



wwPDB EM Validation Summary Report ⓘ

Apr 15, 2026 – 02:13 PM EDT

PDB ID : 9OXA / pdb_00009oxa
EMDB ID : EMD-70964
Title : CryoEM structure of Gi-coupled TAS2R43 with aristolochic acid I
Authors : Kim, Y.; Gumpfer, R.H.; Roth, B.L.
Deposited on : 2025-06-03
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

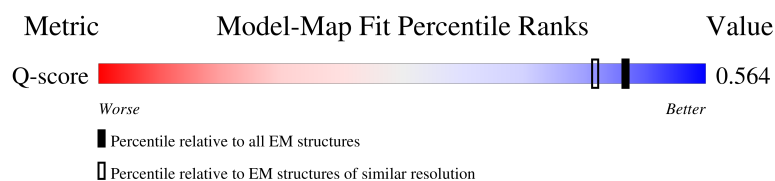
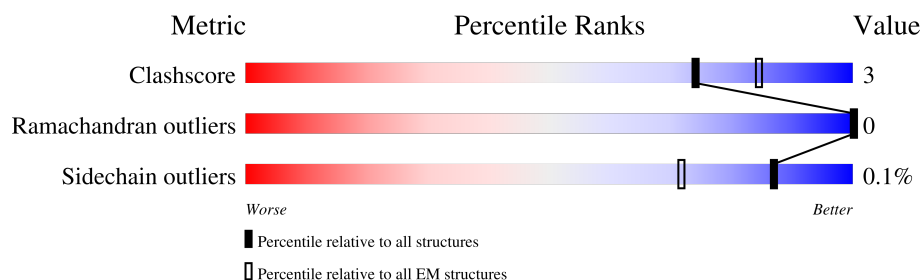
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	645	
2	B	402	
3	C	71	
4	A	354	

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Mol	Chain	Length	Quality of chain
5	D	267	 A horizontal bar chart showing the quality of chain D. The bar is divided into three segments: a green segment representing 76%, a yellow segment representing 11%, and a grey segment representing 13%. A small red dot is visible at the beginning of the green segment.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8645 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 Soluble cytochrome b562,Taste receptor type 2 member 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	284	Total	C	N	O	S	0	0
			2244	1511	360	359	14		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-150	ASP	-	expression tag	UNP P0ABE7
R	-149	TYR	-	expression tag	UNP P0ABE7
R	-148	LYS	-	expression tag	UNP P0ABE7
R	-147	ASP	-	expression tag	UNP P0ABE7
R	-146	ASP	-	expression tag	UNP P0ABE7
R	-145	ASP	-	expression tag	UNP P0ABE7
R	-144	ASP	-	expression tag	UNP P0ABE7
R	-143	ALA	-	expression tag	UNP P0ABE7
R	-142	LYS	-	expression tag	UNP P0ABE7
R	-141	LEU	-	expression tag	UNP P0ABE7
R	-140	GLN	-	expression tag	UNP P0ABE7
R	-139	THR	-	expression tag	UNP P0ABE7
R	-138	MET	-	expression tag	UNP P0ABE7
R	-137	HIS	-	expression tag	UNP P0ABE7
R	-136	HIS	-	expression tag	UNP P0ABE7
R	-135	HIS	-	expression tag	UNP P0ABE7
R	-134	HIS	-	expression tag	UNP P0ABE7
R	-133	HIS	-	expression tag	UNP P0ABE7
R	-132	HIS	-	expression tag	UNP P0ABE7
R	-131	HIS	-	expression tag	UNP P0ABE7
R	-130	HIS	-	expression tag	UNP P0ABE7
R	-129	HIS	-	expression tag	UNP P0ABE7
R	-128	HIS	-	expression tag	UNP P0ABE7
R	-127	GLU	-	expression tag	UNP P0ABE7
R	-126	ASN	-	expression tag	UNP P0ABE7
R	-125	LEU	-	expression tag	UNP P0ABE7
R	-124	TYR	-	expression tag	UNP P0ABE7
R	-123	PHE	-	expression tag	UNP P0ABE7

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-122	GLN	-	expression tag	UNP P0ABE7
R	-121	GLY	-	expression tag	UNP P0ABE7
R	-120	GLY	-	expression tag	UNP P0ABE7
R	-119	THR	-	expression tag	UNP P0ABE7
R	-118	THR	-	expression tag	UNP P0ABE7
R	-117	MET	-	expression tag	UNP P0ABE7
R	-110	TRP	MET	conflict	UNP P0ABE7
R	-15	ILE	HIS	conflict	UNP P0ABE7
R	-11	LEU	-	linker	UNP P0ABE7
R	-10	GLY	-	linker	UNP P0ABE7
R	-9	SER	-	linker	UNP P0ABE7
R	-8	THR	-	linker	UNP P0ABE7
R	-7	LEU	-	linker	UNP P0ABE7
R	-6	GLU	-	linker	UNP P0ABE7
R	-5	VAL	-	linker	UNP P0ABE7
R	-4	LEU	-	linker	UNP P0ABE7
R	-3	PHE	-	linker	UNP P0ABE7
R	-2	GLN	-	linker	UNP P0ABE7
R	-1	GLY	-	linker	UNP P0ABE7
R	0	PRO	-	linker	UNP P0ABE7

- 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
			2537	1569	452	495	21		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	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
B	341	GLY	-	expression tag	UNP P62873
B	342	GLY	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873
B	359	GLY	-	expression tag	UNP P62873
B	360	GLY	-	expression tag	UNP P62873
B	361	GLY	-	expression tag	UNP P62873
B	362	GLY	-	expression tag	UNP P62873
B	363	SER	-	expression tag	UNP P62873
B	364	GLY	-	expression tag	UNP P62873
B	365	GLY	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873
B	367	SER	-	expression tag	UNP P62873
B	368	SER	-	expression tag	UNP P62873
B	369	GLY	-	expression tag	UNP P62873
B	370	GLY	-	expression tag	UNP P62873
B	371	VAL	-	expression tag	UNP P62873
B	372	SER	-	expression tag	UNP P62873
B	373	GLY	-	expression tag	UNP P62873
B	374	TRP	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	375	ARG	-	expression tag	UNP P62873
B	376	LEU	-	expression tag	UNP P62873
B	377	PHE	-	expression tag	UNP P62873
B	378	LYS	-	expression tag	UNP P62873
B	379	LYS	-	expression tag	UNP P62873
B	380	ILE	-	expression tag	UNP P62873
B	381	SER	-	expression tag	UNP P62873
B	382	GLY	-	expression tag	UNP P62873
B	383	GLY	-	expression tag	UNP P62873
B	384	SER	-	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	53	Total	C	N	O	S	0	0
			382	242	65	72	3		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	218	Total	C	N	O	S	0	0
			1713	1097	288	315	13		

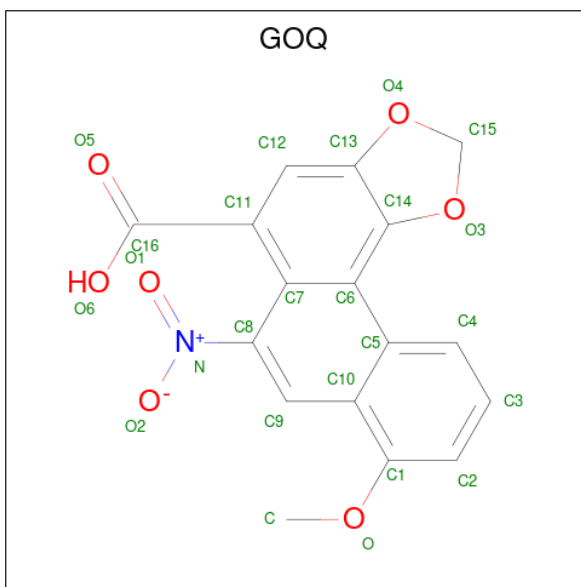
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	ASN	SER	engineered mutation	UNP P63096
A	203	ALA	GLY	engineered mutation	UNP P63096
A	245	ALA	GLU	engineered mutation	UNP P63096
A	326	SER	ALA	engineered mutation	UNP P63096

