WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 11:52 am BST

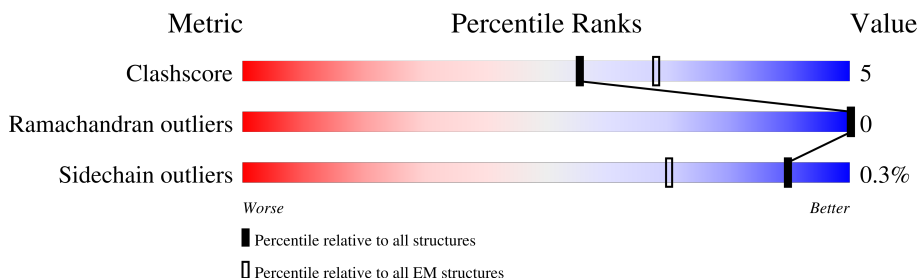|		
PDB ID	:	7OCF
EMDB ID	:	EMD-12806
Title	:	Active state GluA1/A2 AMPA receptor in complex with TARP gamma 8 and CNIH2 (LBD-TMD)
Authors	:	Zhang, D.; Watson, J.F.; Matthews, P.M.; Cais, O.; Greger, I.H.
Deposited on	:	2021-04-26
Resolution	:	3.60 Å(reported)
Based on initial models	:	6QKC, 6PEQ

1   Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.60 Å.

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

Metric	Percentile Ranks	Value
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0.3%

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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 <=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	915	8% 39% 6% 56%
1	C	915	8% 39% 5% 56%
2	B	860	5% 42% • 54%
2	D	860	5% 42% 5% 54%
3	E	188	25% 77% 7% 16%
3	G	188	26% 77% 7% 16%
4	I	423	• 40% • 57%
4	J	423	• 39% • 57%

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 17088 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 Isoform Flip of Glutamate receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	406	Total	C	N	O	S	0	0
			2803	1831	456	504	12		
1	C	406	Total	C	N	O	S	0	0
			2803	1831	456	504	12		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	insertion	UNP P19490
A	-5	TYR	-	insertion	UNP P19490
A	-4	LYS	-	insertion	UNP P19490
A	-3	ASP	-	insertion	UNP P19490
A	-2	ASP	-	insertion	UNP P19490
A	-1	ASP	-	insertion	UNP P19490
A	0	ASP	-	insertion	UNP P19490
A	1	LYS	-	insertion	UNP P19490
C	-6	ASP	-	insertion	UNP P19490
C	-5	TYR	-	insertion	UNP P19490
C	-4	LYS	-	insertion	UNP P19490
C	-3	ASP	-	insertion	UNP P19490
C	-2	ASP	-	insertion	UNP P19490
C	-1	ASP	-	insertion	UNP P19490
C	0	ASP	-	insertion	UNP P19490
C	1	LYS	-	insertion	UNP P19490

- Molecule 2 is a protein called Isoform Flip of Glutamate receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	399	Total	C	N	O	S	0	0
			2878	1870	477	513	18		
2	D	399	Total	C	N	O	S	0	0
			2878	1870	477	513	18		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	586	ARG	GLN	variant	UNP P19491
D	586	ARG	GLN	variant	UNP P19491

- Molecule 3 is a protein called Protein cornichon homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	158	Total	C	N	O	S	0	0
			1222	829	191	190	12		
3	E	158	Total	C	N	O	S	0	0
			1222	829	191	190	12		

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	161	GLU	-	expression tag	UNP Q5BJU5
G	162	ASN	-	expression tag	UNP Q5BJU5
G	163	LEU	-	expression tag	UNP Q5BJU5
G	164	TYR	-	expression tag	UNP Q5BJU5
G	165	PHE	-	expression tag	UNP Q5BJU5
G	166	GLN	-	expression tag	UNP Q5BJU5
G	167	SER	-	expression tag	UNP Q5BJU5
G	168	GLY	-	expression tag	UNP Q5BJU5
G	169	GLY	-	expression tag	UNP Q5BJU5
G	170	SER	-	expression tag	UNP Q5BJU5
G	171	THR	-	expression tag	UNP Q5BJU5
G	172	GLU	-	expression tag	UNP Q5BJU5
G	173	THR	-	expression tag	UNP Q5BJU5
G	174	SER	-	expression tag	UNP Q5BJU5
G	175	GLN	-	expression tag	UNP Q5BJU5
G	176	VAL	-	expression tag	UNP Q5BJU5
G	177	ALA	-	expression tag	UNP Q5BJU5
G	178	PRO	-	expression tag	UNP Q5BJU5
G	179	ALA	-	expression tag	UNP Q5BJU5
G	180	TYR	-	expression tag	UNP Q5BJU5
G	181	PRO	-	expression tag	UNP Q5BJU5
G	182	TYR	-	expression tag	UNP Q5BJU5
G	183	ASP	-	expression tag	UNP Q5BJU5
G	184	VAL	-	expression tag	UNP Q5BJU5
G	185	PRO	-	expression tag	UNP Q5BJU5
G	186	ASP	-	expression tag	UNP Q5BJU5
G	187	TYR	-	expression tag	UNP Q5BJU5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	188	ALA	-	expression tag	UNP Q5BJU5
E	161	GLU	-	expression tag	UNP Q5BJU5
E	162	ASN	-	expression tag	UNP Q5BJU5
E	163	LEU	-	expression tag	UNP Q5BJU5
E	164	TYR	-	expression tag	UNP Q5BJU5
E	165	PHE	-	expression tag	UNP Q5BJU5
E	166	GLN	-	expression tag	UNP Q5BJU5
E	167	SER	-	expression tag	UNP Q5BJU5
E	168	GLY	-	expression tag	UNP Q5BJU5
E	169	GLY	-	expression tag	UNP Q5BJU5
E	170	SER	-	expression tag	UNP Q5BJU5
E	171	THR	-	expression tag	UNP Q5BJU5
E	172	GLU	-	expression tag	UNP Q5BJU5
E	173	THR	-	expression tag	UNP Q5BJU5
E	174	SER	-	expression tag	UNP Q5BJU5
E	175	GLN	-	expression tag	UNP Q5BJU5
E	176	VAL	-	expression tag	UNP Q5BJU5
E	177	ALA	-	expression tag	UNP Q5BJU5
E	178	PRO	-	expression tag	UNP Q5BJU5
E	179	ALA	-	expression tag	UNP Q5BJU5
E	180	TYR	-	expression tag	UNP Q5BJU5
E	181	PRO	-	expression tag	UNP Q5BJU5
E	182	TYR	-	expression tag	UNP Q5BJU5
E	183	ASP	-	expression tag	UNP Q5BJU5
E	184	VAL	-	expression tag	UNP Q5BJU5
E	185	PRO	-	expression tag	UNP Q5BJU5
E	186	ASP	-	expression tag	UNP Q5BJU5
E	187	TYR	-	expression tag	UNP Q5BJU5
E	188	ALA	-	expression tag	UNP Q5BJU5

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-8 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	184	Total	C	N	O	S	0	0
			1322	867	223	226	6		
4	J	184	Total	C	N	O	S	0	0
			1322	867	223	226	6		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	GLY	-	expression tag	UNP Q8VHW5

