C2-C3-O6
3	A	1505	D39	C3-C2-O3-P
3	A	1505	D39	O7-C21-O6-C3
3	A	1505	D39	C35-C36-C37-C38
2	A	1501	Y01	CAJ-CAN-CBA-CAB
3	A	1505	D39	C31-C32-C33-C34
3	A	1505	D39	C6-C5-O4-C4
3	A	1504	D39	C2-C3-C4-O4
3	A	1505	D39	C16-C17-C18-C19
3	A	1505	D39	O5-C5-O4-C4
3	A	1504	D39	C6-C5-O4-C4
3	A	1505	D39	C6-C7-C8-C9
3	A	1505	D39	C9-C10-C11-C12
3	A	1505	D39	C30-C31-C32-C33
3	A	1504	D39	O3-C2-C3-C4
2	A	1503	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
3	A	1505	D39	O3-C2-C3-O6
3	A	1505	D39	C26-C27-C28-C29
3	A	1505	D39	C13-C14-C15-C16
3	A	1504	D39	C12-C13-C14-C15
2	A	1502	Y01	CAJ-CAN-CBA-CAB
3	A	1505	D39	C11-C12-C13-C14
3	A	1505	D39	O3-C2-C3-C4
3	A	1505	D39	C23-C24-C25-C26
3	A	1504	D39	O5-C5-O4-C4
3	A	1505	D39	N-C-C39-O8
3	A	1505	D39	C15-C16-C17-C18
3	A	1504	D39	C16-C17-C18-C19
3	A	1505	D39	C12-C13-C14-C15
2	A	1501	Y01	CAM-CAL-CAX-OAH
3	A	1505	D39	N-C-C39-O9
2	A	1501	Y01	CAM-CAL-CAX-OAF
3	A	1504	D39	C27-C28-C29-C30
3	A	1504	D39	C33-C34-C35-C36
3	A	1505	D39	C17-C18-C19-C20
3	A	1504	D39	C6-C7-C8-C9
3	A	1504	D39	C11-C12-C13-C14
3	A	1505	D39	C29-C30-C31-C32
3	A	1504	D39	C29-C30-C31-C32
3	A	1505	D39	O4-C5-C6-C7
3	A	1505	D39	C7-C8-C9-C10
3	A	1504	D39	C22-C23-C24-C25
3	A	1505	D39	O5-C5-C6-C7

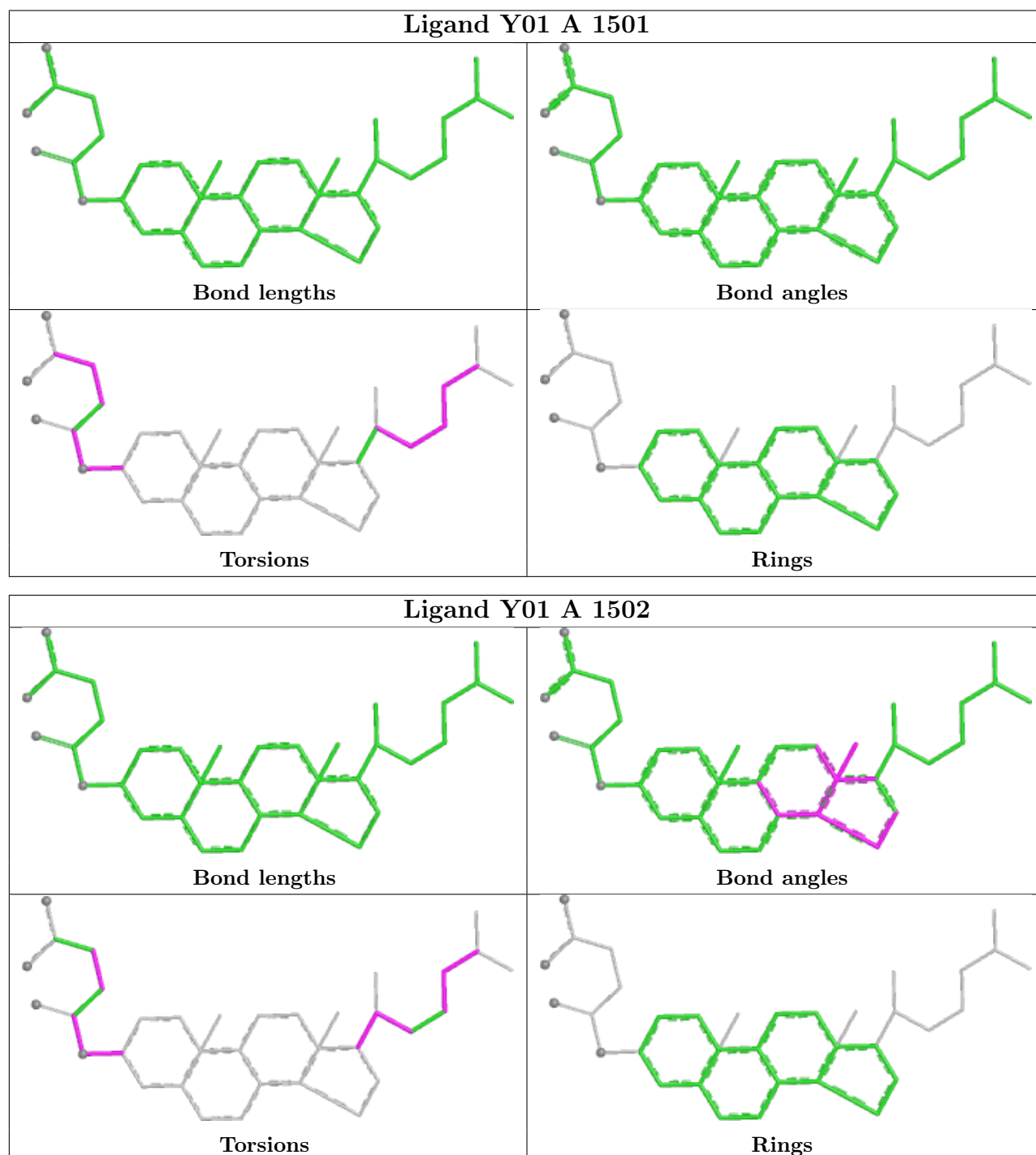
There are no ring outliers.