- Molecule 5 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	232	Total	C	N	O	S	0	0
			1737	1109	290	328	10		

- Molecule 6 is 8-methoxy-6-nitro-naphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (CCD ID: GOQ) (formula: C₁₇H₁₁NO₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			25	17	1	7	

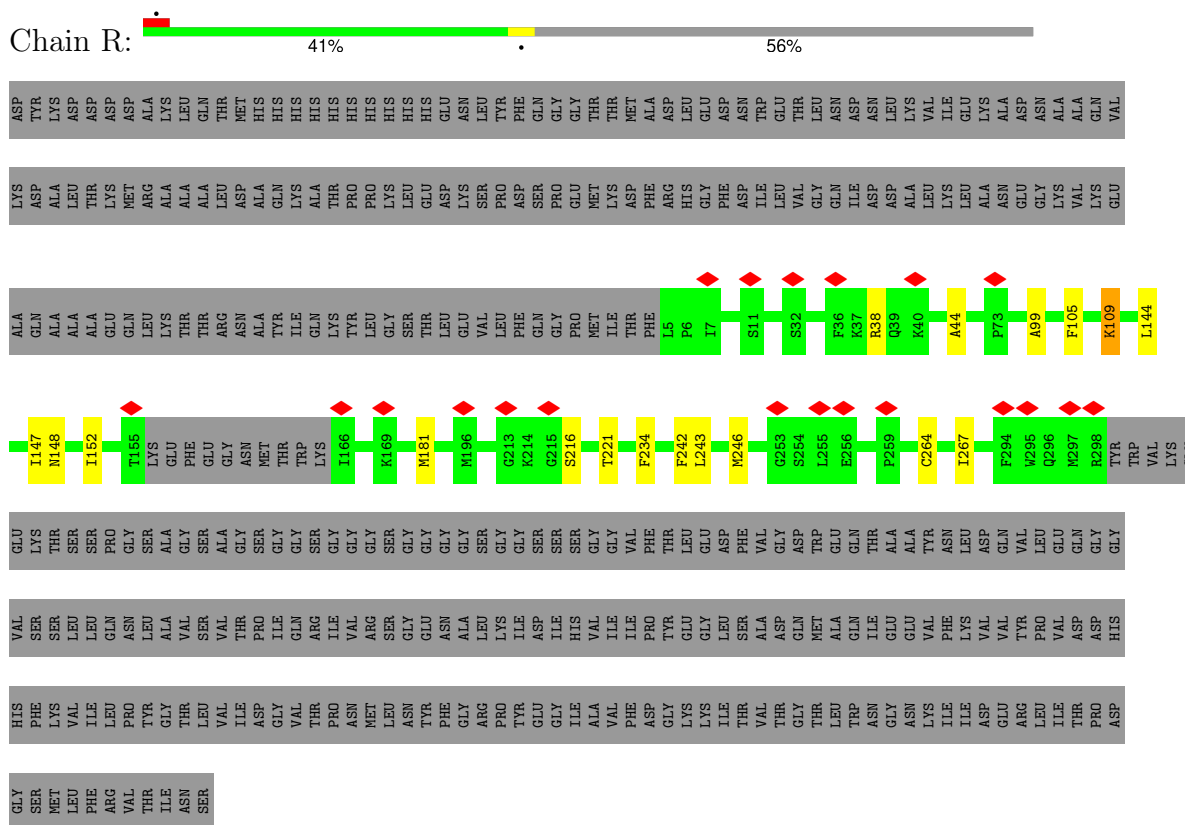
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	R	7	Total	O	0
			7	7	

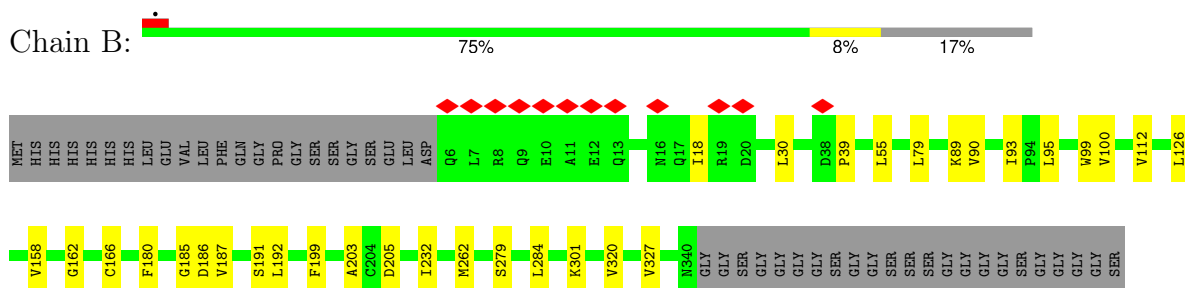
3 Residue-property plots

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: Soluble cytochrome b562, Taste receptor type 2 member 43




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



GLY
GLY
SER
SER
SER
GLY
GLY
VAL
SER
SER
TRP
ARG
LEU
PHE
LYS
LYS
ILE
SER
GLY
GLY
SER

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

Chain C: 

MET
ALA
CYS
ASN
ASN
THR
ALA
SER
ILE
A10
Q11
A12
R13
K14
L15
K20
M21
M24
R27
K62
GLU
LYS
LYS
PHE
PHE
CYS
ALA
ILE
LEU

- Molecule 4: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A: 


MET
GLY
CYS
THR
L5
I19
G27
K35
A41
G42
E43
S44
M47
T48
K51
Q52
M53
K54
ILE
ILE
HIS
GLU
ALA
ALA
TYR
SER
GLU
GLU
GLU
CYS
LYS
GLN
TYR
LYS
LYS
VAL
VAL
TYR
SER
ASN
THR
ILE
GLN
SER
ILE
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ALA
ILE
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ARG
ALA
MET
GLY
ARG

LEU
LYS
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ASP
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GLY
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ALA
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ALA
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ARG
D229
TRP
LYS
ASP
SER
GLY
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GLN
ALA
CYS
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ASN
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GLU
TYR
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ASP
LEU
ASP
ARG
ILE
ALA
GLN
PRO
ASN
TYR
ILE
PRO
THR
GLN
Gln
VAL
ASP
LEU
ARG
THR
VAL
LYS
THR
T182
G183
I184
V218
S228
D229
Y230
L234
ALA
GLU
ASP
GLU
M240
M243
E276
K277
I278
K279
K280
S281
T284
I285

A291
R294
T295
Q304
R313
T316
T321
C325
S326
T327
D328
T329
V332
D341
K345
K349
F354

- Molecule 5: scFv16

Chain D: 

ASP
V2
E6
C22
F27
A40
K43
V64
F68
S88
T91
S99
Y102
P107
T118
V119
S120
S121
GLY
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
GLY
S124
V137
T138
V143
L162
Y163
W164
Q167
P173
Q174

L175
L176
Y177
Y178
F200
Q219
Y223
P224
L225
T226
L233
E234
L235
ALA
ALA
ALA
LEU
VAL
GLU
PHE
GLN
GLY
PRO
HIS
HIS
HIS
HIS
HIS
HIS
HIS

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	583017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.672	Depositor
Minimum map value	-2.159	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	252.288, 252.288, 252.288	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	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: GOQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	R	0.16	0/2304	0.33	0/3136
2	B	0.15	0/2584	0.34	0/3510
3	C	0.11	0/388	0.23	0/528
4	A	0.13	0/1742	0.27	0/2342
5	D	0.14	0/1781	0.30	0/2421
All	All	0.14	0/8799	0.31	0/11937

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2244	0	2323	10	0
2	B	2537	0	2420	21	0
3	C	382	0	373	1	0
4	A	1713	0	1688	11	0
5	D	1737	0	1651	16	0
6	R	25	0	0	0	0
7	R	7	0	0	0	0
All	All	8645	0	8455	54	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 3.

