



## Full wwPDB EM Validation Report ⓘ

May 25, 2026 – 12:12 PM JST

PDB ID : 25NX / pdb\_000025nx  
EMDB ID : EMD-80238  
Title : A complex of PTH1R/Gs bound to a PTHrP analogue with three beta-amino acids  
Authors : Cary, B.P.; Wootten, D.; Sexton, P.M.; Gellman, S.H.; Wook, T.K.; Shin, J.; Gerrard, E.J.  
Deposited on : 2026-04-10  
Resolution : 2.86 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.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

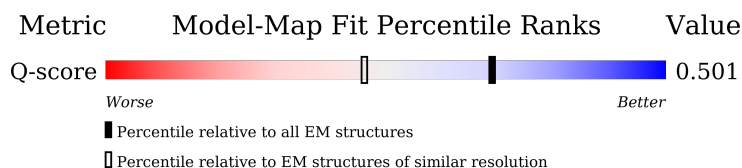
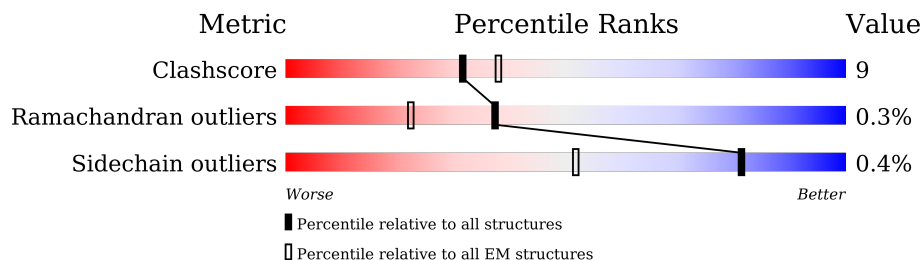
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.86 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	12017 ( 2.36 - 3.36 )

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	394	
2	B	340	
3	G	58	
4	N	156	

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Mol	Chain	Length	Quality of chain
5	P	36	
6	R	616	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	XCP	P	31	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9040 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	238	Total	C	N	O	S	0	0
			1942	1224	351	359	8		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	variant	UNP P63092
A	226	ALA	GLY	variant	UNP P63092
A	268	ALA	GLU	variant	UNP P63092
A	271	LYS	ASN	variant	UNP P63092
A	274	ASP	LYS	variant	UNP P63092
A	280	LYS	ARG	variant	UNP P63092
A	284	ASP	THR	variant	UNP P63092
A	285	THR	ILE	variant	UNP P63092
A	366	SER	ALA	variant	UNP P63092

- 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	337	Total	C	N	O	S	0	0
			2569	1585	461	503	20		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	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	G	56	Total	C	N	O	S	0	0
			425	266	75	81	3		

- Molecule 4 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	126	Total	C	N	O	S	0	0
			953	594	166	187	6		

- Molecule 5 is a protein called Peptide 2 (PTHrP analogue).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	32	Total	C	N	O	S	0	0
			268	171	55	42			

- Molecule 6 is a protein called Parathyroid hormone/parathyroid hormone-related peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	369	Total	C	N	O	S	0	0
			2883	1903	475	484	21		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	MET	-	initiating methionine	UNP Q03431
R	-2	LYS	-	expression tag	UNP Q03431
R	-1	THR	-	expression tag	UNP Q03431
R	0	ILE	-	expression tag	UNP Q03431
R	1	ILE	-	expression tag	UNP Q03431
R	2	ALA	-	expression tag	UNP Q03431
R	3	LEU	-	expression tag	UNP Q03431
R	4	SER	-	expression tag	UNP Q03431
R	5	TYR	-	expression tag	UNP Q03431
R	6	ILE	-	expression tag	UNP Q03431
R	7	PHE	-	expression tag	UNP Q03431
R	8	CYS	-	expression tag	UNP Q03431
R	9	LEU	-	expression tag	UNP Q03431
R	10	VAL	-	expression tag	UNP Q03431
R	11	PHE	-	expression tag	UNP Q03431
R	12	ALA	-	expression tag	UNP Q03431
R	13	ASP	-	expression tag	UNP Q03431
R	14	TYR	-	expression tag	UNP Q03431

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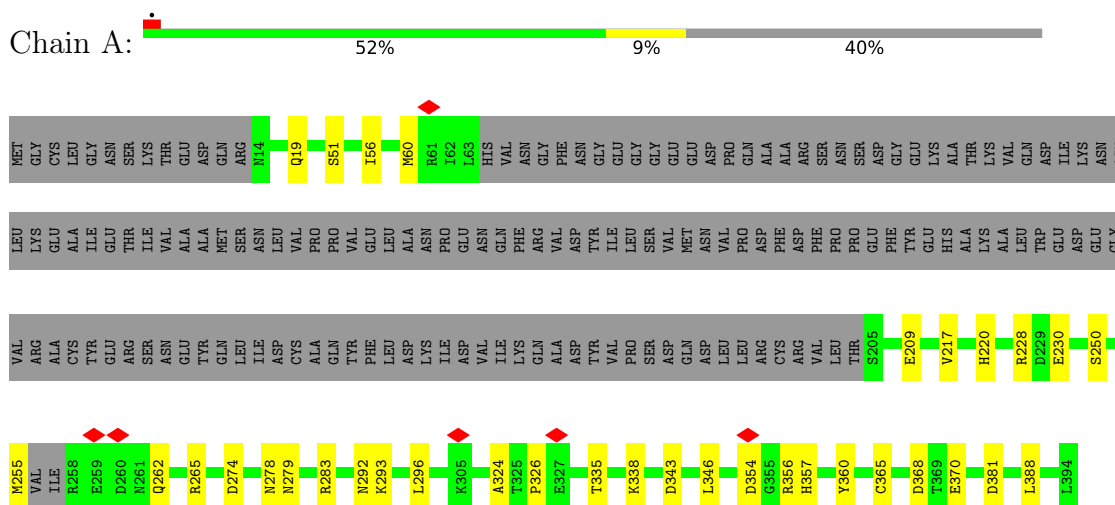
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Chain	Residue	Modelled	Actual	Comment	Reference
R	15	LYS	-	expression tag	UNP Q03431
R	16	ASP	-	expression tag	UNP Q03431
R	17	ASP	-	expression tag	UNP Q03431
R	18	ASP	-	expression tag	UNP Q03431
R	19	ASP	-	expression tag	UNP Q03431
R	20	LEU	-	expression tag	UNP Q03431
R	21	GLU	-	expression tag	UNP Q03431
R	22	VAL	-	expression tag	UNP Q03431
R	23	LEU	-	expression tag	UNP Q03431
R	24	PHE	-	expression tag	UNP Q03431
R	25	GLN	-	expression tag	UNP Q03431
R	26	GLY	-	expression tag	UNP Q03431
R	27	PRO	-	expression tag	UNP Q03431
R	594	PRO	-	expression tag	UNP Q03431
R	595	ALA	-	expression tag	UNP Q03431
R	596	GLY	-	expression tag	UNP Q03431
R	597	LEU	-	expression tag	UNP Q03431
R	598	GLU	-	expression tag	UNP Q03431
R	599	VAL	-	expression tag	UNP Q03431
R	600	LEU	-	expression tag	UNP Q03431
R	601	PHE	-	expression tag	UNP Q03431
R	602	GLN	-	expression tag	UNP Q03431
R	603	GLY	-	expression tag	UNP Q03431
R	604	PRO	-	expression tag	UNP Q03431
R	605	HIS	-	expression tag	UNP Q03431
R	606	HIS	-	expression tag	UNP Q03431
R	607	HIS	-	expression tag	UNP Q03431
R	608	HIS	-	expression tag	UNP Q03431
R	609	HIS	-	expression tag	UNP Q03431
R	610	HIS	-	expression tag	UNP Q03431
R	611	HIS	-	expression tag	UNP Q03431
R	612	HIS	-	expression tag	UNP Q03431

### 3 Residue-property plots

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.

