



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 9J4X / pdb_00009j4x
EMDB ID : EMD-61138
Title : CryoEM structure of human XPR1 in apo state
Authors : Zhang, W.H.; Chen, Y.K.; Guan, Z.Y.; Liu, Z.
Deposited on : 2024-08-10
Resolution : 2.90 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

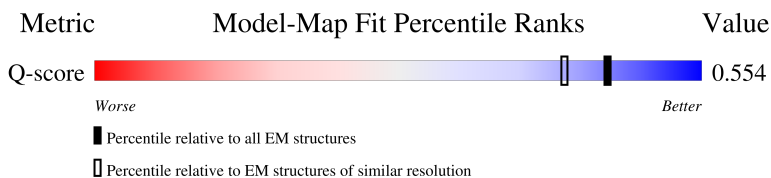
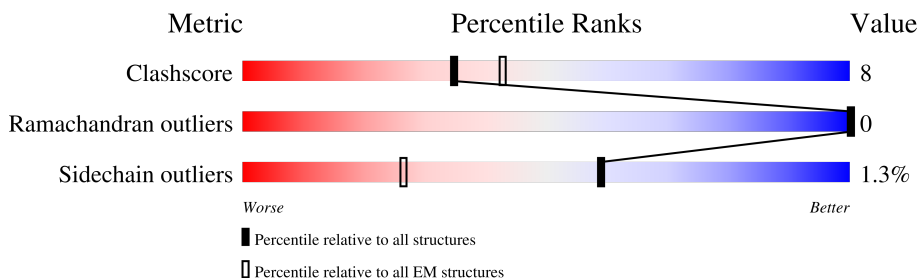
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

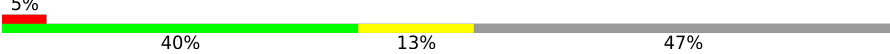
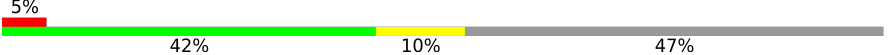
The reported resolution of this entry is 2.90 Å.

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	13054 (2.40 - 3.40)

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	720	
1	B	720	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6588 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 Solute carrier family 53 member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	382	Total	C	N	O	S	0	0
			3186	2143	510	518	15		
1	B	382	Total	C	N	O	S	0	0
			3186	2143	510	518	15		

There are 48 discrepancies between the modelled and reference sequences:

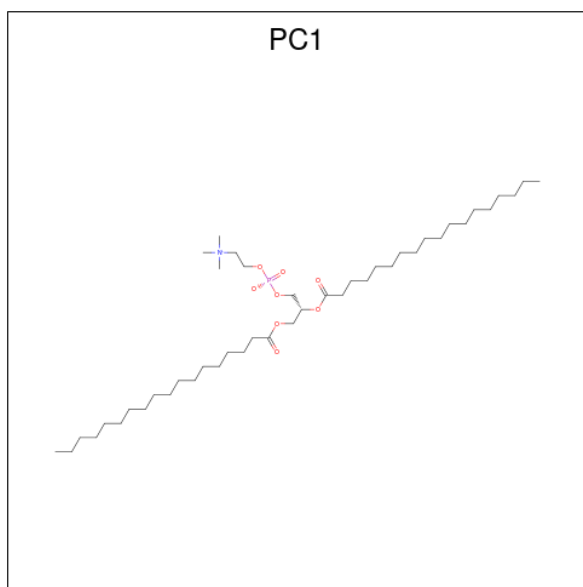
Chain	Residue	Modelled	Actual	Comment	Reference
A	697	LEU	-	expression tag	UNP Q9UBH6
A	698	GLU	-	expression tag	UNP Q9UBH6
A	699	ASP	-	expression tag	UNP Q9UBH6
A	700	TYR	-	expression tag	UNP Q9UBH6
A	701	LYS	-	expression tag	UNP Q9UBH6
A	702	ASP	-	expression tag	UNP Q9UBH6
A	703	HIS	-	expression tag	UNP Q9UBH6
A	704	ASP	-	expression tag	UNP Q9UBH6
A	705	GLY	-	expression tag	UNP Q9UBH6
A	706	ASP	-	expression tag	UNP Q9UBH6
A	707	TYR	-	expression tag	UNP Q9UBH6
A	708	LYS	-	expression tag	UNP Q9UBH6
A	709	ASP	-	expression tag	UNP Q9UBH6
A	710	HIS	-	expression tag	UNP Q9UBH6
A	711	ASP	-	expression tag	UNP Q9UBH6
A	712	ILE	-	expression tag	UNP Q9UBH6
A	713	ASP	-	expression tag	UNP Q9UBH6
A	714	TYR	-	expression tag	UNP Q9UBH6
A	715	LYS	-	expression tag	UNP Q9UBH6
A	716	ASP	-	expression tag	UNP Q9UBH6
A	717	ASP	-	expression tag	UNP Q9UBH6
A	718	ASP	-	expression tag	UNP Q9UBH6
A	719	ASP	-	expression tag	UNP Q9UBH6
A	720	LYS	-	expression tag	UNP Q9UBH6
B	697	LEU	-	expression tag	UNP Q9UBH6
B	698	GLU	-	expression tag	UNP Q9UBH6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	699	ASP	-	expression tag	UNP Q9UBH6
B	700	TYR	-	expression tag	UNP Q9UBH6
B	701	LYS	-	expression tag	UNP Q9UBH6
B	702	ASP	-	expression tag	UNP Q9UBH6
B	703	HIS	-	expression tag	UNP Q9UBH6
B	704	ASP	-	expression tag	UNP Q9UBH6
B	705	GLY	-	expression tag	UNP Q9UBH6
B	706	ASP	-	expression tag	UNP Q9UBH6
B	707	TYR	-	expression tag	UNP Q9UBH6
B	708	LYS	-	expression tag	UNP Q9UBH6
B	709	ASP	-	expression tag	UNP Q9UBH6
B	710	HIS	-	expression tag	UNP Q9UBH6
B	711	ASP	-	expression tag	UNP Q9UBH6
B	712	ILE	-	expression tag	UNP Q9UBH6
B	713	ASP	-	expression tag	UNP Q9UBH6
B	714	TYR	-	expression tag	UNP Q9UBH6
B	715	LYS	-	expression tag	UNP Q9UBH6
B	716	ASP	-	expression tag	UNP Q9UBH6
B	717	ASP	-	expression tag	UNP Q9UBH6
B	718	ASP	-	expression tag	UNP Q9UBH6
B	719	ASP	-	expression tag	UNP Q9UBH6
B	720	LYS	-	expression tag	UNP Q9UBH6

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
2	B	1	Total	C	N	O	P	0
			54	44	1	8	1	

THR	GLU	CYS	ARG	GLU	VAL	GLN	LYS	HIS	THR	GLU	LEU	ALA	LYS	ILE	THR	PHE	TYR	GLU	SER	LYS	GLU	LEU	ALA	GLN	VAL	THR	ILE	ARG	GLN	ASN	TYR	GLN	ASN	GLY	THR	VAL	THR	LEU	SER	HIS	GLU							
GLU	ARG	VAL	ALA	PRO	PHE	HIS	ARG	ASN	ILE	LYS	ASP	ASN	THR	ILE	THR	LYS	LEU	PHE	GLU	SER	GLU	LEU	ALA	TYR	SER	VAL	THR	ILE	ARG	LEU	ARG	ILE	VAL	PRO	LYS	THR	GLY	PHE	ASP	LEU	SER	HIS	VAL					
E260	T261	D262	R263	S264	I265	I271	I279	E280	F281	L285	W292	V300	L305	N306	P307	R308	S309	E318	I319	G324	I325	L331	L332	F336	I339	S340	V341	L351	Y352	M355	V356	I360	Y367	W373	I374	L375	A384	P385	F394	W395								
Q399	S404	M408	L419	E420	L421	K422	W423	D424	E425	S426	K427	Q428	L429	L430	P431	ASN	ASN	SER	GLU	GLU	SER	GLY	ILE	CYS	HIS	LYS	TYR	THR	G446	V447	R448	Q452	P455	A456	W457	L458	R459	F460	I461	R466	R472	K482	T485	T486	F487	F488	M489	K500
E501	R502	G503	H504	S505	D506	T507	M508	Y518	I519	L526	D529	D533	W534	G535	L536	K539	H540	E543	R548	Y559	I563	V567	R570	T574	I579	T580	S581	L584	L585	P586	H587	R611	L612	E613	M614	E615	H616	L617	G621	E622	F623	R624	ALA					
VAL	ARG	ASP	ILE	SER	VAL	VAL	ALA	PRO	ALA	ASN	ASN	THR	ALA	ASP	GLN	THR	LEU	LYS	ASP	GLU	GLN	MET	MET	ASP	GLN	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLN	ASN	SER	ILE	SER	LYS	ALA	ARG	ASP	THR	LYS	VAL			
LEU	ILE	GLU	ASP	THR	ASP	VAL	ASP	ASP	GLU	ALA	ASN	ASN	THR	THR	GLU	GLY	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174844	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.118	Depositor
Minimum map value	-4.352	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.75	Depositor
Map size ($\text{\AA}$)	299.6, 299.6, 299.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	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: PC1

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	0.14	0/3292	0.33	0/4479
1	B	0.14	0/3292	0.29	0/4479
All	All	0.14	0/6584	0.31	0/8958

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3186	0	3186	58	0
1	B	3186	0	3186	46	0
2	A	108	0	176	7	0
2	B	108	0	176	5	0
All	All	6588	0	6724	106	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 8.