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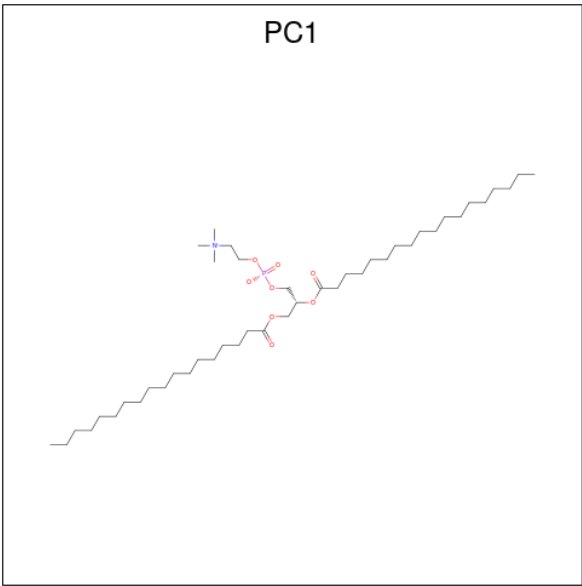| Chain	Residue	Modelled	Actual	Comment	Reference
I	418	LEU	-	expression tag	UNP Q8VHW5
I	419	GLU	-	expression tag	UNP Q8VHW5
I	420	VAL	-	expression tag	UNP Q8VHW5
I	421	LEU	-	expression tag	UNP Q8VHW5
I	422	PHE	-	expression tag	UNP Q8VHW5
I	423	GLN	-	expression tag	UNP Q8VHW5
J	1	GLY	-	expression tag	UNP Q8VHW5
J	418	LEU	-	expression tag	UNP Q8VHW5
J	419	GLU	-	expression tag	UNP Q8VHW5
J	420	VAL	-	expression tag	UNP Q8VHW5
J	421	LEU	-	expression tag	UNP Q8VHW5
J	422	PHE	-	expression tag	UNP Q8VHW5
J	423	GLN	-	expression tag	UNP Q8VHW5

- Molecule 5 is CYCLOTHIAZIDE (three-letter code: CYZ) (formula: $C_{14}H_{16}ClN_3O_4S_2$).
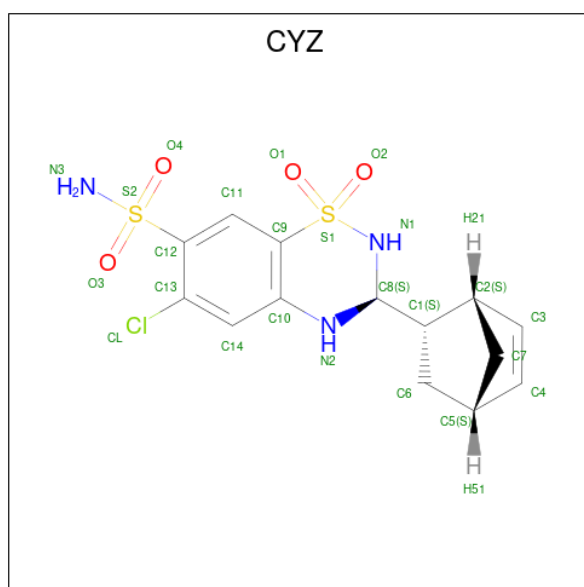
Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	B	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	C	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	
5	D	1	Total	C	Cl	N	O	S	0
			24	14	1	3	4	2	

- Molecule 6 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1)

(formula: $C_{44}H_{88}NO_8P$).

PC1

Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 18	C 16	O 2	0
6	A	1	Total 18	C 16	O 2	0
6	A	1	Total 18	C 16	O 2	0
6	A	1	Total 20	C 18	O 2	0
6	A	1	Total 20	C 18	O 2	0
6	A	1	Total 20	C 18	O 2	0
6	B	1	Total 16	C 14	O 2	0
6	B	1	Total 20	C 18	O 2	0
6	B	1	Total 20	C 18	O 2	0
6	B	1	Total 18	C 16	O 2	0
6	B	1	Total 25	C 21	O 4	0
6	I	1	Total 20	C 18	O 2	0
6	I	1	Total 20	C 18	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
6	C	1	Total 18	C 16	O 2	0
6	C	1	Total 18	C 16	O 2	0
6	C	1	Total 18	C 16	O 2	0
6	C	1	Total 20	C 18	O 2	0
6	C	1	Total 20	C 18	O 2	0
6	C	1	Total 20	C 18	O 2	0
6	E	1	Total 18	C 16	O 2	0
6	J	1	Total 20	C 18	O 2	0
6	J	1	Total 20	C 18	O 2	0
6	D	1	Total 16	C 14	O 2	0
6	D	1	Total 20	C 18	O 2	0
6	D	1	Total 20	C 18	O 2	0
6	D	1	Total 25	C 21	O 4	0

- Molecule 7 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).

GLU

OE1

O

OH OE2

CD

O

CB

CG

CA(S)

C

HO

OXT

NH₂

N
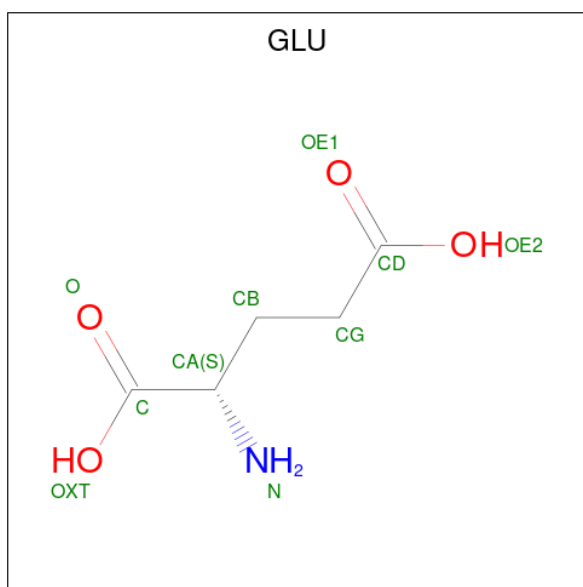
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			9	5	1	3	
7	B	1	Total	C	N	O	0
			9	5	1	3	
7	C	1	Total	C	N	O	0
			9	5	1	3	
7	D	1	Total	C	N	O	0
			9	5	1	3	

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: Isoform Flip of Glutamate receptor 1

GLY SER GLY GLU ASN GLY ARG VAL VAL SER GLN ASP PHE PRO LYS SER MET GLN SER ILE PRO CYS MET SER HIS SER GLY MET PRO LEU GLY ALA THR GLY LEU

• Molecule 1: Isoform Flip of Glutamate receptor 1

Chain C:

MET PRO TYR ILE PHE ALA PHE PHE CYS THR GLY PHE GLY LEU GLY ALA VAL VAL GLY ALA ASP TYR LYS ASP ASP ASP LYS ASN PHE PRO ASN ASN ILE GLN ILE GLY LEU PHE PRO ASN GLN GLN SER GLN GLU HIS ALA ALA PHE ARG PHE ALA LEU SER GLN LEU THR GLU PRO

PRO LYS LEU LEU PRO GLN ILE ASP ILE VAL ASN ILE ASP SER SER PHE GLU MET THR TYR ARG PHE CYS SER GLN PHE SER LYS GLY VAL TYR ALA ILE PHE GLY PHE TYR GLU ARG ARG THR VAL ASN MET LEU THR SER PHE CYS GLY ALA LEU HIS VAL CYS PHE ILE THR PRO SER

PHE PRO VAL ASP THR SER ASN GLN PHE VAL LEU GLN LEU ARG PRO GLU LEU GLN GLU ALA LEU ILE SER ILE ILE ASP HIS TYR LYS TRP GLN THR PHE VAL TYR ILE TYR ASP ALA ASP ARG GLY LEU SER VAL LEU GLN ARG VAL LEU ASP THR ALA ALA GLU LYS ASN TRP GLN VAL

THR ALA VAL ASN ILE LEU THR THR THR GLU GLU GLY TYR ARG MET LEU PHE GLN ASP LEU GLU LYS LYS LYS GLU ARG LEU VAL VAL VAL ASP CYS GLU SER GLU ARG LEU ASN ALA ILE LEU GLY GLN ILE VAL LYS LEU GLU LYS ASN GLY ILE GLY TYR HIS TYR ILE LEU ALA ASN

LEU GLY PHE MET ASP ILE ASP LEU ASN LYS PHE LYS GLU SER GLY ALA ASN VAL THR GLY PHE GLN LEU VAL ASN TYR THR ASP THR ILE PRO ALA ARG ILE MET GLN GLN TRP ARG THR SER ASP SER ARG ASP HIS THR ARG VAL ASP TRP LYS ARG PRO LYS TYR THR SER ALA LEU