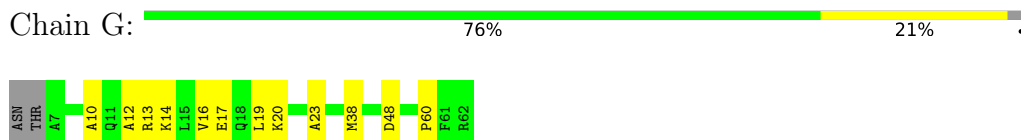
- Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



- 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: Nanobody35

L86	T91	Y94	Y95	C96	A97	P102	R105	D106	V110	Y117	T125	V126	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	L11	L18	R19	C22	F29	N35	W36	Y37	K43	D50	F51	S52	S57	F58	S59	T69	R72	L79	D82	M83				
MET	LYS	TYR	LEU	LEU	PRO	THR	ALA	ALA	GLY	LEU	LEU	LEU	LEU	ALA	ALA	GLN	PRO	ALA	ALA	MET	ALA	G1	V2	Q3	L4	Q5	L11	L18	R19	C22	F29	N35	W36	Y37	K43	D50	F51	S52	S57	F58	S59	T69	R72	L79	D82	M83

- Chain P:  36% 36% 17% 11%

A1		Q6	L7	L8	H9	D10	K11	G12	K13	S14	I15		L18	R21	F22	F23	X24	H25	H26	L27	X28	A29	E30	X31	H32	X33	THR	ALA	GLU	TLE
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- Chain R: 

[illegible]

ILE	MET	GLU	GLY	ASP	LYS	GLY	TRP	THR	SER	ALA	SER	THR	SER	LYS	PRO	ARG	R106	L166	L117	L118	L119	L120	L121
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A122	P123	G124	E125	V126	V127	A128	V129	P130	C131	P132	D133	Y134	I135	Y136		H140	K141	G142	H143	A144	Y145		D149	R150	N151	G152	S153	W154	E155	L156	V157	P158	G159	H160	N161	R162	T163	W164		Y167	S168	E169	C170	V171		L174	T175	N176		E180	R181	F182	V183		G188	M189	I190	Y191
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S198	L215	H216	C217	T218	R219	N220	Y221	L222	F227	M231	S236	S246	GLY	ALA	THR	LEU	ASP	GLU	ALA	GLU	ARG	LEU	THR	GLU	GLU	GLU	GLU	ARG	ALA	IIE	ALA	GLN	ALA	PRO	PRO	PRO	PRO	ALA	ALA	THR	ALA	ALA	A276	C281	T286	F287	F288	L289	Y290	F291	L292	A293
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Category	Count
Y296	1
E302	1
A313	1
F314	1
K319	1
V336	1
W339	1
V342	1
P343	1
A344	1
N348	1
W352	1
S355	1
K359	1
P366	1
P366	1
I367	1
L385	1
L389	1
R396	1
C397	1
D398	1
Q401	1
Q402	1
Y403	1
R404	1
M414	1
P415	1
V419	1
H420	1
Y421	1
Y429	1
T430	1
E431	1
M441	1
M445	1
S449	1

1457	ALA	LEU	ASP	PHE	LYS	ARG	LYS	ALA	ARG	SER	GLY	SER	SER	SER	TYR	TYR	GLY	PRO	MET	VAL	SER	HIS	THR	SER	VAL	THR	ASN	VAL	GLY	PRO	ARG	VAL	GLY	LEU	GLY	LEU	PRO	LEU	PRO	THR	ALA	THR	THR	ASN	GLY	HIS	PRO	ASN
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LEU	PRO	GLY	HIS	ALA	LYS	PRO	GLY	THR	PRO	ALA	LEU	GLU	THR	THR	PRO	PRO	ALA	ALA	ALA	LYS	ASP	ASP	GLY	PHE	LEU	ASN	GLY	GLY	CYS	SER	GLY	LEU	ASP	GLU	GLU	ALA	SER	GLY	PRO	GLU	GLU	ARG	PRO	PRO	ALA	ALA	LEU	LEU	GLN	GLU	GLU	TRP	GLU	THR	THR	VAL	MET
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PRO  
ALA  
GLY  
LEU  
GLU  
VAL  
LEU  
PHE  
GLN  
GLY  
PRO  
HIS  
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	336618	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.897	Depositor
Minimum map value	-0.416	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.16	Depositor
Map size (Å)	247.68001, 247.68001, 247.68001	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: XCP

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	0.20	0/1978	0.33	0/2662
2	B	0.26	0/2616	0.41	0/3551
3	G	0.21	0/431	0.51	0/582
4	N	0.21	0/973	0.34	0/1320
5	P	0.82	0/247	1.10	0/324
6	R	0.31	0/2970	0.50	0/4053
All	All	0.29	0/9215	0.46	0/12492

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	P	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	P	23	PHE	Peptide
5	P	27	LEU	Peptide
5	P	30	GLU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1942	0	1888	24	0
2	B	2569	0	2450	38	0
3	G	425	0	427	13	0
4	N	953	0	911	21	0
5	P	268	0	265	29	0
6	R	2883	0	2732	67	0
All	All	9040	0	8673	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 9.

