



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:48 PM UTC

PDB ID : 8GRS / pdb_00008grs
EMDB ID : EMD-34214
Title : human TMEM63A
Authors : Zhang, M.F.
Deposited on : 2022-09-02
Resolution : 3.30 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

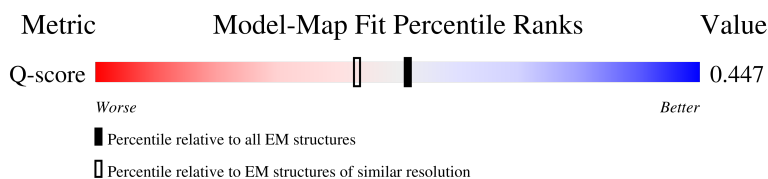
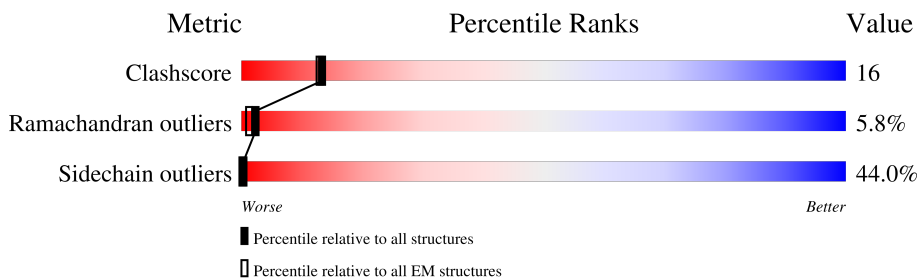
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	807	

2 Entry composition [i](#)

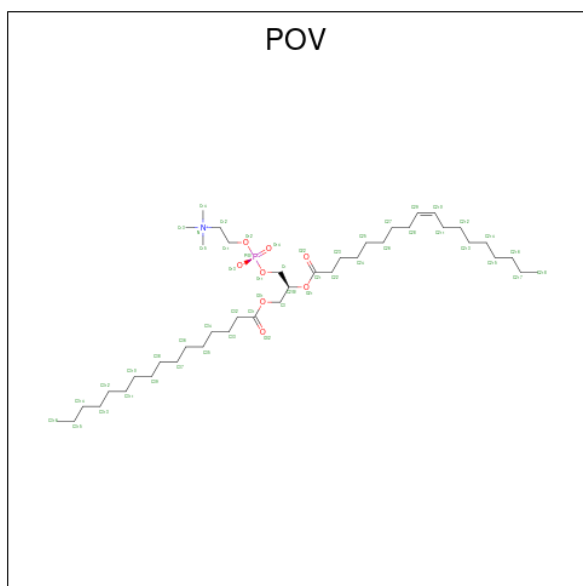
There are 2 unique types of molecules in this entry. The entry contains 5148 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

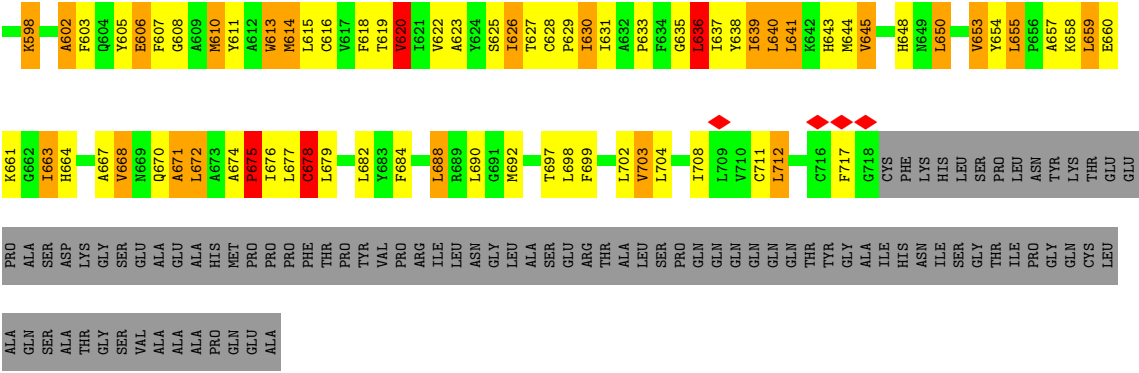
- Molecule 1 is a protein called CSC1-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	626	5096	3369	820	876	31	0	0

- Molecule 2 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (CCD ID: POV) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	52	42	1	8	1	0



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155000	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	2500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.106	Depositor
Minimum map value	-0.697	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.16	Depositor
Map size ($\text{\AA}$)	262.4, 262.4, 262.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82, 0.82, 0.82	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: POV

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	1.20	22/5232 (0.4%)	1.38	93/7104 (1.3%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	511	ILE	CA-C	-10.83	1.40	1.52
1	A	153	VAL	C-O	-8.91	1.14	1.24
1	A	562	ALA	CA-C	-8.44	1.42	1.52
1	A	157	SER	CA-C	-7.97	1.42	1.52
1	A	512	PHE	CA-C	-7.86	1.42	1.52
1	A	512	PHE	C-O	-7.07	1.15	1.24
1	A	563	SER	C-O	-6.89	1.15	1.24
1	A	154	SER	C-O	-6.48	1.16	1.24
1	A	162	LEU	N-CA	-6.38	1.42	1.46
1	A	516	ILE	CA-C	-6.18	1.43	1.52
1	A	508	ILE	C-O	-5.94	1.17	1.24
1	A	507	TYR	C-O	-5.90	1.17	1.24
1	A	501	ILE	C-O	-5.58	1.17	1.24
1	A	559	TYR	C-O	-5.57	1.17	1.24
1	A	517	LEU	CA-C	-5.54	1.45	1.52
1	A	515	LEU	CA-C	-5.46	1.45	1.52
1	A	147	ILE	C-O	-5.39	1.18	1.24
1	A	157	SER	C-O	-5.23	1.17	1.24
1	A	159	CYS	C-O	5.17	1.30	1.24
1	A	150	LEU	C-O	-5.12	1.17	1.24
1	A	436	LEU	C-O	5.11	1.29	1.24
1	A	187	GLN	CA-C	-5.01	1.46	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	ILE	CB-CA-C	-14.34	93.35	111.70
1	A	511	ILE	N-CA-C	-13.68	96.00	110.23
1	A	134	GLU	N-CA-C	-13.27	97.71	114.56
1	A	517	LEU	CA-C-N	-11.81	105.94	119.05
1	A	517	LEU	C-N-CA	-11.81	105.94	119.05
1	A	674	ALA	CA-C-N	-10.98	106.81	119.32
1	A	674	ALA	C-N-CA	-10.98	106.81	119.32
1	A	511	ILE	N-CA-CB	10.57	121.71	110.62
1	A	551	ASP	N-CA-C	-10.45	93.69	110.20
1	A	162	LEU	CA-C-N	-10.29	108.54	119.24
1	A	162	LEU	C-N-CA	-10.29	108.54	119.24
1	A	506	VAL	N-CA-C	-9.79	101.03	110.42
1	A	151	VAL	N-CA-C	-9.33	101.76	110.53
1	A	636	LEU	N-CA-C	-8.94	100.97	112.23
1	A	572	LEU	N-CA-C	-8.84	101.32	112.90
1	A	267	ALA	N-CA-C	8.81	122.76	109.63
1	A	643	HIS	N-CA-C	-8.76	101.82	111.36
1	A	162	LEU	N-CA-C	-8.54	100.56	112.17
1	A	511	ILE	CA-C-O	-8.18	112.90	121.41
1	A	527	PHE	N-CA-C	-8.01	102.56	111.28
1	A	68	PHE	N-CA-C	-8.00	103.47	113.55
1	A	184	ALA	N-CA-C	-7.95	94.94	109.56
1	A	49	GLY	N-CA-C	-7.92	105.11	113.58
1	A	568	ASN	N-CA-C	-7.90	102.28	112.23
1	A	136	ALA	N-CA-C	-7.81	105.72	114.62
1	A	531	TRP	N-CA-C	-7.81	101.87	111.40
1	A	439	PRO	CA-N-CD	-7.74	101.17	112.00
1	A	438	THR	CA-C-N	-7.62	110.31	119.84
1	A	438	THR	C-N-CA	-7.62	110.31	119.84
1	A	478	LEU	N-CA-C	-7.38	103.24	112.90
1	A	477	ALA	N-CA-C	-7.25	104.05	114.12
1	A	180	ARG	N-CA-C	-7.14	103.53	111.82
1	A	571	GLU	N-CA-C	-7.01	104.75	113.38
1	A	81	ILE	N-CA-C	-6.97	106.43	113.47
1	A	663	ILE	O-C-N	-6.94	115.14	121.87
1	A	248	PHE	N-CA-C	-6.84	104.41	112.89
1	A	67	VAL	N-CA-C	-6.81	104.69	111.77
1	A	66	LEU	N-CA-C	-6.80	104.87	113.72
1	A	288	ASN	N-CA-C	-6.75	104.66	113.17
1	A	48	GLY	N-CA-C	-6.75	106.36	113.58
1	A	620	VAL	N-CA-CB	6.71	117.96	110.51
1	A	557	VAL	N-CA-C	-6.63	102.80	111.09
1	A	153	VAL	N-CA-C	-6.59	103.90	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	GLN	N-CA-C	-6.46	103.74	112.26
1	A	688	LEU	N-CA-C	-6.43	103.96	110.97
1	A	511	ILE	O-C-N	6.40	128.88	121.96
1	A	578	LEU	N-CA-C	-6.31	104.40	111.28
1	A	217	SER	N-CA-C	-6.19	107.56	114.62
1	A	397	VAL	N-CA-C	-6.16	97.48	107.28
1	A	163	PRO	CA-N-CD	-6.03	103.56	112.00
1	A	675	PRO	CA-N-CD	-6.03	103.56	112.00
1	A	667	ALA	CA-C-N	-6.01	112.22	120.46
1	A	667	ALA	C-N-CA	-6.01	112.22	120.46
1	A	330	ARG	N-CA-C	-5.95	104.73	112.23
1	A	331	LEU	N-CA-C	-5.86	104.98	111.36
1	A	501	ILE	N-CA-C	-5.85	104.81	110.72
1	A	421	GLN	N-CA-C	-5.78	104.90	111.14
1	A	61	PHE	N-CA-C	-5.75	104.93	111.14
1	A	411	LEU	N-CA-C	-5.73	101.03	109.62
1	A	179	GLY	N-CA-C	-5.67	99.73	113.18
1	A	235	LEU	CA-C-N	-5.67	114.13	119.85
1	A	235	LEU	C-N-CA	-5.67	114.13	119.85
1	A	611	TYR	N-CA-C	-5.62	104.37	111.11
1	A	247	HIS	N-CA-C	-5.58	105.97	112.89
1	A	533	PHE	N-CA-C	-5.56	106.63	113.41
1	A	63	PHE	N-CA-C	-5.49	104.22	111.96
1	A	648	HIS	N-CA-C	-5.47	103.20	111.56
1	A	178	PHE	N-CA-C	-5.46	99.18	110.80
1	A	618	PHE	N-CA-C	-5.45	105.50	111.82
1	A	440	SER	N-CA-C	5.41	116.86	111.07
1	A	220	TYR	N-CA-C	-5.39	101.93	109.96
1	A	137	ILE	N-CA-C	-5.38	104.51	112.04
1	A	270	ILE	CB-CA-C	-5.34	105.14	111.97
1	A	439	PRO	CA-C-N	-5.30	113.55	120.44
1	A	439	PRO	C-N-CA	-5.30	113.55	120.44
1	A	149	LEU	N-CA-C	-5.29	105.59	111.36
1	A	575	LEU	CA-C-N	-5.29	113.23	119.84
1	A	575	LEU	C-N-CA	-5.29	113.23	119.84
1	A	678	CYS	CA-C-N	-5.28	113.15	120.38
1	A	678	CYS	C-N-CA	-5.28	113.15	120.38
1	A	208	VAL	N-CA-C	-5.23	105.40	110.42
1	A	194	TRP	N-CA-C	-5.21	105.68	111.36
1	A	562	ALA	N-CA-C	-5.21	104.66	111.02
1	A	135	ASP	N-CA-C	-5.20	106.70	112.57
1	A	577	GLY	N-CA-C	-5.17	100.94	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	ALA	CA-C-N	-5.16	113.37	120.28
1	A	671	ALA	C-N-CA	-5.16	113.37	120.28
1	A	592	ALA	N-CA-C	-5.15	105.57	111.14
1	A	240	ARG	N-CA-C	5.14	121.74	110.80
1	A	517	LEU	CB-CA-C	5.13	120.28	110.17
1	A	682	LEU	N-CA-C	-5.04	105.68	111.07
1	A	186	LEU	CB-CA-C	-5.02	109.82	115.79
1	A	640	LEU	N-CA-C	-5.01	105.52	111.69

