



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 11:09 AM UTC

PDB ID : 8IEQ / pdb_00008ieq
EMDB ID : EMD-35390
Title : Cryo-EM structure of G-protein free GPR156
Authors : Shin, J.; Park, J.; Cho, Y.
Deposited on : 2023-02-15
Resolution : 2.73 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

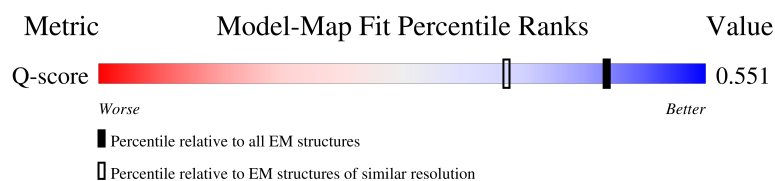
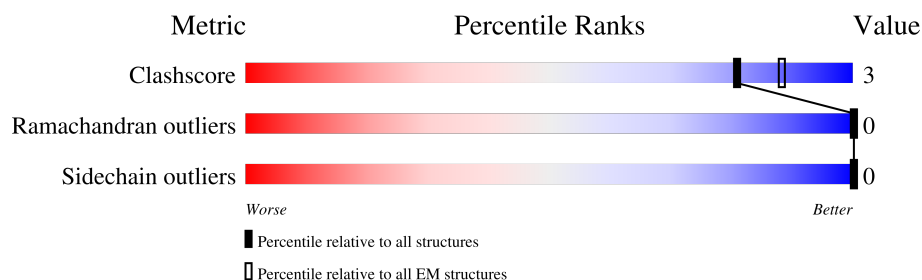
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.73 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	10432 (2.23 - 3.23)

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	598	
1	B	598	
1	C	598	
1	D	598	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8900 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 Probable G-protein coupled receptor 156.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	277	Total	C	N	O	S	0	0
			2135	1406	342	370	17		
1	B	286	Total	C	N	O	S	0	0
			2230	1471	360	381	18		
1	C	278	Total	C	N	O	S	0	0
			2155	1422	344	371	18		
1	D	279	Total	C	N	O	S	0	0
			2172	1433	349	372	18		

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	558	SER	-	expression tag	UNP Q8NFN8
A	559	GLY	-	expression tag	UNP Q8NFN8
A	560	SER	-	expression tag	UNP Q8NFN8
A	561	GLY	-	expression tag	UNP Q8NFN8
A	562	SER	-	expression tag	UNP Q8NFN8
A	563	GLY	-	expression tag	UNP Q8NFN8
A	564	ARG	-	expression tag	UNP Q8NFN8
A	565	GLY	-	expression tag	UNP Q8NFN8
A	566	ARG	-	expression tag	UNP Q8NFN8
A	567	GLY	-	expression tag	UNP Q8NFN8
A	568	GLY	-	expression tag	UNP Q8NFN8
A	569	SER	-	expression tag	UNP Q8NFN8
A	570	GLU	-	expression tag	UNP Q8NFN8
A	571	ASN	-	expression tag	UNP Q8NFN8
A	572	LEU	-	expression tag	UNP Q8NFN8
A	573	TYR	-	expression tag	UNP Q8NFN8
A	574	PHE	-	expression tag	UNP Q8NFN8
A	575	GLN	-	expression tag	UNP Q8NFN8
A	576	GLY	-	expression tag	UNP Q8NFN8
A	577	GLY	-	expression tag	UNP Q8NFN8
A	578	SER	-	expression tag	UNP Q8NFN8
A	579	GLY	-	expression tag	UNP Q8NFN8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	580	SER	-	expression tag	UNP Q8NFN8
A	581	GLY	-	expression tag	UNP Q8NFN8
A	582	GLY	-	expression tag	UNP Q8NFN8
A	583	ASP	-	expression tag	UNP Q8NFN8
A	584	TYR	-	expression tag	UNP Q8NFN8
A	585	LYS	-	expression tag	UNP Q8NFN8
A	586	ASP	-	expression tag	UNP Q8NFN8
A	587	ASP	-	expression tag	UNP Q8NFN8
A	588	ASP	-	expression tag	UNP Q8NFN8
A	589	ASP	-	expression tag	UNP Q8NFN8
A	590	LYS	-	expression tag	UNP Q8NFN8
A	591	ASP	-	expression tag	UNP Q8NFN8
A	592	TYR	-	expression tag	UNP Q8NFN8
A	593	LYS	-	expression tag	UNP Q8NFN8
A	594	ASP	-	expression tag	UNP Q8NFN8
A	595	ASP	-	expression tag	UNP Q8NFN8
A	596	ASP	-	expression tag	UNP Q8NFN8
A	597	ASP	-	expression tag	UNP Q8NFN8
A	598	LYS	-	expression tag	UNP Q8NFN8
B	558	SER	-	expression tag	UNP Q8NFN8
B	559	GLY	-	expression tag	UNP Q8NFN8
B	560	SER	-	expression tag	UNP Q8NFN8
B	561	GLY	-	expression tag	UNP Q8NFN8
B	562	SER	-	expression tag	UNP Q8NFN8
B	563	GLY	-	expression tag	UNP Q8NFN8
B	564	ARG	-	expression tag	UNP Q8NFN8
B	565	GLY	-	expression tag	UNP Q8NFN8
B	566	ARG	-	expression tag	UNP Q8NFN8
B	567	GLY	-	expression tag	UNP Q8NFN8
B	568	GLY	-	expression tag	UNP Q8NFN8
B	569	SER	-	expression tag	UNP Q8NFN8
B	570	GLU	-	expression tag	UNP Q8NFN8
B	571	ASN	-	expression tag	UNP Q8NFN8
B	572	LEU	-	expression tag	UNP Q8NFN8
B	573	TYR	-	expression tag	UNP Q8NFN8
B	574	PHE	-	expression tag	UNP Q8NFN8
B	575	GLN	-	expression tag	UNP Q8NFN8
B	576	GLY	-	expression tag	UNP Q8NFN8
B	577	GLY	-	expression tag	UNP Q8NFN8
B	578	SER	-	expression tag	UNP Q8NFN8
B	579	GLY	-	expression tag	UNP Q8NFN8
B	580	SER	-	expression tag	UNP Q8NFN8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	581	GLY	-	expression tag	UNP Q8NFN8
B	582	GLY	-	expression tag	UNP Q8NFN8
B	583	ASP	-	expression tag	UNP Q8NFN8
B	584	TYR	-	expression tag	UNP Q8NFN8
B	585	LYS	-	expression tag	UNP Q8NFN8
B	586	ASP	-	expression tag	UNP Q8NFN8
B	587	ASP	-	expression tag	UNP Q8NFN8
B	588	ASP	-	expression tag	UNP Q8NFN8
B	589	ASP	-	expression tag	UNP Q8NFN8
B	590	LYS	-	expression tag	UNP Q8NFN8
B	591	ASP	-	expression tag	UNP Q8NFN8
B	592	TYR	-	expression tag	UNP Q8NFN8
B	593	LYS	-	expression tag	UNP Q8NFN8
B	594	ASP	-	expression tag	UNP Q8NFN8
B	595	ASP	-	expression tag	UNP Q8NFN8
B	596	ASP	-	expression tag	UNP Q8NFN8
B	597	ASP	-	expression tag	UNP Q8NFN8
B	598	LYS	-	expression tag	UNP Q8NFN8
C	558	SER	-	expression tag	UNP Q8NFN8
C	559	GLY	-	expression tag	UNP Q8NFN8
C	560	SER	-	expression tag	UNP Q8NFN8
C	561	GLY	-	expression tag	UNP Q8NFN8
C	562	SER	-	expression tag	UNP Q8NFN8
C	563	GLY	-	expression tag	UNP Q8NFN8
C	564	ARG	-	expression tag	UNP Q8NFN8
C	565	GLY	-	expression tag	UNP Q8NFN8
C	566	ARG	-	expression tag	UNP Q8NFN8
C	567	GLY	-	expression tag	UNP Q8NFN8
C	568	GLY	-	expression tag	UNP Q8NFN8
C	569	SER	-	expression tag	UNP Q8NFN8
C	570	GLU	-	expression tag	UNP Q8NFN8
C	571	ASN	-	expression tag	UNP Q8NFN8
C	572	LEU	-	expression tag	UNP Q8NFN8
C	573	TYR	-	expression tag	UNP Q8NFN8
C	574	PHE	-	expression tag	UNP Q8NFN8
C	575	GLN	-	expression tag	UNP Q8NFN8
C	576	GLY	-	expression tag	UNP Q8NFN8
C	577	GLY	-	expression tag	UNP Q8NFN8
C	578	SER	-	expression tag	UNP Q8NFN8
C	579	GLY	-	expression tag	UNP Q8NFN8
C	580	SER	-	expression tag	UNP Q8NFN8
C	581	GLY	-	expression tag	UNP Q8NFN8