THR TYR ASP GLY VAL LYS VAL MET ALA GLU ALA PHE GLN SER LEU ARG ARG GLN ARG ILE ASP ILE SER ARG ARG GLY ASN ALA GLY ASP CYS LEU ALA ASN PRO ALA VAL PRO TRP GLY GLN GLY ILE ASP ILE GLN ARG ALA LEU GLN GLN VAL ARG PHE GLU GLY LEU THR GLY ASN

VAL GLN PHE ASN GLU LYS GLY ARG ARG THR ASN TYR THR LEU HIS VAL ILE GLU MET LYS HIS ASP GLY ILE ARG LYS ILE GLY TYR TRP ASN GLU ASP ASP LYS PHE VAL PRO ALA ALA THR ASP ALA GLN ALA GLY GLY ASP ASN SER SER VAL GLN ASN ARG T390 L397 Y401

GLU ASN GLY ARG VAL VAL SER GLN ASP PHE PRO LYS SER MET GLN SER ILE PRO CYS MET SER HIS SER GLY MET PRO LEU GLY ALA THR GLY LEU

• Molecule 2: Isoform Flip of Glutamate receptor 2

Chain B:

MET GLN LYS ILE MET HIS ILE SER VAL LEU LEU SER PRO VAL LEU TRP GLY LEU ILE PHE GLY VAL SER SER ASN SER ILE GLN ILE GLY GLY LEU PHE PRO ARG GLY ALA ASP GLN GLU TYR SER ALA PHE ARG VAL GLY MET VAL GLN PHE SER THR SER GLU PHE ARG LEU THR PRO

HIS ILE ASP ASN LEU GLU VAL ALA ASN SER PHE ALA VAL THR ASN ALA PHE CYS SER GLN PHE SER ARG GLY VAL TYR ALA ILE PHE GLY PHE TYR ASP LYS LYS SER VAL ASN THR ILE THR SER PHE CYS GLY THR LEU HIS VAL SER PHE ILE THR PRO SER PHE PRO THR ASP GLY

• Molecule 2: Isoform Flip of Glutamate receptor 2

Chain D:

• Molecule 3: Protein cornichon homolog 2

Chain G:

• Molecule 3: Protein cornichon homolog 2

Chain E:

• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

Chain I:

• Molecule 4: Voltage-dependent calcium channel gamma-8 subunit

Chain J:

39%   57%

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	120052	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.198	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, CYZ

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	0.40	0/2870	0.43	0/3937
1	C	0.40	0/2870	0.44	0/3937
2	B	0.39	0/2942	0.44	0/4005
2	D	0.39	0/2942	0.44	0/4005
3	E	0.29	0/1263	0.40	0/1727
3	G	0.29	0/1263	0.40	0/1727
4	I	0.40	0/1346	0.53	1/1833 (0.1%)
4	J	0.40	0/1346	0.53	1/1833 (0.1%)
All	All	0.38	0/16842	0.45	2/23004 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	102	LYS	CD-CE-NZ	-11.02	86.35	111.70
4	J	102	LYS	CD-CE-NZ	-11.00	86.41	111.70

There are no chirality outliers.

There are no planarity outliers.

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	2803	0	2471	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2803	0	2471	34	0
2	B	2878	0	2715	25	0
2	D	2878	0	2715	28	0
3	E	1222	0	1149	9	0
3	G	1222	0	1149	9	0
4	I	1322	0	1296	11	0
4	J	1322	0	1296	12	0
5	A	24	0	10	2	0
5	B	24	0	10	1	0
5	C	24	0	10	2	0
5	D	24	0	10	1	0
6	A	114	0	189	1	0
6	B	99	0	162	2	0
6	C	114	0	189	0	0
6	D	81	0	134	2	0
6	E	18	0	28	0	0
6	I	40	0	70	0	0
6	J	40	0	70	0	0
7	A	9	0	5	1	0
7	B	9	0	5	1	0
7	C	9	0	5	1	0
7	D	9	0	5	1	0
All	All	17088	0	16164	160	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 5.

The worst 5 of 160 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)
2:B:705:GLU:OE1	2:B:705:GLU:N	2.09	0.85
2:D:705:GLU:N	2:D:705:GLU:OE1	2.10	0.84
2:B:654:SER:N	7:B:1407:GLU:O	2.15	0.79
2:D:654:SER:N	7:D:1406:GLU:O	2.15	0.78
2:D:395:VAL:N	2:D:439:LYS:O	2.18	0.76

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	400/915 (44%)	380 (95%)	20 (5%)	0	100	100
1	C	400/915 (44%)	380 (95%)	20 (5%)	0	100	100
2	B	393/860 (46%)	373 (95%)	20 (5%)	0	100	100
2	D	393/860 (46%)	373 (95%)	20 (5%)	0	100	100
3	E	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
3	G	156/188 (83%)	154 (99%)	2 (1%)	0	100	100
4	I	178/423 (42%)	173 (97%)	5 (3%)	0	100	100
4	J	178/423 (42%)	172 (97%)	6 (3%)	0	100	100
All	All	2254/4772 (47%)	2159 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/778 (30%)	235 (100%)	0	100	100
1	C	235/778 (30%)	235 (100%)	0	100	100
2	B	270/737 (37%)	269 (100%)	1 (0%)	89	95
2	D	270/737 (37%)	269 (100%)	1 (0%)	89	95
3	E	114/166 (69%)	114 (100%)	0	100	100
3	G	114/166 (69%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	I	124/309 (40%)	123 (99%)	1 (1%)	79	88
4	J	124/309 (40%)	123 (99%)	1 (1%)	79	88
All	All	1486/3980 (37%)	1482 (100%)	4 (0%)	90	96

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

Mol	Chain	Res	Type
2	B	628	ARG
4	I	102	LYS
4	J	102	LYS
2	D	628	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5　Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6　Ligand geometry ⓘ

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	PC1	D	1405	-	24,24,53	0.78	2 (8%)	25,25,61	1.04	1 (4%)
6	PC1	D	1404	-	19,19,53	0.79	1 (5%)	19,19,61	0.97	0
5	CYZ	A	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.44	16 (42%)
5	CYZ	C	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.45	15 (39%)
6	PC1	I	1802	-	19,19,53	0.76	1 (5%)	19,19,61	1.10	1 (5%)
7	GLU	B	1407	-	7,8,9	0.85	0	4,9,11	1.00	0
6	PC1	D	1402	-	15,15,53	1.70	2 (13%)	15,15,61	1.00	0
6	PC1	A	1402	-	17,17,53	0.80	1 (5%)	17,17,61	1.09	1 (5%)
6	PC1	B	1404	-	19,19,53	0.79	1 (5%)	19,19,61	0.97	0
6	PC1	C	1406	-	19,19,53	0.78	1 (5%)	19,19,61	1.01	0
6	PC1	C	1407	-	19,19,53	0.75	1 (5%)	19,19,61	1.10	0
6	PC1	B	1402	-	15,15,53	1.71	2 (13%)	15,15,61	1.00	0
6	PC1	B	1403	-	19,19,53	0.76	1 (5%)	19,19,61	1.04	0
6	PC1	I	1801	-	19,19,53	0.76	1 (5%)	19,19,61	1.06	0
6	PC1	B	1405	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	0
6	PC1	A	1405	-	19,19,53	0.77	1 (5%)	19,19,61	0.99	0
6	PC1	A	1407	-	19,19,53	0.76	1 (5%)	19,19,61	1.09	0
6	PC1	A	1404	-	17,17,53	0.82	1 (5%)	17,17,61	1.09	1 (5%)
6	PC1	J	1901	-	19,19,53	0.76	1 (5%)	19,19,61	1.09	1 (5%)
7	GLU	A	1408	-	7,8,9	0.86	0	4,9,11	1.02	0
5	CYZ	B	1401	-	26,27,27	7.59	18 (69%)	38,44,44	3.36	13 (34%)
6	PC1	D	1403	-	19,19,53	0.75	1 (5%)	19,19,61	1.05	0
6	PC1	E	1901	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	0
7	GLU	D	1406	-	7,8,9	0.86	0	4,9,11	0.99	0
6	PC1	C	1402	-	17,17,53	0.81	1 (5%)	17,17,61	1.08	1 (5%)
6	PC1	C	1404	-	17,17,53	0.81	1 (5%)	17,17,61	1.09	1 (5%)
6	PC1	C	1405	-	19,19,53	0.77	1 (5%)	19,19,61	0.99	0
6	PC1	A	1403	-	17,17,53	0.81	1 (5%)	17,17,61	1.10	1 (5%)
5	CYZ	D	1401	-	26,27,27	7.60	18 (69%)	38,44,44	3.36	13 (34%)
6	PC1	A	1406	-	19,19,53	0.79	1 (5%)	19,19,61	1.02	0
6	PC1	B	1406	-	24,24,53	0.78	2 (8%)	25,25,61	1.03	1 (4%)
6	PC1	J	1902	-	19,19,53	0.76	1 (5%)	19,19,61	1.06	0
7	GLU	C	1408	-	7,8,9	0.85	0	4,9,11	1.02	0
6	PC1	C	1403	-	17,17,53	0.82	1 (5%)	17,17,61	1.11	1 (5%)

