



wwPDB EM Validation Summary Report ⓘ

Nov 6, 2022 – 12:16 AM JST

PDB ID : 7XJ2
EMDB ID : EMD-33217
Title : Structure of human TRPV3_G573S in complex with Trpvicin in C4 symmetry
Authors : Fan, J.; Yue, Z.; Jiang, D.; Lei, X.
Deposited on : 2022-04-14
Resolution : 3.64 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

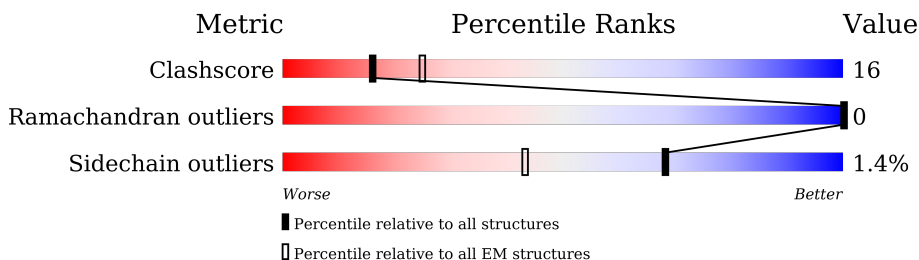
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.64 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	1061	 6% 39% 18% 43%
1	B	1061	 7% 39% 18% 43%
1	C	1061	 6% 39% 18% 43%
1	D	1061	 6% 39% 18% 43%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EQK	A	1101	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EQK	B	1101	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18438 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 Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	607	Total	C	N	O	S	0	0
			4585	3015	763	780	27		
1	C	607	Total	C	N	O	S	0	0
			4575	3011	762	775	27		
1	A	607	Total	C	N	O	S	0	0
			4571	3006	763	775	27		
1	D	607	Total	C	N	O	S	0	0
			4575	3011	762	775	27		

There are 24 discrepancies between the modelled and reference sequences:

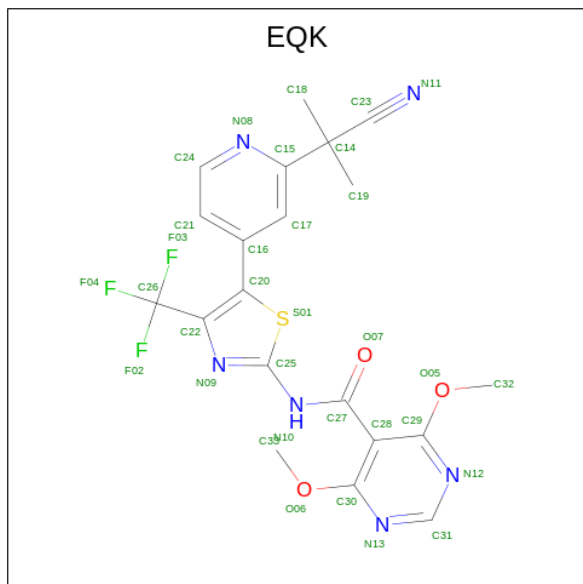
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ILE	VAL	conflict	UNP B2KYM6
B	117	ARG	GLY	conflict	UNP B2KYM6
B	246	LYS	ARG	conflict	UNP B2KYM6
B	247	GLY	GLU	conflict	UNP B2KYM6
B	573	SER	GLY	conflict	UNP B2KYM6
B	772	ASN	ASP	conflict	UNP B2KYM6
C	25	ILE	VAL	conflict	UNP B2KYM6
C	117	ARG	GLY	conflict	UNP B2KYM6
C	246	LYS	ARG	conflict	UNP B2KYM6
C	247	GLY	GLU	conflict	UNP B2KYM6
C	573	SER	GLY	conflict	UNP B2KYM6
C	772	ASN	ASP	conflict	UNP B2KYM6
A	25	ILE	VAL	conflict	UNP B2KYM6
A	117	ARG	GLY	conflict	UNP B2KYM6
A	246	LYS	ARG	conflict	UNP B2KYM6
A	247	GLY	GLU	conflict	UNP B2KYM6
A	573	SER	GLY	conflict	UNP B2KYM6
A	772	ASN	ASP	conflict	UNP B2KYM6
D	25	ILE	VAL	conflict	UNP B2KYM6
D	117	ARG	GLY	conflict	UNP B2KYM6
D	246	LYS	ARG	conflict	UNP B2KYM6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	247	GLY	GLU	conflict	UNP B2KYM6
D	573	SER	GLY	conflict	UNP B2KYM6
D	772	ASN	ASP	conflict	UNP B2KYM6

- Molecule 2 is N-[5-[2-(2-cyanopropan-2-yl)pyridin-4-yl]-4-(trifluoromethyl)-1,3-thiazol-2-yl]-4,6-dimethoxy-pyrimidine-5-carboxamide (three-letter code: EQK) (formula: C₂₀H₁₇F₃N₆O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total 33	C 20	F 3	N 6	O 3	S 1	0
2	C	1	Total 33	C 20	F 3	N 6	O 3	S 1	0
2	A	1	Total 33	C 20	F 3	N 6	O 3	S 1	0
2	D	1	Total 33	C 20	F 3	N 6	O 3	S 1	0

[illegible]

- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP



MET	LYS	ALA	HIS	PRO	LYS	GLU	MET	LEU	GLY	LYS	ARG	VAL	ALA	ALA	PRO	SER	GLY	ASN	PRO	ALA	ILE	LEU	GLU	LYS	ARG	PRO	ALA	ALA	GLU	ILE	THR	PRO	THR	LYS	LYS	SER	ALA	HIS	PHE	PHE	LEU	GLU	ILE	GLU	GLY	PHE	GLU	PRO	PRO	ASN	PRO	THR	VAL	ALA	LYS	THR	SER
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PRO VAL PHE SER LYS PRO MET ASP SER ASN ILE ARG GLN CYS ILE SER GLY ASN CYS ASP ASP MET ASP SER PRO GLN ASP ASP VAL THR THR GLU PRO SER ASN PRO ASN SER PRO SER ALA ALA LEU ALA LYS GLU GLU GLN ARG ARG LYS LYS ARG R118

	E129	G130	C131	V132	E133		V136		V140	R147	R148	R149	H1S	GLU	ASP	P154	P155	D156	F157	L158	M159	H160	K161	L162		D166	T167		L172		L176		N180		T183		V187		L191	A192	F193	A194	E195	E196	N197	D198	I199	L200		F203	L204		Y213	E214	G215	Q216
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L219	C247	A248	F250	G258	F259	T264	A267	R292	G295	N297	N298	L299	L300	H301	A302	L303	V304	A307	E308	Q313	V317	Y321	D322	L325	L326	R330	W331	E332	L333	E334	T335	T336	R337	G341	L342	T343	Q346	L347	A348	A349	K350
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K363
I366
I360
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S362
S363
E364
I365
L373
S374
R375
K376
F377
T378
D379
W380
S387
Y390
D391
L392
T393
D396
T399
D400
V403
L404
E405
V408
V409
N410
R416
H417
E418
M419
L420
T421
L425
W433
K434
K435
F436
A437
M440
F441
F445

Y448	T456	Y460	R464	GLU	GLU	GLU	ALA	ILE	PRO	PRO	PRO	LEU	ALA	LEU	THR	HIS	LYS	MET	G480	W481	L482	Q483	L484	L485	G486	G487	M488	I492	W493	G494	M495	G496	I497	S498	V499	K500	E501	I505	F506	L507	L508	ARG	PRO	SER	ASP	LEU	GLN	SER	ILE	LEU	S518	F522
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V525	F526	F527	F528	F529	F530	F531	F532	F533	F534	F535	F536	F537	F538	F539	F540	F541	F542	F543	F544	F545	F546	F547	F548	F549	F550	F551	F552	F553	F554	F555	F556	F557	F558	F559	F560	F561	F562	F563	F564	F565	F566	F567	F568	F569	F570	F571	F572	F573	F574	F575	F576	F577	F578	F579	F580	F581	F582	F583	F584	F585	F586	F587	F588	F589	F590	F591	F592	F593	F594	F595	F596	F597	F598	F599	F600	F601	F602	F603	F604	F605	F606	F607	F608
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I609	E610	K611	P612	P613	LYS ASP	N616	K617	D618	C619	S620	S621	F625	E631	L632	F633	K634	L635	T636	I637	G638	D641	L642	N643	I644	Q645	Q646	N647	S648	K649	F654	L658	Y661	L664	T665	F666	V667	L668	L669	L670	N671	M672	L673	I674	A675	L676	M677	G678	E679	T680	F681	F682
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[illegible]

