



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 03:52 PM UTC

PDB ID : 9L00 / pdb_00009l00
EMDB ID : EMD-62681
Title : structure of hZnT1-CDDO-ME complex
Authors : Xu, B.; Wang, Y.
Deposited on : 2024-12-11
Resolution : 3.78 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

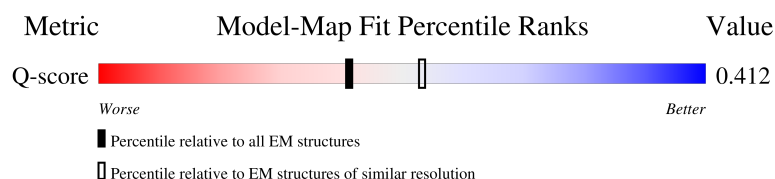
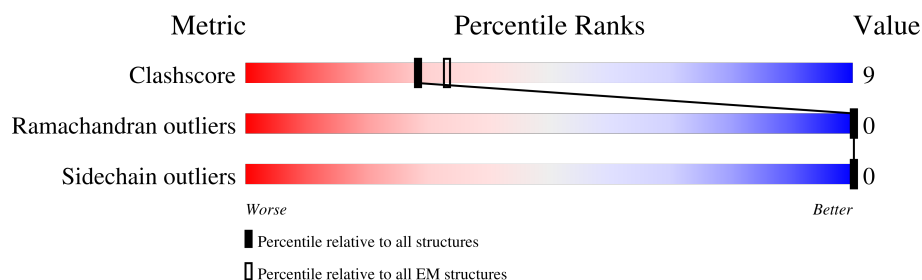
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.78 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	10074 (3.28 - 4.27)

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	507	
1	B	507	

2 Entry composition [i](#)

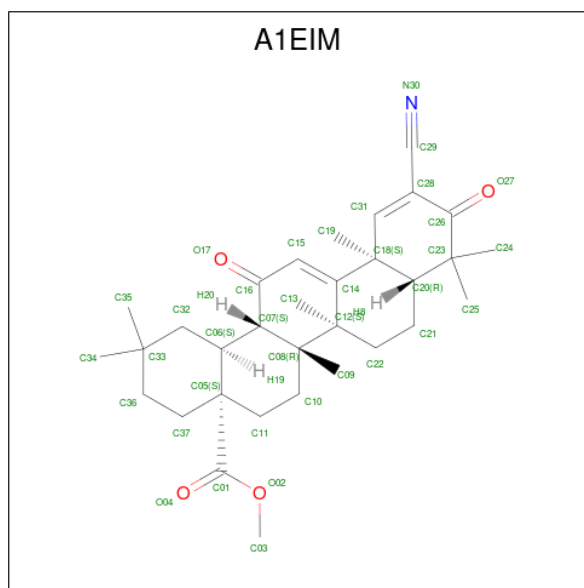
There are 2 unique types of molecules in this entry. The entry contains 4854 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Proton-coupled zinc antiporter SLC30A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	307	Total	C	N	O	S	0	0
			2390	1549	405	415	21		
1	B	307	Total	C	N	O	S	0	0
			2390	1549	405	415	21		

- Molecule 2 is methyl (4aS,6aR,6bS,8aR,12aS,14aS,14bS)-11-cyano-2,2,6a,6b,9,9,12a-heptamethyl-10,14-bis(oxidanylidene)-1,3,4,5,6,7,8,8a,14a,14b-decahydropicene-4a-carboxylate (CCD ID: A1EIM) (formula: $C_{32}H_{43}NO_4$) (labeled as "Ligand of Interest" by depositor).