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	PC1	D	1405	-	-	6/24/24/57	-
6	PC1	D	1404	-	-	3/17/17/57	-
5	CYZ	A	1401	-	-	6/6/42/42	0/5/4/4
5	CYZ	C	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	I	1802	-	-	10/17/17/57	-
7	GLU	B	1407	-	-	2/6/7/9	-
6	PC1	D	1402	-	-	7/13/13/57	-
6	PC1	A	1402	-	-	6/15/15/57	-
6	PC1	B	1404	-	-	3/17/17/57	-
6	PC1	C	1406	-	-	6/17/17/57	-
6	PC1	C	1407	-	-	6/17/17/57	-
6	PC1	B	1402	-	-	7/13/13/57	-
6	PC1	B	1403	-	-	10/17/17/57	-
6	PC1	I	1801	-	-	5/17/17/57	-
6	PC1	B	1405	-	-	7/15/15/57	-
6	PC1	A	1405	-	-	10/17/17/57	-
6	PC1	A	1407	-	-	6/17/17/57	-
6	PC1	A	1404	-	-	5/15/15/57	-
6	PC1	J	1901	-	-	10/17/17/57	-
7	GLU	A	1408	-	-	3/6/7/9	-
5	CYZ	B	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	D	1403	-	-	10/17/17/57	-
6	PC1	E	1901	-	-	7/15/15/57	-
7	GLU	D	1406	-	-	2/6/7/9	-
6	PC1	C	1402	-	-	6/15/15/57	-
6	PC1	C	1404	-	-	5/15/15/57	-
6	PC1	C	1405	-	-	10/17/17/57	-
6	PC1	A	1403	-	-	3/15/15/57	-
5	CYZ	D	1401	-	-	6/6/42/42	0/5/4/4
6	PC1	A	1406	-	-	6/17/17/57	-
6	PC1	B	1406	-	-	6/24/24/57	-
6	PC1	J	1902	-	-	5/17/17/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLU	C	1408	-	-	3/6/7/9	-
6	PC1	C	1403	-	-	3/15/15/57	-

The worst 5 of 102 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1401	CYZ	C2-C3	-18.94	0.99	1.51
5	A	1401	CYZ	C2-C3	-18.92	0.99	1.51
5	B	1401	CYZ	C2-C3	-18.75	1.00	1.51
5	D	1401	CYZ	C2-C3	-18.74	1.00	1.51
5	A	1401	CYZ	C2-C1	-15.57	1.21	1.55

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	1401	CYZ	C9-S1-N1	11.77	118.45	103.43
5	A	1401	CYZ	C9-S1-N1	11.75	118.42	103.43
5	D	1401	CYZ	C9-S1-N1	11.22	117.75	103.43
5	B	1401	CYZ	C9-S1-N1	11.19	117.71	103.43
5	B	1401	CYZ	O4-S2-O3	-10.79	101.03	118.76

There are no chirality outliers.

5 of 202 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1401	CYZ	C11-C12-S2-O4
5	A	1401	CYZ	C11-C12-S2-N3
5	A	1401	CYZ	C13-C12-S2-O3
5	A	1401	CYZ	C13-C12-S2-O4
5	A	1401	CYZ	C13-C12-S2-N3

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	1405	PC1	2	0
5	A	1401	CYZ	2	0
5	C	1401	CYZ	2	0
7	B	1407	GLU	1	0
6	A	1404	PC1	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1408	GLU	1	0
5	B	1401	CYZ	1	0
7	D	1406	GLU	1	0
5	D	1401	CYZ	1	0
6	B	1406	PC1	2	0
7	C	1408	GLU	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

Ligand PC1 D 1405

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 D 1404

Bond lengths

Bond angles

Torsions

Rings

Ligand CYZ A 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand CYZ C 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 I 1802

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 D 1402

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1402

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 1404

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1406

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1407

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 1402

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 1403

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 I 1801

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 1405

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1405

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1407

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1404

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 J 1901

Bond lengths

Bond angles

Torsions

Rings

Ligand CYZ B 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 D 1403

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 E 1901

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1402

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1404

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1405

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1403

Bond lengths

Bond angles

Torsions

Rings

Ligand CYZ D 1401

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 A 1406

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 B 1406

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 J 1902

Bond lengths

Bond angles

Torsions

Rings

Ligand PC1 C 1403

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-12806. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