All (106) 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:B:251:LEU:HD21	1:B:331:LEU:HD23	1.76	0.68
1:A:306:ASN:ND2	1:A:309:SER:OG	2.27	0.67
1:A:251:LEU:HD21	1:A:331:LEU:HD23	1.76	0.67
1:B:385:PRO:HD3	1:B:461:ILE:HD12	1.78	0.65
1:A:611:ARG:NH1	1:A:620:CYS:SG	2.70	0.64
1:A:271:ILE:O	1:A:352:TYR:OH	2.14	0.61
1:A:310:ASN:HA	2:A:801:PC1:H112	1.83	0.60
1:A:272:TYR:OH	1:A:334:CYS:SG	2.60	0.59
1:A:466:ARG:NH2	1:A:621:GLY:O	2.24	0.59
1:B:482:LYS:O	1:B:485:THR:OG1	2.20	0.58
2:A:801:PC1:H342	2:A:801:PC1:H2	1.86	0.58
1:B:373:TRP:HB2	2:B:801:PC1:H153	1.85	0.57
1:A:277:LEU:HD11	1:A:597:ALA:HB1	1.86	0.57
1:B:318:GLU:OE1	1:B:367:TYR:OH	2.23	0.56
1:B:472:ARG:NH2	1:B:622:GLU:OE1	2.37	0.56
1:B:533:ASP:OD1	1:B:611:ARG:NH1	2.39	0.55
1:B:260:GLU:OE1	1:B:263:ARG:NH1	2.40	0.55
1:B:559:TYR:OH	1:B:613:GLU:OE2	2.26	0.54
1:A:385:PRO:O	1:A:465:ARG:NH1	2.38	0.54
1:A:482:LYS:O	1:A:485:THR:OG1	2.25	0.53
2:A:802:PC1:H261	2:A:802:PC1:H352	1.90	0.53
1:A:399:GLN:HG2	1:A:604:ARG:HD2	1.91	0.53
1:A:385:PRO:HD3	1:A:461:ILE:HD12	1.91	0.52
1:B:332:LEU:O	1:B:336:PHE:N	2.37	0.51
1:A:578:SER:O	1:A:582:THR:OG1	2.26	0.51
1:B:281:PHE:HE2	2:B:801:PC1:H381	1.75	0.51
1:B:534:TRP:O	1:B:548:ARG:NH1	2.43	0.50
1:A:364:LYS:HG3	1:A:368:TYR:CD2	2.47	0.50
1:B:395:TRP:O	1:B:399:GLN:HG2	2.12	0.50
1:A:398:ASP:OD2	1:A:604:ARG:NH1	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:LEU:HD21	2:B:801:PC1:H332	1.94	0.49
1:A:300:VAL:HG13	1:A:305:LEU:HB2	1.95	0.49
1:A:279:ILE:HD13	1:A:324:GLY:HA2	1.94	0.49
1:B:236:ARG:NE	1:B:318:GLU:OE2	2.29	0.49
1:A:404:SER:O	1:A:408:MET:HG2	2.12	0.49
1:A:281:PHE:HE2	2:A:801:PC1:H381	1.78	0.49
1:B:404:SER:HB3	1:B:455:PRO:HG2	1.95	0.49
1:A:295:ALA:HB1	1:A:552:VAL:HG12	1.95	0.48
1:B:305:LEU:HD22	2:B:801:PC1:H112	1.95	0.48
1:A:271:ILE:HG12	1:A:413:MET:HG2	1.96	0.48
1:B:457:TRP:HA	1:B:487:PHE:HZ	1.78	0.48
1:B:518:TYR:HD1	1:B:519:ILE:HD12	1.78	0.48
1:B:529:ASP:HA	1:B:533:ASP:HB2	1.96	0.48
1:A:550:GLU:HG3	1:A:617:LEU:HD13	1.97	0.47
1:B:536:LEU:HD13	1:B:563:ILE:HD11	1.97	0.47
1:B:271:ILE:O	1:B:352:TYR:OH	2.25	0.46
1:B:300:VAL:HG13	1:B:305:LEU:HB2	1.96	0.46
1:B:408:MET:HE1	1:B:448:ARG:HG3	1.98	0.46
1:B:279:ILE:HD13	1:B:324:GLY:HA2	1.97	0.46
1:B:356:VAL:O	1:B:360:ILE:HG12	2.15	0.46
1:A:240:PHE:HA	1:A:325:ILE:HD11	1.97	0.46
1:A:548:ARG:HH12	1:A:613:GLU:CD	2.24	0.45
1:B:319:ILE:HD13	2:B:801:PC1:H242	1.98	0.45
1:B:404:SER:O	1:B:408:MET:HG2	2.17	0.45
1:B:452:GLN:HG2	1:B:581:SER:HB3	1.97	0.45
1:A:355:MET:HB3	2:A:801:PC1:H2D2	1.97	0.45
1:A:251:LEU:HD11	1:A:331:LEU:HG	1.98	0.45
1:A:306:ASN:OD1	1:A:306:ASN:N	2.47	0.45
1:B:351:LEU:HD11	1:B:355:MET:HE3	1.98	0.45
1:B:526:LEU:HD21	1:B:567:VAL:HG22	1.99	0.45
1:A:529:ASP:HA	1:A:533:ASP:HB2	1.99	0.45
1:A:536:LEU:HD13	1:A:563:ILE:HD11	1.97	0.45
1:A:559:TYR:OH	1:A:613:GLU:OE2	2.29	0.44
1:A:472:ARG:NH2	1:A:475:PRO:HG3	2.32	0.44
1:A:457:TRP:HA	1:A:487:PHE:HZ	1.80	0.44
1:A:506:ASP:O	1:A:509:VAL:HG22	2.18	0.44
1:B:489:MET:HE1	1:B:574:THR:HG22	2.00	0.44
1:B:306:ASN:ND2	1:B:309:SER:OG	2.46	0.44
1:A:367:TYR:HB3	1:A:370:SER:OG	2.18	0.44
1:A:270:ARG:NH1	1:A:590:ASP:OD1	2.52	0.43
1:B:466:ARG:NH2	1:B:621:GLY:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:O	1:A:261:THR:OG1	2.31	0.43
1:B:263:ARG:HA	1:B:431:PRO:HA	1.99	0.43
1:A:410:LEU:HD21	2:A:801:PC1:H2G1	2.00	0.43
1:B:579:ILE:HG12	1:B:584:LEU:HD21	2.01	0.43
1:A:292:TRP:HE1	1:A:609:PHE:HA	1.84	0.43
1:B:292:TRP:CE2	1:B:612:LEU:HD22	2.54	0.42
1:A:271:ILE:HG23	1:A:413:MET:SD	2.58	0.42
1:A:551:ILE:HD12	1:A:559:TYR:CZ	2.54	0.42
1:A:569:LEU:O	1:A:573:TRP:N	2.49	0.42
1:B:251:LEU:HD11	1:B:331:LEU:HG	2.02	0.42
1:B:459:ARG:HD2	1:B:459:ARG:HA	1.82	0.42
1:A:268:LEU:HD12	1:A:268:LEU:HA	1.94	0.42
1:A:369:LYS:HB3	2:A:801:PC1:H132	2.01	0.42
1:A:366:PHE:O	1:A:371:ARG:NE	2.37	0.42
1:A:489:MET:HE2	1:A:489:MET:HB3	1.97	0.42
1:A:378:LEU:HD23	1:A:396:LEU:HD21	2.02	0.41
1:B:240:PHE:HA	1:B:325:ILE:HD11	2.02	0.41
1:A:552:VAL:HG23	1:A:617:LEU:HD11	2.01	0.41
1:B:242:GLY:O	1:B:246:VAL:HG23	2.20	0.41
1:A:508:MET:HG3	1:A:512:TYR:CE2	2.55	0.41
1:B:611:ARG:NH2	1:B:615:GLU:OE2	2.48	0.41
1:A:356:VAL:O	1:A:360:ILE:HG12	2.20	0.41
1:B:339:ILE:HG22	1:B:341:VAL:HG22	2.03	0.41
1:A:266:TRP:CH2	1:A:591:ILE:HG13	2.56	0.41
1:A:472:ARG:HH21	1:A:622:GLU:CD	2.28	0.41
1:A:484:SER:HA	1:A:487:PHE:CD2	2.56	0.41
1:B:570:ARG:O	1:B:574:THR:OG1	2.36	0.41
1:A:291:GLY:HA3	1:A:609:PHE:HE1	1.84	0.41
1:A:263:ARG:HD2	1:A:431:PRO:HA	2.03	0.41
1:A:459:ARG:HD3	1:A:483:TYR:CZ	2.56	0.41
1:A:457:TRP:O	1:A:461:ILE:HG12	2.21	0.40
1:A:551:ILE:HD13	1:A:551:ILE:HA	1.91	0.40
1:A:496:TYR:CE2	1:A:511:PHE:HB2	2.57	0.40
1:B:617:LEU:HD12	1:B:617:LEU:HA	1.91	0.40
1:B:360:ILE:HA	1:B:375:LEU:HD11	2.04	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	378/720 (52%)	358 (95%)	20 (5%)	0	100	100
1	B	378/720 (52%)	363 (96%)	15 (4%)	0	100	100
All	All	756/1440 (52%)	721 (95%)	35 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	339/644 (53%)	334 (98%)	5 (2%)	57	84
1	B	339/644 (53%)	335 (99%)	4 (1%)	63	86
All	All	678/1288 (53%)	669 (99%)	9 (1%)	59	86