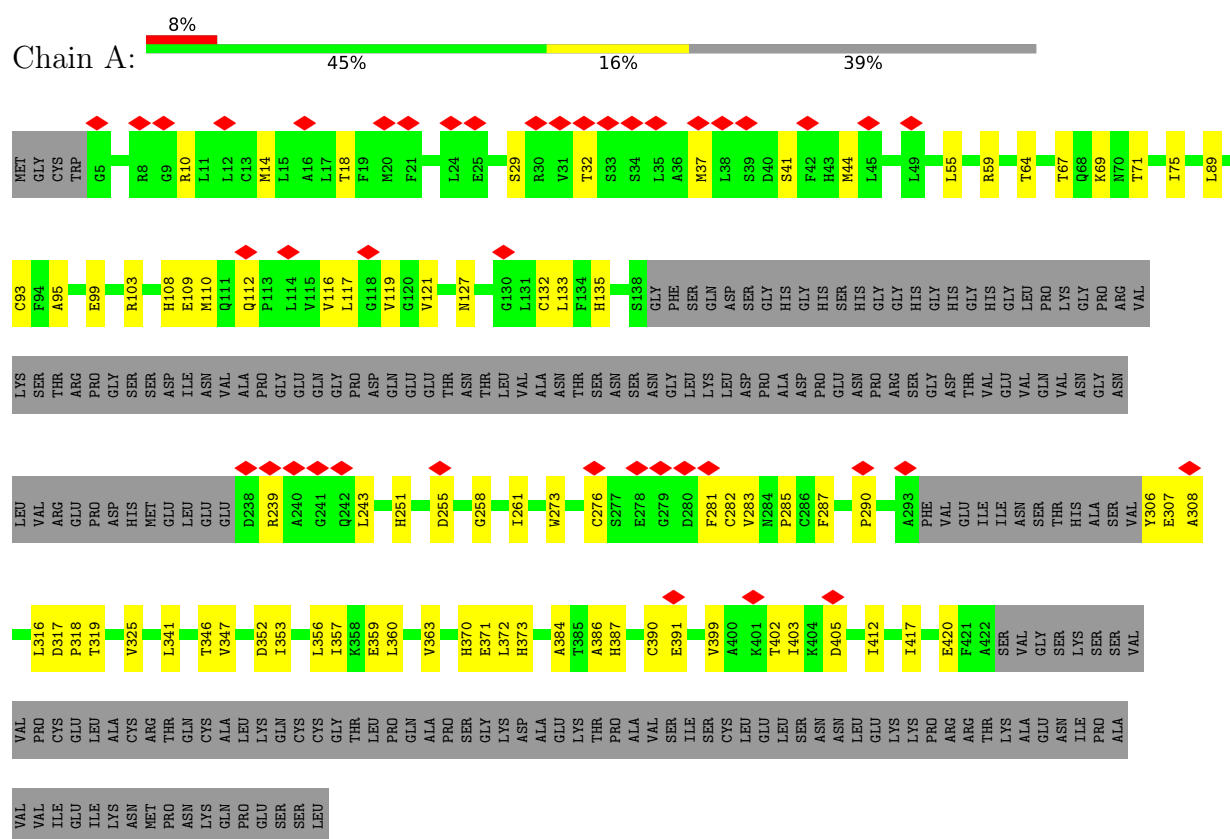


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			37	32	1	4	
2	B	1	Total	C	N	O	0
			37	32	1	4	

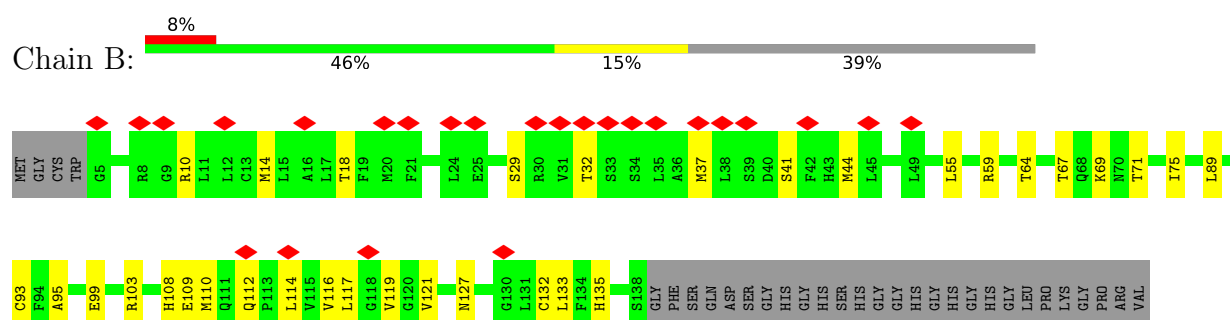
3 Residue-property plots

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: Proton-coupled zinc antiporter SLC30A1



