



# Full wwPDB EM Validation Report ⓘ

Feb 20, 2025 – 02:06 AM EST

PDB ID : 8U4P  
EMDB ID : EMD-41890  
Title : Structure of AMD3100-bound CXCR4/Gi complex  
Authors : Saotome, K.; McGoldrick, L.L.; Franklin, M.C.  
Deposited on : 2023-09-11  
Resolution : 3.15 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.dev117  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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) : 2.41.3

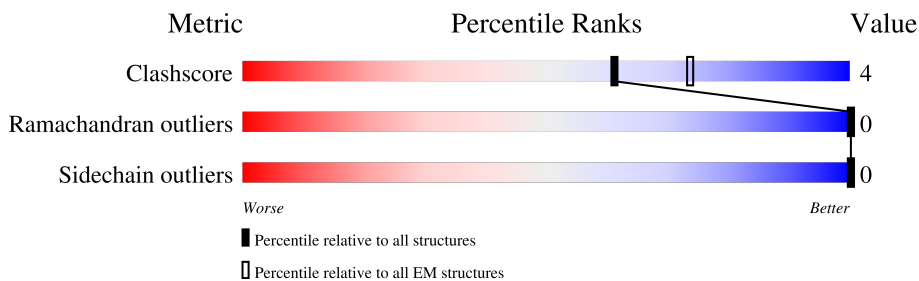
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.15 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	365	
2	B	350	
3	C	71	
4	R	632	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7006 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 Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	221	Total	C	N	O	S	0	0
			1777	1129	295	339	14		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P63096
A	-9	HIS	-	expression tag	UNP P63096
A	-8	HIS	-	expression tag	UNP P63096
A	-7	HIS	-	expression tag	UNP P63096
A	-6	HIS	-	expression tag	UNP P63096
A	-5	HIS	-	expression tag	UNP P63096
A	-4	HIS	-	expression tag	UNP P63096
A	-3	GLY	-	expression tag	UNP P63096
A	-2	GLY	-	expression tag	UNP P63096
A	-1	GLY	-	expression tag	UNP P63096
A	0	GLY	-	expression tag	UNP P63096
A	1	SER	-	expression tag	UNP P63096
A	47	CYS	SER	conflict	UNP P63096
A	202	THR	GLY	conflict	UNP P63096
A	203	ALA	GLY	conflict	UNP P63096
A	245	ALA	GLU	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	335	Total	C	N	O	S	0	0
			2516	1560	448	487	21		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	50	Total	C	N	O	S	0	0
			345	219	60	64	2		

- Molecule 4 is a protein called C-X-C chemokine receptor type 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	286	Total	C	N	O	S	0	0
			2304	1545	368	380	11		

There are 20 discrepancies between the modelled and reference sequences:

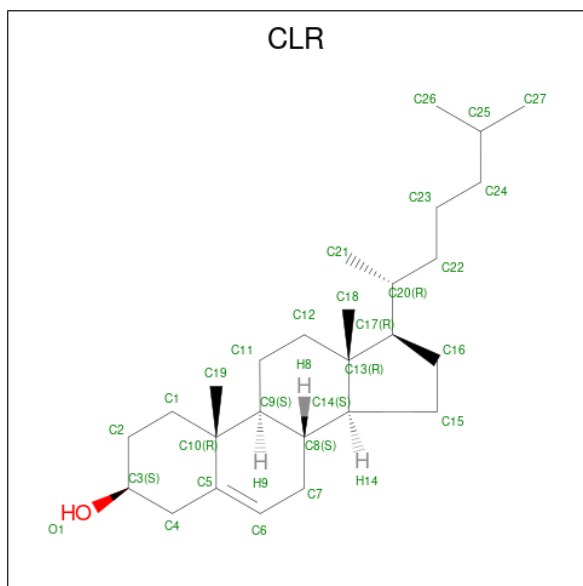
Chain	Residue	Modelled	Actual	Comment	Reference
R	-17	MET	-	initiating methionine	UNP P61073
R	-16	LYS	-	expression tag	UNP P61073
R	-15	THR	-	expression tag	UNP P61073
R	-14	ILE	-	expression tag	UNP P61073
R	-13	ILE	-	expression tag	UNP P61073
R	-12	ALA	-	expression tag	UNP P61073
R	-11	LEU	-	expression tag	UNP P61073
R	-10	SER	-	expression tag	UNP P61073
R	-9	TYR	-	expression tag	UNP P61073
R	-8	ILE	-	expression tag	UNP P61073
R	-7	PHE	-	expression tag	UNP P61073
R	-6	CYS	-	expression tag	UNP P61073
R	-5	LEU	-	expression tag	UNP P61073
R	-4	VAL	-	expression tag	UNP P61073
R	-3	PHE	-	expression tag	UNP P61073

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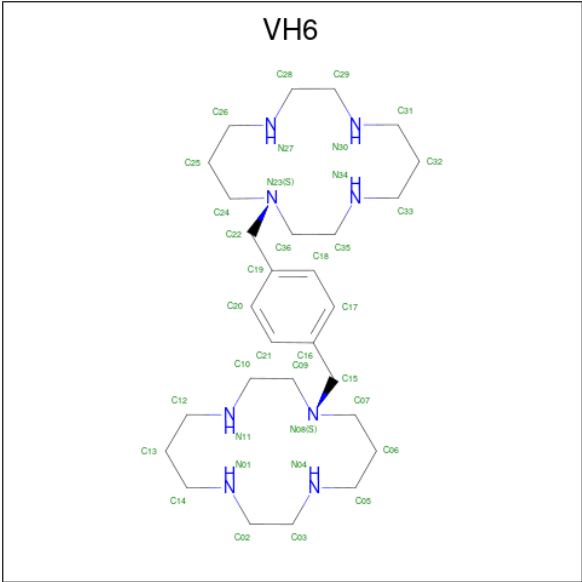
Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	ALA	-	expression tag	UNP P61073
R	-1	GLY	-	expression tag	UNP P61073
R	0	ALA	-	expression tag	UNP P61073
R	1	PRO	-	expression tag	UNP P61073
R	119	SER	ASN	conflict	UNP P61073

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



Mol	Chain	Residues	Atoms			AltConf
5	R	1	Total	C	O	0
			28	27	1	

- Molecule 6 is Plerixafor (three-letter code: VH6) (formula:  $C_{28}H_{54}N_8$ ) (labeled as "Ligand of Interest" by depositor).

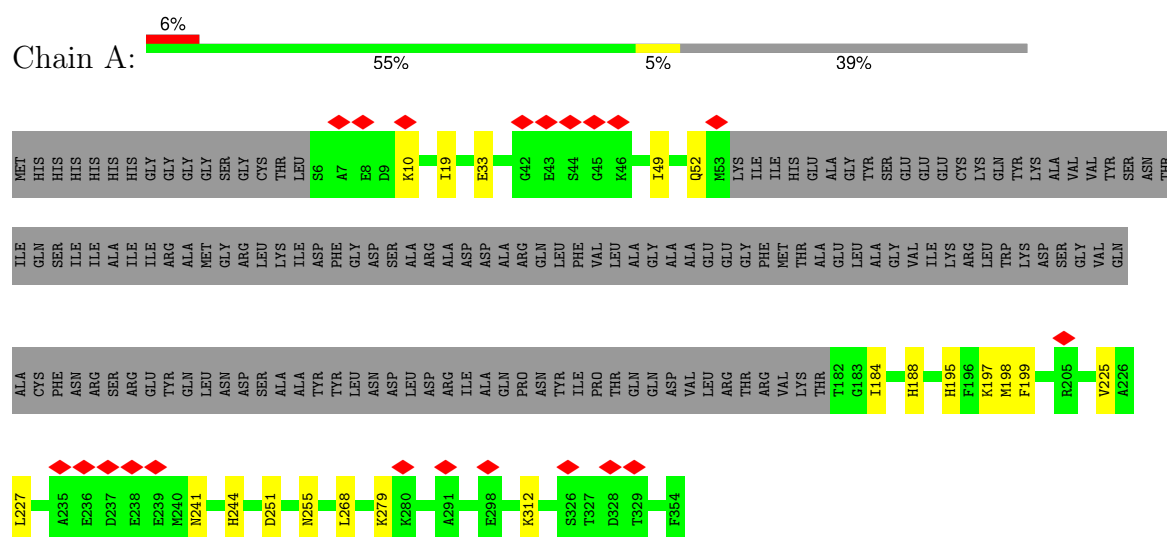


Mol	Chain	Residues	Atoms			AltConf
6	R	1	Total	C	N	0
			36	28	8	

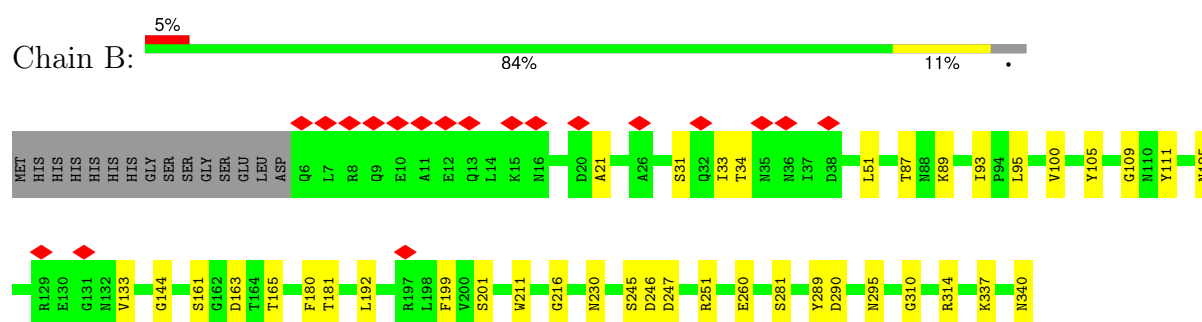
### 3 Residue-property plots [i](#)

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.