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	394	PHE
1	A	509	VAL
1	A	550	GLU
1	A	566	ASP
1	A	618	ASN
1	B	265	ILE
1	B	394	PHE
1	B	489	MET

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Mol	Chain	Res	Type
1	B	574	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	614	ASN
1	A	616	HIS
1	B	452	GLN
1	B	504	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PC1	A	802	-	53,53,53	0.50	0	59,61,61	0.52	1 (1%)
2	PC1	A	801	-	53,53,53	0.49	0	59,61,61	0.50	1 (1%)
2	PC1	B	801	-	53,53,53	0.49	0	59,61,61	0.49	1 (1%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PC1	B	802	-	53,53,53	0.50	0	59,61,61	0.48	1 (1%)

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	PC1	A	802	-	-	23/57/57/57	-
2	PC1	A	801	-	-	23/57/57/57	-
2	PC1	B	801	-	-	17/57/57/57	-
2	PC1	B	802	-	-	24/57/57/57	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	PC1	O12-P-O14	2.50	124.05	112.44
2	B	802	PC1	O12-P-O14	2.49	124.05	112.44
2	A	801	PC1	O12-P-O14	2.46	123.88	112.44
2	B	801	PC1	O12-P-O14	2.38	123.54	112.44

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	PC1	C1-O11-P-O12
2	A	801	PC1	C1-O11-P-O14
2	A	801	PC1	C1-O11-P-O13
2	A	802	PC1	C1-O11-P-O13
2	A	802	PC1	O22-C21-O21-C2
2	A	802	PC1	C22-C21-O21-C2
2	B	801	PC1	C11-O13-P-O12
2	B	801	PC1	C11-O13-P-O14
2	B	801	PC1	C11-O13-P-O11
2	B	802	PC1	C1-O11-P-O13
2	B	802	PC1	C22-C21-O21-C2
2	B	802	PC1	O22-C21-O21-C2
2	B	802	PC1	C32-C31-O31-C3
2	A	801	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	A	801	PC1	O32-C31-O31-C3
2	B	801	PC1	O32-C31-O31-C3
2	B	801	PC1	C32-C31-O31-C3
2	B	802	PC1	O32-C31-O31-C3
2	A	801	PC1	C31-C32-C33-C34
2	A	801	PC1	C35-C36-C37-C38
2	A	801	PC1	C24-C25-C26-C27
2	A	801	PC1	C21-C22-C23-C24
2	B	802	PC1	C21-C22-C23-C24
2	A	802	PC1	C3C-C3D-C3E-C3F
2	B	802	PC1	C3B-C3C-C3D-C3E
2	B	802	PC1	C24-C25-C26-C27
2	B	802	PC1	C2E-C2F-C2G-C2H
2	B	802	PC1	C3A-C3B-C3C-C3D
2	A	801	PC1	C2D-C2E-C2F-C2G
2	A	802	PC1	C23-C24-C25-C26
2	A	802	PC1	C3B-C3C-C3D-C3E
2	B	801	PC1	C31-C32-C33-C34
2	A	802	PC1	C3D-C3E-C3F-C3G
2	B	802	PC1	C2D-C2E-C2F-C2G
2	B	801	PC1	C2B-C2C-C2D-C2E
2	A	802	PC1	C24-C25-C26-C27
2	B	801	PC1	C35-C36-C37-C38
2	A	802	PC1	C25-C26-C27-C28
2	B	802	PC1	C32-C33-C34-C35
2	B	801	PC1	C21-C22-C23-C24
2	B	802	PC1	C23-C24-C25-C26
2	A	802	PC1	C32-C33-C34-C35
2	B	801	PC1	C38-C39-C3A-C3B
2	B	802	PC1	C25-C26-C27-C28
2	A	801	PC1	C38-C39-C3A-C3B
2	B	802	PC1	C3F-C3G-C3H-C3I
2	A	802	PC1	C1-C2-C3-O31
2	B	802	PC1	C2A-C2B-C2C-C2D
2	B	801	PC1	C34-C35-C36-C37
2	A	801	PC1	C11-C12-N-C15
2	B	802	PC1	C28-C29-C2A-C2B
2	A	802	PC1	C2A-C2B-C2C-C2D
2	A	801	PC1	C11-C12-N-C14
2	A	802	PC1	C35-C36-C37-C38
2	A	802	PC1	O13-C11-C12-N
2	B	801	PC1	O13-C11-C12-N

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Mol	Chain	Res	Type	Atoms
2	B	802	PC1	C31-C32-C33-C34
2	A	802	PC1	C29-C2A-C2B-C2C
2	A	801	PC1	C11-C12-N-C13
2	A	802	PC1	O21-C2-C3-O31
2	A	802	PC1	C1-O11-P-O14
2	B	802	PC1	C1-O11-P-O14
2	A	802	PC1	C22-C23-C24-C25
2	B	801	PC1	C24-C25-C26-C27
2	B	802	PC1	C35-C36-C37-C38
2	A	801	PC1	C29-C2A-C2B-C2C
2	B	801	PC1	C27-C28-C29-C2A
2	A	801	PC1	C33-C34-C35-C36
2	A	801	PC1	C2-C1-O11-P
2	A	801	PC1	C34-C35-C36-C37
2	B	802	PC1	C33-C34-C35-C36
2	A	801	PC1	C26-C27-C28-C29
2	A	801	PC1	C27-C28-C29-C2A
2	B	801	PC1	C3B-C3C-C3D-C3E
2	B	802	PC1	O21-C2-C3-O31
2	A	802	PC1	C33-C34-C35-C36
2	A	801	PC1	O31-C31-C32-C33
2	B	801	PC1	O31-C31-C32-C33
2	B	802	PC1	C39-C3A-C3B-C3C
2	A	801	PC1	C28-C29-C2A-C2B
2	A	802	PC1	C39-C3A-C3B-C3C
2	B	801	PC1	O32-C31-C32-C33
2	A	802	PC1	C21-C22-C23-C24
2	A	801	PC1	O32-C31-C32-C33
2	A	802	PC1	C3E-C3F-C3G-C3H
2	B	802	PC1	C1-C2-C3-O31
2	A	802	PC1	O21-C21-C22-C23