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GLU	LEU	D317	D339	D352	D366	D379	D393	D407	D421	D435	D449	D463	D477	D491	D505	D519	D533	D547	D561	D575	D589	D603	D617	D631	D645	D659	D673	D687	D701	D715	D729	D743	D757	D771	D785	D799	D813	D827	D841	D855	D869	D883	D897	D911	D925	D939	D953	D967	D981	D995	E009	E023	E037	E051	E065	E079	E093	E107	E121	E135	E149	E163	E177	E191	E205	E219	E233	E247	E261	E275	E289	E303	E317	E331	E345	E359	E373	E387	E401	E415	E429	E443	E457	E471	E485	E499	E513	E527	E541	E555	E569	E583	E597	E611	E625	E639	E653	E667	E681	E695	E709	E723	E737	E751	E765	E779	E793	E807	E821	E835	E849	E863	E877	E891	E905	E919	E933	E947	E961	E975	E989	F003	F017	F031	F045	F059	F073	F087	F101	F115	F129	F143	F157	F171	F185	F199	F213	F227	F241	F255	F269	F283	F297	F311	F325	F339	F353	F367	F381	F395	F409	F423	F437	F451	F465	F479	F493	F507	F521	F535	F549	F563	F577	F591	F605	F619	F633	F647	F661	F675	F689	F703	F717	F731	F745	F759	F773	F787	F801	F815	F829	F843	F857	F871	F885	F899	F913	F927	F941	F955	F969	F983	F997	G001	G015	G029	G043	G057	G071	G085	G099	G113	G127	G141	G155	G169	G183	G197	G211	G225	G239	G253	G267	G281	G295	G309	G323	G337	G351	G365	G379	G393	G407	G421	G435	G449	G463	G477	G491	G505	G519	G533	G547	G561	G575	G589	G603	G617	G631	G645	G659	G673	G687	G701	G715	G729	G743	G757	G771	G785	G799	G813	G827	G841	G855	G869	G883	G897	G911	G925	G939	G953	G967	G981	G995	H009	H023	H037	H051	H065	H079	H093	H107	H121	H135	H149	H163	H177	H191	H205	H219	H233	H247	H261	H275	H289	H303	H317	H331	H345	H359	H373	H387	H401	H415	H429	H443	H457	H471	H485	H499	H513	H527	H541	H555	H569	H583	H597	H611	H625	H639	H653	H667	H681	H695	H709	H723	H737	H751	H765	H779	H793	H807	H821	H835	H849	H863	H877	H891	H905	H919	H933	H947	H961	H975	H989	I003	I017	I031	I045	I059	I073	I087	I101	I115	I129	I143	I157	I171	I185	I199	I213	I227	I241	I255	I269	I283	I297	I311	I325	I339	I353	I367	I381	I395	I409	I423	I437	I451	I465	I479	I493	I507	I521	I535	I549	I563	I577	I591	I605	I619	I633	I647	I661	I675	I689	I703	I717	I731	I745	I759	I773	I787	I801	I815	I829	I843	I857	I871	I885	I899	I913	I927	I941	I955	I969	I983	I997	L001	L015	L029	L043	L057	L071	L085	L099	L113	L127	L141	L155	L169	L183	L197	L211	L225	L239	L253	L267	L281	L295	L309	L323	L337	L351	L365	L379	L393	L407	L421	L435	L449	L463	L477	L491	L505	L519	L533	L547	L561	L575	L589	L603	L617	L631	L645	L659	L673	L687	L701	L715	L729	L743	L757	L771	L785	L799	L813	L827	L841	L855	L869	L883	L897	L911	L925	L939	L953	L967	L981	L995	M009	M023	M037	M051	M065	M079	M093	M107	M121	M135	M149	M163	M177	M191	M205	M219	M233	M247	M261	M275	M289	M303	M317	M331	M345	M359	M373	M387	M401	M415	M429	M443	M457	M471	M485	M499	M513	M527	M541	M555	M569	M583	M597	M611	M625	M639	M653	M667	M681	M695	M709	M723	M737	M751	M765	M779	M793	M807	M821	M835	M849	M863	M877	M891	M905	M919	M933	M947	M961	M975	M989	N003	N017	N031	N045	N059	N073	N087	N101	N115	N129	N143	N157	N171	N185	N199	N213	N227	N241	N255	N269	N283	N297	N311	N325	N339	N353	N367	N381	N395	N409	N423	N437	N451	N465	N479	N493	N507	N521	N535	N549	N563	N577	N591	N605	N619	N633	N647	N661	N675	N689	N703	N717	N731	N745	N759	N773	N787	N801	N815	N829	N843	N857	N871	N885	N899	N913	N927	N941	N955	N969	N983	N997	O001	O015	O029	O043	O057	O071	O085	O099	O113	O127	O141	O155	O169	O183	O197	O211	O225	O239	O253	O267	O281	O295	O309	O323	O337	O351	O365	O379	O393	O407	O421	O435	O449	O463	O477	O491	O505	O519	O533	O547	O561	O575	O589	O603	O617	O631	O645	O659	O673	O687	O701	O715	O729	O743	O757	O771	O785	O799	O813	O827	O841	O855	O869	O883	O897	O911	O925	O939	O953	O967	O981	O995	P009	P023	P037	P051	P065	P079	P093	P107	P121	P135	P149	P163	P177	P191	P205	P219	P233	P247	P261	P275	P289	P303	P317	P331	P345	P359	P373	P387	P401	P415	P429	P443	P457	P471	P485	P499	P513	P527	P541	P555	P569	P583	P597	P611	P625	P639	P653	P667	P681	P695	P709	P723	P737	P751	P765	P779	P793	P807	P821	P835	P849	P863	P877	P891	P905	P919	P933	P947	P961	P975	P989	Q003	Q017	Q031	Q045	Q059	Q073	Q087	Q101	Q115	Q129	Q143	Q157	Q171	Q185	Q199	Q213	Q227	Q241	Q255	Q269	Q283	Q297	Q311	Q325	Q339	Q353	Q367	Q381	Q395	Q409	Q423	Q437	Q451	Q465	Q479	Q493	Q507	Q521	Q535	Q549	Q563	Q577	Q591	Q605	Q619	Q633	Q647	Q661	Q675	Q689	Q703	Q717	Q731	Q745	Q759	Q773	Q787	Q801	Q815	Q829	Q843	Q857	Q871	Q885	Q899	Q913	Q927	Q941	Q955	Q969	Q983	Q997	R001	R015	R029	R043	R057	R071	R085	R099	R113	R127	R141	R155	R169	R183	R197	R211	R225	R239	R253	R267	R281	R295	R309	R323	R337	R351	R365	R379	R393	R407	R421	R435	R449	R463	R477	R491	R505	R519	R533	R547	R561	R575	R589	R603	R617	R631	R645	R659	R673	R687	R701	R715	R729	R743	R757	R771	R785	R799	R813	R827	R841	R855	R869	R883	R897	R911	R925	R939	R953	R967	R981	R995	S009	S023	S037	S051	S065	S079	S093	S107	S121	S135	S149	S163	S177	S191	S205	S219	S233	S247	S261	S275	S289	S303	S317	S331	S345	S359	S373	S387	S401	S415	S429	S443	S457	S471	S485	S499	S513	S527	S541	S555	S569	S583	S597	S611	S625	S639	S653	S667	S681	S695	S709	S723	S737	S751	S765	S779	S793	S807	S821	S835	S849	S863	S877	S891	S905	S919	S933	S947	S961	S975	S989	T003	T017	T031	T045	T059	T073	T087	T101	T115	T129	T143	T157	T171	T185	T199	T213	T227	T241	T255	T269	T283	T297	T311	T325	T339	T353	T367	T381	T395	T409	T423	T437	T451	T465	T479	T493	T507	T521	T535	T549	T563	T577	T591	T605	T619	T633	T647	T661	T675	T689	T703	T717	T731	T745	T759	T773	T787	T801	T815	T829	T843	T857	T871	T885	T899	T913	T927	T941	T955	T969	T983	T997	U001	U015	U029	U043	U057	U071	U085	U099	U113	U127	U141	U155	U169	U183	U197	U211	U225	U239	U253	U267	U281	U295	U309	U323	U337	U351	U365	U379	U393	U407	U421	U435	U449	U463	U477	U491	U505	U519	U533	U547	U561	U575	U589	U603	U617	U631	U645	U659	U673	U687	U701	U715	U729	U743	U757	U771	U785	U799	U813	U827	U841	U855	U869	U883	U897	U911	U925	U939	U953	U967	U981	U995	V009	V023	V037	V051	V065	V079	V093	V107	V121	V135	V149	V163	V177	V191	V205	V219	V233	V247	V261	V275	V289	V303	V317	V331	V345	V359	V373	V387	V401	V415	V429	V443	V457	V471	V485	V499	V513	V527	V541	V555	V569	V583	V597	V611	V625	V639	V653	V667	V681	V695	V709	V723	V737	V751	V765	V779	V793	V807	V821	V835	V849	V863	V877	V891	V905	V919	V933	V947	V961	V975	V989	W003	W017	W031	W045	W059	W073	W087	W101	W115	W129	W143	W157	W171	W185	W199	W213	W227	W241	W255	W269	W283	W297	W311	W325	W339	W353	W367	W381	W395	W409	W423	W437	W451	W465	W479	W493	W507	W521	W535	W549	W563	W577	W591	W605	W619	W633	W647	W661	W675	W689	W703	W717	W731	W745	W759	W773	W787	W801	W815	W829	W843	W857	W871	W885	W899	W913	W927	W941	W955	W969	W983	W997	X001	X015	X029	X043	X057	X071	X085	X099	X113	X127	X141	X155	X169	X183	X197	X211	X225	X239	X253	X267	X281	X295	X309	X323	X337	X351	X365	X379	X393	X407	X421	X435	X449	X463	X477	X491	X505	X519	X533	X547	X561	X575	X589	X603	X617	X631	X645	X659	X673	X687	X701	X715	X729	X743	X757	X771	X785	X799	X813	X827	X841	X855	X869	X883	X897	X911	X925	X939	X953	X967	X981	X995	Y009	Y023	Y037	Y051	Y065	Y079	Y093	Y107	Y121	Y135	Y149	Y163	Y177	Y191	Y205	Y219	Y233	Y247	Y261	Y275	Y289	Y303	Y317	Y331	Y345	Y359	Y373	Y387	Y401	Y415	Y429	Y443	Y457	Y471	Y485	Y499	Y513	Y527	Y541	Y555	Y569	Y583	Y597	Y611	Y625	Y639	Y653	Y667	Y681	Y695	Y709	Y723	Y737	Y751	Y765	Y779	Y793	Y807	Y821	Y835	Y849	Y863	Y877	Y891	Y905	Y919	Y933	Y947	Y961	Y975	Y989	Z003	Z017	Z031	Z045	Z059	Z073	Z087	Z101	Z115	Z129	Z143	Z157	Z171	Z185	Z199	Z213	Z227	Z241	Z255	Z269	Z283	Z297	Z311	Z325	Z339	Z353	Z367	Z381	Z395	Z409	Z423	Z437	Z451	Z465	Z479	Z493	Z507	Z521	Z535	Z549	Z563	Z577	Z591	Z605	Z619	Z633	Z647	Z661	Z675	Z689	Z703	Z717	Z731	Z745	Z759	Z773	Z787	Z801	Z815	Z829	Z843	Z857	Z871	Z885	Z899	Z913	Z927	Z941	Z955	Z969	Z983	Z997
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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	350390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	1.147	Depositor
Minimum map value	-0.675	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1EIM