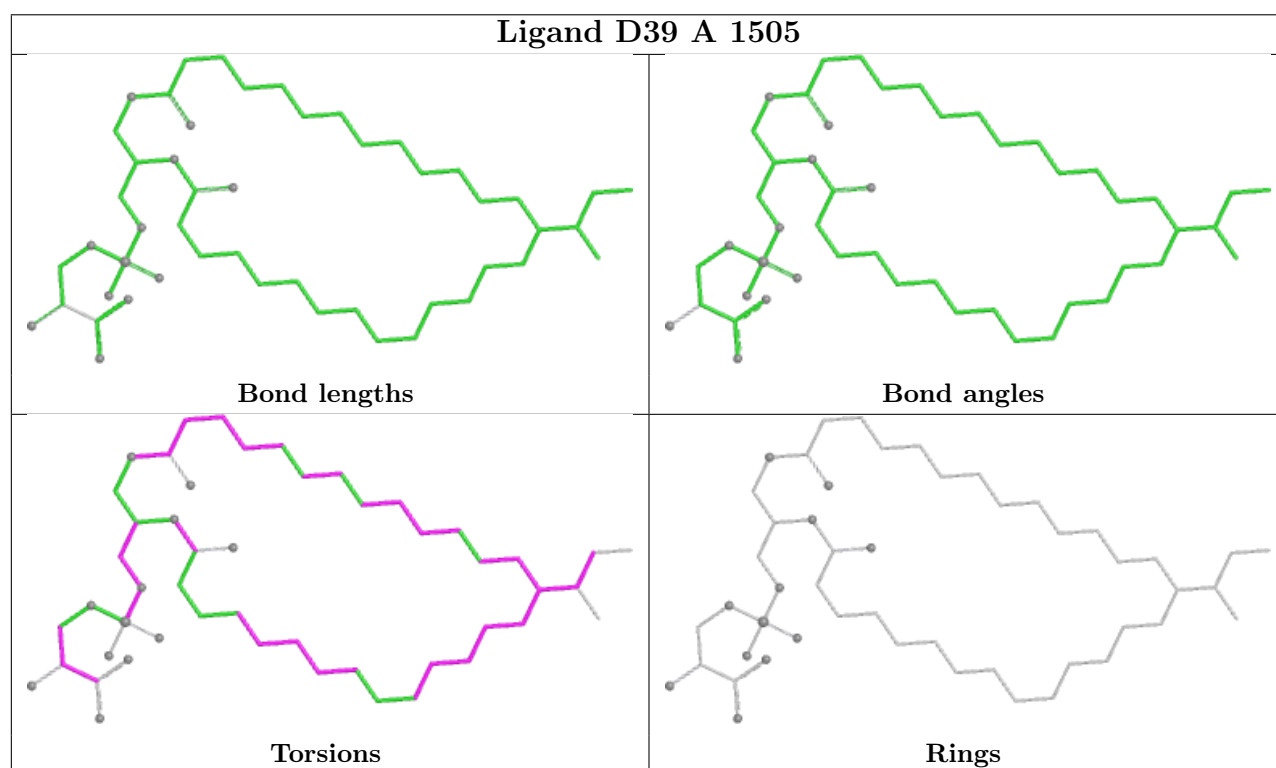
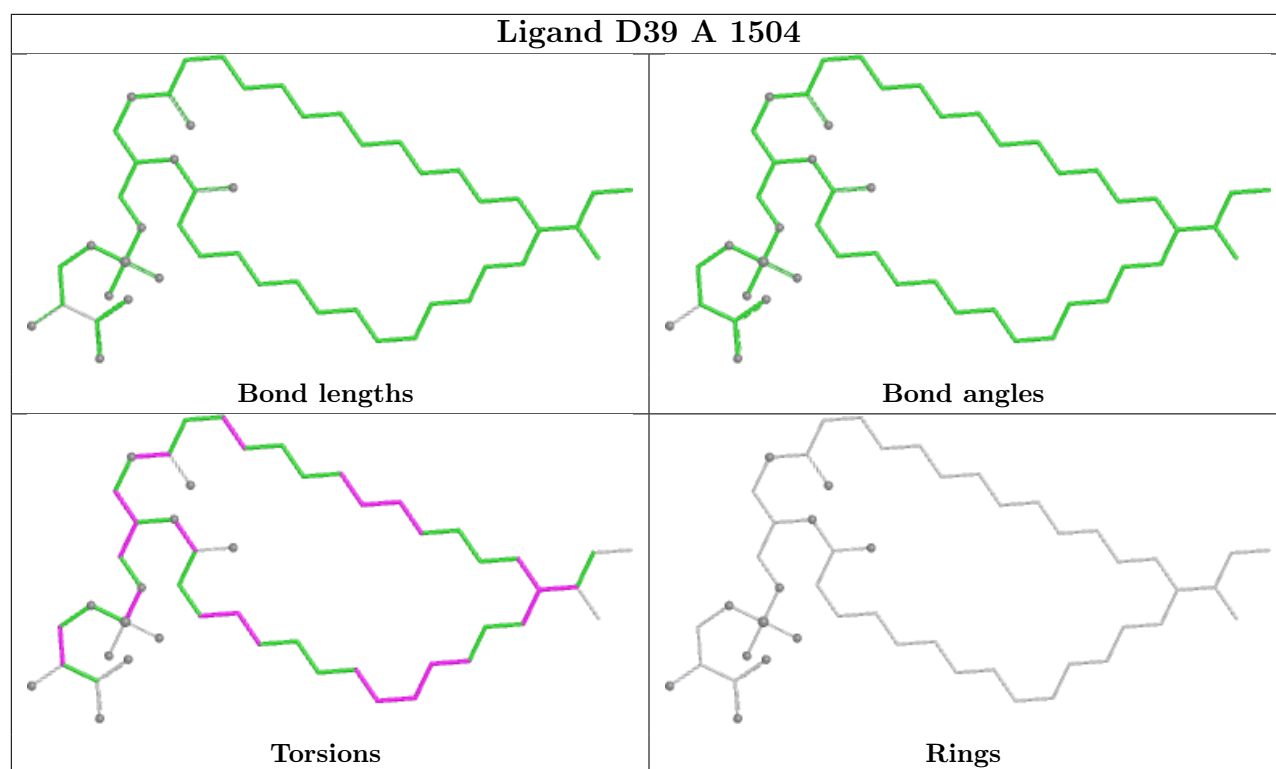
3 monomers are involved in 19 short contacts:

