



## Full wwPDB EM Validation Report ⓘ

Jun 9, 2025 – 01:53 PM EDT

PDB ID : 8TIO / pdb\_00008tio  
EMDB ID : EMD-41297  
Title : Human ACKR3 with C tail extended by 12 glycines phosphorylated by GRK5  
in complex with Arrestin2 reconstructed without receptor/micelle  
Authors : Chen, Q.; Tesmer, J.J.G.  
Deposited on : 2023-07-19  
Resolution : 3.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

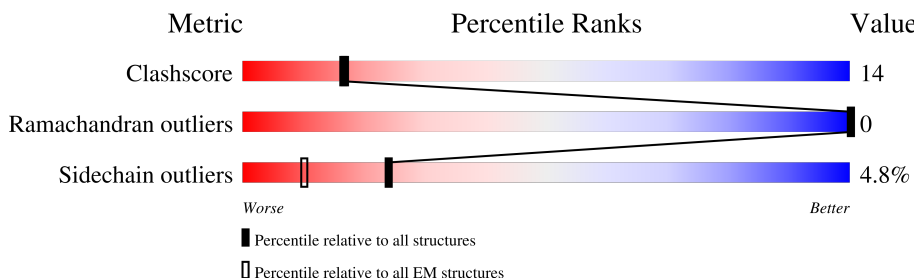
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*




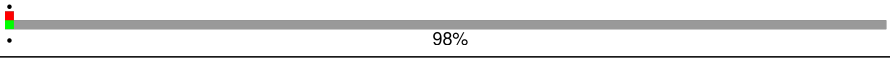
The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	418	
2	H	240	
3	L	215	
4	R	405	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11164 atoms, of which 5573 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 Beta-arrestin-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	299	Total	C	H	N	O	S	0	0
			4840	1531	2455	413	432	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	386	ALA	ILE	conflict	UNP P17870
A	387	ALA	VAL	conflict	UNP P17870
A	388	ALA	PHE	conflict	UNP P17870

- Molecule 2 is a protein called Fab7 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	H	204	Total	C	H	N	O	S	0	0
			3087	1007	1517	260	296	7		

- Molecule 3 is a protein called Fab7 light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	L	204	Total	C	H	N	O	S	0	0
			3115	992	1539	262	317	5		

- Molecule 4 is a protein called Atypical chemokine receptor 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	R	7	Total	C	H	N	O	P	0	0
			122	34	62	9	15	2		

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	GLY	-	expression tag	UNP P25106

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Chain	Residue	Modelled	Actual	Comment	Reference
R	2	ALA	-	expression tag	UNP P25106
R	3	PRO	-	expression tag	UNP P25106
R	337	GLY	-	insertion	UNP P25106
R	338	GLY	-	insertion	UNP P25106
R	339	GLY	-	insertion	UNP P25106
R	340	GLY	-	insertion	UNP P25106
R	341	GLY	-	insertion	UNP P25106
R	342	GLY	-	insertion	UNP P25106
R	343	GLY	-	insertion	UNP P25106
R	344	GLY	-	insertion	UNP P25106
R	345	GLY	-	insertion	UNP P25106
R	346	GLY	-	insertion	UNP P25106
R	347	GLY	-	insertion	UNP P25106
R	348	GLY	-	insertion	UNP P25106
R	377	GLY	-	expression tag	UNP P25106
R	378	ARG	-	expression tag	UNP P25106
R	379	PRO	-	expression tag	UNP P25106
R	380	LEU	-	expression tag	UNP P25106
R	381	GLU	-	expression tag	UNP P25106
R	382	VAL	-	expression tag	UNP P25106
R	383	LEU	-	expression tag	UNP P25106
R	384	PHE	-	expression tag	UNP P25106
R	385	GLN	-	expression tag	UNP P25106
R	386	GLY	-	expression tag	UNP P25106
R	387	PRO	-	expression tag	UNP P25106
R	388	HIS	-	expression tag	UNP P25106
R	389	HIS	-	expression tag	UNP P25106
R	390	HIS	-	expression tag	UNP P25106
R	391	HIS	-	expression tag	UNP P25106
R	392	HIS	-	expression tag	UNP P25106
R	393	HIS	-	expression tag	UNP P25106
R	394	HIS	-	expression tag	UNP P25106
R	395	HIS	-	expression tag	UNP P25106
R	396	HIS	-	expression tag	UNP P25106
R	397	HIS	-	expression tag	UNP P25106
R	398	ASP	-	expression tag	UNP P25106
R	399	TYR	-	expression tag	UNP P25106
R	400	LYS	-	expression tag	UNP P25106
R	401	ASP	-	expression tag	UNP P25106
R	402	ASP	-	expression tag	UNP P25106
R	403	ASP	-	expression tag	UNP P25106
R	404	ASP	-	expression tag	UNP P25106

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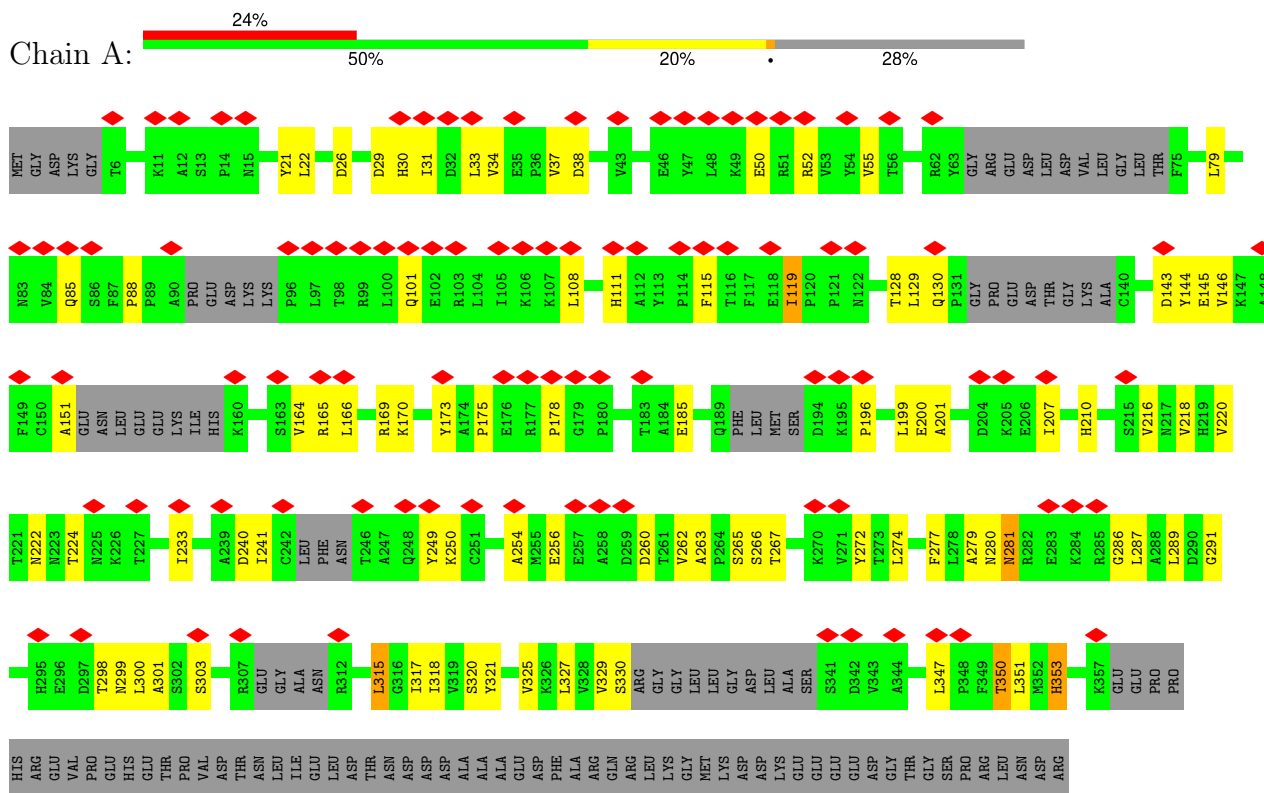
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Chain	Residue	Modelled	Actual	Comment	Reference
R	405	LYS	-	expression tag	UNP P25106

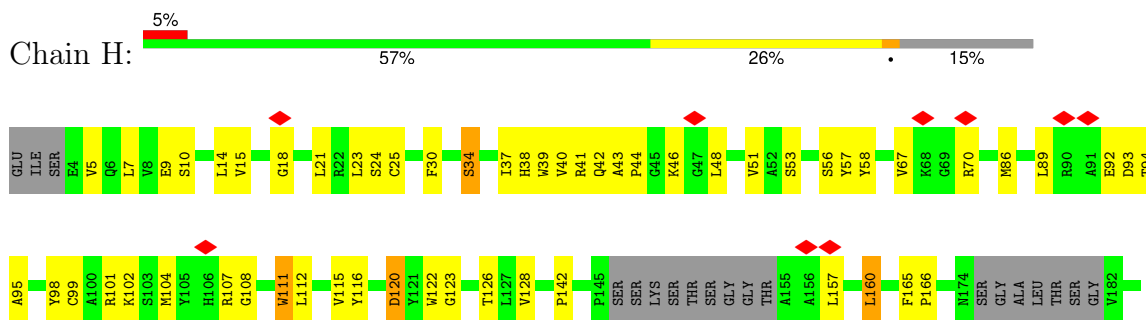
### 3 Residue-property plots [i](#)