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	0.16	0/2441	0.37	0/3318
1	B	0.16	0/2441	0.37	0/3318
All	All	0.16	0/4882	0.37	0/6636

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

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	2390	0	2429	48	0
1	B	2390	0	2429	46	0
2	A	37	0	0	0	0
2	B	37	0	0	0	0
All	All	4854	0	4858	92	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 9.

The worst 5 of 92 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:387:HIS:ND1	1:B:420:GLU:OE1	2.26	0.69
1:A:285:PRO:HD3	1:A:307:GLU:HB2	1.76	0.68
1:B:285:PRO:HD3	1:B:307:GLU:HB2	1.76	0.68
1:A:387:HIS:ND1	1:A:420:GLU:OE1	2.26	0.66
1:B:37:MET:HE1	1:B:119:VAL:HG21	1.78	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	301/507 (59%)	280 (93%)	21 (7%)	0	100	100
1	B	301/507 (59%)	279 (93%)	22 (7%)	0	100	100
All	All	602/1014 (59%)	559 (93%)	43 (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	262/433 (60%)	262 (100%)	0	100	100
1	B	262/433 (60%)	262 (100%)	0	100	100
All	All	524/866 (60%)	524 (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 (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	HIS
1	B	410	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](#)

2 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	A1EIM	B	601	-	38,41,41	1.73	7 (18%)	54,71,71	2.94	23 (42%)
2	A1EIM	A	601	-	38,41,41	1.72	7 (18%)	54,71,71	2.94	23 (42%)

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	A1EIM	B	601	-	-	0/8/107/107	0/5/5/5
2	A1EIM	A	601	-	-	0/8/107/107	0/5/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	A1EIM	C07-C06	-5.24	1.48	1.55
2	A	601	A1EIM	C07-C06	-5.20	1.48	1.55
2	B	601	A1EIM	C08-C12	4.33	1.65	1.59
2	A	601	A1EIM	C08-C12	4.28	1.65	1.59
2	B	601	A1EIM	C12-C14	3.55	1.58	1.53

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1EIM	C12-C08-C07	11.12	116.61	107.96
2	B	601	A1EIM	C12-C08-C07	11.11	116.59	107.96
2	A	601	A1EIM	C09-C08-C12	7.28	118.24	109.98
2	B	601	A1EIM	C09-C08-C12	7.22	118.17	109.98
2	B	601	A1EIM	C13-C12-C14	-5.18	99.53	107.33

There are no chirality outliers.

