



## Full wwPDB EM Validation Report ⓘ

Oct 20, 2025 – 12:14 PM JST

PDB ID : 8ZMZ / pdb\_00008zmz  
EMDB ID : EMD-60263  
Title : Cryo-EM structure of R-eLACCO2 in the lactate-bound state  
Authors : Kamijo, Y.; Kusakizako, T.; Nureki, O.; Campbell, R.E.; Nasu, Y.  
Deposited on : 2024-05-24  
Resolution : 2.70 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.dev129  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

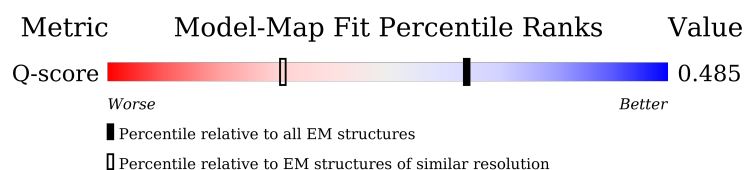
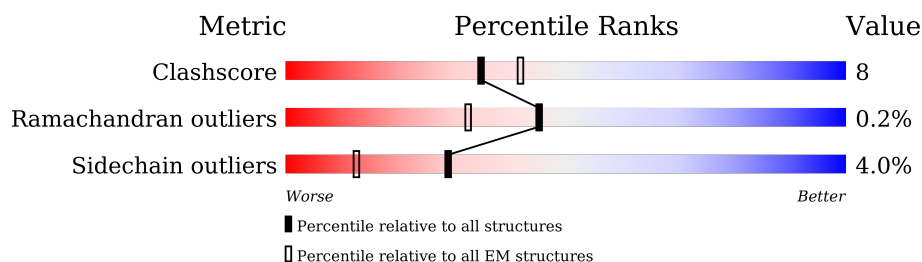
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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	620	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4425 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 Lactate-binding periplasmic protein TTHA0766, Red fluorescent protein drFP583.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	548	4418	2854	760	788	16	0	0

There are 131 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	MET	-	initiating methionine	UNP Q5SK82
A	-34	GLY	-	expression tag	UNP Q5SK82
A	-33	GLY	-	expression tag	UNP Q5SK82
A	-32	SER	-	expression tag	UNP Q5SK82
A	-31	HIS	-	expression tag	UNP Q5SK82
A	-30	HIS	-	expression tag	UNP Q5SK82
A	-29	HIS	-	expression tag	UNP Q5SK82
A	-28	HIS	-	expression tag	UNP Q5SK82
A	-27	HIS	-	expression tag	UNP Q5SK82
A	-26	HIS	-	expression tag	UNP Q5SK82
A	-25	GLY	-	expression tag	UNP Q5SK82
A	-24	MET	-	expression tag	UNP Q5SK82
A	-23	ALA	-	expression tag	UNP Q5SK82
A	-22	SER	-	expression tag	UNP Q5SK82
A	-21	MET	-	expression tag	UNP Q5SK82
A	-20	THR	-	expression tag	UNP Q5SK82
A	-19	GLY	-	expression tag	UNP Q5SK82
A	-18	GLY	-	expression tag	UNP Q5SK82
A	-17	GLN	-	expression tag	UNP Q5SK82
A	-16	GLN	-	expression tag	UNP Q5SK82
A	-15	MET	-	expression tag	UNP Q5SK82
A	-14	GLY	-	expression tag	UNP Q5SK82
A	-13	ARG	-	expression tag	UNP Q5SK82
A	-12	ASP	-	expression tag	UNP Q5SK82
A	-11	LEU	-	expression tag	UNP Q5SK82
A	-10	TYR	-	expression tag	UNP Q5SK82
A	-9	ASP	-	expression tag	UNP Q5SK82

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	ASP	-	expression tag	UNP Q5SK82
A	-7	ASP	-	expression tag	UNP Q5SK82
A	-6	ASP	-	expression tag	UNP Q5SK82
A	-5	LYS	-	expression tag	UNP Q5SK82
A	-4	ASP	-	expression tag	UNP Q5SK82
A	-3	PRO	-	expression tag	UNP Q5SK82
A	-2	SER	-	expression tag	UNP Q5SK82
A	-1	SER	-	expression tag	UNP Q5SK82
A	0	ARG	-	expression tag	UNP Q5SK82
A	1	MET	-	expression tag	UNP Q5SK82
A	5	MET	LEU	engineered mutation	UNP Q5SK82
A	14	LYS	ARG	engineered mutation	UNP Q5SK82
A	51	LEU	PHE	engineered mutation	UNP Q5SK82
A	83	GLU	GLY	engineered mutation	UNP Q5SK82
A	116	ASN	ILE	engineered mutation	UNP Q5SK82
A	138	THR	ILE	engineered mutation	UNP Q5SK82
A	190	ALA	VAL	engineered mutation	UNP Q5SK82
A	191	VAL	ILE	engineered mutation	UNP Q5SK82
A	192	THR	-	linker	UNP Q5SK82
A	193	ALA	-	linker	UNP Q5SK82
A	194	VAL	SER	engineered mutation	UNP Q9U6Y8
A	195	SER	THR	engineered mutation	UNP Q9U6Y8
A	198	MET	LEU	engineered mutation	UNP Q9U6Y8
A	201	GLU	ARG	engineered mutation	UNP Q9U6Y8
A	204	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	207	SER	GLY	engineered mutation	UNP Q9U6Y8
A	210	LYS	HIS	engineered mutation	UNP Q9U6Y8
A	212	GLY	ALA	engineered mutation	UNP Q9U6Y8
A	214	ARG	LYS	engineered mutation	UNP Q9U6Y8
A	222	ALA	LEU	engineered mutation	UNP Q9U6Y8
A	223	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	224	VAL	GLU	engineered mutation	UNP Q9U6Y8
A	225	VAL	PHE	engineered mutation	UNP Q9U6Y8
A	227	THR	SER	engineered mutation	UNP Q9U6Y8
A	228	THR	ILE	engineered mutation	UNP Q9U6Y8
A	230	LYS	MET	engineered mutation	UNP Q9U6Y8
A	240	ALA	TYR	engineered mutation	UNP Q9U6Y8
A	242	VAL	TYR	engineered mutation	UNP Q9U6Y8
A	245	ILE	SER	engineered mutation	UNP Q9U6Y8
A	246	GLN	LYS	engineered mutation	UNP Q9U6Y8
A	250	VAL	THR	engineered mutation	UNP Q9U6Y8
A	262	CYS	TYR	engineered mutation	UNP Q9U6Y8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ALA	THR	engineered mutation	UNP Q9U6Y8
A	270	SER	-	linker	UNP Q9U6Y8
A	271	THR	-	linker	UNP Q9U6Y8
A	272	GLY	-	linker	UNP Q9U6Y8
A	273	GLY	-	linker	UNP Q9U6Y8
A	274	VAL	-	linker	UNP Q9U6Y8
A	275	VAL	-	linker	UNP Q9U6Y8
A	276	GLU	-	linker	UNP Q9U6Y8
A	277	LEU	-	linker	UNP Q9U6Y8
A	278	ASP	-	linker	UNP Q9U6Y8
A	279	LYS	-	linker	UNP Q9U6Y8
A	280	GLY	-	linker	UNP Q9U6Y8
A	281	GLY	-	linker	UNP Q9U6Y8
A	282	THR	-	linker	UNP Q9U6Y8
A	283	GLY	-	linker	UNP Q9U6Y8
A	284	GLY	-	linker	UNP Q9U6Y8
A	285	SER	-	linker	UNP Q9U6Y8
A	286	LEU	-	linker	UNP Q9U6Y8
A	287	VAL	-	linker	UNP Q9U6Y8
A	288	SER	-	linker	UNP Q9U6Y8
A	289	LYS	-	linker	UNP Q9U6Y8
A	290	GLY	-	linker	UNP Q9U6Y8
A	291	GLU	-	linker	UNP Q9U6Y8
A	292	GLU	-	linker	UNP Q9U6Y8
A	293	ASP	-	linker	UNP Q9U6Y8
A	294	ASP	-	linker	UNP Q9U6Y8
A	295	MET	-	linker	UNP Q9U6Y8
A	296	ALA	-	linker	UNP Q9U6Y8
A	297	ILE	-	linker	UNP Q9U6Y8
A	298	VAL	ILE	engineered mutation	UNP Q9U6Y8
A	307	HIS	ARG	engineered mutation	UNP Q9U6Y8
A	311	SER	THR	engineered mutation	UNP Q9U6Y8
A	330	ALA	GLY	engineered mutation	UNP Q9U6Y8
A	331	PHE	HIS	engineered mutation	UNP Q9U6Y8
A	332	GLN	ASN	engineered mutation	UNP Q9U6Y8
A	334	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	357	NRQ	GLN	chromophore	UNP Q9U6Y8
A	357	NRQ	TYR	chromophore	UNP Q9U6Y8
A	357	NRQ	GLY	chromophore	UNP Q9U6Y8
A	361	ALA	VAL	engineered mutation	UNP Q9U6Y8
A	363	ILE	VAL	engineered mutation	UNP Q9U6Y8
A	373	PHE	LYS	engineered mutation	UNP Q9U6Y8