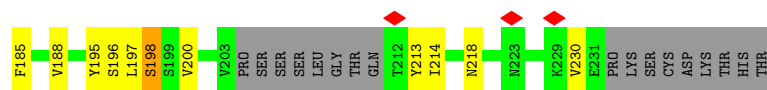
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Beta-arrestin-1

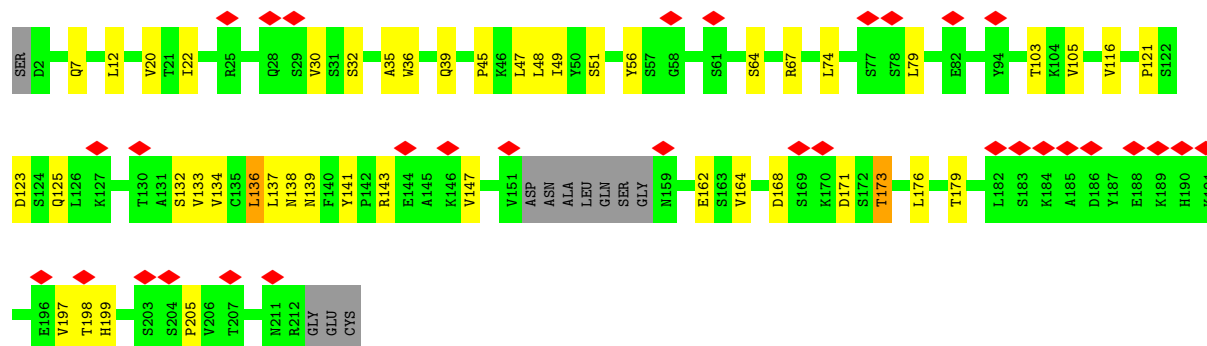
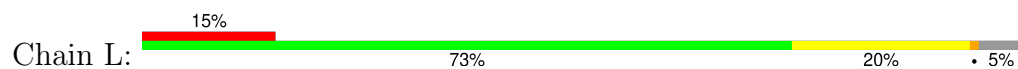


#### • Molecule 2: Fab7 heavy chain

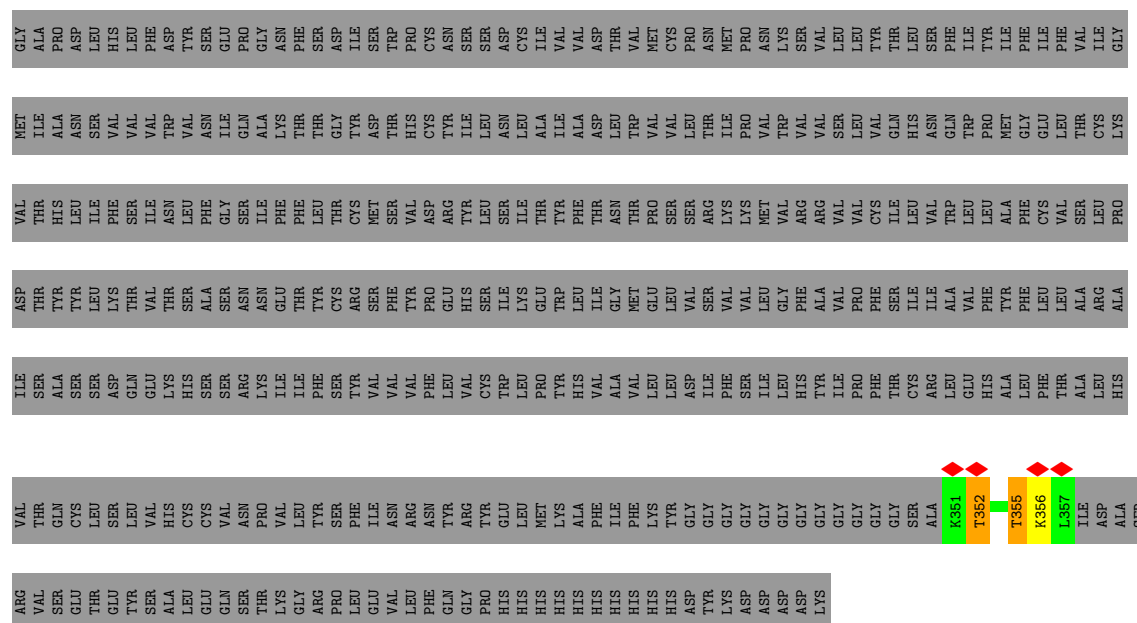




• Molecule 3: Fab7 light chain



• Molecule 4: Atypical chemokine receptor 3



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285430	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 ( $e^-/\text{\AA}^2$ )	56	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.273	Depositor
Minimum map value	-1.554	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.258	Depositor
Map size ( $\text{\AA}$ )	337.28, 337.28, 337.28	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.054, 1.054, 1.054	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: 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	A	0.13	0/2431	0.27	0/3288
2	H	0.18	0/1613	0.33	0/2197
3	L	0.15	0/1611	0.30	0/2187
4	R	0.05	0/35	0.15	0/40
All	All	0.15	0/5690	0.29	0/7712

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	A	2385	2455	2453	68	0
2	H	1570	1517	1514	59	0
3	L	1576	1539	1539	37	0
4	R	60	62	61	2	0
All	All	5591	5573	5567	154	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 14.