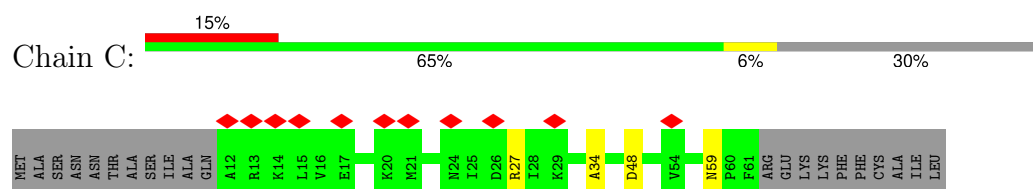
- Molecule 1: Guanine nucleotide-binding protein G(i) subunit alpha-1



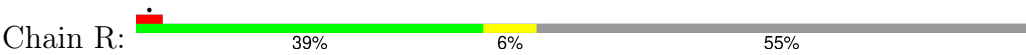
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 4: C-X-C chemokine receptor type 4



LEU	VAL	GLN	GLY	ASP	TRP	GLY	P211	K67	MET
LYS	GLN	LEU	THR	LEU	TRP	GLY	P211	K68	LYS
ASP	ALA	LEU	THR	LEU	TRP	GLY	P254	L69	THR
TYR	ASP	LEU	VAL	LEU	LEU	SER	I259	R70	ILE
ASP	HIS	THR	ARG	THR	THR	SER	E268	S71	ALA
ASP	THR	THR	ILE	THR	THR	LYS	E268	M72	LEU
ASP	GLN	GLN	GLY	LEU	LEU	GLY	T73	T73	SER
ASP	ASN	LEU	LEU	THR	THR	GLU	D74	D74	TYR
LYS	THR	LYS	TYR	TYR	TYR	GLU	K271	L78	ILE
	PRO	PRO	GLY	GLY	GLY	LEU	Q272	L78	CYS
	ILE	ILE	ILE	VAL	VAL	PHE	Q272	L85	THR
	GLY	GLY	ASP	GLN	GLN	THR	T287	L86	VAL
	ASP	ASP	PHE	CYS	CYS	GLY	T287	F87	PHE
	PRO	PRO	LYS	PHE	PHE	VAL	T318	V88	ALA
	VAL	VAL	GLY	SER	SER	VAL	SER	I89	GLY
	ASP	ASP	PRO	ARG	ARG	PRO	VAL	T90	ALA
	LEU	LEU	GLY	TYR	TYR	ILE	SER		PRO
	LEU	LEU	ASN	ASN	ASN	ASP	ARG	V96	GLU
	PRO	PRO	ILE	PRO	PRO	VAL	GLY		GLY
	ASN	ASN	LEU	HIS	HIS	LEU	SER	A100	ILE
	ASP	ASP	GLY	GLY	GLY	LEU	SER	N101	SER
	HIS	HIS	HIS	LYS	LYS	ASP	LEU	N101	ILE
	TYR	TYR	LYS	GLN	GLN	GLY	LYS	F104	TYR
	LEU	LEU	LEU	HIS	HIS	ASP	ILE		THR
	SER	SER	GLY	ASP	ASP	VAL	ASP	L108	SER
	GLN	GLN	TYR	PHE	PHE	VAL	LEU	C109	ASP
	LYS	LYS	ASN	PHE	PHE	GLY	SER	K110	ASN
	LEU	LEU	SER	LYS	LYS	HIS	LYS		TYR
	SER	SER	ASN	SER	SER	PHE	LYS	I126	THR
	LEU	LEU	HIS	ALA	ALA	ASP	GLY		GLU
	LYS	LYS	ASN	PRO	PRO	VAL	ARG	S144	MET
	ASP	ASP	VAL	GLY	GLY	VAL	HIS		GLY
	PRO	PRO	TYR	GLY	GLY	GLY	SER	K149	SER
	ASN	ASN	ILE	TYR	TYR	GLY	SER		GLY
	GLY	GLY	MET	VAL	VAL	GLY	VAL	A152	ASP
	ARG	ARG	ALA	GLN	GLN	GLU	GLY	E153	TYR
	LYS	LYS	ASP	ASP	ASP	GLY	THR		ASP
	HIS	HIS	LYS	ARG	ARG	ASP	GLU	V156	MET
	MET	MET	GLN	THR	THR	ALA	SER		LYS
	VAL	VAL	LYS	ILE	ILE	THR	GLU	V160	GLU
	LEU	LEU	ASN	PHE	PHE	TYR	SER		PRO
	GLY	GLY	GLY	PHE	PHE	GLY	SER	A175	CYS
	LEU	LEU	ILE	ASP	ASP	LYS	SER	N176	PHE
	GLY	GLY	VAL	VAL	VAL	LEU	PHE		ARG
	VAL	VAL	ASN	ASN	ASN	LEU	HIS	E179	GLU
	THR	THR	PHE	ASN	ASN	LEU	SER	A180	ARG
	ALA	ALA	LYS	LYS	TYR	PHE	GLY	D181	N33
	GLY	GLY	ILE	THR	THR	ILE	ARG	D182	A34
	ILE	ILE	ARG	ARG	ARG	CYS	PRO	R183	N35
	THR	THR	HIS	THR	THR	THR	LEU		
	LEU	LEU	ASN	ALA	ALA	THR	GLY	Y190	K38
	GLY	GLY	ILE	GLY	GLY	VAL	VAL		
	MET	MET	GLY	VAL	VAL	LYS	LEU	V196	I39
	ASP	ASP	ASP	LYS	LYS	LEU	PHE		
	GLY	GLY	GLY	PHE	PHE	PRO	GLN	I204	G52
						VAL	VAL	M205	
						PRO	PRO		N56
								I209	



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193216	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	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	2.197	Depositor
Minimum map value	-1.471	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.24	Depositor
Map size (Å)	255.0, 255.0, 255.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: CLR, VH6

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	0.24	0/1807	0.44	0/2425
2	B	0.24	0/2563	0.51	0/3483
3	C	0.23	0/351	0.39	0/480
4	R	0.26	0/2368	0.44	0/3225
All	All	0.25	0/7089	0.47	0/9613

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	1777	0	1757	13	0
2	B	2516	0	2392	24	0
3	C	345	0	320	4	0
4	R	2304	0	2383	22	0
5	R	28	0	46	2	0
6	R	36	0	0	0	0
All	All	7006	0	6898	58	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 4.

