



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 10:28 AM UTC

PDB ID : 8JRU / pdb_00008jru
EMDB ID : EMD-36606
Title : Cryo-EM structure of the glucagon receptor bound to beta-arrestin 1 in ligand-free state
Authors : Chen, K.; Zhang, C.; Lin, S.; Zhao, Q.; Wu, B.
Deposited on : 2023-06-17
Resolution : 3.50 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

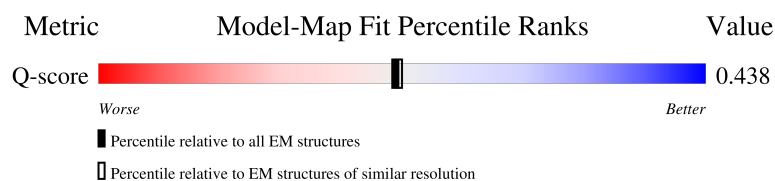
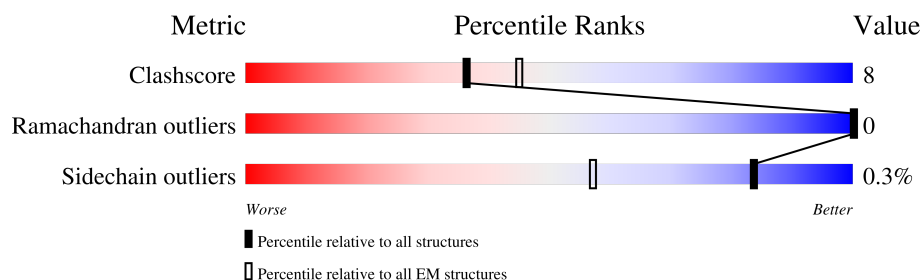
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

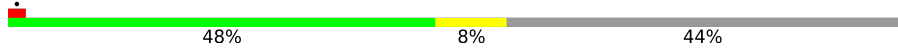
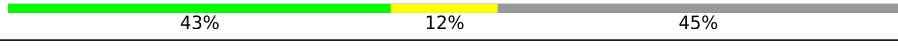
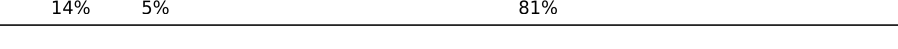
The reported resolution of this entry is 3.50 Å.

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	13950 (3.00 - 4.00)

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	R	478	
2	A	627	
2	H	627	
2	L	627	

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Mol	Chain	Length	Quality of chain
3	B	126	64% 22% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7120 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 HA signal peptide,HPC4 purification tag,Glucagon receptor,C-terminal tail of Vasopressin V2 receptor.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	R	267	Total	C	N	O	P	S	0	0
			2008	1319	332	346	5	6		

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-16	GLY	-	expression tag	UNP P03435
R	-15	SER	-	expression tag	UNP P03435
R	2	GLY	-	linker	UNP P03435
R	3	ALA	-	linker	UNP P03435
R	4	PRO	-	linker	UNP P03435
R	17	GLY	-	linker	UNP P04070
R	18	SER	-	linker	UNP P04070
R	19	GLY	-	linker	UNP P04070
R	20	SER	-	linker	UNP P04070
R	21	ALA	-	linker	UNP P04070
R	22	GLY	-	linker	UNP P04070
R	23	SER	-	linker	UNP P04070
R	24	ALA	-	linker	UNP P04070
R	25	GLY	-	linker	UNP P04070
R	26	SER	-	linker	UNP P04070

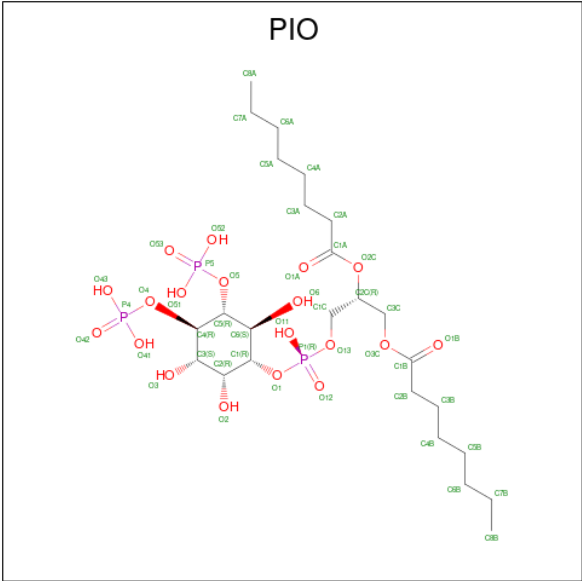
- Molecule 2 is a protein called Beta-arrestin 1 and single-chain fragment variable 30 (scFv30).

Mol	Chain	Residues	Atoms						AltConf	Trace
2	A	346	Total	C	N	O	S		0	0
			2576	1657	442	474	3			
2	H	117	Total	C	N	O	S		0	0
			891	569	150	170	2			
2	L	107	Total	C	N	O	S		0	0
			790	501	130	157	2			

- Molecule 3 is a protein called Nanobody 32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	110	815	507	145	159	4	0	0

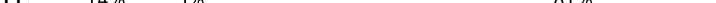
- Molecule 4 is [(2R)-2-octanoyloxy-3-[oxidanyl-[(1R,2R,3S,4R,5R,6S)-2,3,6-tris(oxidanyl)-4,5-diphosphonooxy-cyclohexyl]oxy-phosphoryl]oxy-propyl] octanoate (CCD ID: PIO) (formula: C₂₅H₄₉O₁₉P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	40	18	19	3	0

[illegible]

- Molecule 2: Beta-arrestin 1 and single-chain fragment variable 30 (scFv30)

Chain H:  14% 5% 81%

M86	VAL	PRO	ALA	ILE	GLN	PRO	GLN	PRO	PHE	MET
L89	ILE	LYS	SER	VAL	VAL	HIS	PRO	SER	ARG	GLY
D93	GLY	LEU	VAL	THR	LEU	ARG	THR	LEU	TYR	ASN
T94	THR	ILE	GLU	THR	LEU	VAL	THR	SER	GLY	THR
A95	THR	SER	PRO	GLU	LEU	GLY	ALA	VAL	ASP	ARG
V96	ALA	HIS	ARG	GLU	ARG	HIS	GLN	THR	LEU	VAL
	ALA	SER	GLU	GLY	GLY	GLU	TYR	GLY	ASP	PHE
R101	SER	SER	THR	ALA	LYS	THR	LYS	GLN	VAL	LYS
	GLY	LEU	ASN	VAL	VAL	PRO	VAL	PRO	LEU	LYS
W106	SER	TYR	VAL	ARG	PRO	VAL	MET	GLY	GLY	ALA
	SER	SER	ASP	GLU	VAL	ASP	SER	PRO	LEU	SER
Y112	GLY	GLY	ILE	ILE	VAL	THR	ALA	GLU	PHE	VAL
	GLY	VAL	ASN	LEU	MET	ASP	LYS	ASP	THR	THR
Q115	SER	PRO	GLY	GLY	GLU	PRO	PRO	THR	ARG	GLY
	SER	SER	ILE	ILE	GLU	LEU	HIS	LYS	LYS	LYS
L118	SER	ARG	ASP	ILE	ALA	ASP	HIS	LYS	ASP	LEU
	GLY	PHE	ILE	VAL	ASP	ILE	LEU	ALA	LEU	THR
V121	ALA	SER	GLN	SER	ASP	GLN	GLU	ILE	PHE	VAL
SER	GLY	GLY	MET	TYR	THR	THR	SER	GLY	VAL	TYR
SER	V5	SER	THR	LYS	VAL	VAL	VAL	VAL	ALA	LEU
HIS		ARG	GLN	VAL	ALA	GLN	ALA	ASN	ASN	GLY
ALA		GLY	SER	LYS	VAL	SER	PRO	TYR	VAL	GLY
HIS		THR	VAL	VAL	VAL	PRO	VAL	ASP	GLN	VAL
HIS		THR	THR	THR	THR	SER	SER	LYS	VAL	GLY
HIS		ASP	VAL	VAL	VAL	SER	ILE	ALA	ALA	THR
HIS		PHE	VAL	PHE	PHE	LEU	THR	THR	PRO	ASP
HIS		THR	VAL	THR	THR	SER	VAL	PHE	PRO	ASP
HIS		LEU	ALA	SER	SER	ALA	HIS	VAL	ALA	HIS
		THR	SER	ARG	VAL	THR	GLY	ALA	PRO	ILE
		ILE	VAL	GLY	VAL	VAL	THR	GLU	GLU	ILE
		SER	GLY	GLY	THR	GLY	ILE	ASP	ASP	LEU
		SER	LEU	LEU	LEU	GLY	PRO	ASN	GLY	VAL
		SER	GLY	GLY	THR	THR	THR	ASN	LYS	GLY
		LEU	GLY	THR	THR	VAL	VAL	ASN	VAL	VAL
		PRO	ALA	THR	THR	THR	THR	GLN	GLY	LEU
		GLU	THR	ILE	THR	THR	VAL	ASN	ARG	VAL
		SER	ALA	ALA	ARG	ALA	GLY	ASN	GLY	VAL
		THR	SER	THR	THR	THR	ALA	THR	ILE	VAL
		TYR	GLN	VAL	VAL	GLN	THR	VAL	GLY	VAL
		CYS	VAL	GLU	ARG	VAL	LYS	ASN	ILE	PRO
		GLN	VAL	GLY	THR	GLY	THR	LEU	LYS	TYR
		GLN	SER	LEU	LEU	ALA	THR	VAL	LYS	LEU
		TYR	SER	PRO	THR	SER	VAL	ILE	LEU	GLY
		LYS	ALA	PHE	THR	THR	LYS	GLU	GLY	LYS
		THR	THR	THR	THR	THR	VAL	GLY	GLY	LYS
		VAL	THR	THR	THR	THR	THR	VAL	GLY	GLY
		VAL	THR	THR	THR	THR	THR	THR	THR	THR
		THR	GLN	PRO	LYS	LYS	LYS	ALA	PRO	TYR
		PHE	GLN	LYS	THR	HIS	VAL	PRO	PHE	THR
		GLY	THR	PRO	GLY	GLY	GLY	GLY	THR	THR
		GLN	GLY	LYS	THR	THR	THR	GLY	PHE	THR
		THR	LYS	ALA	ASN	ASN	ASN	GLY	GLY	ALA
		LYS	PRO	PRO	PRO	PRO	ASN	PRO	ILE	ALA