All (154) 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:249:TYR:OH	1:A:286:GLY:O	1.89	0.90
1:A:299:ASN:OD1	1:A:353:HIS:NE2	2.15	0.80
3:L:125:GLN:OE1	3:L:132:SER:N	2.16	0.78
2:H:42:GLN:OE1	3:L:39:GLN:NE2	2.17	0.77
1:A:301:ALA:O	1:A:321:TYR:OH	2.04	0.74
2:H:48:LEU:HD11	3:L:45:PRO:CG	2.19	0.73
1:A:143:ASP:OD1	1:A:144:TYR:N	2.23	0.72
1:A:260:ASP:OD2	1:A:272:TYR:OH	2.06	0.72
3:L:171:ASP:O	3:L:173:THR:OG1	2.09	0.70
3:L:30:VAL:O	3:L:67:ARG:NH2	2.24	0.70
3:L:164:VAL:HG22	3:L:176:LEU:HG	1.72	0.69
2:H:9:GLU:OE2	2:H:99:CYS:N	2.26	0.69
1:A:210:HIS:NE2	1:A:300:LEU:O	2.25	0.69
1:A:37:VAL:HG11	1:A:146:VAL:HG21	1.75	0.67
1:A:199:LEU:HD22	1:A:327:LEU:HD11	1.78	0.66
2:H:70:ARG:NH1	2:H:93:ASP:OD2	2.30	0.64
3:L:143:ARG:NH2	3:L:164:VAL:HG21	2.12	0.64
1:A:196:PRO:O	1:A:224:THR:HG23	1.95	0.64
1:A:79:LEU:HD21	1:A:315:LEU:HD13	1.79	0.64
3:L:20:VAL:HG21	3:L:79:LEU:HD22	1.81	0.63
2:H:142:PRO:HB3	2:H:230:VAL:HG22	1.81	0.63
2:H:38:HIS:HD1	2:H:53:SER:HG	1.47	0.63
1:A:29:ASP:OD2	1:A:170:LYS:NZ	2.20	0.62
2:H:86:MET:HB3	2:H:89:LEU:HD21	1.82	0.62
2:H:120:ASP:N	2:H:120:ASP:OD1	2.32	0.62
1:A:50:GLU:N	1:A:50:GLU:OE1	2.33	0.61
1:A:263:ALA:O	1:A:266:SER:OG	2.13	0.61
1:A:199:LEU:HD22	1:A:327:LEU:CD1	2.31	0.61
3:L:121:PRO:HD3	3:L:133:VAL:HG12	1.81	0.61
1:A:37:VAL:HG11	1:A:146:VAL:CG2	2.32	0.59
2:H:142:PRO:CB	2:H:230:VAL:HG22	2.33	0.59
2:H:99:CYS:O	2:H:123:GLY:N	2.36	0.59
3:L:116:VAL:HG21	3:L:197:VAL:HG11	1.84	0.58
2:H:10:SER:OG	2:H:24:SER:OG	2.20	0.58
2:H:42:GLN:NE2	2:H:46:LYS:O	2.36	0.58
1:A:52:ARG:O	1:A:151:ALA:N	2.38	0.57
2:H:14:LEU:HD11	2:H:165:PHE:HE1	1.70	0.57
1:A:199:LEU:HD22	1:A:327:LEU:CG	2.35	0.57
2:H:41:ARG:NH2	2:H:92:GLU:O	2.38	0.56
1:A:22:LEU:HD12	1:A:166:LEU:HD23	1.87	0.56
1:A:199:LEU:HD12	1:A:200:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:137:LEU:HD21	3:L:147:VAL:CG1	2.35	0.55
2:H:51:VAL:HG13	2:H:67:VAL:HG11	1.88	0.55
2:H:30:PHE:CE2	2:H:37:ILE:HD11	2.41	0.55
2:H:48:LEU:HD21	3:L:45:PRO:HG2	1.90	0.54
2:H:86:MET:HE1	2:H:128:VAL:HG11	1.89	0.54
1:A:279:ALA:HB2	2:H:56:SER:O	2.08	0.54
1:A:22:LEU:CD1	1:A:166:LEU:HD23	2.38	0.53
3:L:79:LEU:CD2	3:L:105:VAL:HG11	2.39	0.53
3:L:143:ARG:HH22	3:L:164:VAL:HG21	1.71	0.53
1:A:199:LEU:HD22	1:A:327:LEU:HG	1.90	0.53
1:A:303:SER:OG	1:A:351:LEU:N	2.42	0.52
2:H:101:ARG:NH1	2:H:120:ASP:OD2	2.42	0.52
3:L:162:GLU:HB3	3:L:176:LEU:HD21	1.91	0.52
1:A:129:LEU:HD21	1:A:317:ILE:HD13	1.91	0.52
2:H:5:VAL:HG13	2:H:30:PHE:CD1	2.45	0.52
2:H:40:VAL:HG21	2:H:122:TRP:CH2	2.45	0.52
1:A:21:TYR:CE1	1:A:108:LEU:HD21	2.45	0.51
1:A:281:ASN:OD1	1:A:281:ASN:N	2.42	0.51
2:H:200:VAL:HG21	3:L:136:LEU:CD1	2.40	0.51
2:H:7:LEU:HD23	2:H:25:CYS:SG	2.51	0.51
3:L:141:TYR:O	3:L:199:HIS:NE2	2.44	0.50
1:A:254:ALA:HB1	1:A:274:LEU:HD22	1.93	0.50
2:H:185:PHE:HE1	2:H:200:VAL:HG22	1.77	0.50
2:H:107:ARG:HA	2:H:112:LEU:HD11	1.93	0.49
1:A:256:GLU:HB2	1:A:274:LEU:HD21	1.94	0.49
1:A:318:ILE:HD12	1:A:318:ILE:N	2.27	0.49
1:A:233:ILE:O	1:A:274:LEU:HD11	2.12	0.49
1:A:30:HIS:O	1:A:33:LEU:O	2.31	0.49
1:A:21:TYR:CZ	1:A:108:LEU:HD21	2.48	0.49
1:A:145:GLU:OE2	1:A:165:ARG:NE	2.41	0.49
1:A:22:LEU:HD12	1:A:166:LEU:CD2	2.43	0.48
4:R:355:TPO:OG1	4:R:356:LYS:N	2.36	0.48
1:A:216:VAL:HG21	1:A:233:ILE:HG21	1.96	0.48
1:A:303:SER:HB2	1:A:350:THR:HG23	1.95	0.48
3:L:79:LEU:HD21	3:L:105:VAL:HG11	1.96	0.48
2:H:30:PHE:CZ	2:H:37:ILE:HD11	2.49	0.48
2:H:197:LEU:C	2:H:197:LEU:HD12	2.39	0.48
2:H:42:GLN:NE2	3:L:39:GLN:OE1	2.47	0.47
2:H:214:ILE:HD12	2:H:214:ILE:N	2.30	0.47
3:L:134:VAL:HG22	3:L:179:THR:HG23	1.96	0.47
1:A:233:ILE:HG22	1:A:274:LEU:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:48:LEU:HD11	3:L:45:PRO:CB	2.45	0.47
1:A:287:LEU:HD21	1:A:300:LEU:HD22	1.97	0.47
3:L:138:ASN:OD1	3:L:139:ASN:N	2.47	0.47
1:A:101:GLN:NE2	1:A:115:PHE:O	2.48	0.47
2:H:48:LEU:HD21	3:L:45:PRO:CG	2.44	0.46
1:A:128:THR:O	1:A:289:LEU:N	2.49	0.46
2:H:48:LEU:HD11	3:L:45:PRO:HG3	1.92	0.46
2:H:7:LEU:N	2:H:7:LEU:HD12	2.30	0.46
1:A:287:LEU:HD21	1:A:300:LEU:CD2	2.46	0.46
1:A:317:ILE:C	1:A:318:ILE:HD12	2.42	0.45
2:H:38:HIS:CG	2:H:53:SER:HG	2.34	0.45
3:L:137:LEU:HD12	3:L:137:LEU:N	2.32	0.45
1:A:222:ASN:O	1:A:265:SER:N	2.49	0.45
3:L:198:THR:HG22	3:L:205:PRO:HB3	1.99	0.45
1:A:169:ARG:NH1	1:A:291:GLY:O	2.44	0.45
3:L:47:LEU:HD23	3:L:56:TYR:CD1	2.52	0.45
1:A:173:TYR:OH	2:H:108:GLY:O	2.27	0.45
3:L:136:LEU:C	3:L:137:LEU:HD12	2.42	0.45
1:A:30:HIS:O	1:A:31:ILE:C	2.59	0.45
2:H:34:SER:O	2:H:34:SER:OG	2.26	0.45
2:H:7:LEU:HD23	2:H:99:CYS:SG	2.57	0.44
2:H:213:TYR:C	2:H:214:ILE:HD12	2.43	0.44
1:A:277:PHE:O	1:A:281:ASN:ND2	2.50	0.44
2:H:58:TYR:HH	2:H:111:TRP:CD1	2.35	0.44
1:A:240:ASP:OD1	1:A:241:ILE:N	2.50	0.44
1:A:262:VAL:HG12	1:A:266:SER:OG	2.18	0.44
2:H:112:LEU:HB3	2:H:115:VAL:HG13	2.00	0.44
2:H:115:VAL:HG23	2:H:116:TYR:N	2.33	0.44
3:L:64:SER:O	3:L:74:LEU:HD12	2.18	0.44
2:H:37:ILE:O	2:H:53:SER:HA	2.18	0.43
2:H:160:LEU:HD23	3:L:125:GLN:HE22	1.82	0.43
2:H:107:ARG:HB2	2:H:112:LEU:HG	1.99	0.43
2:H:195:TYR:O	2:H:196:SER:OG	2.29	0.43
3:L:35:ALA:HA	3:L:49:ILE:O	2.18	0.43
1:A:199:LEU:HD12	1:A:200:GLU:N	2.34	0.43
1:A:279:ALA:N	2:H:57:TYR:O	2.52	0.43
2:H:39:TRP:O	2:H:51:VAL:N	2.48	0.43
4:R:352:TPO:O3P	4:R:352:TPO:N	2.45	0.43
1:A:300:LEU:HD12	1:A:351:LEU:HD21	2.00	0.43
1:A:79:LEU:CD2	1:A:315:LEU:HD13	2.47	0.43
3:L:7:GLN:OE1	3:L:22:ILE:HG21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ASP:OD1	1:A:169:ARG:NE	2.41	0.43
1:A:303:SER:HG	1:A:321:TYR:HD1	1.60	0.42
2:H:102:LYS:HE3	2:H:115:VAL:HG21	2.02	0.42
1:A:199:LEU:HD13	1:A:220:VAL:HG22	2.01	0.42
2:H:14:LEU:HD23	2:H:15:VAL:N	2.34	0.42
3:L:32:SER:O	3:L:51:SER:C	2.62	0.42
3:L:123:ASP:OD1	3:L:123:ASP:N	2.53	0.42
1:A:85:GLN:NE2	1:A:88:PRO:O	2.53	0.41
1:A:329:VAL:HG12	1:A:330:SER:N	2.35	0.41
1:A:201:ALA:HB2	1:A:325:VAL:HG21	2.02	0.41
2:H:165:PHE:CE1	2:H:166:PRO:HB3	2.55	0.41
2:H:51:VAL:CG1	2:H:67:VAL:HG11	2.51	0.41
3:L:103:THR:O	3:L:103:THR:HG22	2.21	0.41
2:H:43:ALA:HB1	2:H:44:PRO:CD	2.51	0.41
1:A:218:VAL:HG21	1:A:233:ILE:HD11	2.02	0.41
1:A:350:THR:O	1:A:350:THR:HG22	2.20	0.41
3:L:36:TRP:O	3:L:48:LEU:N	2.47	0.41
1:A:34:VAL:HG11	1:A:119:ILE:HD12	2.02	0.41
1:A:175:PRO:HB2	1:A:207:ILE:HD11	2.03	0.41
1:A:201:ALA:CB	1:A:325:VAL:HG21	2.50	0.41
1:A:130:GLN:N	1:A:287:LEU:O	2.43	0.40
2:H:94:THR:O	2:H:95:ALA:HB2	2.21	0.40
2:H:18:GLY:N	2:H:89:LEU:O	2.44	0.40
2:H:197:LEU:HD12	2:H:198:SER:N	2.36	0.40
3:L:12:LEU:HD11	3:L:105:VAL:HG13	2.03	0.40
1:A:178:PRO:HA	1:A:207:ILE:HD12	2.04	0.40
1:A:277:PHE:CE1	1:A:279:ALA:HB3	2.56	0.40
2:H:23:LEU:HB3	2:H:39:TRP:CH2	2.56	0.40
1:A:128:THR:HG22	1:A:129:LEU:N	2.37	0.40
2:H:14:LEU:HD11	2:H:165:PHE:CE1	2.52	0.40
2:H:157:LEU:HD21	2:H:230:VAL:HB	2.03	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	281/418 (67%)	256 (91%)	25 (9%)	0	100	100
2	H	196/240 (82%)	177 (90%)	19 (10%)	0	100	100
3	L	200/215 (93%)	182 (91%)	18 (9%)	0	100	100
4	R	3/405 (1%)	3 (100%)	0	0	100	100
All	All	680/1278 (53%)	618 (91%)	62 (9%)	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	270/369 (73%)	254 (94%)	16 (6%)	16	45
2	H	170/200 (85%)	159 (94%)	11 (6%)	14	42
3	L	182/190 (96%)	179 (98%)	3 (2%)	58	76
4	R	4/361 (1%)	4 (100%)	0	100	100
All	All	626/1120 (56%)	596 (95%)	30 (5%)	24	51