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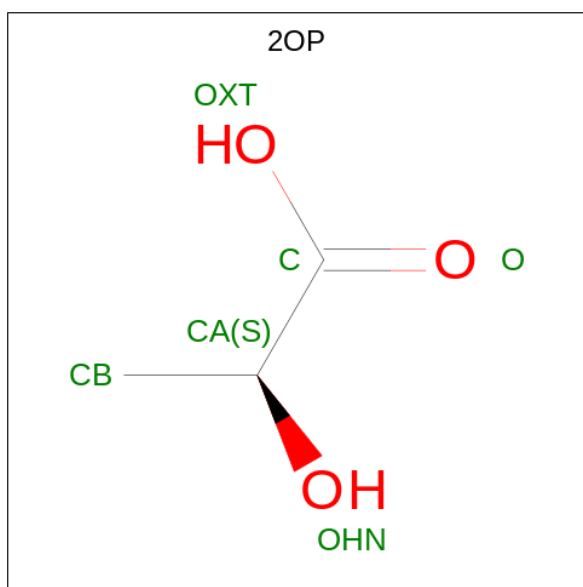
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Chain	Residue	Modelled	Actual	Comment	Reference
A	382	ARG	LYS	engineered mutation	UNP Q9U6Y8
A	388	TYR	ASN	engineered mutation	UNP Q9U6Y8
A	394	ILE	VAL	engineered mutation	UNP Q9U6Y8
A	395	ILE	VAL	engineered mutation	UNP Q9U6Y8
A	396	HIS	THR	engineered mutation	UNP Q9U6Y8
A	398	ASP	THR	engineered mutation	UNP Q9U6Y8
A	407	VAL	CYS	engineered mutation	UNP Q9U6Y8
A	414	LEU	PHE	engineered mutation	UNP Q9U6Y8
A	415	ARG	ILE	engineered mutation	UNP Q9U6Y8
A	417	THR	VAL	engineered mutation	UNP Q9U6Y8
A	421	PRO	SER	engineered mutation	UNP Q9U6Y8
A	434	GLU	-	linker	UNP Q9U6Y8
A	435	ARG	-	linker	UNP Q9U6Y8
A	436	GLY	-	linker	UNP Q9U6Y8
A	437	ARG	-	linker	UNP Q9U6Y8
A	438	SER	ASP	engineered mutation	UNP Q5SK82
A	456	GLU	VAL	engineered mutation	UNP Q5SK82
A	534	GLY	SER	engineered mutation	UNP Q5SK82
A	571	ARG	LYS	engineered mutation	UNP Q5SK82
A	575	HIS	TYR	engineered mutation	UNP Q5SK82

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Ca 1 1	0

- Molecule 3 is (2S)-2-HYDROXYPROPANOIC ACID (CCD ID: 2OP) (formula: C<sub>3</sub>H<sub>6</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
3	A	1	6	3	3	0





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	146454	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.262	Depositor
Minimum map value	-0.135	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	298.8, 298.8, 298.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: NRQ, ZOP, CA

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	0.63	0/4519	1.00	6/6114 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	431	MET	CB-CA-C	-6.13	101.99	111.74
1	A	184	PRO	N-CA-C	-5.93	105.29	113.53
1	A	329	GLU	N-CA-C	-5.57	106.49	113.28
1	A	42	THR	CB-CA-C	-5.41	101.34	110.64
1	A	518	GLU	CB-CG-CD	5.38	121.75	112.60
1	A	580	GLU	N-CA-C	-5.17	105.77	111.71

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	4418	0	4337	68	0
2	A	1	0	0	0	0
3	A	6	0	4	0	0
All	All	4425	0	4341	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (68) 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:51:LEU:HD13	1:A:56:VAL:CG2	1.81	1.09
1:A:155:LYS:HE3	1:A:175:VAL:HG13	1.46	0.97
1:A:51:LEU:HD13	1:A:56:VAL:HG21	1.54	0.90
1:A:155:LYS:CE	1:A:175:VAL:HG13	2.08	0.82
1:A:194:VAL:CG1	1:A:211:LYS:HE2	2.09	0.82
1:A:155:LYS:HE3	1:A:175:VAL:CG1	2.10	0.82
1:A:194:VAL:HG13	1:A:211:LYS:HE2	1.62	0.81
1:A:51:LEU:CD1	1:A:56:VAL:HG21	2.10	0.81
1:A:51:LEU:HD13	1:A:56:VAL:HG23	1.59	0.80
1:A:155:LYS:CE	1:A:175:VAL:CG1	2.63	0.76
1:A:307:HIS:ND1	1:A:320:GLU:OE1	2.17	0.75
1:A:38:VAL:O	1:A:42:THR:HG23	1.88	0.74
1:A:213:LEU:HD12	1:A:432:GLY:O	1.97	0.64
1:A:215:LEU:HD11	1:A:221:TYR:HB2	1.80	0.63
1:A:152:LYS:NZ	1:A:390:GLU:OE2	2.32	0.63
1:A:326:ARG:O	1:A:330:ALA:N	2.33	0.61
1:A:216:LYS:HA	1:A:431:MET:HE2	1.81	0.60
1:A:155:LYS:HE2	1:A:175:VAL:CG1	2.31	0.60
1:A:214:ARG:O	1:A:431:MET:N	2.34	0.59
1:A:550:PHE:O	1:A:554:LYS:HG3	2.04	0.58
1:A:194:VAL:HG21	1:A:436:GLY:CA	2.34	0.57
1:A:196:GLU:CB	1:A:209:ILE:HG12	2.35	0.56
1:A:51:LEU:CD1	1:A:56:VAL:CG2	2.65	0.56
1:A:196:GLU:HB2	1:A:209:ILE:HG12	1.87	0.56
1:A:262:CYS:HB3	1:A:333:THR:HG23	1.89	0.55
1:A:229:TYR:OH	1:A:360:LYS:HE2	2.09	0.53
1:A:194:VAL:HG12	1:A:211:LYS:HE2	1.87	0.53
1:A:155:LYS:HE2	1:A:175:VAL:HG11	1.90	0.52
1:A:183:TYR:N	1:A:184:PRO:HD2	2.25	0.52
1:A:320:GLU:HG3	1:A:339:THR:HG21	1.90	0.52
1:A:332:GLN:HE22	1:A:359:SER:HB3	1.74	0.52
1:A:135:ASP:OD1	1:A:136:LEU:N	2.43	0.51
1:A:136:LEU:C	1:A:136:LEU:HD12	2.35	0.51
1:A:491:LYS:N	1:A:492:PRO:CD	2.74	0.50
1:A:576:VAL:HG11	1:A:581:LEU:HD21	1.94	0.50
1:A:132:VAL:HG13	1:A:505:SER:HA	1.94	0.50
1:A:198:MET:CE	1:A:205:LEU:HG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:O	1:A:35:THR:HG23	2.11	0.49
1:A:247:LEU:HD21	1:A:352:SER:HB2	1.94	0.49
1:A:581:LEU:HA	1:A:584:LEU:HD12	1.94	0.49
1:A:197:ARG:HG2	1:A:208:GLU:O	2.11	0.49
1:A:214:ARG:NH1	1:A:431:MET:HB2	2.27	0.49
1:A:217:ASP:OD1	1:A:217:ASP:C	2.56	0.48
1:A:34:PHE:HB2	1:A:504:TYR:CD1	2.49	0.48
1:A:196:GLU:HG2	1:A:243:VAL:HB	1.97	0.47
1:A:198:MET:HE2	1:A:205:LEU:HG	1.98	0.46
1:A:156:LEU:HA	1:A:439:ALA:O	2.15	0.46
1:A:35:THR:HG21	1:A:50:PRO:HB3	1.98	0.45
1:A:330:ALA:HB2	1:A:364:LYS:N	2.32	0.45
1:A:39:LYS:HG3	1:A:44:GLY:HA2	1.99	0.45
1:A:198:MET:HE2	1:A:205:LEU:CD2	2.48	0.44
1:A:198:MET:HE2	1:A:205:LEU:HD21	1.99	0.44
1:A:262:CYS:CB	1:A:333:THR:HG23	2.47	0.44
1:A:434:GLU:HG3	1:A:436:GLY:H	1.83	0.43
1:A:142:LYS:HB3	1:A:142:LYS:HE2	1.72	0.43
1:A:185:ALA:O	1:A:186:LEU:C	2.62	0.42
1:A:211:LYS:O	1:A:211:LYS:HG3	2.19	0.42
1:A:14:LYS:N	1:A:14:LYS:HD2	2.34	0.42
1:A:352:SER:N	1:A:353:PRO:CD	2.82	0.42
1:A:135:ASP:CG	1:A:136:LEU:N	2.77	0.42
1:A:567:LEU:HG	1:A:571:ARG:HD3	2.02	0.42
1:A:31:PHE:HE1	1:A:479:PHE:CZ	2.37	0.41
1:A:247:LEU:HD12	1:A:262:CYS:O	2.19	0.41
1:A:28:TYR:O	1:A:32:GLN:HG3	2.21	0.41
1:A:198:MET:HE2	1:A:205:LEU:CG	2.51	0.41
1:A:244:ASP:O	1:A:265:ALA:HA	2.21	0.41
1:A:214:ARG:HB2	1:A:431:MET:O	2.21	0.40
1:A:198:MET:HE3	1:A:206:LYS:O	2.21	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	541/620 (87%)	526 (97%)	14 (3%)	1 (0%)	44 68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	VAL