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	5096	0	5158	168	0
2	A	52	0	82	0	0
All	All	5148	0	5240	168	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 16.

All (168) 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:437:THR:HG21	1:A:517:LEU:HB3	1.40	1.02
1:A:342:VAL:O	1:A:346:PRO:HD2	1.88	0.74
1:A:563:SER:O	1:A:564:ALA:C	2.32	0.71
1:A:671:ALA:O	1:A:675:PRO:HD2	1.90	0.71
1:A:18:ARG:HA	1:A:21:LEU:HD23	1.71	0.70
1:A:512:PHE:O	1:A:513:MET:C	2.31	0.70
1:A:513:MET:O	1:A:518:PRO:HD2	1.95	0.66
1:A:259:ASP:HA	1:A:360:ALA:HA	1.76	0.66
1:A:147:ILE:HG12	1:A:639:ILE:HG23	1.81	0.63
1:A:239:ALA:HA	1:A:355:GLN:HB3	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:HG12	1:A:185:ASN:HD21	1.62	0.62
1:A:280:GLU:HB3	1:A:334:ARG:HG3	1.81	0.62
1:A:435:PHE:O	1:A:439:PRO:HD2	2.00	0.62
1:A:157:SER:O	1:A:158:LEU:C	2.41	0.60
1:A:269:LEU:HB3	1:A:345:GLN:HG2	1.84	0.60
1:A:257:VAL:HG13	1:A:364:LEU:HD13	1.84	0.60
1:A:572:LEU:HG	1:A:645:VAL:HG22	1.84	0.59
1:A:623:ALA:HA	1:A:678:CYS:HB2	1.83	0.59
1:A:513:MET:O	1:A:514:VAL:C	2.45	0.59
1:A:437:THR:HG23	1:A:518:PRO:HD3	1.85	0.58
1:A:239:ALA:HB3	1:A:395:TRP:HB3	1.86	0.58
1:A:74:ARG:O	1:A:75:PHE:C	2.48	0.57
1:A:218:ILE:HD12	1:A:664:HIS:HB2	1.85	0.57
1:A:30:SER:O	1:A:31:TYR:C	2.48	0.56
1:A:158:LEU:O	1:A:159:CYS:C	2.43	0.56
1:A:437:THR:CG2	1:A:518:PRO:HD3	2.36	0.56
1:A:63:PHE:O	1:A:67:VAL:HG23	2.07	0.55
1:A:270:ILE:HD13	1:A:346:PRO:HD3	1.88	0.54
1:A:54:LEU:HD13	1:A:561:ILE:HD13	1.89	0.54
1:A:514:VAL:O	1:A:515:LEU:C	2.47	0.54
1:A:438:THR:O	1:A:439:PRO:C	2.49	0.53
1:A:512:PHE:O	1:A:513:MET:O	2.26	0.53
1:A:155:PHE:O	1:A:156:LEU:C	2.51	0.53
1:A:530:ARG:HH12	1:A:543:ARG:HG3	1.73	0.53
1:A:240:ARG:HA	1:A:395:TRP:CD1	2.44	0.52
1:A:344:ASP:O	1:A:347:LEU:HB2	2.10	0.52
1:A:619:THR:O	1:A:620:VAL:C	2.50	0.52
1:A:71:ILE:HD13	1:A:578:LEU:HD22	1.91	0.52
1:A:523:THR:HG21	1:A:684:PHE:HE2	1.75	0.51
1:A:523:THR:HG21	1:A:684:PHE:CE2	2.46	0.51
1:A:405:ASP:O	1:A:406:ILE:C	2.54	0.51
1:A:154:SER:O	1:A:155:PHE:C	2.53	0.51
1:A:392:THR:O	1:A:393:SER:C	2.51	0.51
1:A:348:GLY:HA2	1:A:351:PHE:HD2	1.76	0.51
1:A:204:LEU:HD21	1:A:679:LEU:HD12	1.91	0.50
1:A:425:ILE:HD11	1:A:489:LEU:O	2.12	0.50
1:A:510:LEU:O	1:A:511:ILE:C	2.54	0.49
1:A:159:CYS:O	1:A:163:PRO:HD2	2.12	0.49
1:A:261:GLN:H	1:A:359:MET:HB2	1.77	0.49
1:A:585:MET:HA	1:A:588:ALA:HB2	1.95	0.49
1:A:622:VAL:HG11	1:A:675:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:PHE:O	1:A:252:TYR:HB2	2.12	0.48
1:A:511:ILE:O	1:A:512:PHE:O	2.31	0.48
1:A:153:VAL:O	1:A:154:SER:C	2.56	0.48
1:A:159:CYS:O	1:A:160:VAL:C	2.56	0.48
1:A:443:LEU:O	1:A:446:MET:HG2	2.13	0.48
1:A:215:THR:HG22	1:A:668:VAL:HG11	1.95	0.48
1:A:240:ARG:CZ	1:A:393:SER:HB3	2.43	0.48
1:A:581:TYR:CZ	1:A:585:MET:HE1	2.49	0.48
1:A:278:LYS:HD2	1:A:278:LYS:HA	1.81	0.48
1:A:162:LEU:O	1:A:163:PRO:C	2.53	0.47
1:A:250:ASP:HB3	1:A:388:ARG:HG3	1.95	0.47
1:A:615:LEU:HD23	1:A:615:LEU:HA	1.72	0.47
1:A:164:VAL:HG13	1:A:192:LEU:HB3	1.95	0.47
1:A:72:ARG:HE	1:A:72:ARG:HB3	1.47	0.47
1:A:586:ILE:HD13	1:A:586:ILE:HA	1.70	0.47
1:A:162:LEU:HD11	1:A:181:THR:HB	1.96	0.47
1:A:562:ALA:O	1:A:563:SER:C	2.58	0.47
1:A:393:SER:C	1:A:395:TRP:H	2.21	0.47
1:A:605:TYR:OH	1:A:610:MET:HG2	2.14	0.47
1:A:598:LYS:HB3	1:A:598:LYS:HE2	1.27	0.47
1:A:146:ILE:HG12	1:A:211:MET:HE1	1.97	0.46
1:A:242:GLU:H	1:A:242:GLU:HG2	1.46	0.46
1:A:236:PRO:HA	1:A:399:PHE:O	2.15	0.46
1:A:321:ILE:H	1:A:321:ILE:HG13	1.32	0.46
1:A:33:TYR:HB3	1:A:40:THR:HG21	1.97	0.46
1:A:445:THR:C	1:A:447:ASP:H	2.24	0.46
1:A:18:ARG:H	1:A:18:ARG:HG2	1.47	0.46
1:A:522:LEU:HB3	1:A:550:PRO:HD2	1.97	0.46
1:A:77:ASP:H	1:A:581:TYR:HE2	1.64	0.46
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.76	0.46
1:A:162:LEU:HB3	1:A:163:PRO:CD	2.46	0.46
1:A:522:LEU:O	1:A:550:PRO:HD3	2.16	0.46
1:A:573:LEU:HD23	1:A:573:LEU:HA	1.83	0.46
1:A:248:PHE:C	1:A:250:ASP:H	2.24	0.45
1:A:425:ILE:CD1	1:A:489:LEU:O	2.64	0.45
1:A:505:LYS:O	1:A:506:VAL:C	2.57	0.45
1:A:606:GLU:C	1:A:608:GLY:H	2.24	0.45
1:A:513:MET:O	1:A:514:VAL:O	2.34	0.45
1:A:13:LYS:HB3	1:A:13:LYS:HE3	1.35	0.45
1:A:672:LEU:HD12	1:A:672:LEU:HA	1.78	0.45
1:A:614:MET:HB3	1:A:614:MET:HE3	1.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:VAL:HA	1:A:364:LEU:HD22	1.99	0.45
1:A:518:PRO:HB2	1:A:556:PHE:CZ	2.52	0.45
1:A:602:ALA:HB1	1:A:655:LEU:HD13	1.98	0.45
1:A:177:SER:O	1:A:178:PHE:C	2.60	0.45
1:A:503:MET:HE2	1:A:503:MET:HB2	1.73	0.45
1:A:574:ARG:HH22	1:A:653:VAL:HG21	1.82	0.45
1:A:503:MET:HG3	1:A:504:THR:N	2.28	0.45
1:A:289:LEU:HA	1:A:294:GLY:H	1.82	0.45
1:A:265:ASN:HD22	1:A:355:GLN:HG3	1.82	0.44
1:A:506:VAL:O	1:A:507:TYR:C	2.56	0.44
1:A:572:LEU:HD23	1:A:572:LEU:HA	1.76	0.44
1:A:158:LEU:HD12	1:A:158:LEU:HA	1.75	0.44
1:A:220:TYR:HD1	1:A:220:TYR:HA	1.73	0.44
1:A:575:LEU:HB3	1:A:576:PRO:HD3	1.98	0.44
1:A:365:LYS:H	1:A:365:LYS:HG3	1.35	0.44
1:A:607:PHE:CE2	1:A:650:LEU:HD21	2.53	0.44
1:A:24:GLY:O	1:A:25:ASP:C	2.60	0.44
1:A:517:LEU:O	1:A:518:PRO:C	2.52	0.44
1:A:150:LEU:HD12	1:A:150:LEU:HA	1.82	0.44
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.90	0.44
1:A:677:LEU:HD23	1:A:677:LEU:HA	1.83	0.43
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.53	0.43
1:A:186:LEU:HD13	1:A:186:LEU:HA	1.85	0.43
1:A:530:ARG:HD2	1:A:530:ARG:HA	1.71	0.43
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.89	0.43
1:A:66:LEU:HD22	1:A:66:LEU:HA	1.67	0.43
1:A:628:CYS:O	1:A:629:PRO:C	2.59	0.43
1:A:45:VAL:O	1:A:46:THR:C	2.61	0.43
1:A:201:VAL:HG22	1:A:703:VAL:HG11	1.99	0.43
1:A:164:VAL:HG12	1:A:185:ASN:ND2	2.31	0.43
1:A:280:GLU:HB3	1:A:334:ARG:CG	2.49	0.43
1:A:712:LEU:HD12	1:A:712:LEU:HA	1.71	0.43
1:A:554:ALA:O	1:A:555:PHE:C	2.60	0.43
1:A:641:LEU:HD12	1:A:641:LEU:HA	1.74	0.43
1:A:398:THR:O	1:A:399:PHE:C	2.62	0.42
1:A:329:ASP:HA	1:A:332:LEU:HB2	2.00	0.42
1:A:473:TRP:CD1	1:A:613:TRP:HH2	2.38	0.42
1:A:80:ARG:H	1:A:80:ARG:HG3	1.59	0.42
1:A:626:ILE:H	1:A:626:ILE:HG13	1.44	0.42
1:A:187:GLN:HB3	1:A:188:THR:H	1.36	0.42
1:A:232:ILE:O	1:A:233:THR:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LYS:O	1:A:14:ALA:C	2.61	0.42
1:A:74:ARG:HB3	1:A:75:PHE:H	1.61	0.42
1:A:388:ARG:HA	1:A:388:ARG:HD3	1.83	0.42
1:A:446:MET:HB2	1:A:446:MET:HE2	1.80	0.42
1:A:507:TYR:O	1:A:511:ILE:HG13	2.19	0.42
1:A:364:LEU:H	1:A:364:LEU:HG	1.40	0.42
1:A:416:LEU:O	1:A:417:ARG:C	2.60	0.42
1:A:615:LEU:HD13	1:A:670:GLN:HB2	2.02	0.42
1:A:178:PHE:HE1	1:A:630:ILE:HG13	1.85	0.42
1:A:636:LEU:HD23	1:A:636:LEU:HA	1.94	0.42
1:A:607:PHE:HE1	1:A:657:ALA:HB3	1.84	0.41
1:A:535:LYS:H	1:A:535:LYS:HG3	1.33	0.41
1:A:551:ASP:O	1:A:553:GLY:N	2.54	0.41
1:A:564:ALA:HA	1:A:638:TYR:HD1	1.85	0.41
1:A:144:ARG:HA	1:A:147:ILE:HD12	2.01	0.41
1:A:284:THR:HB	1:A:331:LEU:HA	1.77	0.41
1:A:607:PHE:HD1	1:A:659:LEU:HD21	1.84	0.41
1:A:361:THR:HB	1:A:362:TYR:H	1.51	0.41
1:A:415:GLY:O	1:A:416:LEU:C	2.63	0.41
1:A:202:ILE:HD13	1:A:202:ILE:HA	1.85	0.41
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.75	0.41
1:A:281:LYS:HE3	1:A:281:LYS:HB3	1.45	0.41
1:A:574:ARG:O	1:A:575:LEU:C	2.62	0.41
1:A:175:PRO:HB2	1:A:176:TYR:H	1.68	0.41
1:A:198:ILE:HG22	1:A:699:PHE:HE2	1.86	0.41
1:A:479:LEU:O	1:A:480:PRO:C	2.59	0.41
1:A:633:PRO:C	1:A:635:GLY:H	2.27	0.41
1:A:442:ILE:O	1:A:443:LEU:C	2.60	0.41
1:A:431:LEU:HD12	1:A:431:LEU:HA	1.84	0.40
1:A:434:PHE:O	1:A:435:PHE:C	2.60	0.40
1:A:562:ALA:O	1:A:563:SER:O	2.39	0.40
1:A:510:LEU:HD23	1:A:510:LEU:HA	1.80	0.40
1:A:581:TYR:O	1:A:582:THR:C	2.65	0.40
1:A:156:LEU:HD23	1:A:156:LEU:HA	1.76	0.40
1:A:357:LYS:HZ3	1:A:357:LYS:HG3	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	616/807 (76%)	449 (73%)	131 (21%)	36 (6%)	1 9