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:255:MET:SD	4:N:43:LYS:NZ	2.54	0.81
5:P:28:XCP:HGA	6:R:115:ILE:HG13	1.62	0.80
5:P:31:XCP:HD	6:R:115:ILE:HG12	1.65	0.79
6:R:180:GLU:HA	6:R:183:VAL:HG12	1.65	0.77
2:B:18:ILE:HD11	3:G:23:ALA:HA	1.68	0.74
5:P:27:LEU:HG	6:R:115:ILE:HD11	1.70	0.73
5:P:18:LEU:O	5:P:21:ARG:HG3	1.90	0.70
2:B:325:MET:O	2:B:340:ASN:ND2	2.24	0.69
6:R:215:LEU:O	6:R:220:ASN:ND2	2.26	0.68
2:B:45:MET:HE3	2:B:308:LEU:HD21	1.78	0.65
5:P:18:LEU:HD11	6:R:181:ARG:NH1	2.12	0.65
2:B:146:LEU:HD11	2:B:159:THR:HB	1.79	0.64
6:R:40:LEU:HD21	6:R:134:TYR:HB2	1.79	0.64
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.30	0.64
6:R:296:TYR:HE1	6:R:421:TYR:CZ	2.14	0.64
2:B:245:SER:OG	2:B:247:ASP:OD1	2.15	0.64
5:P:31:XCP:CG	6:R:114:HIS:HB2	2.28	0.64
4:N:83:MET:HB3	4:N:86:LEU:HD21	1.82	0.62
1:A:51:SER:O	1:A:292:ASN:ND2	2.27	0.61
4:N:22:CYS:HB3	4:N:79:LEU:HB3	1.82	0.61
1:A:228:ARG:NH2	1:A:230:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:THR:HG22	3:G:38:MET:HE2	1.83	0.60
2:B:325:MET:HE2	3:G:60:PRO:HD2	1.84	0.59
5:P:28:XCP:CG	6:R:115:ILE:HG13	2.29	0.59
6:R:188:GLY:HA2	6:R:191:TYR:CE2	2.37	0.59
2:B:71:VAL:HG12	2:B:81:ILE:HG12	1.84	0.59
6:R:227:PHE:O	6:R:231:MET:HG3	2.03	0.57
4:N:50:ASP:OD1	4:N:59:SER:OG	2.20	0.57
5:P:9:HIS:CD2	6:R:355:SER:HB2	2.39	0.57
1:A:283:ARG:O	1:A:357:HIS:ND1	2.38	0.57
5:P:21:ARG:HH22	6:R:176:ASN:HA	1.70	0.57
2:B:213:VAL:HG23	2:B:214:ARG:HD3	1.86	0.57
3:G:16:VAL:HG12	3:G:20:LYS:NZ	2.21	0.56
1:A:56:ILE:HG22	1:A:60:MET:HE3	1.88	0.56
1:A:279:ASN:HA	4:N:106:ASP:OD2	2.07	0.55
2:B:22:ARG:NH1	2:B:258:ASP:O	2.39	0.55
1:A:354:ASP:OD2	1:A:356:ARG:NH2	2.39	0.55
2:B:137:ARG:NH1	2:B:172:GLU:O	2.35	0.54
1:A:274:ASP:OD1	1:A:278:ASN:ND2	2.40	0.54
3:G:17:GLU:HA	3:G:20:LYS:NZ	2.23	0.54
5:P:28:XCP:HE	6:R:171:VAL:HG11	1.89	0.54
1:A:228:ARG:NH1	2:B:186:ASP:OD1	2.41	0.54
2:B:247:ASP:HA	4:N:102:PRO:HG3	1.90	0.54
5:P:31:XCP:HDA	6:R:113:ASP:OD2	2.08	0.54
3:G:12:ALA:O	3:G:16:VAL:HG23	2.08	0.54
3:G:16:VAL:HG12	3:G:20:LYS:HZ2	1.73	0.53
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.90	0.53
5:P:31:XCP:C	6:R:167:TYR:HE2	2.22	0.53
3:G:17:GLU:HA	3:G:20:LYS:HZ3	1.72	0.53
6:R:286:THR:HG22	6:R:339:TRP:HZ3	1.73	0.53
6:R:156:LEU:HD22	6:R:161:ASN:HA	1.90	0.53
5:P:14:SER:OG	6:R:181:ARG:NH2	2.42	0.52
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.92	0.52
5:P:23:PHE:CD2	6:R:34:LYS:HE3	2.44	0.52
6:R:217:CYS:SG	6:R:218:THR:N	2.83	0.51
5:P:23:PHE:CG	6:R:34:LYS:HE3	2.45	0.51
1:A:209:GLU:OE2	1:A:220:HIS:NE2	2.33	0.51
4:N:3:GLN:OE1	4:N:5:GLN:NE2	2.40	0.51
6:R:296:TYR:CE1	6:R:421:TYR:CZ	2.99	0.50
6:R:414:MET:HG3	6:R:419:VAL:HB	1.93	0.50
6:R:431:GLU:H	6:R:431:GLU:CD	2.20	0.50
2:B:290:ASP:OD1	2:B:314:ARG:NE	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:31:XCP:C	6:R:167:TYR:CE2	2.96	0.49
6:R:290:TYR:HA	6:R:336:VAL:HG21	1.95	0.49
1:A:19:GLN:NE2	2:B:83:ASP:OD2	2.45	0.49
1:A:370:GLU:N	1:A:370:GLU:OE1	2.46	0.48
6:R:105:GLY:N	6:R:150:ARG:O	2.46	0.48
6:R:222:ILE:HG22	6:R:302:GLU:OE2	2.14	0.48
1:A:19:GLN:OE1	2:B:88:ASN:ND2	2.34	0.47
6:R:398:ASP:HB3	6:R:401:GLN:HG3	1.96	0.47
5:P:7:LEU:HD13	6:R:441:MET:HE2	1.96	0.47
5:P:32:HIS:CE1	6:R:167:TYR:HD2	2.32	0.47
4:N:11:LEU:HD13	4:N:125:THR:HG23	1.98	0.46
5:P:11:LYS:O	5:P:15:ILE:HG12	2.15	0.46
1:A:388:LEU:HD22	6:R:385:LEU:HD21	1.96	0.46
6:R:130:PRO:HA	6:R:143:HIS:HA	1.96	0.46
4:N:35:ASN:HD22	4:N:110:VAL:HG11	1.80	0.46
6:R:132:PRO:HG2	6:R:135:ILE:HD12	1.98	0.46
3:G:13:ARG:O	3:G:17:GLU:OE1	2.32	0.46
5:P:31:XCP:HD	6:R:115:ILE:CG1	2.39	0.46
6:R:236:SER:HB2	6:R:291:PHE:HD2	1.81	0.46
4:N:69:THR:HB	4:N:82:GLN:HB3	1.98	0.45
6:R:198:SER:OG	6:R:449:SER:O	2.34	0.45
6:R:281:CYS:SG	6:R:352:TRP:N	2.90	0.45
1:A:360:TYR:OH	1:A:381:ASP:OD2	2.26	0.45
4:N:29:PHE:O	4:N:72:ARG:NH2	2.50	0.45
4:N:35:ASN:ND2	4:N:110:VAL:HG11	2.31	0.45
2:B:54:HIS:NE2	2:B:72:SER:OG	2.37	0.45
2:B:75:GLN:OE1	2:B:99:TRP:HE3	1.98	0.45
2:B:112:VAL:HG13	2:B:126:LEU:HD11	1.98	0.45
6:R:401:GLN:HA	6:R:404:ARG:HE	1.81	0.45
5:P:31:XCP:HEA	6:R:167:TYR:OH	2.17	0.44
6:R:158:PRO:HD3	6:R:164:TRP:CD1	2.52	0.44
2:B:118:ASP:N	2:B:118:ASP:OD1	2.47	0.44
4:N:91:THR:HG22	4:N:125:THR:HA	1.99	0.44
5:P:13:LYS:HD2	5:P:13:LYS:HA	1.75	0.44
6:R:389:LEU:HB3	6:R:402:GLN:HG3	1.99	0.44
2:B:79:LEU:HB2	2:B:93:ILE:HB	1.98	0.44
6:R:128:ALA:HA	6:R:145:TYR:HA	1.98	0.44
2:B:12:GLU:O	2:B:16:ASN:ND2	2.51	0.44
4:N:18:LEU:HD12	4:N:19:ARG:H	1.82	0.44
1:A:324:ALA:O	1:A:326:PRO:HD3	2.17	0.44
4:N:105:ARG:HB2	4:N:105:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:249:THR:OG1	2:B:251:ARG:NH1	2.50	0.44
6:R:414:MET:HB3	6:R:415:PRO:HD3	1.99	0.44
4:N:37:VAL:HG23	4:N:95:TYR:HB2	2.00	0.44
6:R:293:ALA:HB2	6:R:367:ILE:HD11	2.00	0.44
6:R:344:ALA:HA	6:R:348:ASN:HB2	2.00	0.44
6:R:471:LYS:HA	6:R:471:LYS:HD2	1.70	0.43
4:N:52:SER:HB3	4:N:57:SER:HB3	1.99	0.43
5:P:21:ARG:O	5:P:22:PHE:C	2.61	0.43
1:A:335:THR:O	1:A:338:LYS:HG2	2.19	0.43
5:P:31:XCP:HG	6:R:114:HIS:HB2	1.98	0.43
5:P:23:PHE:CG	5:P:24:XCP:N	2.85	0.43
2:B:317:CYS:SG	2:B:330:GLY:HA3	2.59	0.43
6:R:32:MET:HG2	6:R:136:TYR:CD2	2.54	0.43
2:B:204:CYS:O	4:N:117:TYR:OH	2.37	0.43
5:P:9:HIS:CG	6:R:355:SER:HB2	2.54	0.43
6:R:441:MET:HE3	6:R:445:MET:HE3	2.01	0.43
2:B:180:PHE:CE1	2:B:216:GLY:HA2	2.54	0.42
4:N:52:SER:O	4:N:72:ARG:NH1	2.50	0.42
6:R:319:LYS:HD2	6:R:319:LYS:HA	1.80	0.42
3:G:14:LYS:HD2	3:G:17:GLU:OE2	2.18	0.42
2:B:57:LYS:HE2	2:B:75:GLN:HG3	2.01	0.42
6:R:292:LEU:HD12	6:R:292:LEU:C	2.44	0.42
2:B:14:LEU:HB3	3:G:19:LEU:HD21	2.00	0.42
6:R:236:SER:OG	6:R:288:PHE:HA	2.19	0.42
1:A:343:ASP:OD1	6:R:396:ARG:NH2	2.52	0.42
1:A:262:GLN:OE1	1:A:265:ARG:NH1	2.52	0.42
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.82	0.42
2:B:6:GLN:HG2	2:B:7:LEU:N	2.34	0.42
2:B:253:PHE:HA	2:B:260:GLU:HA	2.02	0.42
2:B:310:GLY:O	2:B:337:LYS:NZ	2.36	0.42
3:G:10:ALA:HA	3:G:13:ARG:NH1	2.35	0.42
1:A:293:LYS:HD2	1:A:296:LEU:HD12	2.02	0.41
4:N:83:MET:HE1	4:N:94:TYR:CZ	2.55	0.41
2:B:253:PHE:CE2	2:B:260:GLU:HB3	2.55	0.41
1:A:365:CYS:N	1:A:368:ASP:OD2	2.53	0.41
4:N:35:ASN:HB2	4:N:97:ALA:HB3	2.02	0.41
1:A:217:VAL:HG21	6:R:314:PHE:CD2	2.56	0.41
6:R:189:MET:HE2	6:R:189:MET:HB3	1.96	0.41
2:B:13:GLN:HA	2:B:16:ASN:HD22	1.86	0.41
3:G:48:ASP:OD1	3:G:48:ASP:N	2.48	0.41
6:R:180:GLU:CA	6:R:183:VAL:HG12	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:292:LEU:CD1	6:R:296:TYR:HE2	2.33	0.41
6:R:342:VAL:HG12	6:R:359:LYS:HE3	2.03	0.41
1:A:250:SER:OG	1:A:293:LYS:O	2.39	0.41
5:P:31:XCP:HEA	6:R:167:TYR:CZ	2.56	0.41
6:R:365:VAL:HB	6:R:366:PRO:HD3	2.02	0.41
6:R:454:PHE:HA	6:R:457:ILE:HG22	2.03	0.41
5:P:6:GLN:HG3	6:R:429:TYR:CD2	2.56	0.40
5:P:31:XCP:CD	6:R:114:HIS:HB2	2.51	0.40
2:B:166:CYS:SG	2:B:187:VAL:HG11	2.62	0.40
2:B:235:PHE:CG	2:B:236:PRO:HD2	2.56	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	232/394 (59%)	232 (100%)	0	0	100	100
2	B	335/340 (98%)	320 (96%)	15 (4%)	0	100	100
3	G	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
4	N	124/156 (80%)	121 (98%)	3 (2%)	0	100	100
5	P	27/36 (75%)	22 (82%)	2 (7%)	3 (11%)	0	0
6	R	363/616 (59%)	355 (98%)	8 (2%)	0	100	100
All	All	1135/1600 (71%)	1103 (97%)	29 (3%)	3 (0%)	37	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	P	29	ALA
5	P	30	GLU
5	P	25	HIS