All (58) 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:251:ASP:OD1	1:A:255:ASN:ND2	2.31	0.63
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.31	0.61
4:R:205:MET:HA	4:R:209:ILE:HD13	1.82	0.61
2:B:340:ASN:ND2	3:C:59:ASN:OD1	2.36	0.59
4:R:110:LYS:NZ	4:R:175:ALA:O	2.36	0.59
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.84	0.58
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.86	0.58
4:R:52:GLY:O	4:R:56:ASN:ND2	2.36	0.57
2:B:31:SER:HA	2:B:34:THR:HG22	1.85	0.57
4:R:210:LEU:HB2	4:R:211:PRO:HD3	1.86	0.56
4:R:104:PHE:HB3	4:R:108:LEU:HD23	1.87	0.56
1:A:19:ILE:HD11	2:B:89:LYS:HB2	1.88	0.55
4:R:70:ARG:HG3	4:R:74:ASP:HB2	1.88	0.55
2:B:281:SER:OG	3:C:48:ASP:OD2	2.24	0.54
2:B:251:ARG:NH1	2:B:260:GLU:OE2	2.32	0.53
4:R:204:ILE:HD11	4:R:259:ILE:HG22	1.90	0.53
4:R:78:LEU:HD23	5:R:701:CLR:H191	1.91	0.52
2:B:165:THR:HG22	2:B:181:THR:HG22	1.92	0.52
2:B:310:GLY:O	2:B:337:LYS:NZ	2.33	0.51
2:B:93:ILE:HG12	2:B:133:VAL:HG21	1.92	0.51
1:A:33:GLU:HG2	1:A:195:HIS:HB3	1.93	0.50
1:A:184:ILE:HD11	1:A:199:PHE:HB3	1.93	0.50
4:R:254:PRO:HB2	4:R:287:THR:HG21	1.92	0.50
2:B:245:SER:OG	2:B:247:ASP:OD1	2.25	0.50
1:A:241:ASN:HB3	1:A:244:HIS:HB2	1.93	0.49
4:R:152:ALA:HA	4:R:156:VAL:HG23	1.97	0.47
2:B:105:TYR:HE2	2:B:109:GLY:HA2	1.80	0.47
4:R:96:VAL:O	4:R:100:ALA:N	2.43	0.47
4:R:268:GLU:HG3	4:R:271:LYS:HE3	1.98	0.46
2:B:201:SER:OG	2:B:211:TRP:NE1	2.34	0.46
4:R:149:LYS:O	4:R:153:GLU:HG2	2.16	0.46
1:A:312:LYS:HA	1:A:312:LYS:HD3	1.76	0.46
2:B:289:TYR:HE1	2:B:295:ASN:HB2	1.81	0.45
4:R:85:LEU:O	4:R:89:ILE:HG23	2.16	0.45
1:A:225:VAL:HB	1:A:268:LEU:HD23	2.00	0.44
4:R:144:SER:OG	4:R:144:SER:O	2.35	0.44
4:R:190:TYR:CD2	4:R:196:VAL:HG22	2.53	0.44
1:A:198:MET:HE2	1:A:198:MET:HB3	1.54	0.44
2:B:21:ALA:HB3	3:C:27:ARG:HH21	1.82	0.43
4:R:87:PHE:O	4:R:90:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:126:ILE:HG13	4:R:160:VAL:HG11	2.01	0.43
1:A:10:LYS:HD2	1:A:10:LYS:HA	1.75	0.43
2:B:163:ASP:OD1	2:B:165:THR:OG1	2.37	0.43
2:B:192:LEU:HD23	2:B:199:PHE:HB3	2.01	0.43
2:B:180:PHE:HE1	2:B:216:GLY:HA2	1.84	0.43
1:A:279:LYS:HE2	1:A:279:LYS:HB3	1.83	0.42
1:A:49:ILE:HG23	1:A:52:GLN:HE21	1.85	0.42
2:B:33:ILE:HD11	3:C:34:ALA:HB3	2.01	0.42
2:B:180:PHE:CE1	2:B:216:GLY:HA2	2.55	0.42
4:R:110:LYS:NZ	4:R:176:ASN:OD1	2.48	0.42
1:A:188:HIS:NE2	1:A:197:LYS:HE3	2.36	0.41
1:A:227:LEU:HG	1:A:268:LEU:HB3	2.02	0.41
4:R:71:SER:OG	4:R:72:MET:N	2.54	0.41
2:B:144:GLY:O	2:B:161:SER:OG	2.38	0.41
4:R:70:ARG:HH12	5:R:701:CLR:H42	1.85	0.41
2:B:51:LEU:HD23	2:B:87:THR:HG23	2.02	0.40
2:B:111:TYR:HD2	2:B:125:ASN:HA	1.87	0.40
4:R:85:LEU:HD12	4:R:85:LEU:HA	1.95	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	217/365 (60%)	210 (97%)	7 (3%)	0	100	100
2	B	333/350 (95%)	323 (97%)	10 (3%)	0	100	100
3	C	48/71 (68%)	47 (98%)	1 (2%)	0	100	100
4	R	284/632 (45%)	273 (96%)	11 (4%)	0	100	100
All	All	882/1418 (62%)	853 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	195/313 (62%)	195 (100%)	0	100	100
2	B	264/291 (91%)	264 (100%)	0	100	100
3	C	30/58 (52%)	30 (100%)	0	100	100
4	R	252/552 (46%)	252 (100%)	0	100	100
All	All	741/1214 (61%)	741 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	340	ASN
3	C	59	ASN

### 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](#)

2 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	$\# Z  > 2$
5	CLR	R	701	-	31,31,31	1.11	2 (6%)	48,48,48	1.33	7 (14%)
6	VH6	R	702	-	38,38,38	1.20	4 (10%)	44,44,44	1.36	8 (18%)

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
5	CLR	R	701	-	-	2/10/68/68	0/4/4/4
6	VH6	R	702	-	-	18/40/40/40	2/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	702	VH6	C22-N23	3.35	1.54	1.47
6	R	702	VH6	C24-N23	2.53	1.53	1.47
5	R	701	CLR	C18-C13	-2.41	1.50	1.54
5	R	701	CLR	C7-C6	2.26	1.54	1.50
6	R	702	VH6	C36-N23	2.23	1.52	1.47
6	R	702	VH6	C15-N08	2.19	1.51	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	702	VH6	C18-C19-C20	-4.18	112.02	118.23
6	R	702	VH6	C21-C16-C17	-3.79	112.61	118.23
5	R	701	CLR	C22-C20-C17	-2.93	104.26	110.33
6	R	702	VH6	C16-C15-N08	2.66	118.59	113.15
5	R	701	CLR	C18-C13-C12	2.46	114.23	110.61
6	R	702	VH6	C17-C18-C19	2.40	124.15	121.00
5	R	701	CLR	C21-C20-C22	-2.32	106.75	110.34
5	R	701	CLR	C7-C8-C14	-2.22	107.79	110.93

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	702	VH6	C21-C20-C19	2.14	123.81	121.00
6	R	702	VH6	C22-C19-C20	2.13	124.67	120.75
5	R	701	CLR	C13-C17-C20	-2.07	116.30	119.50
6	R	702	VH6	C18-C17-C16	2.07	123.72	121.00
6	R	702	VH6	C20-C21-C16	2.05	123.70	121.00
5	R	701	CLR	C24-C23-C22	-2.05	104.11	113.28
5	R	701	CLR	C11-C12-C13	-2.00	109.36	112.74

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	702	VH6	C35-C36-N23-C22
6	R	702	VH6	C16-C15-N08-C07
6	R	702	VH6	C03-C02-N01-C14
6	R	702	VH6	N34-C35-C36-N23
6	R	702	VH6	C19-C22-N23-C36
6	R	702	VH6	C19-C22-N23-C24
6	R	702	VH6	C12-C13-C14-N01
6	R	702	VH6	C05-C06-C07-N08
6	R	702	VH6	N01-C02-C03-N04
6	R	702	VH6	N23-C24-C25-C26
6	R	702	VH6	N04-C05-C06-C07
6	R	702	VH6	N30-C31-C32-C33
6	R	702	VH6	C02-C03-N04-C05
6	R	702	VH6	C09-C10-N11-C12
6	R	702	VH6	C36-C35-N34-C33
6	R	702	VH6	N08-C09-C10-N11
5	R	701	CLR	C13-C17-C20-C21
6	R	702	VH6	C16-C15-N08-C09
6	R	702	VH6	C25-C26-N27-C28
5	R	701	CLR	C21-C20-C22-C23

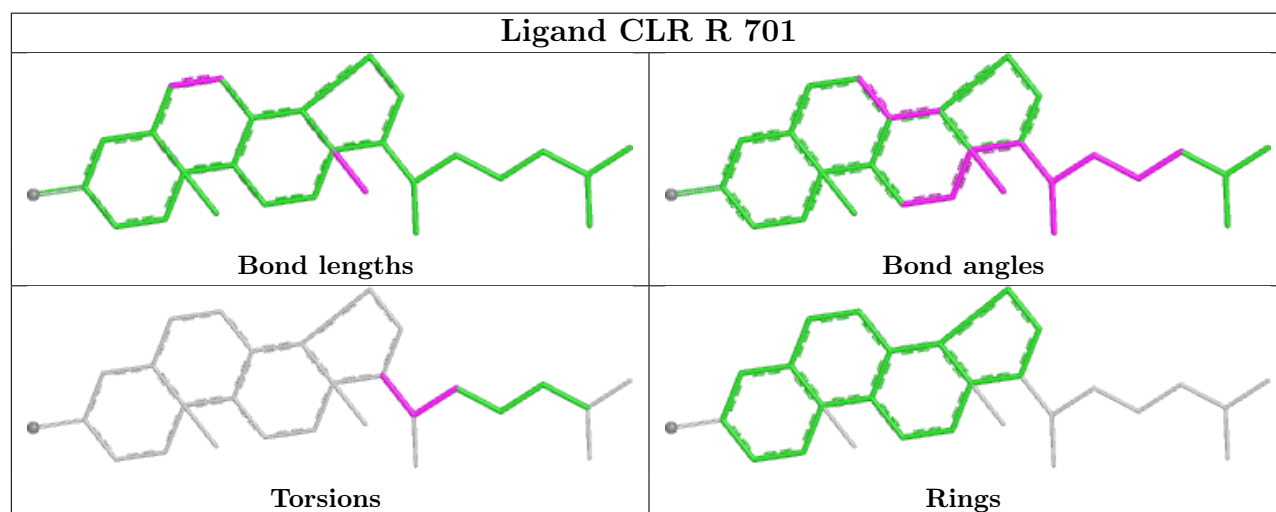
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	702	VH6	C02-C03-C05-C06-C07-C09-C10-C12-C13-C14-N01-N04-N08-N11
6	R	702	VH6	C24-C25-C26-C28-C29-C31-C32-C33-C35-C36-N23-N27-N30-N34