- Molecule 2: Beta-arrestin 1 and single-chain fragment variable 30 (scFv30)

Chain L: 15% . 83%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250907	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.929	Depositor
Minimum map value	-1.537	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.060	Depositor
Recommended contour level	0.35	Depositor
Map size ($\text{\AA}$)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.071, 1.071, 1.071	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: SEP, PIO, TPO

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	R	0.09	0/2000	0.28	0/2726
2	A	0.08	0/2635	0.24	0/3606
2	H	0.08	0/915	0.24	0/1246
2	L	0.13	0/808	0.28	0/1103
3	B	0.13	0/829	0.36	0/1126
All	All	0.10	0/7187	0.27	0/9807

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2008	0	1906	20	0
2	A	2576	0	2492	47	0
2	H	891	0	833	20	0
2	L	790	0	742	8	0
3	B	815	0	765	18	0
4	A	40	0	24	0	0
All	All	7120	0	6762	107	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 (107) 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)
3:B:34:MET:HG3	3:B:78:VAL:HG11	1.63	0.78
1:R:241:TRP:HE3	1:R:271:GLY:HA3	1.58	0.67
2:A:37:VAL:HB	2:A:117:PHE:HB2	1.77	0.66
2:L:91:GLN:HE21	2:L:98:THR:H	1.41	0.66
1:R:406:GLU:N	1:R:406:GLU:OE2	2.30	0.64
2:L:34:VAL:HB	2:L:52:ALA:HB2	1.81	0.62
2:H:94:THR:HG22	2:H:121:VAL:H	1.63	0.62
2:H:26:ALA:HA	2:H:81:THR:HG22	1.82	0.61
2:H:5:VAL:N	2:H:28:SER:O	2.33	0.61
2:H:46:LYS:N	2:H:46:LYS:HE2	2.15	0.61
2:A:188:ARG:HE	2:A:343:VAL:HG22	1.66	0.61
3:B:29:PHE:O	3:B:71:ARG:NH2	2.34	0.61
2:A:83:ASN:HD21	2:A:154:LEU:HD21	1.66	0.60
2:A:8:VAL:HG11	2:A:104:LEU:HD21	1.84	0.60
2:A:39:GLY:O	2:A:101:GLN:NE2	2.35	0.59
3:B:62:SER:O	3:B:66:ARG:NH2	2.35	0.59
2:H:64:ALA:HB3	2:H:67:VAL:HG22	1.85	0.58
2:A:130:GLN:HE22	2:A:282:ARG:HA	1.70	0.57
2:A:277:PHE:O	2:A:281:ASN:ND2	2.37	0.57
1:R:186:LEU:HD21	1:R:230:PHE:HB3	1.86	0.56
2:A:235:VAL:HG22	2:A:323:VAL:HG22	1.87	0.56
2:H:101:ARG:HD2	2:H:112:TYR:HD2	1.70	0.56
2:A:129:LEU:HB2	2:A:140:ILE:HG13	1.88	0.56
2:A:243:LEU:HD12	2:A:244:PHE:CD1	2.40	0.56
1:R:225:ARG:HA	1:R:295:TRP:HH2	1.71	0.56
2:A:251:VAL:HG11	2:A:287:LEU:HD13	1.87	0.56
2:A:128:THR:HA	2:A:141:GLY:HA3	1.88	0.55
2:A:24:LYS:NZ	2:A:26:ASP:O	2.36	0.55
3:B:36:TRP:HZ3	3:B:93:TYR:HB3	1.71	0.55
1:R:399:LEU:HD13	1:R:403:LEU:HD13	1.89	0.54
2:A:42:LEU:HD23	3:B:99:VAL:HA	1.90	0.53
2:H:43:ALA:HB3	2:H:46:LYS:HB2	1.91	0.53
1:R:280:VAL:HG23	1:R:281:PRO:HD3	1.89	0.52
2:A:204:ASP:OD2	2:A:215:SER:OG	2.27	0.52
3:B:90:THR:HG23	3:B:111:THR:HA	1.91	0.52
3:B:61:ASP:N	3:B:61:ASP:OD1	2.41	0.51
2:A:252:PRO:O	2:A:284:LYS:NZ	2.43	0.51
2:A:236:ARG:NH2	2:A:238:TYR:OH	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:72:THR:O	2:H:85:GLN:N	2.42	0.50
2:A:235:VAL:HB	2:A:254:ALA:HB3	1.93	0.50
3:B:2:VAL:HG11	3:B:102:LEU:HD12	1.93	0.50
3:B:15:GLY:HA2	3:B:84:SER:HA	1.92	0.50
2:H:44:PRO:HD3	2:H:95:ALA:HA	1.94	0.49
3:B:56:THR:HG22	3:B:56:THR:O	2.12	0.49
2:L:62:ARG:NE	2:L:83:ASP:OD2	2.46	0.49
1:R:404:ASN:HB3	1:R:407:VAL:HG12	1.95	0.49
3:B:32:VAL:O	3:B:71:ARG:NH1	2.43	0.49
1:R:151:LEU:HD23	1:R:151:LEU:H	1.78	0.49
2:A:29:ASP:OD2	2:A:170:LYS:NZ	2.36	0.49
2:A:214:ILE:HB	2:A:274:LEU:HB2	1.95	0.49
2:H:22:ARG:NE	2:H:85:GLN:OE1	2.42	0.48
2:L:5:MET:HE1	2:L:91:GLN:HB3	1.95	0.48
1:R:144:MET:HE1	1:R:386:LEU:HD23	1.94	0.48
2:A:292:LYS:HG2	2:A:296:GLU:O	2.13	0.48
1:R:225:ARG:HA	1:R:295:TRP:CH2	2.48	0.48
2:A:356:PRO:HB3	2:H:106:TRP:NE1	2.29	0.47
1:R:313:LEU:O	1:R:317:ILE:HG13	2.13	0.47
2:A:185:GLU:HG2	2:A:200:GLU:HB3	1.94	0.47
2:L:25:ARG:HD2	2:L:71:ASP:HB3	1.95	0.47
2:A:12:ALA:HB1	3:B:101:SER:HB2	1.97	0.47
2:A:222:ASN:O	2:A:265:SER:N	2.45	0.47
2:H:22:ARG:HH11	2:H:83:TYR:HD2	1.62	0.47
3:B:39:ARG:HG2	3:B:40:ALA:H	1.80	0.47
1:R:286:LYS:HZ3	1:R:295:TRP:CD1	2.33	0.46
2:A:278:LEU:HA	2:A:281:ASN:HB2	1.97	0.46
2:H:86:MET:SD	2:H:89:LEU:HD21	2.56	0.46
2:H:35:SER:OG	2:H:101:ARG:NH2	2.46	0.46
1:R:236:VAL:HG21	1:R:307:LEU:HD22	1.98	0.46
2:A:365:VAL:HB	2:A:366:PRO:HD3	1.97	0.46
2:A:293:LEU:HD21	2:A:362:HIS:HB3	1.99	0.45
2:A:176:GLU:H	2:A:176:GLU:CD	2.23	0.45
1:R:410:GLU:OE2	1:R:414:ARG:NH2	2.50	0.45
2:A:178:PRO:HA	2:A:207:ILE:HD12	1.99	0.45
2:A:213:PRO:HD3	2:H:31:ASN:ND2	2.32	0.45
2:H:96:VAL:HG22	2:H:118:LEU:HD13	1.98	0.44
2:H:41:ARG:NH1	2:H:93:ASP:OD1	2.49	0.44
2:A:222:ASN:ND2	2:A:226:LYS:O	2.42	0.44
2:L:84:PHE:C	2:L:84:PHE:CD1	2.96	0.44
1:R:139:SER:OG	1:R:140:SER:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:279:VAL:HA	1:R:307:LEU:HD21	1.98	0.44
2:A:182:PRO:HG2	2:A:203:LEU:HD12	2.00	0.44
2:A:356:PRO:HB3	2:H:106:TRP:HE1	1.82	0.43
2:H:63:TYR:HE1	2:H:71:PHE:HB2	1.84	0.43
2:A:34:VAL:HG11	2:A:119:ILE:HB	2.01	0.43
2:A:263:ALA:O	2:A:266:SER:OG	2.27	0.43
1:R:411:LEU:HD23	1:R:411:LEU:HA	1.90	0.42
2:A:228:VAL:HB	2:A:262:VAL:HB	2.01	0.42
2:A:278:LEU:H	2:A:278:LEU:HD23	1.84	0.42
2:A:14:PRO:HG2	2:A:161:ARG:HA	2.01	0.42
2:A:206:GLU:HG2	2:A:207:ILE:HG13	2.00	0.42
2:A:241:ILE:HG23	2:A:317:ILE:HG12	2.00	0.42
1:R:322:PHE:O	1:R:326:VAL:HG22	2.20	0.42
3:B:33:THR:O	3:B:98:PHE:N	2.45	0.41
3:B:4:LEU:HD13	3:B:24:VAL:HG22	2.01	0.41
2:A:367:GLU:O	2:L:95:VAL:N	2.53	0.41
1:R:244:VAL:HG13	1:R:267:TYR:CD1	2.55	0.41
2:A:88:PRO:N	2:A:89:PRO:HD2	2.36	0.41
3:B:6:GLU:HA	3:B:22:CYS:HA	2.01	0.41
3:B:52:THR:HG22	3:B:56:THR:HB	2.02	0.41
2:A:238:TYR:OH	2:A:346:GLU:OE2	2.24	0.41
2:L:33:ALA:HB3	2:L:93:LYS:HB2	2.02	0.40
2:A:242:VAL:HB	2:A:246:THR:HA	2.02	0.40
2:H:115:GLN:HA	2:H:115:GLN:OE1	2.21	0.40
3:B:76:ASN:OD1	3:B:76:ASN:O	2.39	0.40
1:R:422:LYS:HA	1:R:422:LYS:HD3	1.86	0.40
2:A:80:PHE:CZ	2:A:82:ALA:HB2	2.56	0.40
2:A:123:LEU:HD23	2:A:123:LEU:HA	1.90	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	R	252/478 (53%)	239 (95%)	13 (5%)	0	100	100
2	A	338/627 (54%)	317 (94%)	21 (6%)	0	100	100
2	H	115/627 (18%)	113 (98%)	2 (2%)	0	100	100
2	L	105/627 (17%)	98 (93%)	7 (7%)	0	100	100
3	B	106/126 (84%)	98 (92%)	8 (8%)	0	100	100
All	All	916/2485 (37%)	865 (94%)	51 (6%)	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	R	182/404 (45%)	182 (100%)	0	100	100
2	A	264/538 (49%)	264 (100%)	0	100	100
2	H	89/538 (16%)	88 (99%)	1 (1%)	65	74
2	L	82/538 (15%)	82 (100%)	0	100	100
3	B	83/104 (80%)	82 (99%)	1 (1%)	63	73
All	All	700/2122 (33%)	698 (100%)	2 (0%)	84	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	79	LYS
3	B	4	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	142	GLN
1	R	291	ASN
1	R	361	HIS