| X | Y | Z |
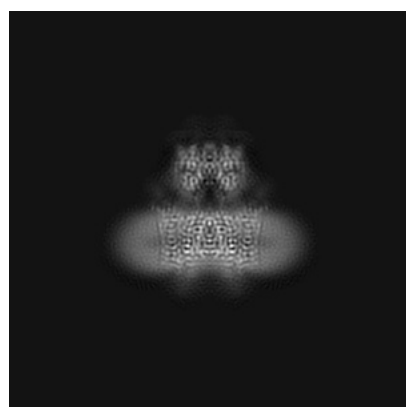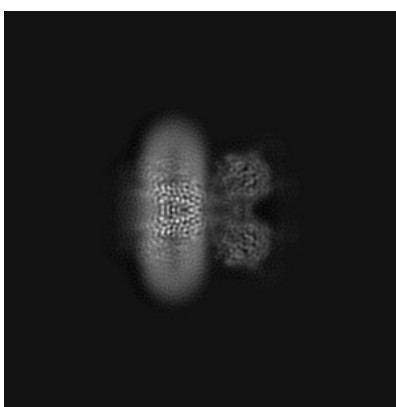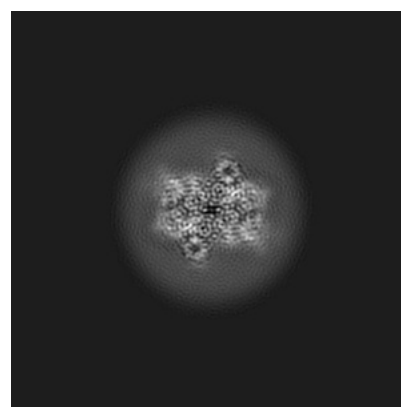
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
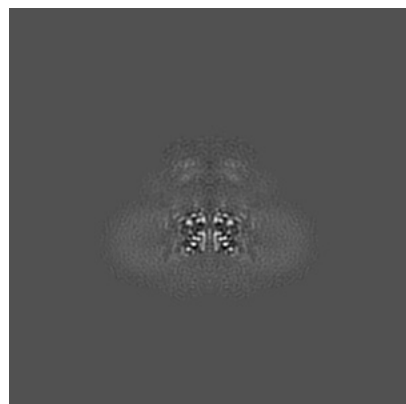
6.2.1 Primary map
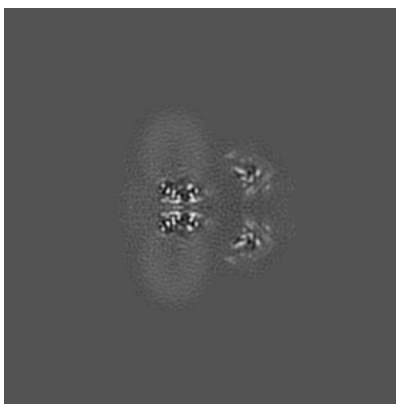
X Index: 160   Y Index: 160   Z Index: 160
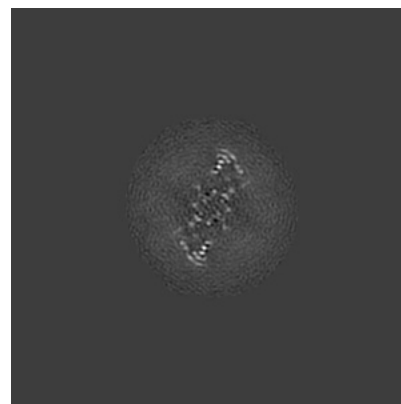
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
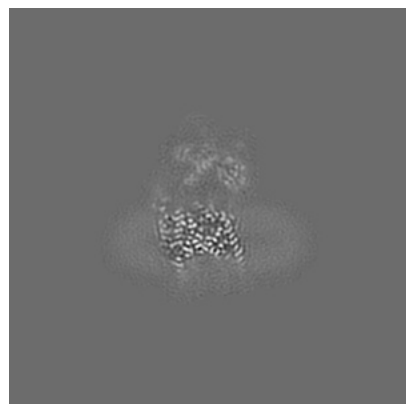
6.3.1 Primary map
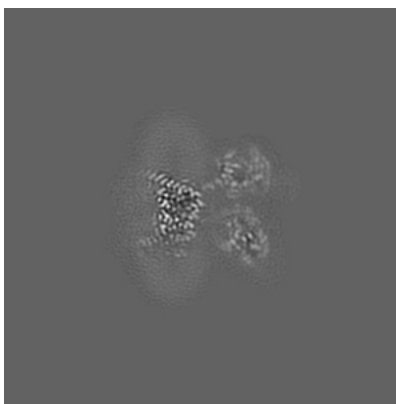
| X Index: 147 | Y Index: 174 | Z Index: 127 |
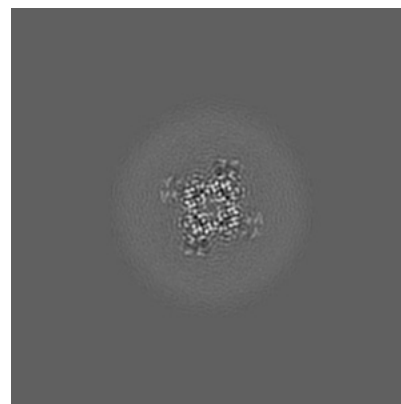
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map