### 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	205/350 (59%)	205 (100%)	0	100	100
2	B	274/283 (97%)	272 (99%)	2 (1%)	76	87
3	G	43/47 (92%)	43 (100%)	0	100	100
4	N	102/126 (81%)	102 (100%)	0	100	100
5	P	25/29 (86%)	25 (100%)	0	100	100
6	R	285/523 (54%)	283 (99%)	2 (1%)	76	87
All	All	934/1358 (69%)	930 (100%)	4 (0%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	59	TYR
2	B	317	CYS
6	R	292	LEU
6	R	430	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
5	P	25	HIS
6	R	307	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 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
5	XCP	P	31	5	8,8,9	1.47	1 (12%)	4,10,12	1.60	1 (25%)
5	XCP	P	28	5	8,8,9	1.36	1 (12%)	4,10,12	1.68	1 (25%)
5	XCP	P	24	5	8,8,9	1.31	1 (12%)	4,10,12	1.37	1 (25%)

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	XCP	P	31	5	-	1/1/12/14	0/1/1/1
5	XCP	P	28	5	-	1/1/12/14	0/1/1/1
5	XCP	P	24	5	-	1/1/12/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	31	XCP	CA-CB	-3.35	1.51	1.55
5	P	28	XCP	CA-CB	-3.02	1.51	1.55
5	P	24	XCP	CA-CB	-3.02	1.51	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	28	XCP	O-C-CA	-2.83	118.55	125.16
5	P	31	XCP	O-C-CA	-2.79	118.64	125.16
5	P	24	XCP	O-C-CA	-2.09	120.28	125.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	P	31	XCP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
5	P	24	XCP	O-C-CA-CB
5	P	28	XCP	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	31	XCP	10	0
5	P	28	XCP	3	0
5	P	24	XCP	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.

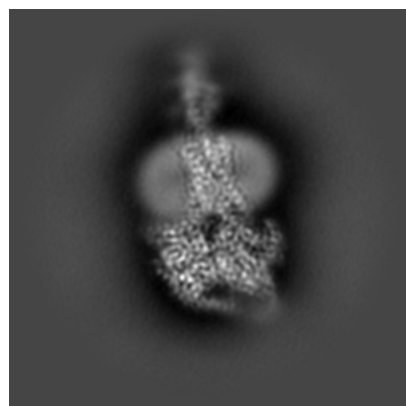
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-80238. These allow visual inspection of the internal detail of the map and identification of artifacts.

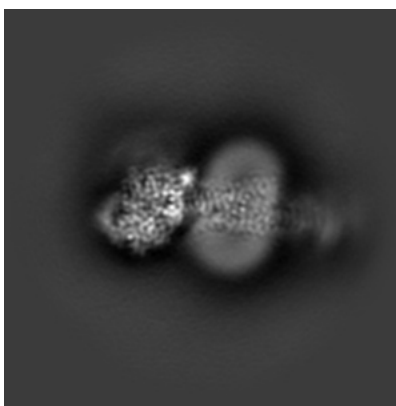
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

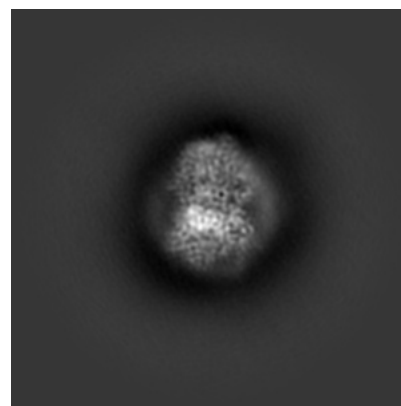
#### 6.1.1 Primary map



X

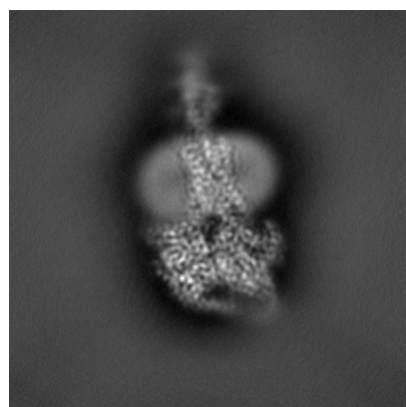


Y

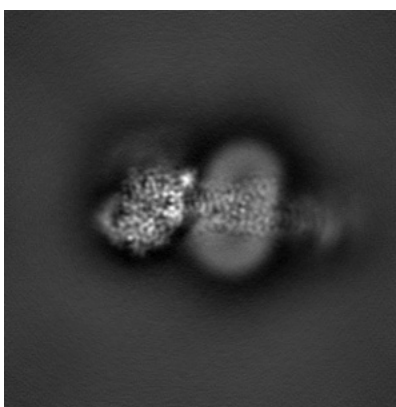


Z

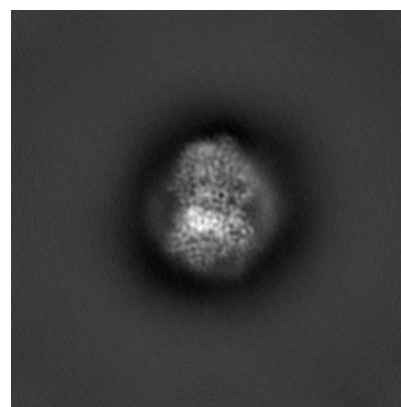
#### 6.1.2 Raw map



X



Y

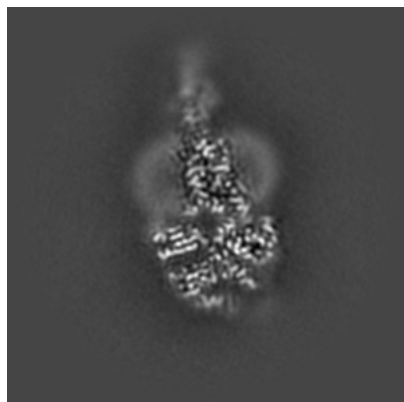


Z

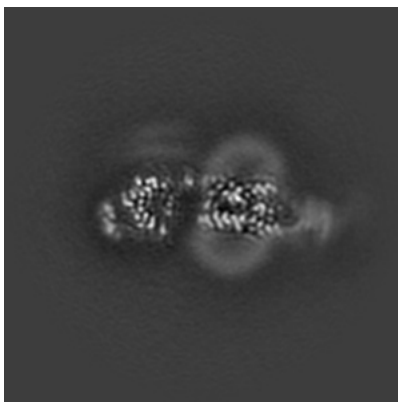
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

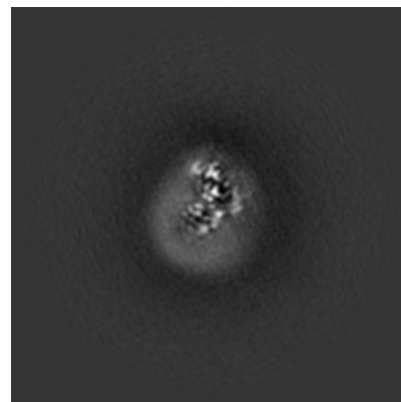
### 6.2.1 Primary map



X Index: 144

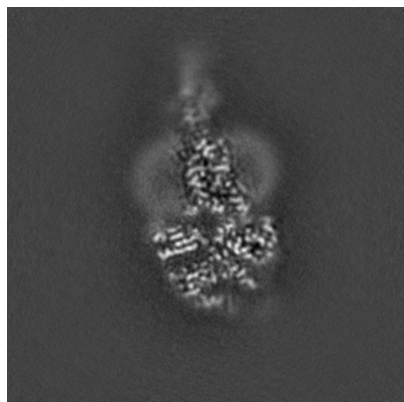


Y Index: 144

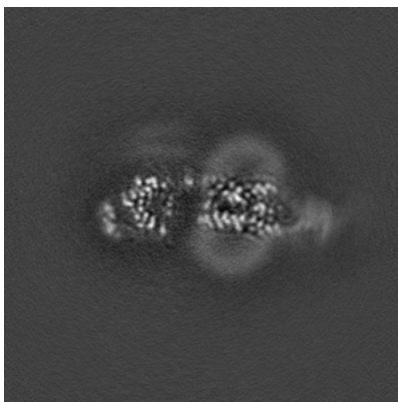


Z Index: 144

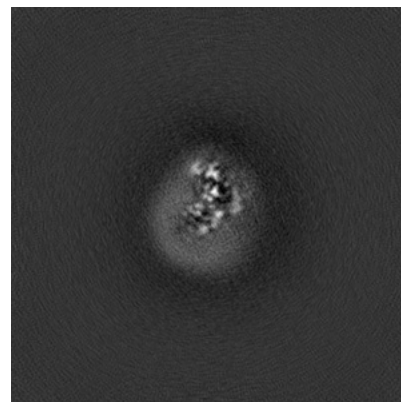
### 6.2.2 Raw map



X Index: 144



Y Index: 144

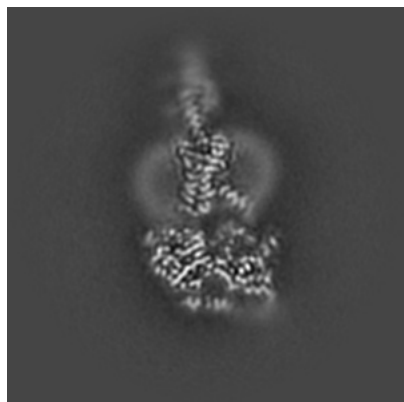


Z Index: 144

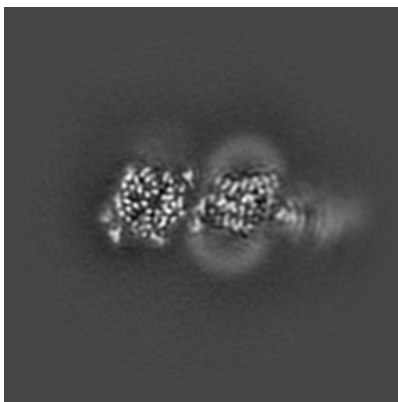
The images above show central slices of the map in three orthogonal directions.