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	55	VAL
1	A	111	HIS
1	A	119	ILE
1	A	164	VAL
1	A	185	GLU
1	A	250	LYS
1	A	267	THR
1	A	280	ASN
1	A	281	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	298	THR
1	A	315	LEU
1	A	320	SER
1	A	347	LEU
1	A	350	THR
1	A	353	HIS
2	H	21	LEU
2	H	34	SER
2	H	98	TYR
2	H	104	MET
2	H	111	TRP
2	H	120	ASP
2	H	126	THR
2	H	160	LEU
2	H	188	VAL
2	H	198	SER
2	H	218	ASN
3	L	136	LEU
3	L	168	ASP
3	L	173	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	L	148	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
4	TPO	R	355	4	8,10,11	1.64	1 (12%)	10,14,16	2.09	1 (10%)
4	TPO	R	352	4	8,10,11	1.11	0	10,14,16	2.02	1 (10%)

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	TPO	R	355	4	-	1/9/11/13	-
4	TPO	R	352	4	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	R	355	TPO	P-O1P	3.51	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	355	TPO	P-OG1-CB	-6.04	106.91	123.33
4	R	352	TPO	P-OG1-CB	-5.79	107.58	123.33

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	355	TPO	N-CA-CB-OG1
4	R	352	TPO	C-CA-CB-CG2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	355	TPO	1	0
4	R	352	TPO	1	0



## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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.

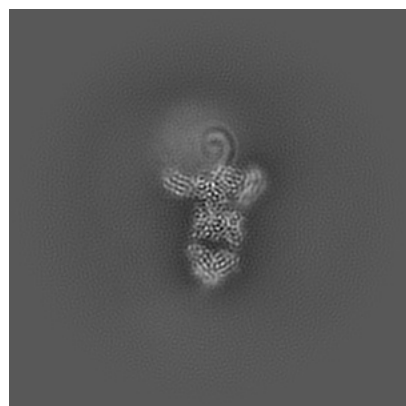
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41297. These allow visual inspection of the internal detail of the map and identification of artifacts.

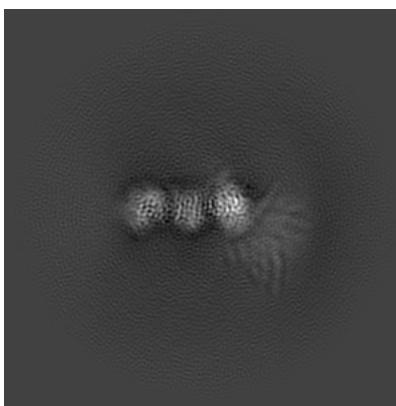
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

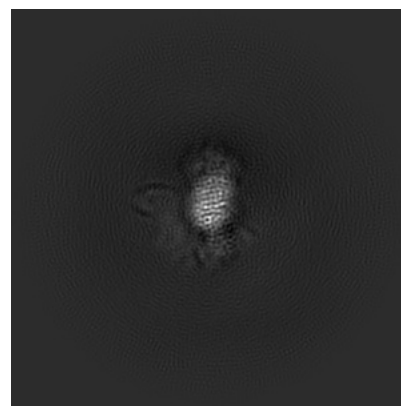
#### 6.1.1 Primary map



X

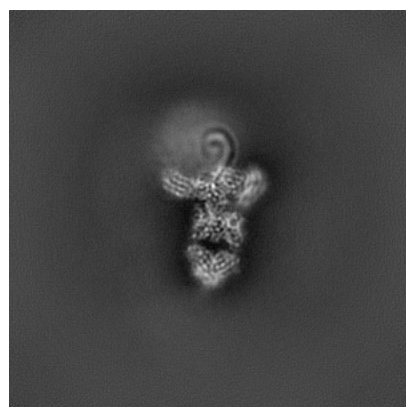


Y

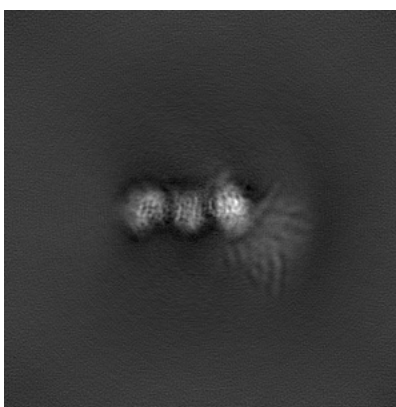


Z

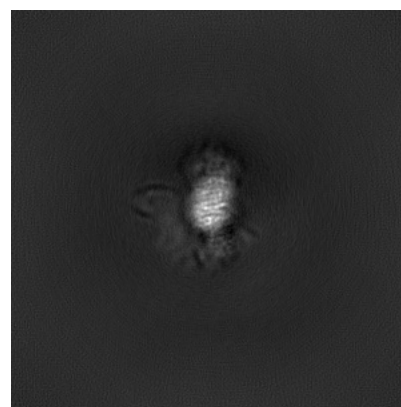
#### 6.1.2 Raw map



X



Y

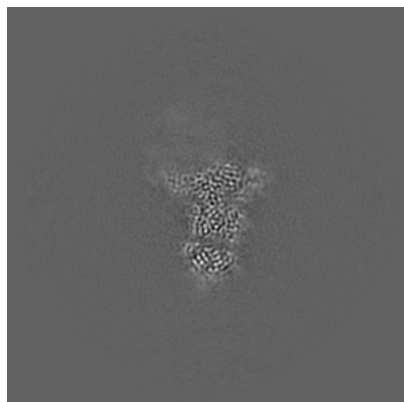


Z

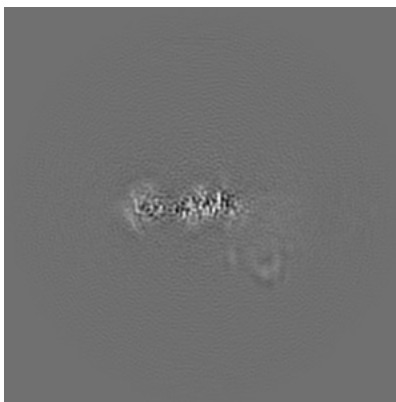
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