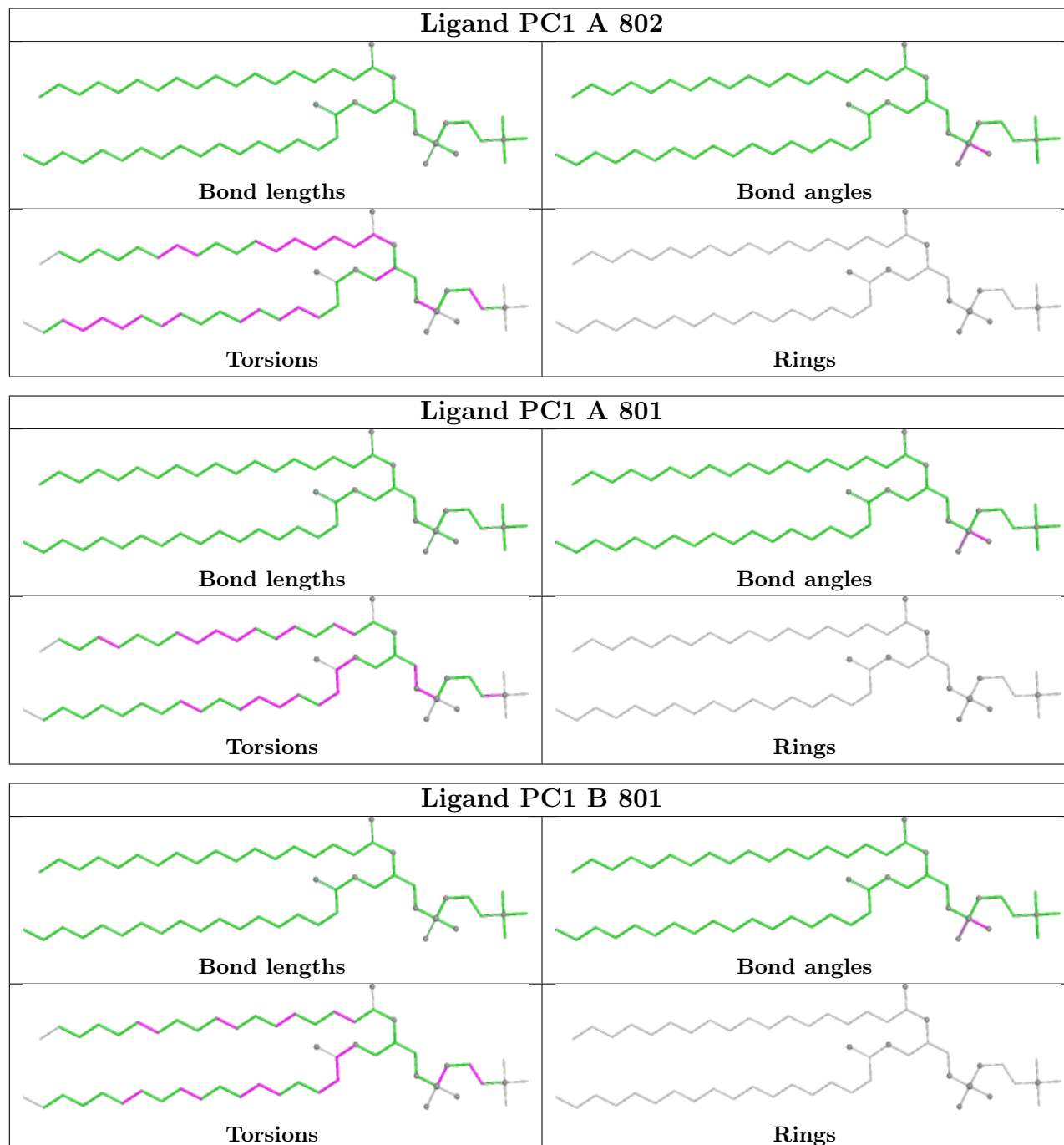
There are no ring outliers.

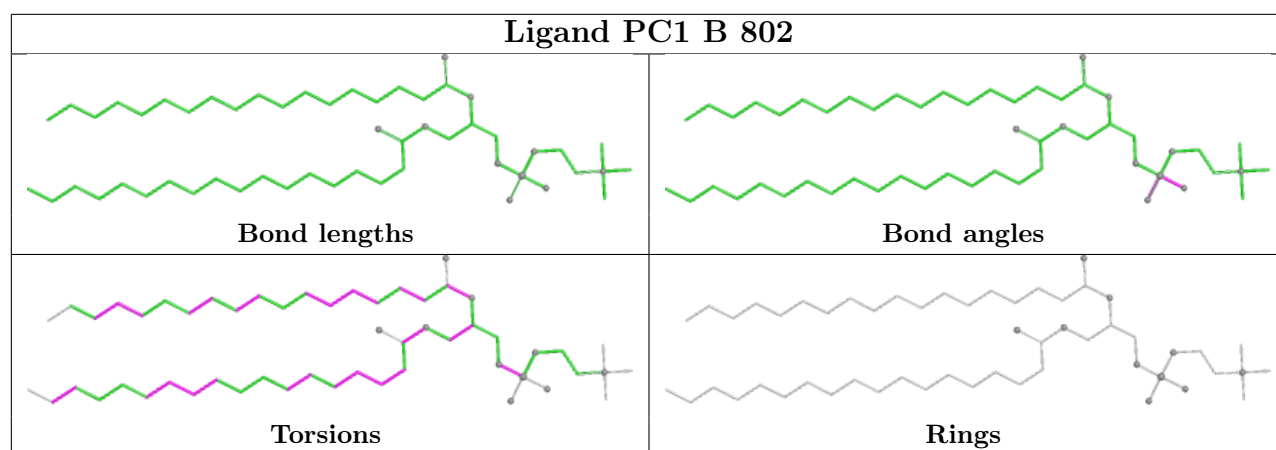
3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	802	PC1	1	0
2	A	801	PC1	6	0
2	B	801	PC1	5	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.

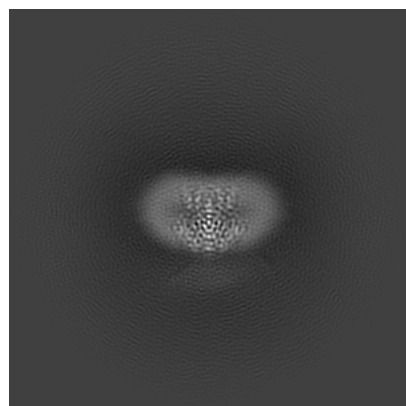
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61138. 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](#)

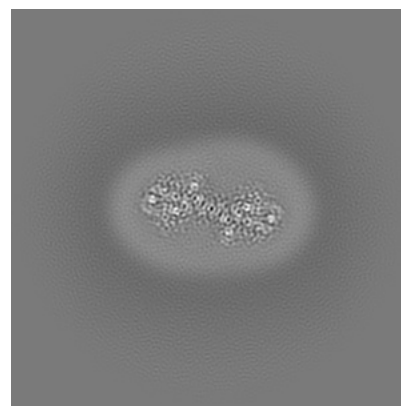
6.1.1 Primary map



X

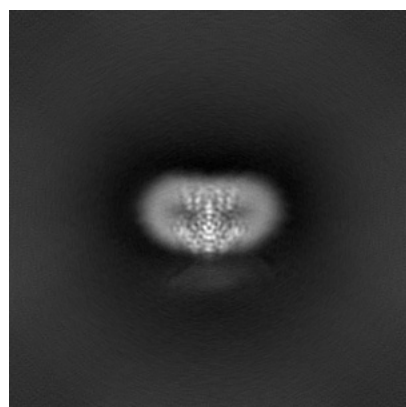


Y

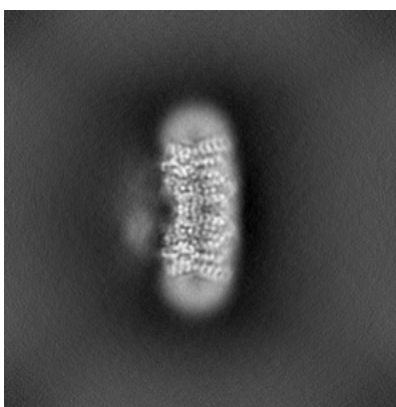


Z

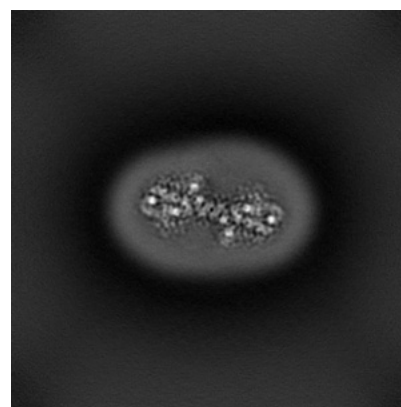
6.1.2 Raw map



X



Y

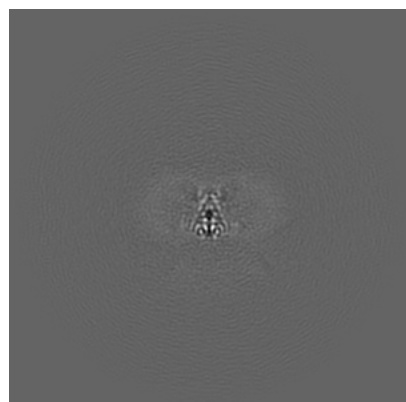


Z

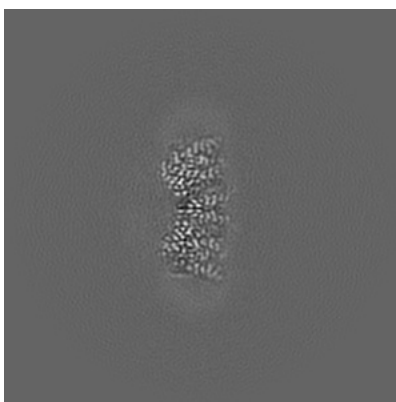
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