Continued on next page...

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Mol	Chain	Res	Type
1	R	392	GLN
1	R	408	GLN
2	A	30	HIS
2	A	83	ASN
2	A	281	ASN
2	H	42	GLN
2	L	91	GLN
3	B	76	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues 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$
1	TPO	R	1360	1	8,10,11	1.64	1 (12%)	10,14,16	2.06	1 (10%)
1	SEP	R	1363	1	8,9,10	1.62	1 (12%)	7,12,14	1.34	1 (14%)
1	SEP	R	1357	1	8,9,10	1.62	1 (12%)	7,12,14	1.41	1 (14%)
1	SEP	R	1362	1	8,9,10	1.61	1 (12%)	7,12,14	1.25	1 (14%)
1	SEP	R	1364	1	8,9,10	1.61	1 (12%)	7,12,14	1.24	1 (14%)

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
1	TPO	R	1360	1	-	1/9/11/13	-
1	SEP	R	1363	1	-	1/6/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	R	1357	1	-	3/6/8/10	-
1	SEP	R	1362	1	-	1/6/8/10	-
1	SEP	R	1364	1	-	2/6/8/10	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1357	SEP	P-O1P	3.55	1.61	1.50
1	R	1363	SEP	P-O1P	3.54	1.61	1.50
1	R	1364	SEP	P-O1P	3.53	1.61	1.50
1	R	1360	TPO	P-O1P	3.52	1.61	1.50
1	R	1362	SEP	P-O1P	3.51	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	1360	TPO	P-OG1-CB	-6.02	106.98	123.33
1	R	1357	SEP	OG-CB-CA	3.14	111.20	108.14
1	R	1363	SEP	OG-CB-CA	2.93	110.99	108.14
1	R	1362	SEP	OG-CB-CA	2.67	110.74	108.14
1	R	1364	SEP	OG-CB-CA	2.62	110.69	108.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	R	1357	SEP	CA-CB-OG-P
1	R	1357	SEP	CB-OG-P-O1P
1	R	1363	SEP	N-CA-CB-OG
1	R	1360	TPO	C-CA-CB-CG2
1	R	1362	SEP	CB-OG-P-O1P
1	R	1364	SEP	N-CA-CB-OG
1	R	1357	SEP	CB-OG-P-O3P
1	R	1364	SEP	C-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
4	PIO	A	701	-	40,40,47	0.83	1 (2%)	55,58,65	1.15	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PIO	A	701	-	-	20/37/61/68	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	PIO	P4-O4	2.46	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	PIO	O2C-C1A-C2A	4.14	120.44	111.48
4	A	701	PIO	C2C-O2C-C1A	4.06	127.52	117.80
4	A	701	PIO	O2C-C2C-C3C	3.13	119.57	108.34
4	A	701	PIO	C3A-C2A-C1A	2.38	122.41	113.69
4	A	701	PIO	O2C-C1A-O1A	-2.11	118.77	123.70

There are no chirality outliers.

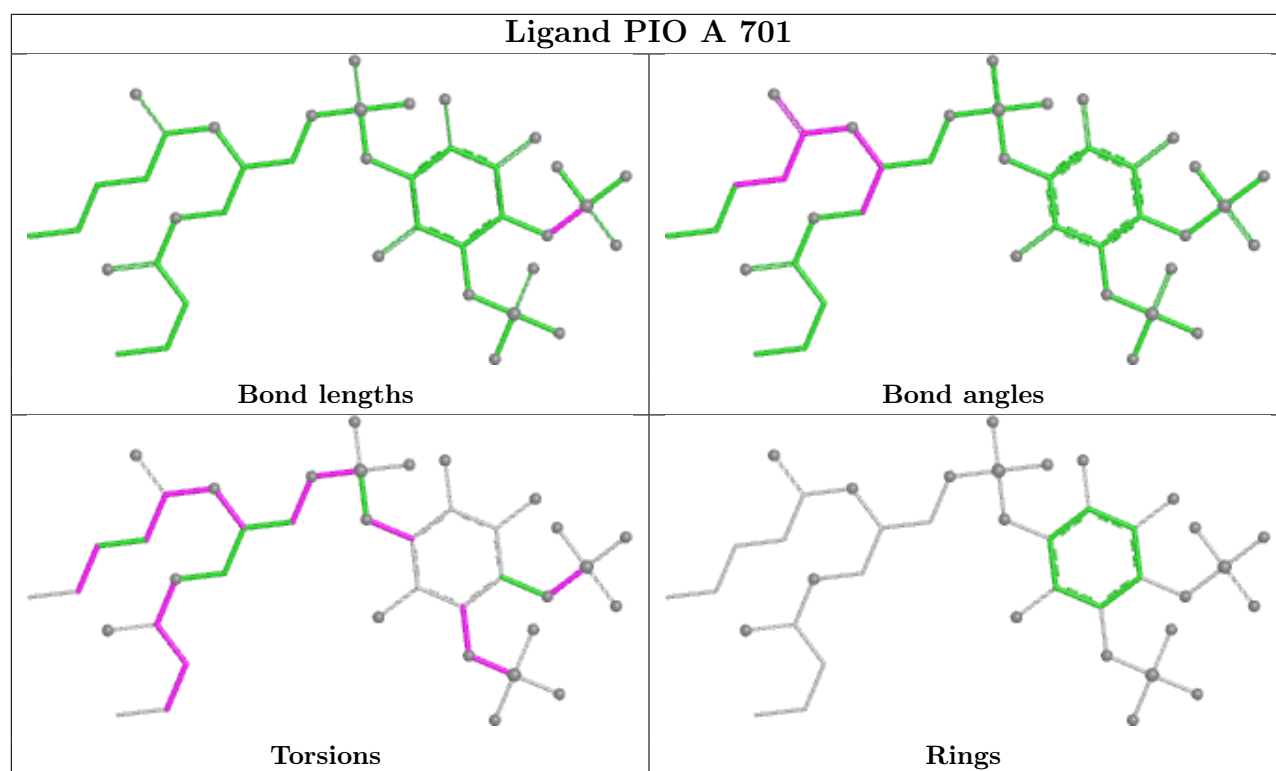
All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	PIO	C2-C1-O1-P1
4	A	701	PIO	C1C-O13-P1-O1
4	A	701	PIO	C1C-O13-P1-O11
4	A	701	PIO	C1C-O13-P1-O12
4	A	701	PIO	C4-C5-O5-P5
4	A	701	PIO	C6-C5-O5-P5
4	A	701	PIO	C2A-C1A-O2C-C2C
4	A	701	PIO	O1A-C1A-O2C-C2C
4	A	701	PIO	C3C-C2C-O2C-C1A
4	A	701	PIO	C2B-C1B-O3C-C3C
4	A	701	PIO	C2A-C3A-C4A-C5A
4	A	701	PIO	O1B-C1B-O3C-C3C
4	A	701	PIO	C5-O5-P5-O53
4	A	701	PIO	C1B-C2B-C3B-C4B
4	A	701	PIO	O3C-C1B-C2B-C3B
4	A	701	PIO	O2C-C1A-C2A-C3A
4	A	701	PIO	C6-C1-O1-P1
4	A	701	PIO	C4-O4-P4-O41
4	A	701	PIO	O1A-C1A-C2A-C3A
4	A	701	PIO	C2C-C1C-O13-P1