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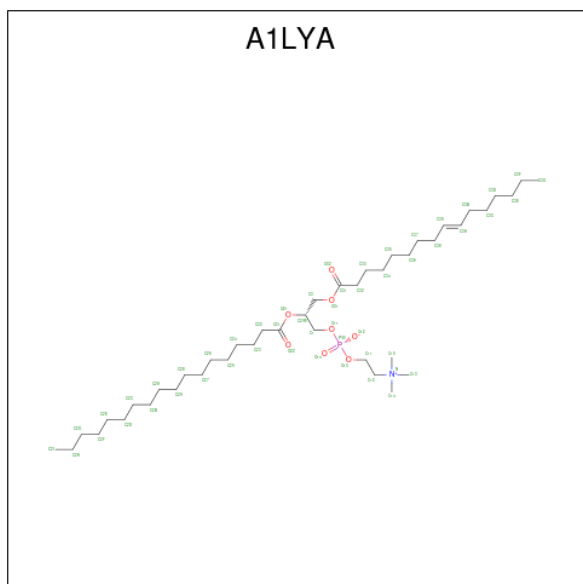
Chain	Residue	Modelled	Actual	Comment	Reference
C	582	GLY	-	expression tag	UNP Q8NFN8
C	583	ASP	-	expression tag	UNP Q8NFN8
C	584	TYR	-	expression tag	UNP Q8NFN8
C	585	LYS	-	expression tag	UNP Q8NFN8
C	586	ASP	-	expression tag	UNP Q8NFN8
C	587	ASP	-	expression tag	UNP Q8NFN8
C	588	ASP	-	expression tag	UNP Q8NFN8
C	589	ASP	-	expression tag	UNP Q8NFN8
C	590	LYS	-	expression tag	UNP Q8NFN8
C	591	ASP	-	expression tag	UNP Q8NFN8
C	592	TYR	-	expression tag	UNP Q8NFN8
C	593	LYS	-	expression tag	UNP Q8NFN8
C	594	ASP	-	expression tag	UNP Q8NFN8
C	595	ASP	-	expression tag	UNP Q8NFN8
C	596	ASP	-	expression tag	UNP Q8NFN8
C	597	ASP	-	expression tag	UNP Q8NFN8
C	598	LYS	-	expression tag	UNP Q8NFN8
D	558	SER	-	expression tag	UNP Q8NFN8
D	559	GLY	-	expression tag	UNP Q8NFN8
D	560	SER	-	expression tag	UNP Q8NFN8
D	561	GLY	-	expression tag	UNP Q8NFN8
D	562	SER	-	expression tag	UNP Q8NFN8
D	563	GLY	-	expression tag	UNP Q8NFN8
D	564	ARG	-	expression tag	UNP Q8NFN8
D	565	GLY	-	expression tag	UNP Q8NFN8
D	566	ARG	-	expression tag	UNP Q8NFN8
D	567	GLY	-	expression tag	UNP Q8NFN8
D	568	GLY	-	expression tag	UNP Q8NFN8
D	569	SER	-	expression tag	UNP Q8NFN8
D	570	GLU	-	expression tag	UNP Q8NFN8
D	571	ASN	-	expression tag	UNP Q8NFN8
D	572	LEU	-	expression tag	UNP Q8NFN8
D	573	TYR	-	expression tag	UNP Q8NFN8
D	574	PHE	-	expression tag	UNP Q8NFN8
D	575	GLN	-	expression tag	UNP Q8NFN8
D	576	GLY	-	expression tag	UNP Q8NFN8
D	577	GLY	-	expression tag	UNP Q8NFN8
D	578	SER	-	expression tag	UNP Q8NFN8
D	579	GLY	-	expression tag	UNP Q8NFN8
D	580	SER	-	expression tag	UNP Q8NFN8
D	581	GLY	-	expression tag	UNP Q8NFN8
D	582	GLY	-	expression tag	UNP Q8NFN8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	583	ASP	-	expression tag	UNP Q8NFN8
D	584	TYR	-	expression tag	UNP Q8NFN8
D	585	LYS	-	expression tag	UNP Q8NFN8
D	586	ASP	-	expression tag	UNP Q8NFN8
D	587	ASP	-	expression tag	UNP Q8NFN8
D	588	ASP	-	expression tag	UNP Q8NFN8
D	589	ASP	-	expression tag	UNP Q8NFN8
D	590	LYS	-	expression tag	UNP Q8NFN8
D	591	ASP	-	expression tag	UNP Q8NFN8
D	592	TYR	-	expression tag	UNP Q8NFN8
D	593	LYS	-	expression tag	UNP Q8NFN8
D	594	ASP	-	expression tag	UNP Q8NFN8
D	595	ASP	-	expression tag	UNP Q8NFN8
D	596	ASP	-	expression tag	UNP Q8NFN8
D	597	ASP	-	expression tag	UNP Q8NFN8
D	598	LYS	-	expression tag	UNP Q8NFN8

- Molecule 2 is [(2R)-3-[(E)-hexadec-9-enoyl]oxy-2-octadecanoyloxy-propyl] 2-(trimethylazaniumyl)ethyl phosphate (CCD ID: A1LYA) (formula: C₄₂H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	B	1	Total	C	N	O	P	0
			52	42	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
2	D	1	Total	C	N	O	P	0
			52	42	1	8	1	

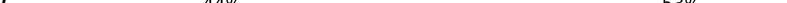
[illegible]

- Molecule 1: Probable G-protein coupled receptor 156

Chain C: 43% 5% 52%

[illegible]

- Molecule 1: Probable G-protein coupled receptor 156

Chain D:  44% 53%

Protein	Residue	Score	Category
Protein 1	PRO ASN	L127	High
	GLU LYS	S132	High
	GLY SER	Y146	High
	ALA PHE	Y146	High
	ALA HIS	T150	High
	PRO THR	Q151	High
	GLN GLN	R152	High
	ALA TYR	VAL	High
	GLY GLY	PRO	High
	GLU ASP	ASP	High
Protein 2	GLU GLY	R161	High
	ALA ARG	T202	High
	GLU GLY	G203	High
	ALA SER	K204	High
	GLN LYS	D205	High
	GLY MET	V206	High
	ALA THR	S207	High
	GLN THR	S210	High
	GLY GLY	D222	High
	PRO ASN	K232	High
Protein 3	GLY VAL	L236	High
	GLU SER	V264	High
	ALA LEU	L267	High
	GLN GLN	L274	High
	GLY VAL	V277	High
	ASN ASN	T278	High
	ALA ALA	R279	High
	GLY GLY	L286	High
	LYS ILE	E320	High
	VAL ARG	Q323	High
Protein 4	LEU MET	T324	High
	SER SER	I325	High
	PRO ALA	R326	High
	GLU SER	K327	High
	THR THR	M328	High
	TYR TYR	A329	High
	ASP ASP	K330	High
	GLN GLN	Y331	High
	THR THR	F332	High
	GLY GLY	S115	High
Protein 5	GLU MET	S44	High
	PRO PRO	S83	High
	GLY ILE	S84	High
	ASN ASN	T98	High
	CYS SER	F105	High
	GLU GLU	D109	High
	GLY GLY	V110	High
	GLY GLY	L111	High
	GLY GLY	V112	High
	GLY GLY	S115	High

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

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	493410	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 ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	12.102	Depositor
Minimum map value	-8.143	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.189	Depositor
Recommended contour level	0.96	Depositor
Map size ($\text{\AA}$)	332.1, 332.1, 332.1	wwPDB
Map dimensions	410, 410, 410	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.81, 0.81, 0.81	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: A1LYA