The worst 5 of 54 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)
5:D:175:LEU:HD21	5:D:178:TYR:HB3	1.73	0.69
4:A:304:GLN:HG3	4:A:321:THR:HG21	1.81	0.63
5:D:40:ALA:HB3	5:D:43:LYS:HB2	1.81	0.62
4:A:53:MET:HG3	4:A:332:VAL:HG22	1.83	0.60
2:B:162:GLY:HA2	2:B:186:ASP:HB2	1.89	0.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	R	280/645 (43%)	277 (99%)	3 (1%)	0	100	100
2	B	333/402 (83%)	314 (94%)	19 (6%)	0	100	100
3	C	51/71 (72%)	51 (100%)	0	0	100	100
4	A	212/354 (60%)	206 (97%)	6 (3%)	0	100	100
5	D	228/267 (85%)	225 (99%)	3 (1%)	0	100	100
All	All	1104/1739 (64%)	1073 (97%)	31 (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	R	246/556 (44%)	245 (100%)	1 (0%)	84	94
2	B	270/319 (85%)	270 (100%)	0	100	100
3	C	37/58 (64%)	37 (100%)	0	100	100
4	A	182/305 (60%)	182 (100%)	0	100	100
5	D	183/216 (85%)	183 (100%)	0	100	100
All	All	918/1454 (63%)	917 (100%)	1 (0%)	87	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	109	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	333	GLN
4	A	269	ASN
4	A	22	ASN
2	B	295	ASN
4	A	244	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](#)

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

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	GOQ	R	501	-	28,28,28	0.96	2 (7%)	30,42,42	1.74	5 (16%)

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
6	GOQ	R	501	-	-	6/8/16/16	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	GOQ	O2-N	-2.13	1.21	1.35
6	R	501	GOQ	O6-C16	-2.00	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	501	GOQ	C8-C7-C6	-5.31	115.06	118.69
6	R	501	GOQ	C1-C10-C5	4.16	121.53	118.94
6	R	501	GOQ	C12-C11-C16	-3.14	112.37	117.67
6	R	501	GOQ	O5-C16-C11	-2.86	114.89	122.31
6	R	501	GOQ	O6-C16-O5	2.26	128.22	123.35

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	501	GOQ	C7-C8-N-O1

Continued on next page...

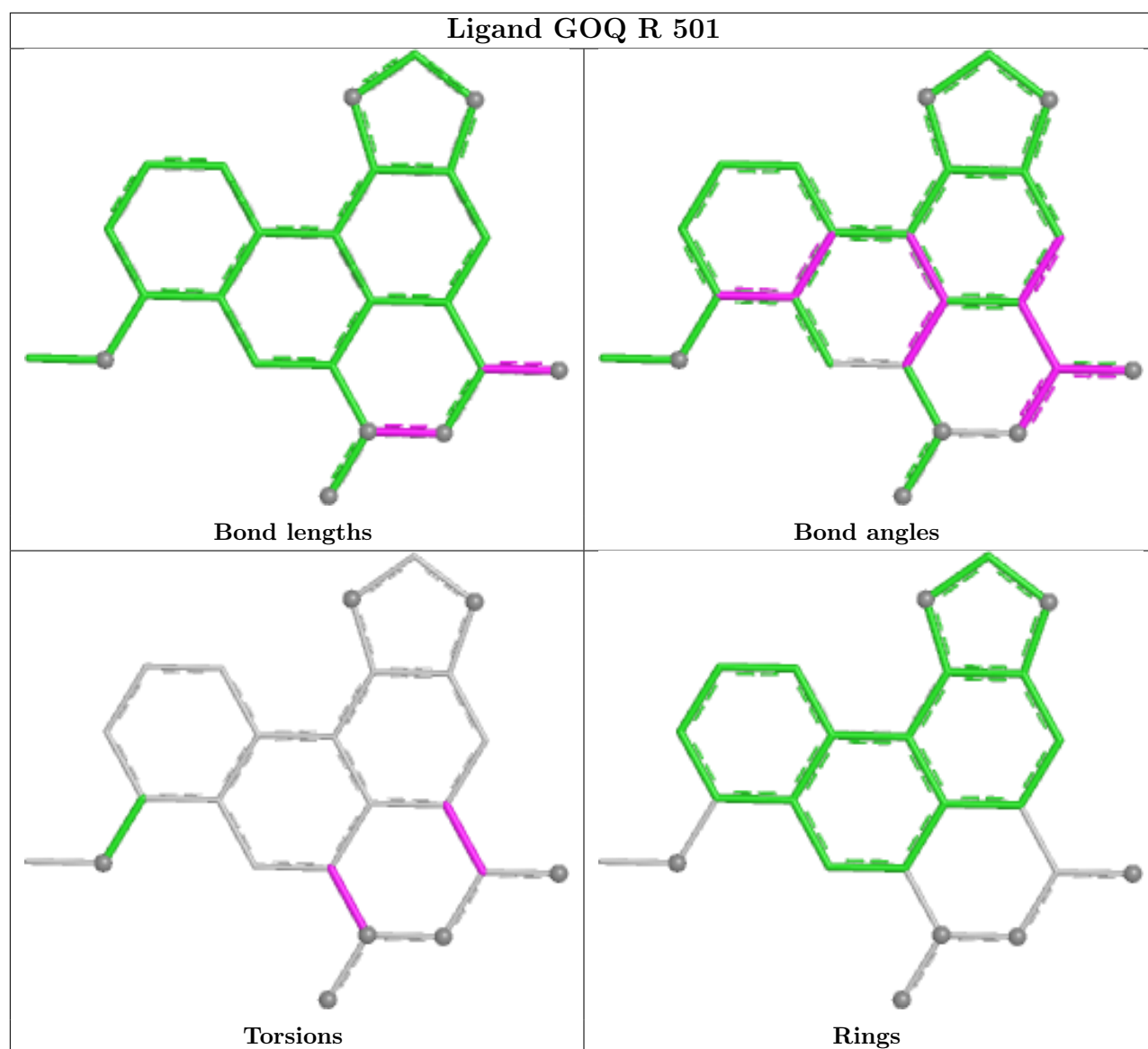
Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	R	501	GOQ	C9-C8-N-O1
6	R	501	GOQ	C12-C11-C16-O5
6	R	501	GOQ	C7-C11-C16-O5
6	R	501	GOQ	C7-C11-C16-O6

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.

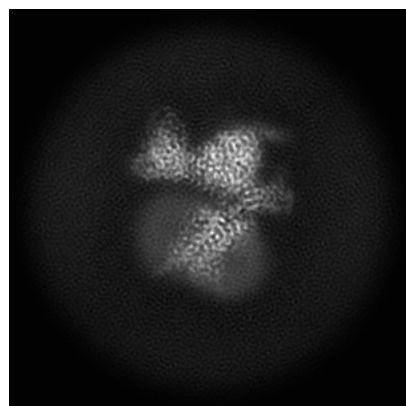
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70964. These allow visual inspection of the internal detail of the map and identification of artifacts.

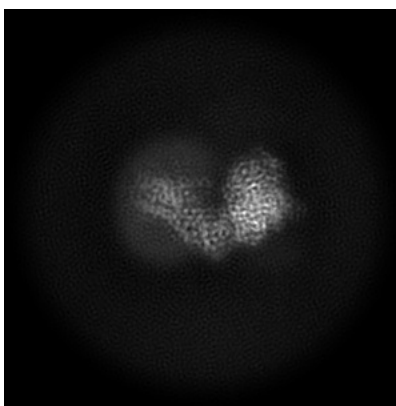
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