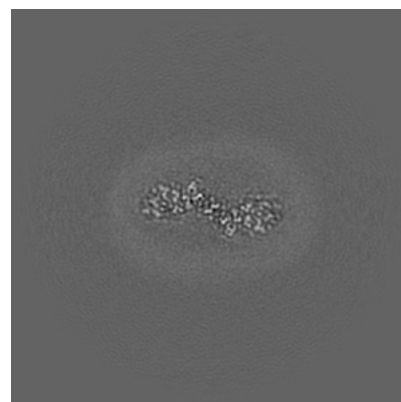
6.2.1 Primary map



X Index: 140

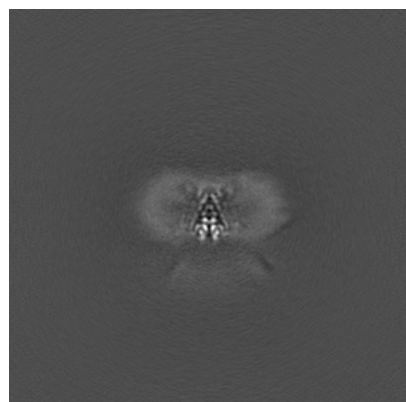


Y Index: 140

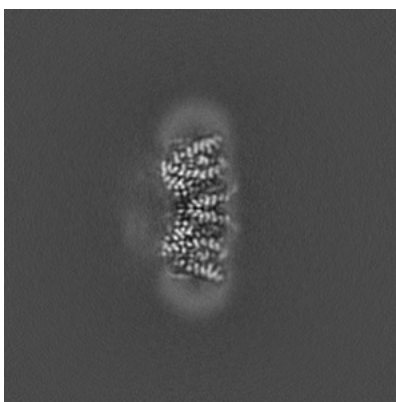


Z Index: 140

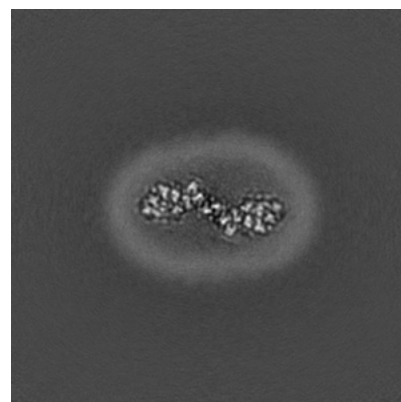
6.2.2 Raw map



X Index: 140



Y Index: 140

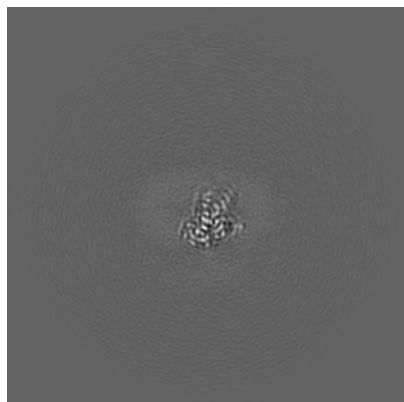


Z Index: 140

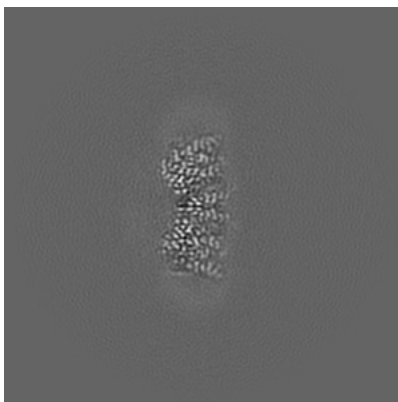
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

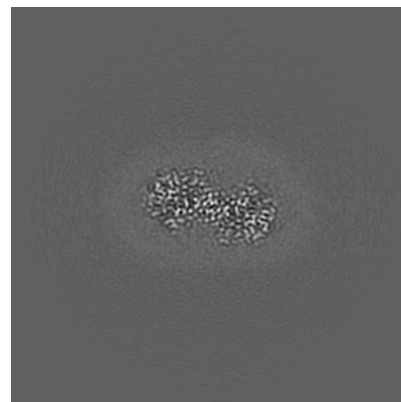
6.3.1 Primary map



X Index: 114

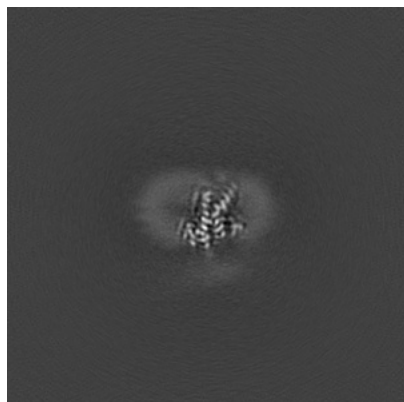


Y Index: 140

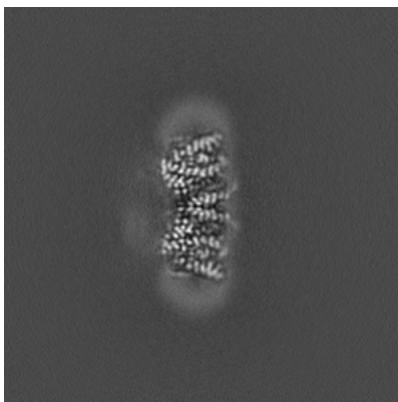


Z Index: 127

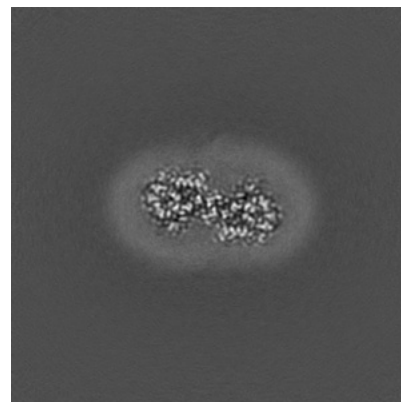
6.3.2 Raw map



X Index: 114



Y Index: 140

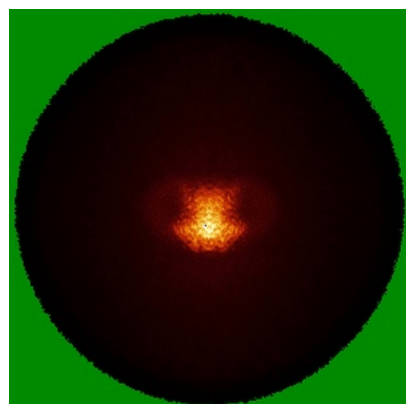


Z Index: 124

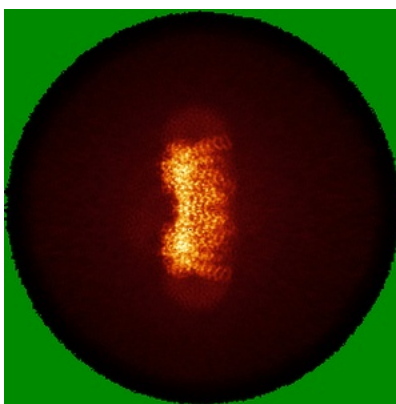
The images above show the largest variance slices of the map in three orthogonal directions.