THR	THR	LEU	LEU	ASN	ALA	PHE	GLU	GLU	VAL	GLU	PHE	PRO	GLU	THR	SER	VAL	LEU	GLU	VAL	PHE	GLN	GLY	PRO	SER	LYS	GLY	GLU	GLU	LEU	PHE	THR	GLY	VAL	VAL	PRO	PRO	ILE	LEU	LEU	VAL	GLU	LEU	ASP	GLY	ASP	VAL	ASN	GLY	HIS	LYS	PHE	SER	VAL	ARG	GLY	GLU	GLY	GLU	GLY	ASP
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ALA	THR	ASN	GLY	LYS	LEU	THR	LEU	LEU	PHE	ILE	CYS	THR	THR	GLY	LYS	LEU	LEU	PRO	PRO	TRP	PRO	THR	THR	LEU	VAL	LEU	THR	THR	TYR	GLY	VAL	GLN	CYS	CYS	PHE	SER	ARG	ARG	TYR	PRO	PRO	ASP	HIS	HIS	MET	LYS	ARG	HIS	ASP	PHE	PHE	PHE	LYS	SER	ALA	ALA	MET	PRO	PRO	GLU	GLY	TYR	VAL	GLN	VAL	GLU	GLU	ARG
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- Molecule 1: Fusion protein of Transient receptor potential cation channel subfamily V member 3 and 3C-GFP



PRO	ASN	GLU	LYS	ARG	ASP	HIS	MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	HIS	GLY	MET	ASP	GLU	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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- Chain D:  6% 39% 18% 43%

[illegible]

Q277 I230 I230 F249 F250 F258 F259 Y260 T264 T267 A267 L268 D288 S291 R292 R295 G296 N297 N298 I299 L300 L300 H301 A302 L303 V304 A307 E308 Q313 Q317 V317 Y321 L326 R327 R328 G329 N330 N331 A331 E332 L333 E334 T335 T336 R337 T343 Q346 L347 A348 Q349

K350	K353	I356	I360	R363	E364	I365	L373	S374	F377	T378	D379	W380	S387	Y390	D391	L392	T393	D396	V403	L404	E405	V408	Y409	N410	R416	H417	E418	M419	L420	T421	L425	K432	W433	K434	K435	F436	A437	M440	F441	S444	F445
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[illegible]

Year	Value	Category
1952	1526	Green
1953	1533	Green
1954	1539	Green
1955	1540	Green
1956	1541	Green
1957	1542	Green
1958	1543	Green
1959	1544	Green
1960	1545	Green
1961	1546	Green
1962	1547	Green
1963	1548	Green
1964	1552	Green
1965	1553	Green
1966	1554	Green
1967	1559	Green
1968	1562	Green
1969	1565	Green
1970	1566	Green
1971	1567	Green
1972	1568	Green
1973	1569	Green
1974	1570	Green
1975	1571	Green
1976	1572	Green
1977	1573	Green
1978	1577	Green
1979	1581	Green
1980	1582	Green
1981	1583	Green
1982	1586	Green
1983	1587	Green
1984	1588	Green
1985	1589	Green
1986	1590	Green
1987	1597	Orange
1988	1598	Orange
1989	1599	Orange
1990	1605	Orange
1991	1606	Orange
1992	1607	Orange
1993	1603	Orange
1994	1604	Orange
1995	1605	Orange
1996	1606	Orange
1997	1607	Orange

L608	L609	E610	K611	C612	P613	LYS	ASP	N616	K617	D618	C619	S620	S621	Y622	F625	A628	E631	L632	T636	G638	L639	G640	D641	T644	G645	G646	M647	S648	K649	F654	Y661	L664	T665	F666	L668	L669	L670	M671	M672	L673	L674	A675	L676	M677	G678	E679	T680	V681	S682
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E687	R690	I691	W692	Q695	R696	A697	R698	L701	F702	F703	E704	L707	W710	L711	L712	S713	R714	F715	R716	M717	V723	A724	E725	R729	I734	L749	G75A	PRO	VAL	ARG	ARG	THR	THR	ALA	ASP	PHE	ASN	LYS	ILE	GLN	ASP	SER	SER	ARG	ASN	ASN	SER	LYS	THR
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THR	LEU	ASN	ALA	PHE	GLU	GLU	VAL	GLU	PHE	PRO	THR	GLU	LEU	VAL	GLN	GLY	GLY	LYS	SER	PRO	GLU	GLU	LEU	VAL	GLN	GLY	GLY	THR	PHE	GLU	GLU	VAL	VAL	VAL	PRO	ILE	LEU	VAL	VAL	GLU	GLU	LEU	ASP	GLY	ASP	GLY	VAL	ASN	GLY	HIS	LYS	PHE	SER	VAL	VAL	ARG	GLY	GLU	GLY	GLY	GLY	ASP	ALA
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THR	ASN	GLY	LYS	LEU	THR	LEU	LYS	PHE	ILE	CYS	THR	THR	GLY	LEU	PRO	VAL	PRO	PRO	THR	THR	LEU	VAL	THR	THR	THR	TYR	GLY	VAL	GLN	CYS	PHE	SER	ARG	TYR	PRO	ASP	HIS	HIS	MET	MET	LYS	ARG	HIS	ASP	PHE	PHE	LYS	SER	ALA	MET	PRO	PRO	GLU	GLY	TYR	VAL	GLN	GLU	ARG	THR
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ILE	SER	PHE	ASP	LYS	ASP	GLY	THR	TYR	THR	ARG	ALA	GLU	VAL	LYS	PHE	GLU	GLY	ASP	THR	LEU	VAL	ASN	ARG	ILE	GLU	LEU	LYS	GLY	ILE	ASP	PHE	LYS	GLU	ASP	ASN	GLY	HIS	LYS	LEU	GLU	TYR	ASN	ASN	PHE	ASN	HIS	SER	HIS	ASN	VAL	TYR	ILE	THR	ALA	ASP	LYS	GLN
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LYS ASN GLY ILE LYS LYS ASN PHE LYS ILE ARG HIS ASN VAL GLU ASP GLY SER VAL GLN LEU ALA ASP HIS ASP TYR GLN GLN ASN THR THR PRO PRO ILE GLY ASP GLY PRO VAL LEU LEU LEU LEU ASP ASP ASN HIS TYR LEU LEU THR THR GLN SER VAL VAL LEU LEU SER SER LYS LYS ASN ASN GLU GLU LYS LYS ARG ASP ASP HIS

MET	VAL	LEU	LEU	GLU	PHE	VAL	THR	ALA	ALA	GLY	ILE	THR	HIS	GLY	MET	ASP	GLU	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS	GLY	GLY	GLY	SER	GLY	GLY	SER	GLY	GLY	SER	GLY	SER	ALA	TRP	SER	HIS	PRO	GLN	PHE	GLU	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	48492	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.076	Depositor
Minimum map value	-1.208	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.36	Depositor
Map size (\AA)	266.24, 266.24, 266.24	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.04, 1.04, 1.04	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: EQK

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	0.30	0/4668	0.45	0/6353
1	B	0.28	0/4683	0.43	0/6373
1	C	0.28	0/4673	0.43	0/6360
1	D	0.30	0/4673	0.43	0/6360
All	All	0.29	0/18697	0.43	0/25446

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4571	0	4409	155	0
1	B	4585	0	4422	143	0
1	C	4575	0	4412	155	0
1	D	4575	0	4412	147	0
2	A	33	0	0	10	0
2	B	33	0	0	11	0
2	C	33	0	0	7	0
2	D	33	0	0	0	0
All	All	18438	0	17655	579	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 16.