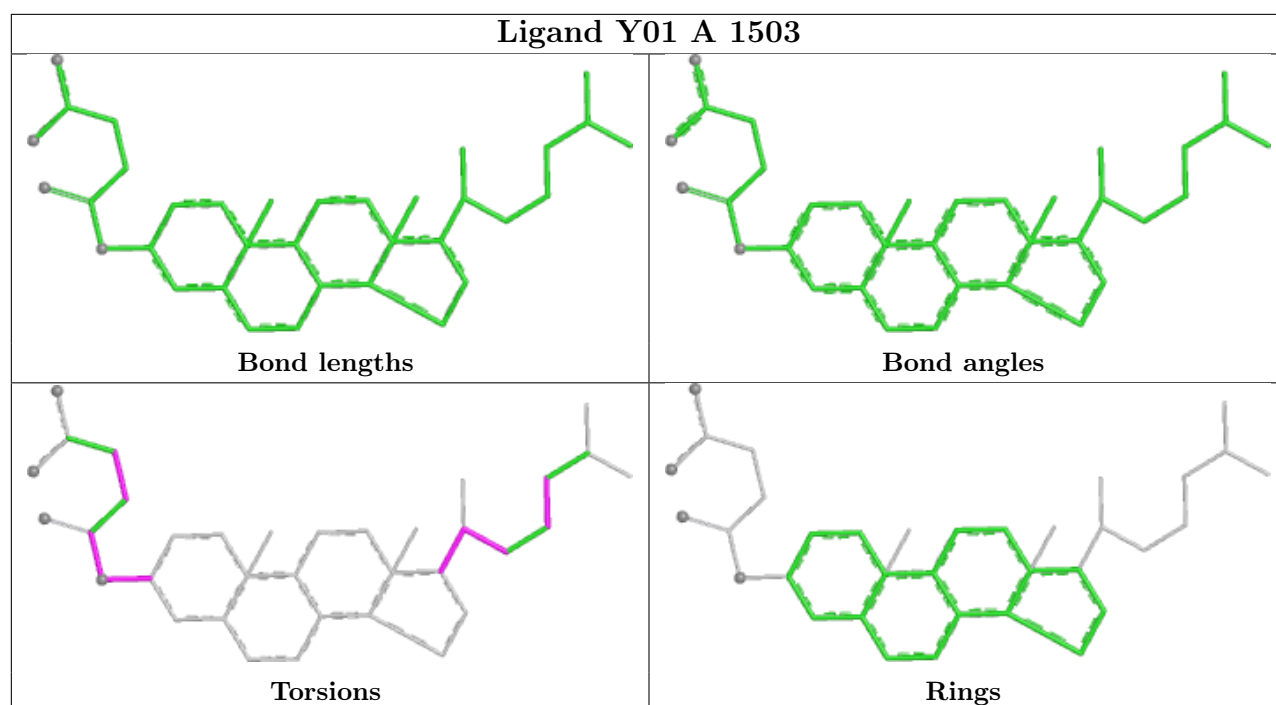
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1501	Y01	9	0
2	A	1502	Y01	2	0
2	A	1503	Y01	8	0

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.

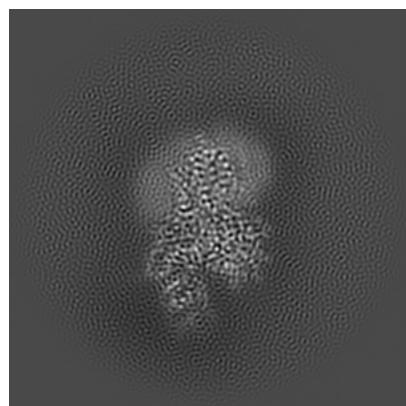
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36995. These allow visual inspection of the internal detail of the map and identification of artifacts.

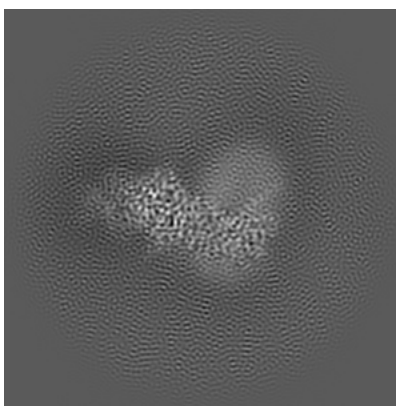
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

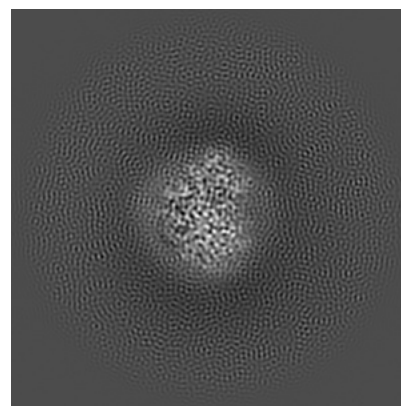
6.1.1 Primary map



X

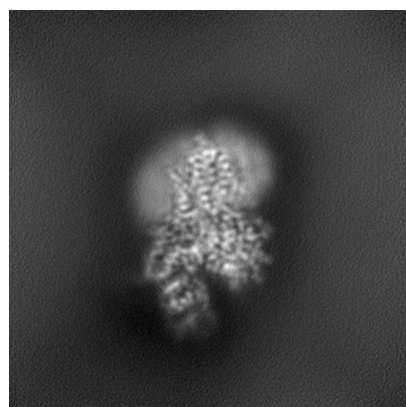


Y

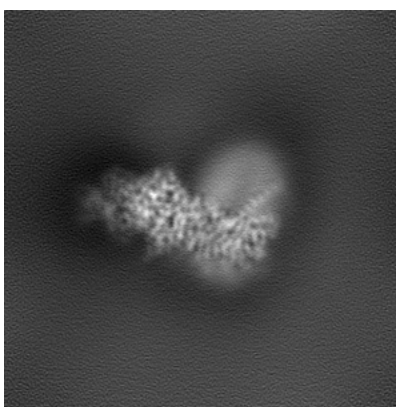


Z

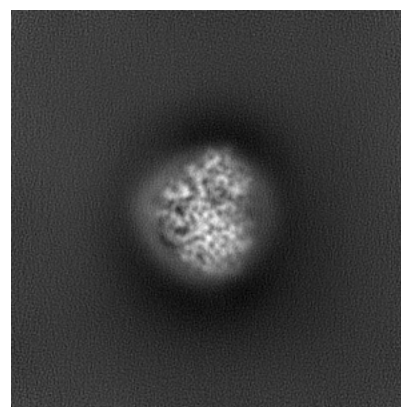
6.1.2 Raw map



X



Y

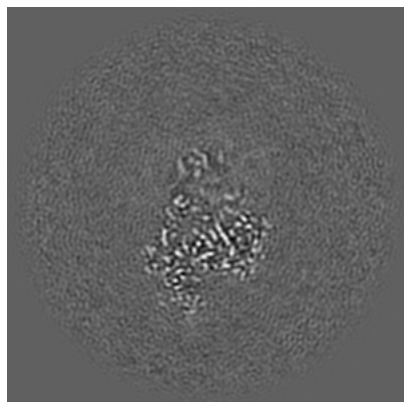


Z

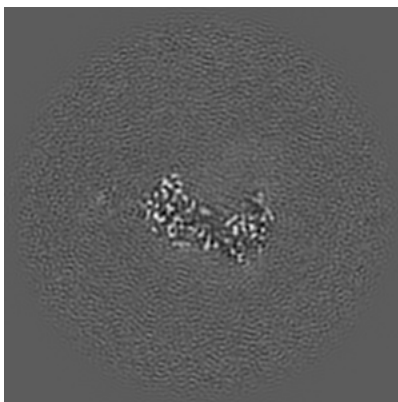
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