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	VAL
1	A	383	PRO
1	A	406	ILE
1	A	412	SER
1	A	512	PHE
1	A	513	MET
1	A	514	VAL
1	A	654	TYR
1	A	32	CYS
1	A	157	SER
1	A	175	PRO
1	A	413	ILE
1	A	450	ASN
1	A	552	GLN
1	A	563	SER
1	A	46	THR
1	A	75	PHE
1	A	159	CYS
1	A	446	MET
1	A	564	ALA
1	A	602	ALA
1	A	76	TRP
1	A	77	ASP
1	A	84	VAL
1	A	158	LEU
1	A	240	ARG
1	A	290	GLN
1	A	402	ASP

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Mol	Chain	Res	Type
1	A	415	GLY
1	A	459	ASN
1	A	543	ARG
1	A	625	SER
1	A	399	PHE
1	A	51	PRO
1	A	266	VAL
1	A	403	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	561/717 (78%)	314 (56%)	247 (44%)	0 0

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	GLN
1	A	12	SER
1	A	13	LYS
1	A	15	VAL
1	A	17	ILE
1	A	18	ARG
1	A	20	GLN
1	A	21	LEU
1	A	23	LEU
1	A	26	ARG
1	A	28	ASN
1	A	32	CYS
1	A	35	SER
1	A	37	LYS
1	A	40	THR
1	A	41	VAL
1	A	42	LEU

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Mol	Chain	Res	Type
1	A	43	GLN
1	A	45	VAL
1	A	50	ILE
1	A	52	THR
1	A	55	LEU
1	A	58	VAL
1	A	59	SER
1	A	62	LEU
1	A	66	LEU
1	A	69	SER
1	A	71	ILE
1	A	72	ARG
1	A	74	ARG
1	A	77	ASP
1	A	80	ARG
1	A	81	ILE
1	A	83	LEU
1	A	86	GLU
1	A	135	ASP
1	A	137	ILE
1	A	143	GLN
1	A	144	ARG
1	A	146	ILE
1	A	149	LEU
1	A	150	LEU
1	A	161	ILE
1	A	163	PRO
1	A	171	LEU
1	A	172	ASP
1	A	173	LYS
1	A	176	TYR
1	A	181	THR
1	A	186	LEU
1	A	190	ASN
1	A	191	ASP
1	A	193	LEU
1	A	195	LEU
1	A	198	ILE
1	A	199	PHE
1	A	204	LEU
1	A	211	MET
1	A	212	ARG

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Mol	Chain	Res	Type
1	A	217	SER
1	A	218	ILE
1	A	219	LYS
1	A	220	TYR
1	A	221	LYS
1	A	223	GLU
1	A	224	ASN
1	A	232	ILE
1	A	235	LEU
1	A	237	ARG
1	A	241	LYS
1	A	242	GLU
1	A	244	VAL
1	A	250	ASP
1	A	252	TYR
1	A	253	PRO
1	A	258	VAL
1	A	259	ASP
1	A	261	GLN
1	A	262	LEU
1	A	264	TYR
1	A	266	VAL
1	A	268	LYS
1	A	270	ILE
1	A	274	LYS
1	A	277	LYS
1	A	278	LYS
1	A	280	GLU
1	A	281	LYS
1	A	283	LEU
1	A	286	TYR
1	A	287	THR
1	A	289	LEU
1	A	291	VAL
1	A	292	LYS
1	A	293	THR
1	A	321	ILE
1	A	327	MET
1	A	328	LYS
1	A	330	ARG
1	A	331	LEU
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	335	ILE
1	A	337	GLU
1	A	338	GLU
1	A	340	ARG
1	A	352	VAL
1	A	353	THR
1	A	355	GLN
1	A	356	GLU
1	A	357	LYS
1	A	358	SER
1	A	359	MET
1	A	361	THR
1	A	363	ILE
1	A	364	LEU
1	A	365	LYS
1	A	371	LYS
1	A	382	GLN
1	A	390	LEU
1	A	393	SER
1	A	394	LYS
1	A	396	THR
1	A	398	THR
1	A	399	PHE
1	A	404	GLU
1	A	406	ILE
1	A	407	CYS
1	A	409	LYS
1	A	411	LEU
1	A	412	SER
1	A	413	ILE
1	A	417	ARG
1	A	420	LEU
1	A	423	LEU
1	A	425	ILE
1	A	426	ASN
1	A	428	THR
1	A	429	LEU
1	A	431	LEU
1	A	435	PHE
1	A	436	LEU
1	A	437	THR
1	A	439	PRO