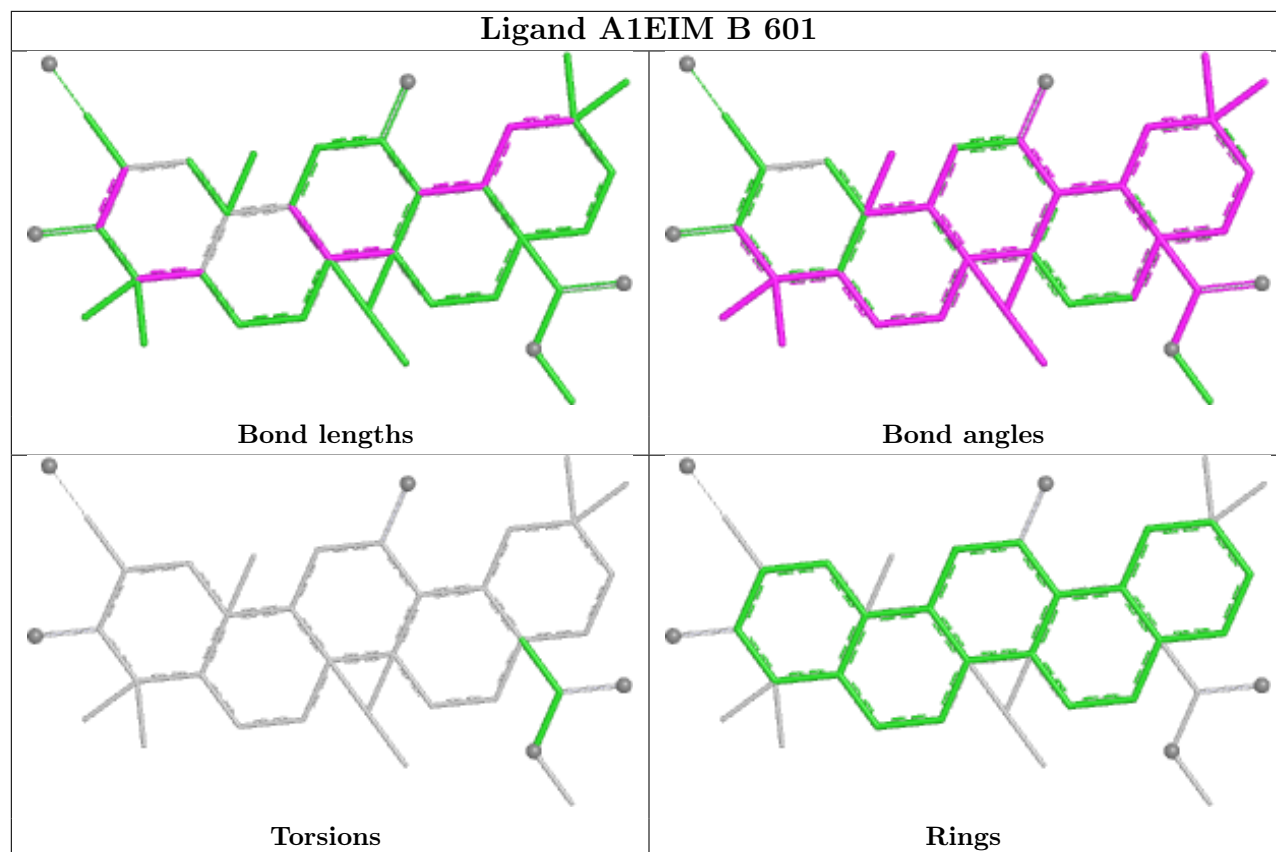
There are no torsion outliers.

There are no ring outliers.

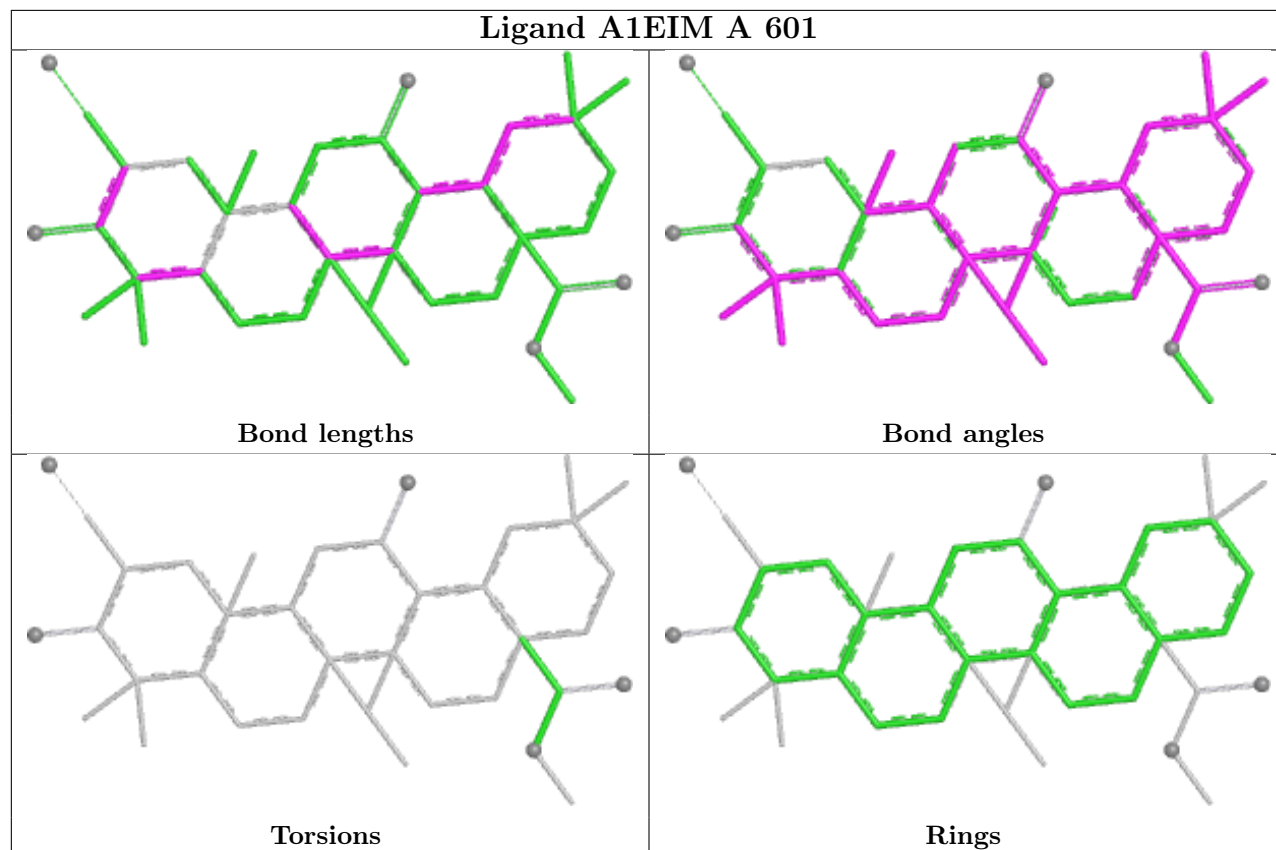
No monomer is involved in short contacts.