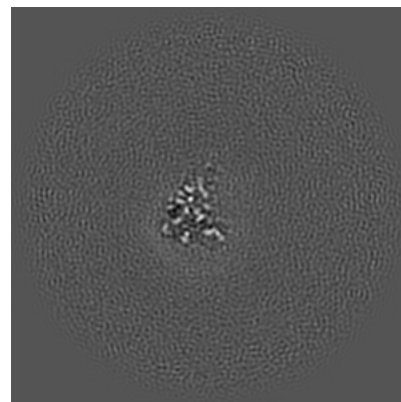
6.2.1 Primary map



X Index: 140

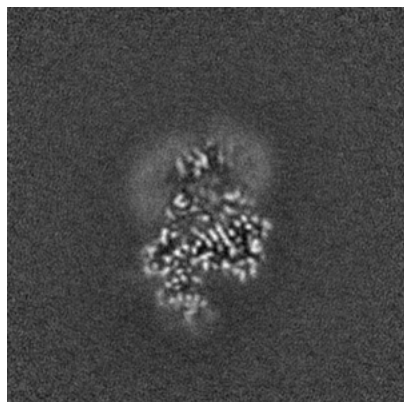


Y Index: 140

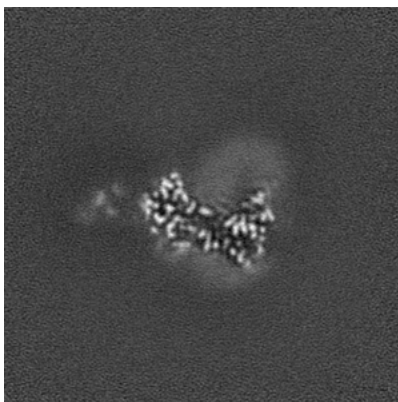


Z Index: 140

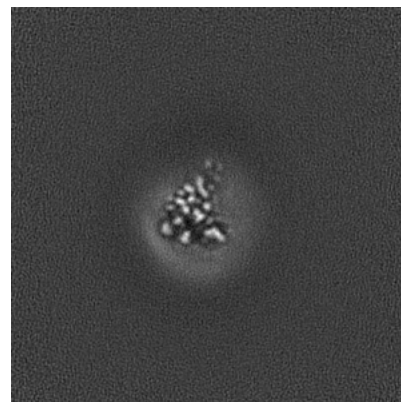
6.2.2 Raw map



X Index: 140



Y Index: 140

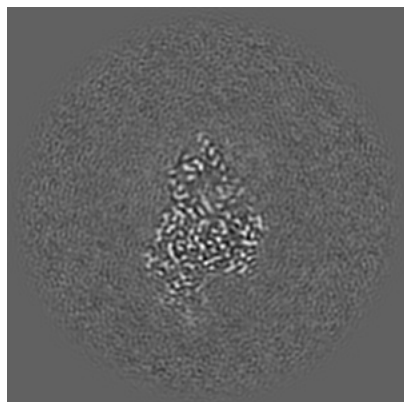


Z Index: 140

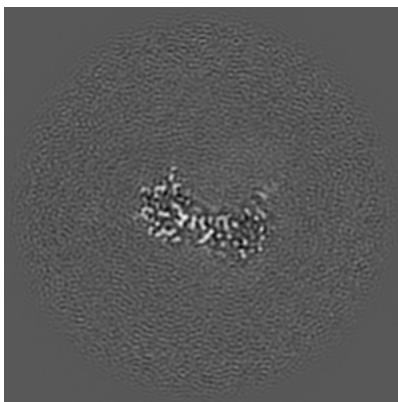
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

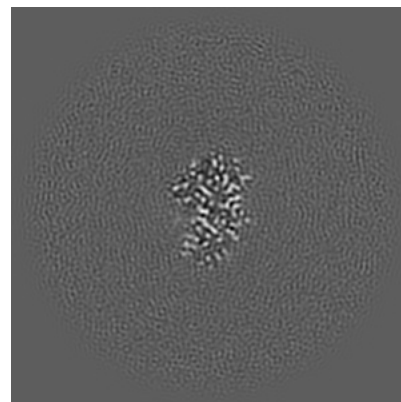
6.3.1 Primary map



X Index: 136

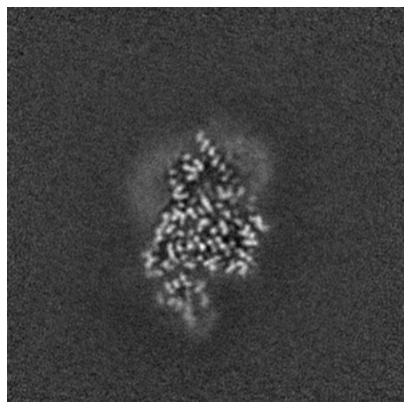


Y Index: 144

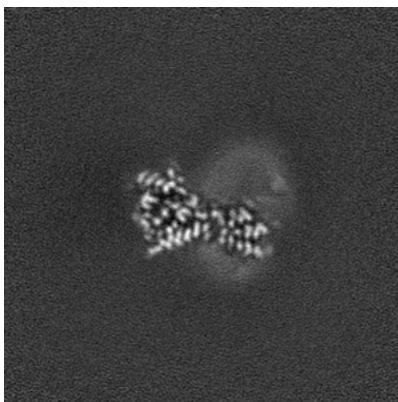


Z Index: 112

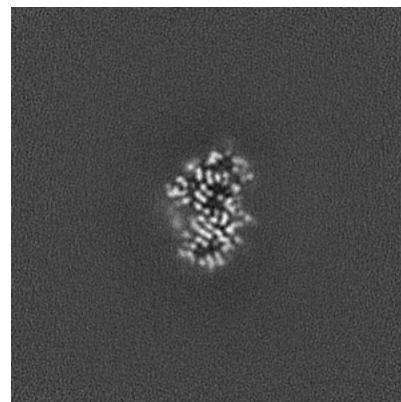
6.3.2 Raw map



X Index: 136



Y Index: 151

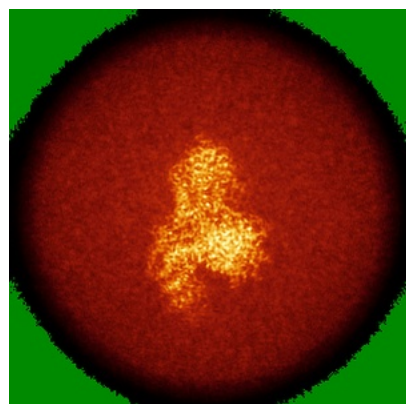


Z Index: 110

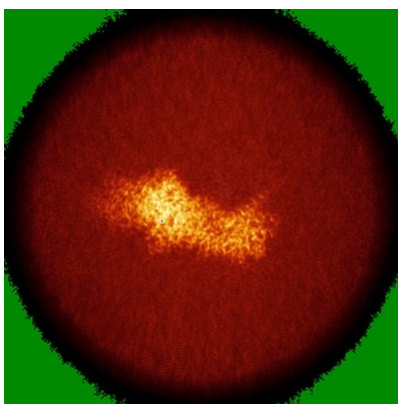
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