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Mol	Chain	Res	Type
1	A	441	ILE
1	A	442	ILE
1	A	443	LEU
1	A	446	MET
1	A	447	ASP
1	A	448	LYS
1	A	451	VAL
1	A	455	ILE
1	A	458	LEU
1	A	459	ASN
1	A	460	ASN
1	A	462	ILE
1	A	463	ILE
1	A	468	PRO
1	A	471	LEU
1	A	479	LEU
1	A	481	SER
1	A	486	SER
1	A	491	SER
1	A	494	THR
1	A	495	LYS
1	A	496	SER
1	A	500	GLN
1	A	501	ILE
1	A	502	MET
1	A	503	MET
1	A	504	THR
1	A	505	LYS
1	A	512	PHE
1	A	513	MET
1	A	516	ILE
1	A	517	LEU
1	A	518	PRO
1	A	522	LEU
1	A	523	THR
1	A	524	SER
1	A	525	LEU
1	A	530	ARG
1	A	531	TRP
1	A	534	ASP
1	A	535	LYS
1	A	539	GLU

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Mol	Chain	Res	Type
1	A	541	SER
1	A	542	ILE
1	A	543	ARG
1	A	549	LEU
1	A	551	ASP
1	A	561	ILE
1	A	566	ILE
1	A	570	MET
1	A	572	LEU
1	A	573	LEU
1	A	574	ARG
1	A	575	LEU
1	A	579	ILE
1	A	583	PHE
1	A	585	MET
1	A	586	ILE
1	A	595	ARG
1	A	598	LYS
1	A	603	PHE
1	A	606	GLU
1	A	610	MET
1	A	613	TRP
1	A	614	MET
1	A	616	CYS
1	A	620	VAL
1	A	626	ILE
1	A	627	THR
1	A	630	ILE
1	A	631	ILE
1	A	636	LEU
1	A	637	ILE
1	A	639	ILE
1	A	640	LEU
1	A	641	LEU
1	A	644	MET
1	A	645	VAL
1	A	650	LEU
1	A	653	VAL
1	A	655	LEU
1	A	658	LYS
1	A	659	LEU
1	A	660	GLU

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Mol	Chain	Res	Type
1	A	661	LYS
1	A	663	ILE
1	A	668	VAL
1	A	672	LEU
1	A	675	PRO
1	A	676	ILE
1	A	678	CYS
1	A	688	LEU
1	A	690	LEU
1	A	692	MET
1	A	697	THR
1	A	698	LEU
1	A	702	LEU
1	A	703	VAL
1	A	704	LEU
1	A	708	ILE
1	A	711	CYS
1	A	712	LEU
1	A	717	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	143	GLN
1	A	185	ASN
1	A	187	GLN
1	A	214	HIS
1	A	224	ASN
1	A	261	GLN
1	A	410	ASN
1	A	450	ASN
1	A	459	ASN
1	A	568	ASN
1	A	596	ASN
1	A	604	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](#)

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$
2	POV	A	901	-	51,51,51	0.94	2 (3%)	57,59,59	1.12	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	POV	A	901	-	-	28/55/55/55	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	POV	O31-C31	4.33	1.46	1.33
2	A	901	POV	O21-C21	3.82	1.45	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	POV	O21-C21-C22	3.89	119.90	111.48
2	A	901	POV	O21-C21-O22	-3.66	115.14	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	POV	O31-C31-C32	2.73	120.16	111.83
2	A	901	POV	C11-C12-N	2.31	123.23	115.82

There are no chirality outliers.

All (28) torsion outliers are listed below:

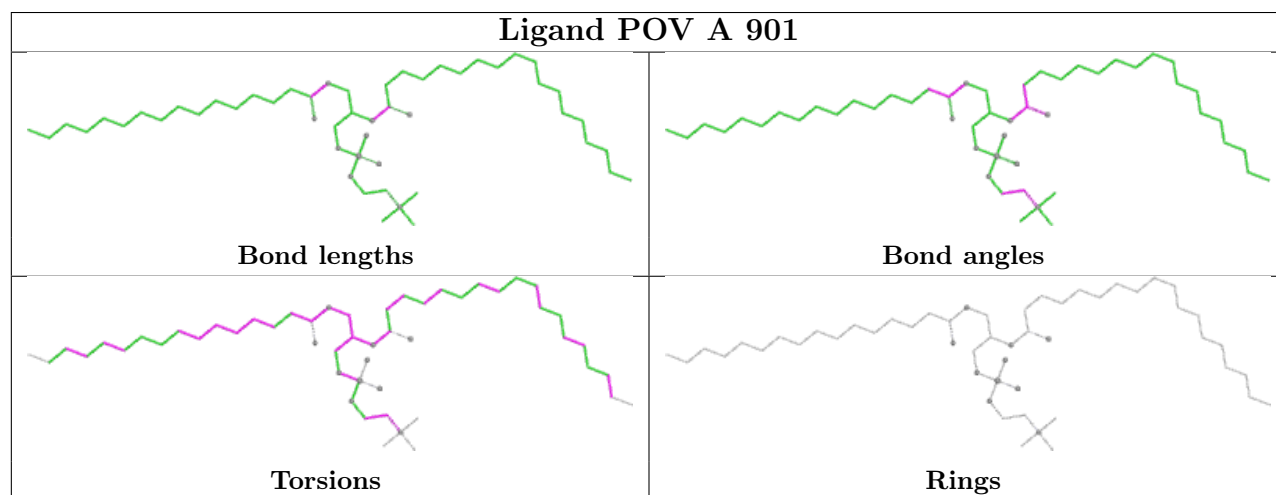
Mol	Chain	Res	Type	Atoms
2	A	901	POV	C1-O11-P-O14
2	A	901	POV	O12-C11-C12-N
2	A	901	POV	C22-C21-O21-C2
2	A	901	POV	O22-C21-O21-C2
2	A	901	POV	C2-C3-O31-C31
2	A	901	POV	C36-C37-C38-C39
2	A	901	POV	C21-C22-C23-C24
2	A	901	POV	C212-C213-C214-C215
2	A	901	POV	O21-C2-C3-O31
2	A	901	POV	C34-C35-C36-C37
2	A	901	POV	C11-C12-N-C15
2	A	901	POV	C310-C311-C312-C313
2	A	901	POV	C1-C2-O21-C21
2	A	901	POV	C26-C27-C28-C29
2	A	901	POV	C23-C24-C25-C26
2	A	901	POV	C312-C313-C314-C315
2	A	901	POV	C215-C216-C217-C218
2	A	901	POV	O11-C1-C2-O21
2	A	901	POV	C11-C12-N-C13
2	A	901	POV	C1-C2-C3-O31
2	A	901	POV	C11-C12-N-C14
2	A	901	POV	C33-C34-C35-C36
2	A	901	POV	C32-C33-C34-C35
2	A	901	POV	C29-C210-C211-C212
2	A	901	POV	C32-C31-O31-C3
2	A	901	POV	O31-C31-C32-C33
2	A	901	POV	O32-C31-O31-C3
2	A	901	POV	C35-C36-C37-C38

There are no ring outliers.

No monomer is involved in short contacts.

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.

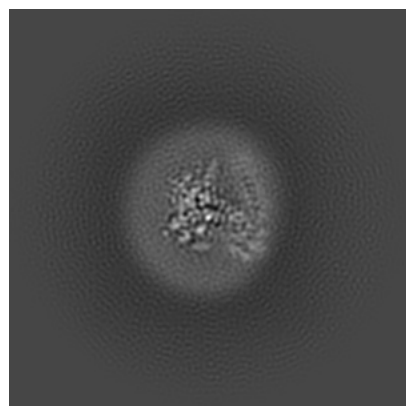
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34214. These allow visual inspection of the internal detail of the map and identification of artifacts.