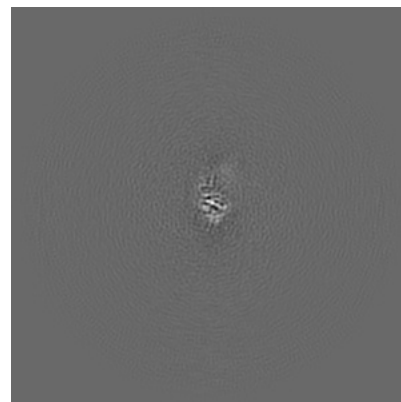
### 6.2.1 Primary map



X Index: 160

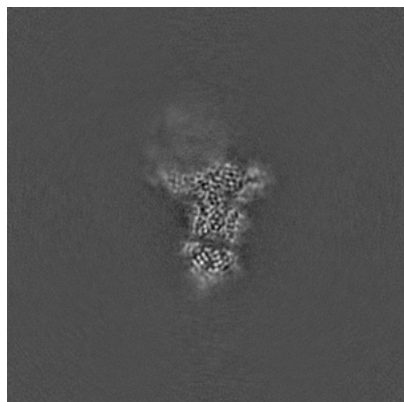


Y Index: 160

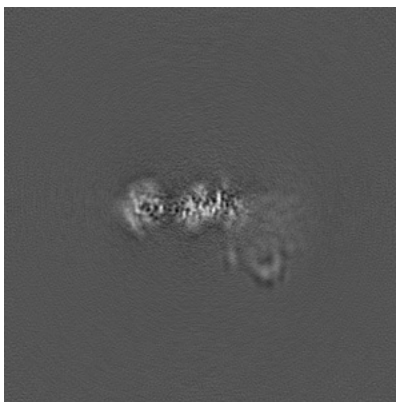


Z Index: 160

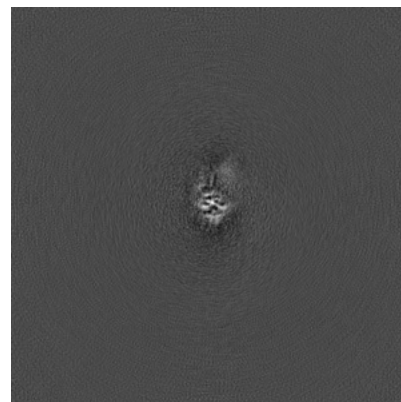
### 6.2.2 Raw map



X Index: 160



Y Index: 160

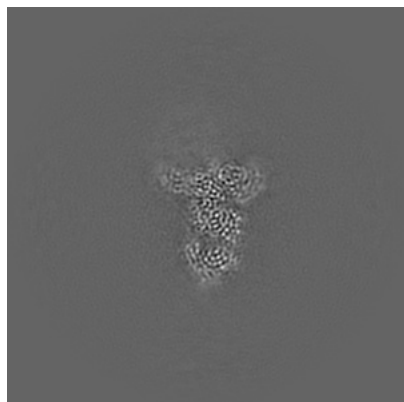


Z Index: 160

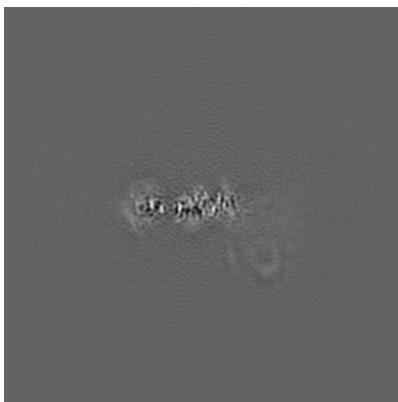
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

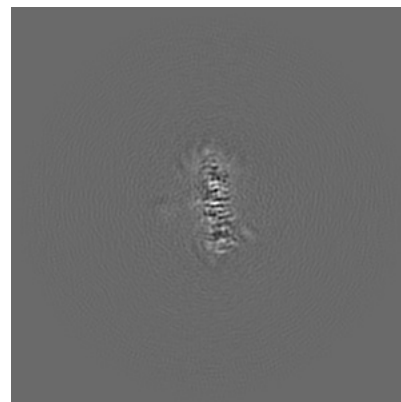
### 6.3.1 Primary map



X Index: 163

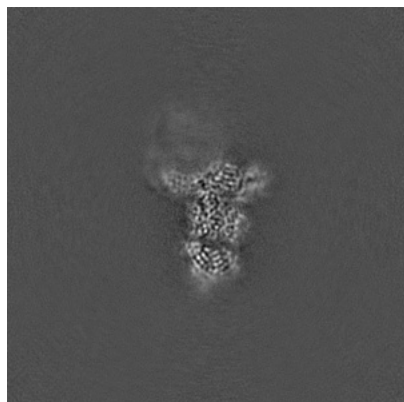


Y Index: 159

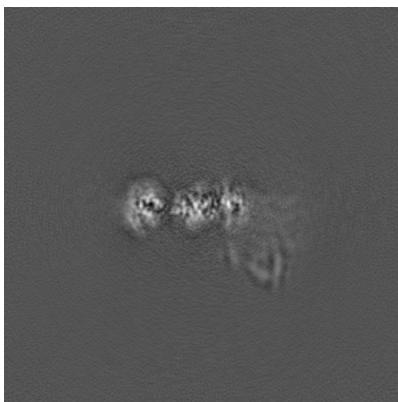


Z Index: 179

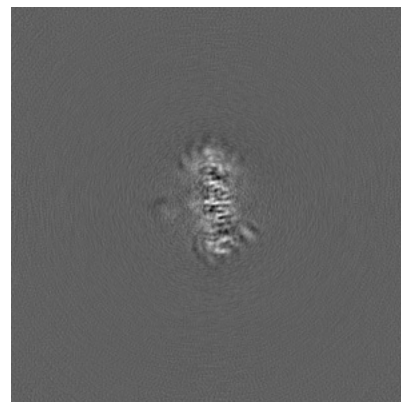
### 6.3.2 Raw map



X Index: 159



Y Index: 162



Z Index: 178

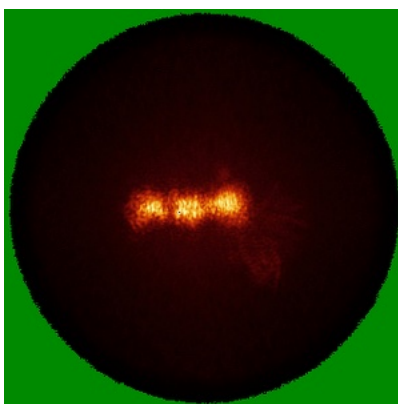
The images above show the largest variance slices of the map in three orthogonal directions.

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

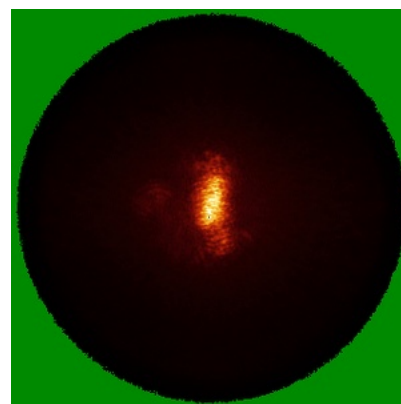
### 6.4.1 Primary map



X

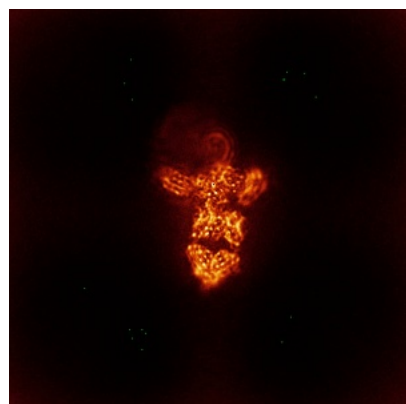


Y

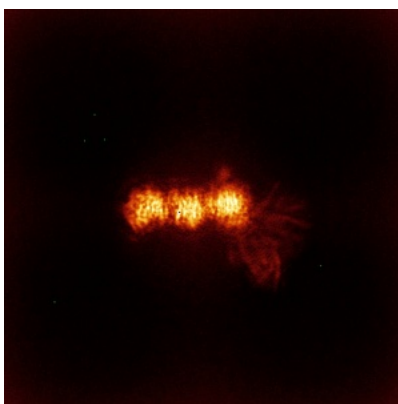


Z

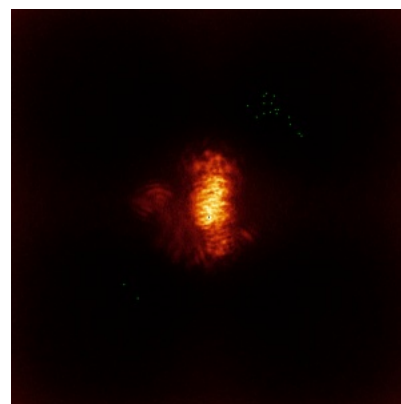
### 6.4.2 Raw map



X



Y

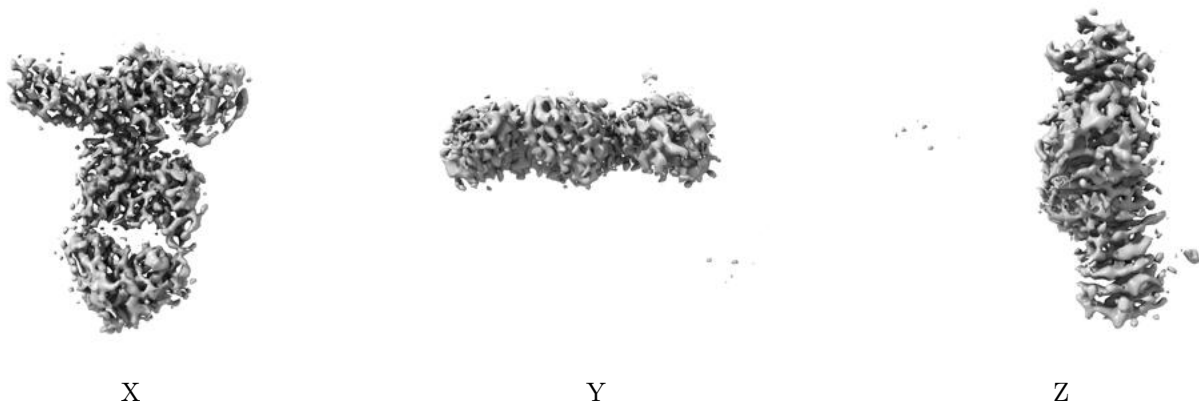


Z

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.