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

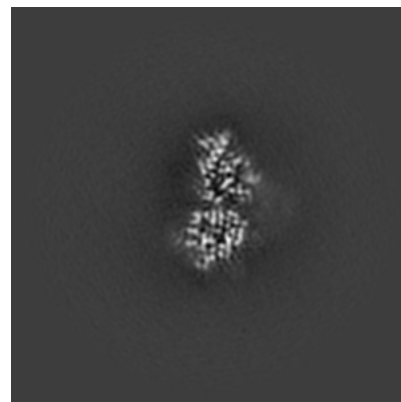
### 6.3.1 Primary map



X Index: 135

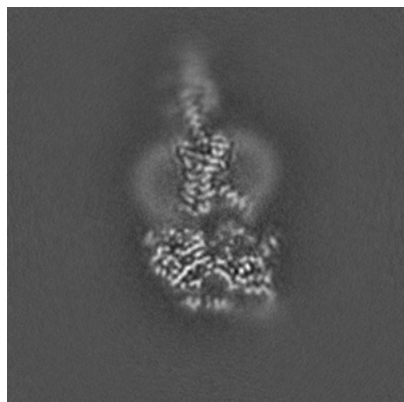


Y Index: 135

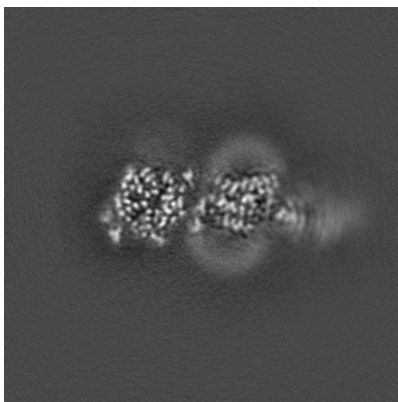


Z Index: 121

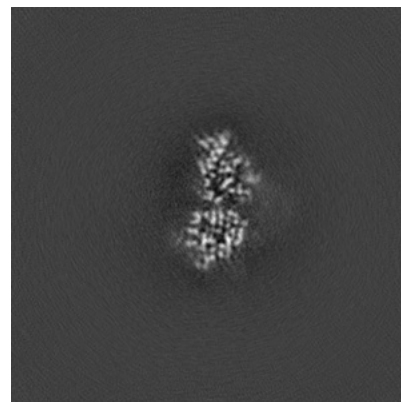
### 6.3.2 Raw map



X Index: 135



Y Index: 135

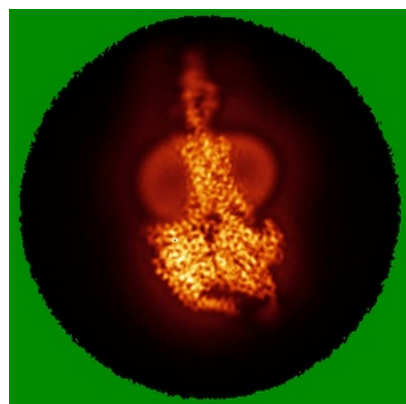


Z Index: 121

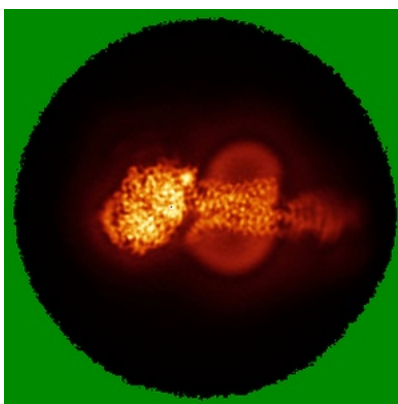
The images above show the largest variance slices of the map in three orthogonal directions.

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

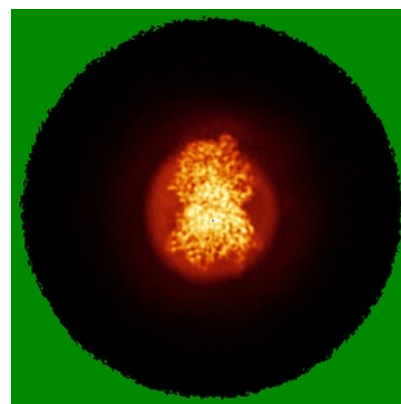
### 6.4.1 Primary map



X

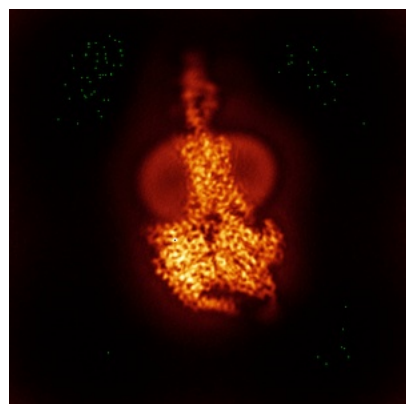


Y

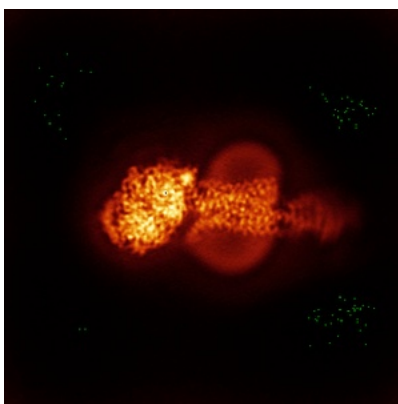


Z

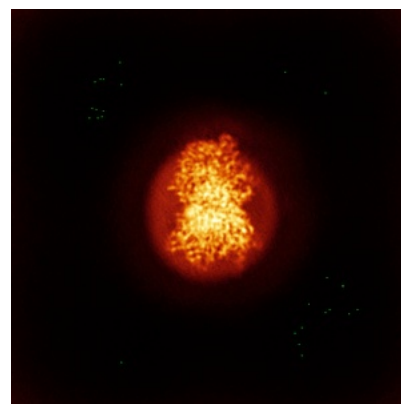
### 6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

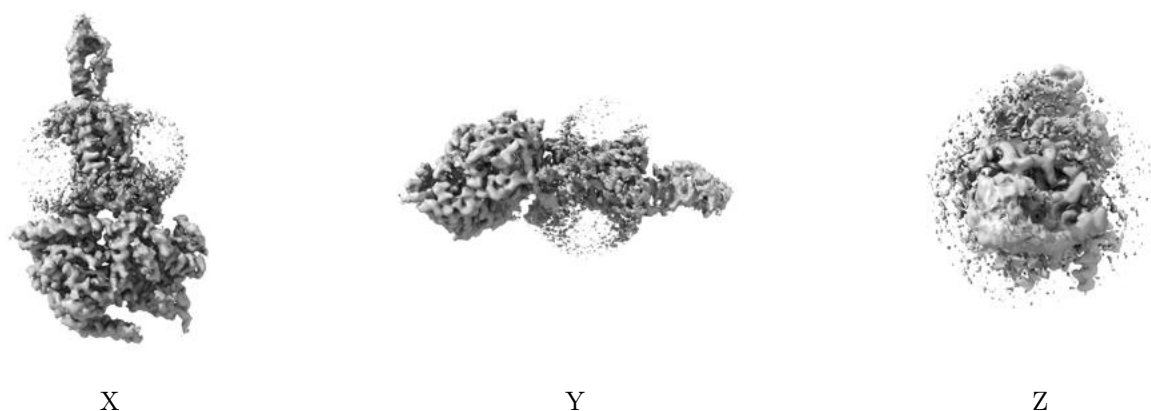
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.16. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



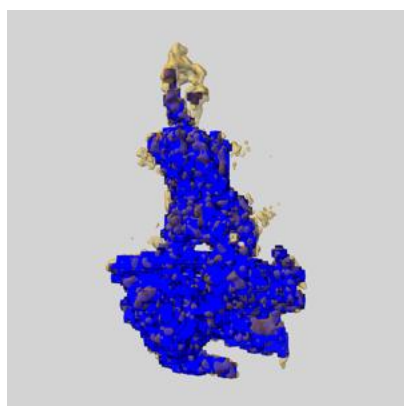
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