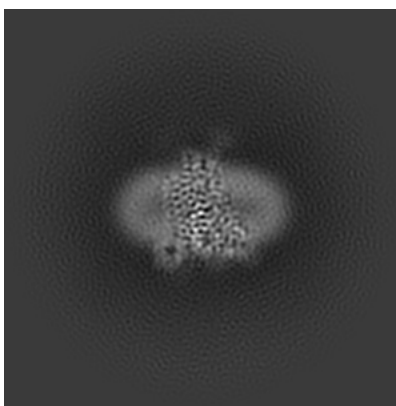
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

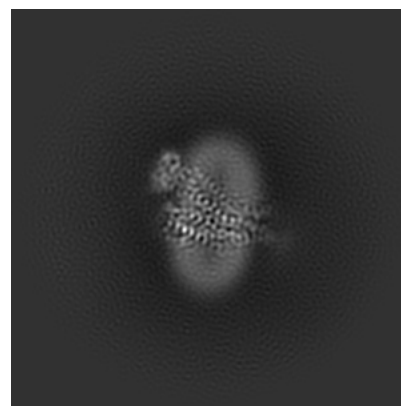
6.1.1 Primary map



X

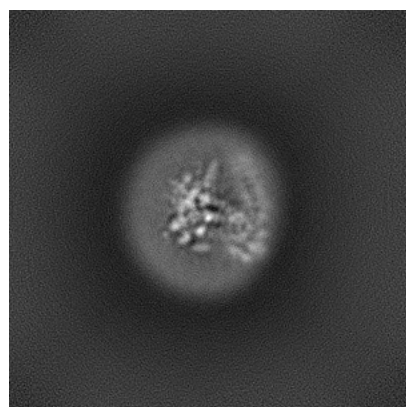


Y

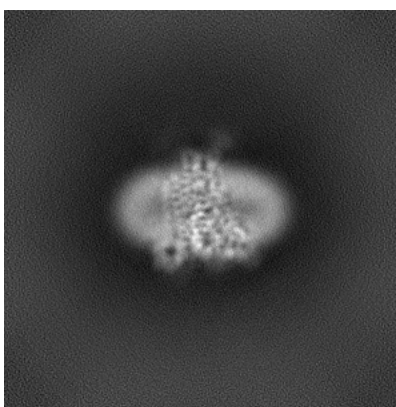


Z

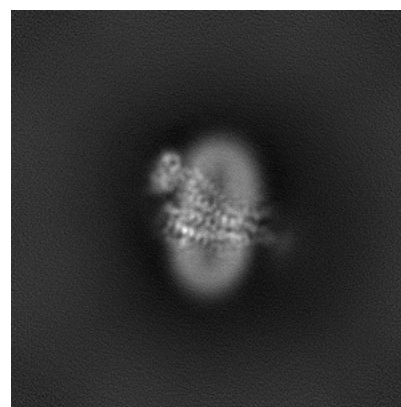
6.1.2 Raw map



X



Y

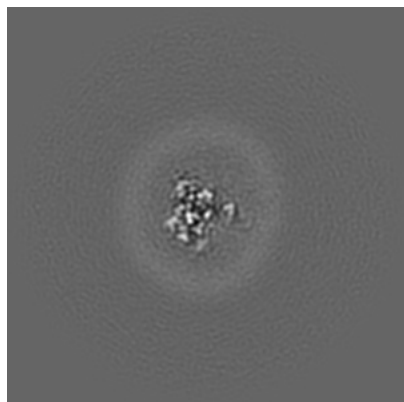


Z

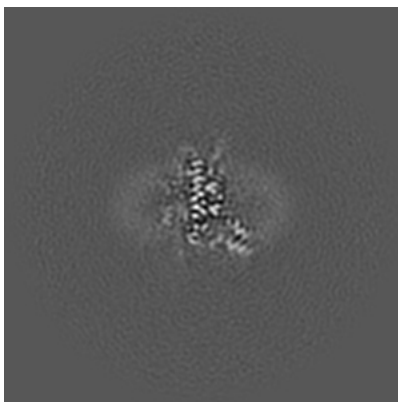
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

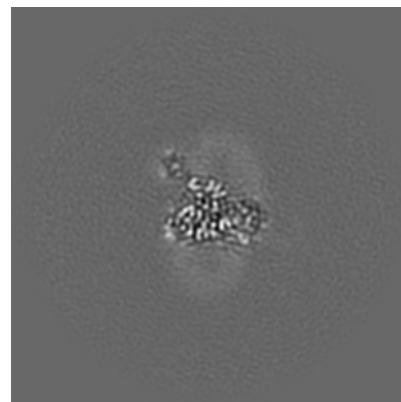
6.2.1 Primary map



X Index: 160

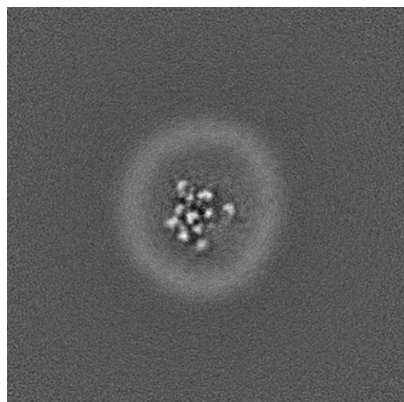


Y Index: 160

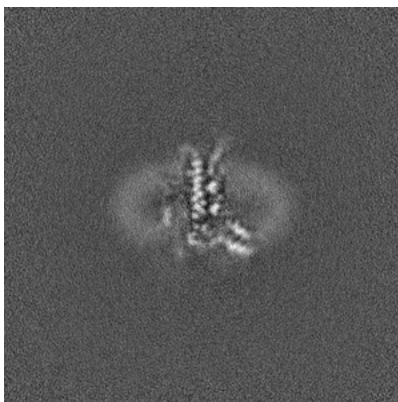


Z Index: 160

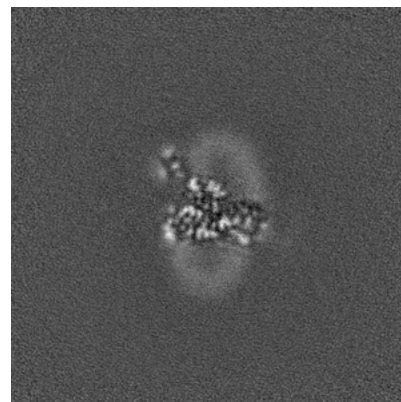
6.2.2 Raw map



X Index: 160



Y Index: 160

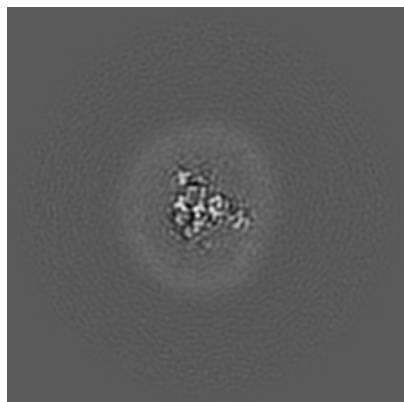


Z Index: 160

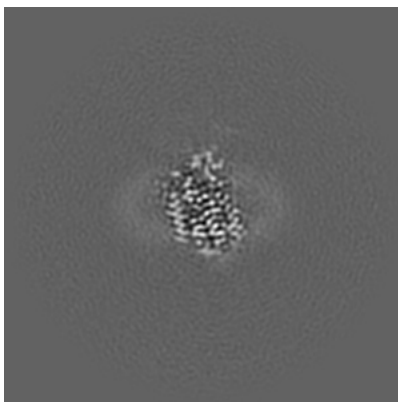
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

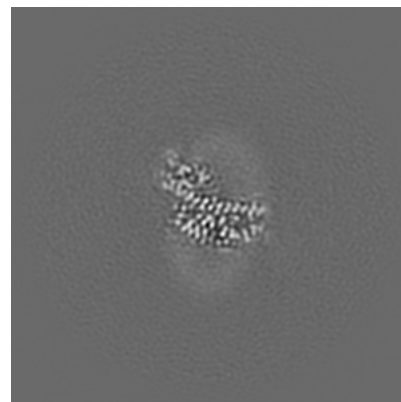
6.3.1 Primary map



X Index: 150

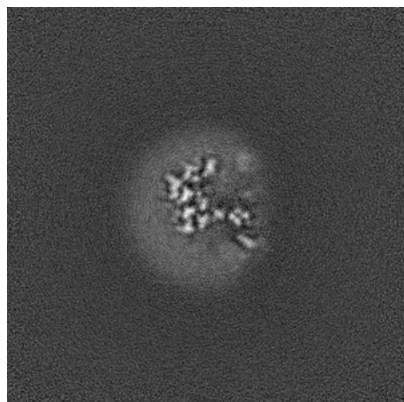


Y Index: 143

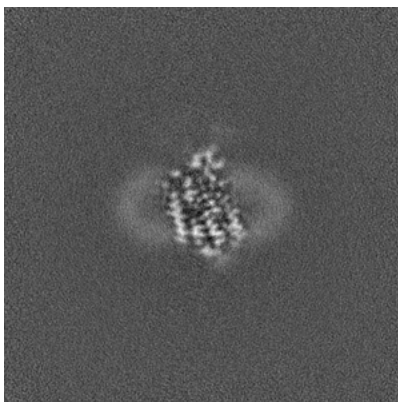


Z Index: 152

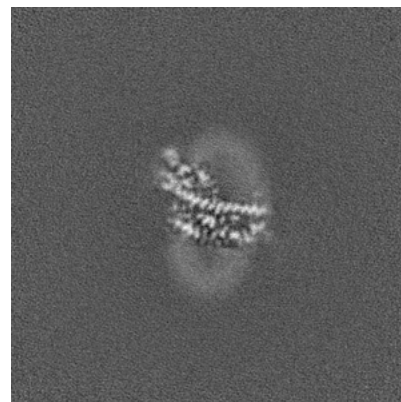
6.3.2 Raw map



X Index: 138



Y Index: 143

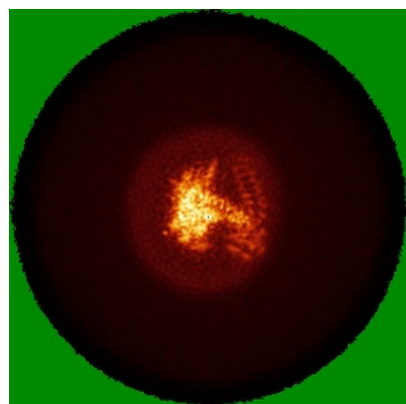


Z Index: 153

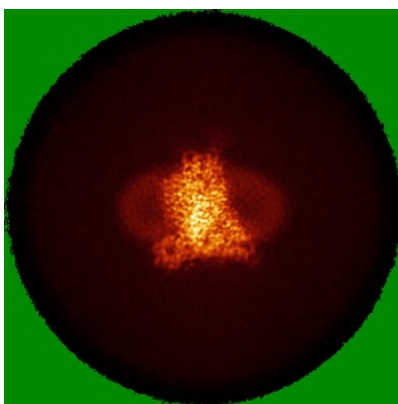
The images above show the largest variance slices of the map in three orthogonal directions.