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.

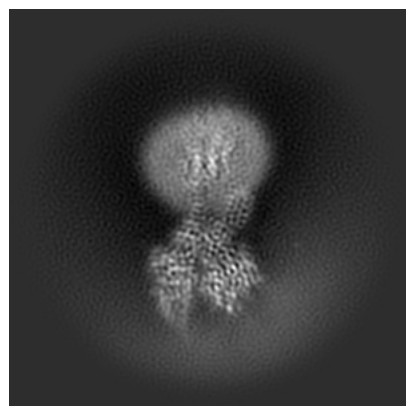
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36606. These allow visual inspection of the internal detail of the map and identification of artifacts.

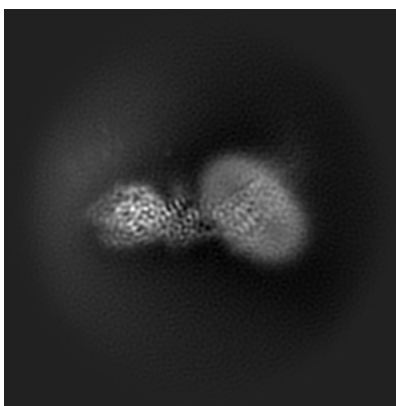
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

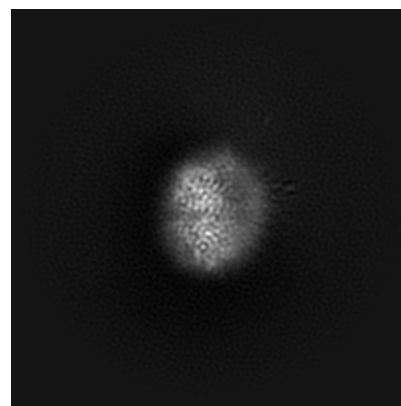
6.1.1 Primary map



X

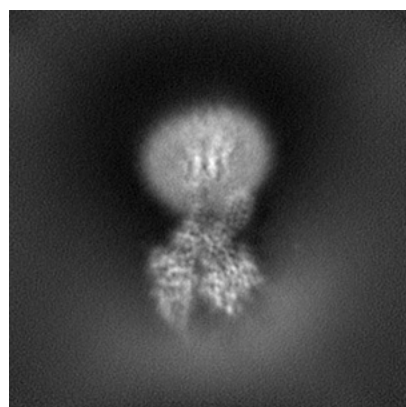


Y

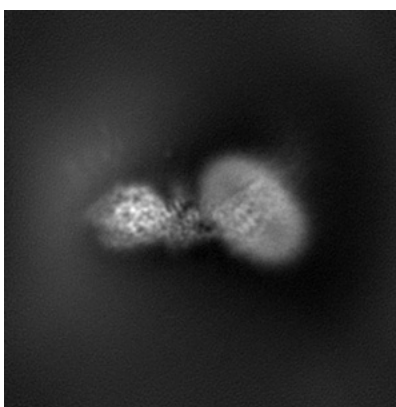


Z

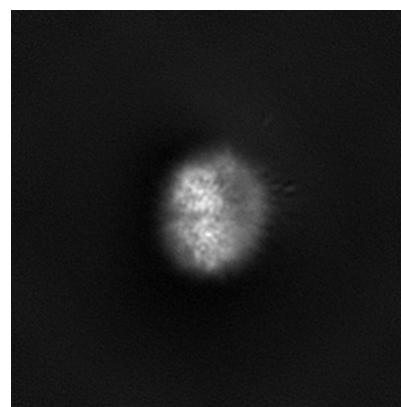
6.1.2 Raw map



X



Y

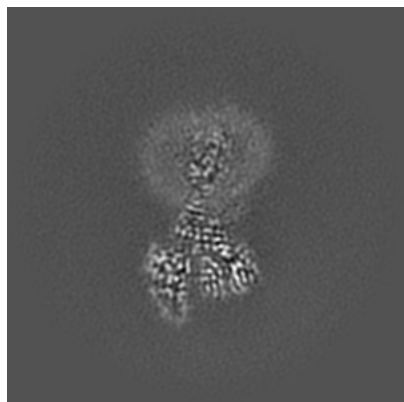


Z

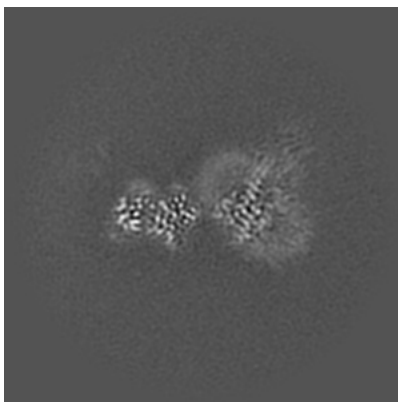
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