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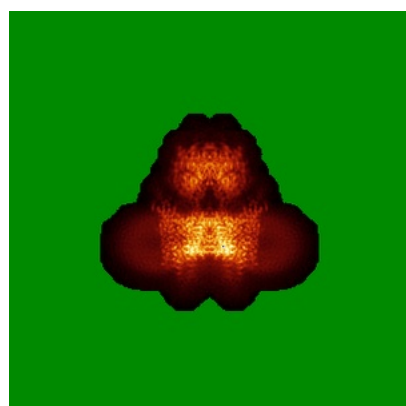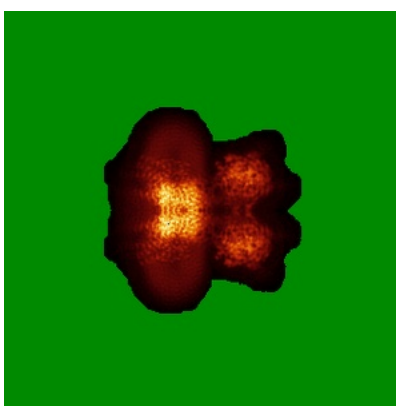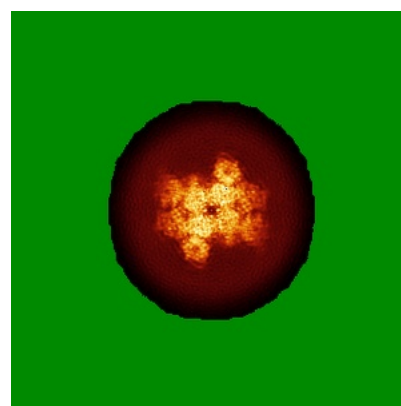
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |
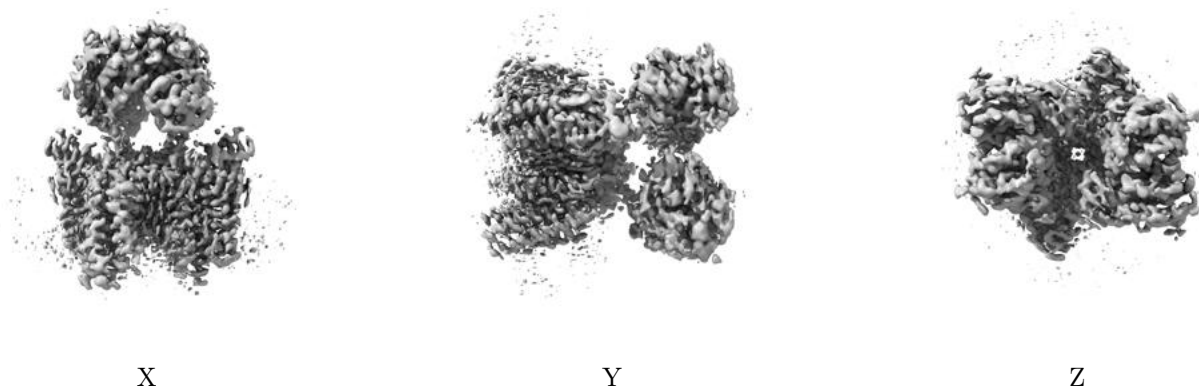
The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ
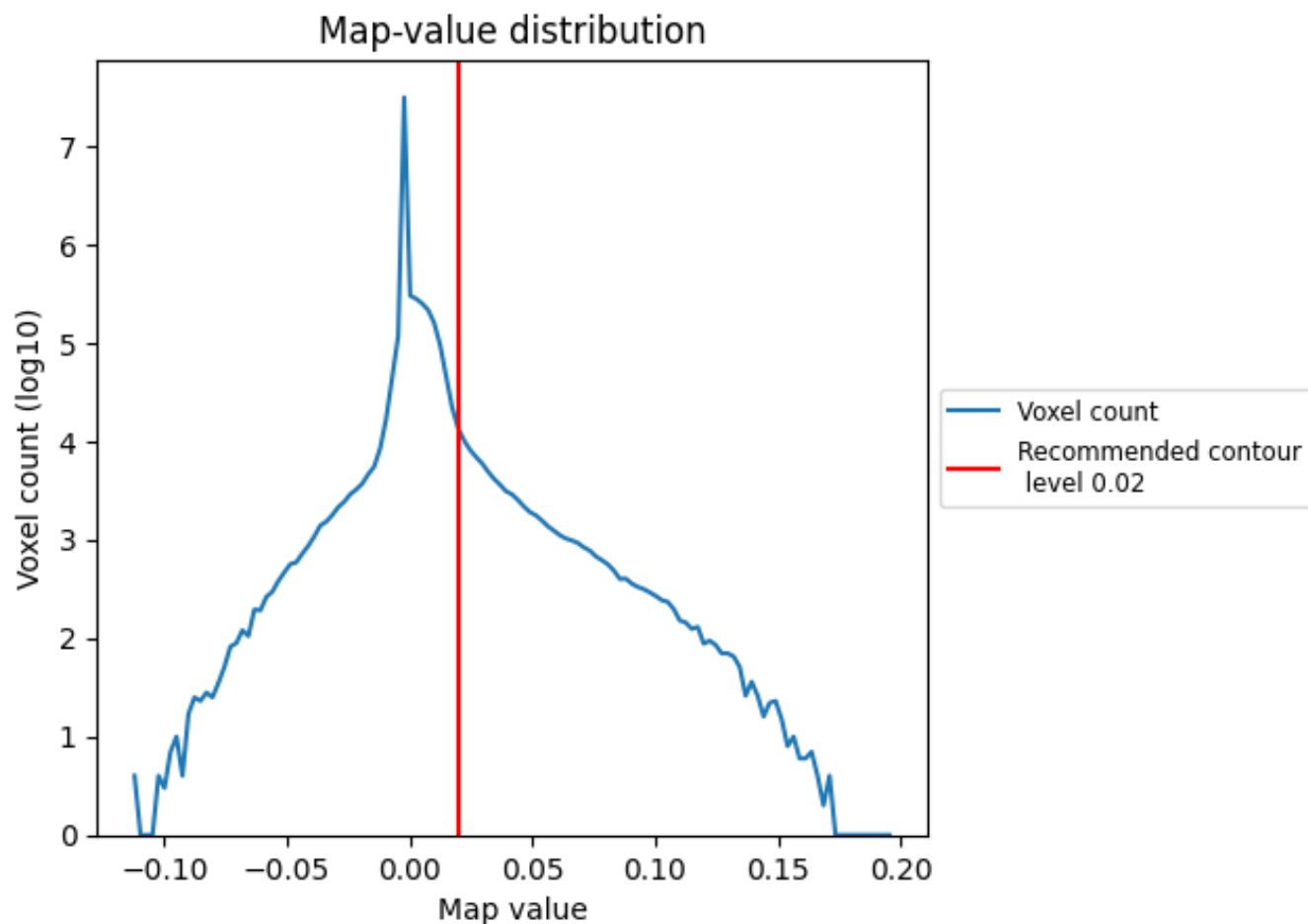
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate ⓘ
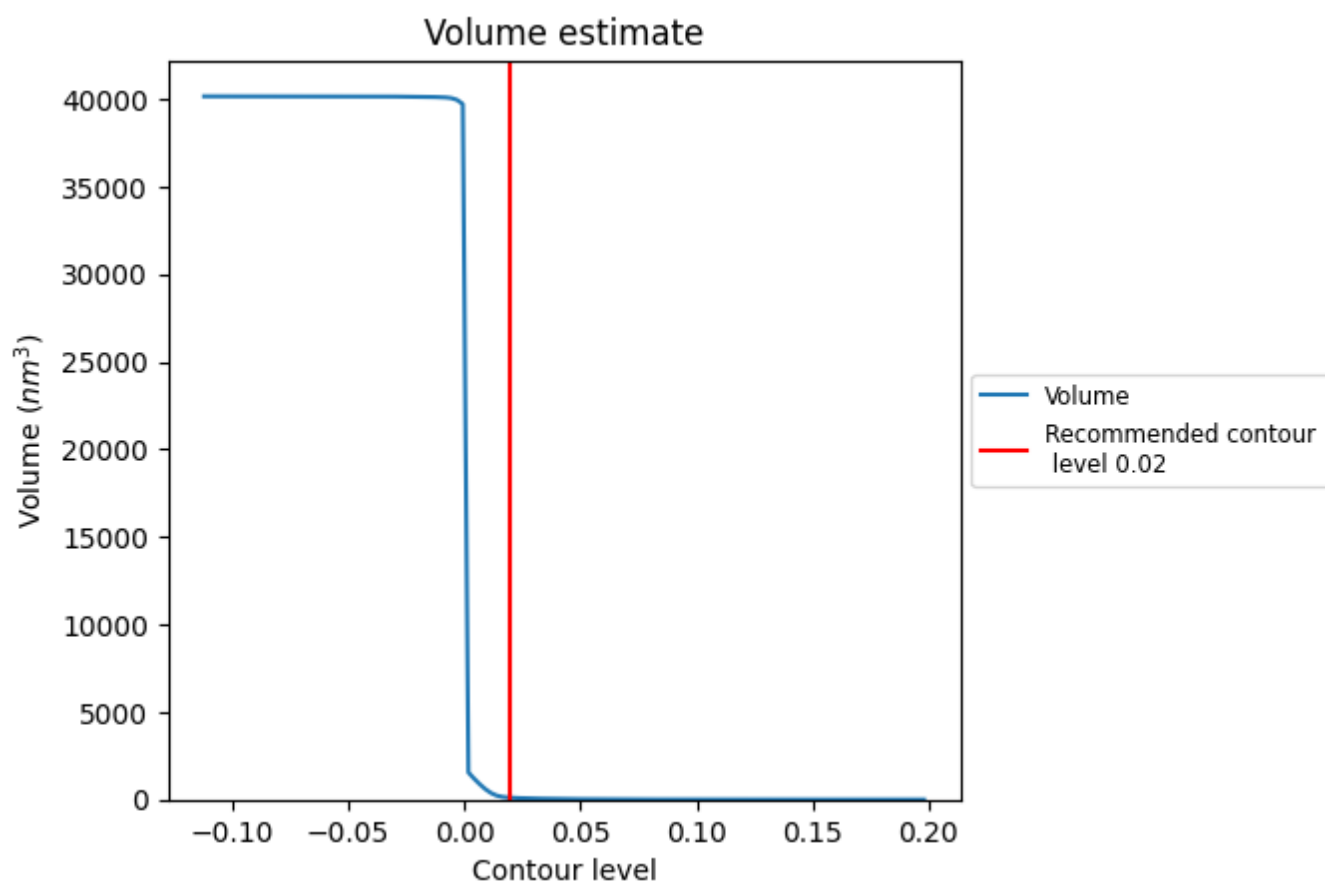
Volume estimate