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	0.17	0/2180	0.34	0/2971
1	B	0.17	0/2278	0.36	0/3100
1	C	0.18	0/2201	0.35	0/2996
1	D	0.17	0/2218	0.34	0/3017
All	All	0.17	0/8877	0.35	0/12084

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	2135	0	2232	11	0
1	B	2230	0	2348	12	0
1	C	2155	0	2248	14	0
1	D	2172	0	2279	9	0
2	A	52	0	0	0	0
2	B	52	0	0	0	0
2	C	52	0	0	0	0
2	D	52	0	0	1	0
All	All	8900	0	9107	46	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 46 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:C:236:LEU:HD11	1:C:267:LEU:HD23	1.64	0.80
1:D:236:LEU:HD22	1:D:264:VAL:HG12	1.68	0.75
1:A:84:SER:OG	1:A:144:ARG:NH2	2.23	0.72
1:A:236:LEU:HD22	1:A:264:VAL:HG12	1.73	0.71
1:C:58:SER:HG	1:C:103:TYR:HH	1.39	0.66

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	273/598 (46%)	262 (96%)	11 (4%)	0	100	100
1	B	282/598 (47%)	272 (96%)	10 (4%)	0	100	100
1	C	272/598 (46%)	262 (96%)	10 (4%)	0	100	100
1	D	273/598 (46%)	266 (97%)	7 (3%)	0	100	100
All	All	1100/2392 (46%)	1062 (96%)	38 (4%)	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	243/523 (46%)	243 (100%)	0	100	100
1	B	254/523 (49%)	254 (100%)	0	100	100
1	C	244/523 (47%)	244 (100%)	0	100	100
1	D	247/523 (47%)	247 (100%)	0	100	100
All	All	988/2092 (47%)	988 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	214	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 [i](#)

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	A1LYA	B	601	-	51,51,51	1.17	4 (7%)	57,59,59	0.75	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1LYA	D	601	-	51,51,51	1.17	4 (7%)	57,59,59	0.74	2 (3%)
2	A1LYA	C	601	-	51,51,51	1.17	4 (7%)	57,59,59	0.75	2 (3%)
2	A1LYA	A	601	-	51,51,51	1.16	4 (7%)	57,59,59	0.77	2 (3%)

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	A1LYA	B	601	-	-	19/55/55/55	-
2	A1LYA	D	601	-	-	19/55/55/55	-
2	A1LYA	C	601	-	-	19/55/55/55	-
2	A1LYA	A	601	-	-	20/55/55/55	-

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	A1LYA	O31-C31	3.35	1.43	1.33
2	A	601	A1LYA	O31-C31	3.32	1.43	1.33
2	C	601	A1LYA	O31-C31	3.28	1.42	1.33
2	B	601	A1LYA	O31-C31	3.27	1.42	1.33
2	A	601	A1LYA	O21-C2	-3.06	1.39	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	A1LYA	O21-C21-C22	3.43	118.91	111.48
2	C	601	A1LYA	O21-C21-C22	3.39	118.81	111.48
2	A	601	A1LYA	O21-C21-C22	3.36	118.75	111.48
2	D	601	A1LYA	O21-C21-C22	3.34	118.72	111.48
2	A	601	A1LYA	O31-C31-C32	2.61	119.80	111.83

There are no chirality outliers.

5 of 77 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1LYA	O13-C11-C12-N
2	B	601	A1LYA	O13-C11-C12-N
2	C	601	A1LYA	O13-C11-C12-N

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Continued from previous page...

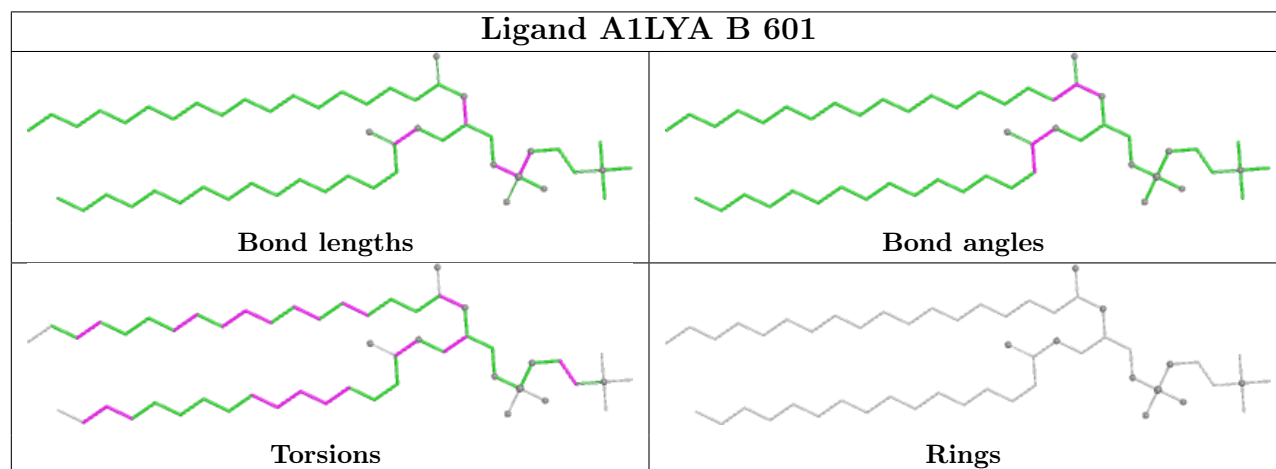
Mol	Chain	Res	Type	Atoms
2	D	601	A1LYA	O13-C11-C12-N
2	A	601	A1LYA	O32-C31-O31-C3

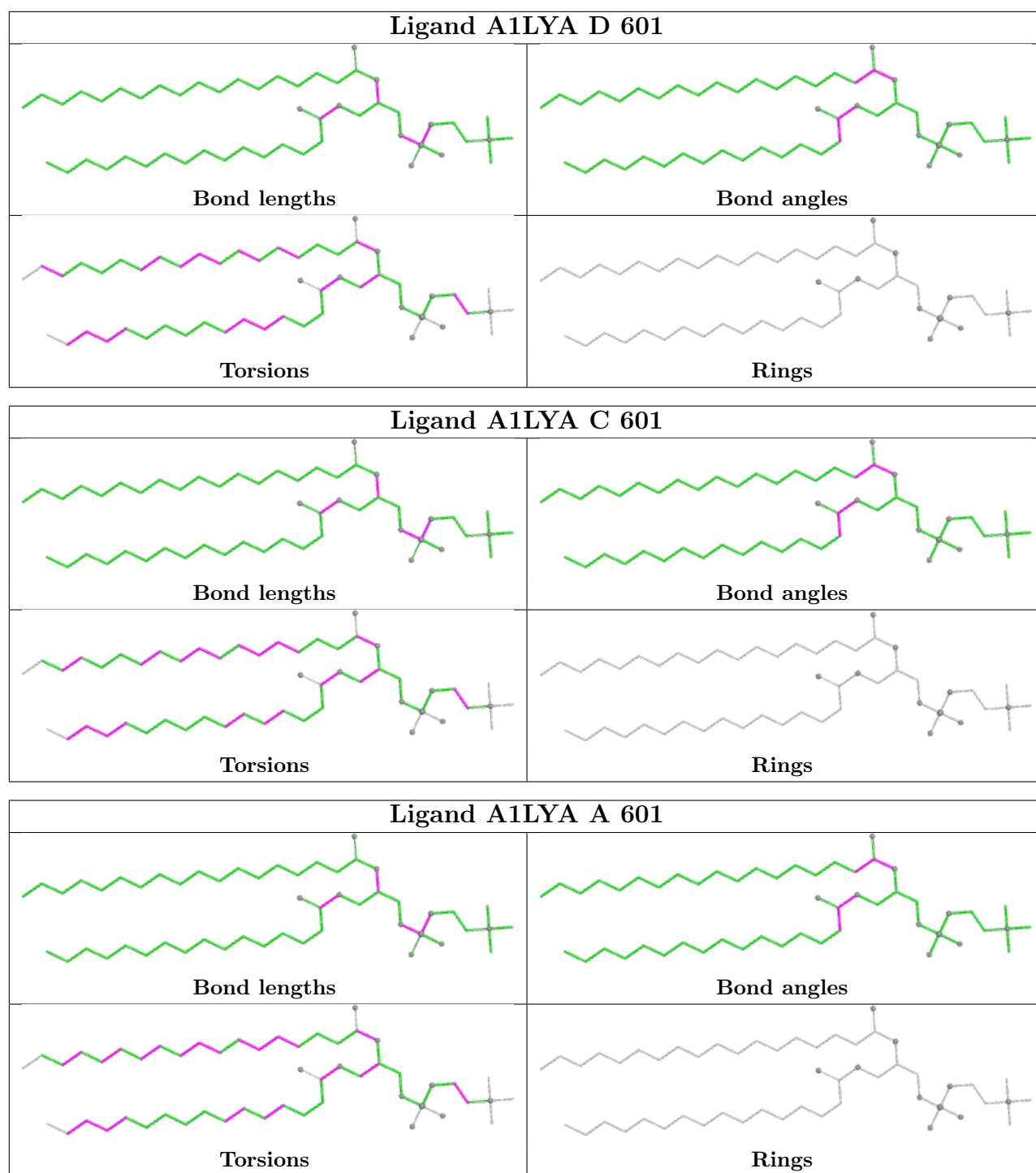
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	A1LYA	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 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.