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

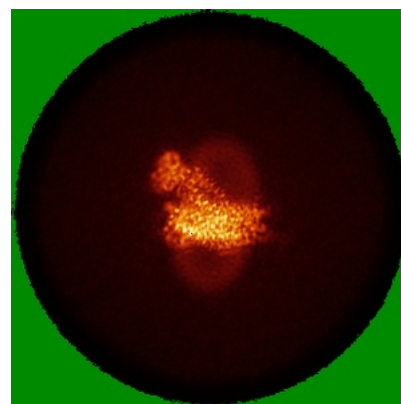
6.4.1 Primary map



X

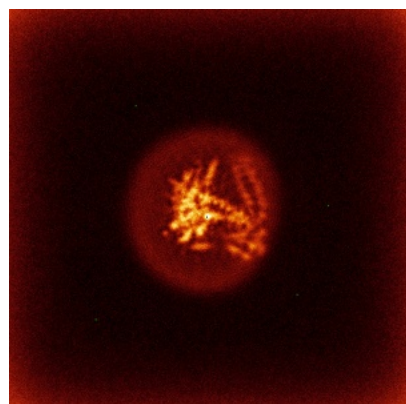


Y

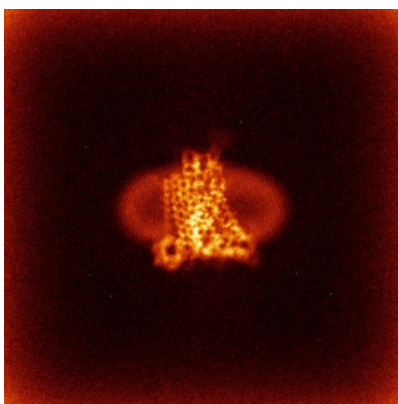


Z

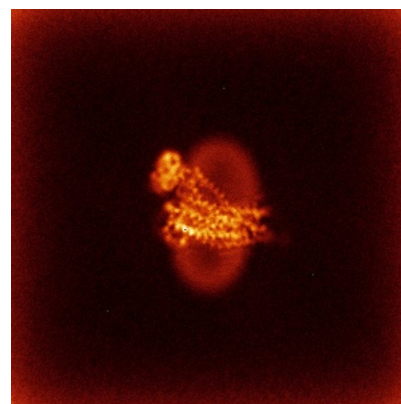
6.4.2 Raw map



X



Y

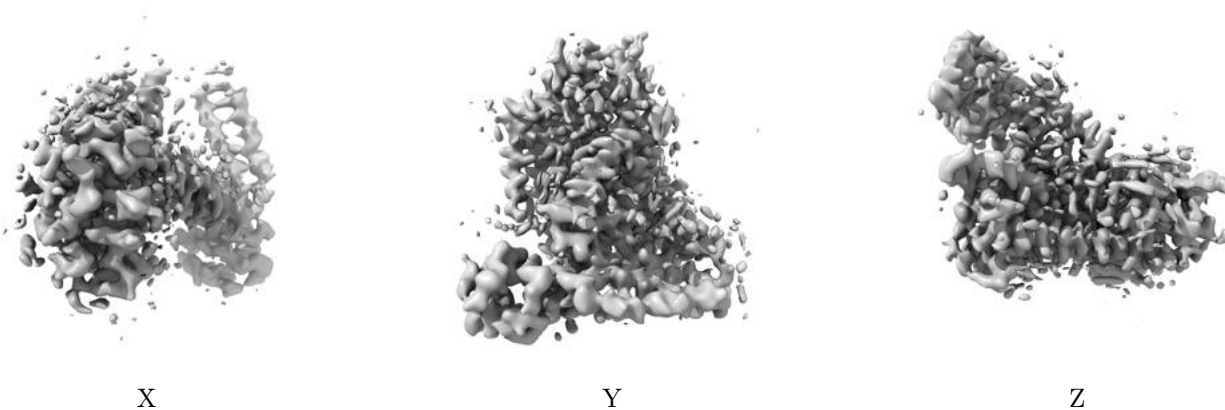


Z

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.

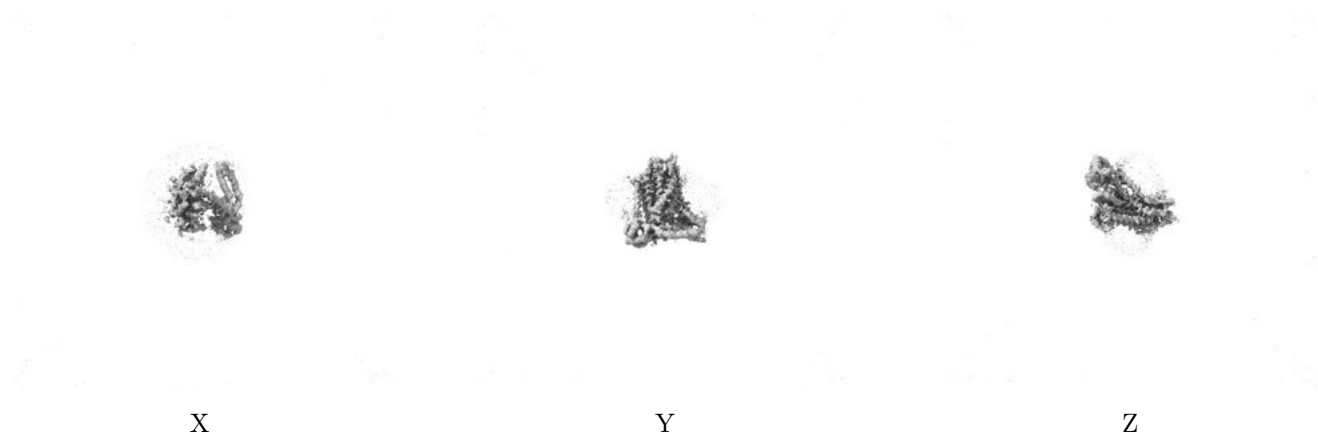
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. 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.

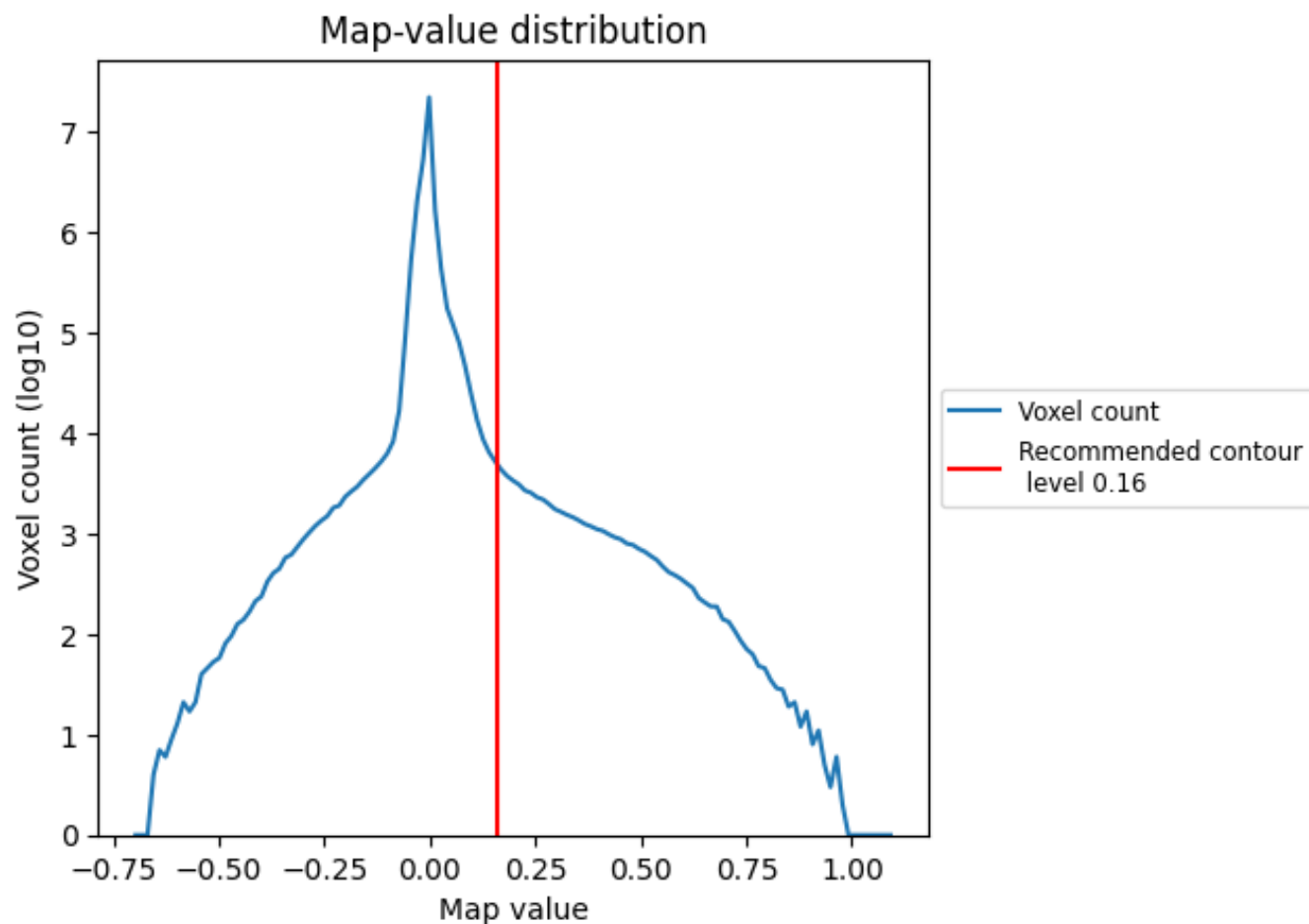
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