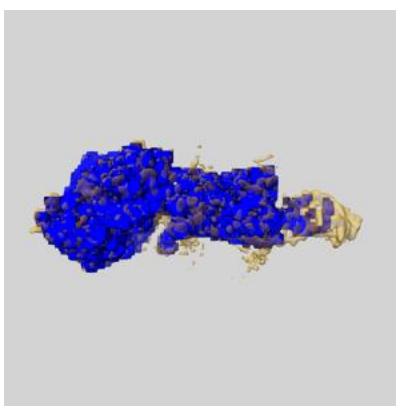
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

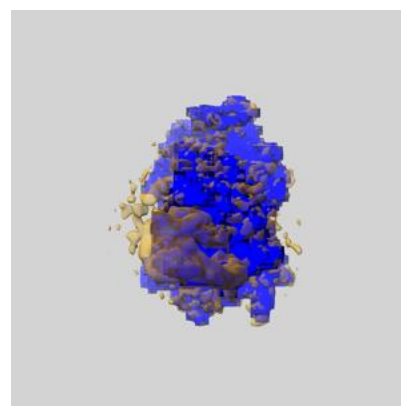
### 6.6.1 emd\_80238\_msk\_1.map [i](#)



X



Y



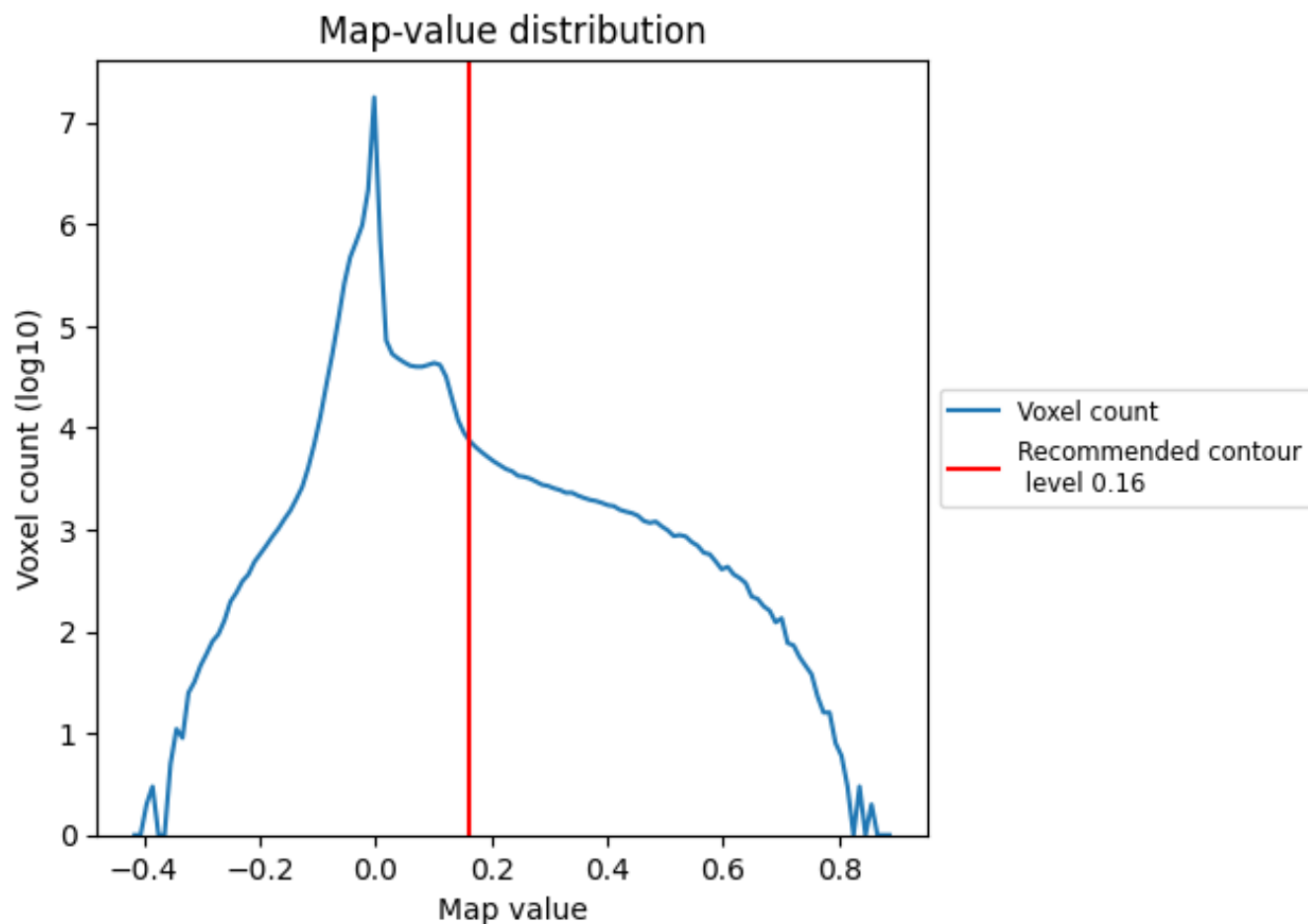
Z



## 7 Map analysis [i](#)

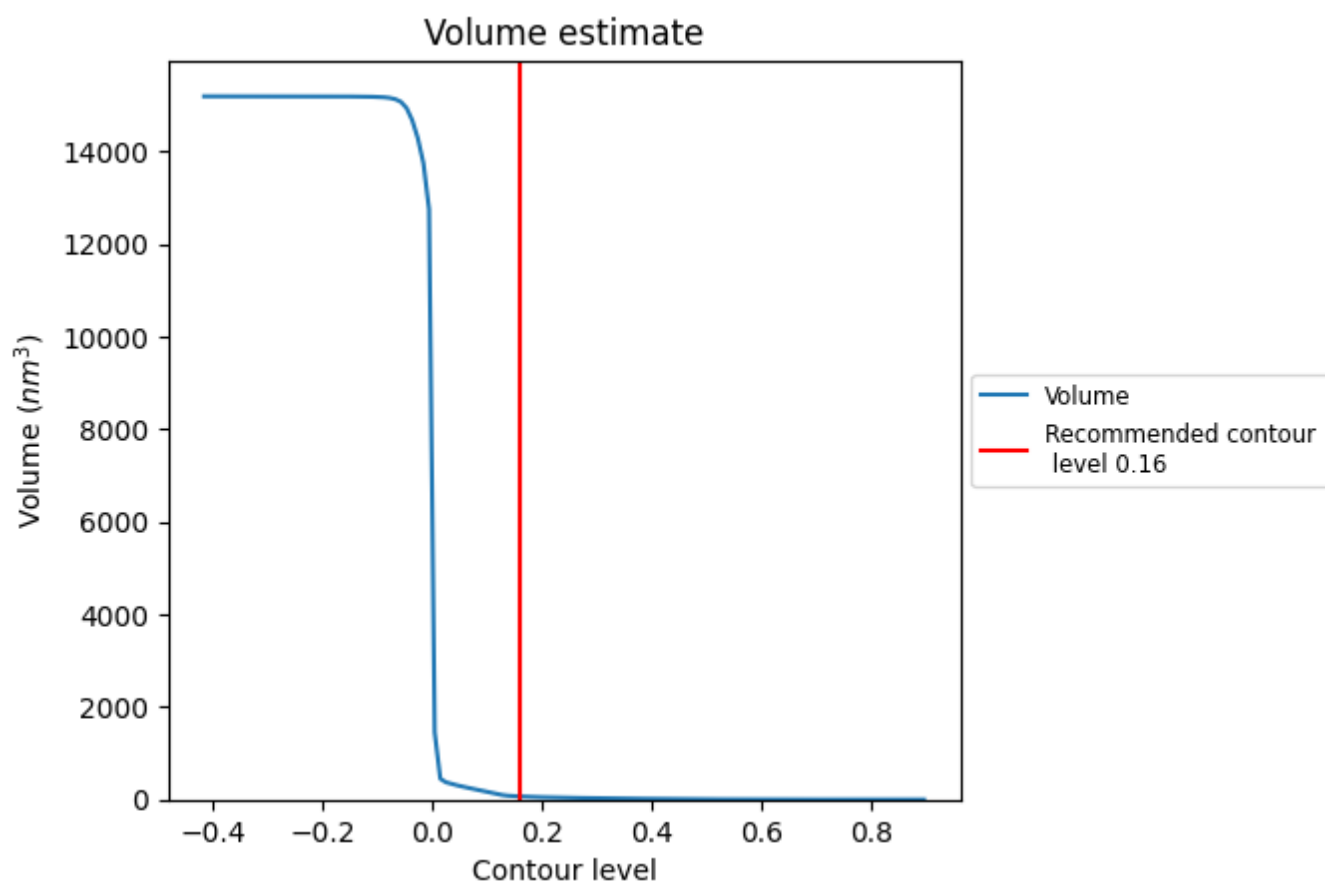
This section contains the results of statistical analysis of the map.