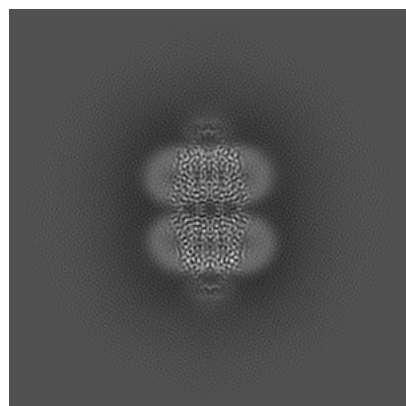
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35390. These allow visual inspection of the internal detail of the map and identification of artifacts.

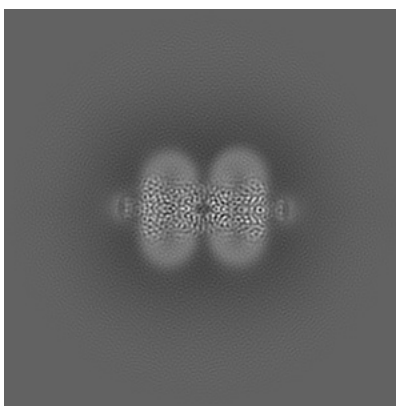
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

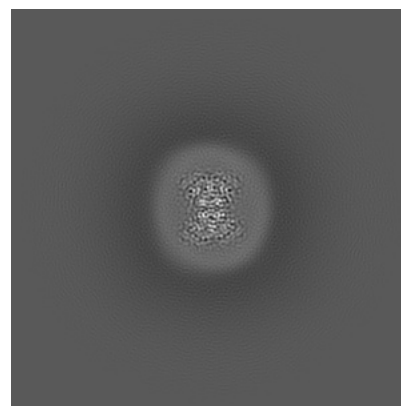
6.1.1 Primary map



X

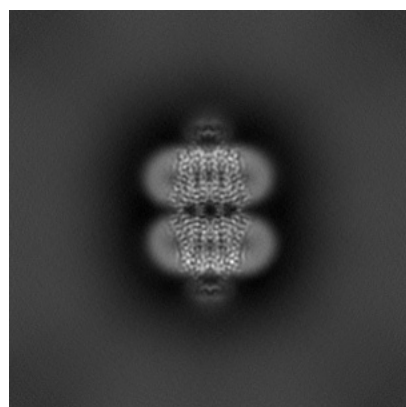


Y

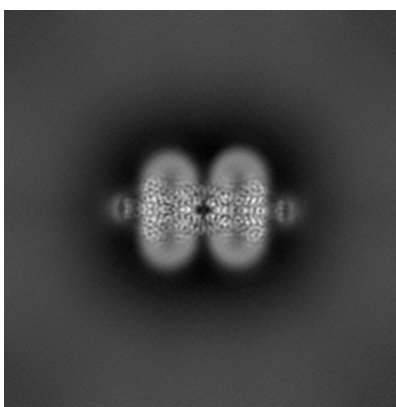


Z

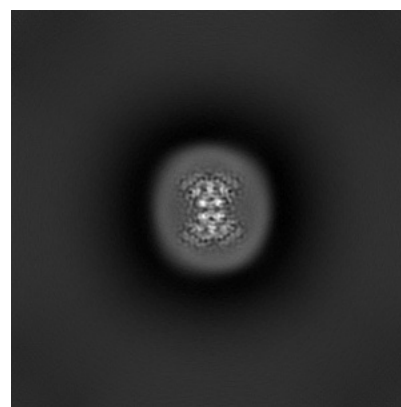
6.1.2 Raw map



X



Y

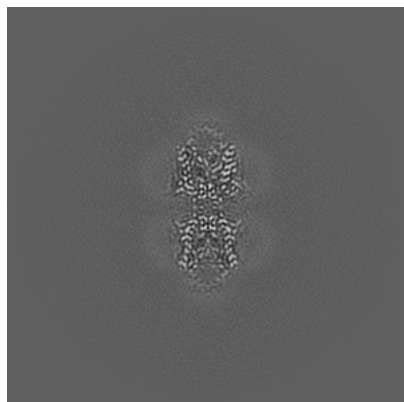


Z

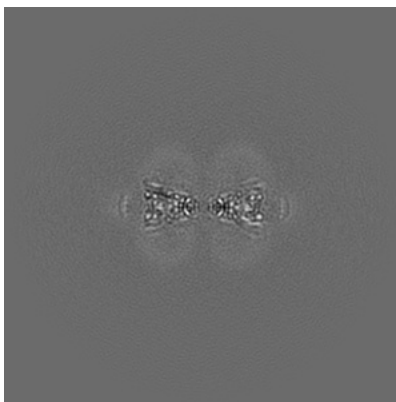
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