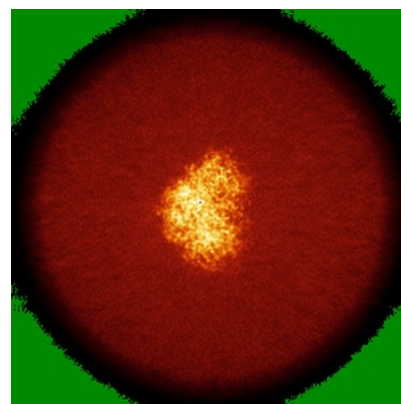
6.4.1 Primary map



X

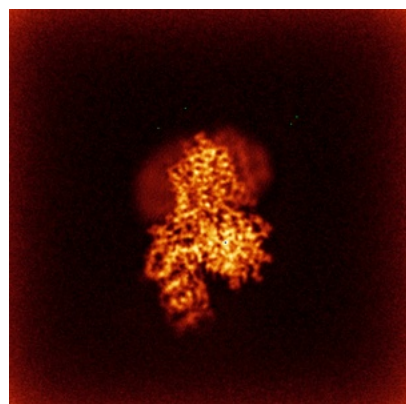


Y

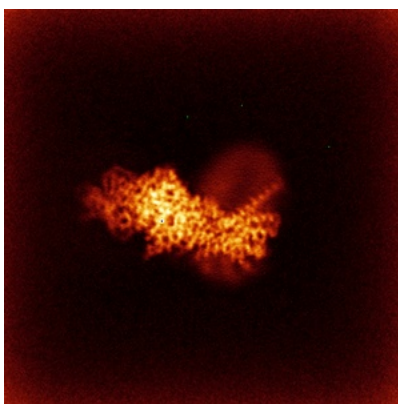


Z

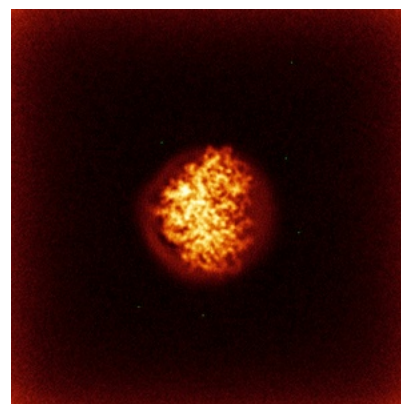
6.4.2 Raw map



X



Y

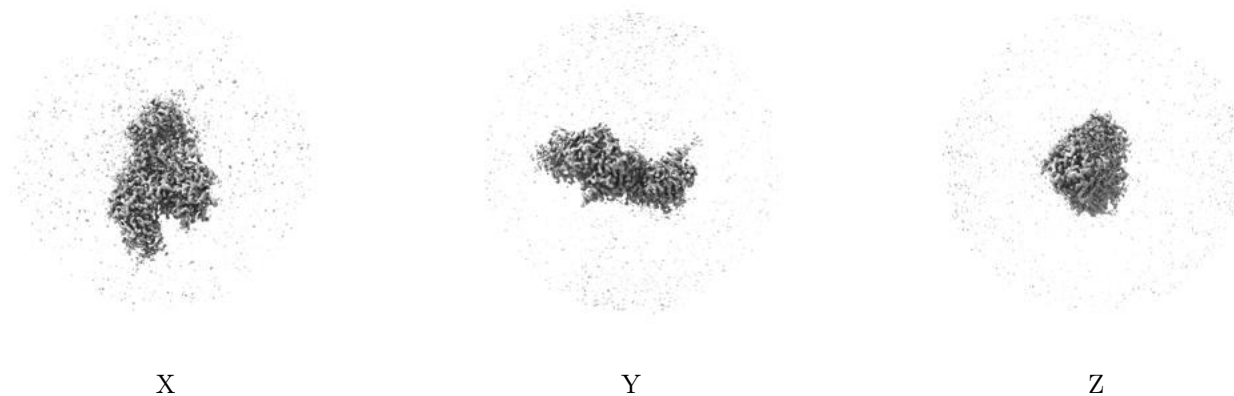


Z

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.

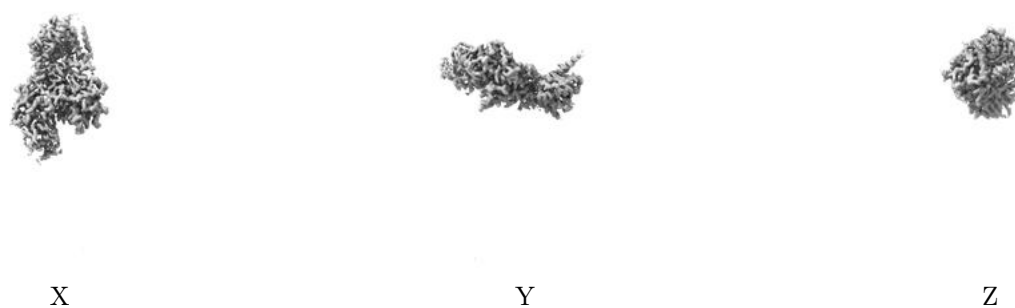
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.743. 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



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.

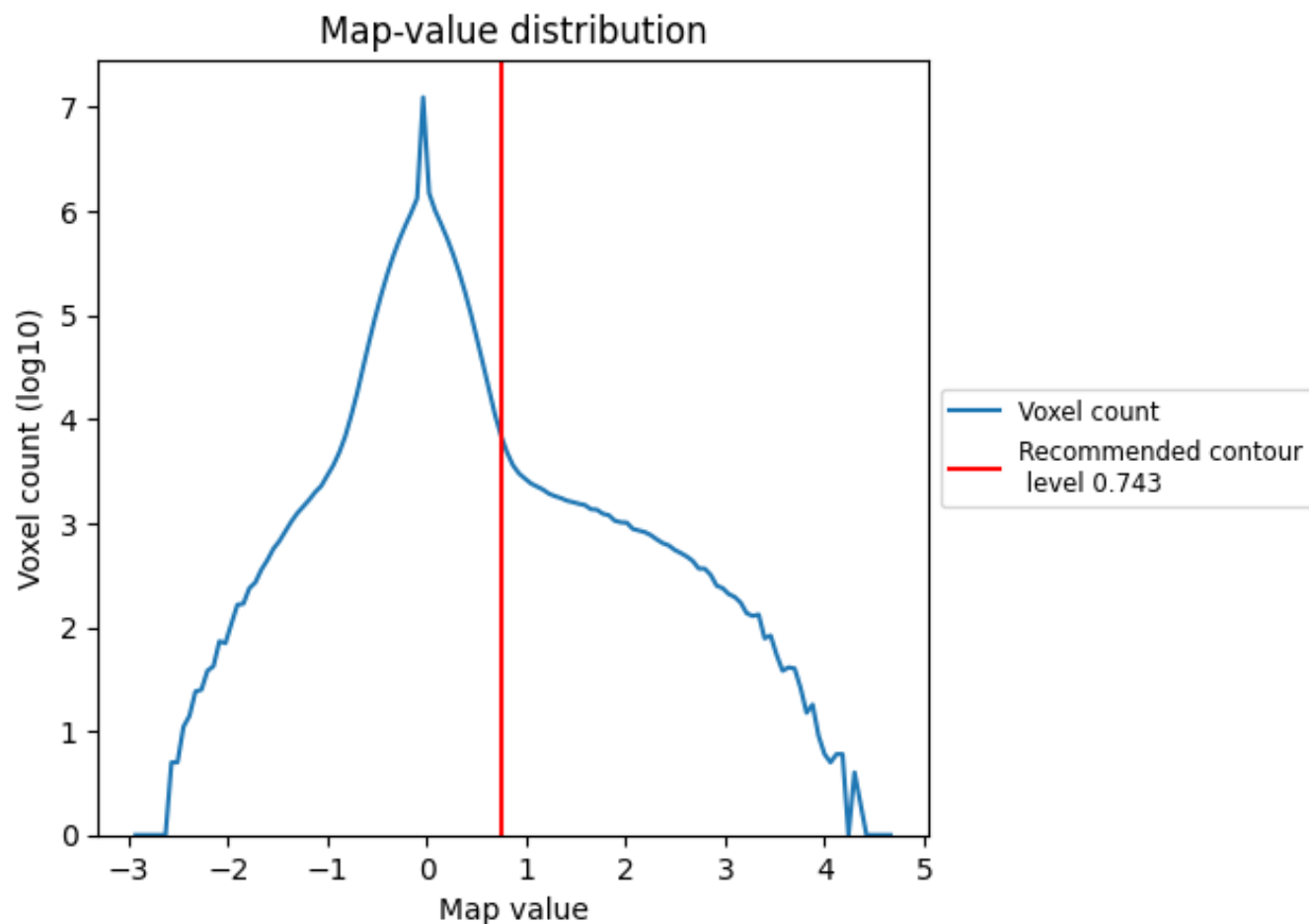
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