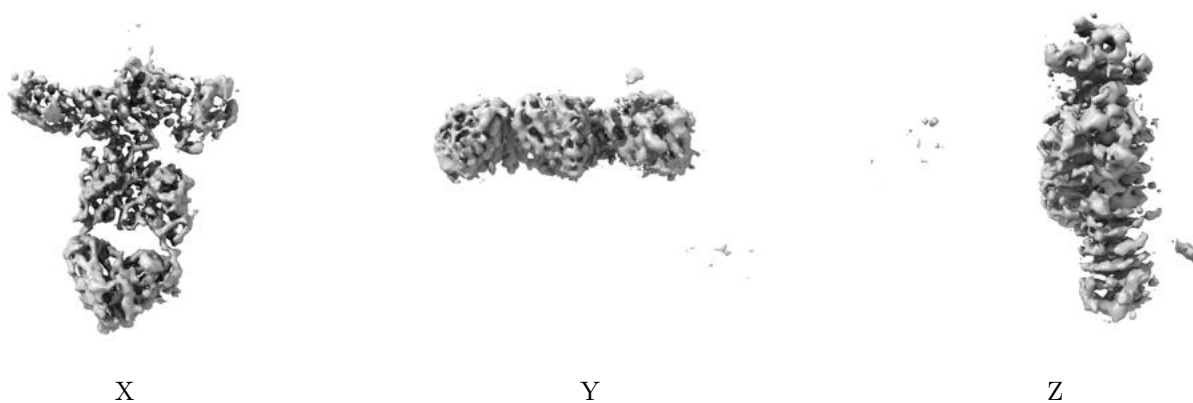
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.258. 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.

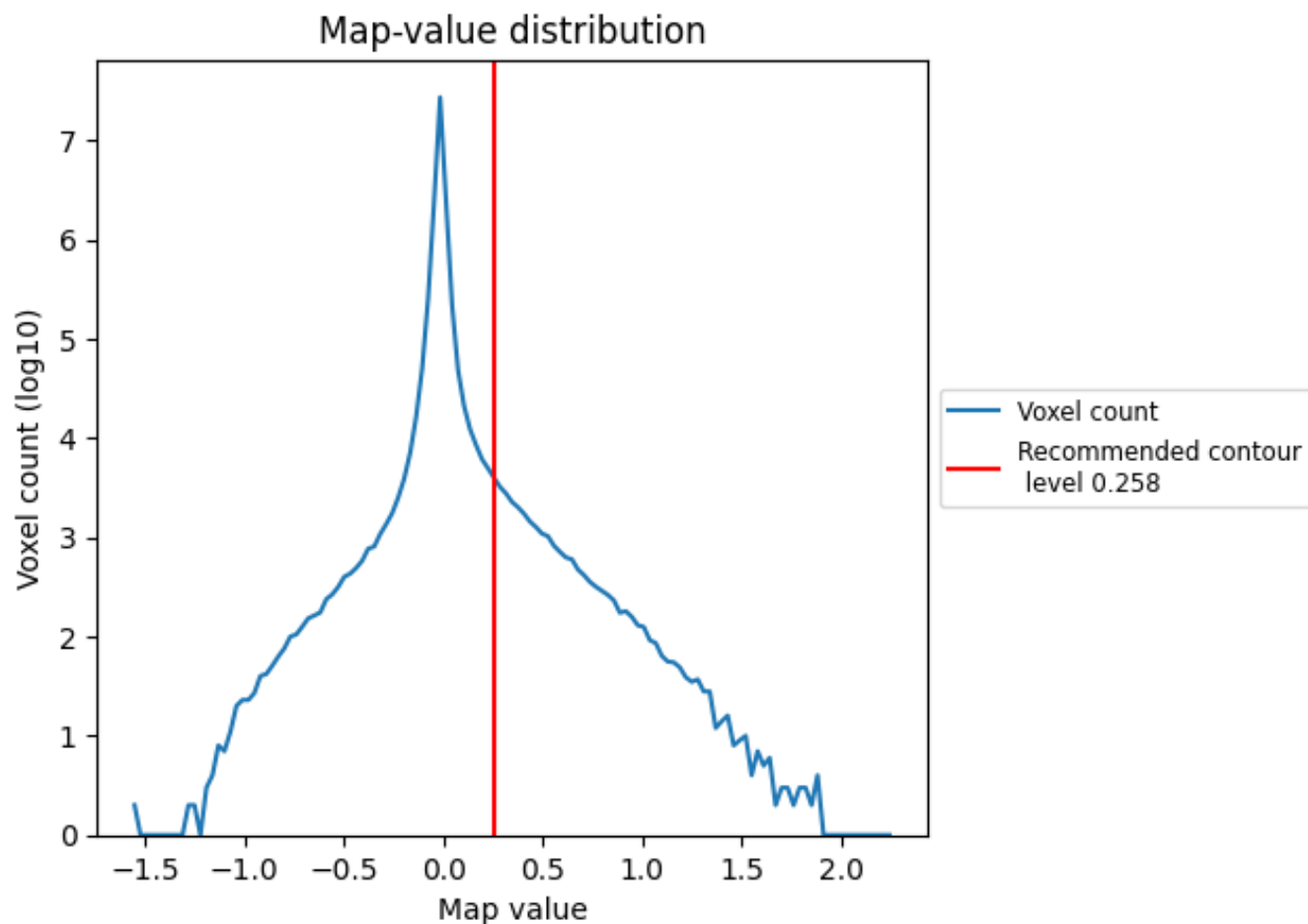
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

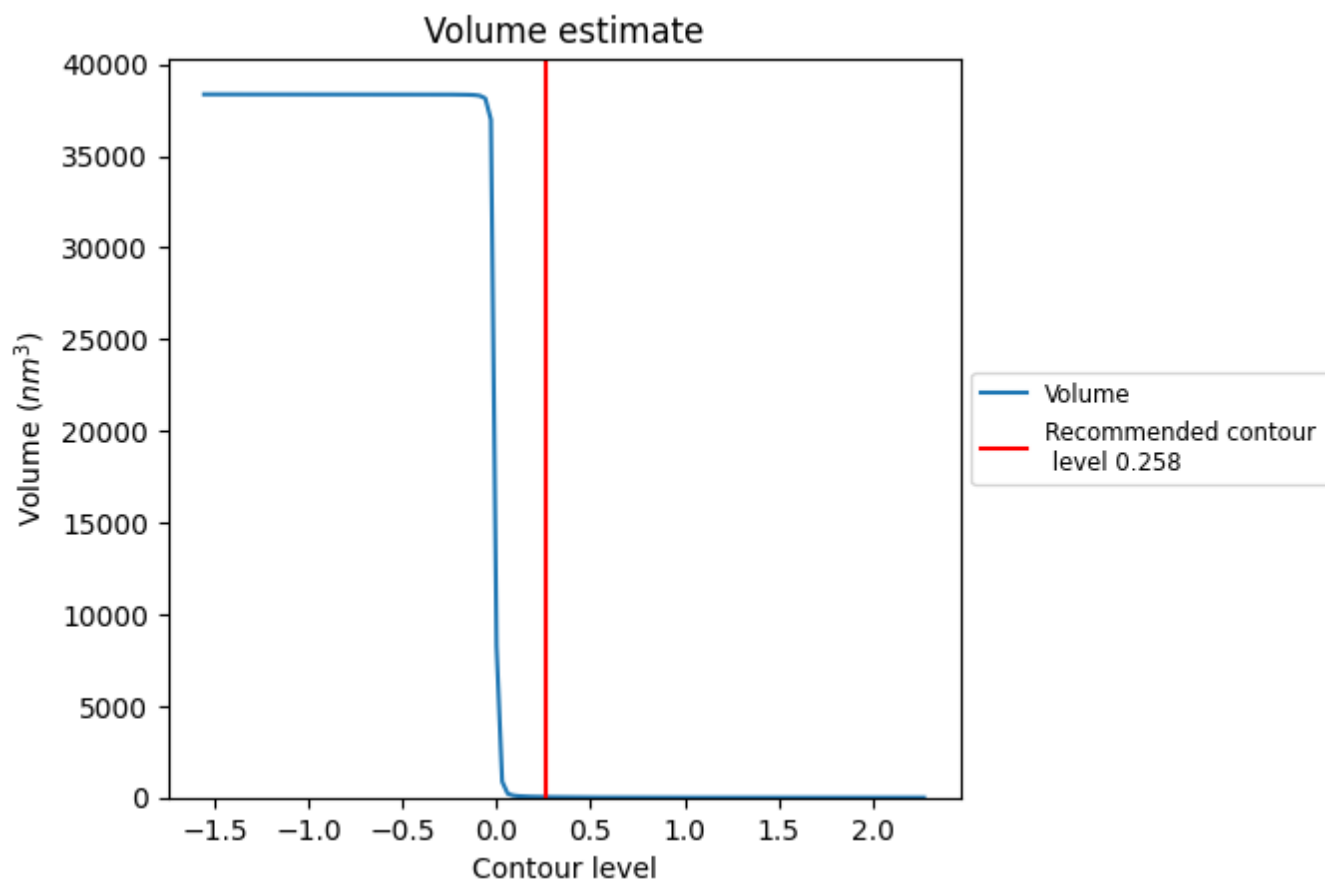
This section contains the results of statistical analysis of the map.