### 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	452/507 (89%)	434 (96%)	18 (4%)	27 55

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	33	LYS
1	A	83	GLU
1	A	142	LYS
1	A	155	LYS
1	A	158	VAL
1	A	186	LEU
1	A	197	ARG
1	A	246	GLN
1	A	260	GLU
1	A	263	GLU
1	A	329	GLU
1	A	333	THR
1	A	390	GLU
1	A	405	ASP
1	A	411	LYS
1	A	434	GLU
1	A	577	THR

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

Mol	Chain	Res	Type
1	A	75	ASN
1	A	116	ASN
1	A	418	ASN
1	A	484	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	NRQ	A	357	1	23,24,25	1.05	2 (8%)	23,32,34	2.29	4 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	A	357	1	-	4/9/31/32	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	357	NRQ	CA2-C2	-2.76	1.45	1.48
1	A	357	NRQ	C1-N2	2.29	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	NRQ	CA2-C2-N3	8.92	107.59	103.37
1	A	357	NRQ	O3-C3-CA3	-3.81	114.88	126.39
1	A	357	NRQ	O2-C2-CA2	-2.97	129.29	130.96
1	A	357	NRQ	CA3-N3-C1	2.47	133.05	128.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	357	NRQ	CA1-CB1-CG1-SD
1	A	357	NRQ	C1-CA1-CB1-CG1
1	A	357	NRQ	CB1-CG1-SD-CE
1	A	357	NRQ	C3-CA3-N3-C1

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
3	2OP	A	602	2	5,5,5	1.00	0	4,6,6	0.83	0

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
3	2OP	A	602	2	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

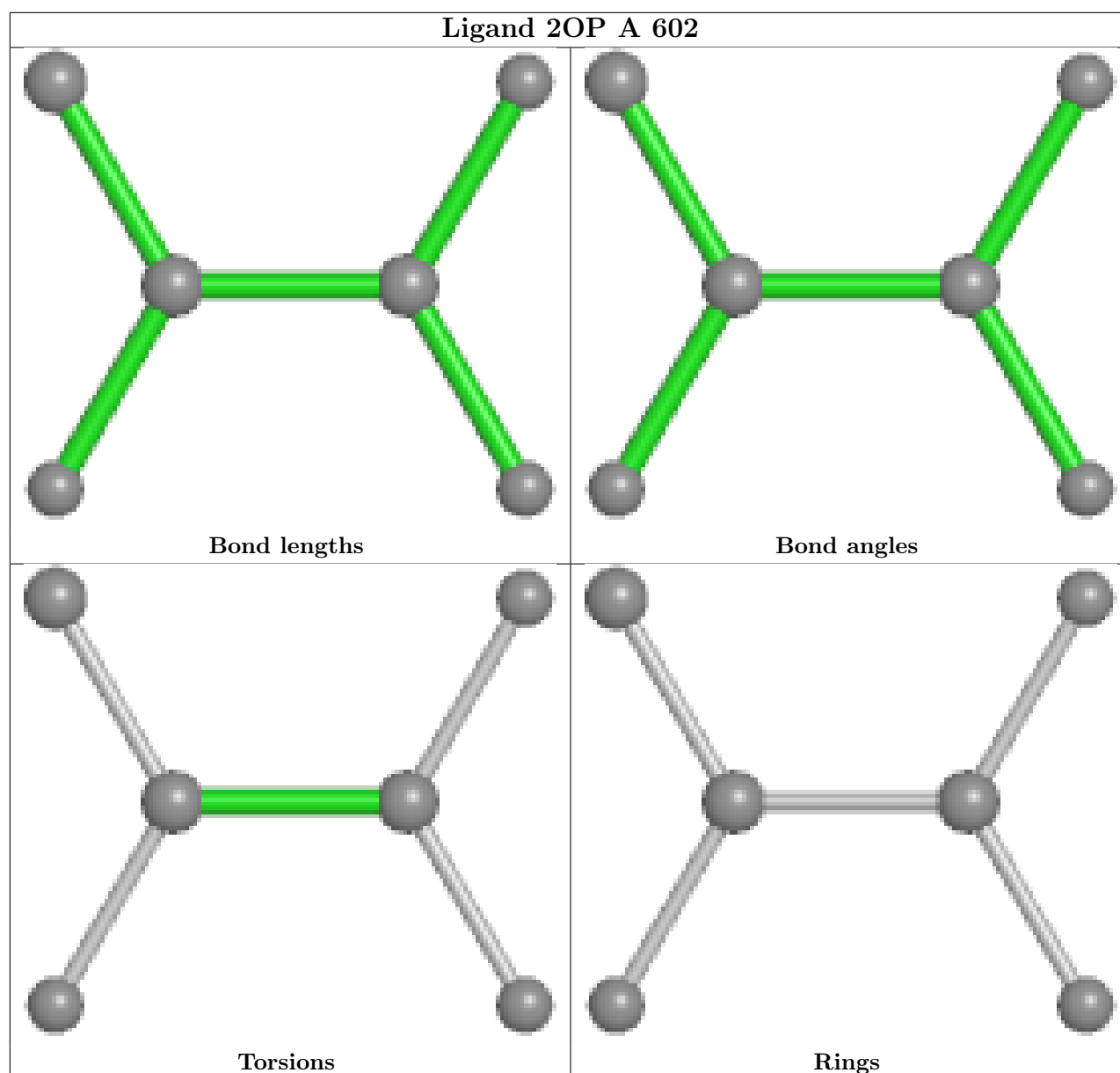
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

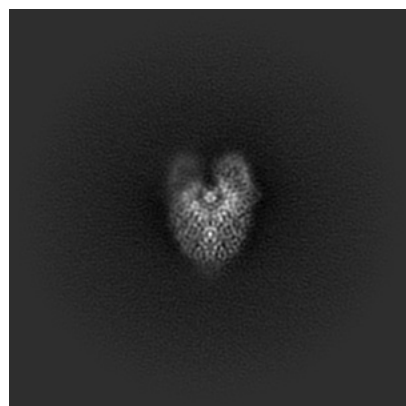
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60263. These allow visual inspection of the internal detail of the map and identification of artifacts.