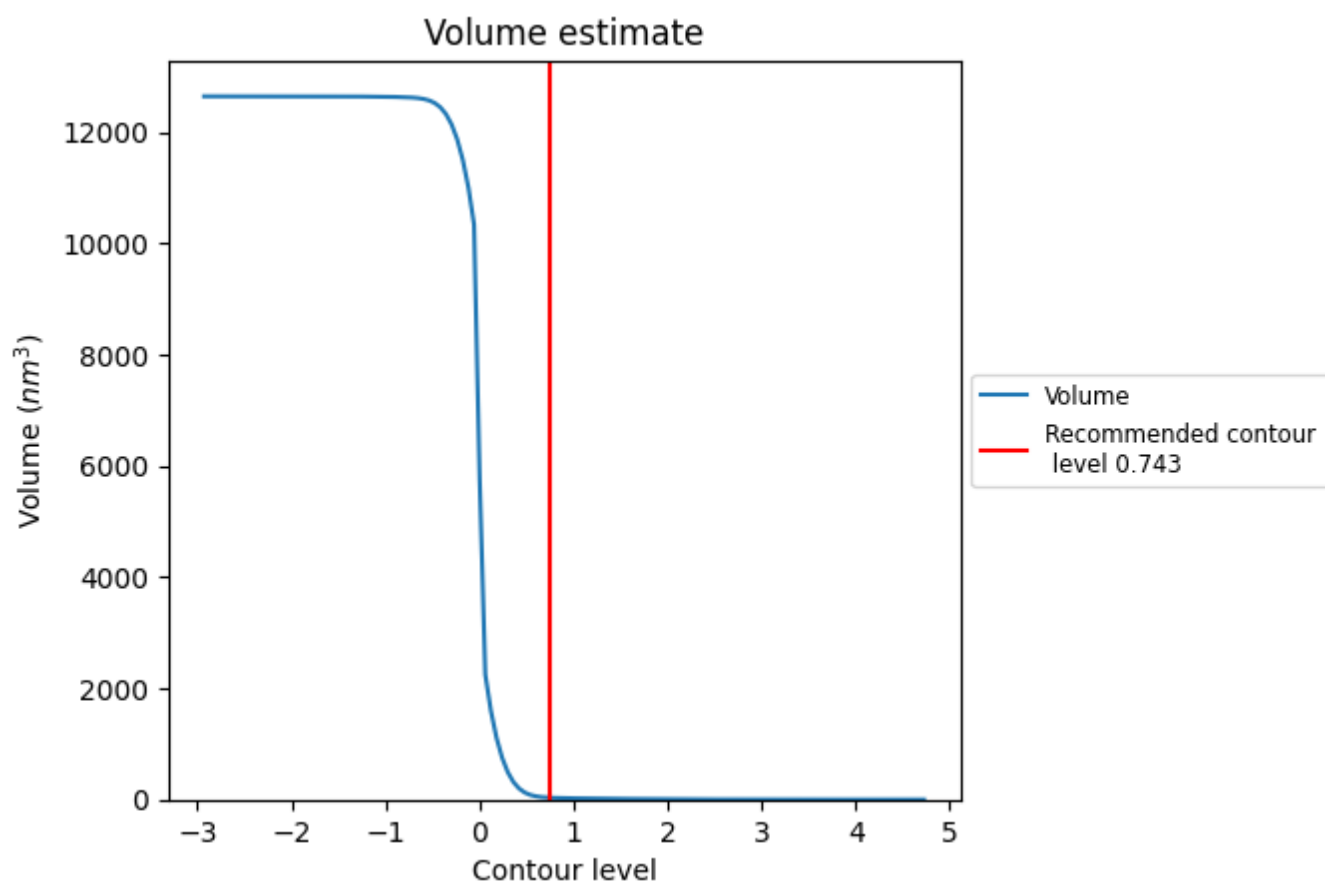
This section contains the results of statistical analysis of the map.

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.