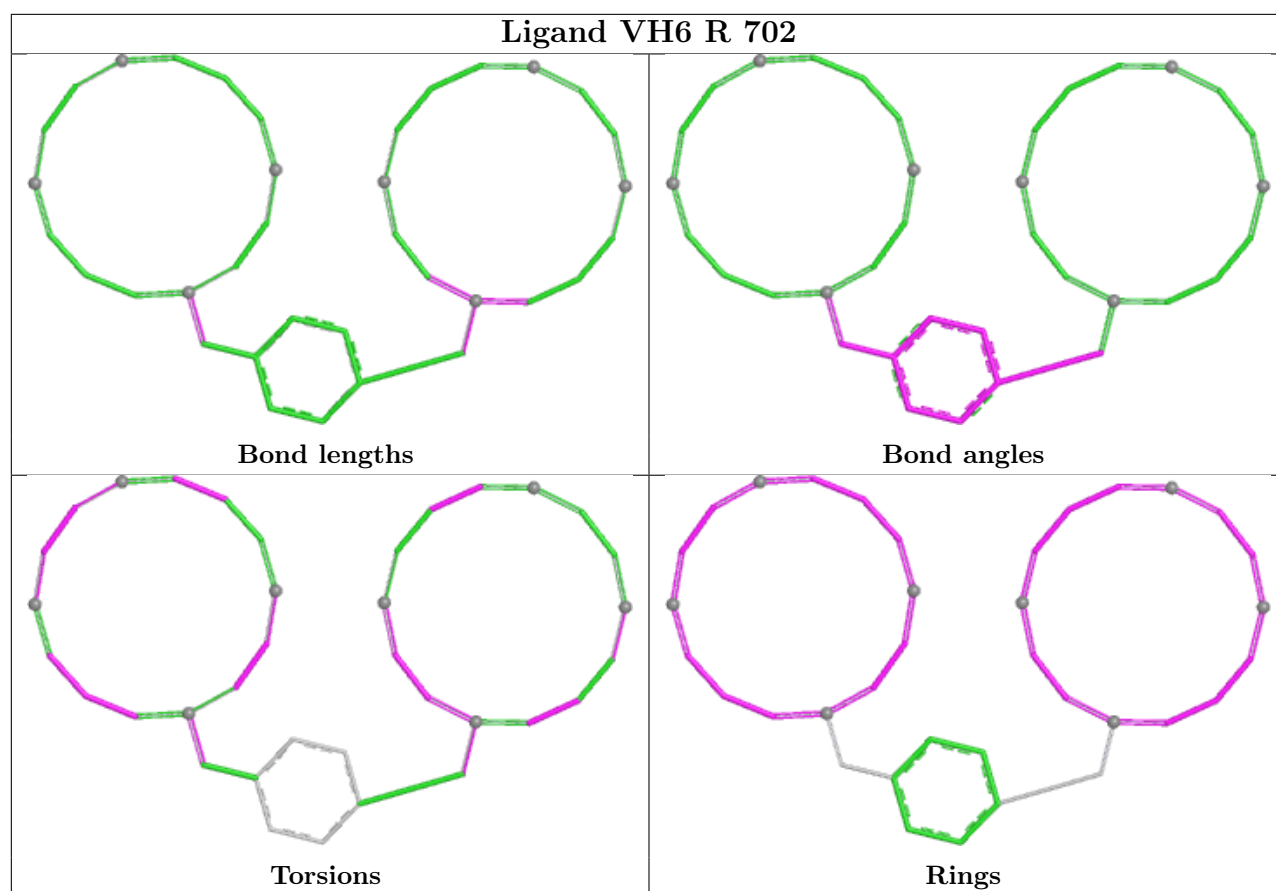
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	701	CLR	2	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.

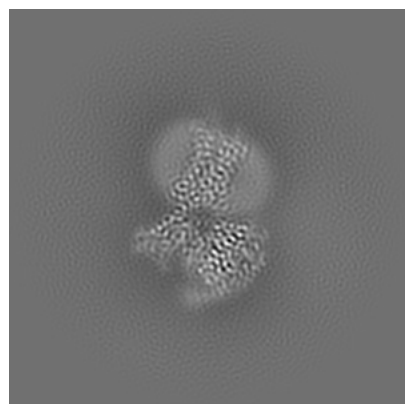
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-41890. These allow visual inspection of the internal detail of the map and identification of artifacts.

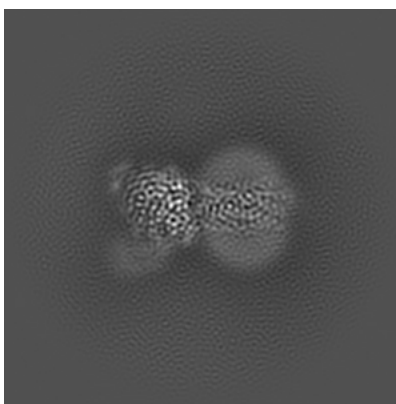
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

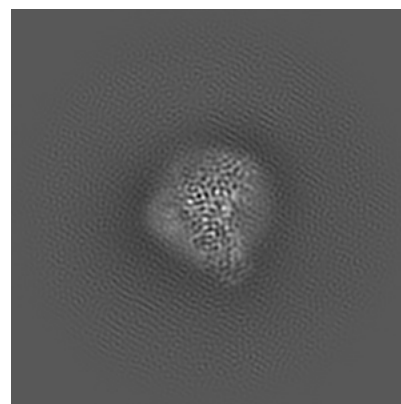
#### 6.1.1 Primary map



X

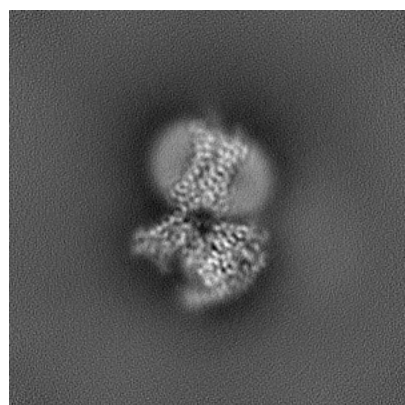


Y

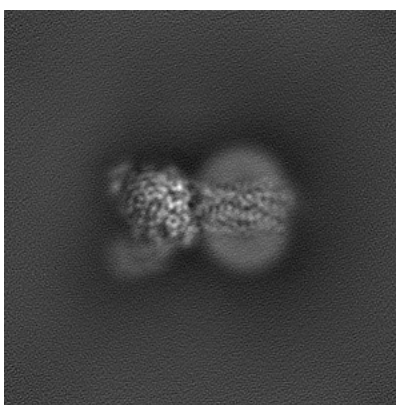


Z

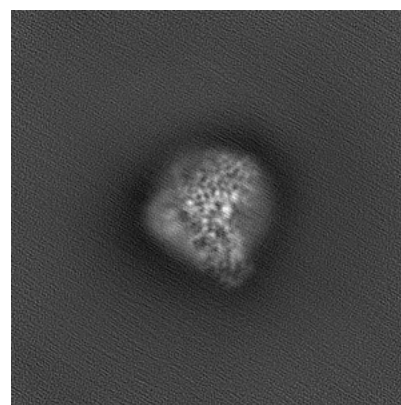
#### 6.1.2 Raw map



X



Y

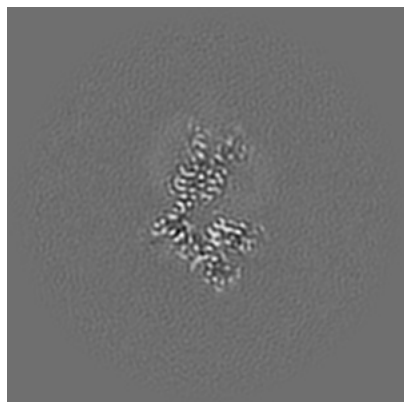


Z

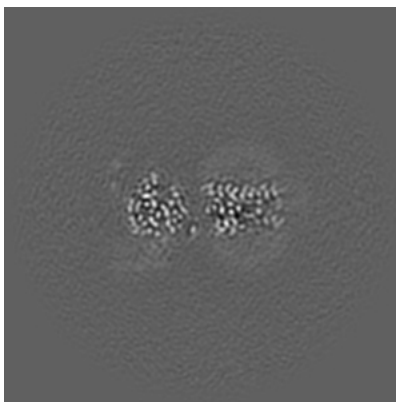
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