The volume at the recommended contour level is 108 nm^3; this corresponds to an approximate mass of 97 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ
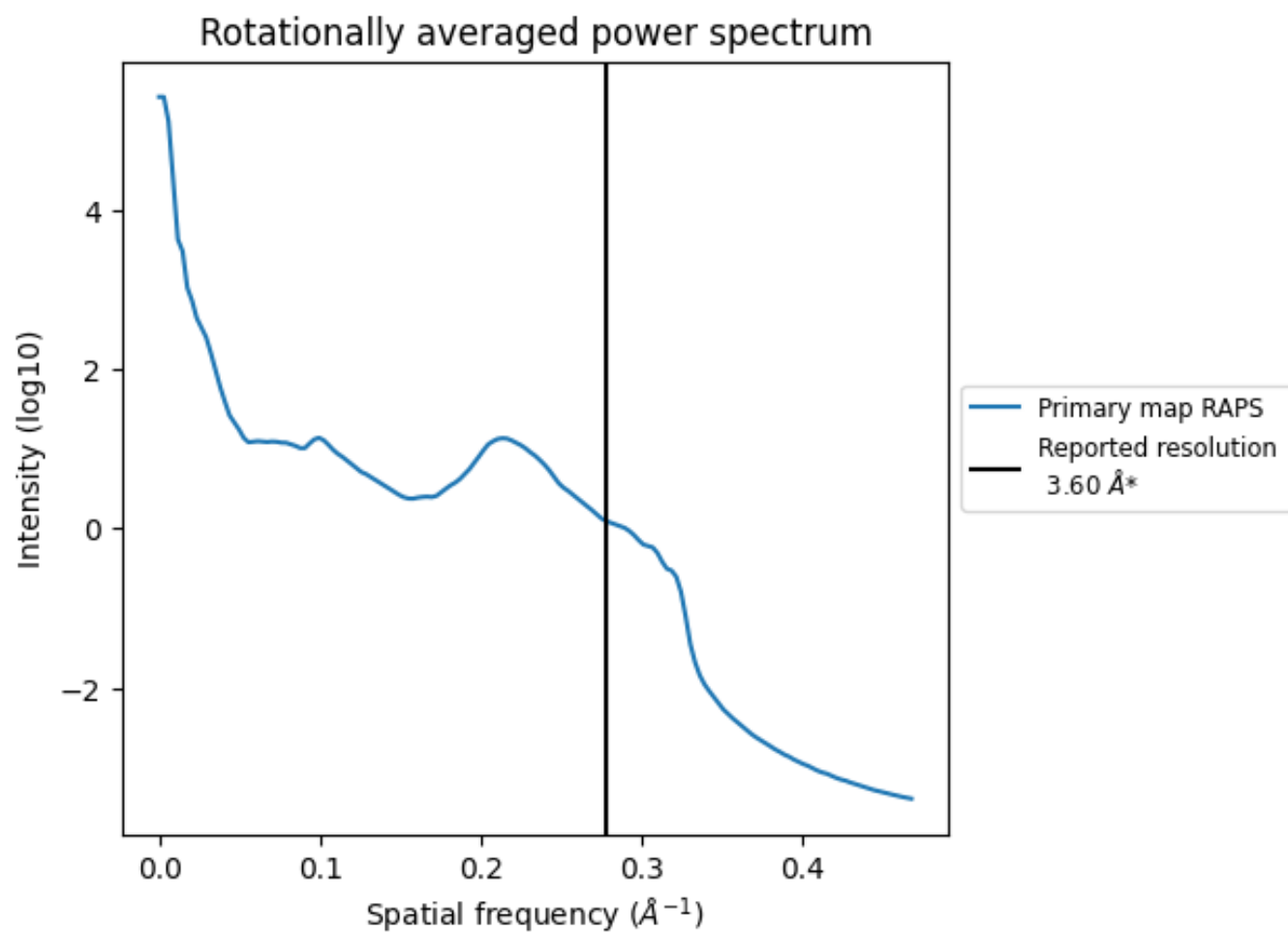
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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)
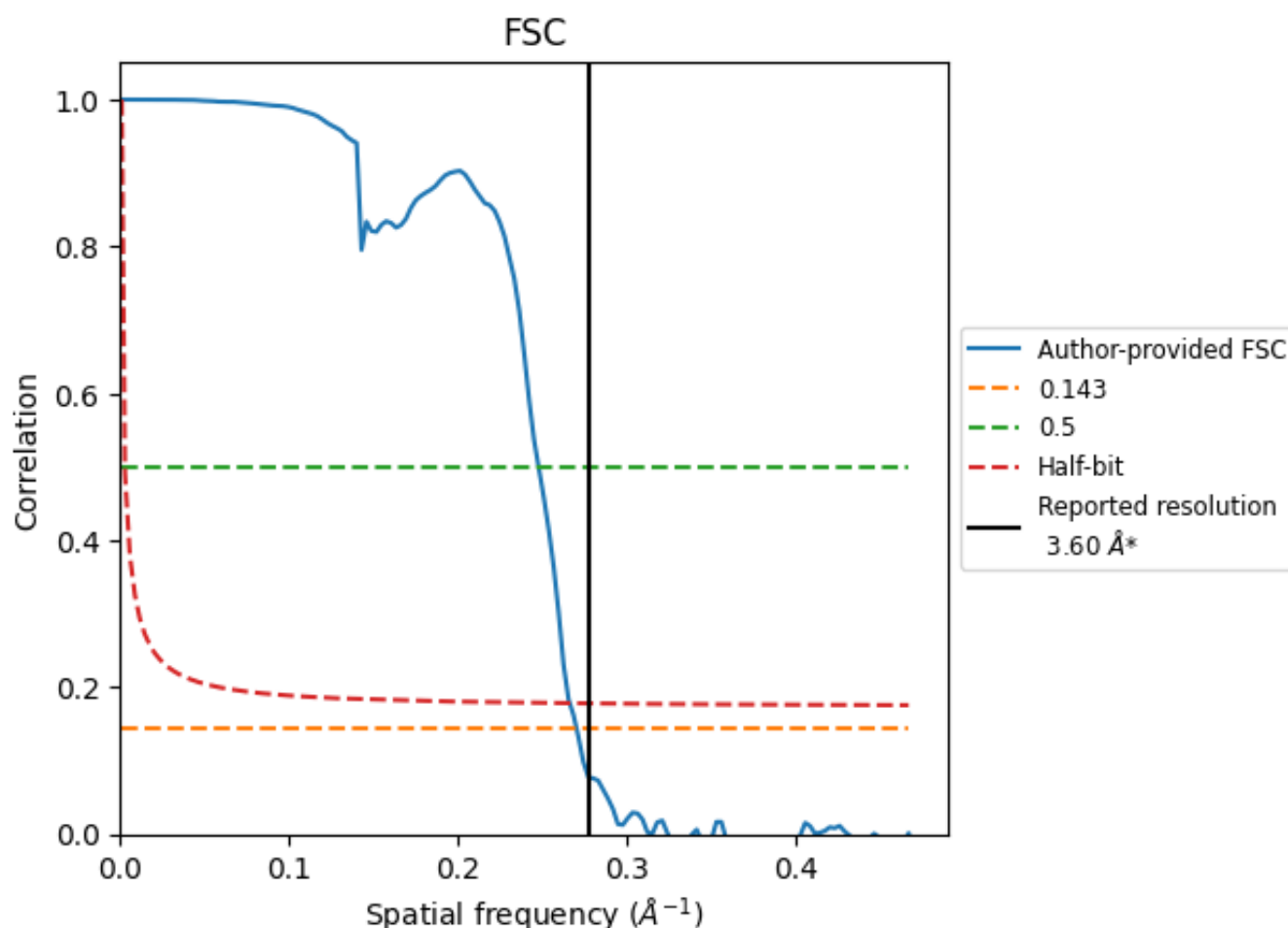
*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates ⓘ

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.70	4.03	3.75
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9   Map-model fit   ⓘ

This section contains information regarding the fit between EMDB map EMD-12806 and PDB model 7OCF. Per-residue inclusion information can be found in section 3 on page 10.

9.1   Map-model overlay   ⓘ
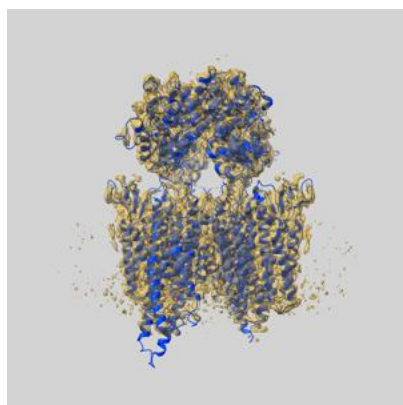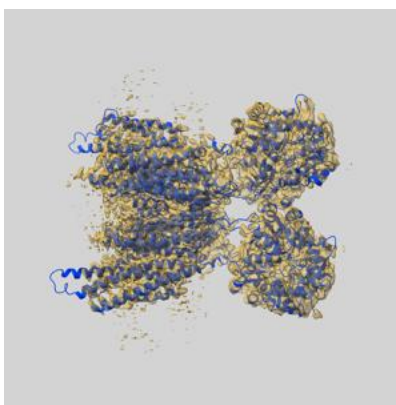
X   Y   Z
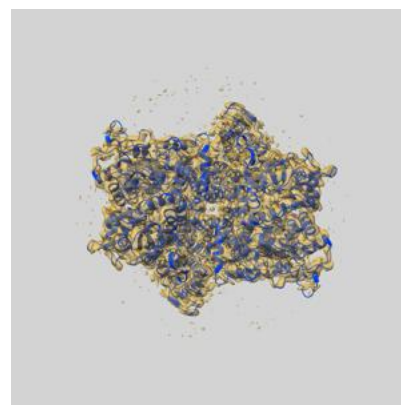
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2   Q-score mapped to coordinate model ⓘ