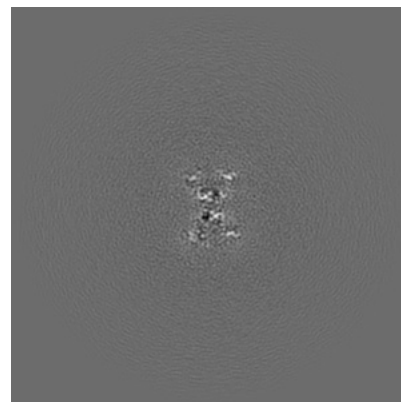
6.2.1 Primary map



X Index: 205

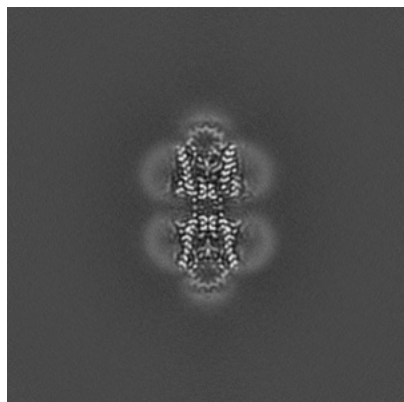


Y Index: 205

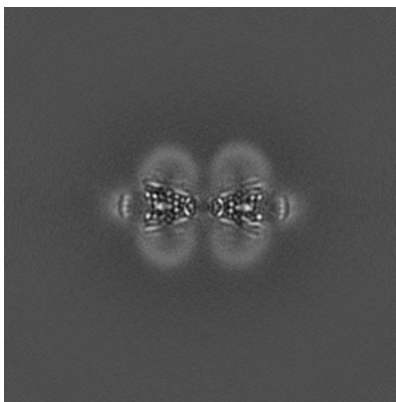


Z Index: 205

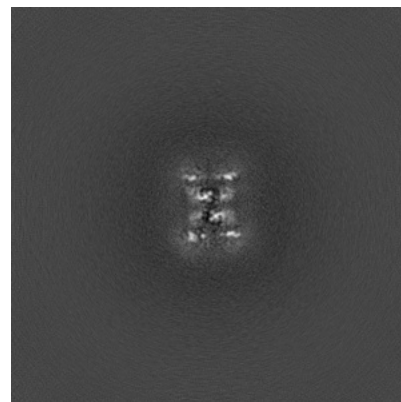
6.2.2 Raw map



X Index: 205



Y Index: 205

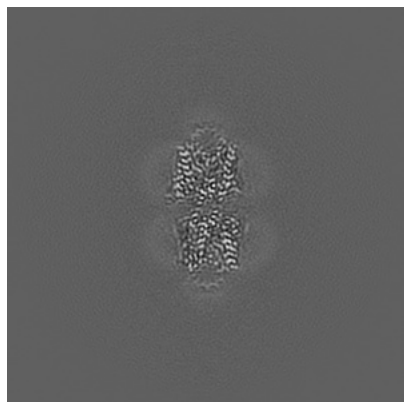


Z Index: 205

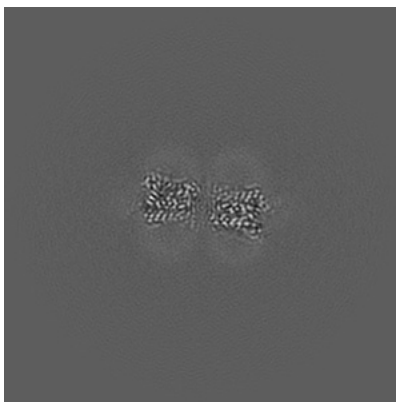
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

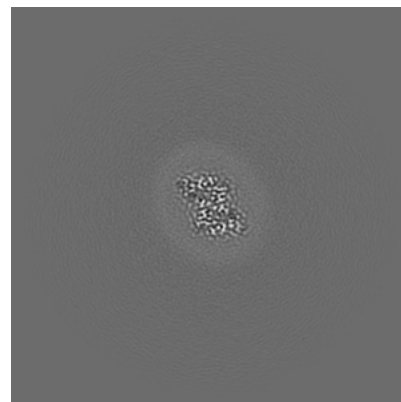
6.3.1 Primary map



X Index: 202

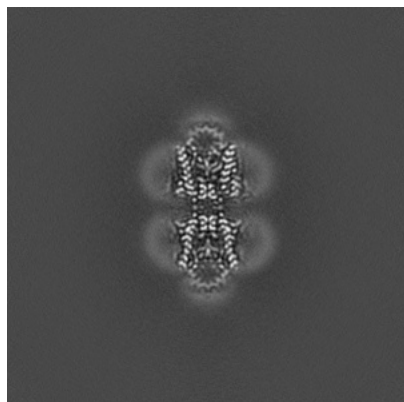


Y Index: 185

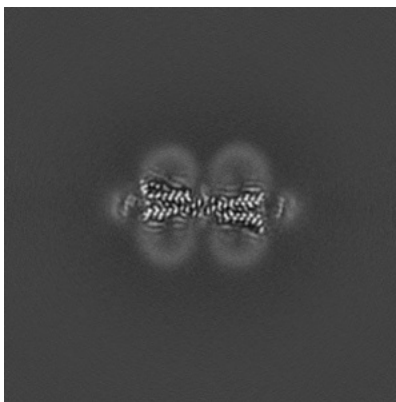


Z Index: 154

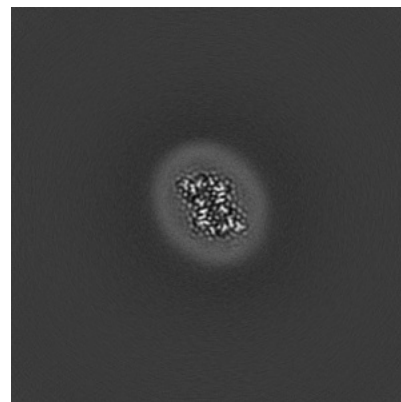
6.3.2 Raw map



X Index: 205



Y Index: 198

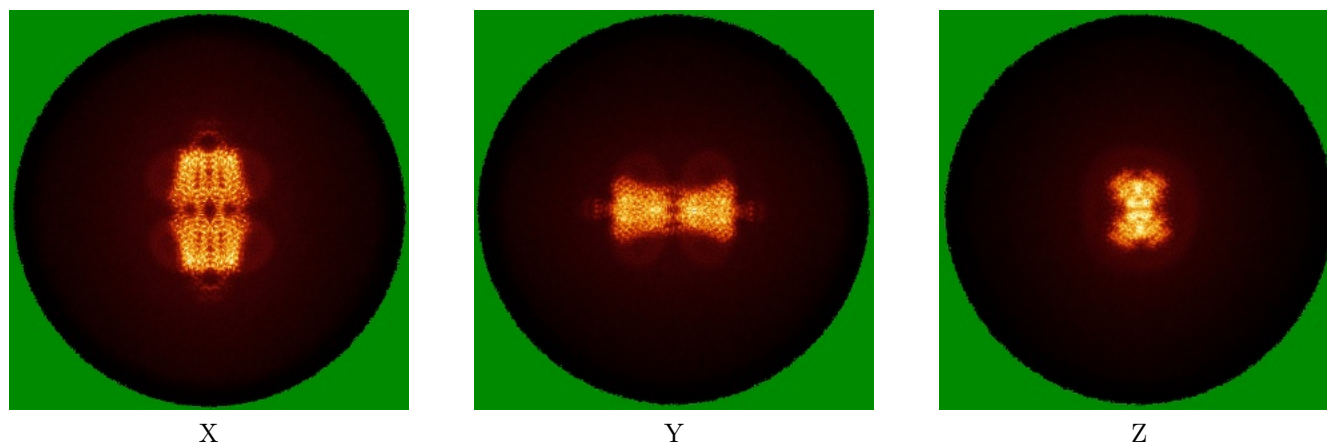


Z Index: 153

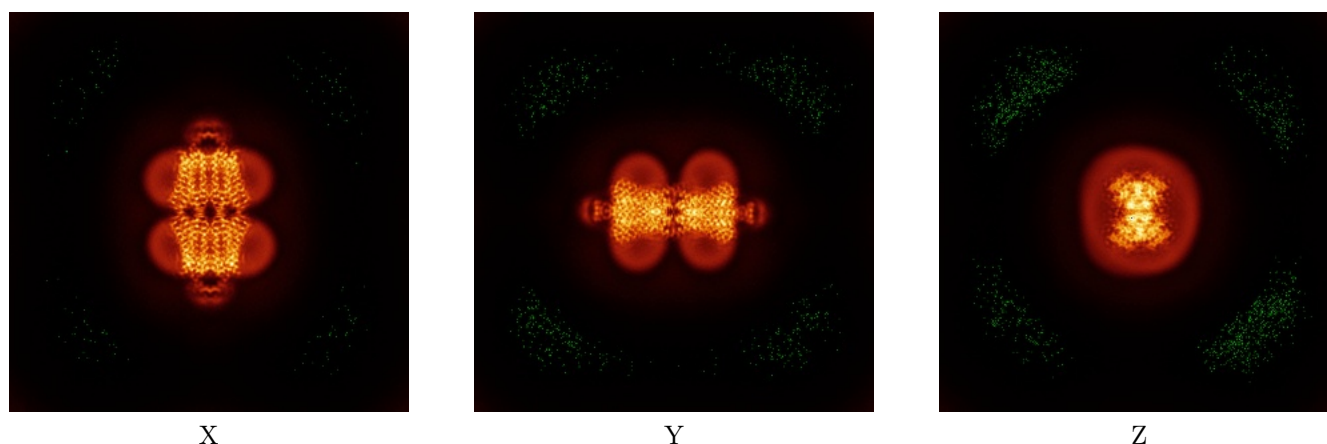
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