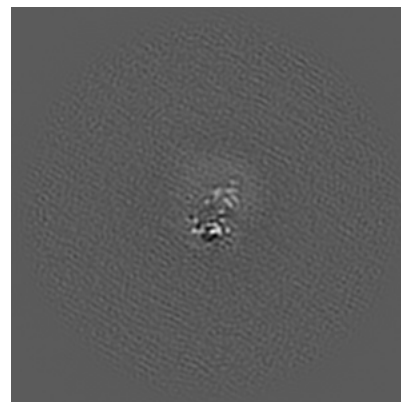
### 6.2.1 Primary map



X Index: 150

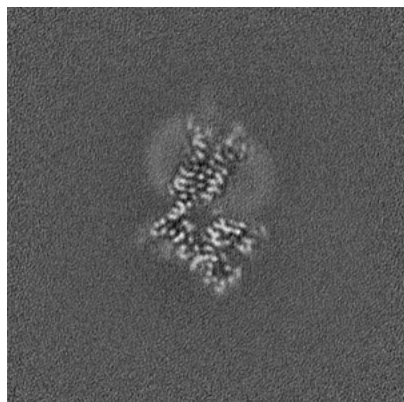


Y Index: 150

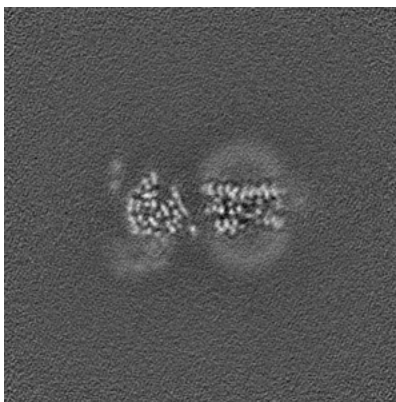


Z Index: 150

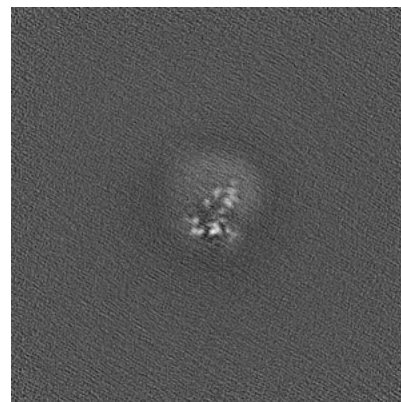
### 6.2.2 Raw map



X Index: 150



Y Index: 150

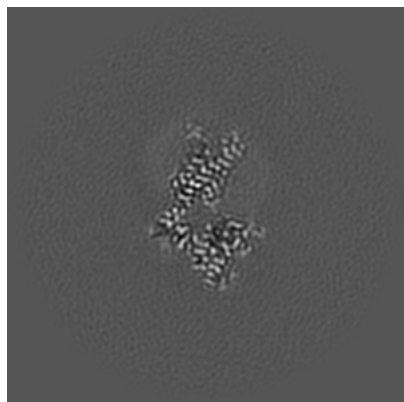


Z Index: 150

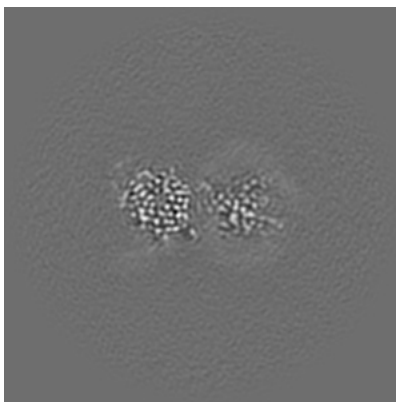
The images above show central slices of the map in three orthogonal directions.