The worst 5 of 579 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:B:583:ILE:HG23	2:B:1101:EQK:C18	1.76	1.15
1:A:620:SER:OG	1:A:646:GLN:HA	1.54	1.06
1:B:583:ILE:HD12	2:B:1101:EQK:C18	1.89	1.02
1:B:583:ILE:CG2	2:B:1101:EQK:C18	2.42	0.97
1:A:620:SER:HG	1:A:646:GLN:HA	1.31	0.94

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	A	597/1061 (56%)	556 (93%)	41 (7%)	0	100	100
1	B	597/1061 (56%)	555 (93%)	42 (7%)	0	100	100
1	C	597/1061 (56%)	557 (93%)	40 (7%)	0	100	100
1	D	597/1061 (56%)	554 (93%)	43 (7%)	0	100	100
All	All	2388/4244 (56%)	2222 (93%)	166 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/934 (46%)	424 (98%)	9 (2%)	53	77
1	B	436/934 (47%)	435 (100%)	1 (0%)	93	98
1	C	433/934 (46%)	426 (98%)	7 (2%)	62	82
1	D	433/934 (46%)	425 (98%)	8 (2%)	59	80
All	All	1735/3736 (46%)	1710 (99%)	25 (1%)	68	84

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	676	LEU
1	D	213	TYR
1	D	692	TRP
1	A	704	GLU
1	D	264	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	205	ASN
1	D	570	GLN
1	D	279	GLN
1	D	313	GLN
1	C	284	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

4 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
2	EQK	C	1101	-	29,35,35	4.87	19 (65%)	33,52,52	2.33	13 (39%)
2	EQK	B	1101	-	29,35,35	4.87	19 (65%)	33,52,52	2.28	13 (39%)
2	EQK	A	1101	-	29,35,35	4.86	19 (65%)	33,52,52	2.28	13 (39%)
2	EQK	D	1101	-	29,35,35	4.81	19 (65%)	33,52,52	2.16	10 (30%)

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
2	EQK	C	1101	-	-	3/26/31/31	0/3/3/3
2	EQK	B	1101	-	-	4/26/31/31	0/3/3/3
2	EQK	A	1101	-	-	6/26/31/31	0/3/3/3
2	EQK	D	1101	-	-	8/26/31/31	0/3/3/3

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	EQK	C31-N12	8.46	1.49	1.33
2	B	1101	EQK	C31-N12	8.44	1.49	1.33
2	A	1101	EQK	C31-N12	8.44	1.49	1.33
2	C	1101	EQK	C31-N13	8.40	1.49	1.33
2	A	1101	EQK	C31-N13	8.40	1.49	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	EQK	N13-C31-N12	-5.78	119.55	128.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	EQK	N13-C31-N12	-5.73	119.63	128.60
2	B	1101	EQK	N13-C31-N12	-5.71	119.67	128.60
2	A	1101	EQK	N13-C31-N12	-5.69	119.69	128.60
2	C	1101	EQK	C26-C22-N09	5.29	126.01	119.69

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

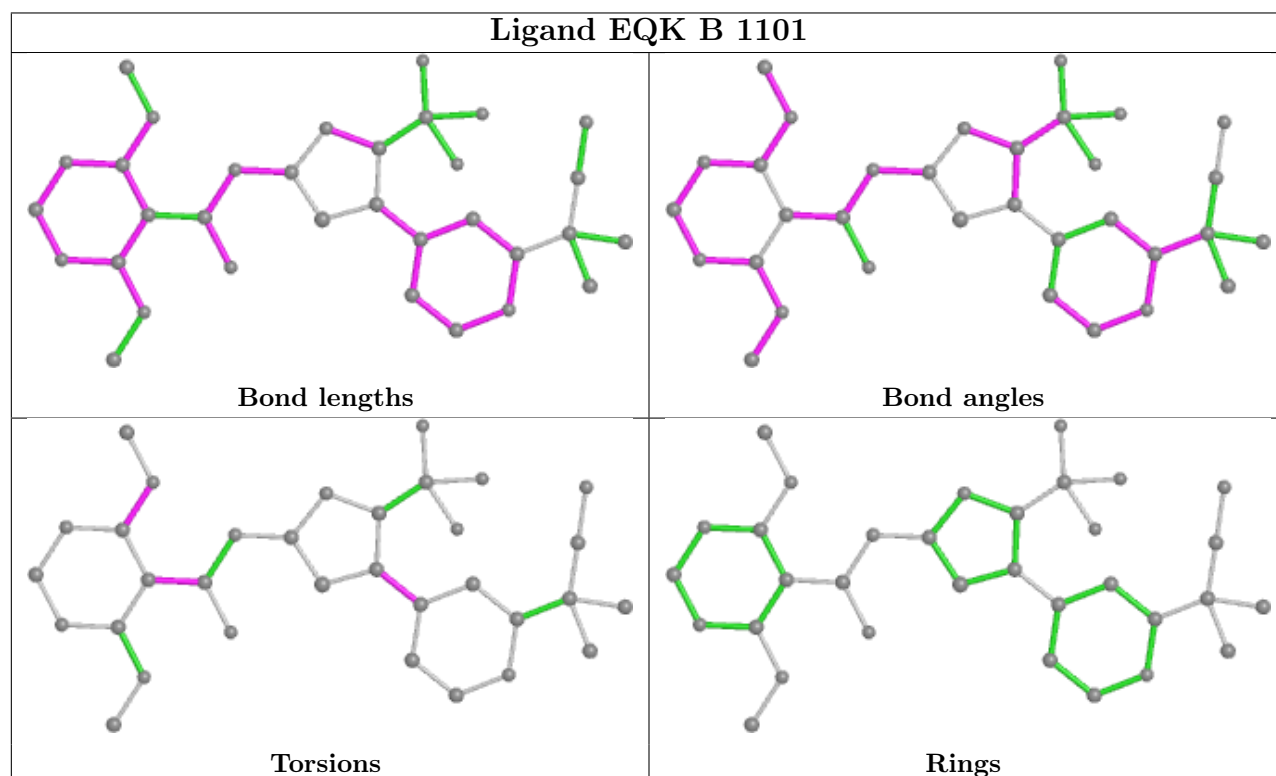
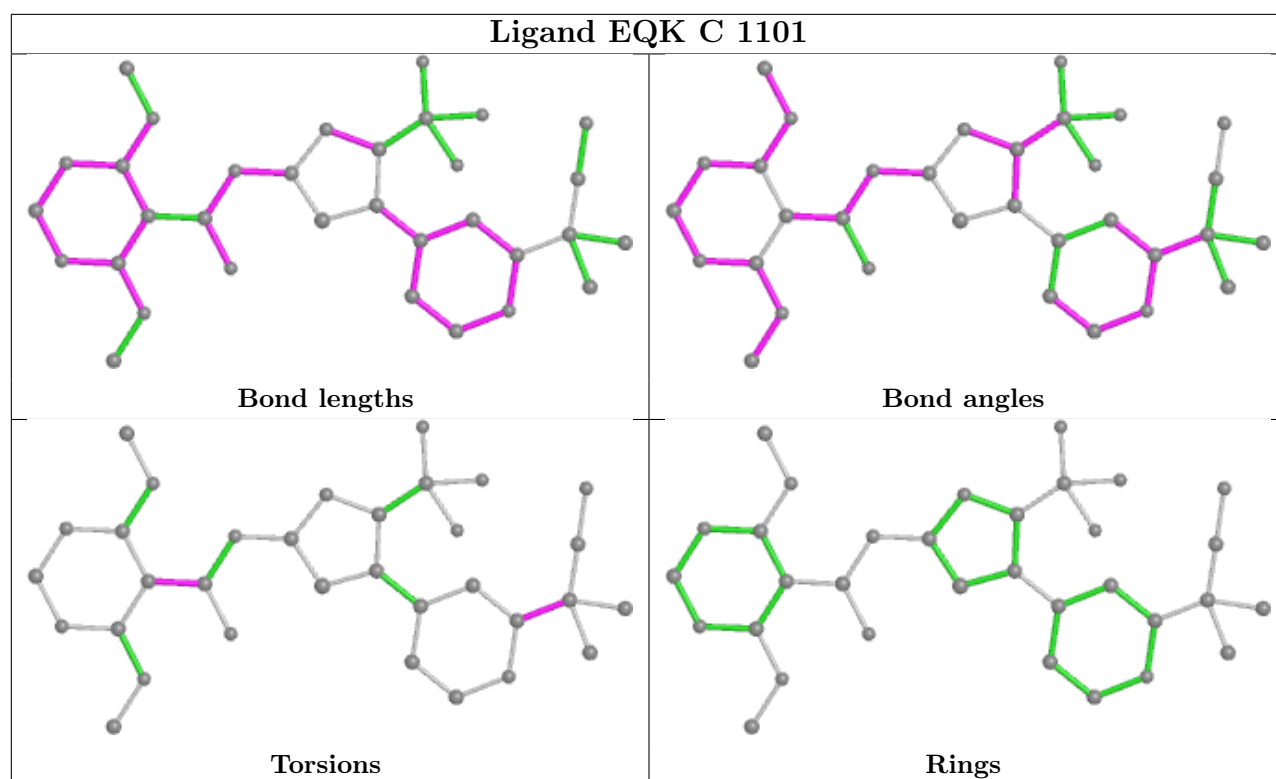
Mol	Chain	Res	Type	Atoms
2	B	1101	EQK	N12-C29-O05-C32
2	C	1101	EQK	O07-C27-C28-C29
2	A	1101	EQK	C28-C29-O05-C32
2	D	1101	EQK	N09-C22-C26-F04
2	B	1101	EQK	C28-C29-O05-C32