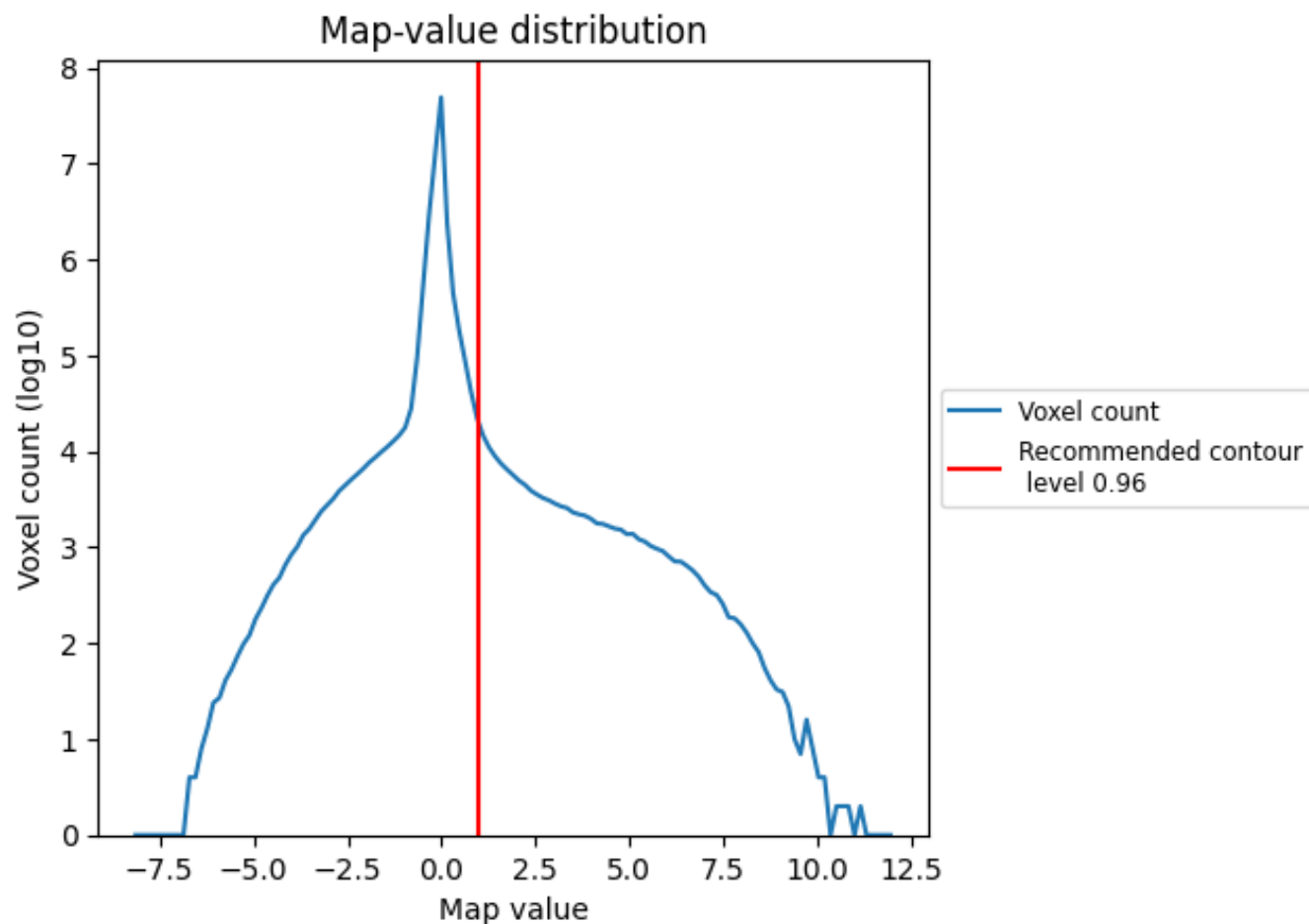
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

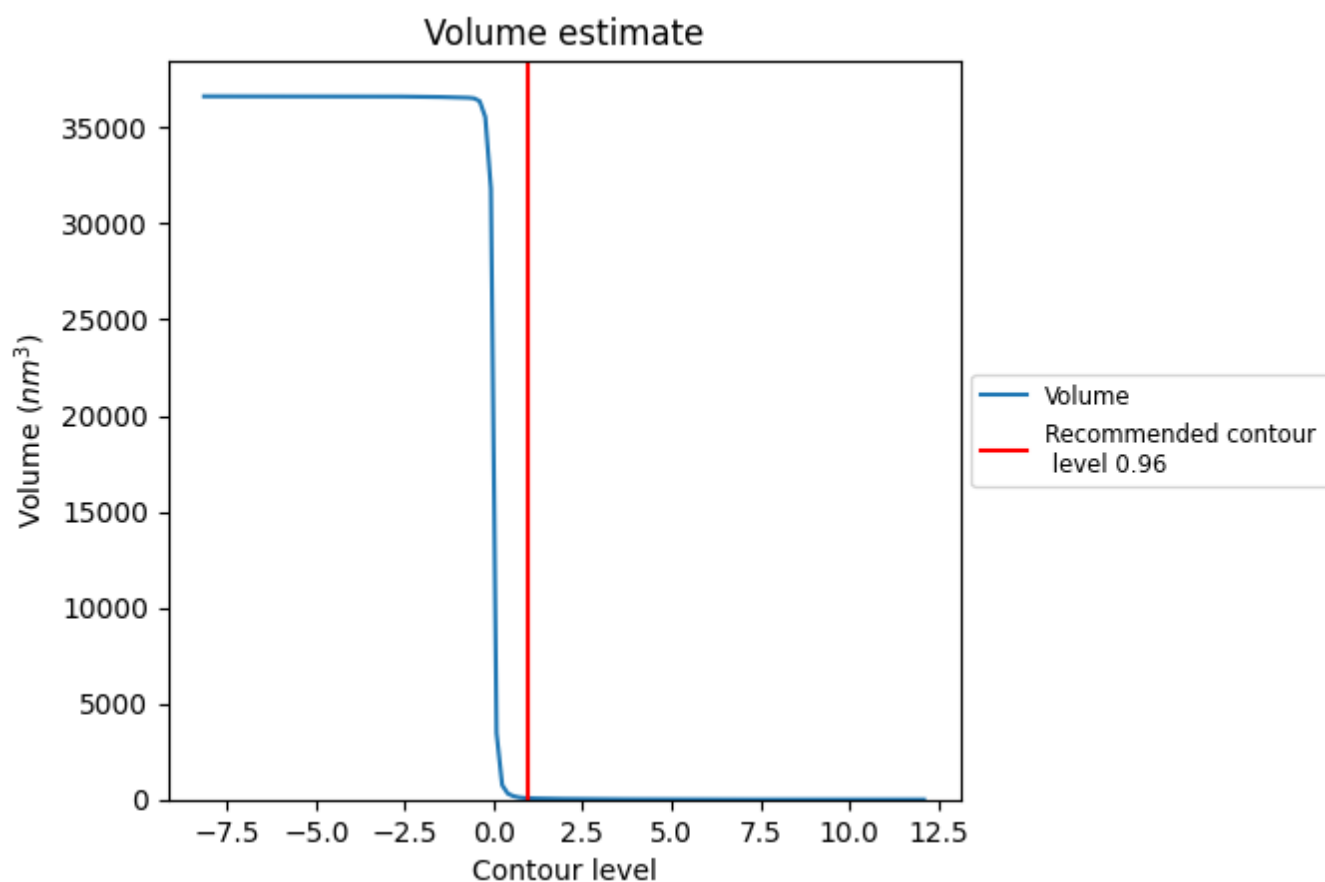
This section contains the results of statistical analysis of the map.

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.