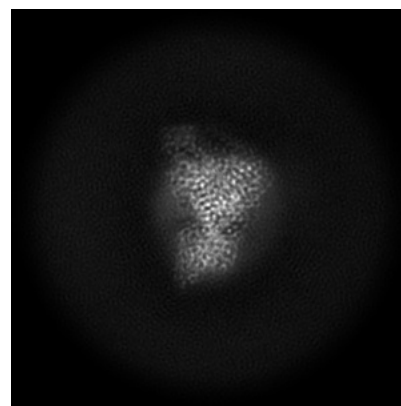
6.1.1 Primary map



X

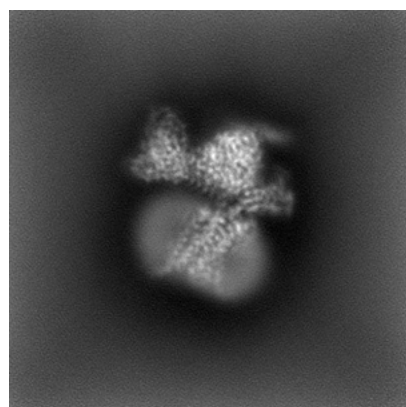


Y

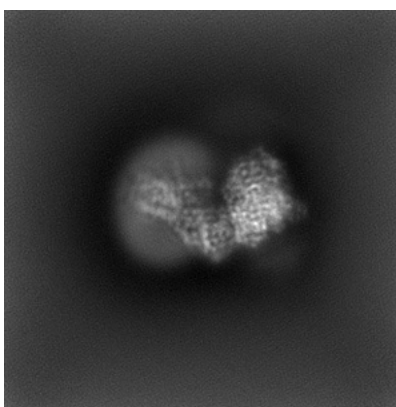


Z

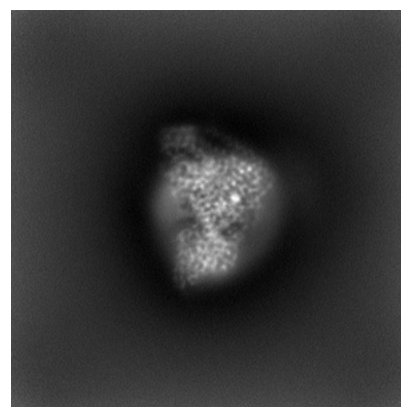
6.1.2 Raw map



X



Y

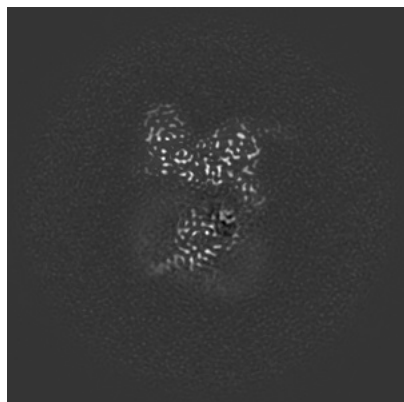


Z

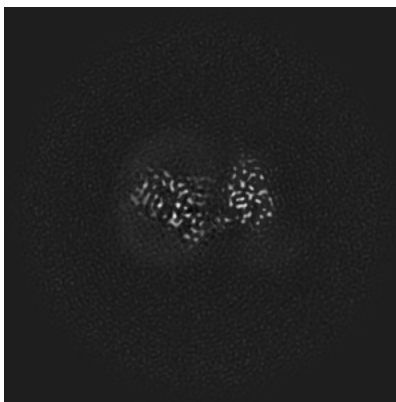
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

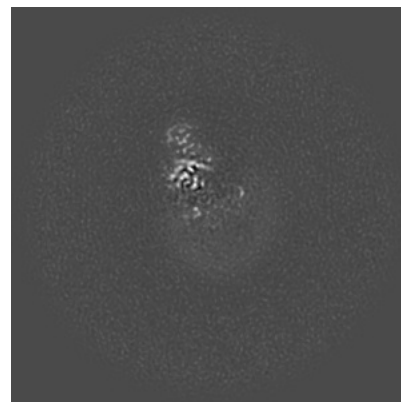
6.2.1 Primary map



X Index: 144

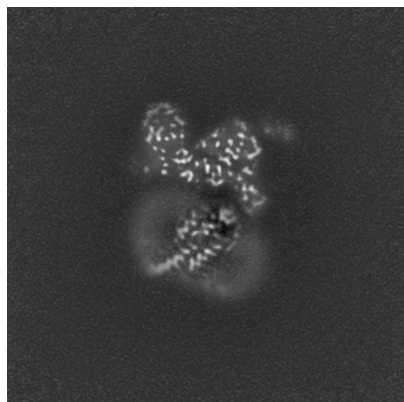


Y Index: 144

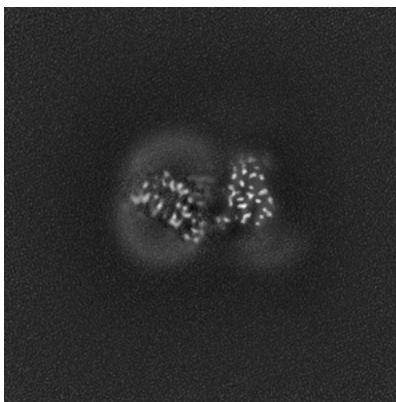


Z Index: 144

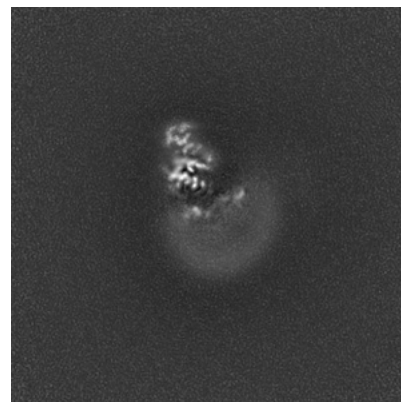
6.2.2 Raw map



X Index: 144



Y Index: 144

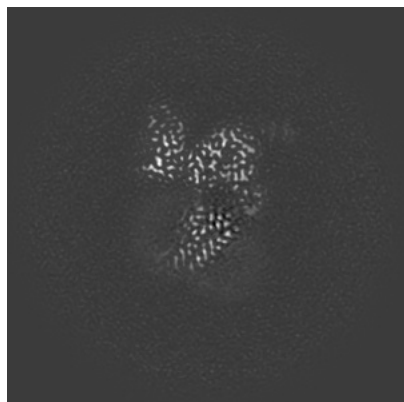


Z Index: 144

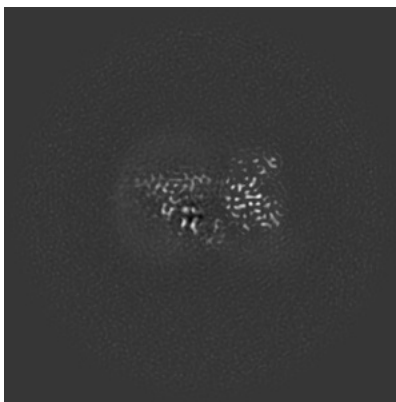
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