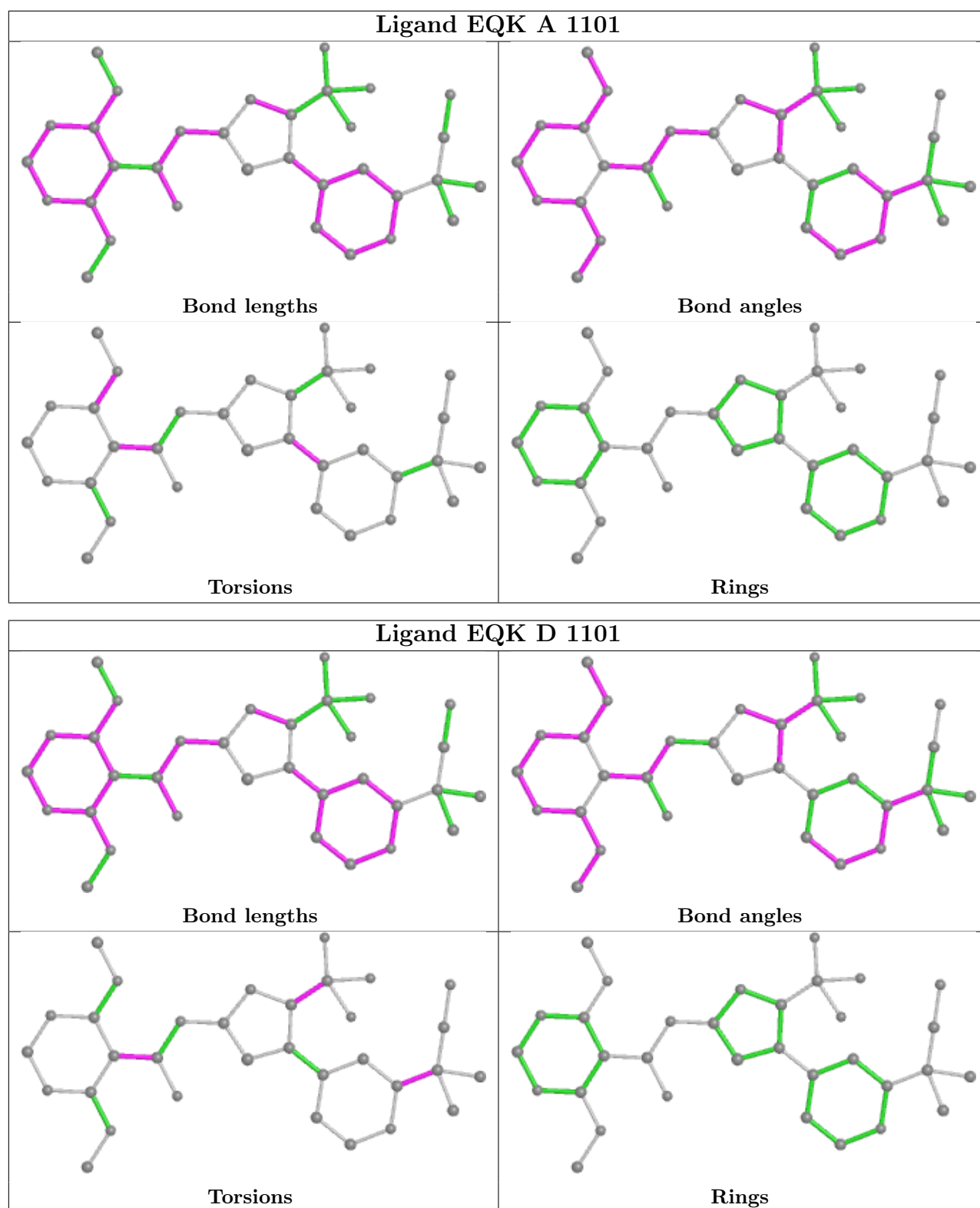
There are no ring outliers.

3 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	EQK	7	0
2	B	1101	EQK	11	0
2	A	1101	EQK	10	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

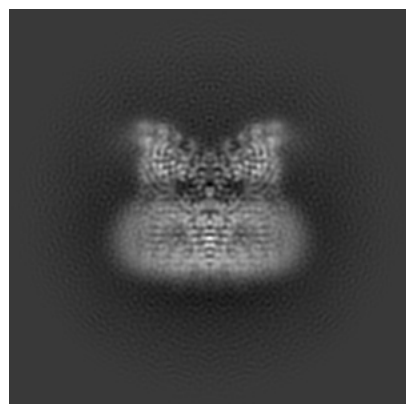
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33217. These allow visual inspection of the internal detail of the map and identification of artifacts.

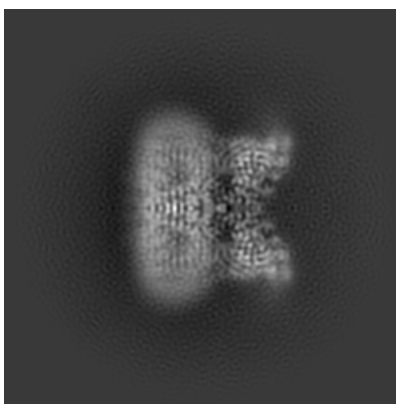
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

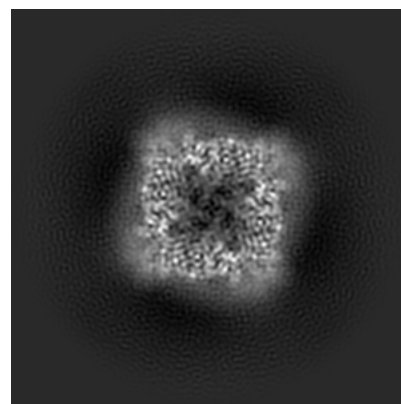
6.1.1 Primary map



X

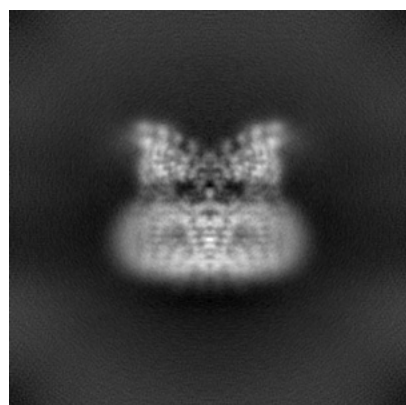


Y

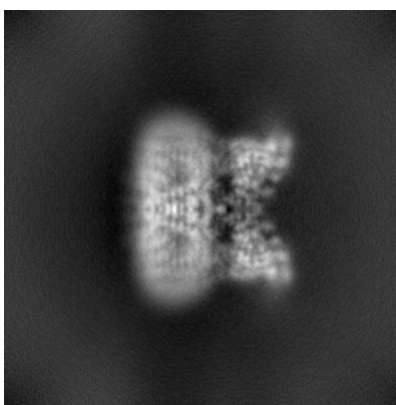


Z

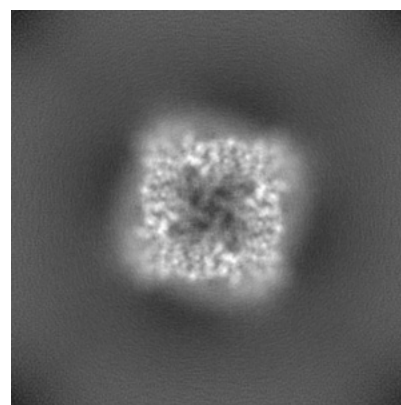
6.1.2 Raw map



X



Y

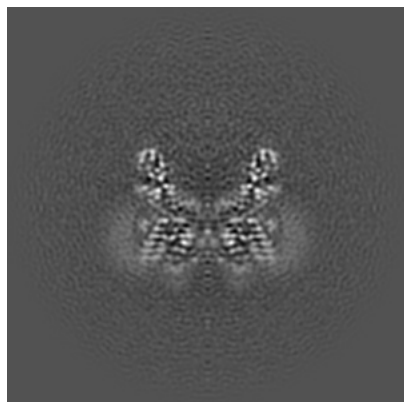


Z

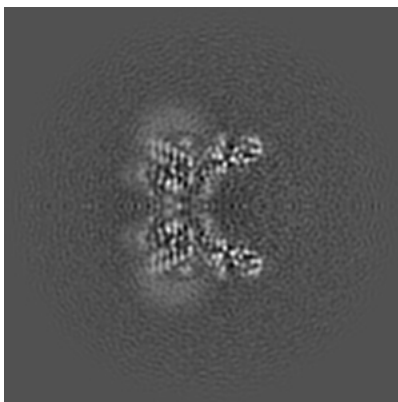
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