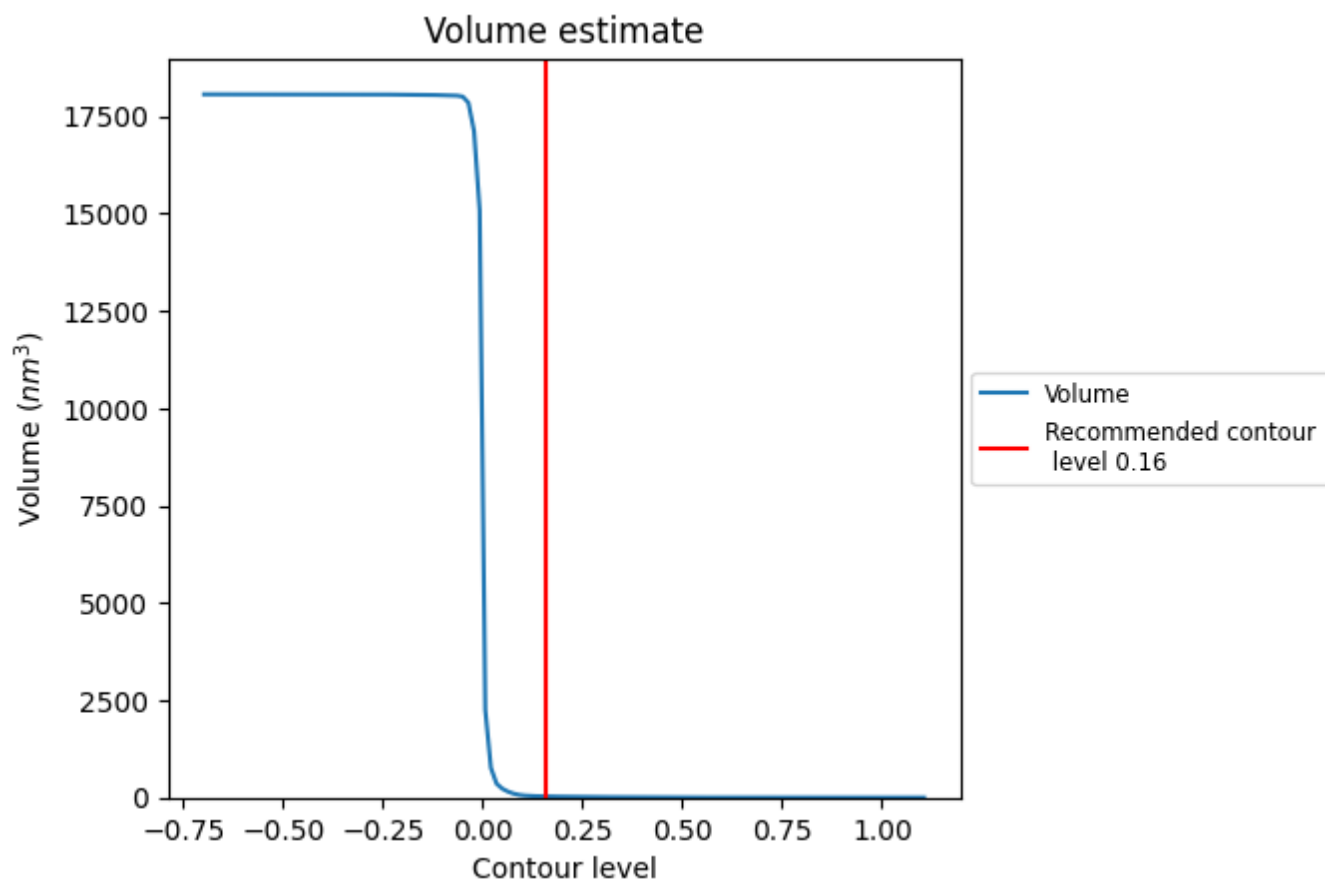
This section contains the results of statistical analysis of the map.

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.

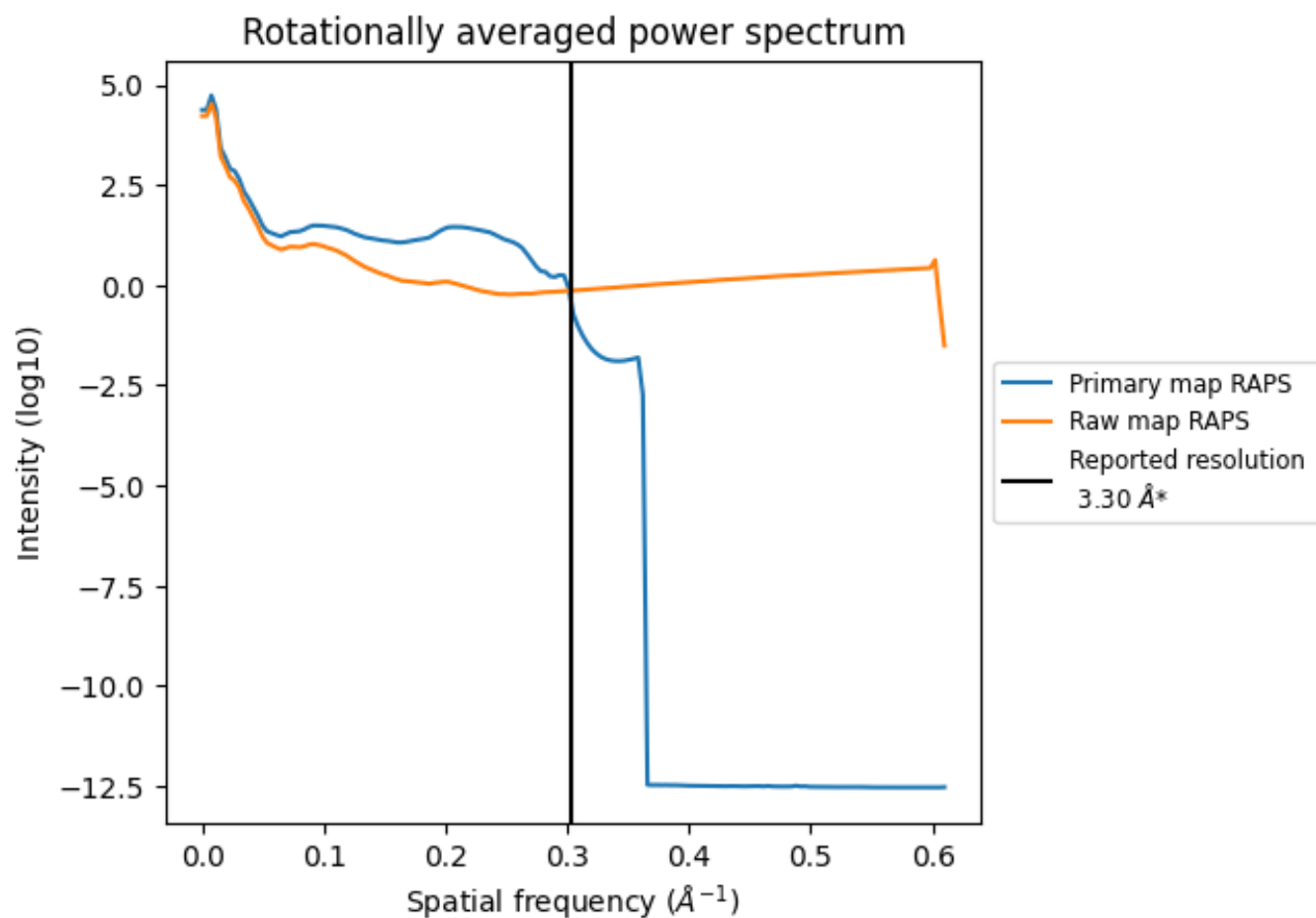
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29 nm³; this corresponds to an approximate mass of 26 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 ⓘ

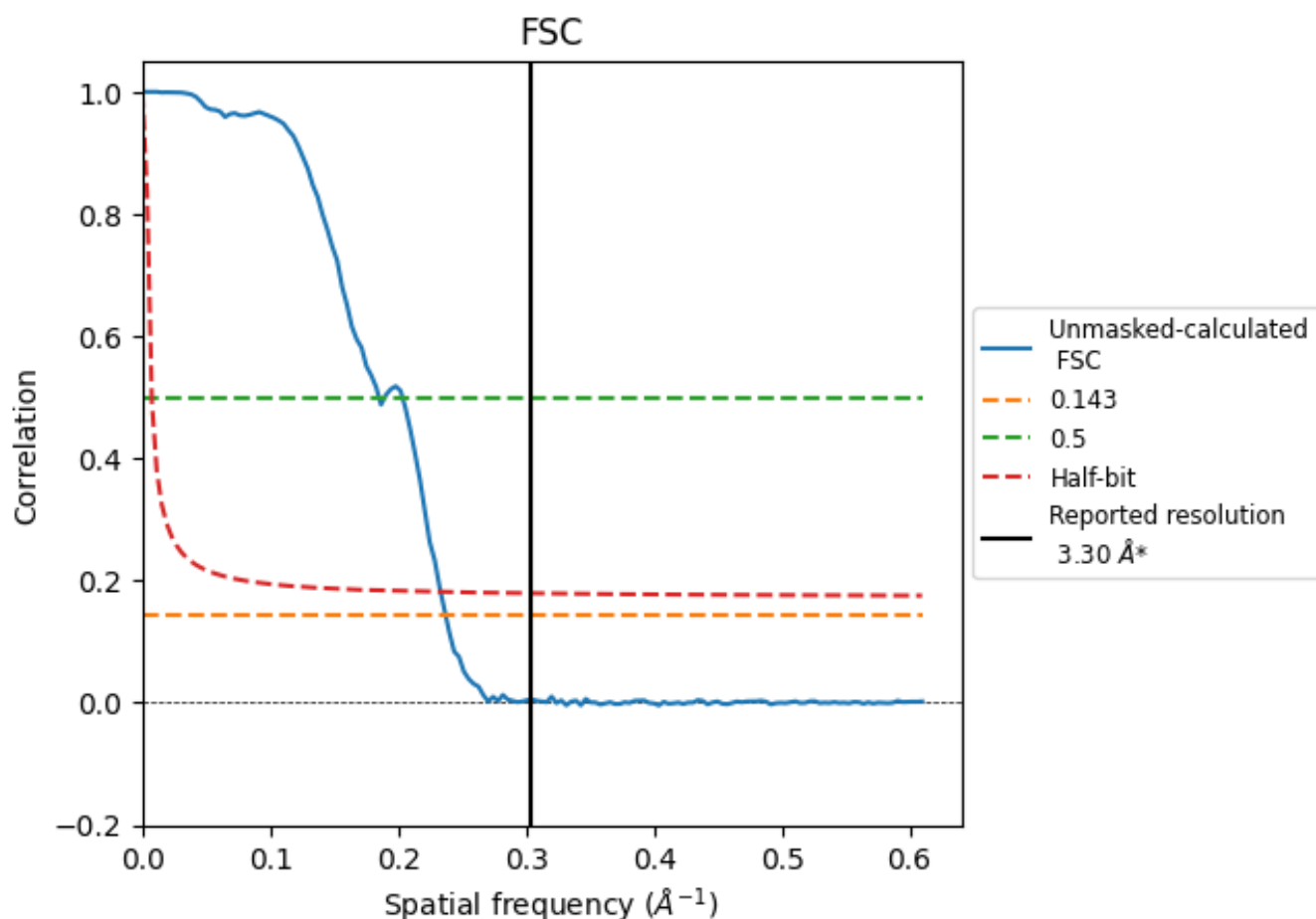


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

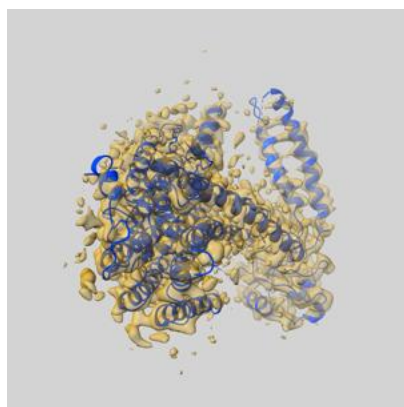
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.21	5.40	4.29