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

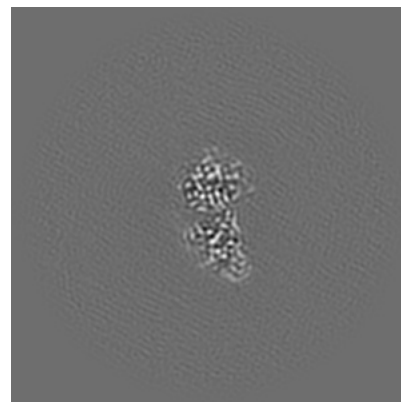
### 6.3.1 Primary map



X Index: 147

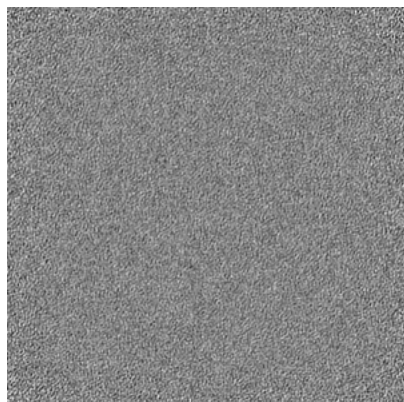


Y Index: 157

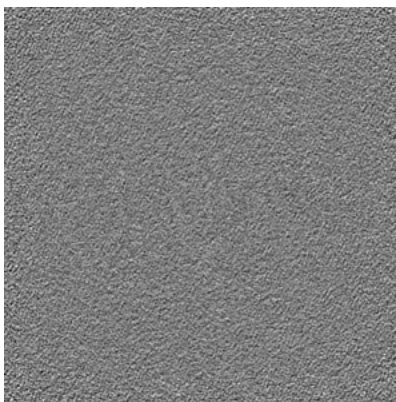


Z Index: 130

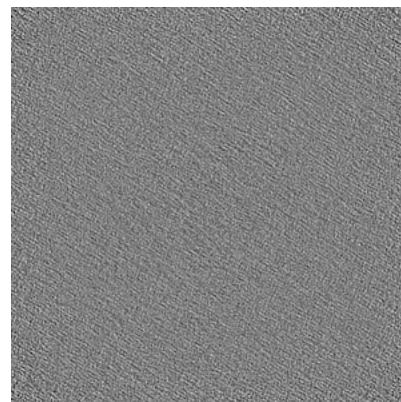
### 6.3.2 Raw map



X Index: 0



Y Index: 0



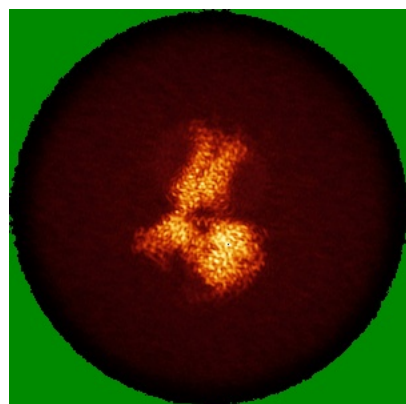
Z Index: 0

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

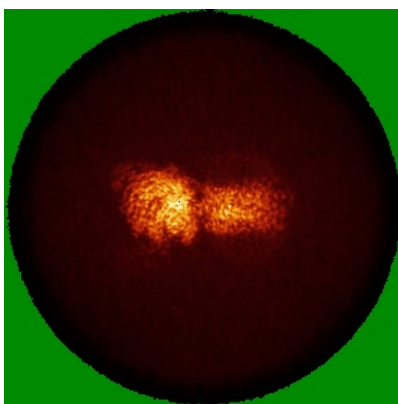


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

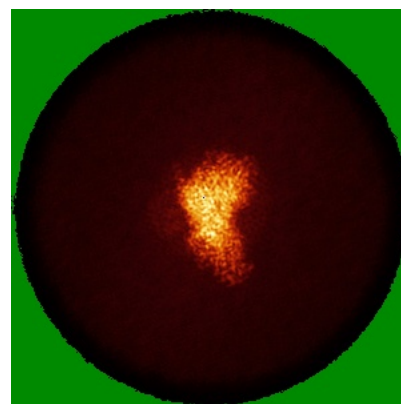
### 6.4.1 Primary map



X

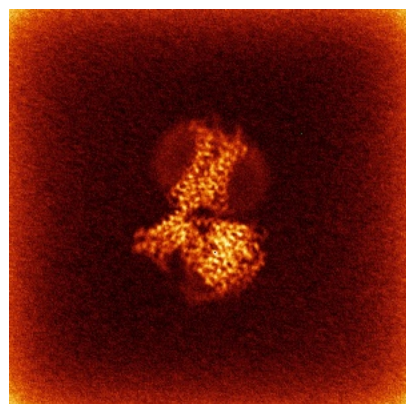


Y

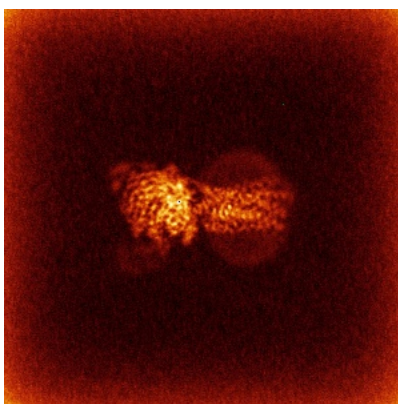


Z

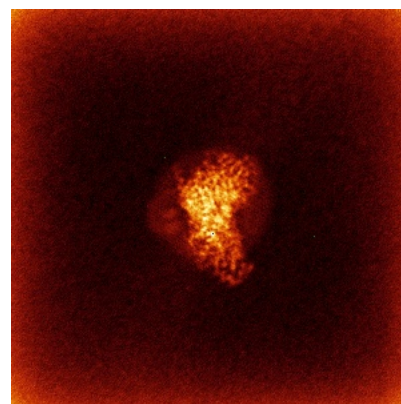
### 6.4.2 Raw map



X



Y

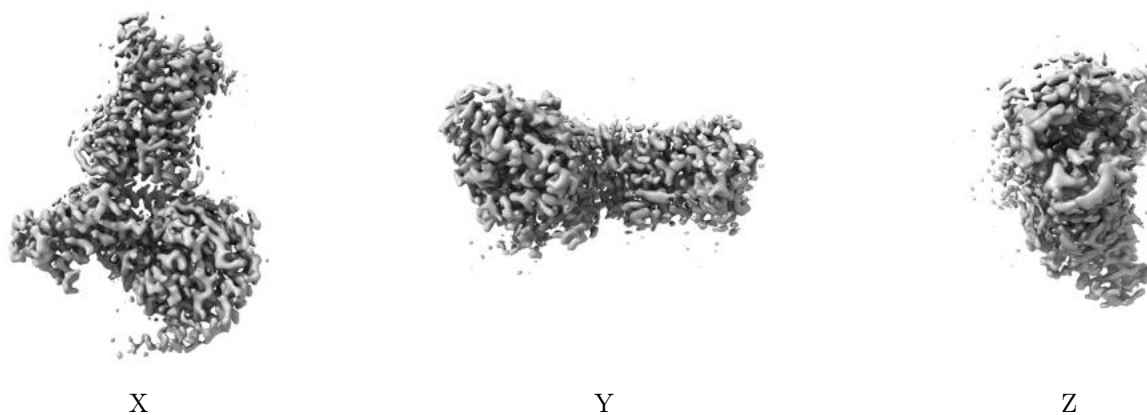


Z

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.

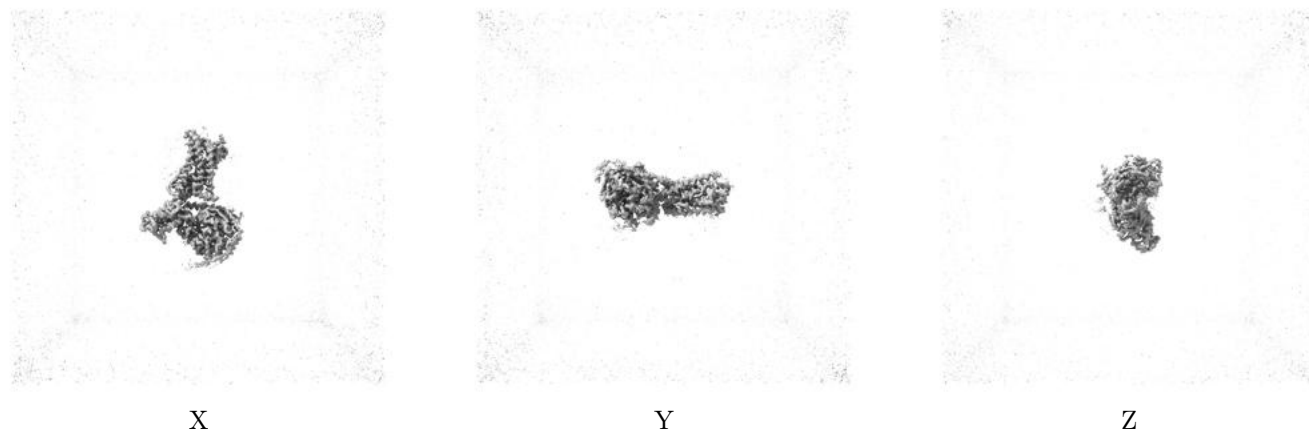
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.24. 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.

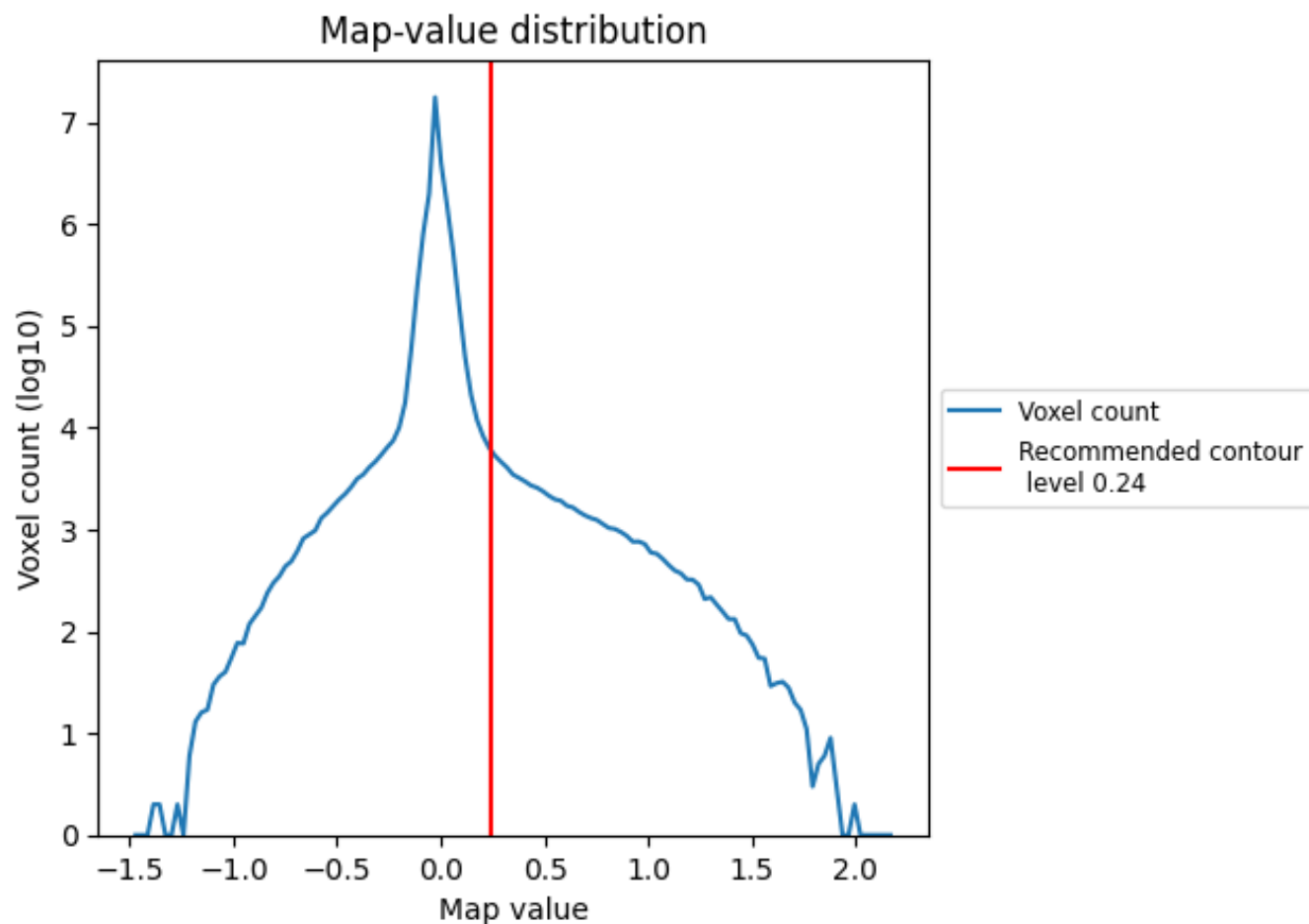
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