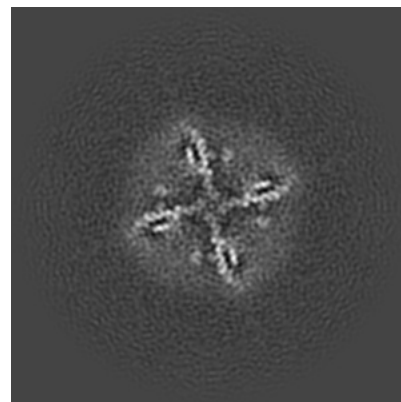
6.2.1 Primary map



X Index: 128

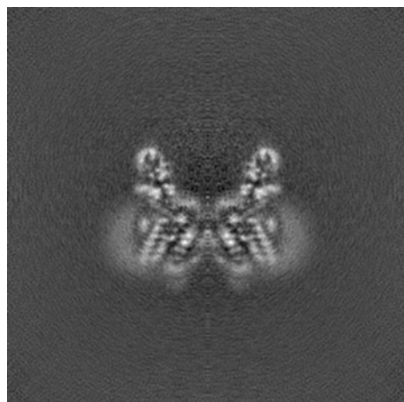


Y Index: 128

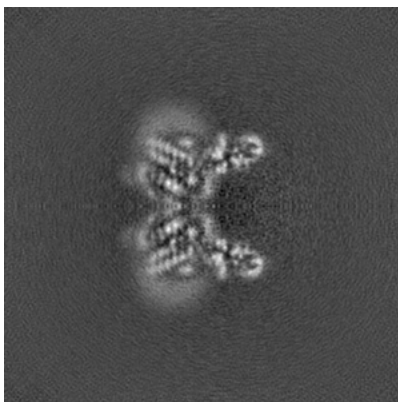


Z Index: 128

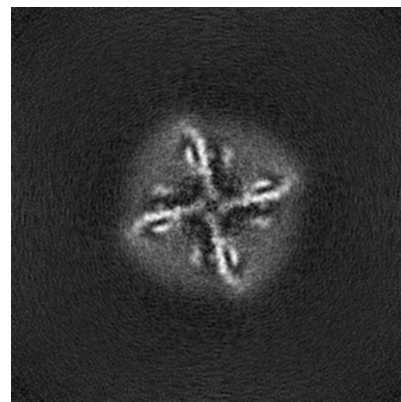
6.2.2 Raw map



X Index: 128



Y Index: 128

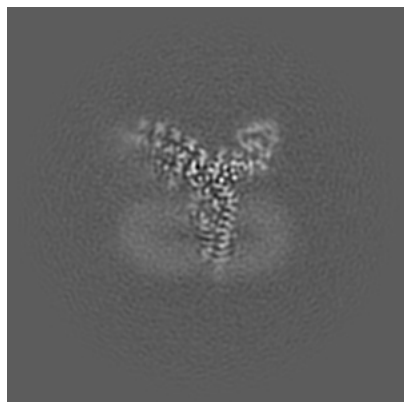


Z Index: 128

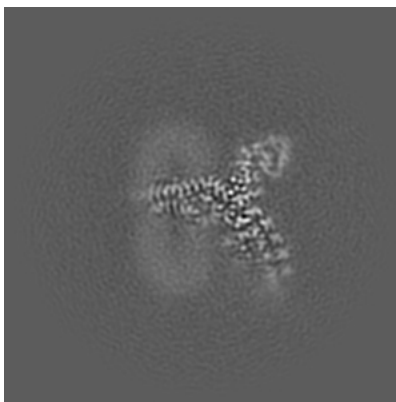
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

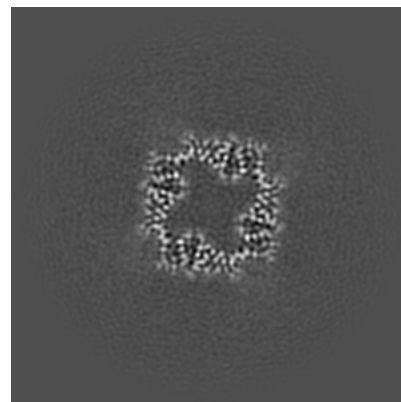
6.3.1 Primary map



X Index: 159

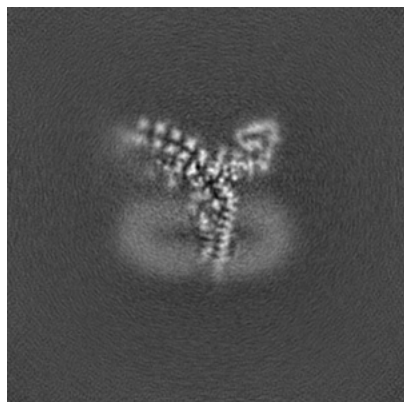


Y Index: 97

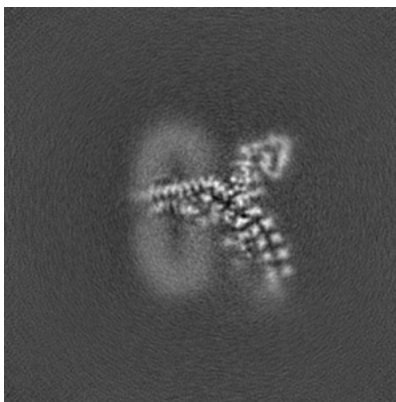


Z Index: 155

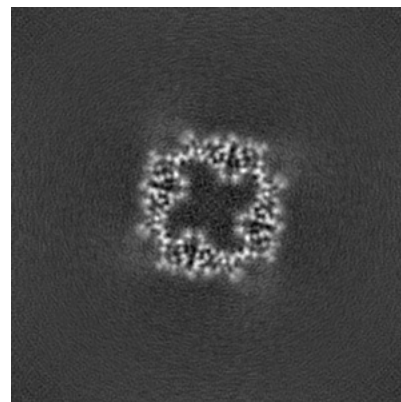
6.3.2 Raw map



X Index: 159



Y Index: 97

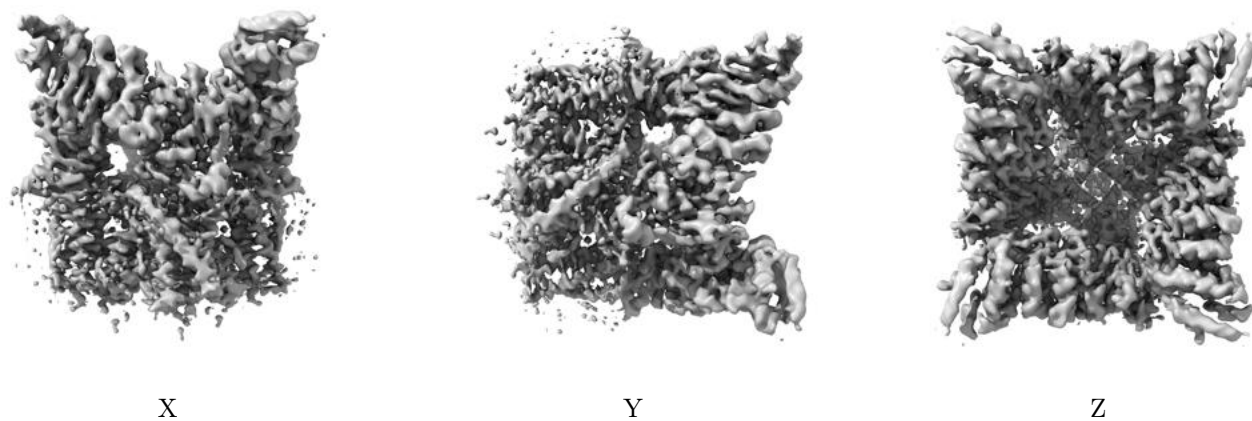


Z Index: 155

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

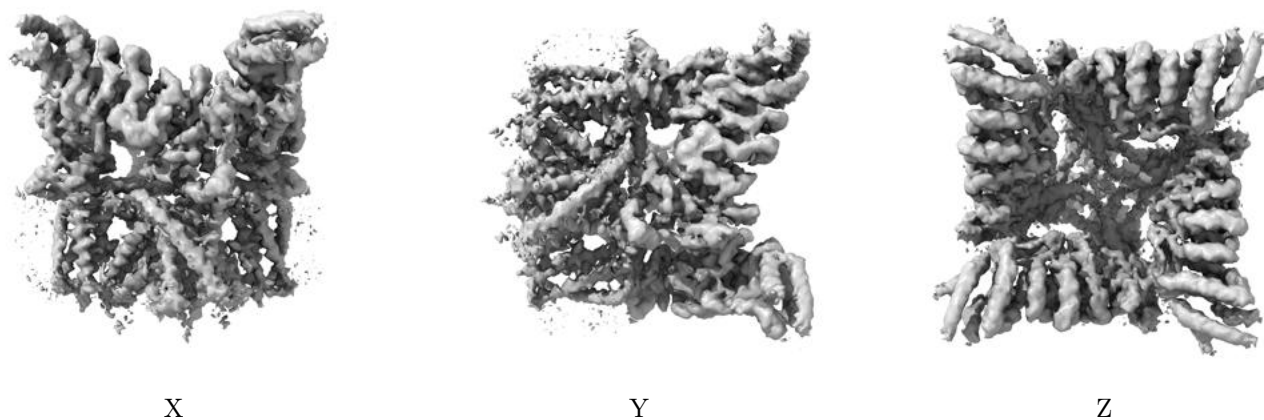
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