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

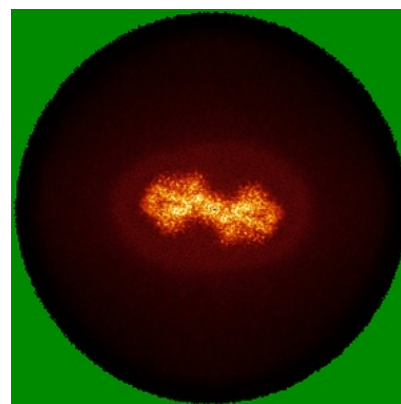
6.4.1 Primary map



X

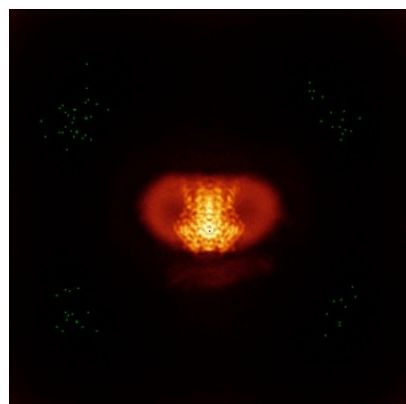


Y

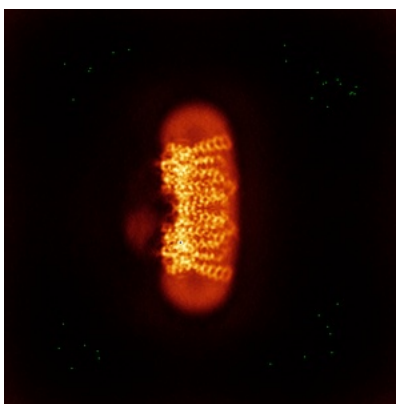


Z

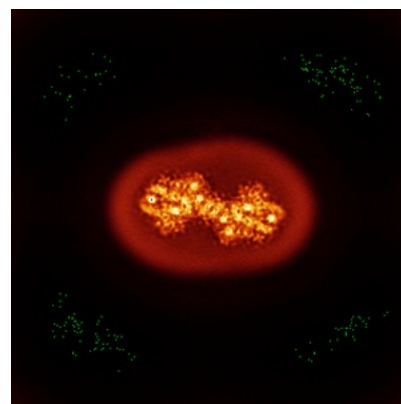
6.4.2 Raw map



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 0.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

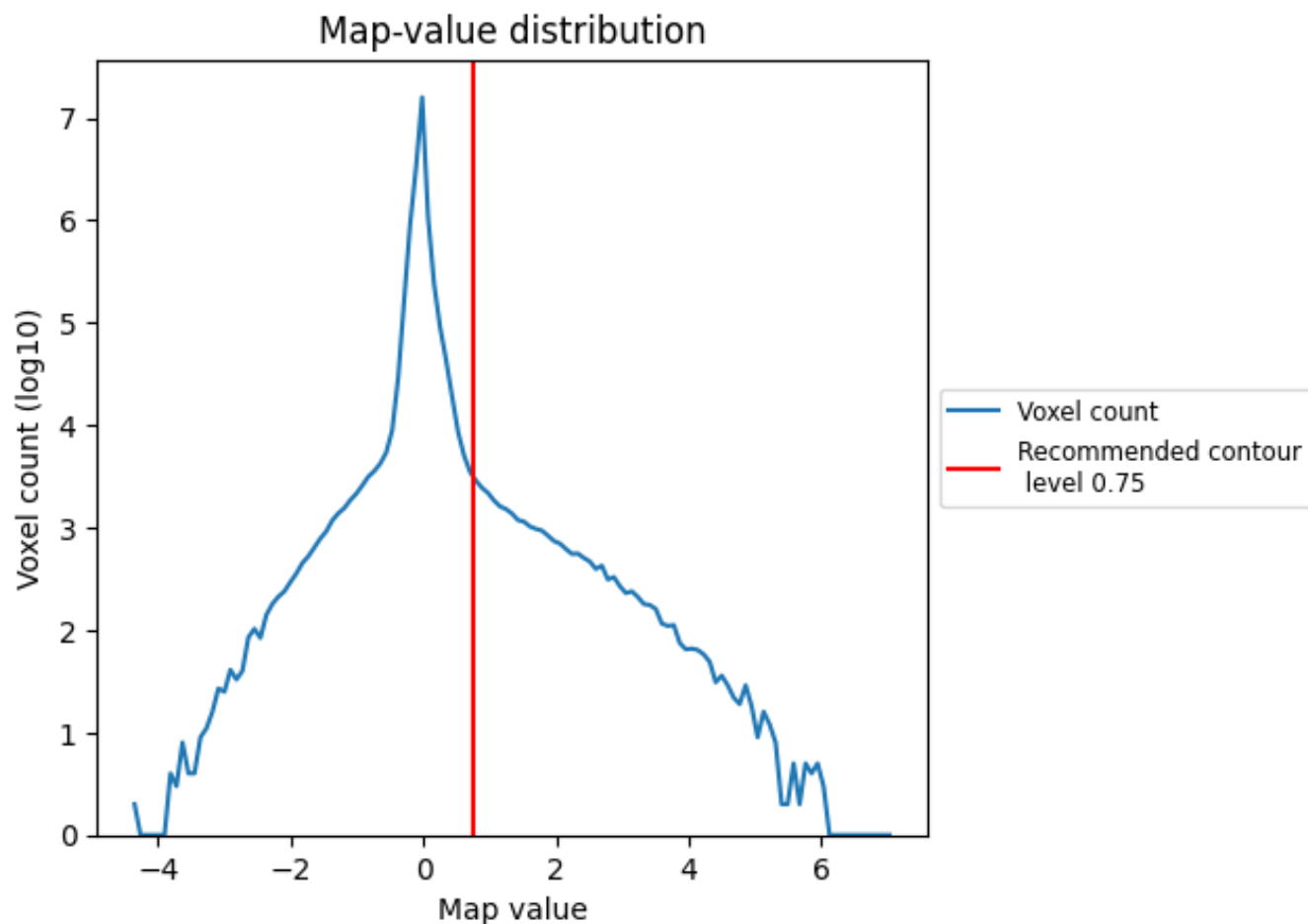
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

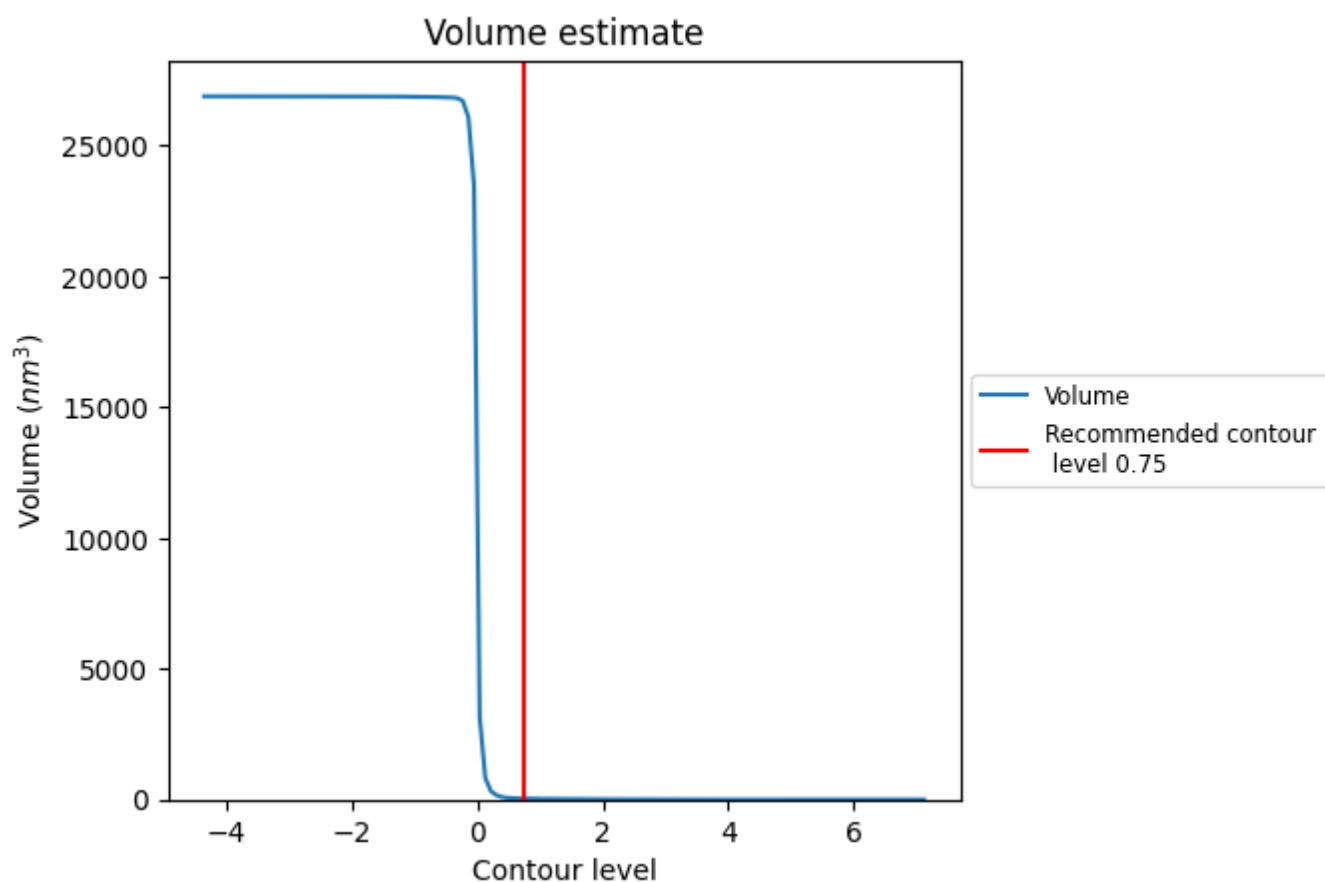
This section contains the results of statistical analysis of the map.