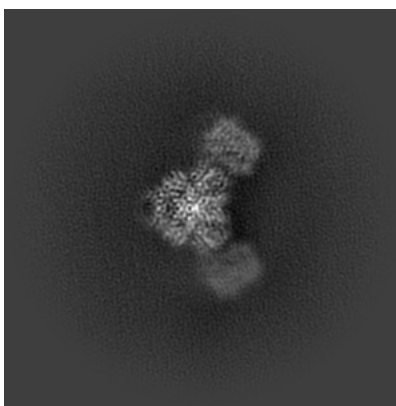
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

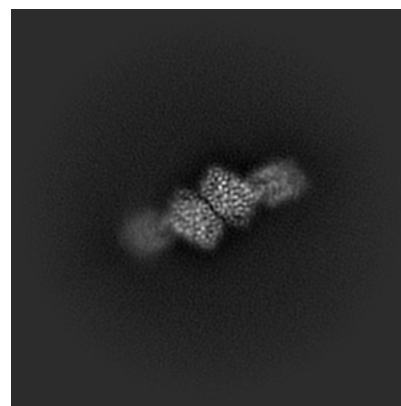
#### 6.1.1 Primary map



X

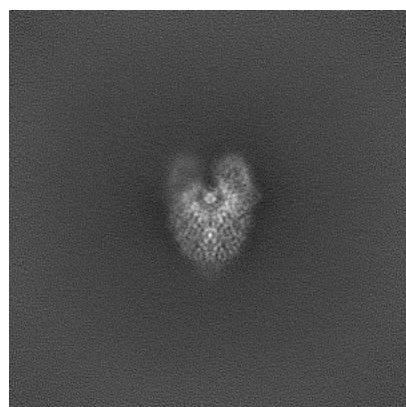


Y

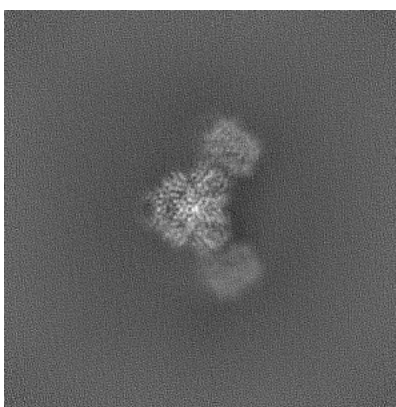


Z

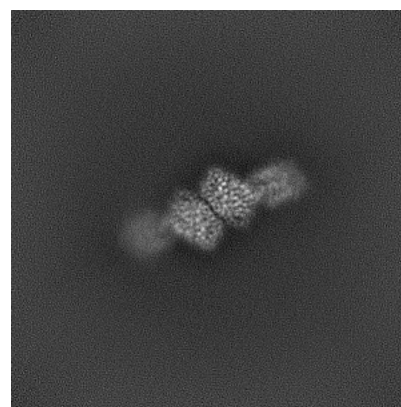
#### 6.1.2 Raw map



X



Y

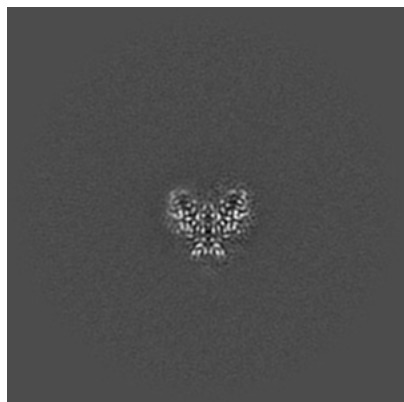


Z

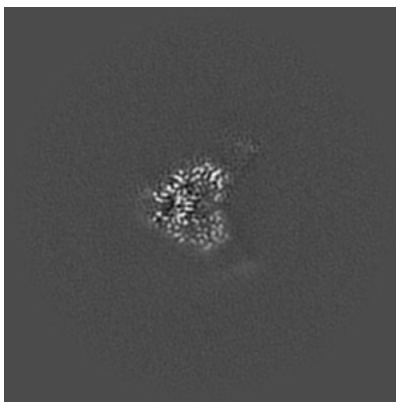
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

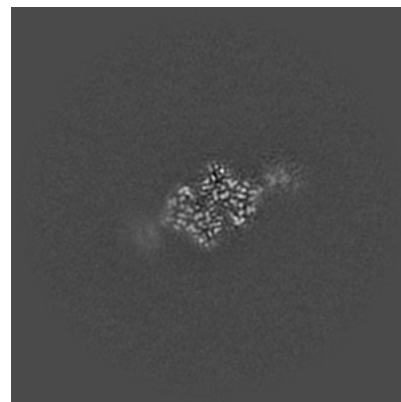
### 6.2.1 Primary map



X Index: 180

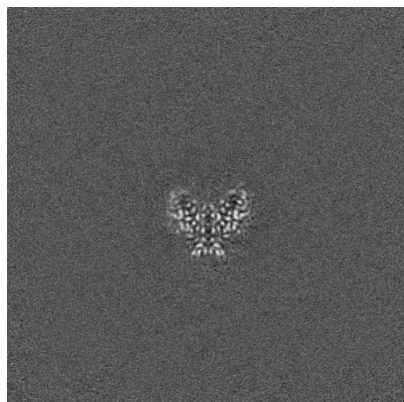


Y Index: 180

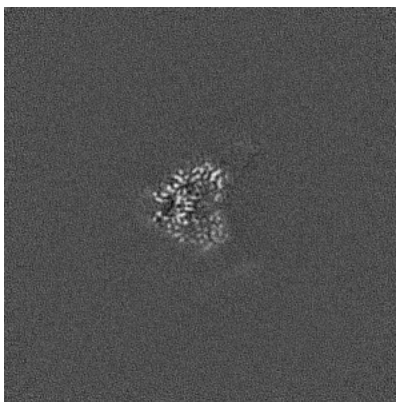


Z Index: 180

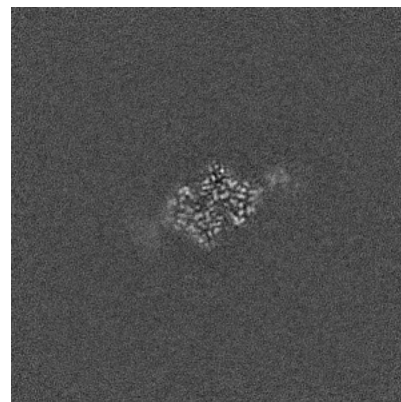
### 6.2.2 Raw map



X Index: 180



Y Index: 180

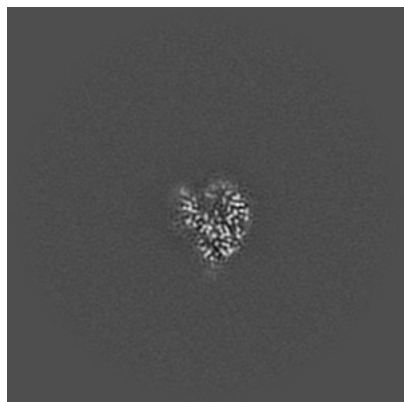


Z Index: 180

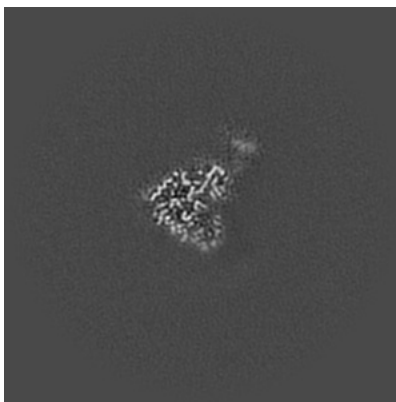
The images above show central slices of the map in three orthogonal directions.