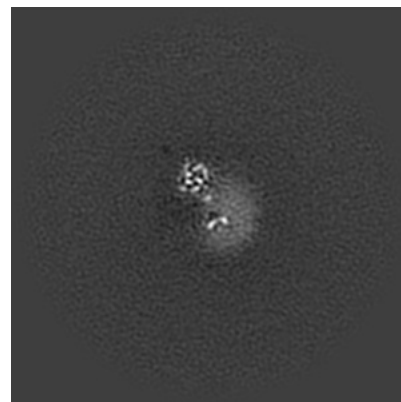
6.2.1 Primary map



X Index: 128

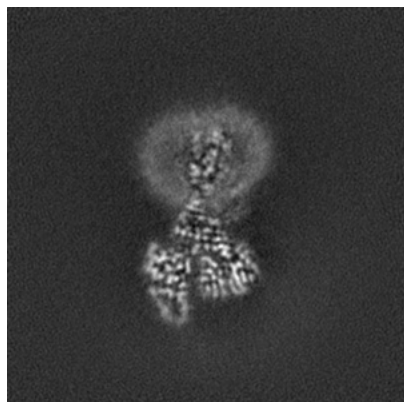


Y Index: 128

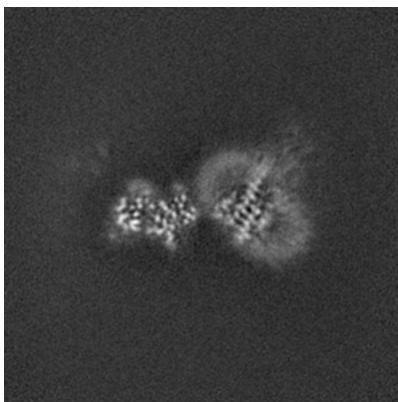


Z Index: 128

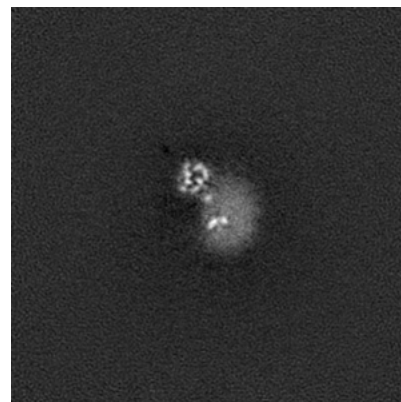
6.2.2 Raw map



X Index: 128



Y Index: 128

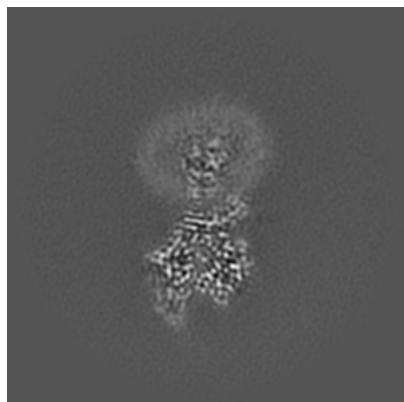


Z Index: 128

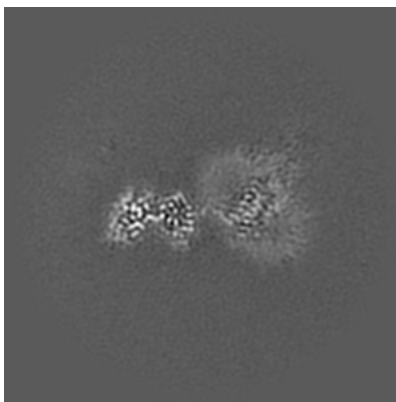
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

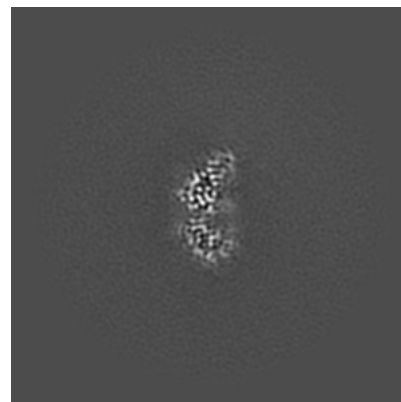
6.3.1 Primary map



X Index: 123

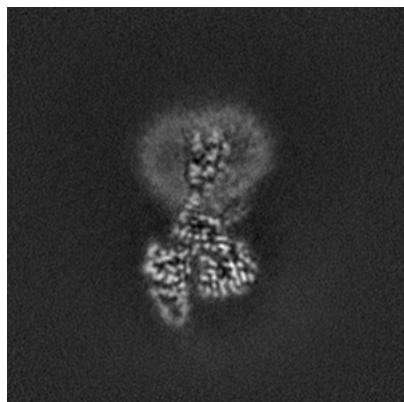


Y Index: 132

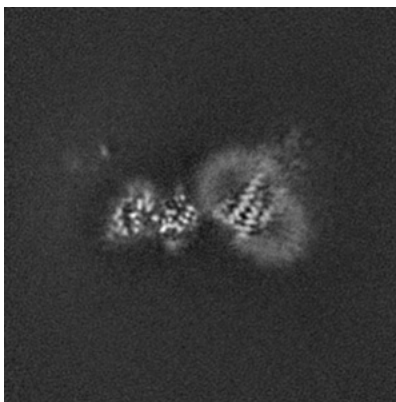


Z Index: 82

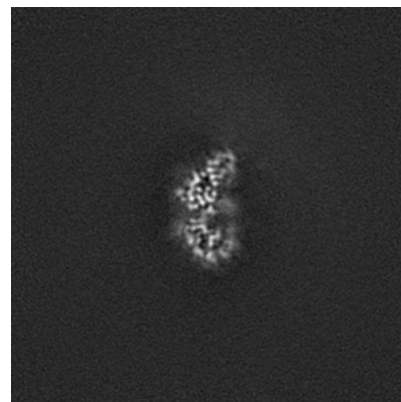
6.3.2 Raw map



X Index: 127



Y Index: 130

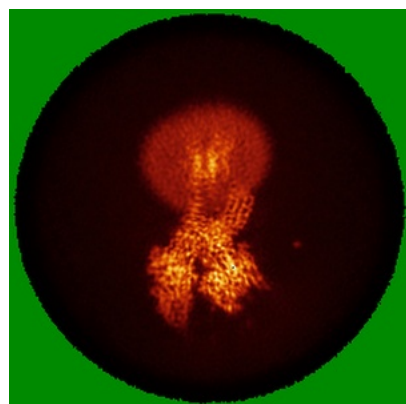


Z Index: 82

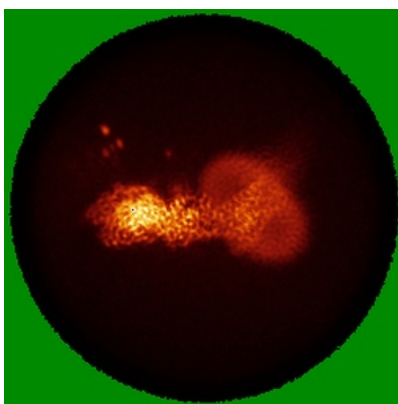
The images above show the largest variance slices of the map in three orthogonal directions.

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

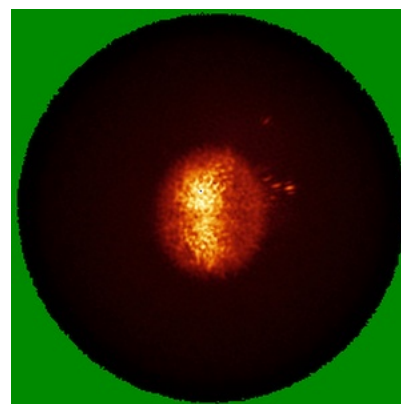
6.4.1 Primary map



X

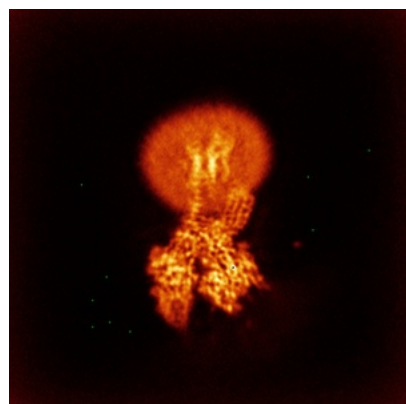


Y

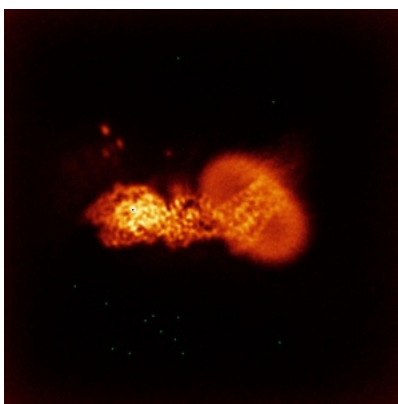


Z

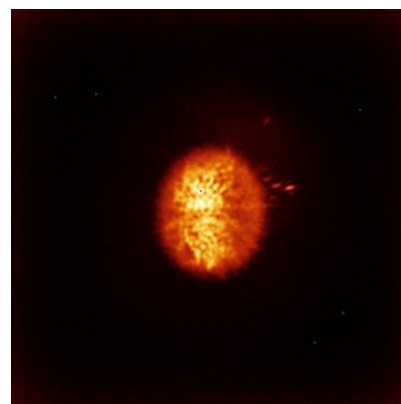
6.4.2 Raw map



X



Y

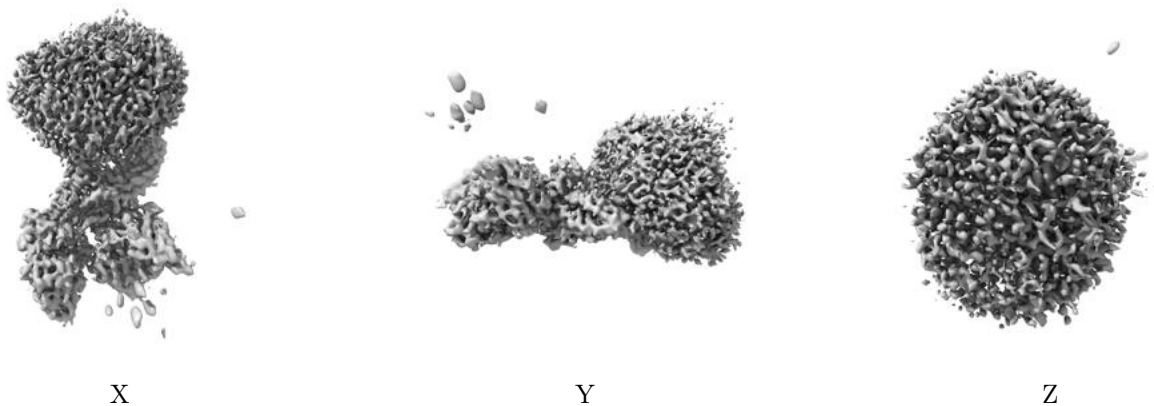


Z

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.