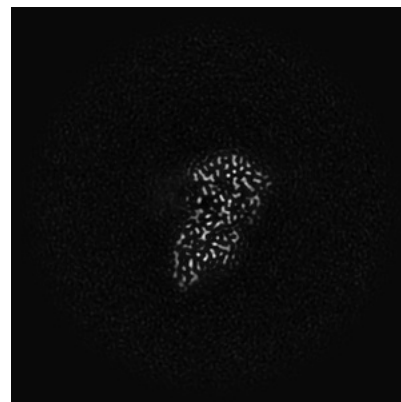
6.3.1 Primary map



X Index: 141

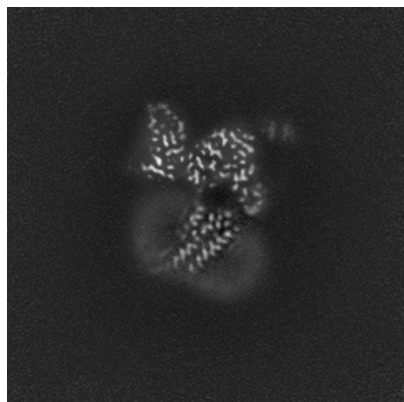


Y Index: 152

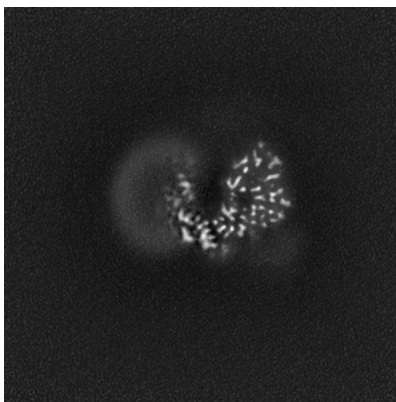


Z Index: 179

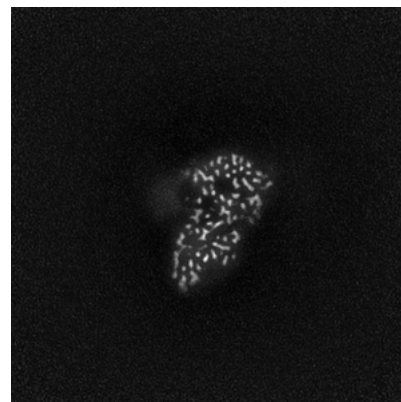
6.3.2 Raw map



X Index: 141



Y Index: 165

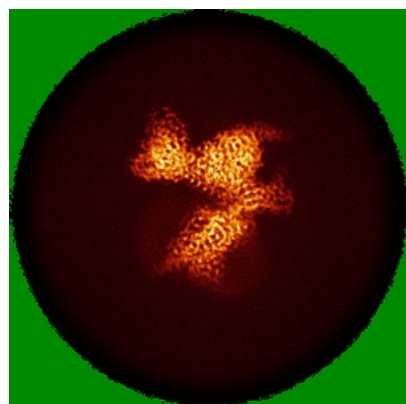


Z Index: 179

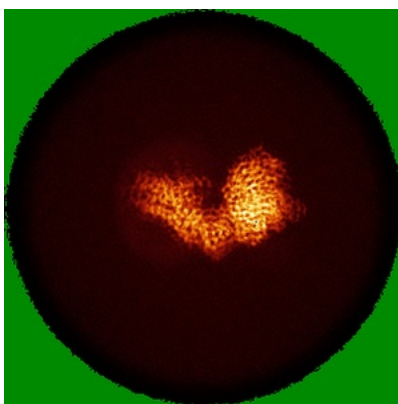
The images above show the largest variance slices of the map in three orthogonal directions.

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

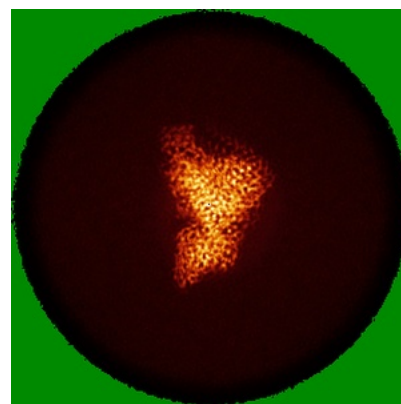
6.4.1 Primary map



X

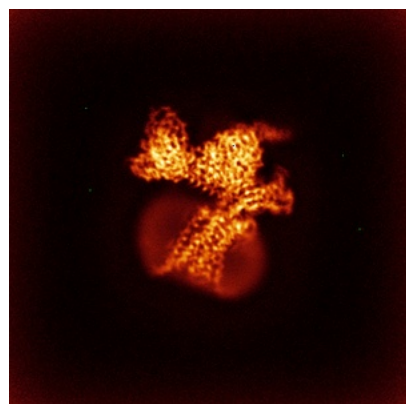


Y

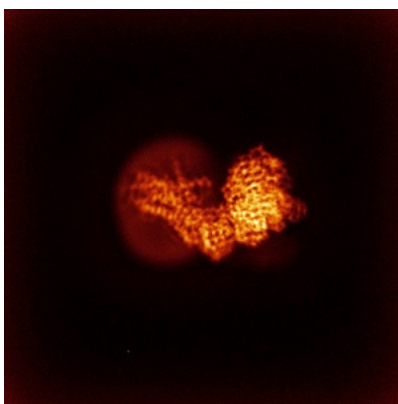


Z

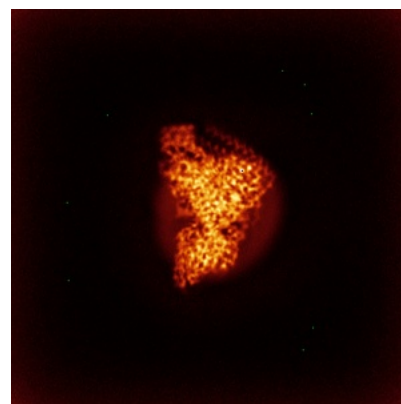
6.4.2 Raw map



X



Y

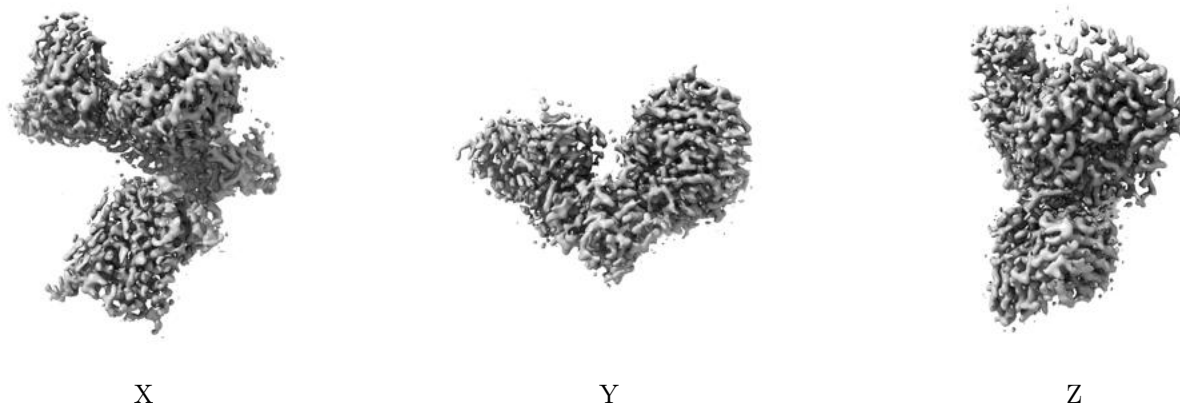


Z

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.

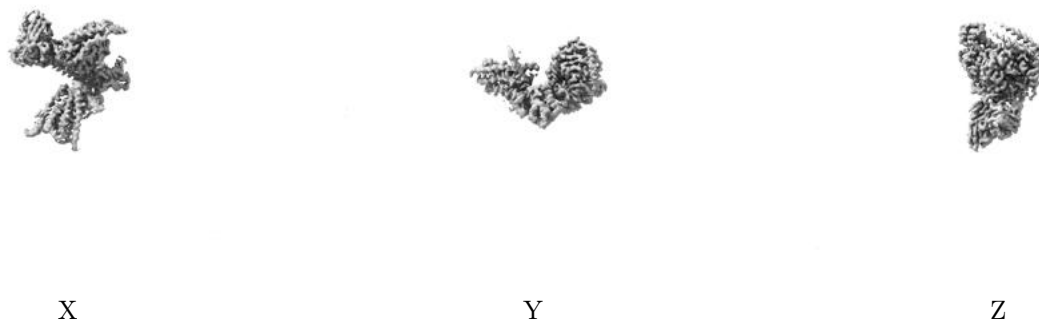
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.6. 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.