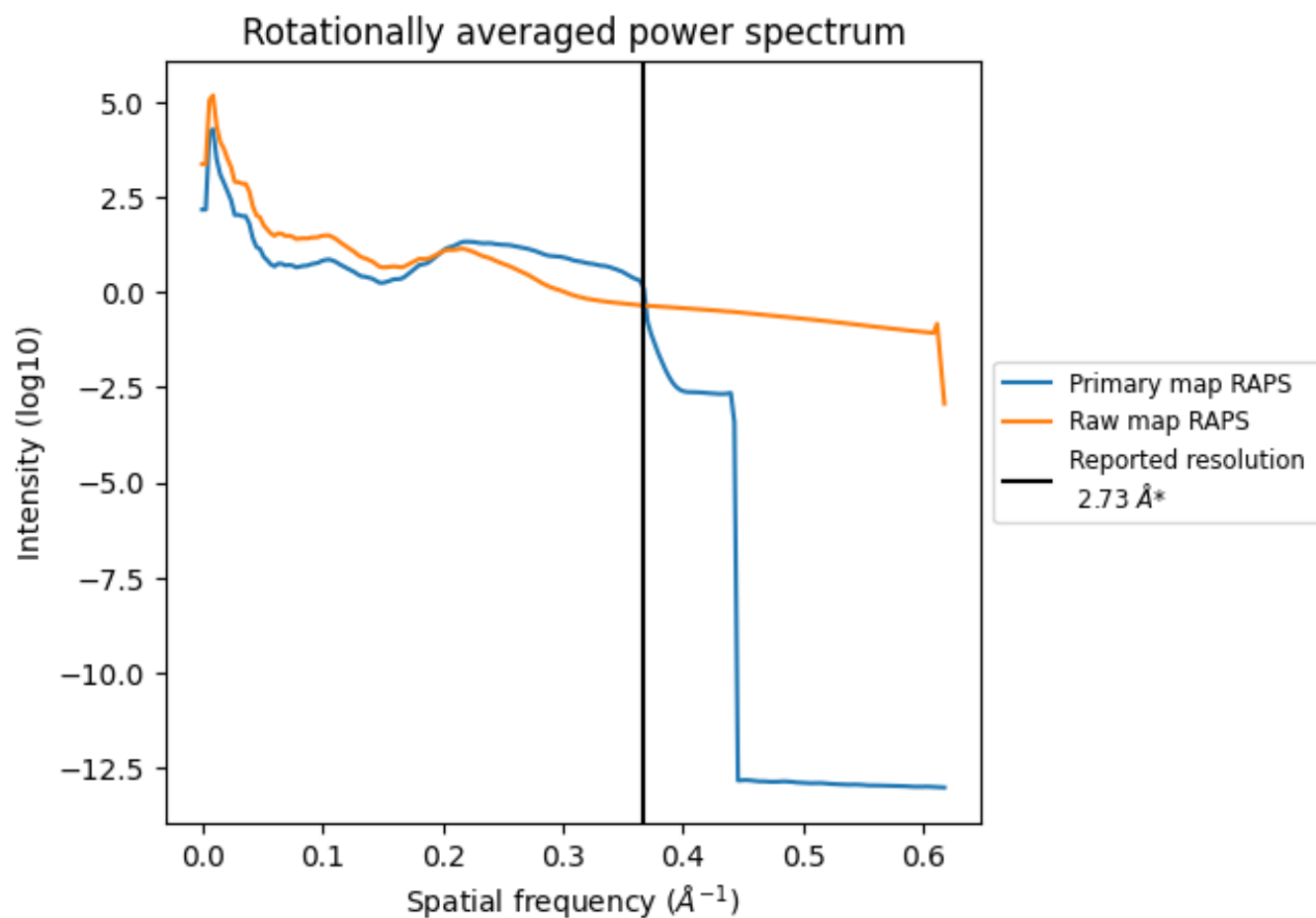
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 74 nm^3 ; this corresponds to an approximate mass of 67 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 ⓘ

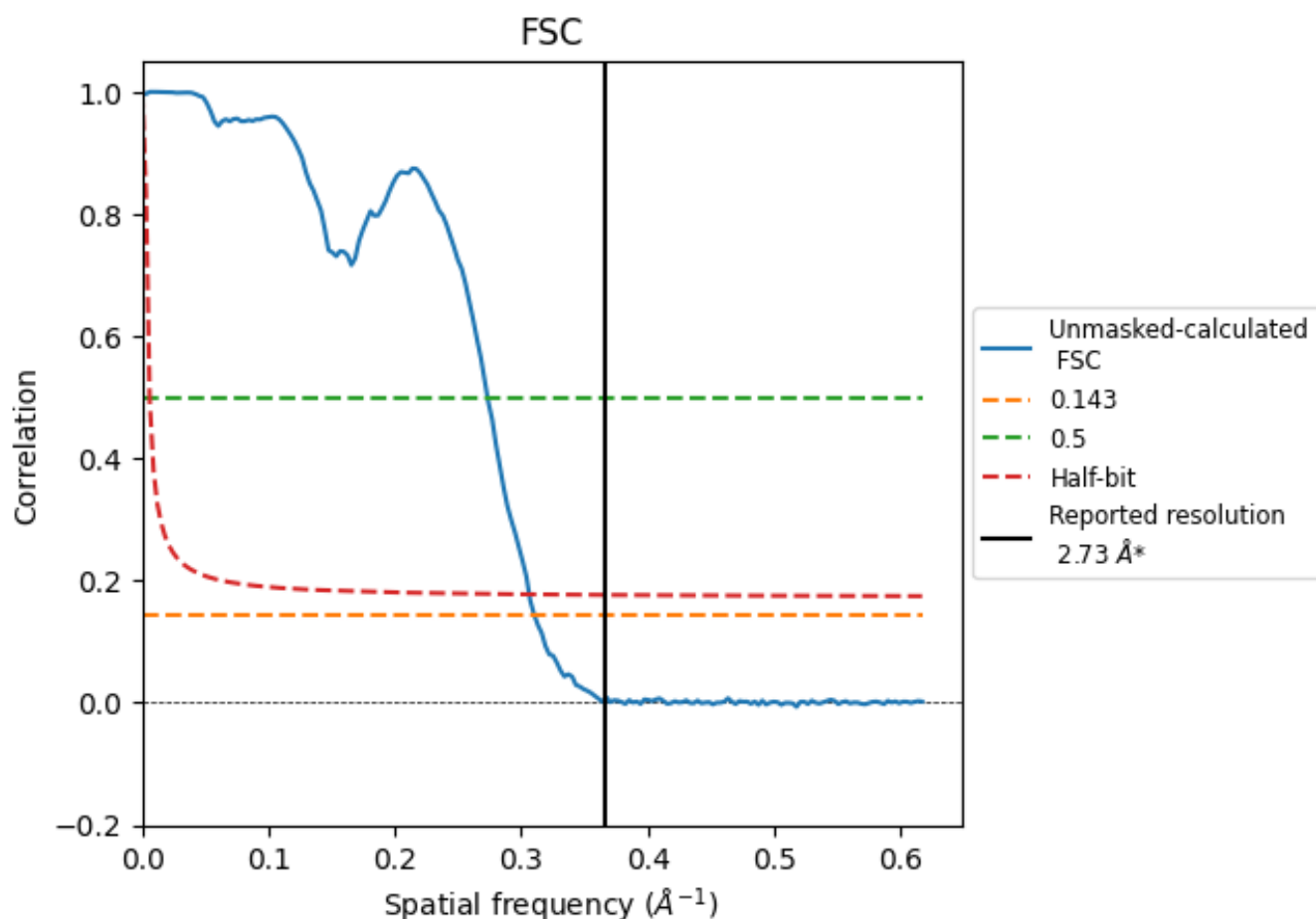


*Reported resolution corresponds to spatial frequency of 0.366 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

8.2 Resolution estimates [i](#)

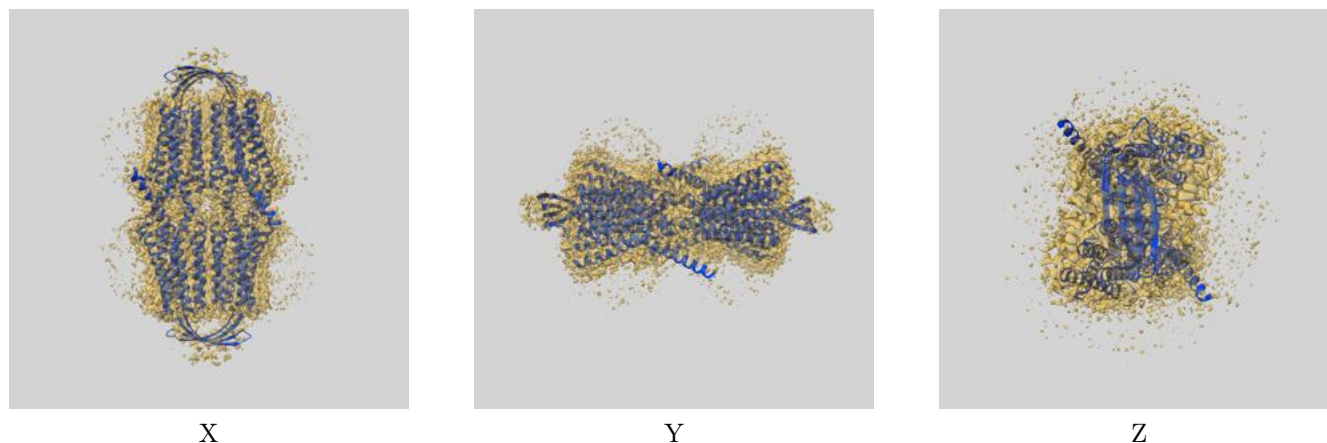
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.22	3.66	3.26