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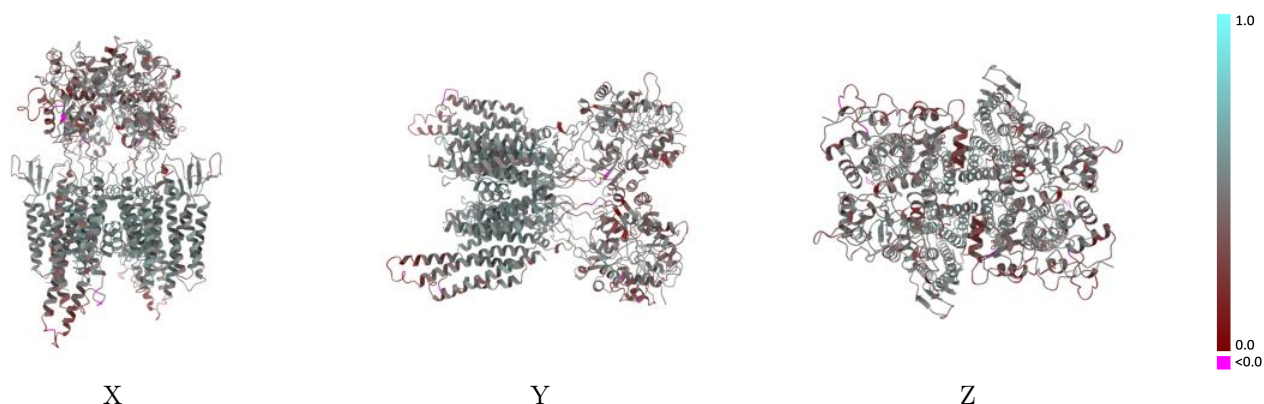
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z
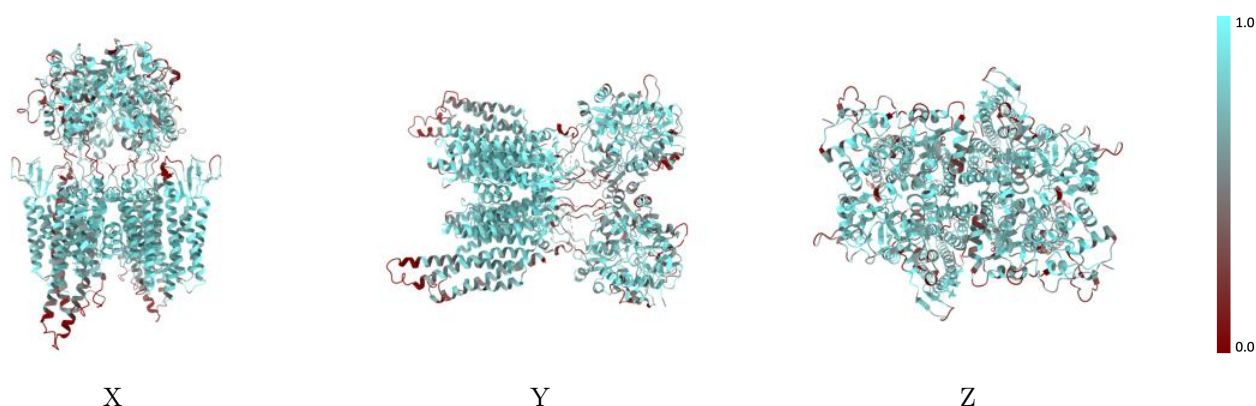
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)
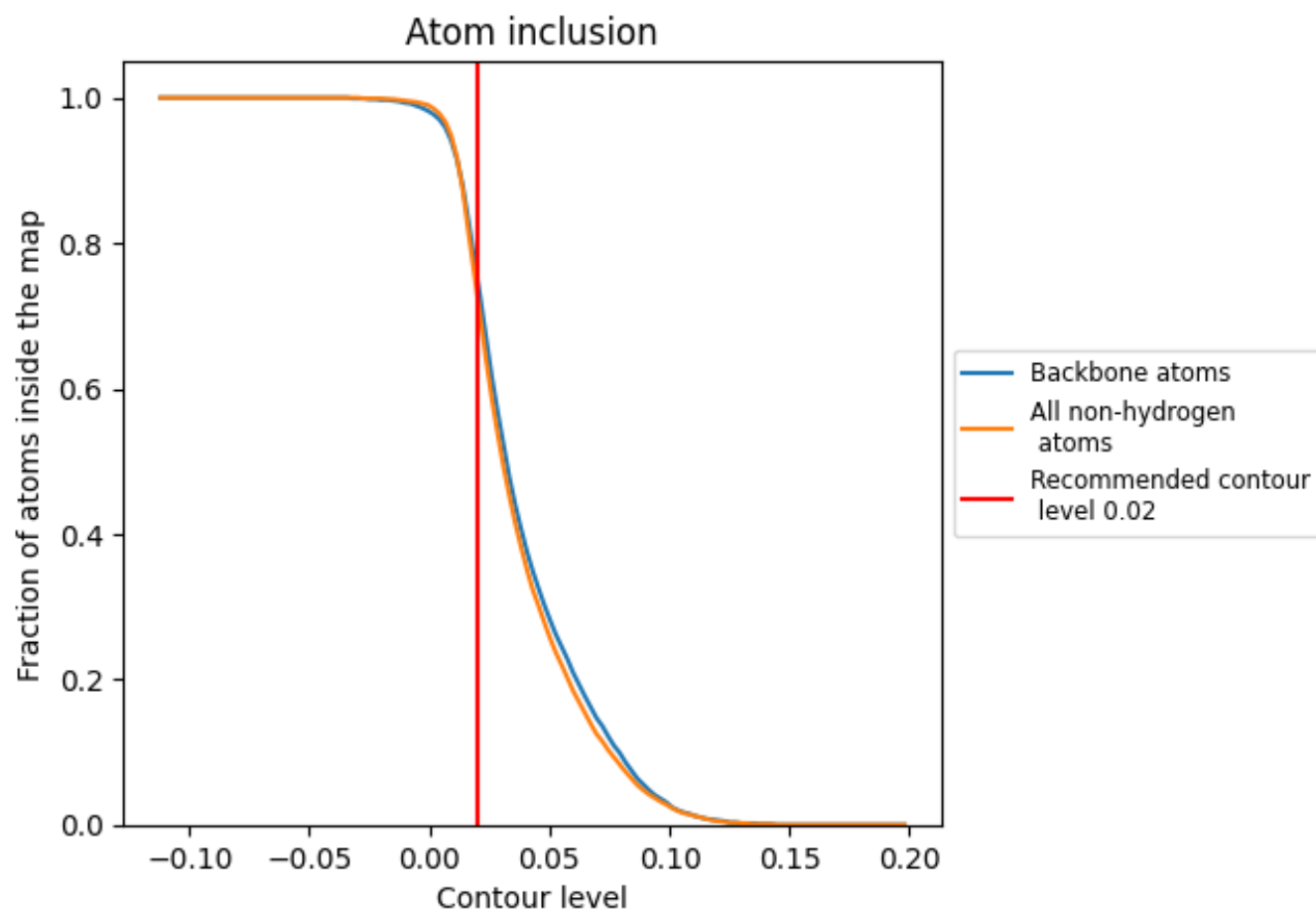
At the recommended contour level, 75% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7280	0.4650
A	0.7220	0.4520
B	0.7700	0.4800
C	0.7260	0.4520
D	0.7770	0.4820
E	0.5740	0.4310
G	0.5490	0.4250
I	0.7860	0.4880
J	0.7860	0.4880

1.0

0.0

<0.0