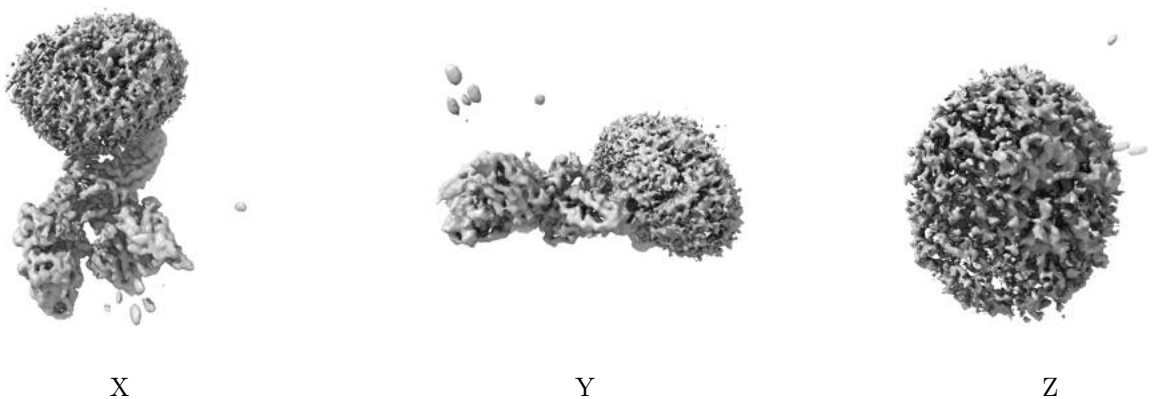
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.35. 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.

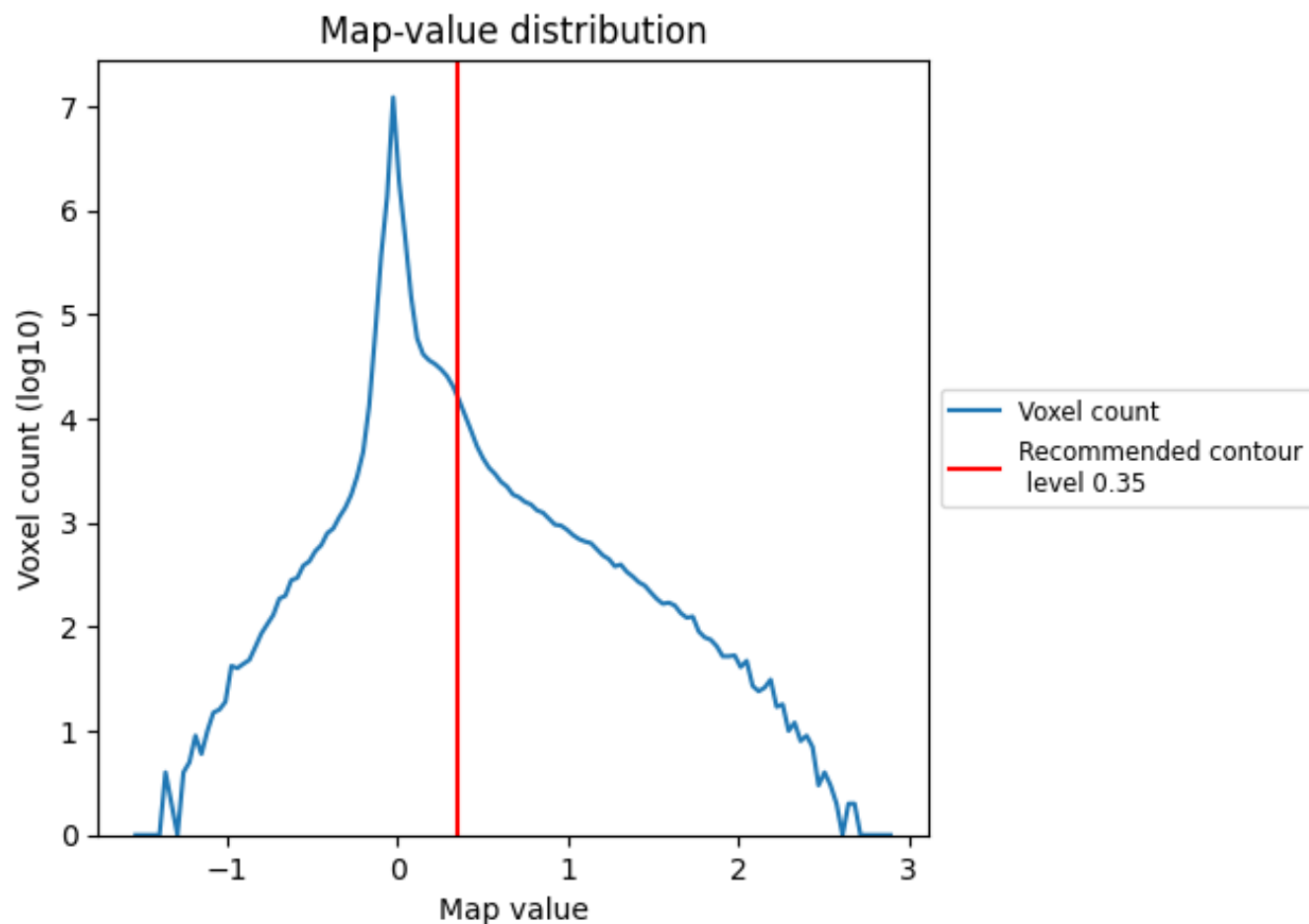
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

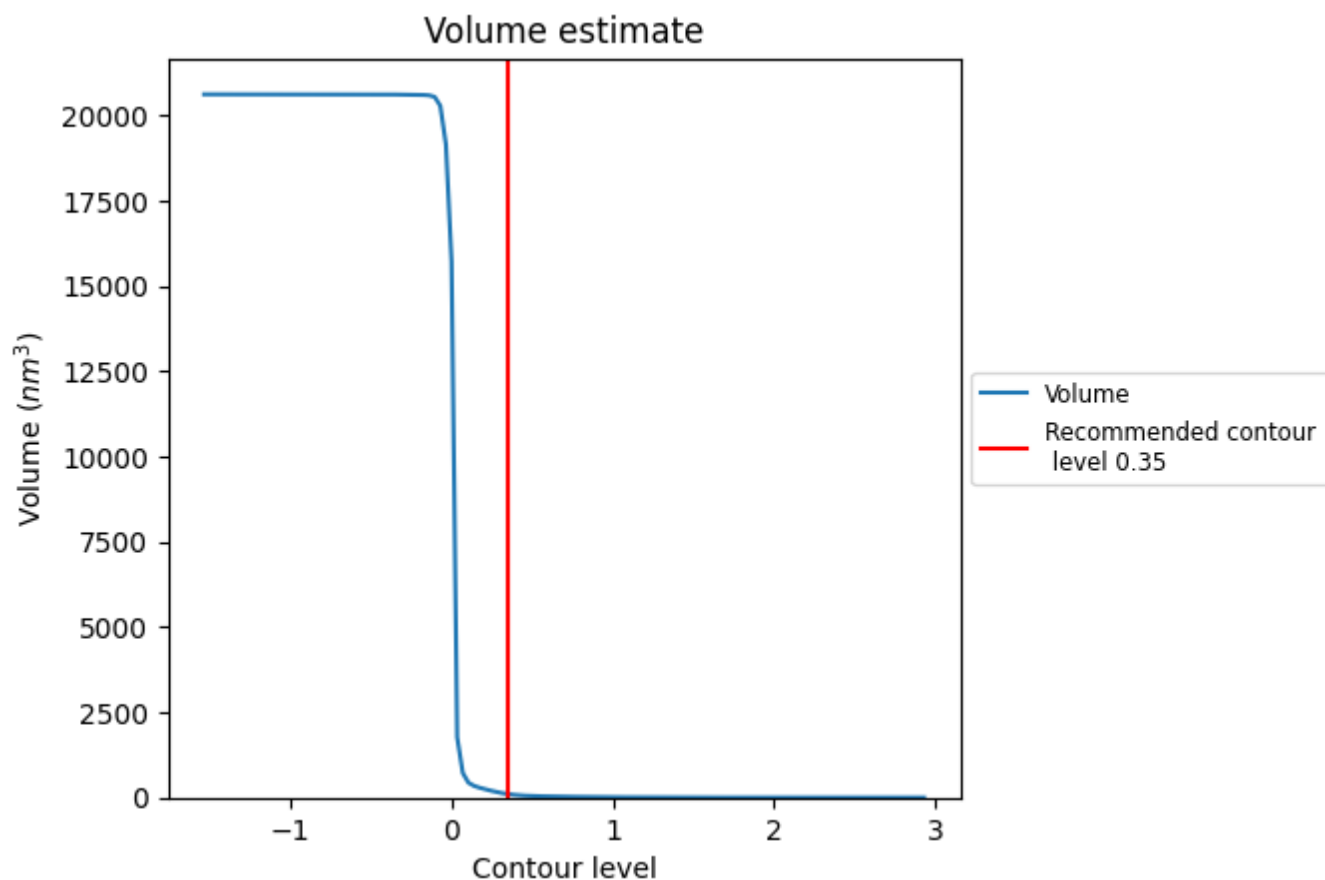
This section contains the results of statistical analysis of the map.