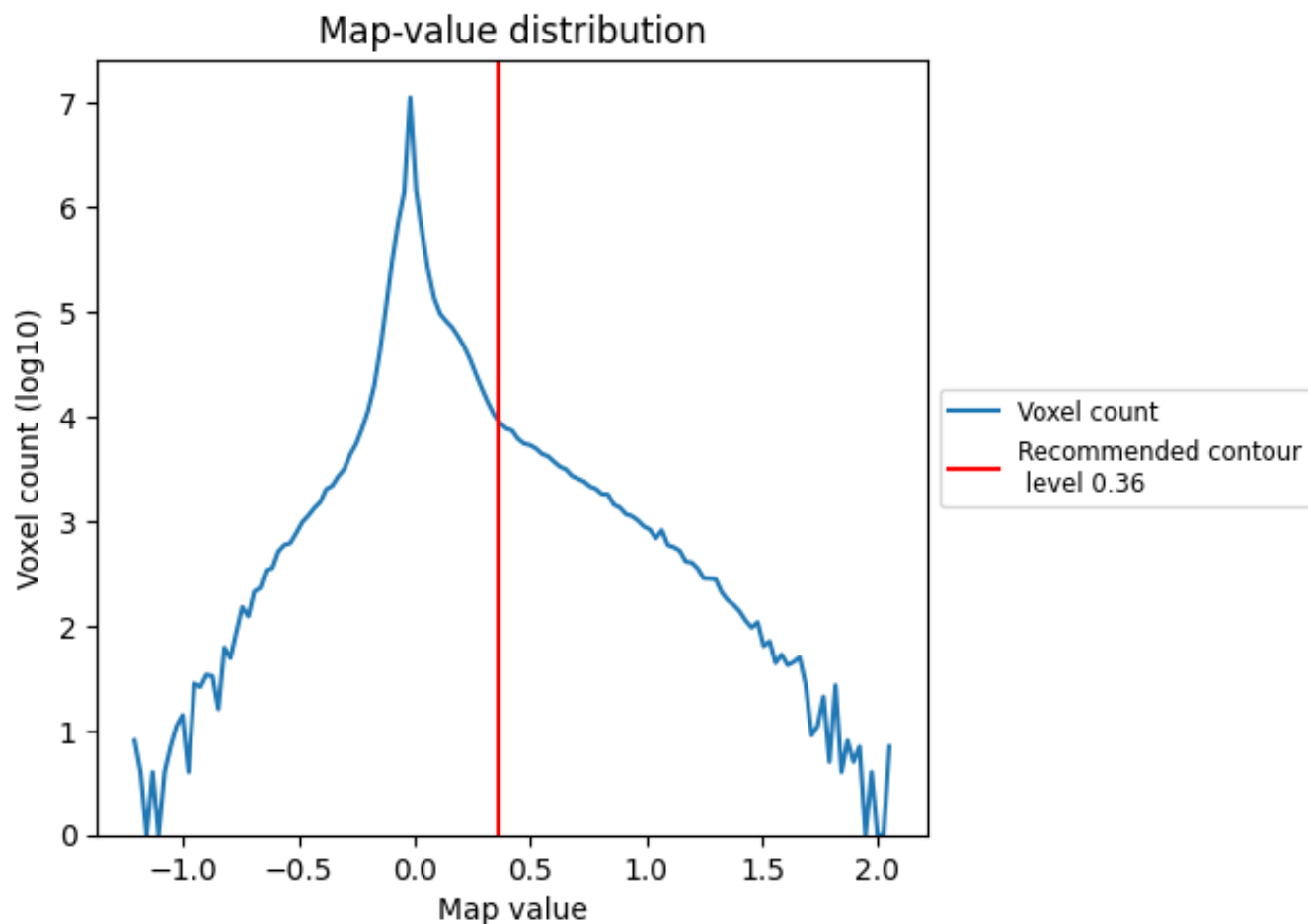
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

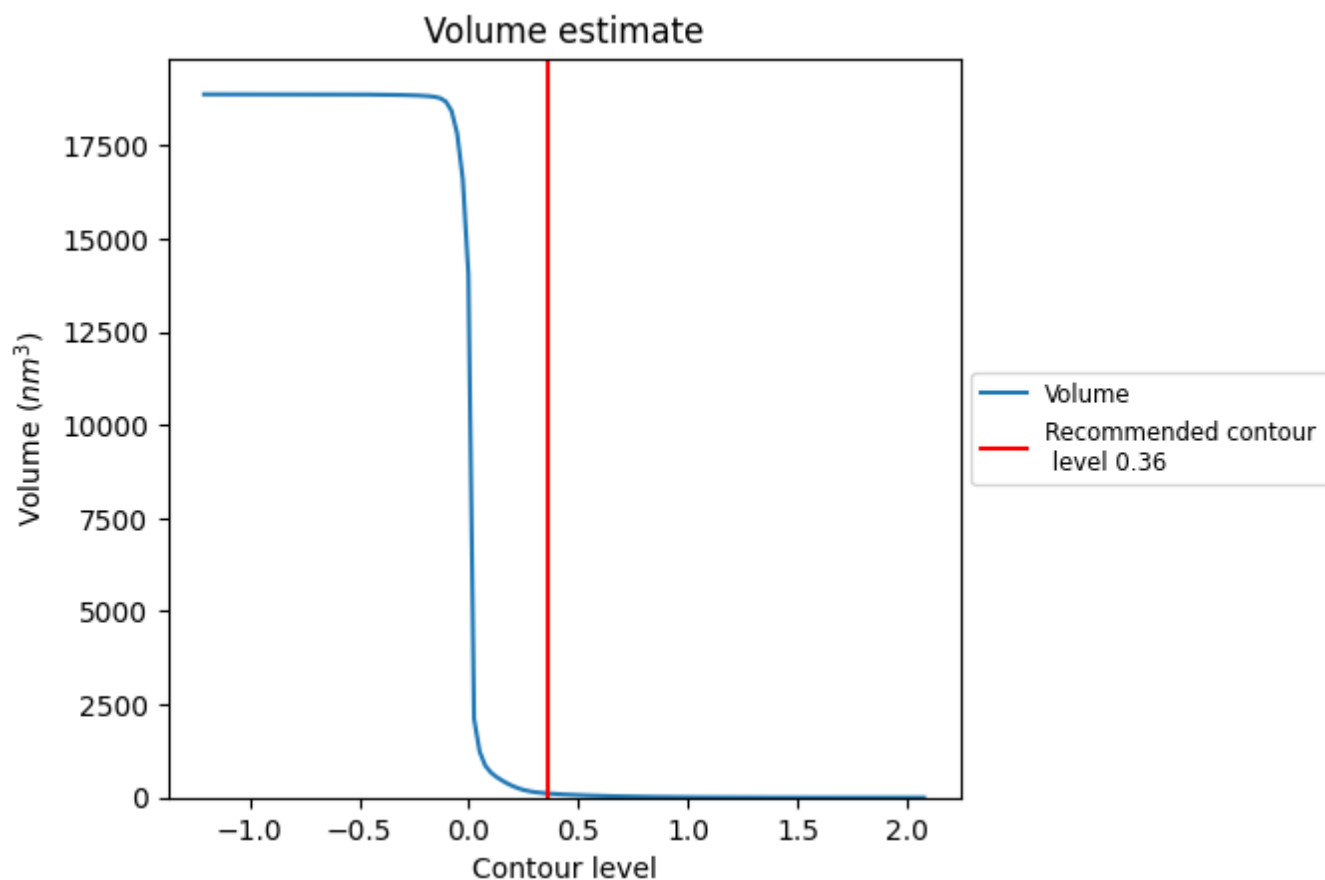
This section contains the results of statistical analysis of the map.

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.