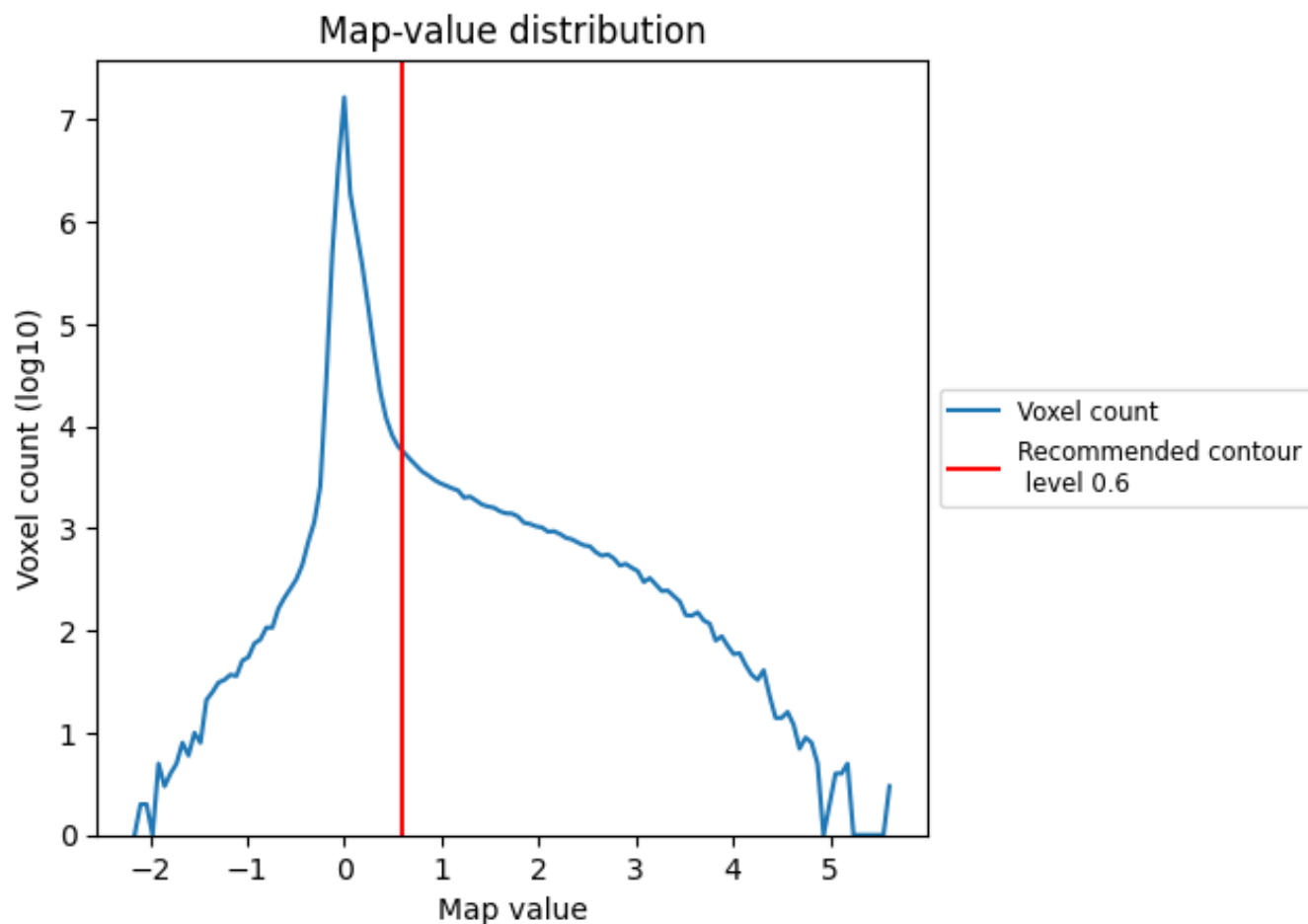
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

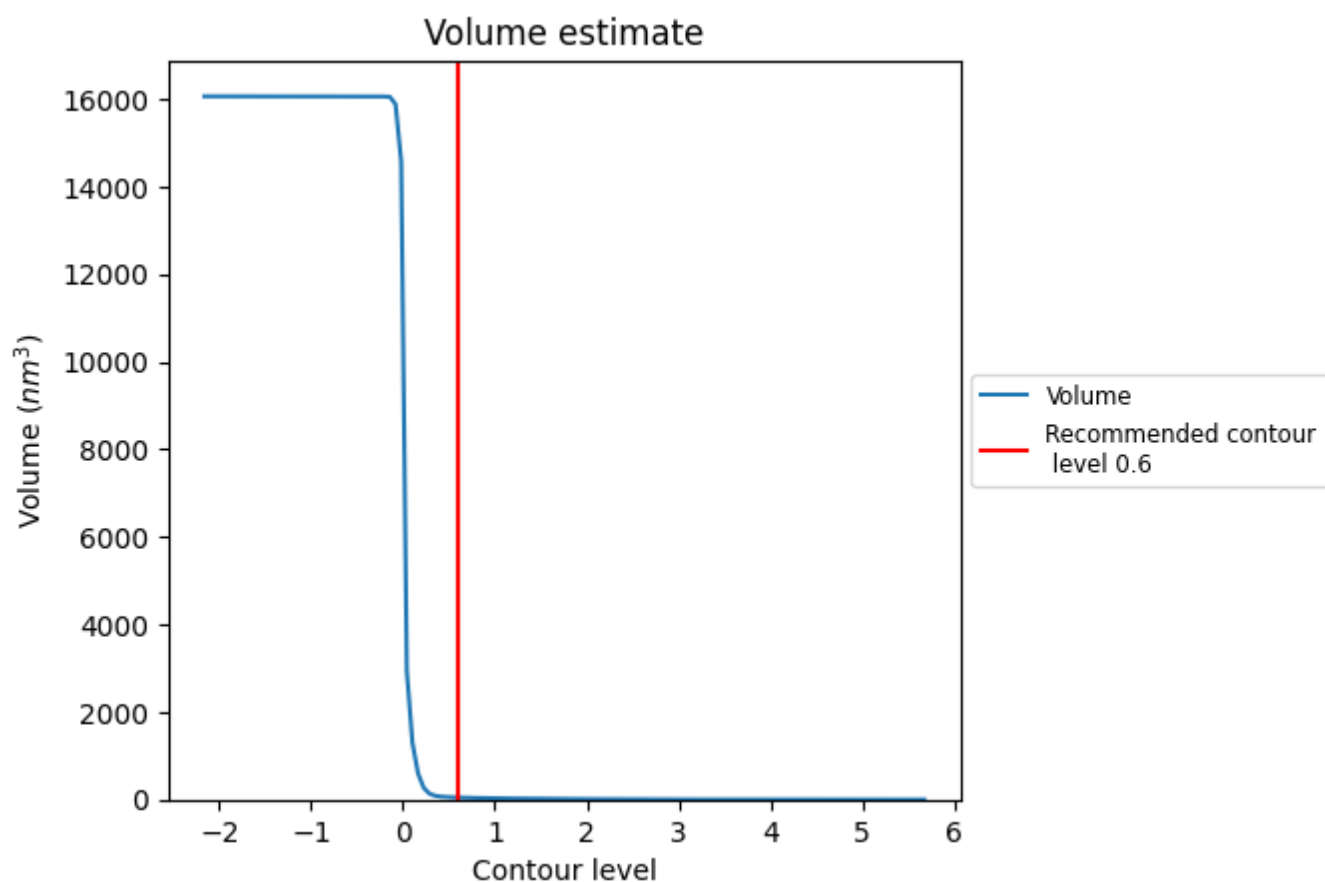
This section contains the results of statistical analysis of the map.

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.