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

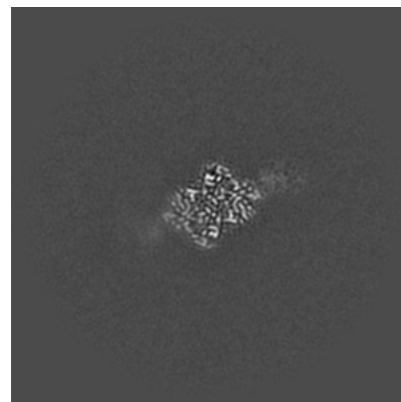
### 6.3.1 Primary map



X Index: 187

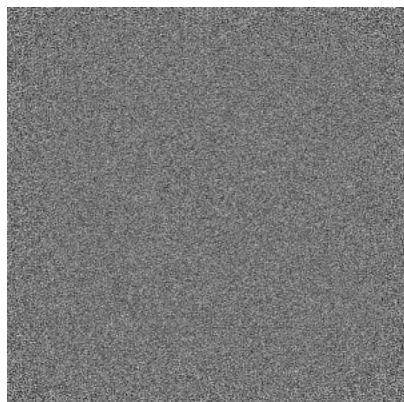


Y Index: 184

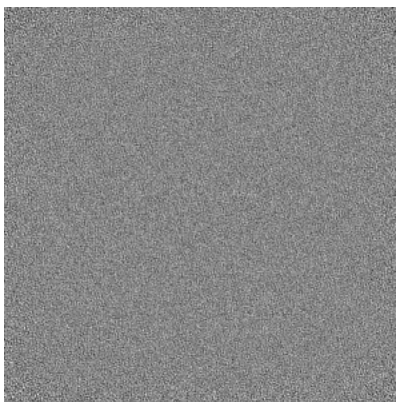


Z Index: 175

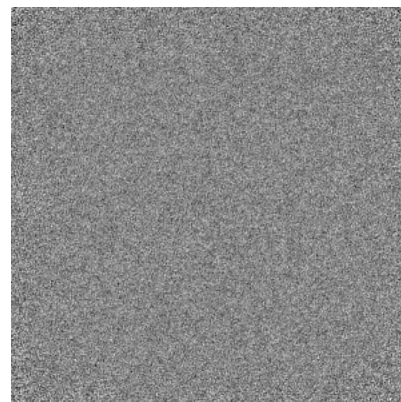
### 6.3.2 Raw map



X Index: 0



Y Index: 0



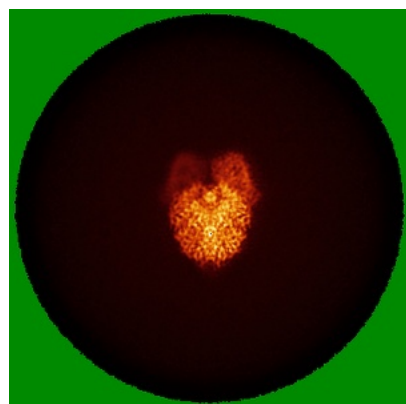
Z Index: 0

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

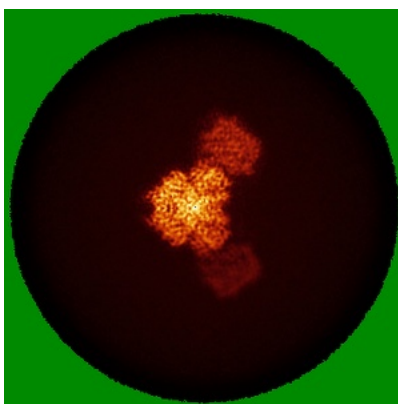


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

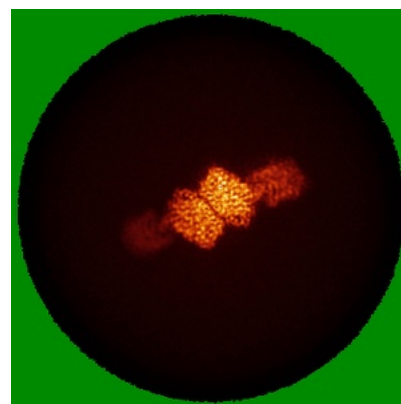
### 6.4.1 Primary map



X

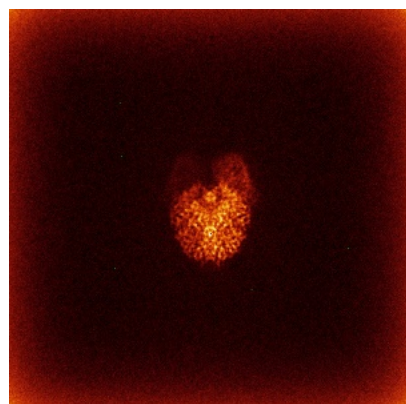


Y

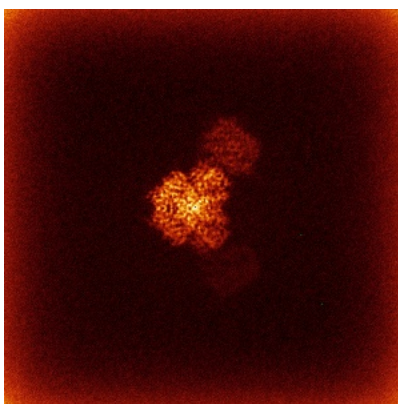


Z

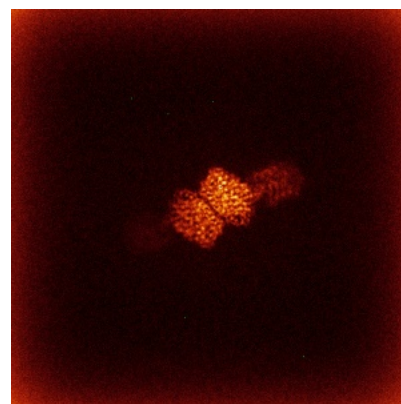
### 6.4.2 Raw map



X



Y

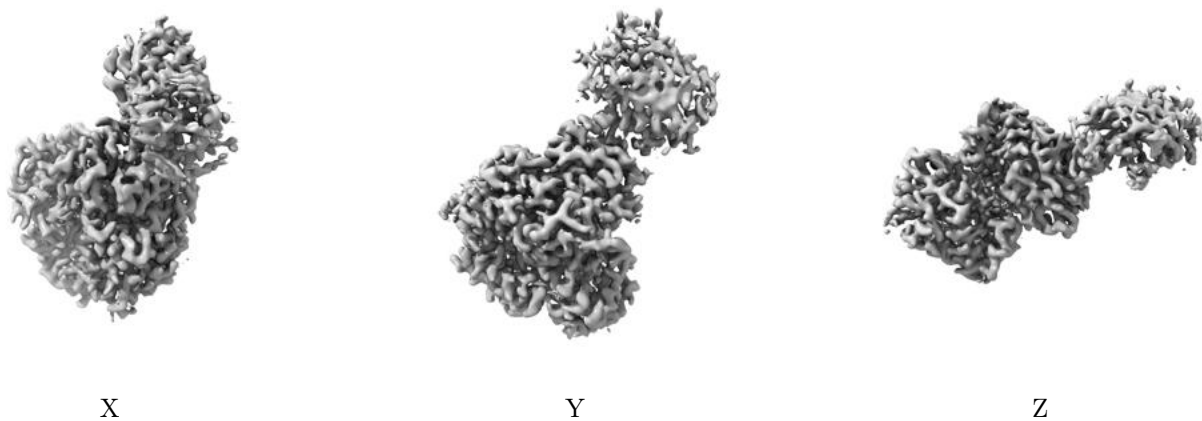


Z

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.

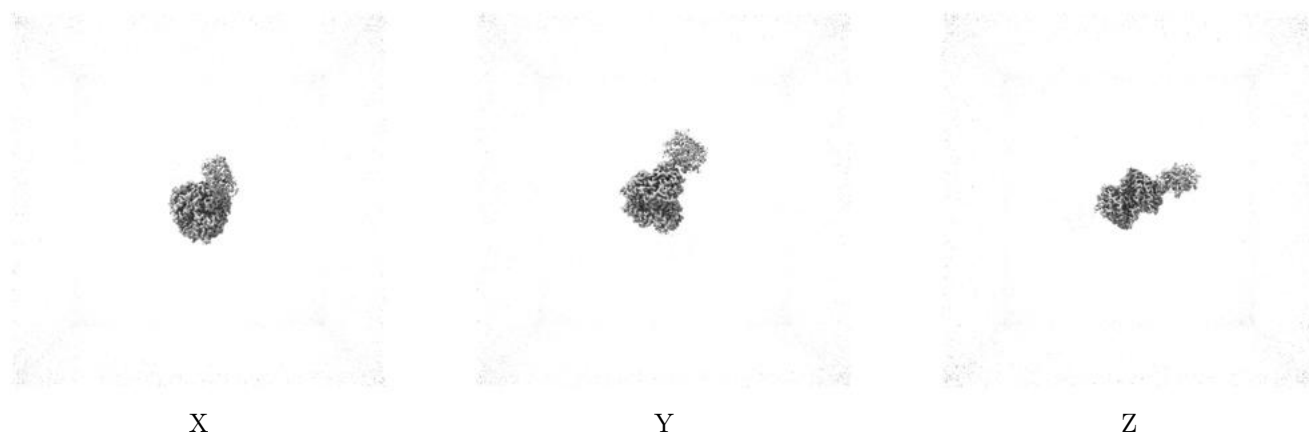
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