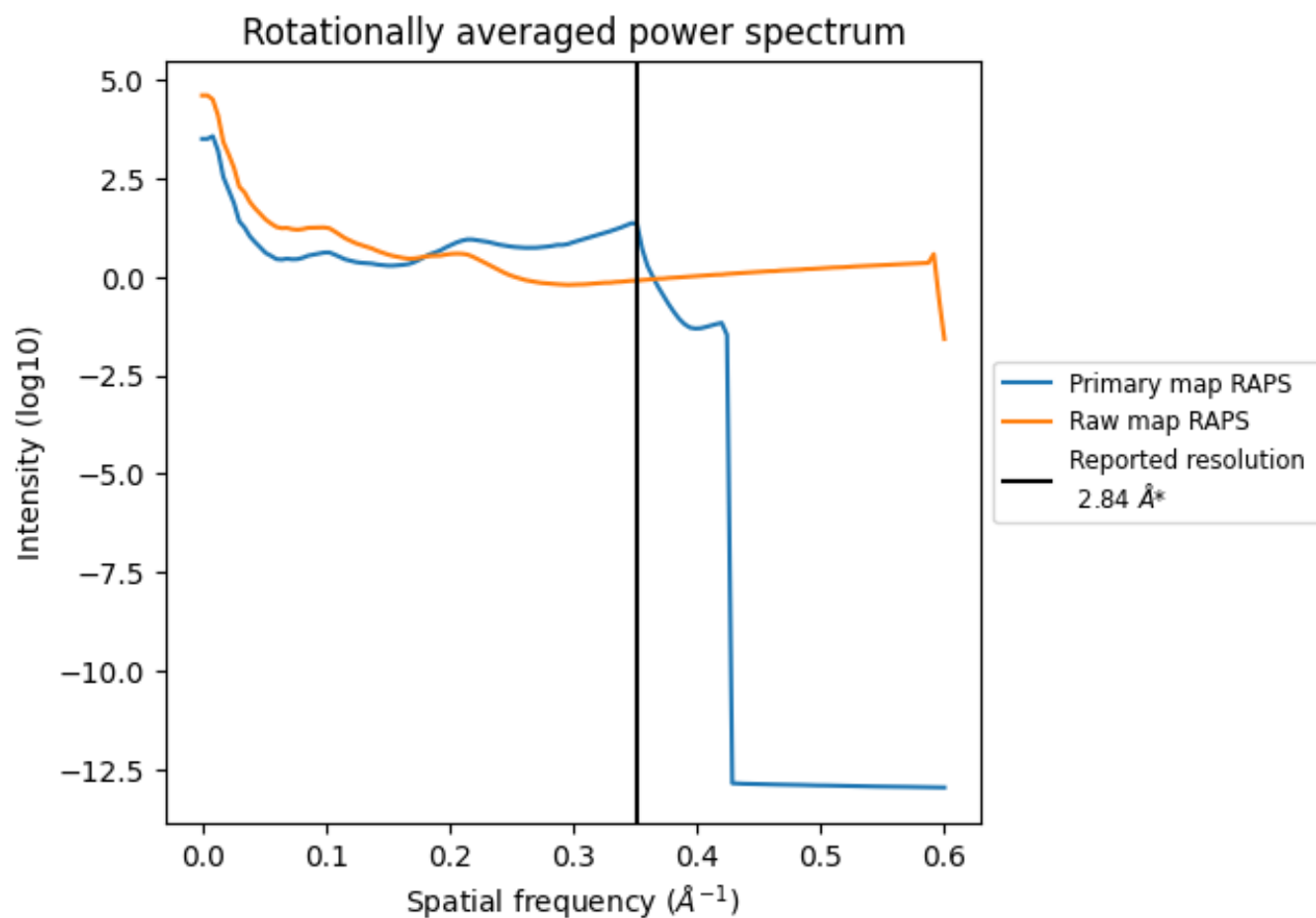
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 34 nm³; this corresponds to an approximate mass of 31 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 ⓘ

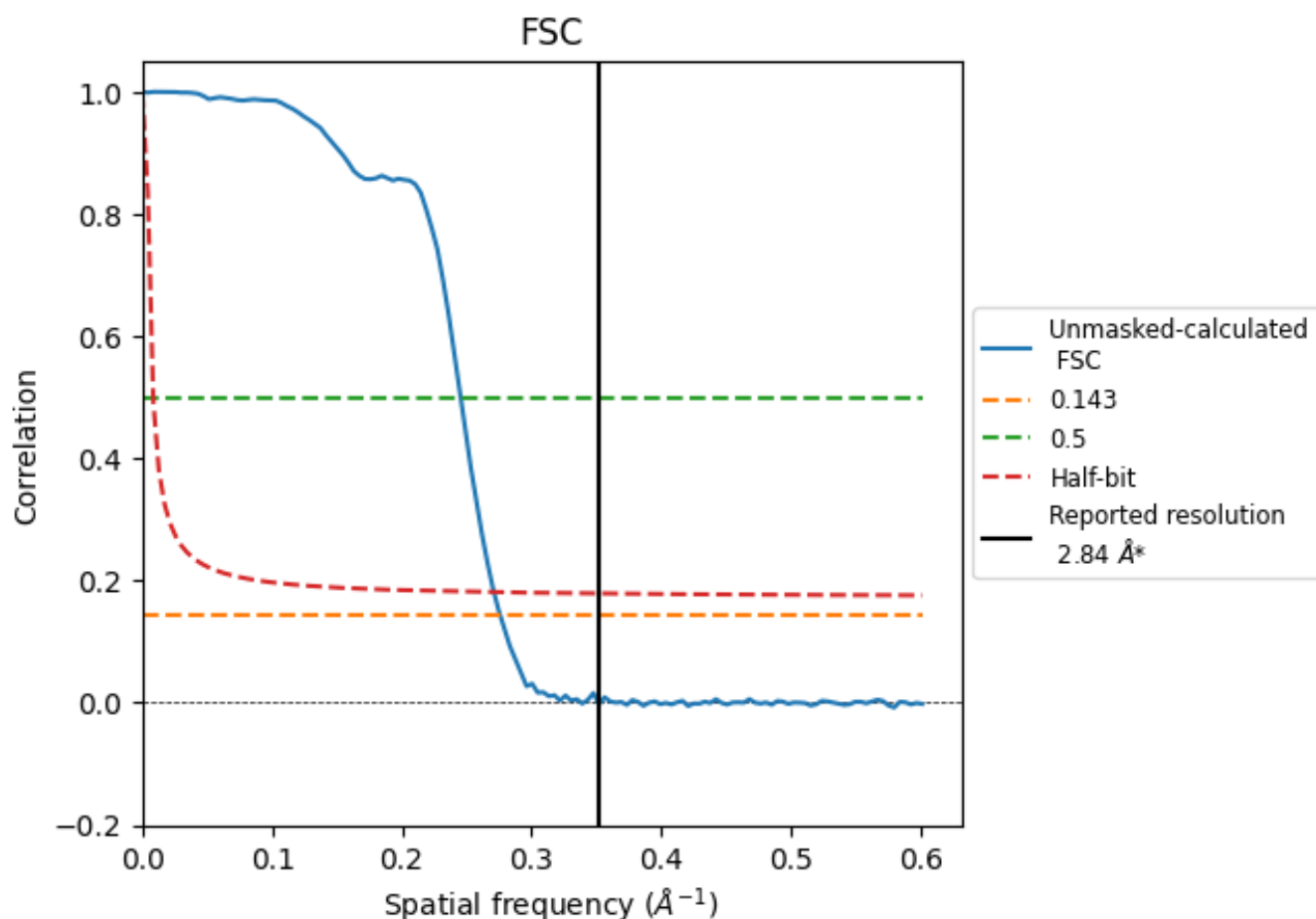


*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

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 $0.352 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	4.08	3.69

*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 3.62 differs from the reported value 2.84 by more than 10 %