*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 4.21 differs from the reported value 3.3 by more than 10 %

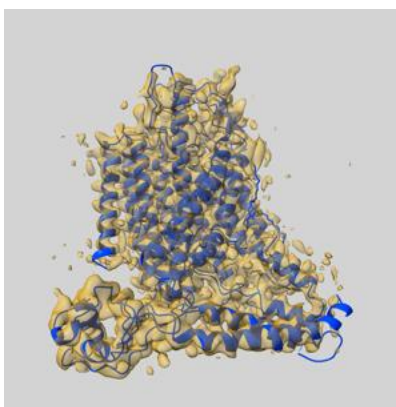
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34214 and PDB model 8GRS. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

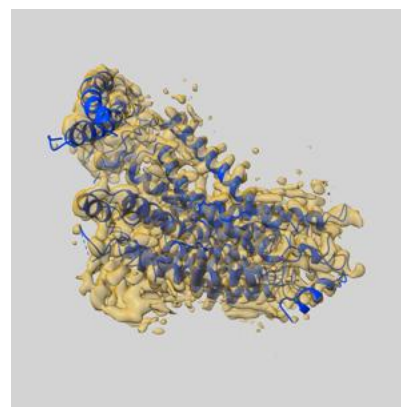
9.1 Map-model overlay [i](#)



X



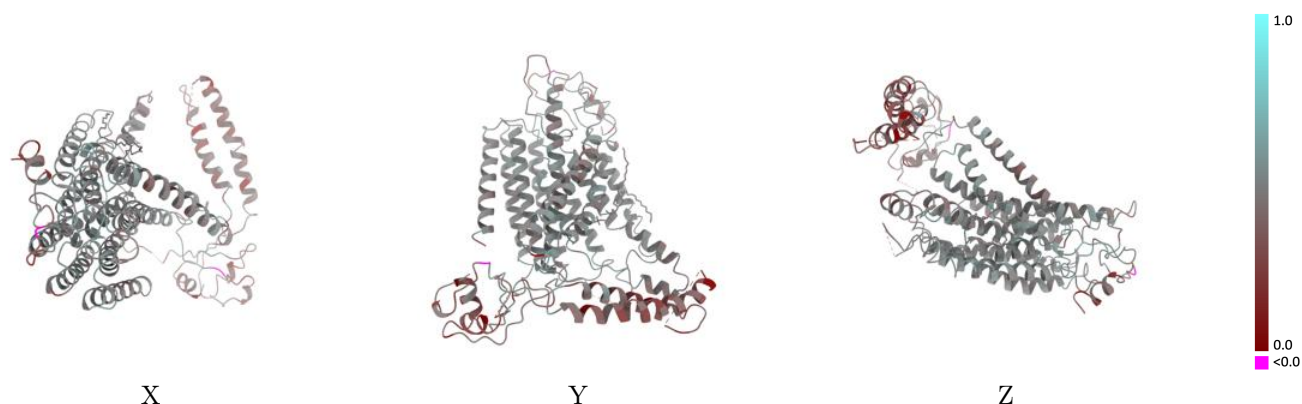
Y



Z

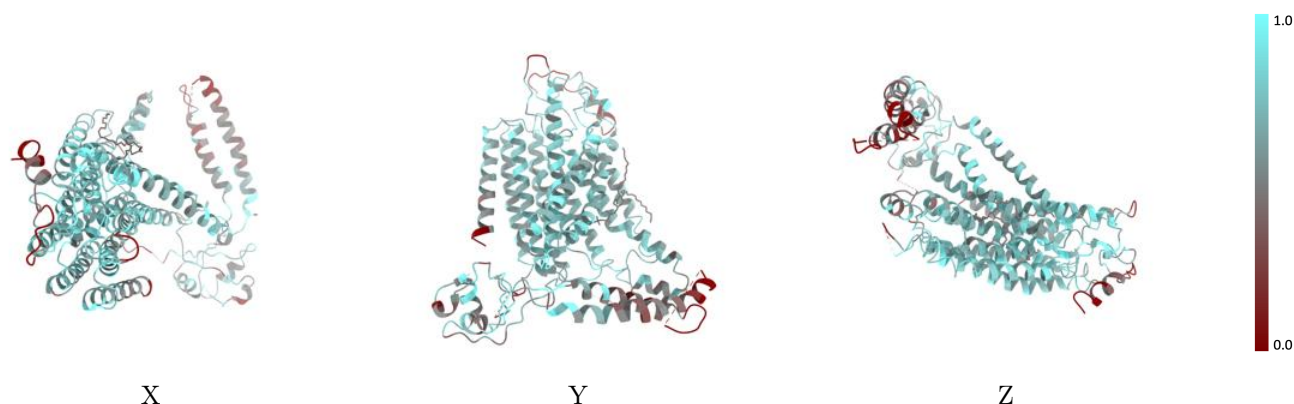
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



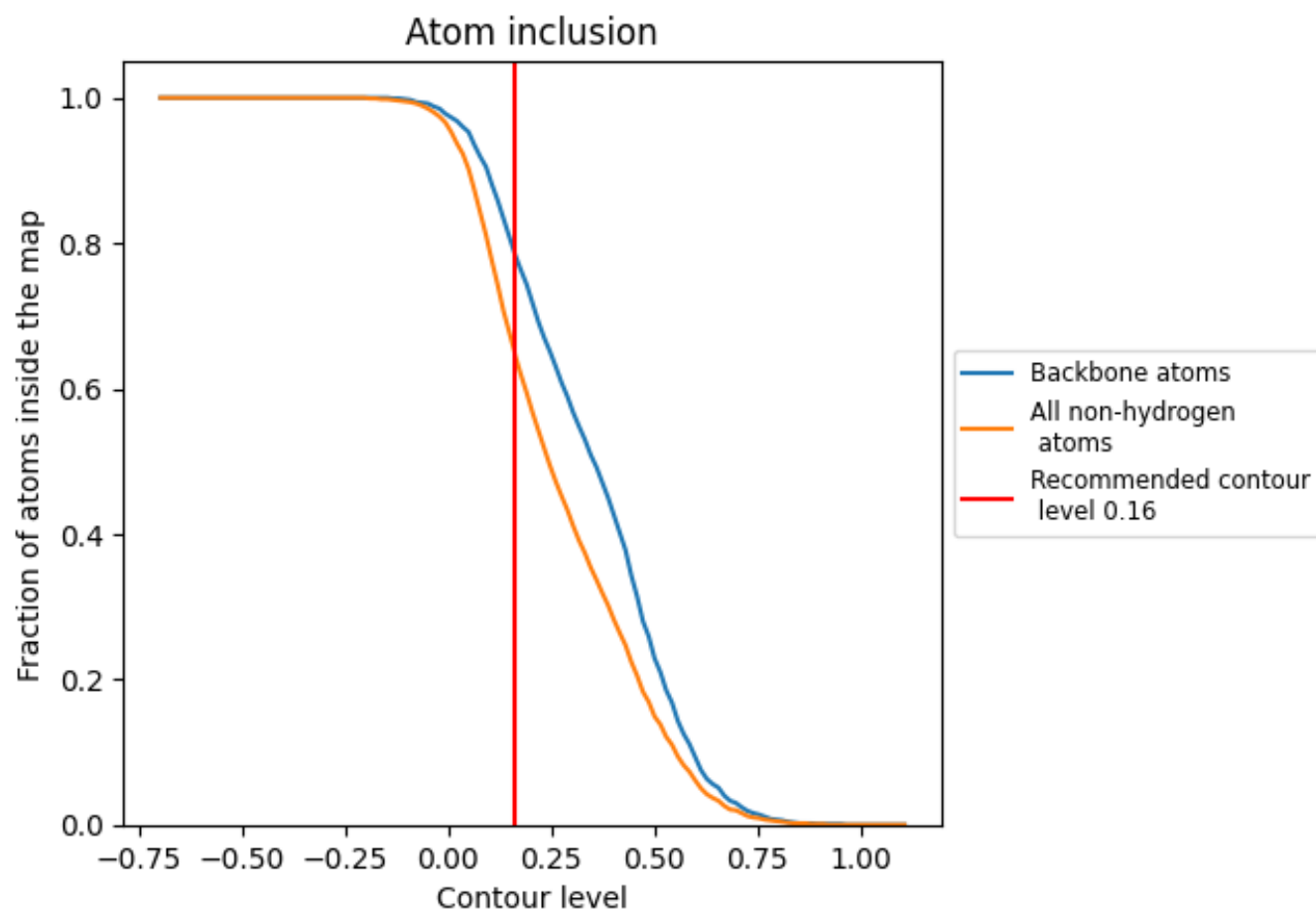
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.16).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 65% 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 (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6520	0.4470
A	0.6520	0.4470