### 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](#)

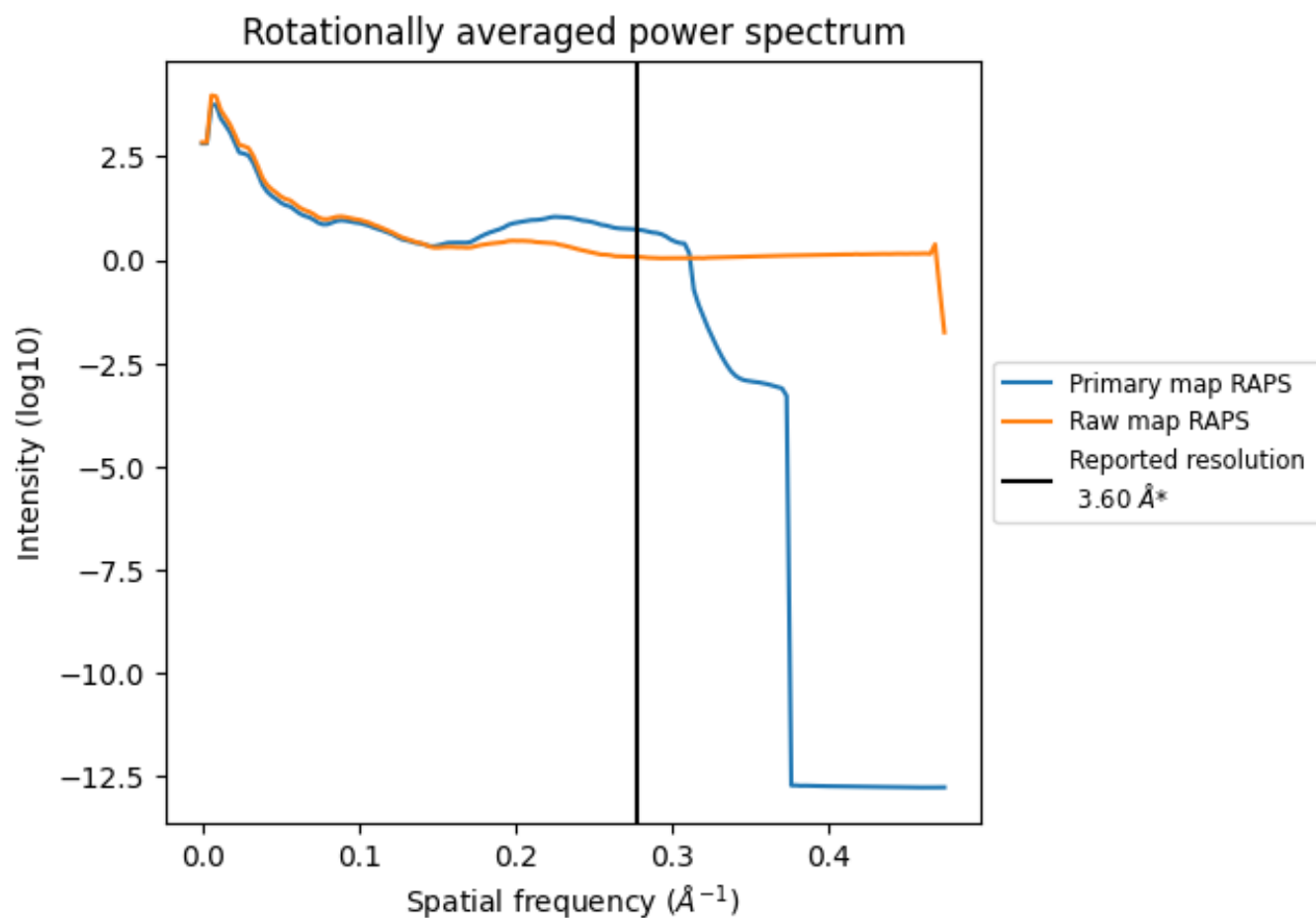


The volume at the recommended contour level is 32 nm<sup>3</sup>; this corresponds to an approximate mass of 28 kDa.

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 ⓘ

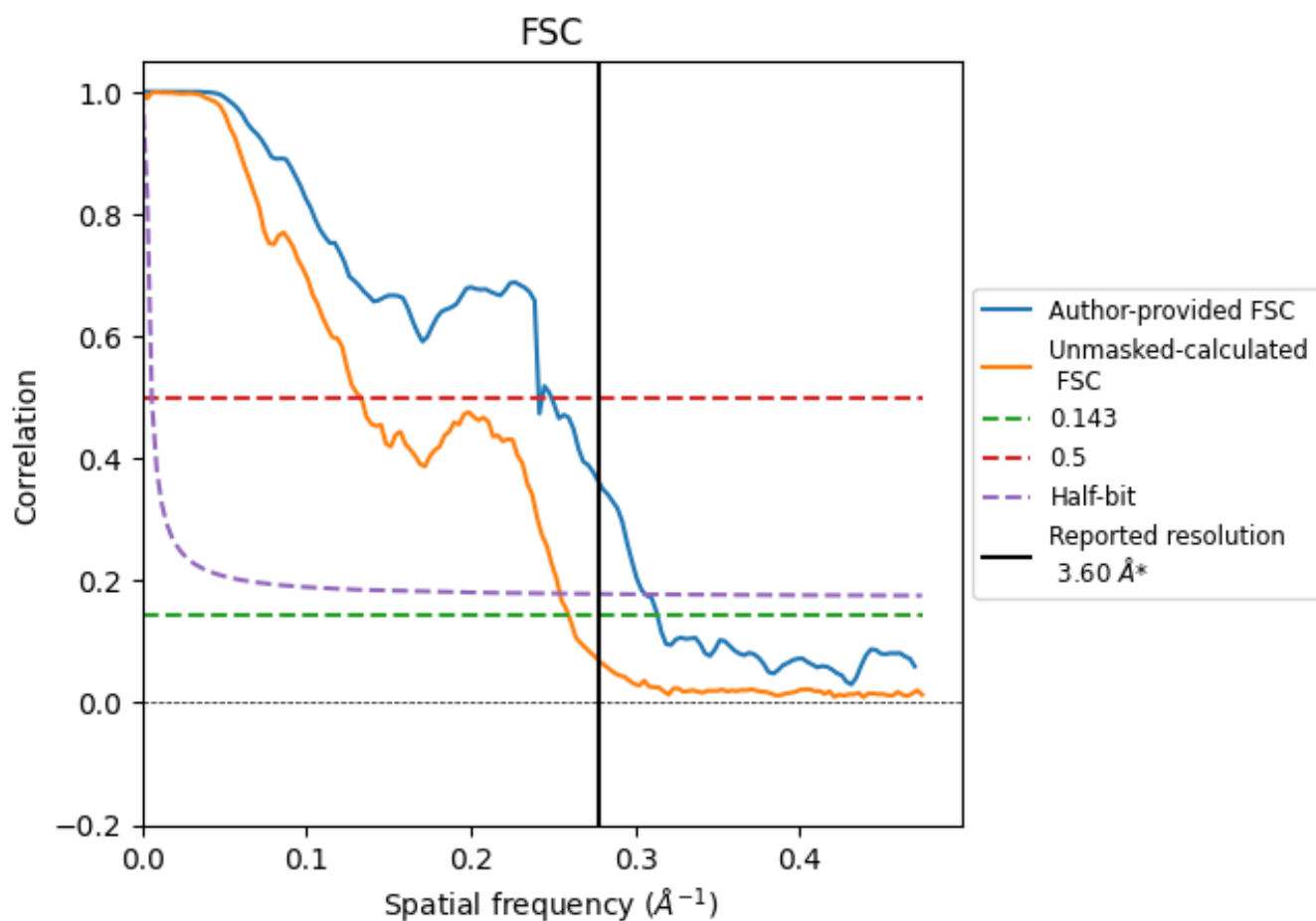


\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 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 0.278  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