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.

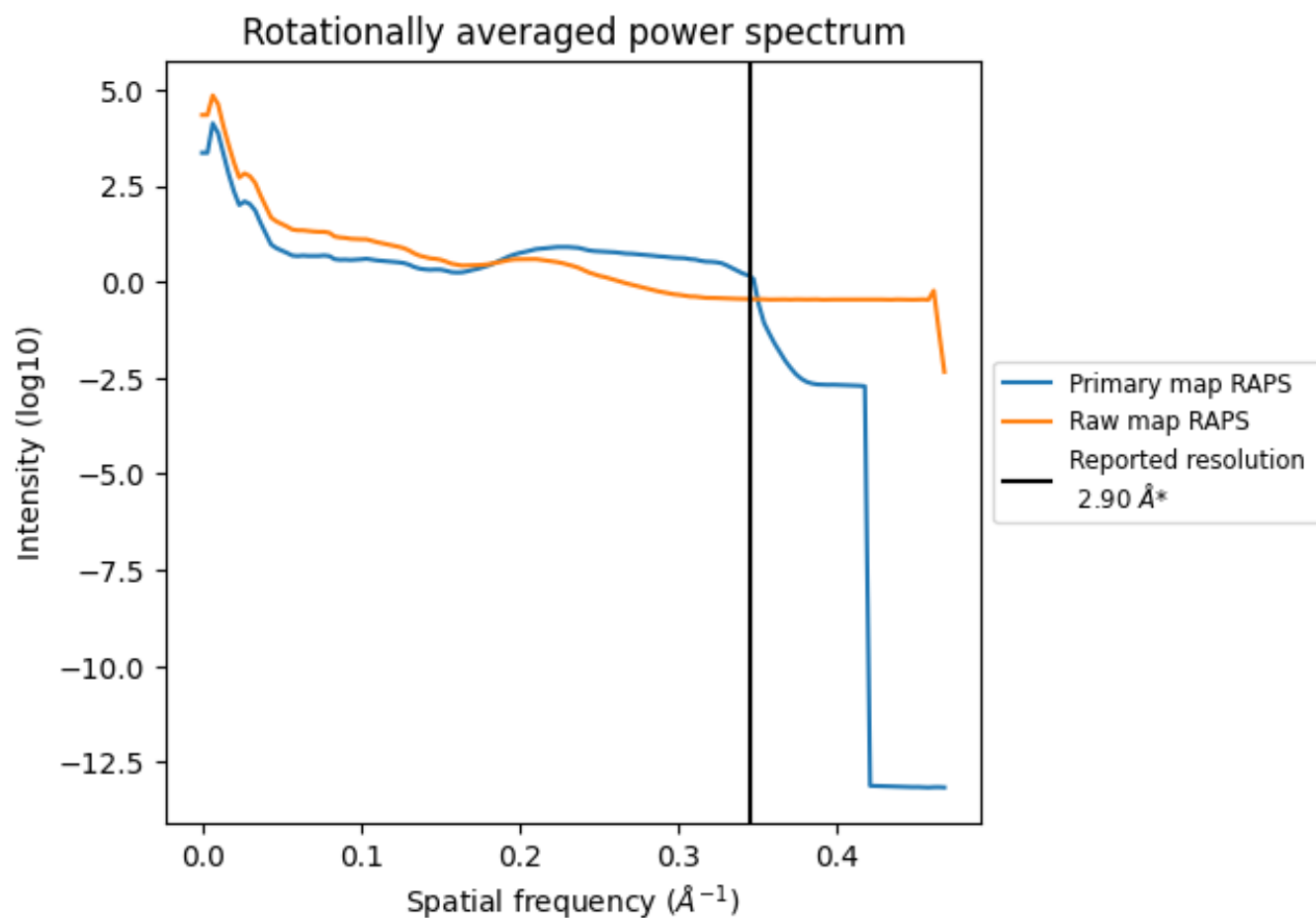
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 36 nm³; this corresponds to an approximate mass of 33 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 ⓘ

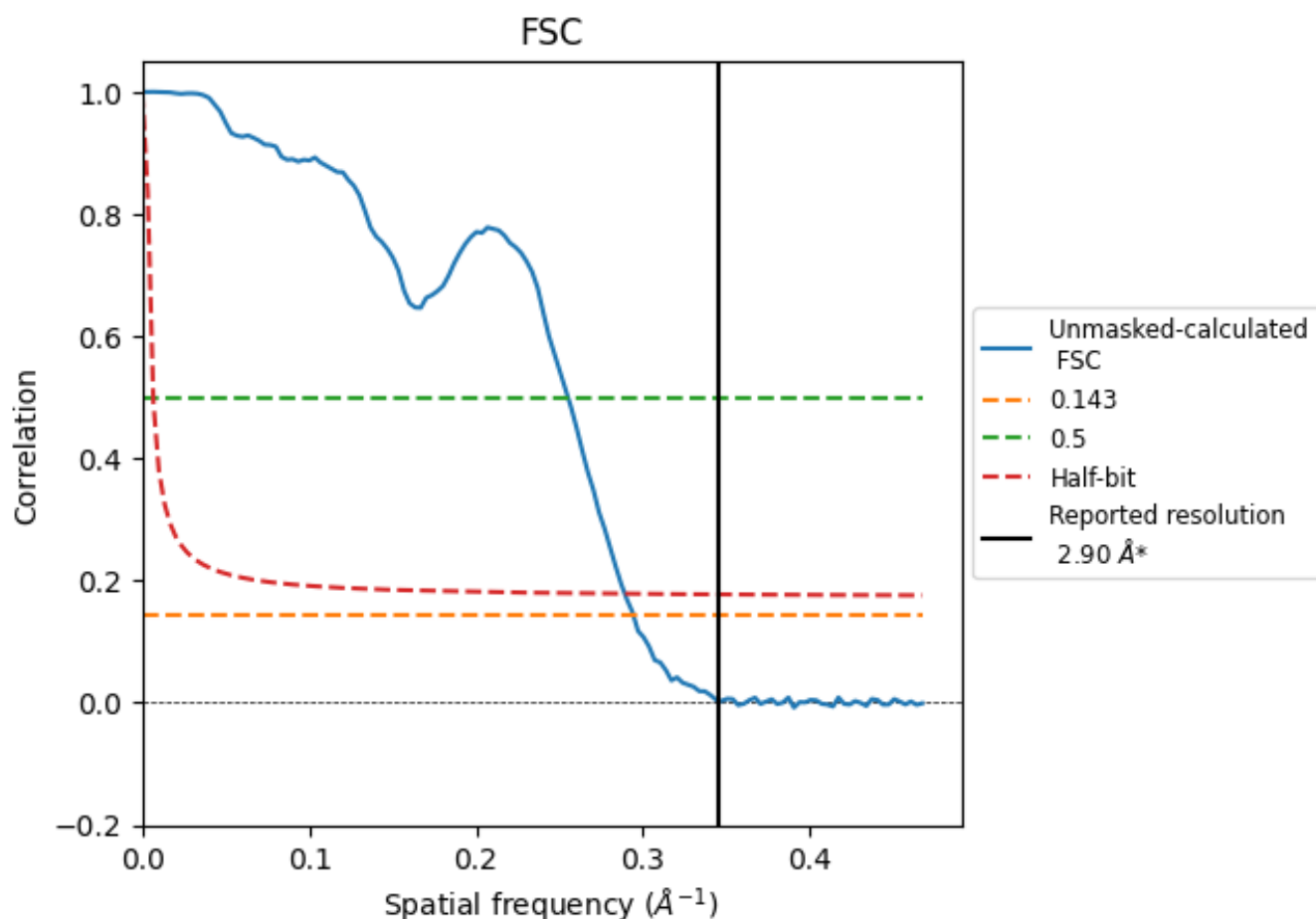


*Reported resolution corresponds to spatial frequency of $0.345 \text{ \AA}^{-1}$

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 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

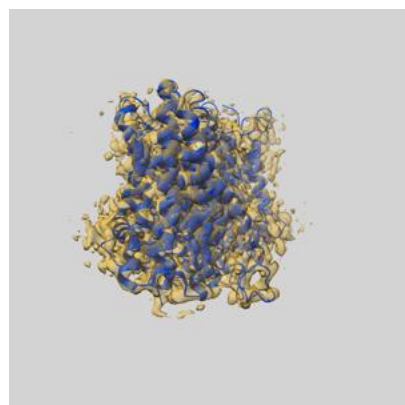
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.40	3.92	3.46

*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 3.40 differs from the reported value 2.9 by more than 10 %

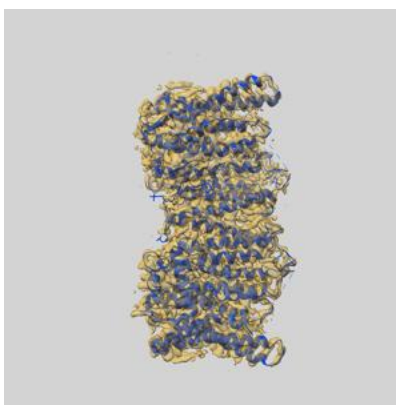
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61138 and PDB model 9J4X. Per-residue inclusion information can be found in section [3](#) on page [6](#).