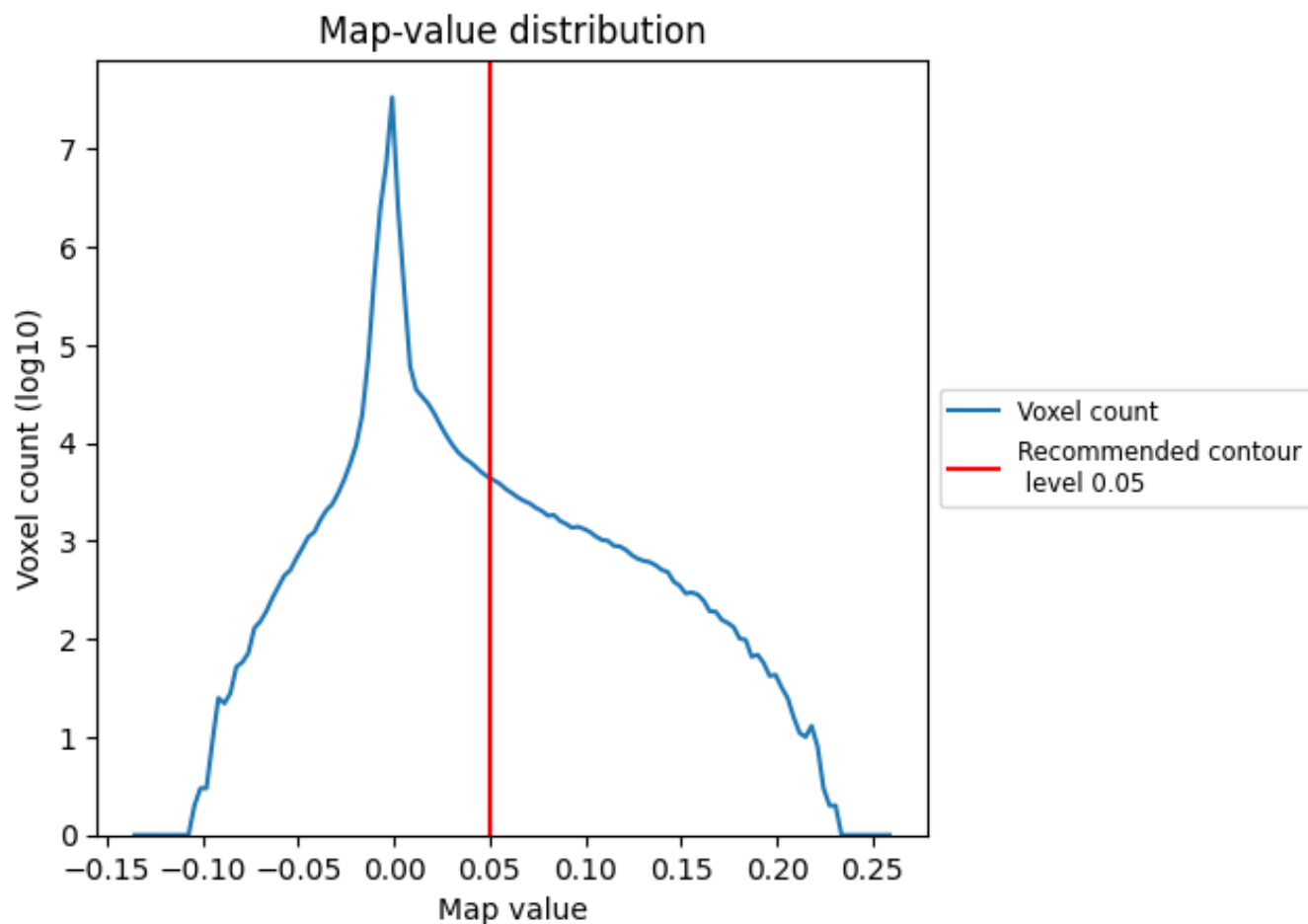
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

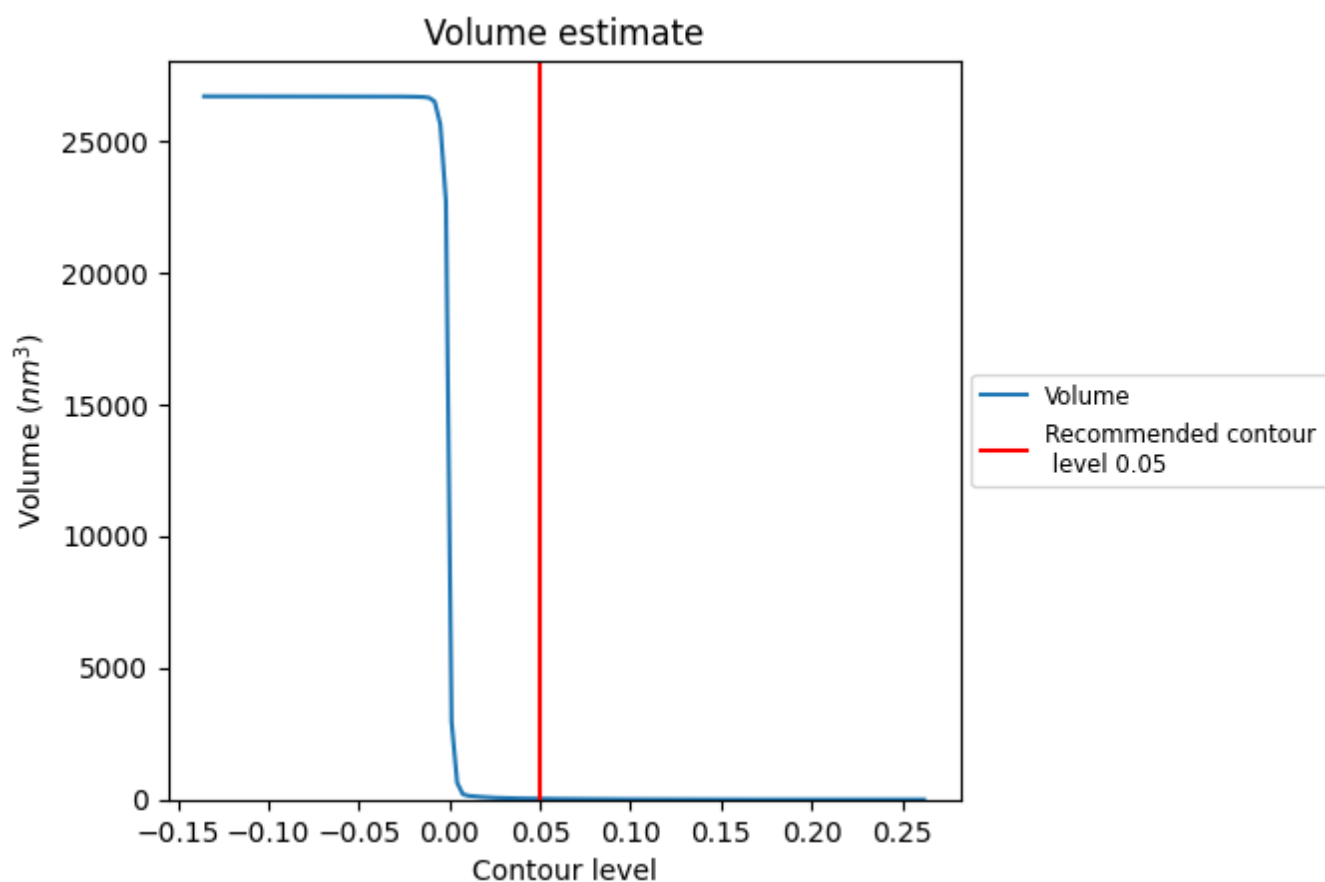
This section contains the results of statistical analysis of the map.