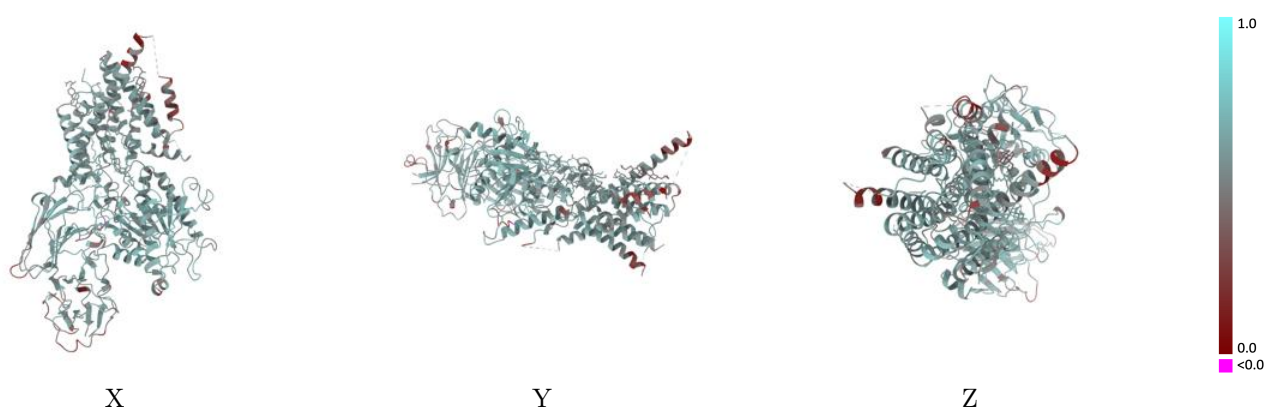
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-36995 and PDB model 8K9Q. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

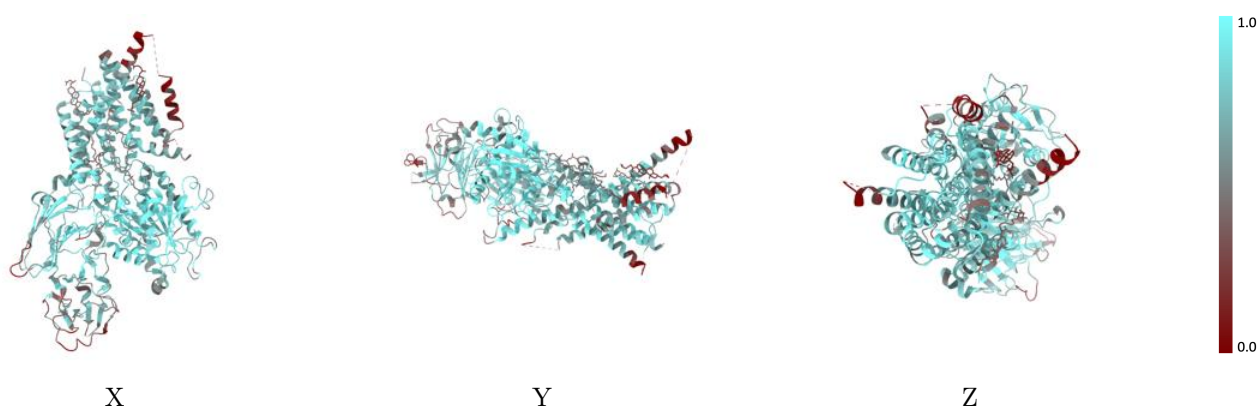
This section was not generated.

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



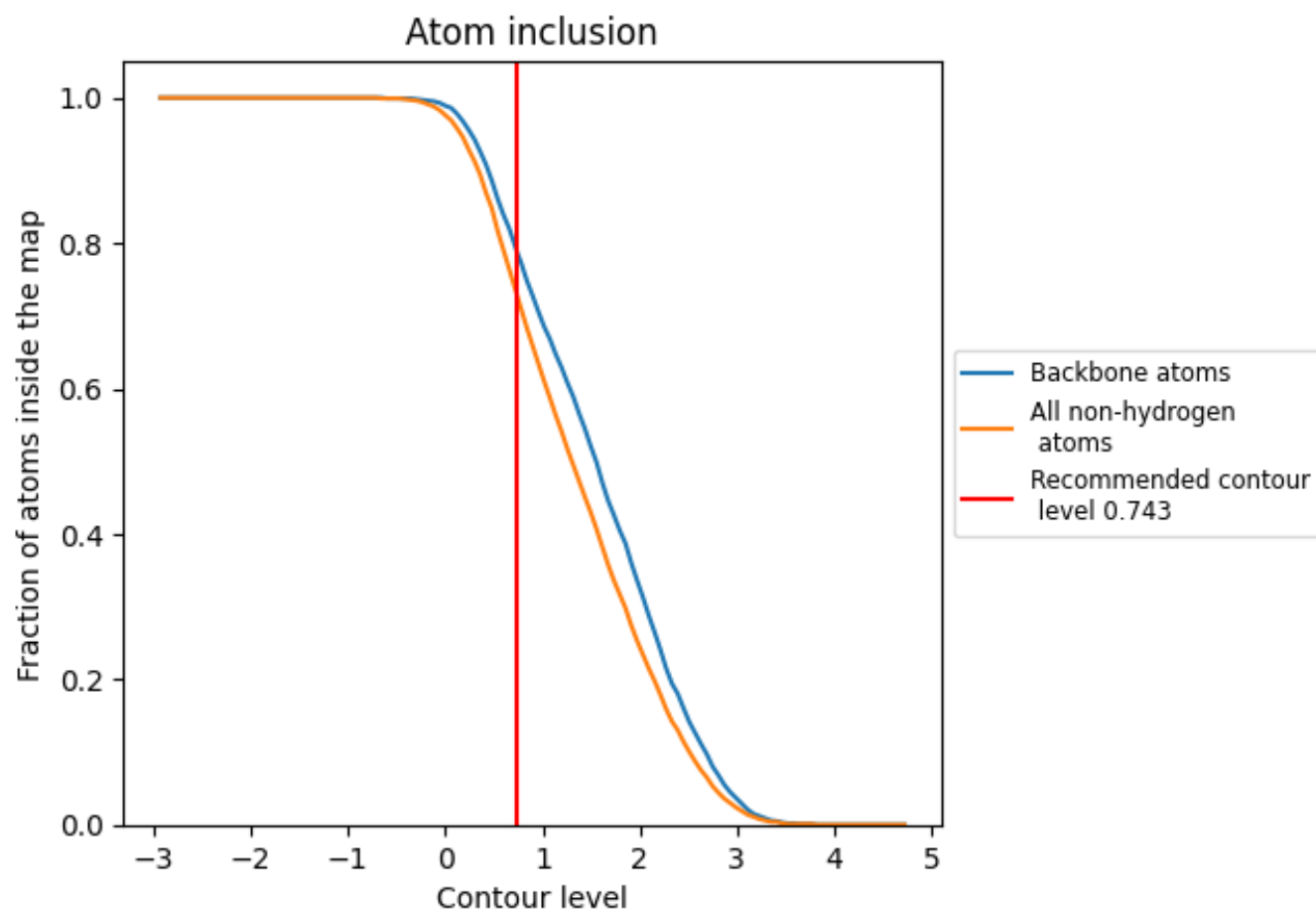
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.743).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.743) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.5630
A	0.7260	0.5630