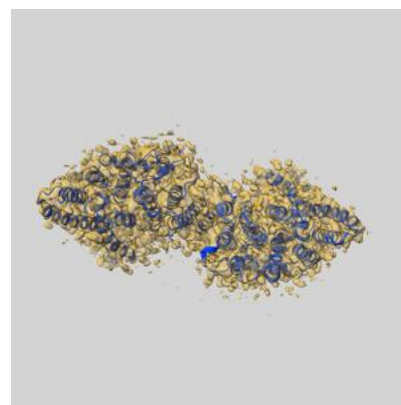
9.1 Map-model overlay [i](#)



X



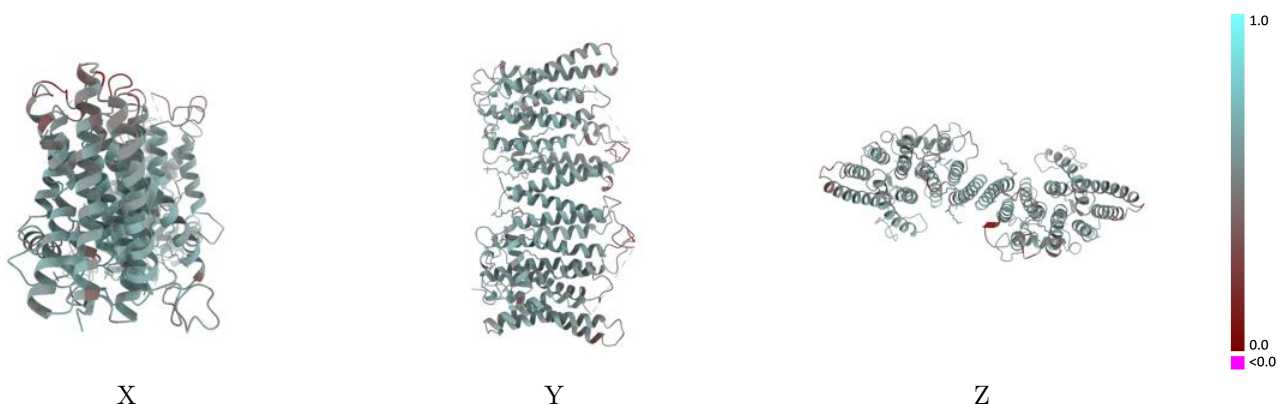
Y



Z

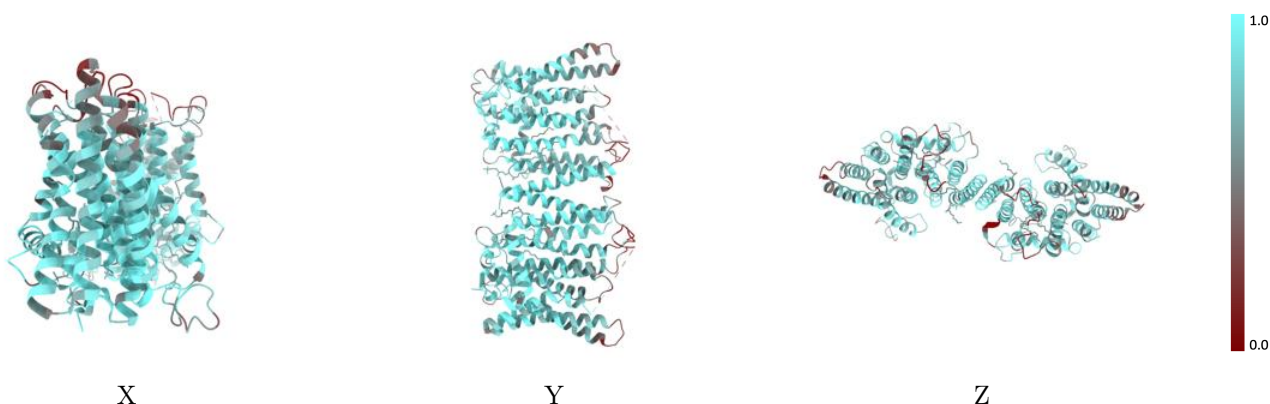
The images above show the 3D surface view of the map at the recommended contour level 0.75 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



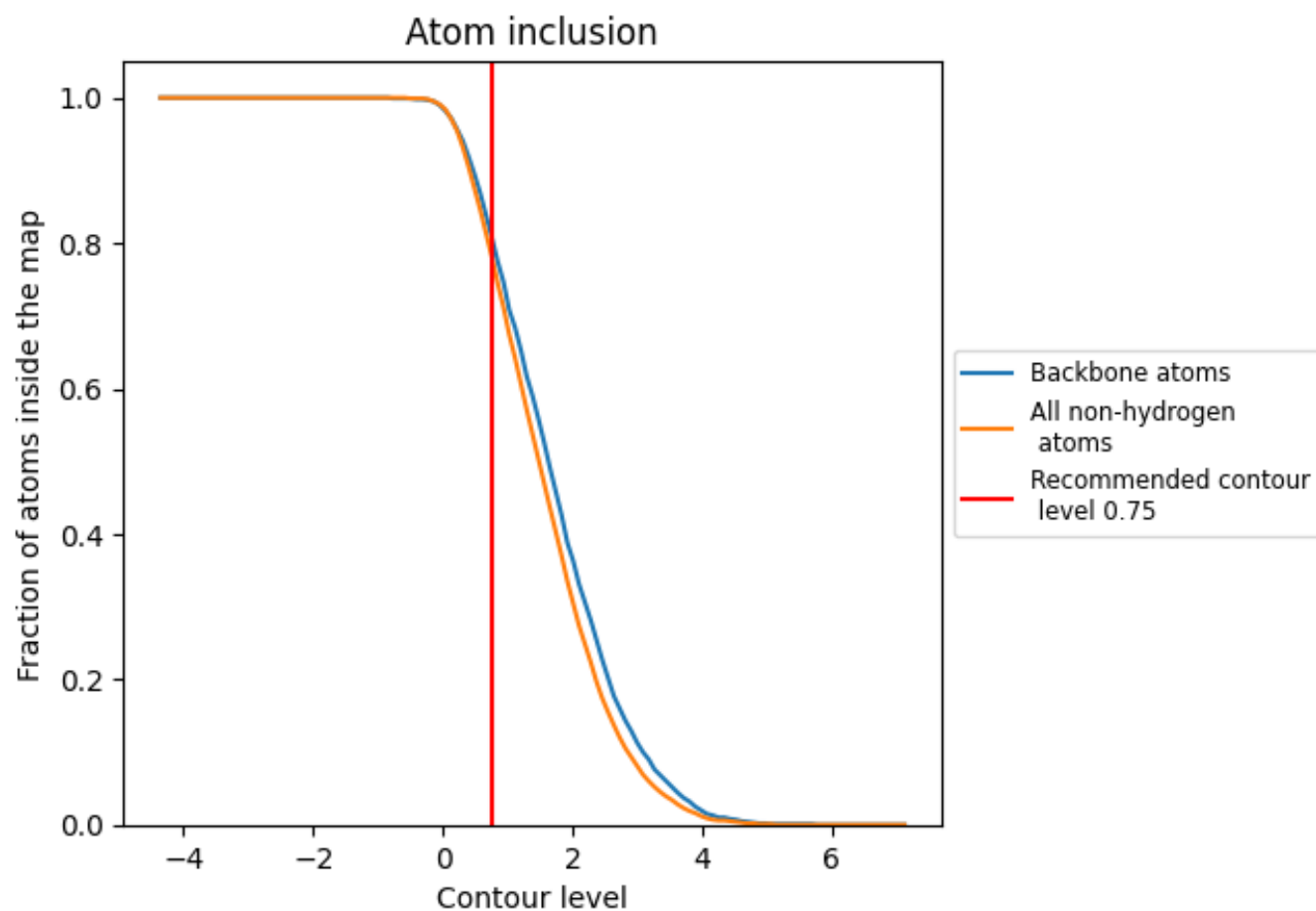
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.75).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 78% 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 (0.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7820	0.5540
A	0.7810	0.5490
B	0.7840	0.5590