### 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](#)

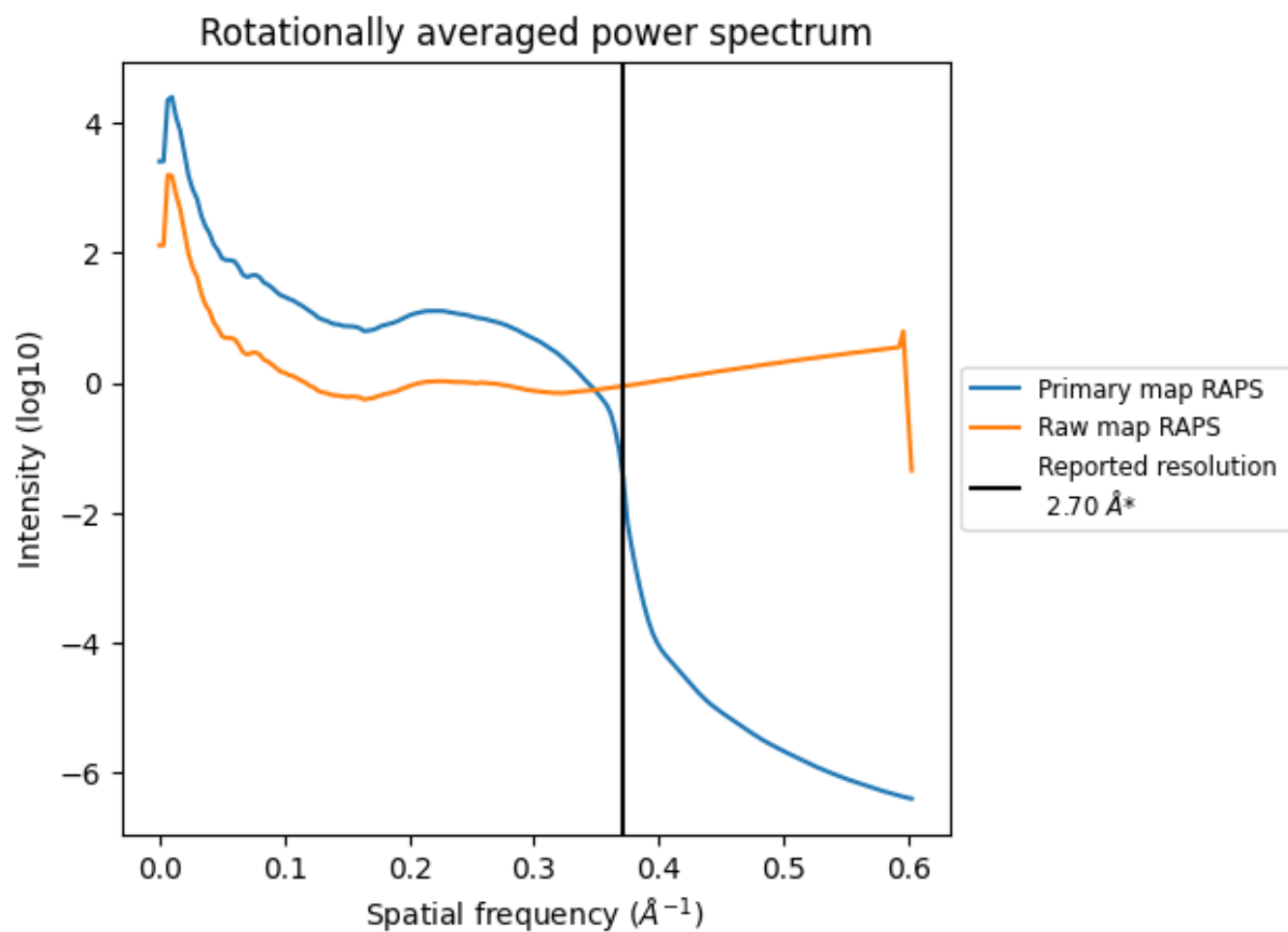


The volume at the recommended contour level is 31  $\text{nm}^3$ ; this corresponds to an approximate mass of 28 kDa.

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 ⓘ

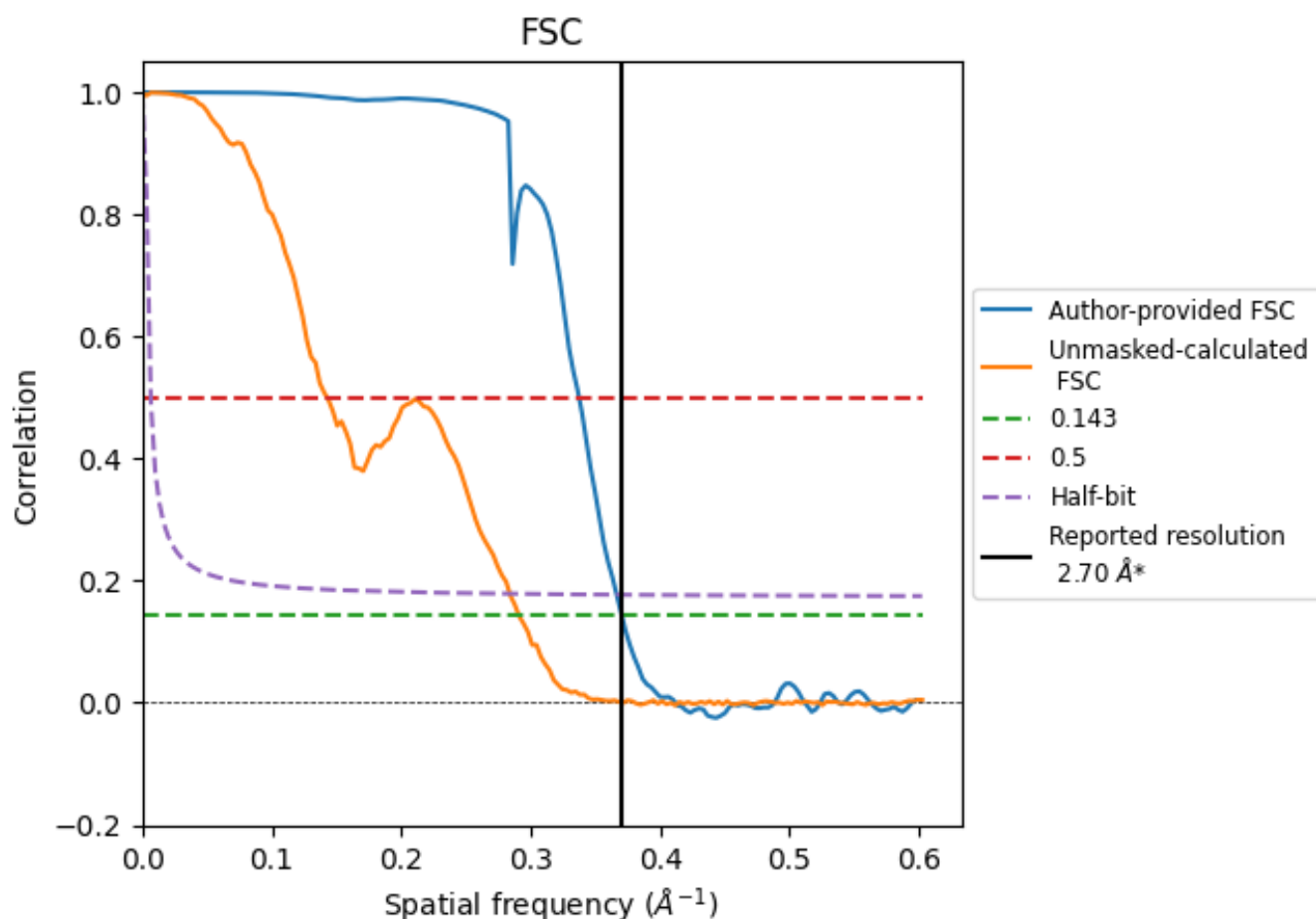


\*Reported resolution corresponds to spatial frequency of  $0.370 \text{ \AA}^{-1}$

## 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  $0.370 \text{ \AA}^{-1}$

## 8.2 Resolution estimates [i](#)

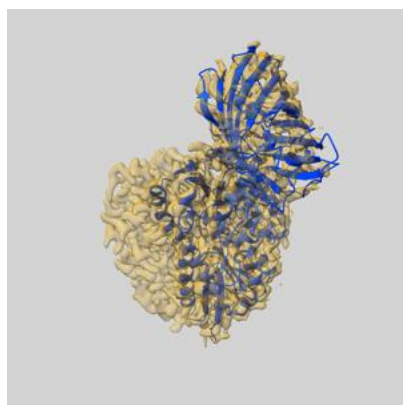
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	2.96	2.73
Unmasked-calculated*	3.44	7.00	3.52

\*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 3.44 differs from the reported value 2.7 by more than 10 %

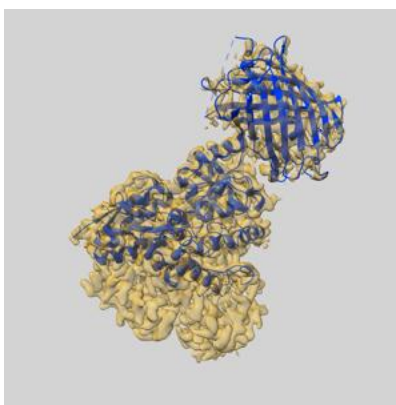
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60263 and PDB model 8ZMZ. Per-residue inclusion information can be found in section [3](#) on page [8](#).