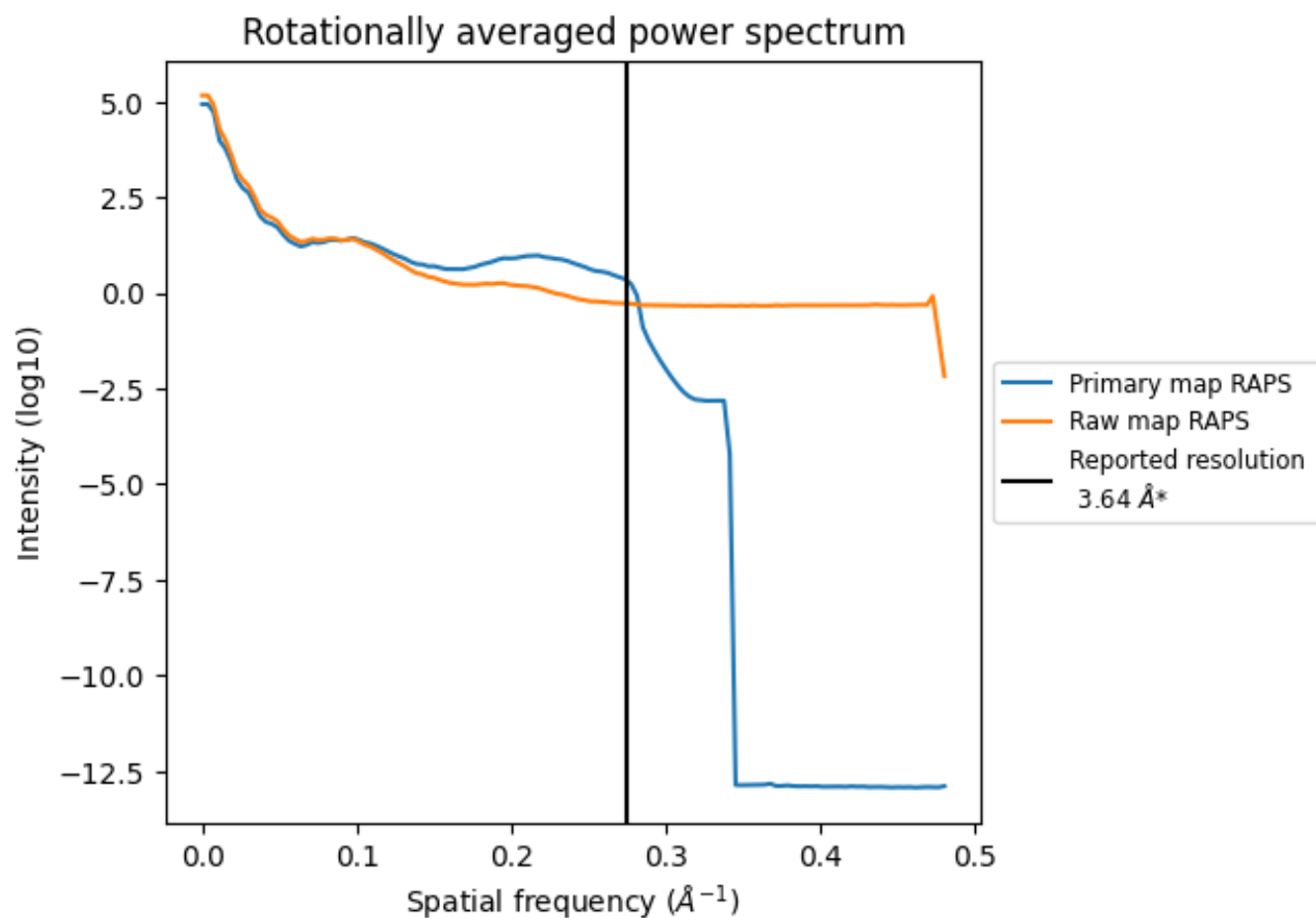
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 110 nm³; this corresponds to an approximate mass of 99 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 ⓘ

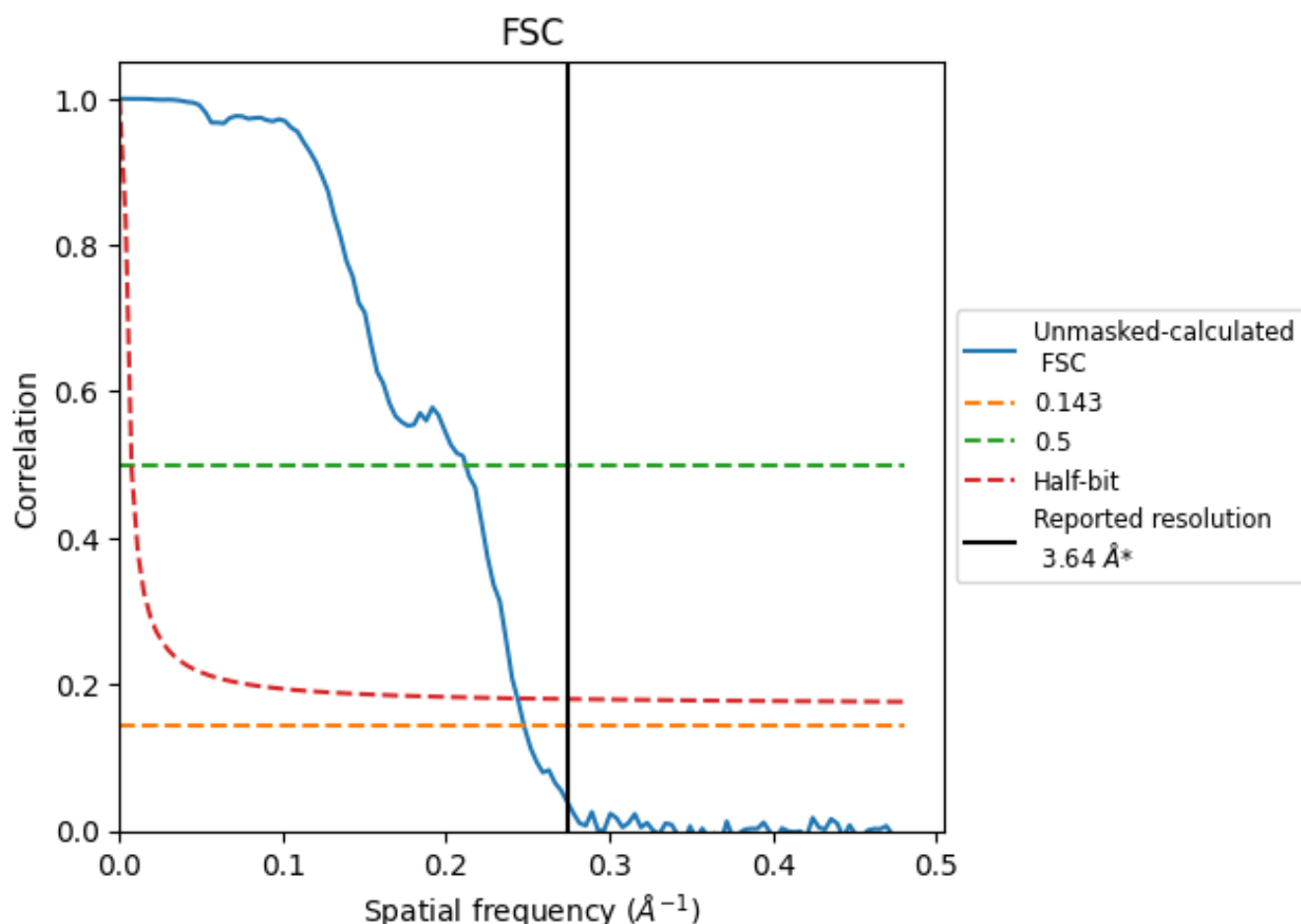


*Reported resolution corresponds to spatial frequency of 0.275 Å⁻¹

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 0.275 Å⁻¹

8.2 Resolution estimates [i](#)

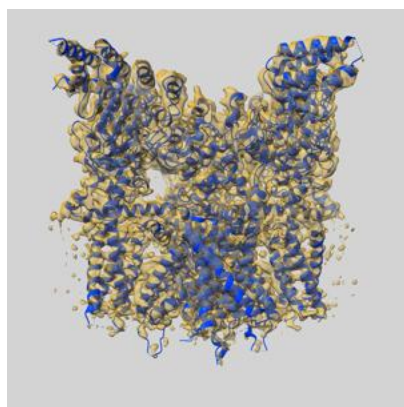
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.64	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.04	4.72	4.10

*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 4.04 differs from the reported value 3.64 by more than 10 %