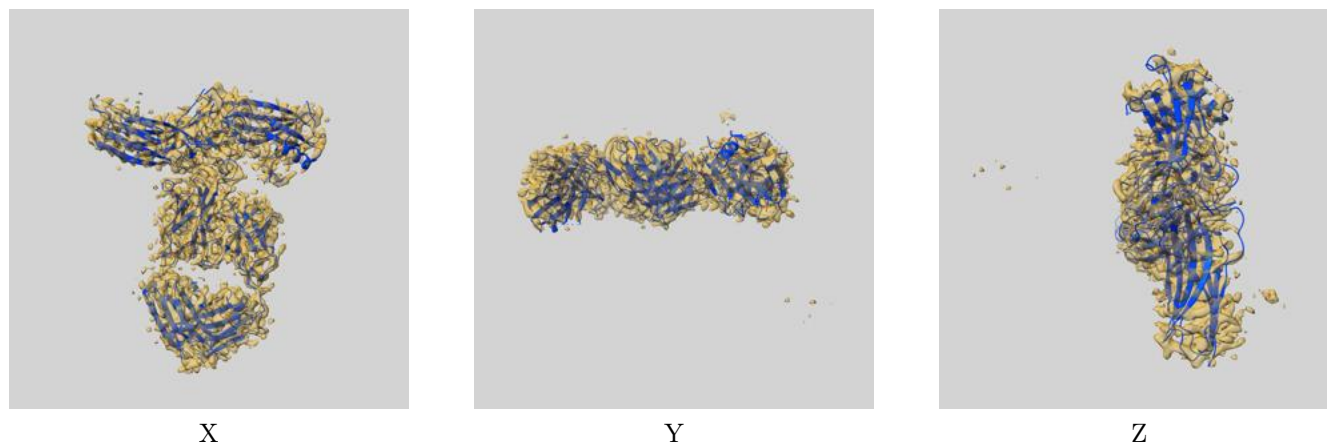
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.19	4.15	3.27
Unmasked-calculated*	3.86	7.52	3.94

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 3.6 by more than 10 %

## 9 Map-model fit [i](#)

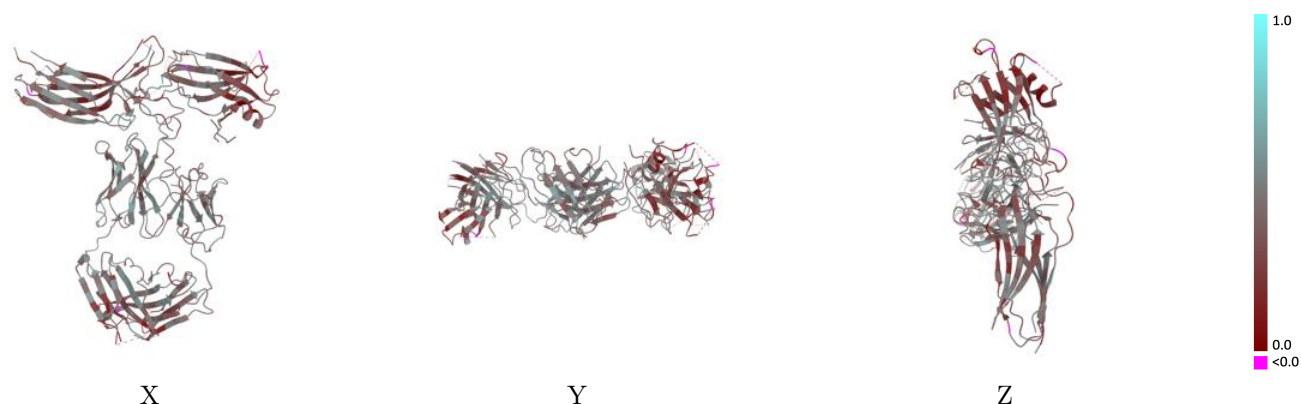
This section contains information regarding the fit between EMDB map EMD-41297 and PDB model 8TIO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

### 9.1 Map-model overlay [i](#)



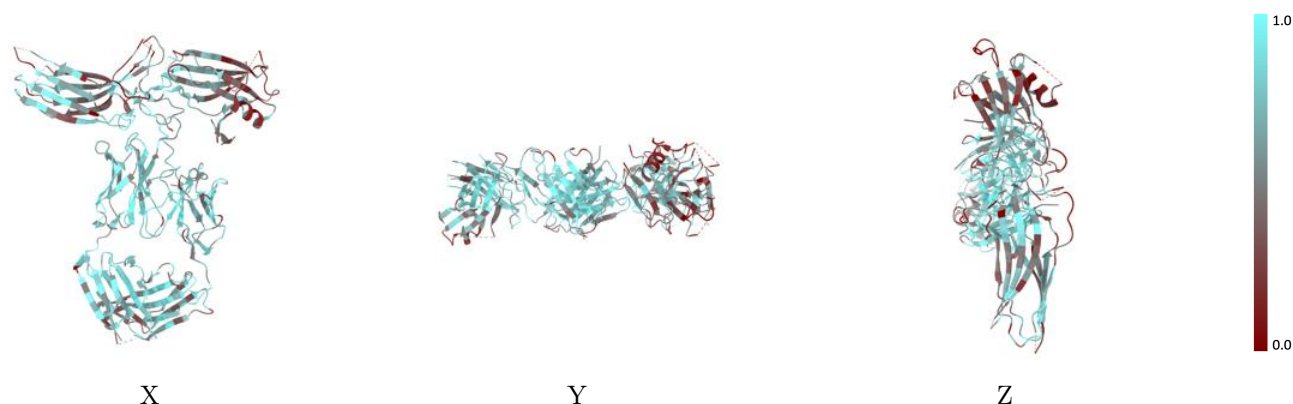
The images above show the 3D surface view of the map at the recommended contour level 0.258 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



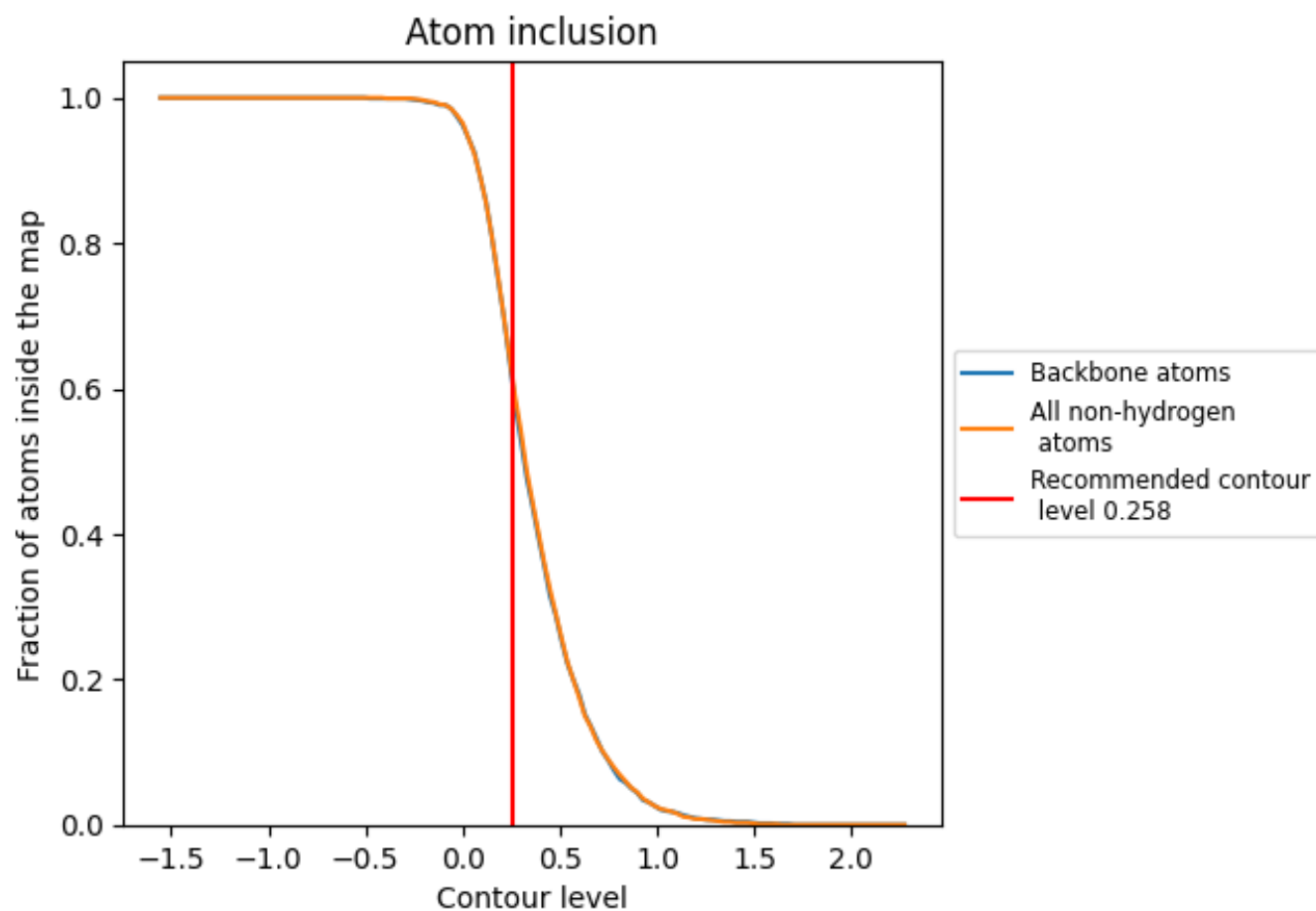
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.258).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 61% 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 (0.258) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6110	<div></div> 0.3980
A	<div></div> 0.5160	<div></div> 0.3660
H	<div></div> 0.7400	<div></div> 0.4390
L	<div></div> 0.6550	<div></div> 0.4050
R	<div></div> 0.4170	<div></div> 0.3710