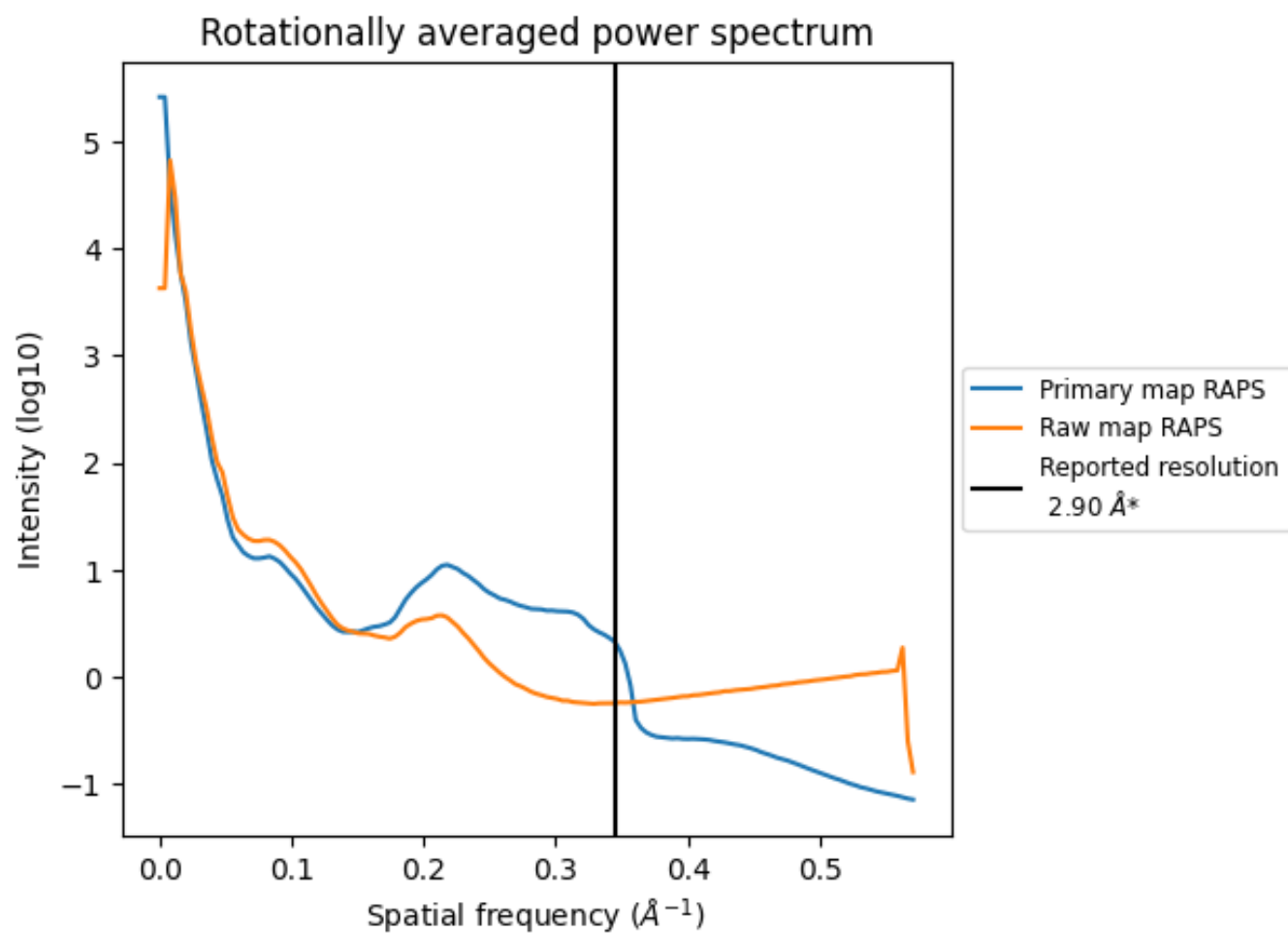
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm^3 ; this corresponds to an approximate mass of 43 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 ⓘ

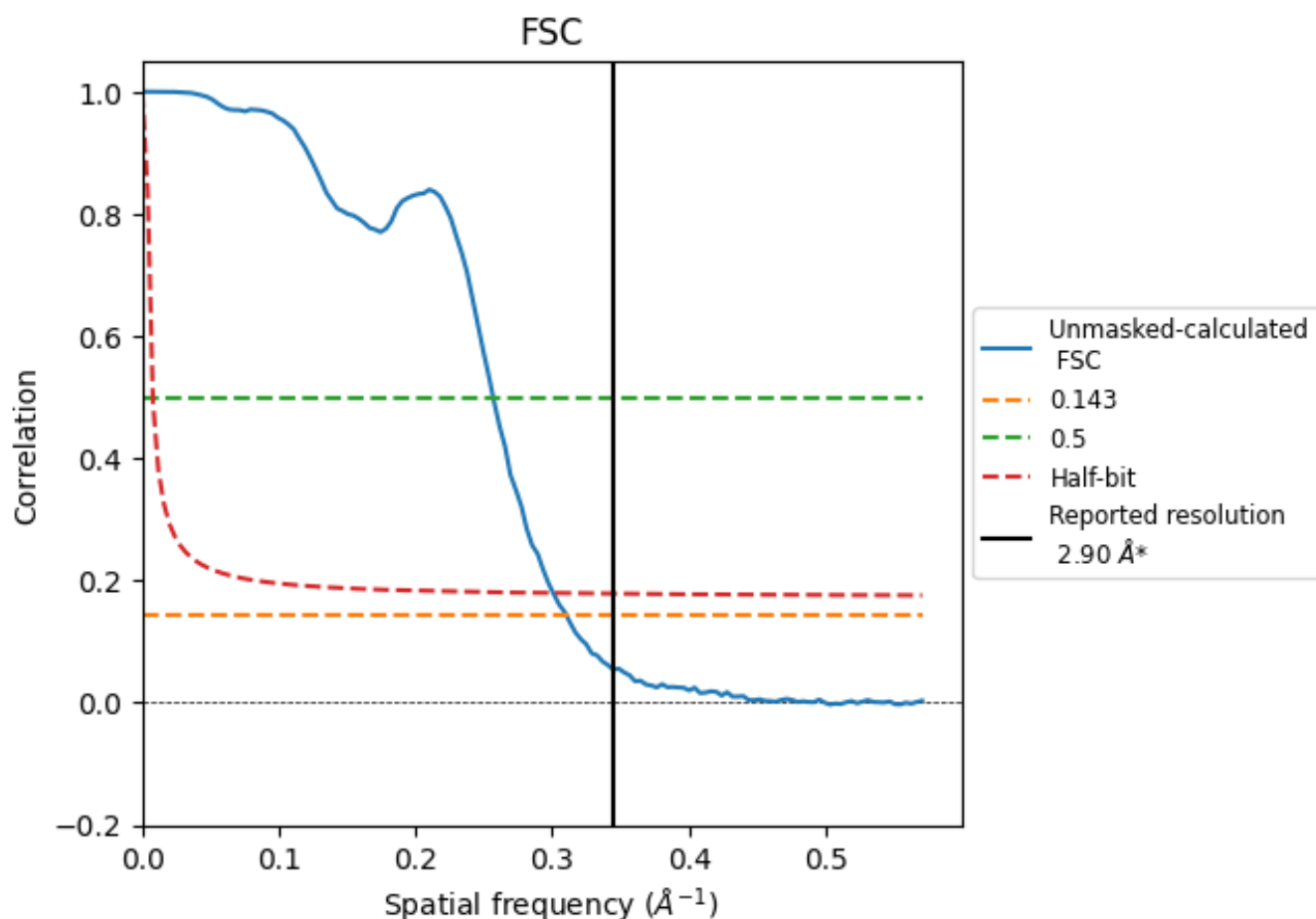


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8.2 Resolution estimates [i](#)

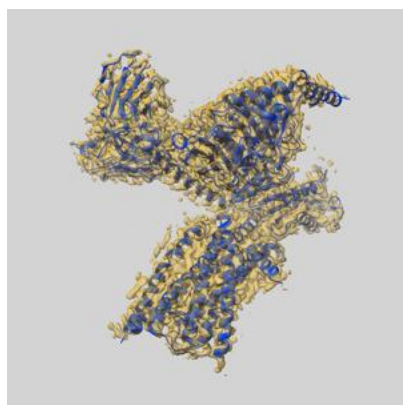
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.89	3.32

*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 3.22 differs from the reported value 2.9 by more than 10 %

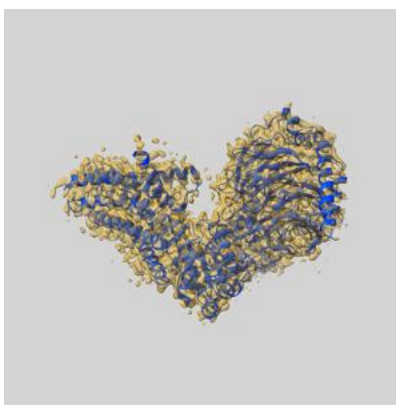
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-70964 and PDB model 9OXA. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

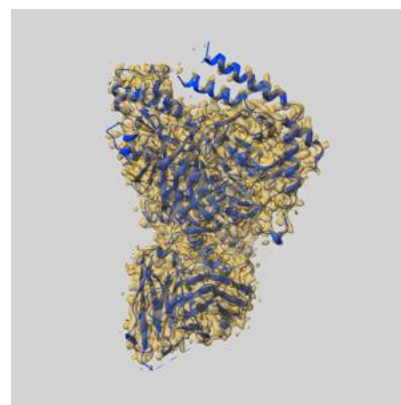
9.1 Map-model overlay [i](#)