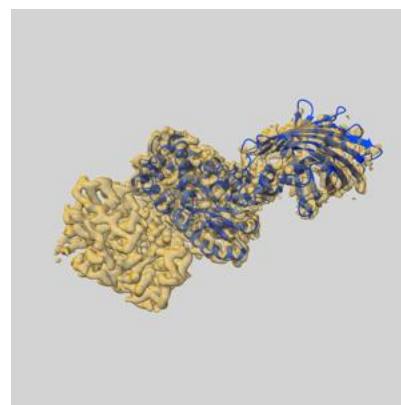
### 9.1 Map-model overlay [i](#)



X



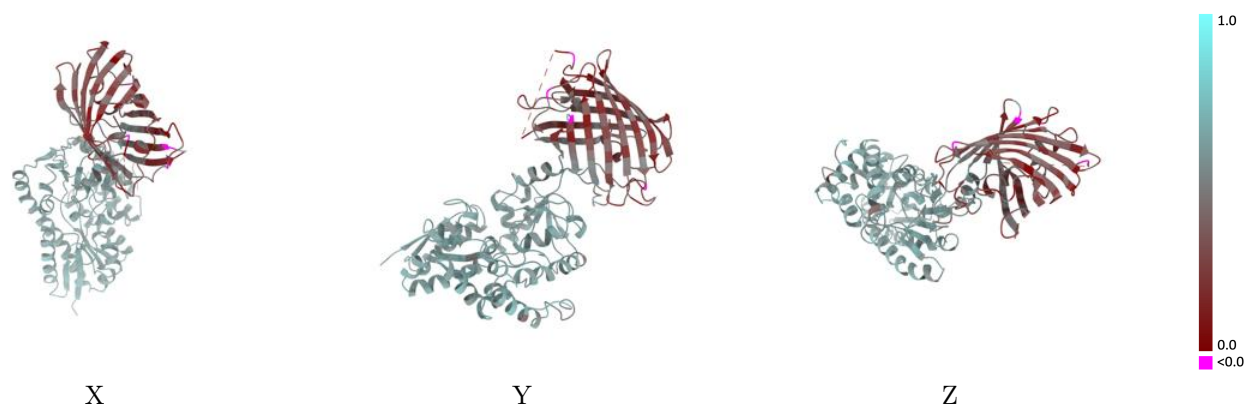
Y



Z

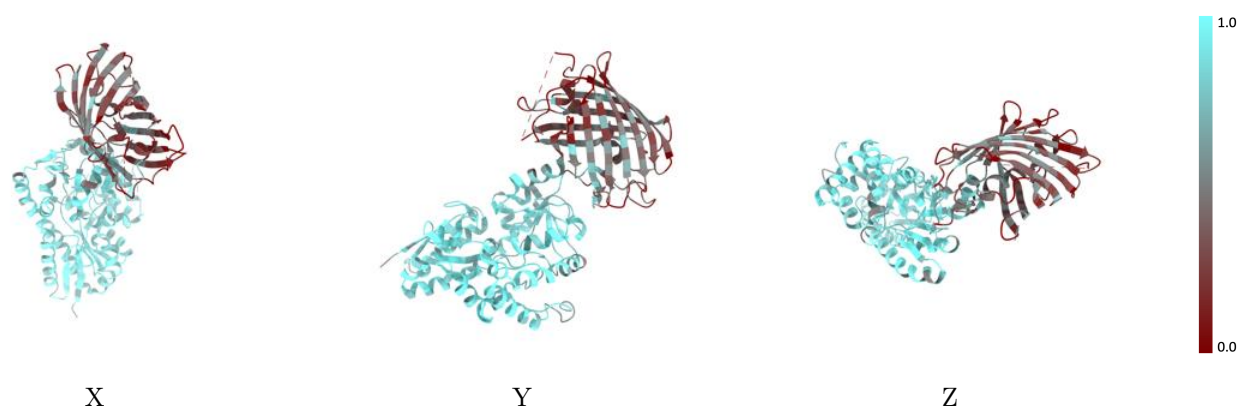
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



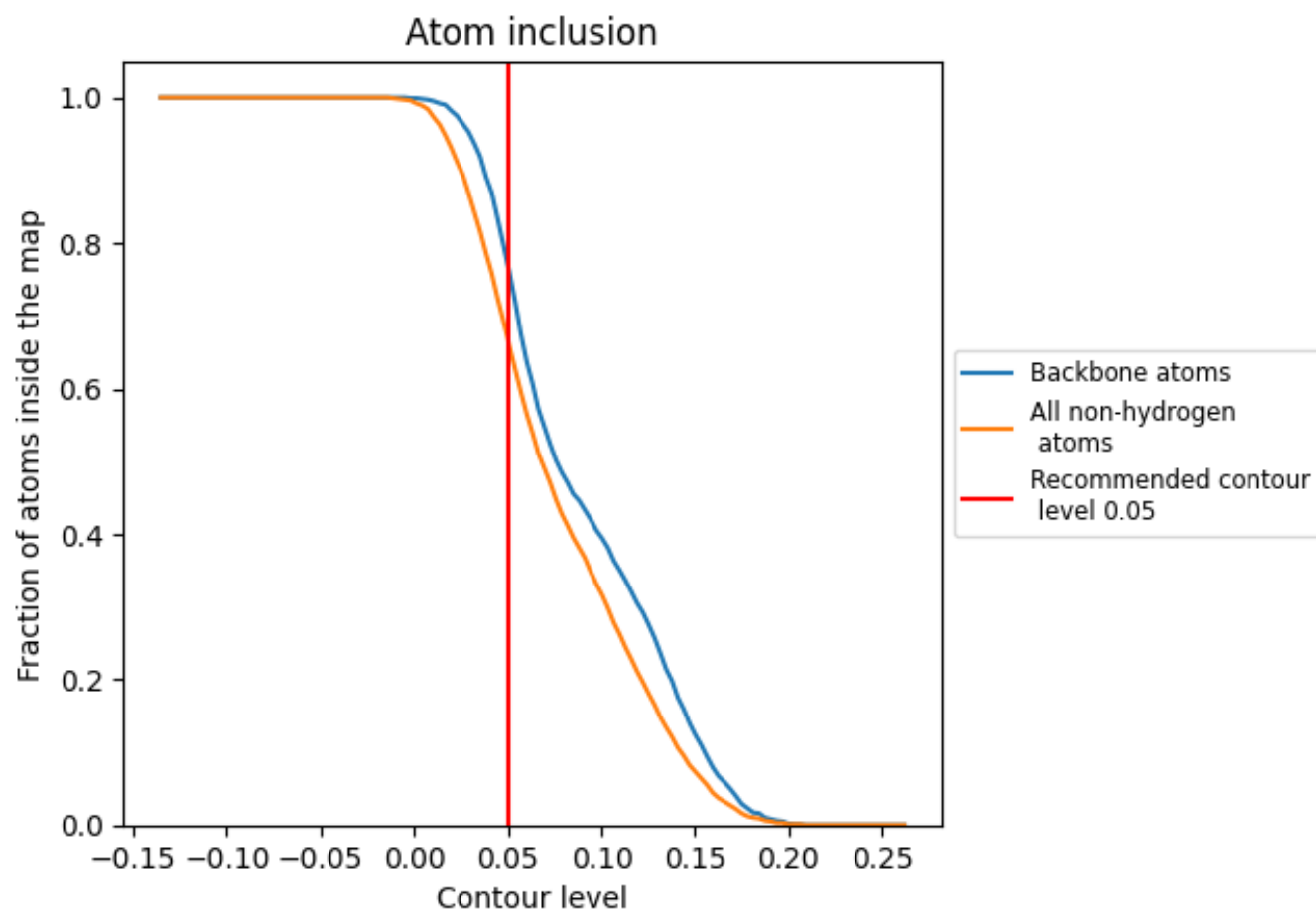
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6700	<div></div> 0.4850
A	<div></div> 0.6700	<div></div> 0.4850