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

Ligand A1EIM B 601



Ligand A1EIM A 601



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-62681. These allow visual inspection of the internal detail of the map and identification of artifacts.

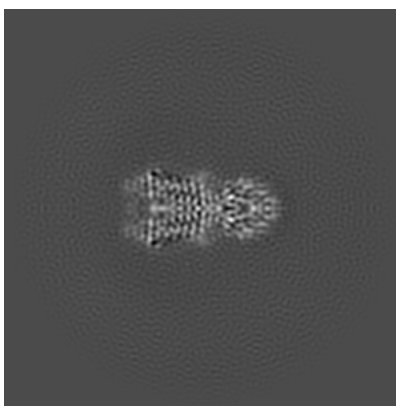
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

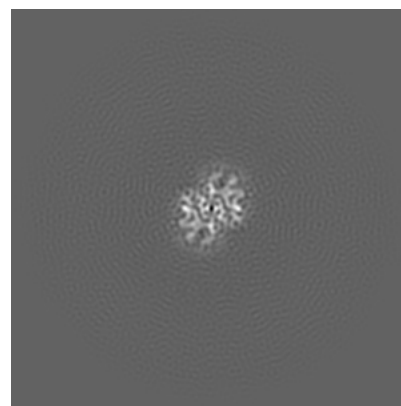
6.1.1 Primary map



X

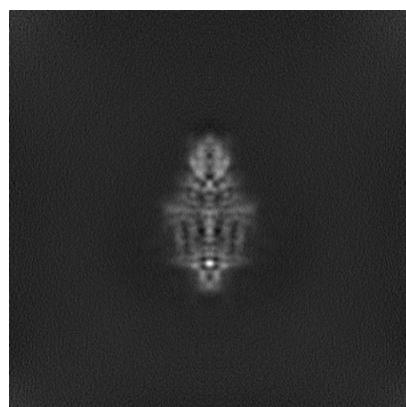


Y

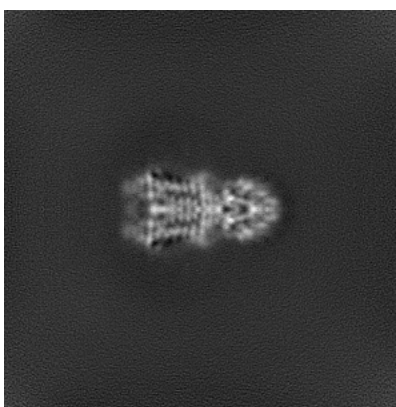


Z

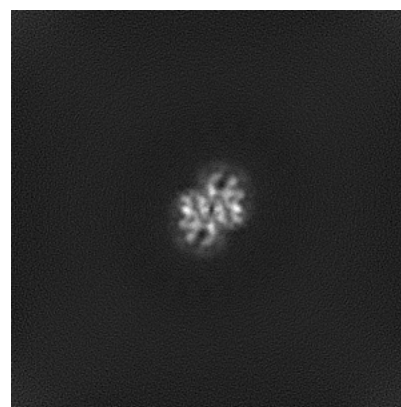
6.1.2 Raw map



X



Y

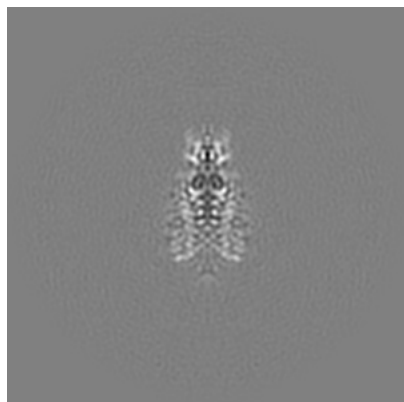


Z

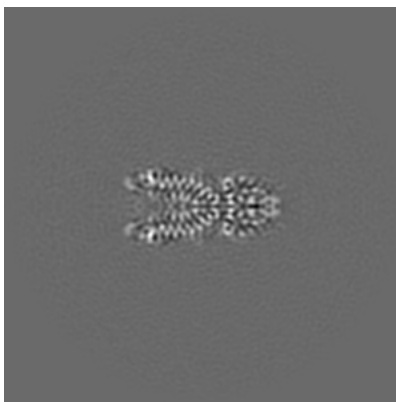
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