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.

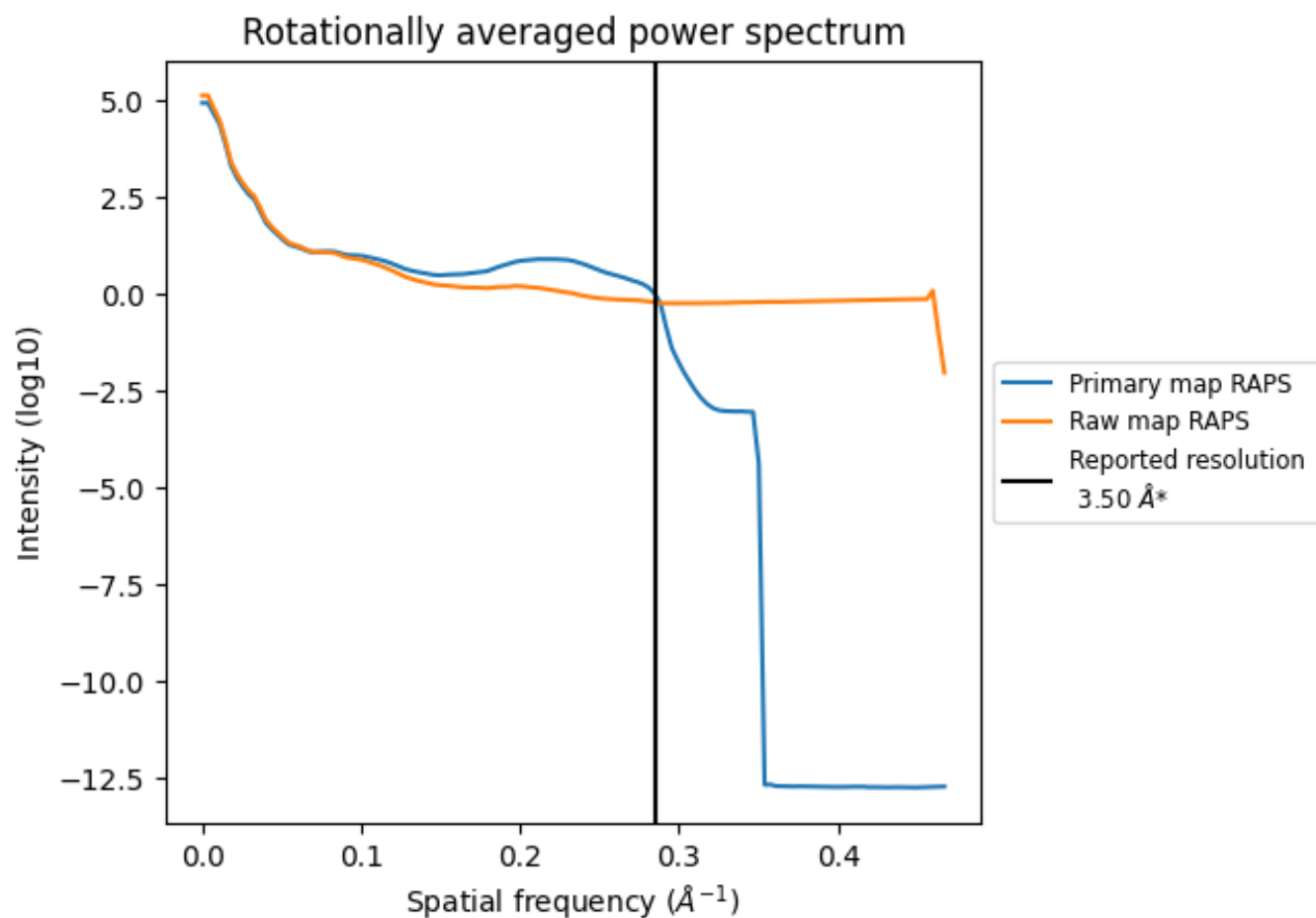
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 100 nm³; this corresponds to an approximate mass of 90 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 ⓘ

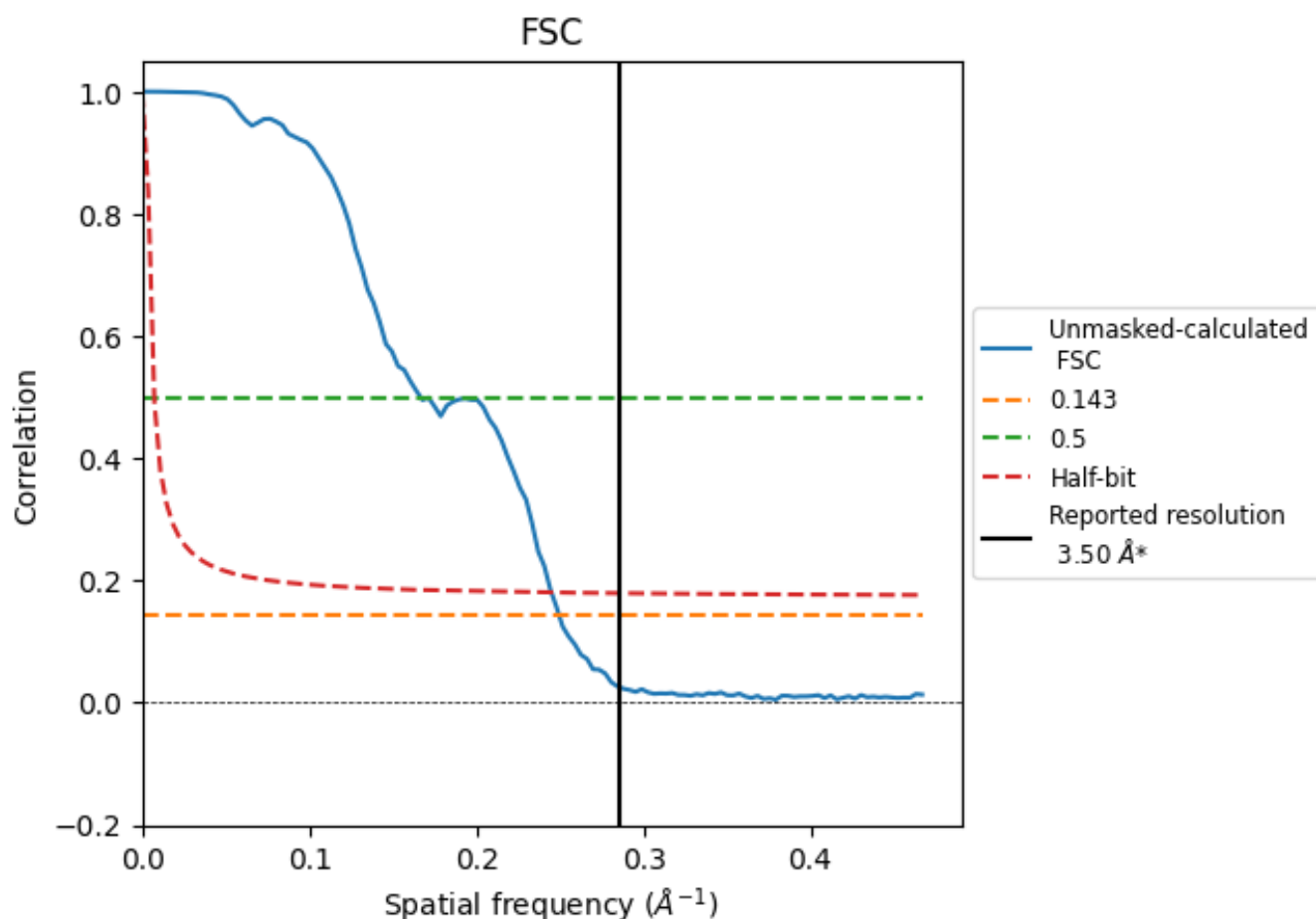


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

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 $0.286 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