### 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.

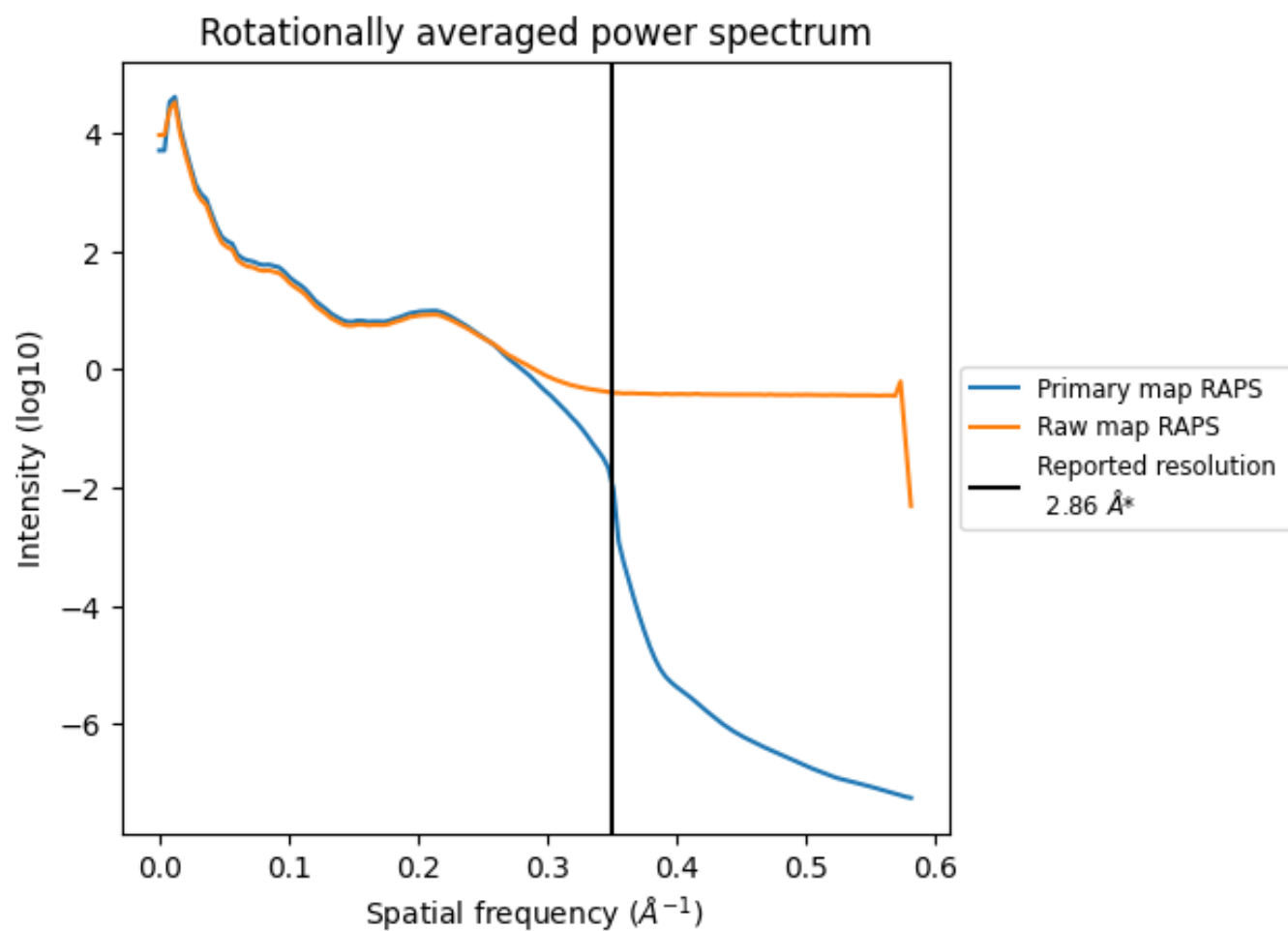
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm<sup>3</sup>; this corresponds to an approximate mass of 61 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 ⓘ

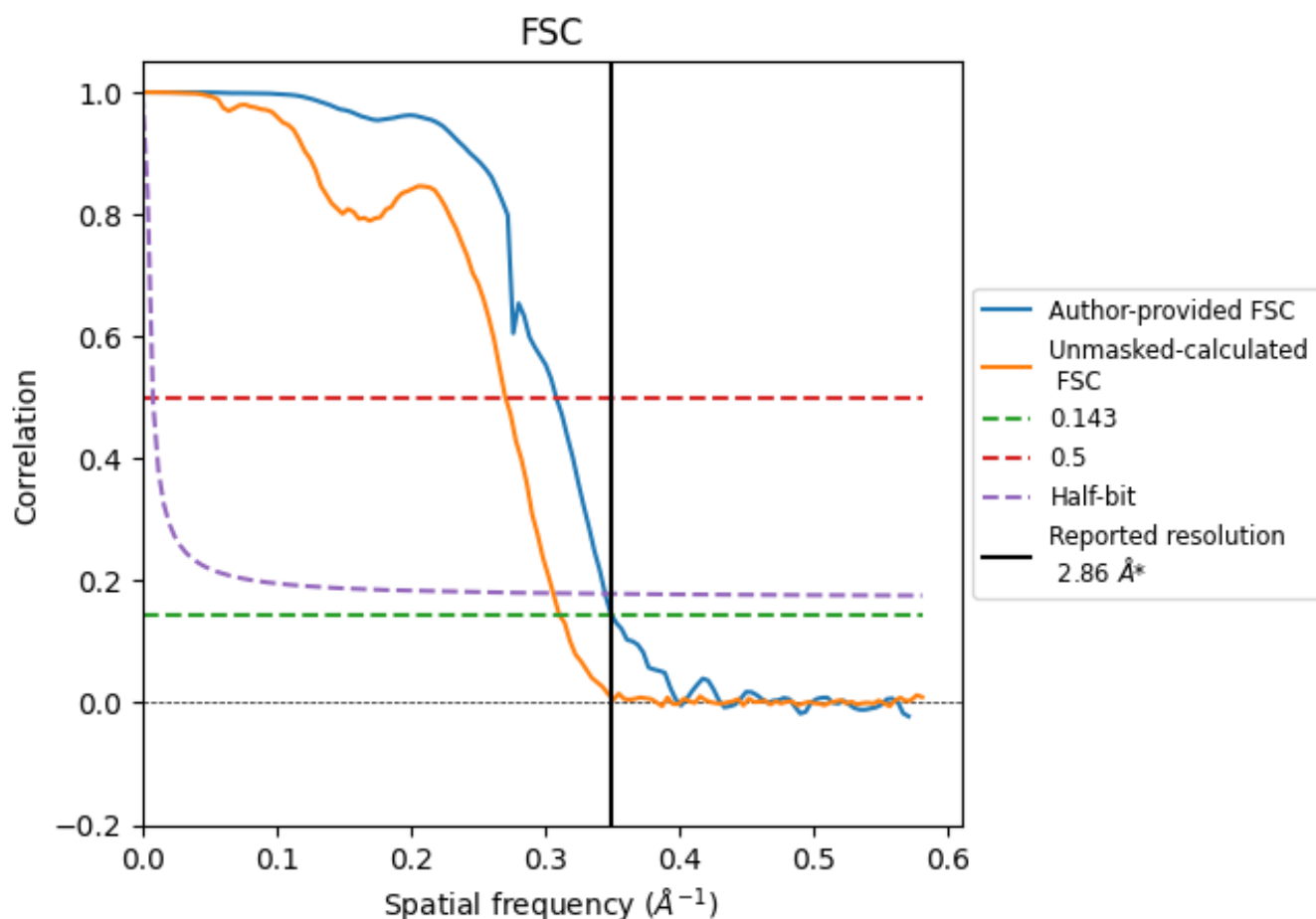


\*Reported resolution corresponds to spatial frequency of 0.350  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.350 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

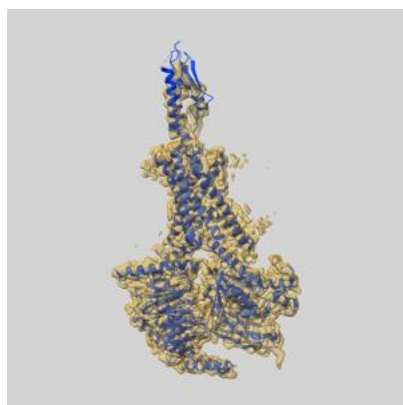
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.86	-	-
Author-provided FSC curve	2.86	3.24	2.90
Unmasked-calculated*	3.21	3.69	3.26

\*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 3.21 differs from the reported value 2.86 by more than 10 %

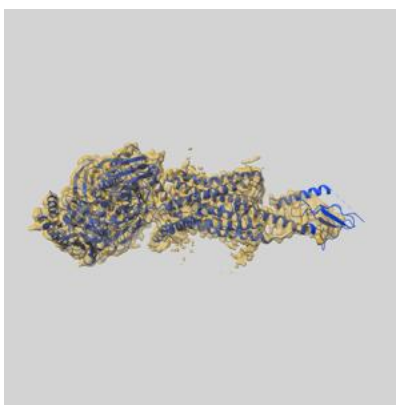
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-80238 and PDB model 25NX. Per-residue inclusion information can be found in section [3](#) on page [7](#).