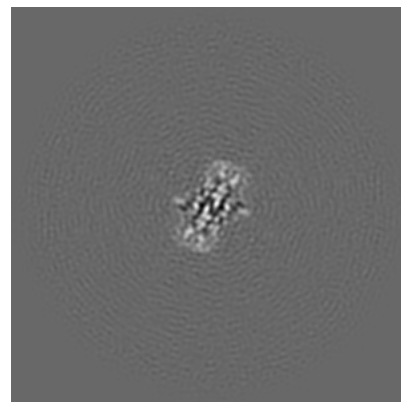
6.2.1 Primary map



X Index: 160

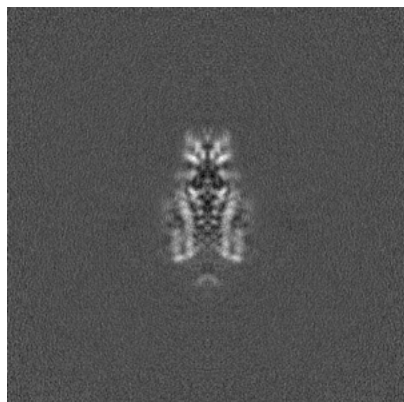


Y Index: 160

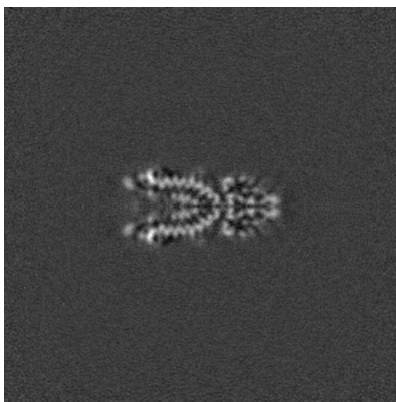


Z Index: 160

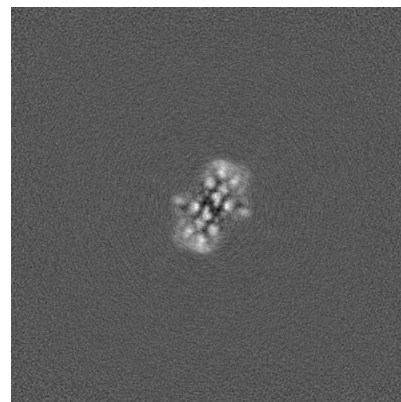
6.2.2 Raw map



X Index: 160



Y Index: 160

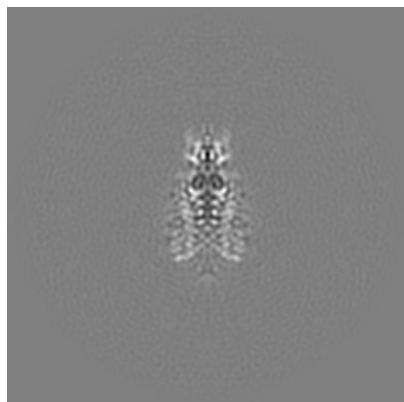


Z Index: 160

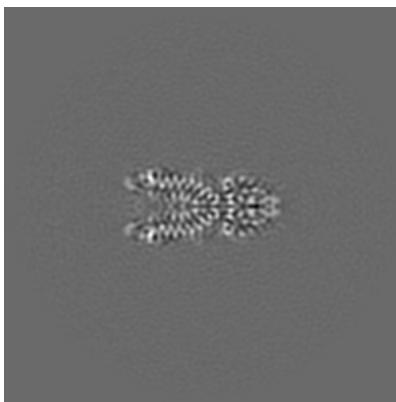
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

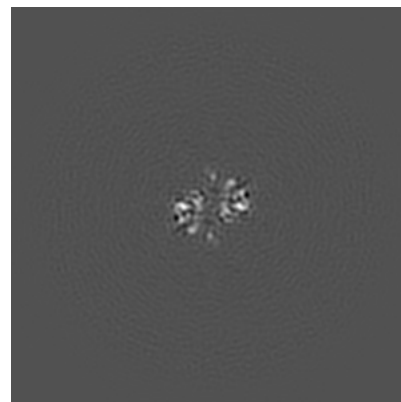
6.3.1 Primary map



X Index: 160

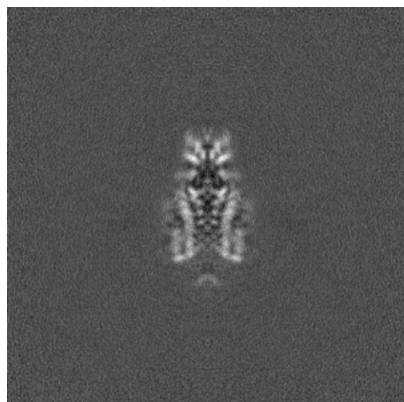


Y Index: 160

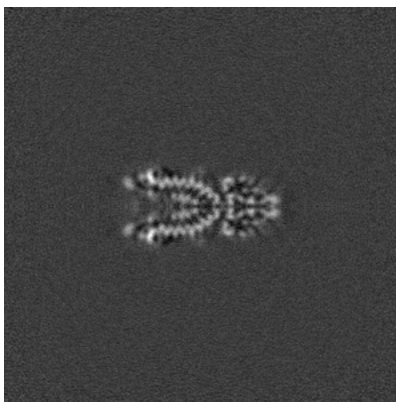


Z Index: 117

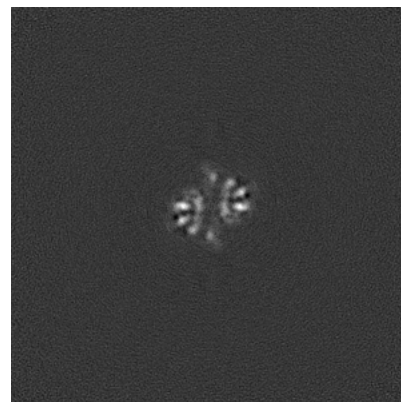
6.3.2 Raw map



X Index: 160



Y Index: 160

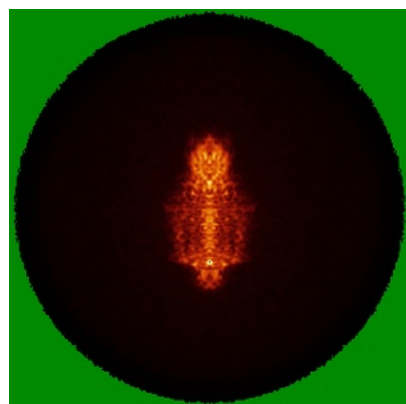


Z Index: 117

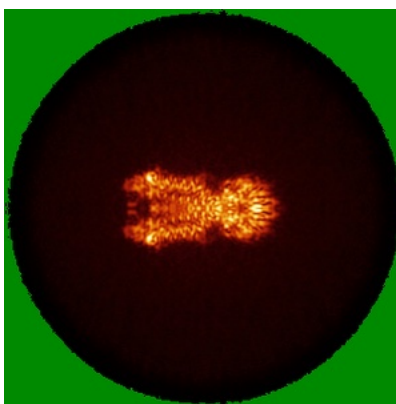
The images above show the largest variance slices of the map in three orthogonal directions.