X



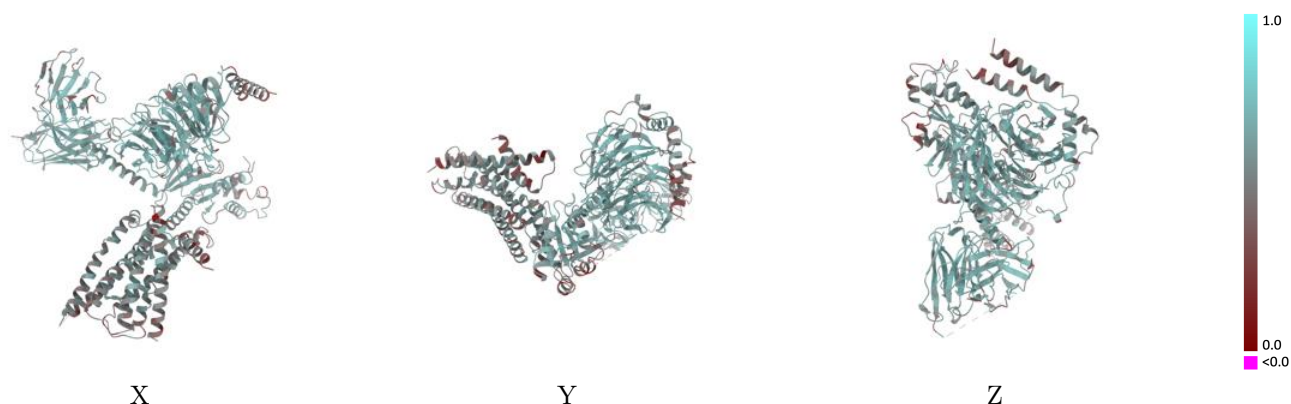
Y



Z

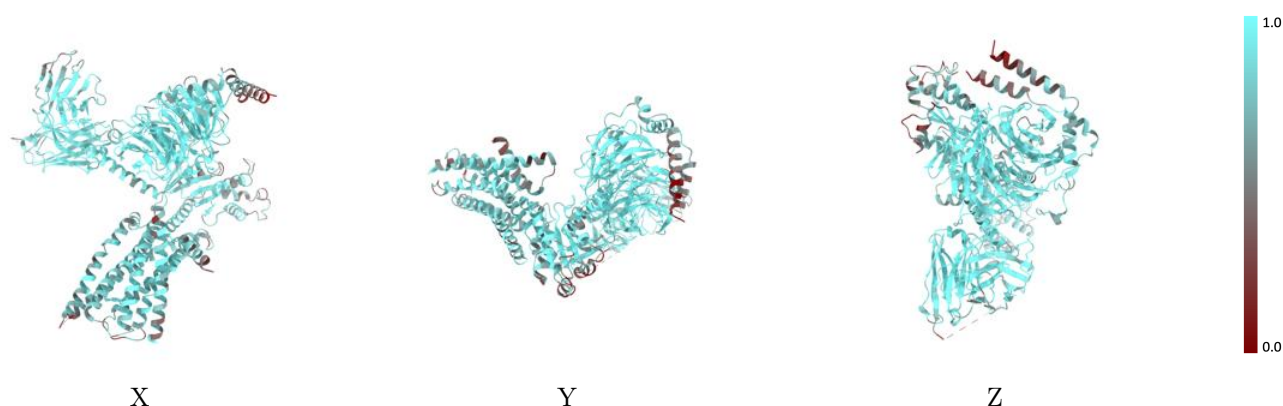
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



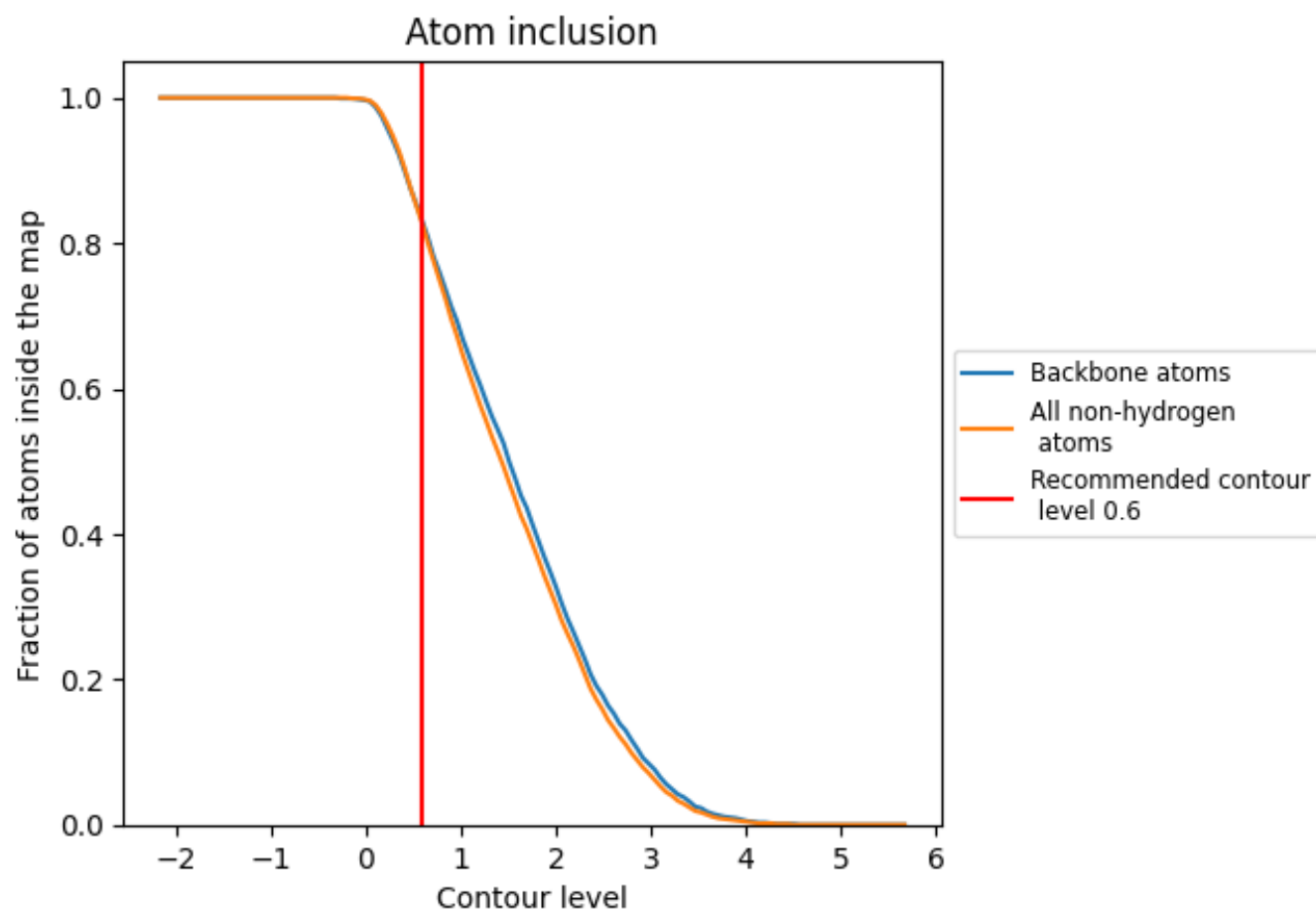
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8250	<div><div></div></div> 0.5640
A	<div><div></div></div> 0.7730	<div><div></div></div> 0.5480
B	<div><div></div></div> 0.9030	<div><div></div></div> 0.6170
C	<div><div></div></div> 0.6830	<div><div></div></div> 0.5340
D	<div><div></div></div> 0.8860	<div><div></div></div> 0.6030
R	<div><div></div></div> 0.7670	<div><div></div></div> 0.4910