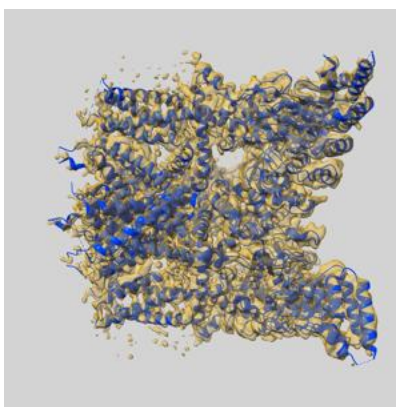
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-33217 and PDB model 7XJ2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

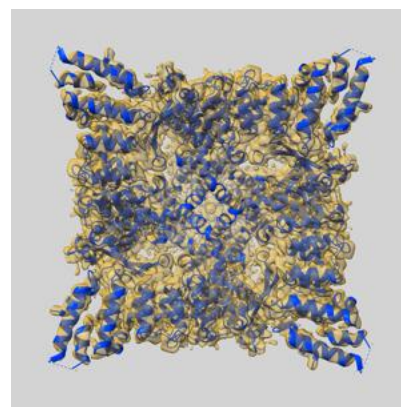
9.1 Map-model overlay [i](#)



X



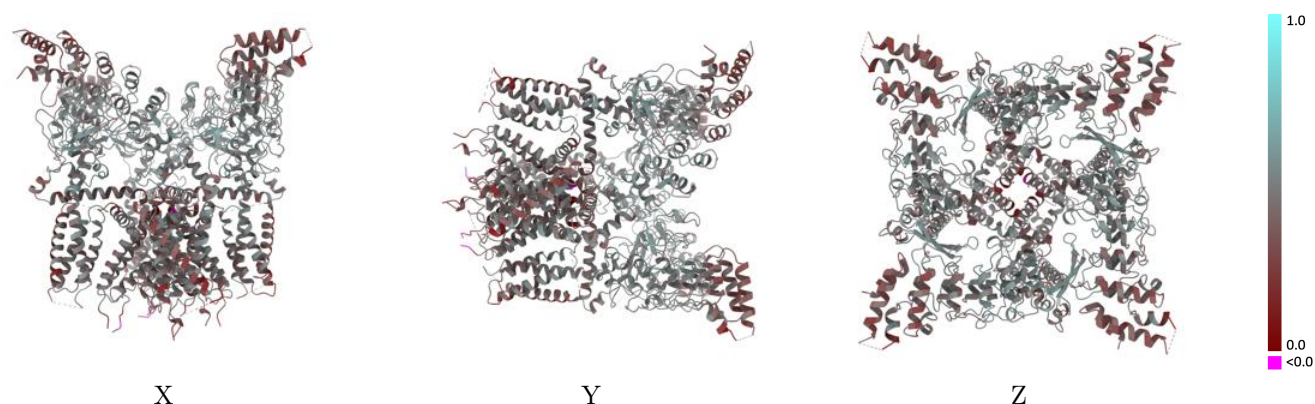
Y



Z

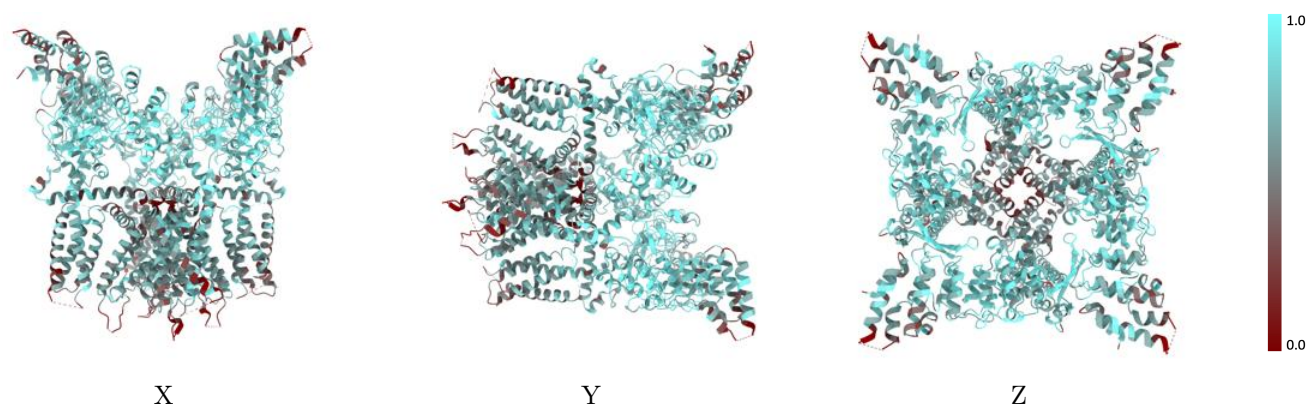
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



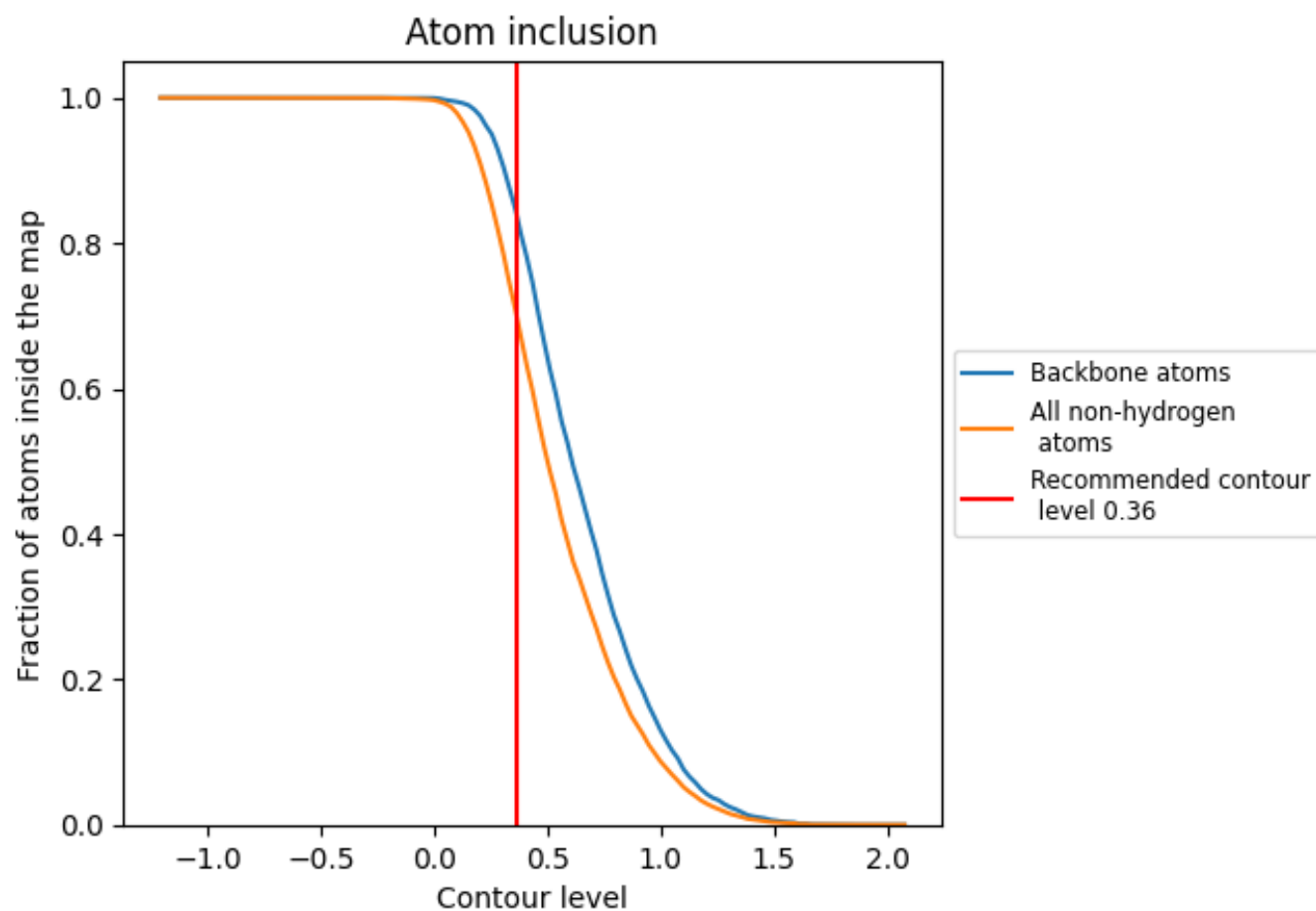
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 71% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7062	<div></div> 0.4470
A	<div></div> 0.7087	<div></div> 0.4490
B	<div></div> 0.7014	<div></div> 0.4440
C	<div></div> 0.7076	<div></div> 0.4460
D	<div></div> 0.7072	<div></div> 0.4480