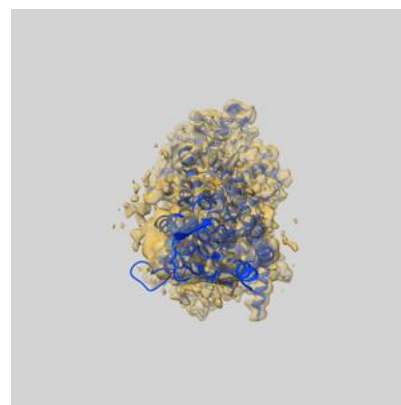
### 9.1 Map-model overlay [i](#)



X



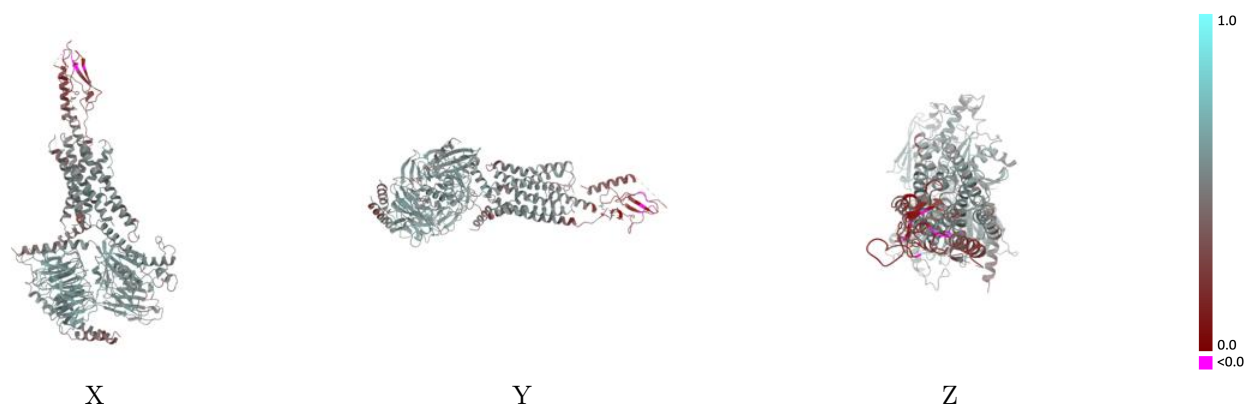
Y



Z

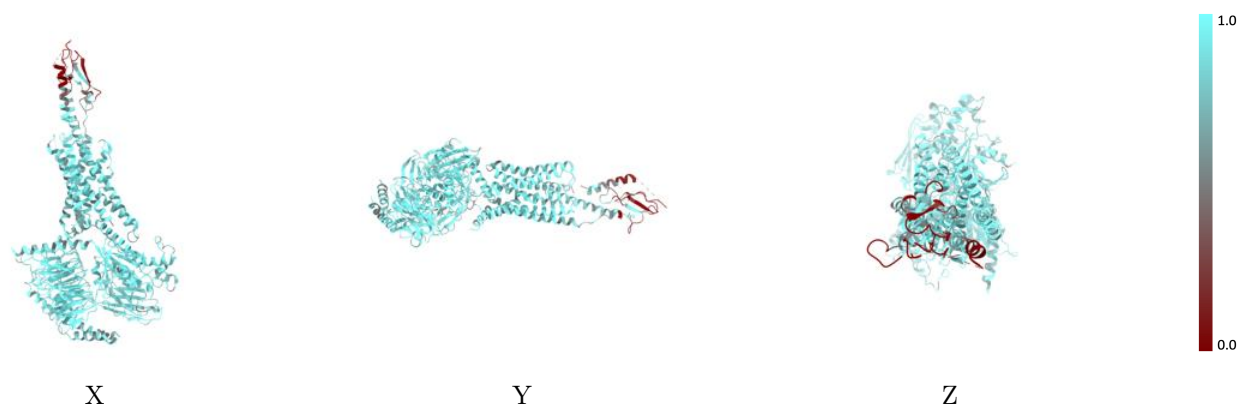
The images above show the 3D surface view of the map at the recommended contour level 0.16 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



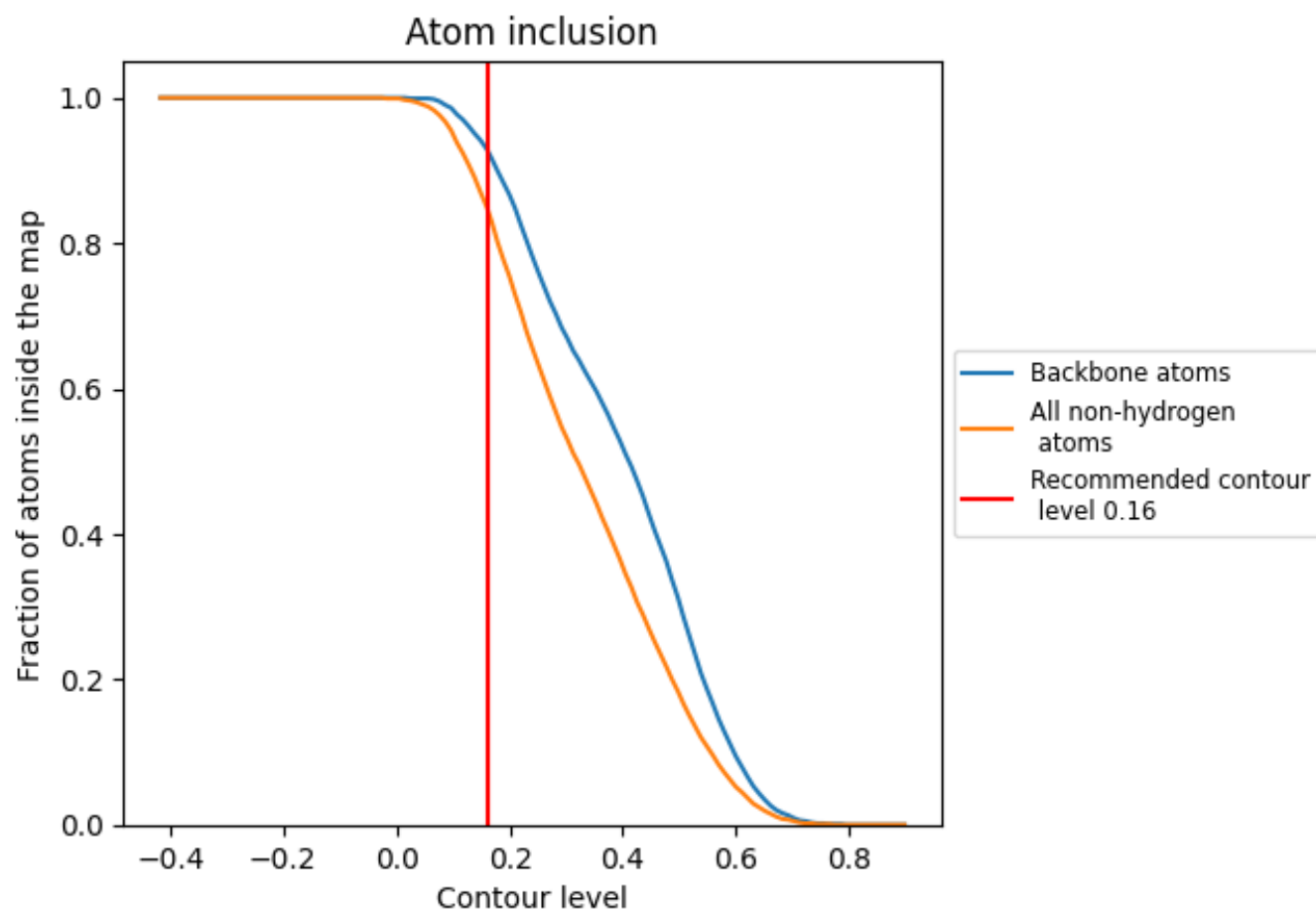
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.16) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8490	<div><div></div></div> 0.5010
A	<div><div></div></div> 0.8650	<div><div></div></div> 0.5220
B	<div><div></div></div> 0.9250	<div><div></div></div> 0.5590
G	<div><div></div></div> 0.8040	<div><div></div></div> 0.4710
N	<div><div></div></div> 0.9210	<div><div></div></div> 0.5580
P	<div><div></div></div> 0.7980	<div><div></div></div> 0.4100
R	<div><div></div></div> 0.7570	<div><div></div></div> 0.4310

1.0

0.0

<0.0