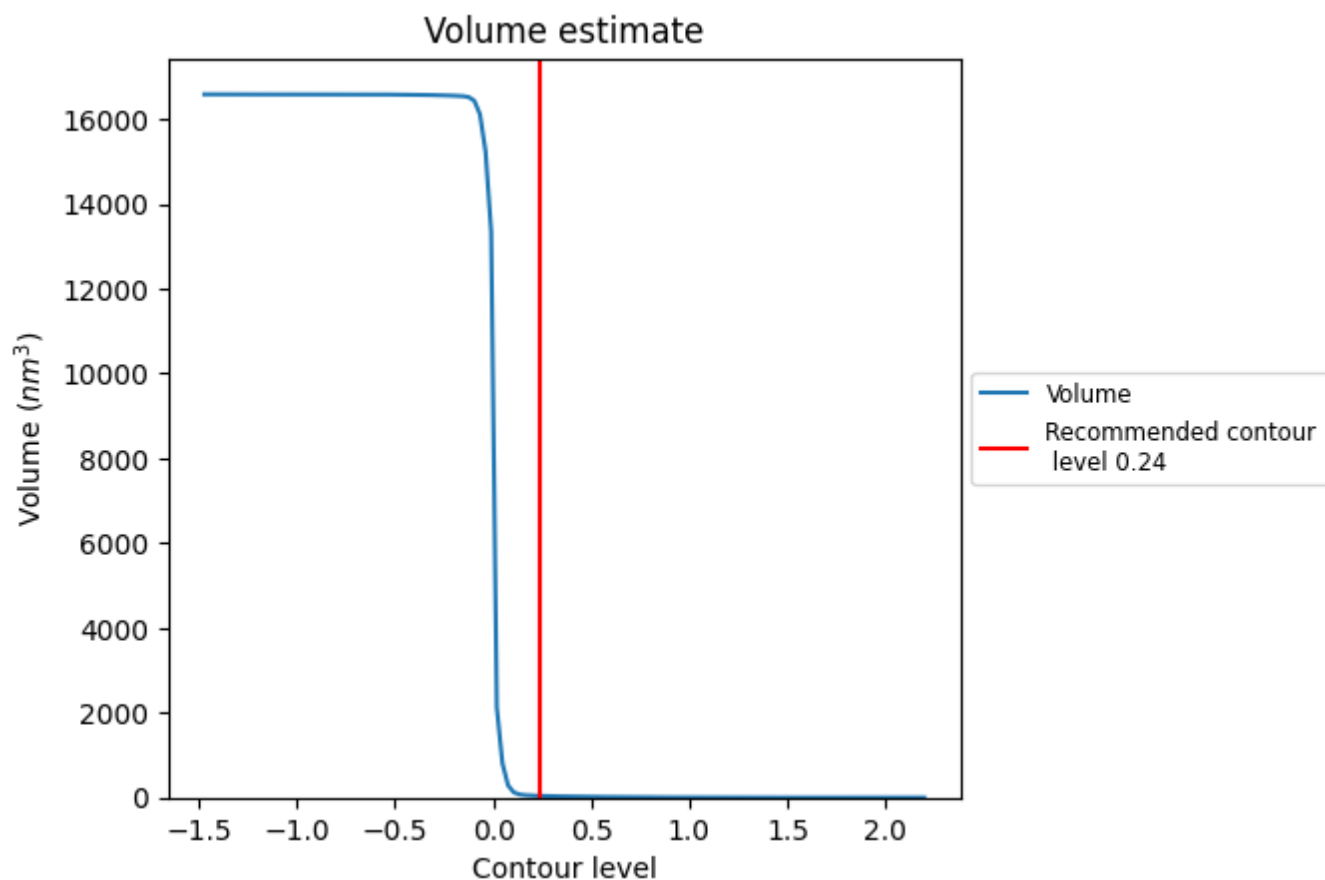
This section contains the results of statistical analysis of the map.

### 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](#)

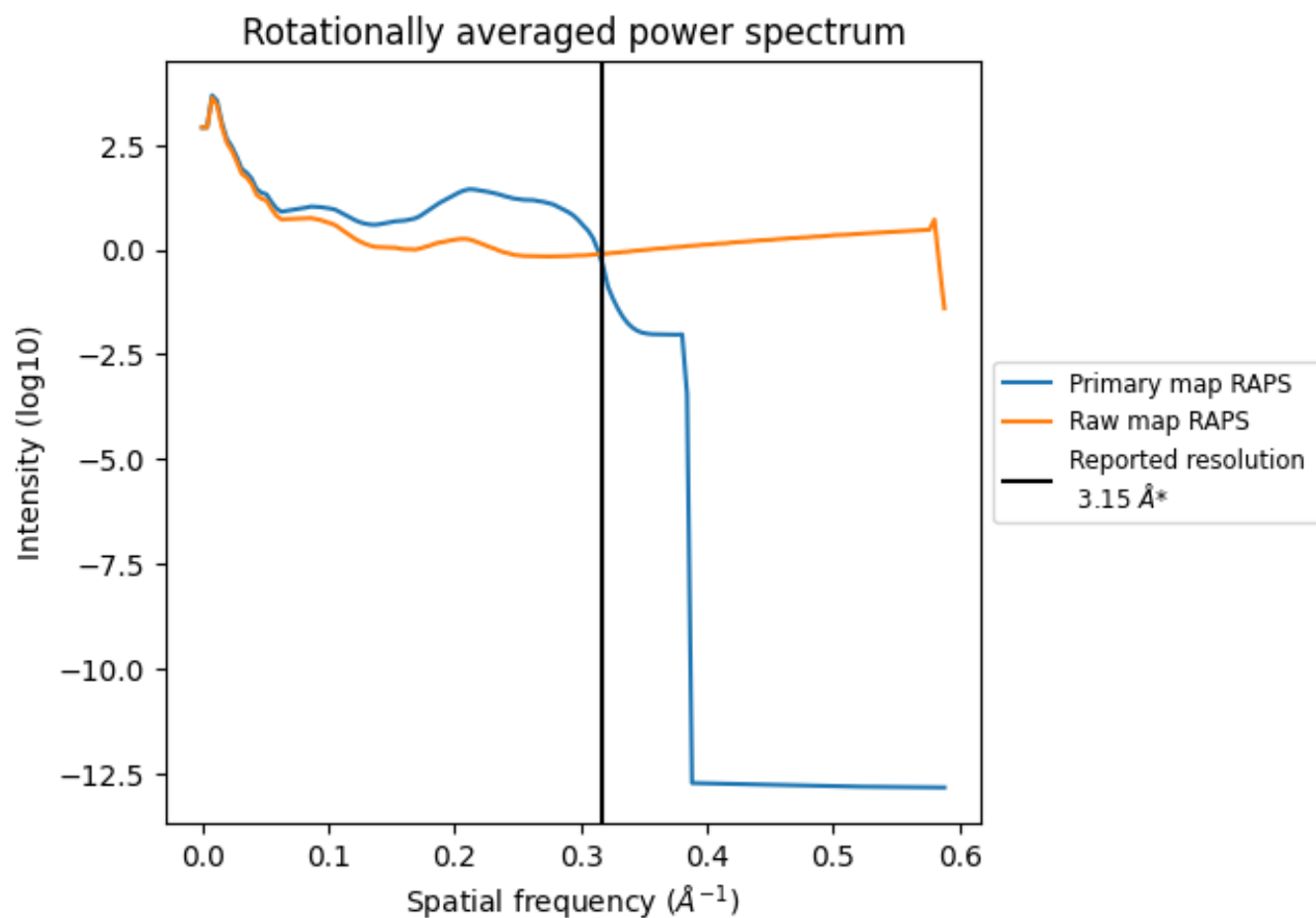


The volume at the recommended contour level is 39  $\text{nm}^3$ ; this corresponds to an approximate mass of 35 kDa.