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.22 differs from the reported value 2.73 by more than 10 %

9 Map-model fit [i](#)

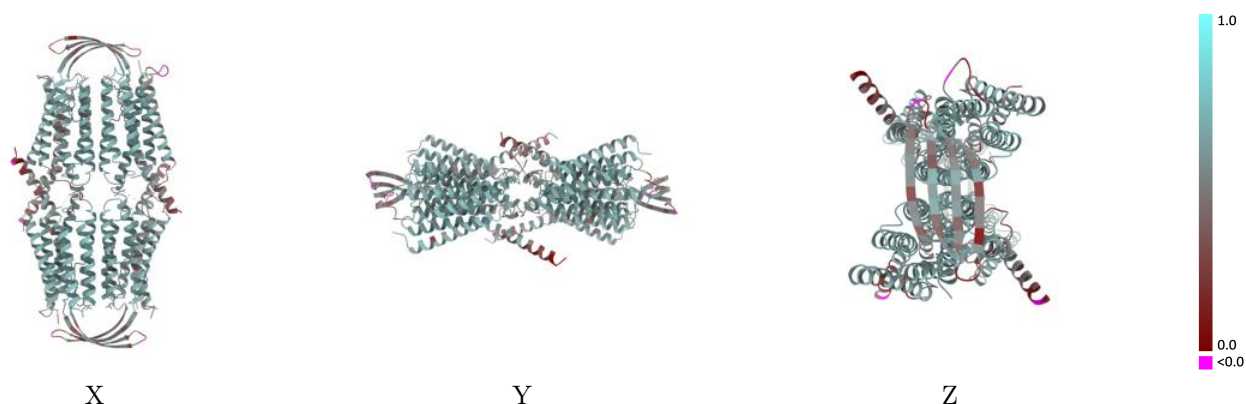
This section contains information regarding the fit between EMDB map EMD-35390 and PDB model 8IEQ. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



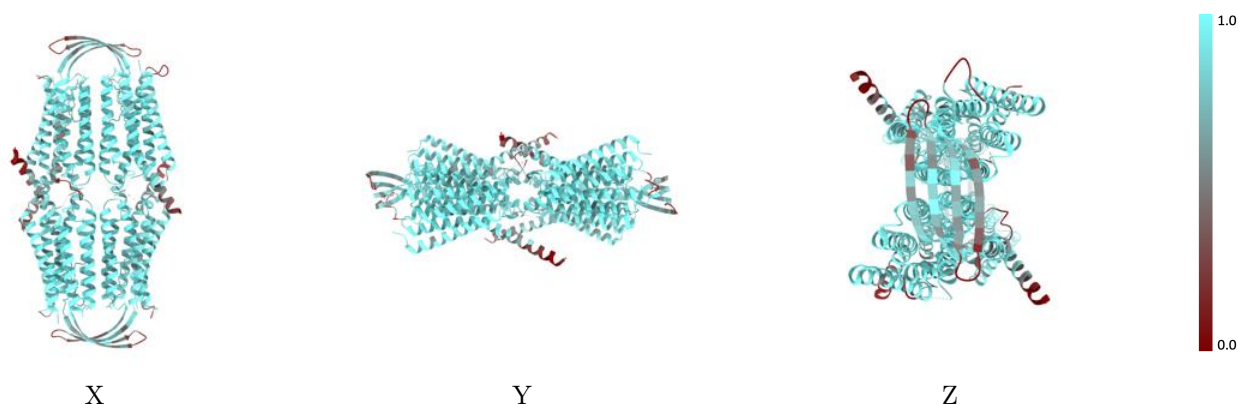
The images above show the 3D surface view of the map at the recommended contour level 0.96 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



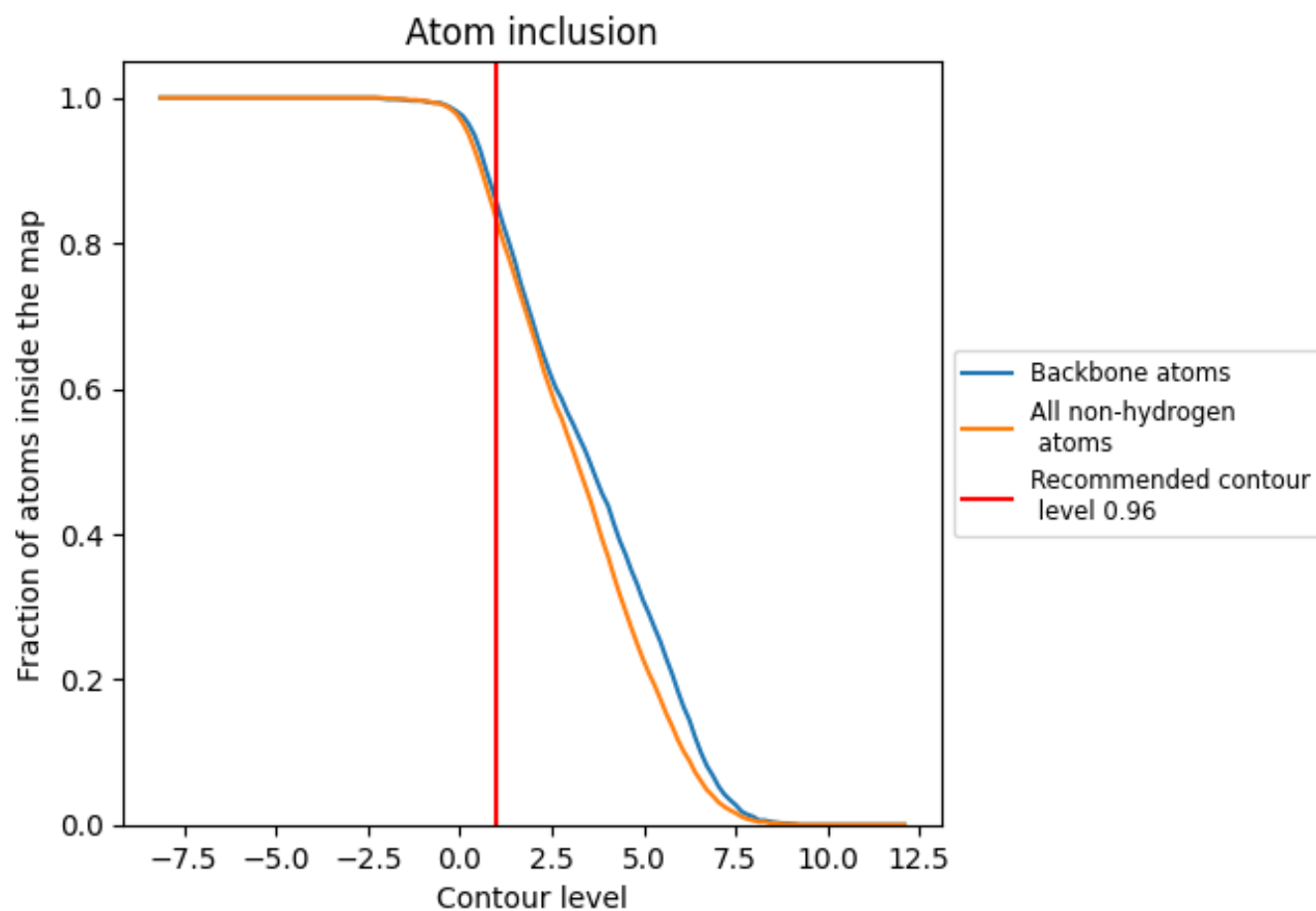
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.96).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.96) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8400	0.5510
A	0.8510	0.5550
B	0.8210	0.5430
C	0.8480	0.5530
D	0.8420	0.5520