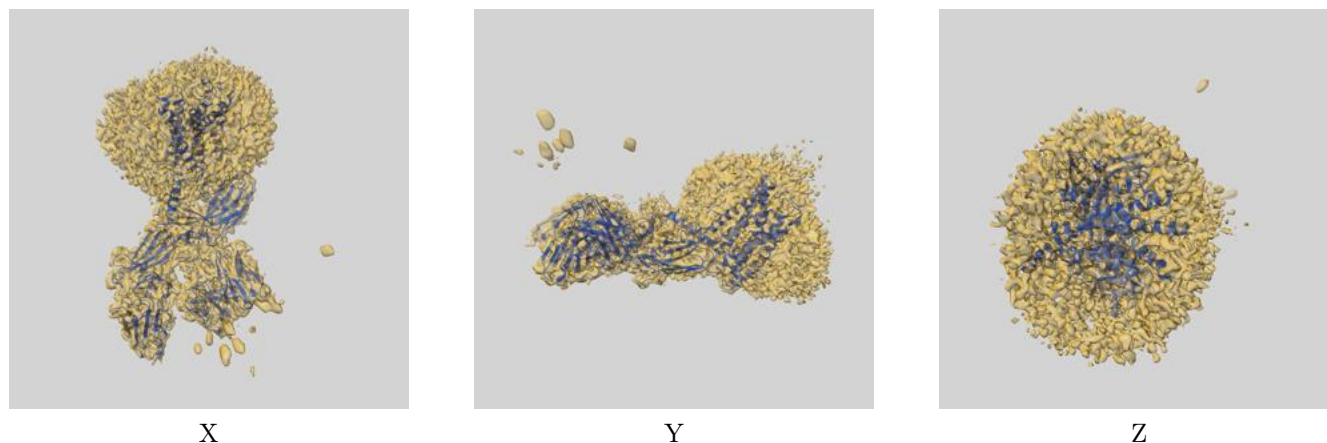
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.00	4.08

*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 4.01 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

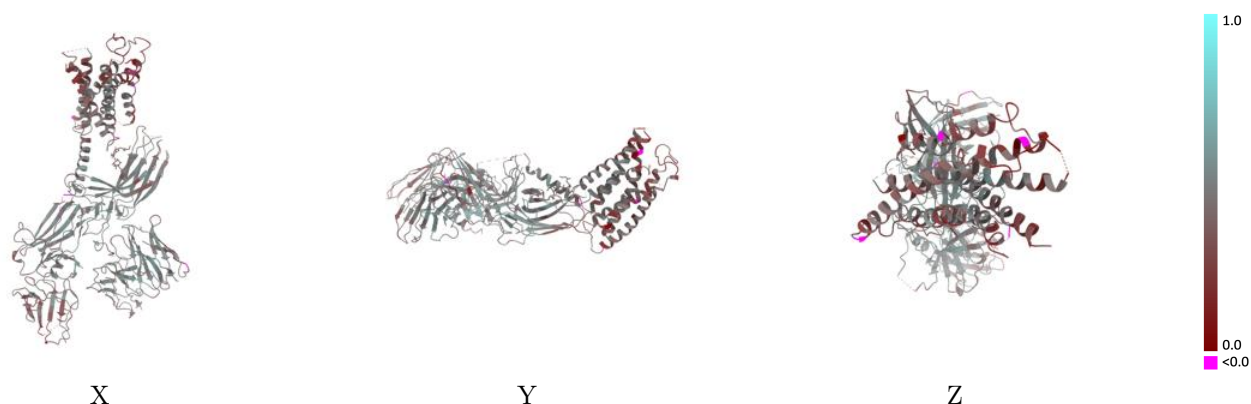
This section contains information regarding the fit between EMDB map EMD-36606 and PDB model 8JRU. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



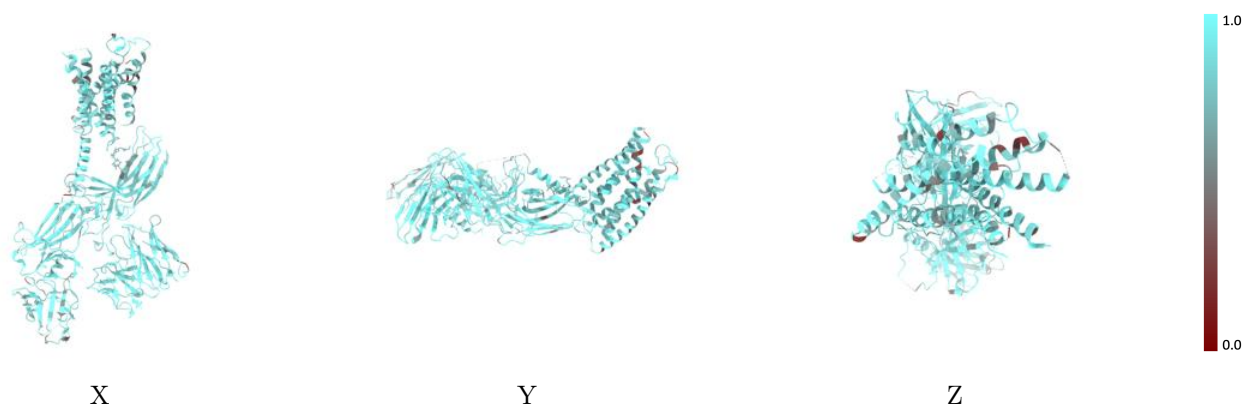
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



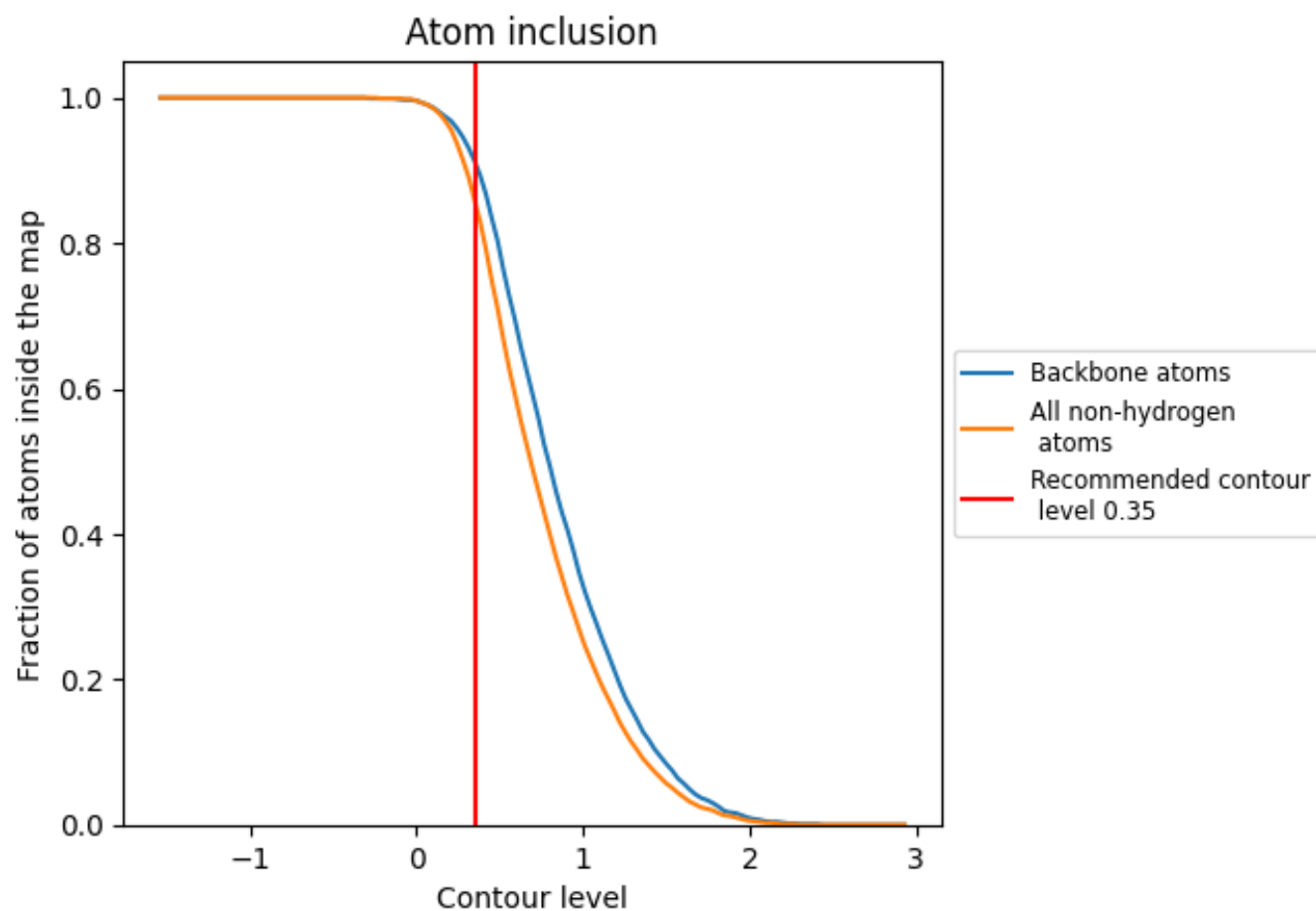
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 86% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8580	0.4380
A	0.8780	0.4700
B	0.8060	0.4150
H	0.8910	0.4690
L	0.9160	0.4830
R	0.8170	0.3720