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 ⓘ

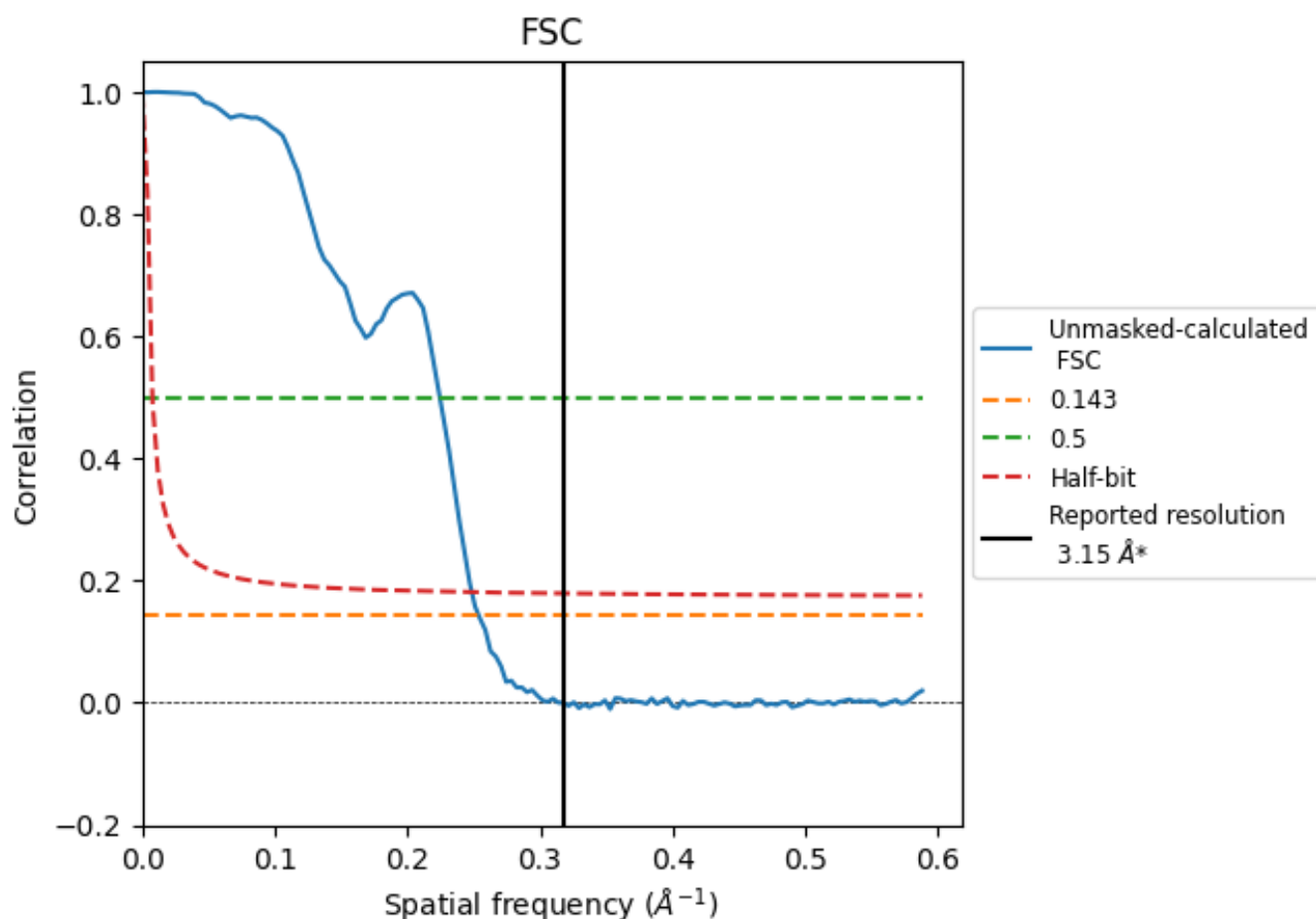


\*Reported resolution corresponds to spatial frequency of 0.317 Å<sup>-1</sup>

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

## 8.2 Resolution estimates [i](#)

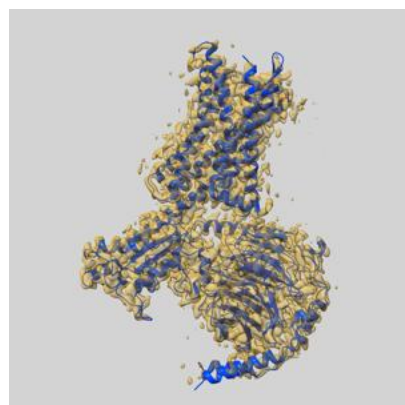
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.94	4.45	4.02

\*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 3.94 differs from the reported value 3.15 by more than 10 %

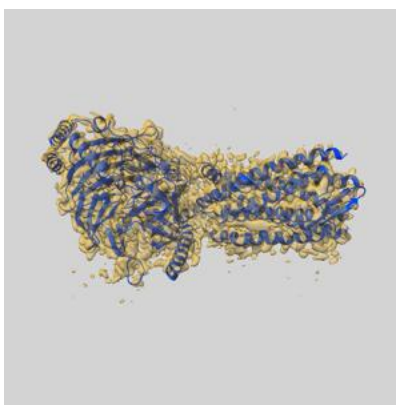
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-41890 and PDB model 8U4P. Per-residue inclusion information can be found in section [3](#) on page [7](#).

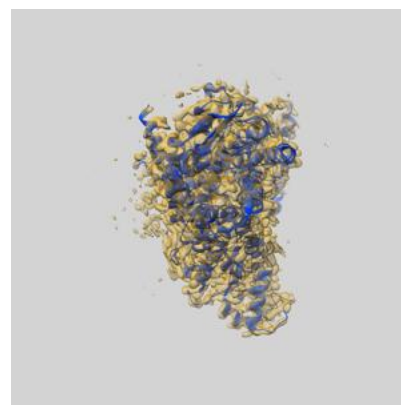
### 9.1 Map-model overlay [i](#)



X



Y



Z

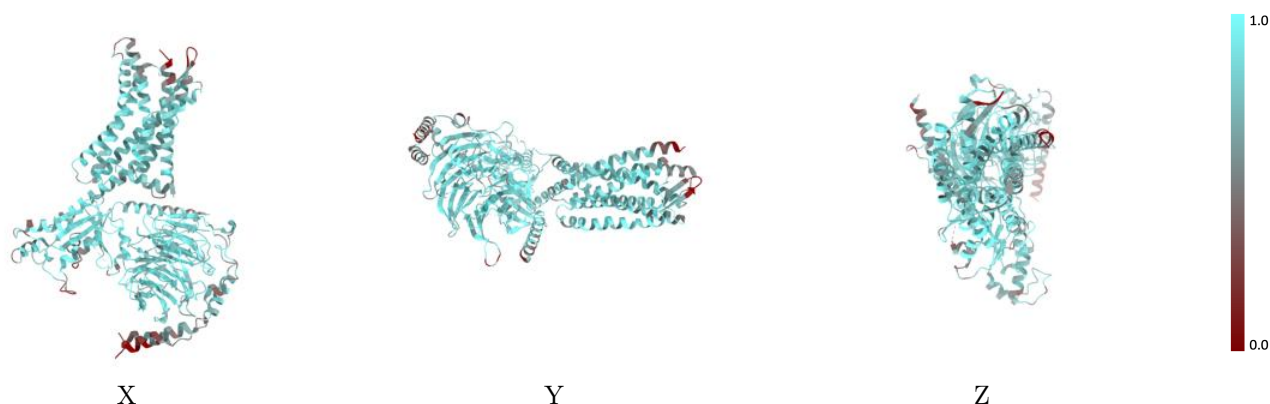
The images above show the 3D surface view of the map at the recommended contour level 0.24 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



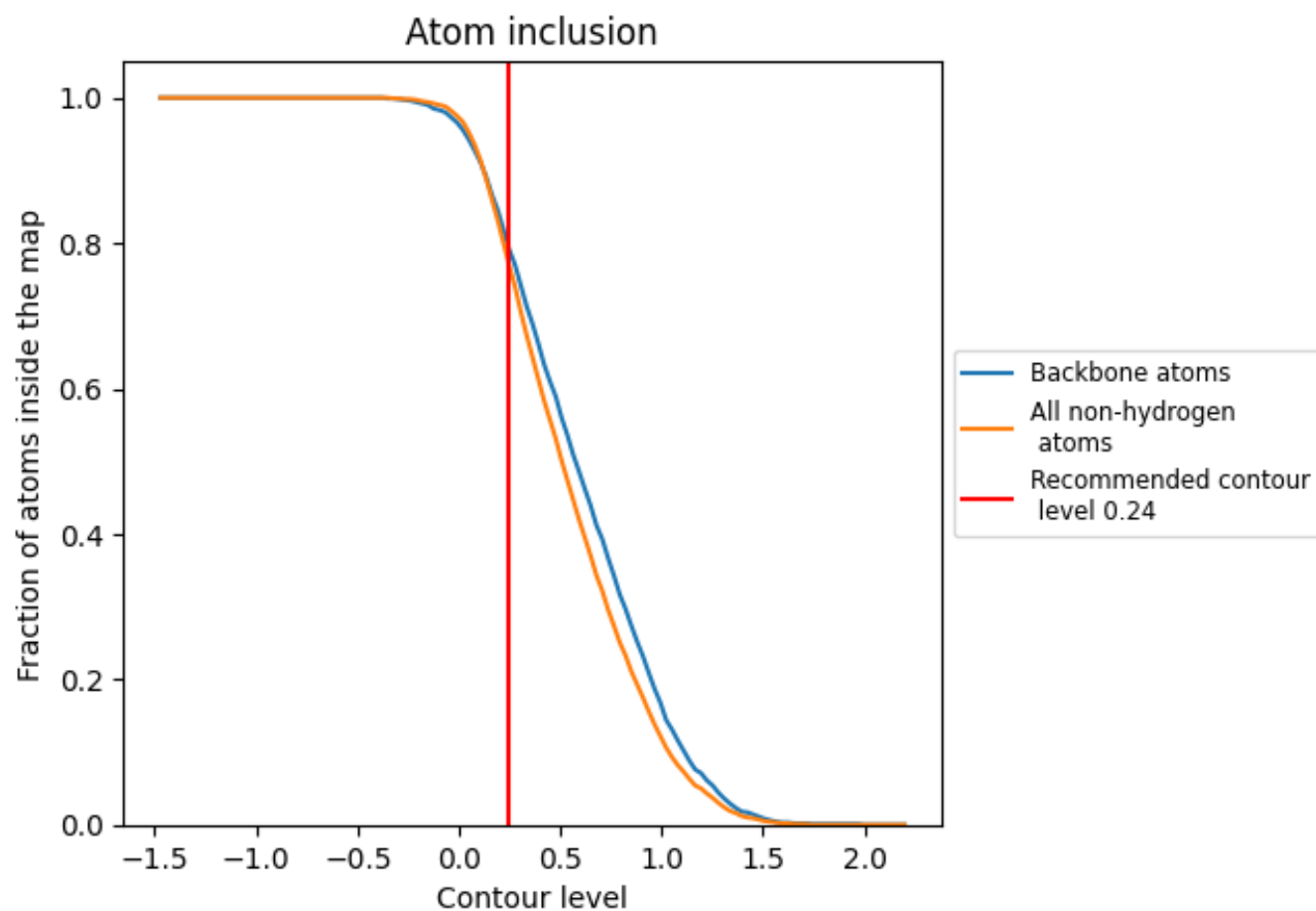
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.24).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% 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 (0.24) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.5320
A	<div></div> 0.7570	<div></div> 0.5200
B	<div></div> 0.8200	<div></div> 0.5600
C	<div></div> 0.6750	<div></div> 0.5210
R	<div></div> 0.7650	<div></div> 0.5130