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

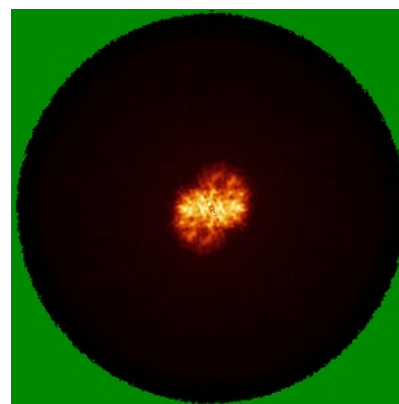
6.4.1 Primary map



X

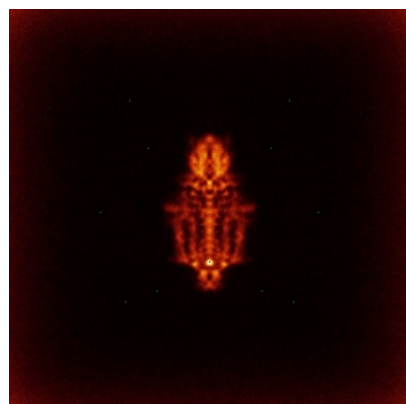


Y

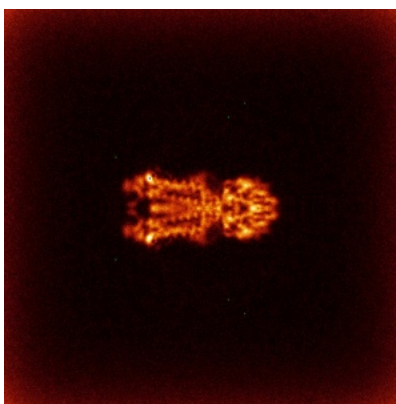


Z

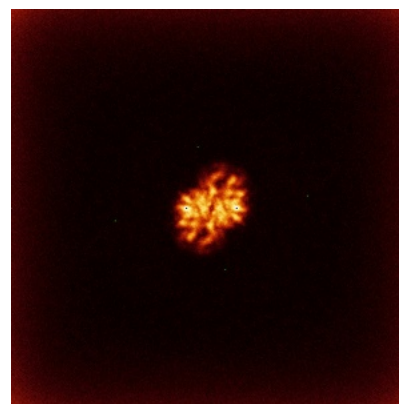
6.4.2 Raw map



X



Y

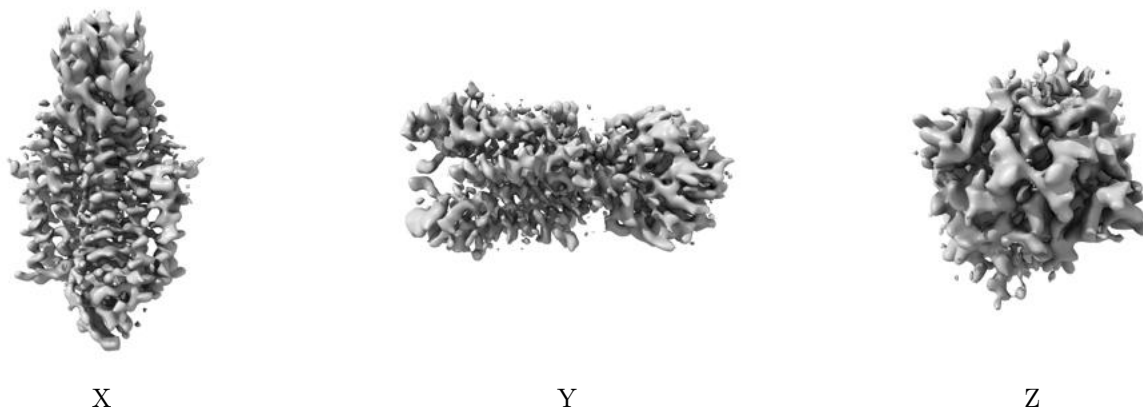


Z

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

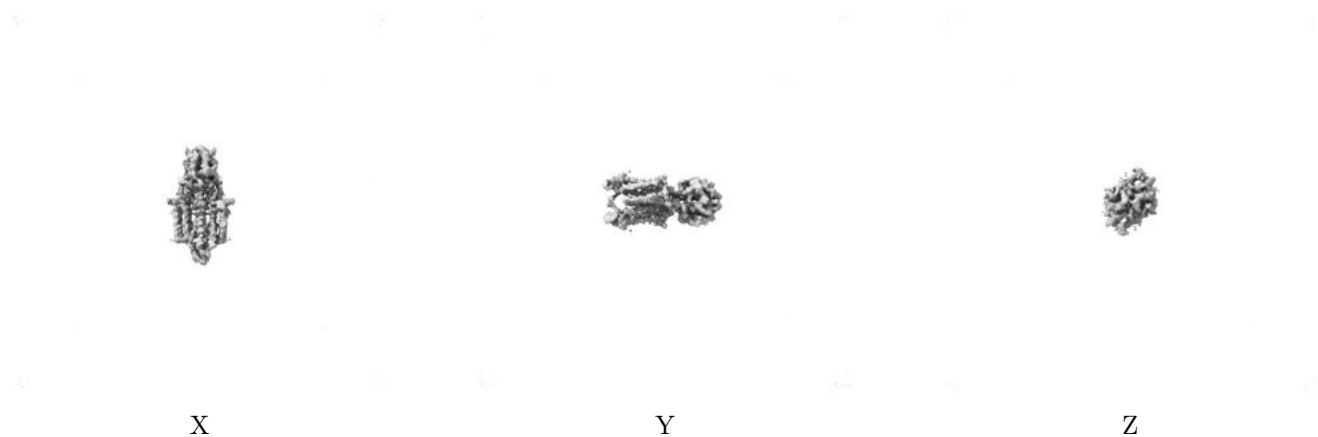
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

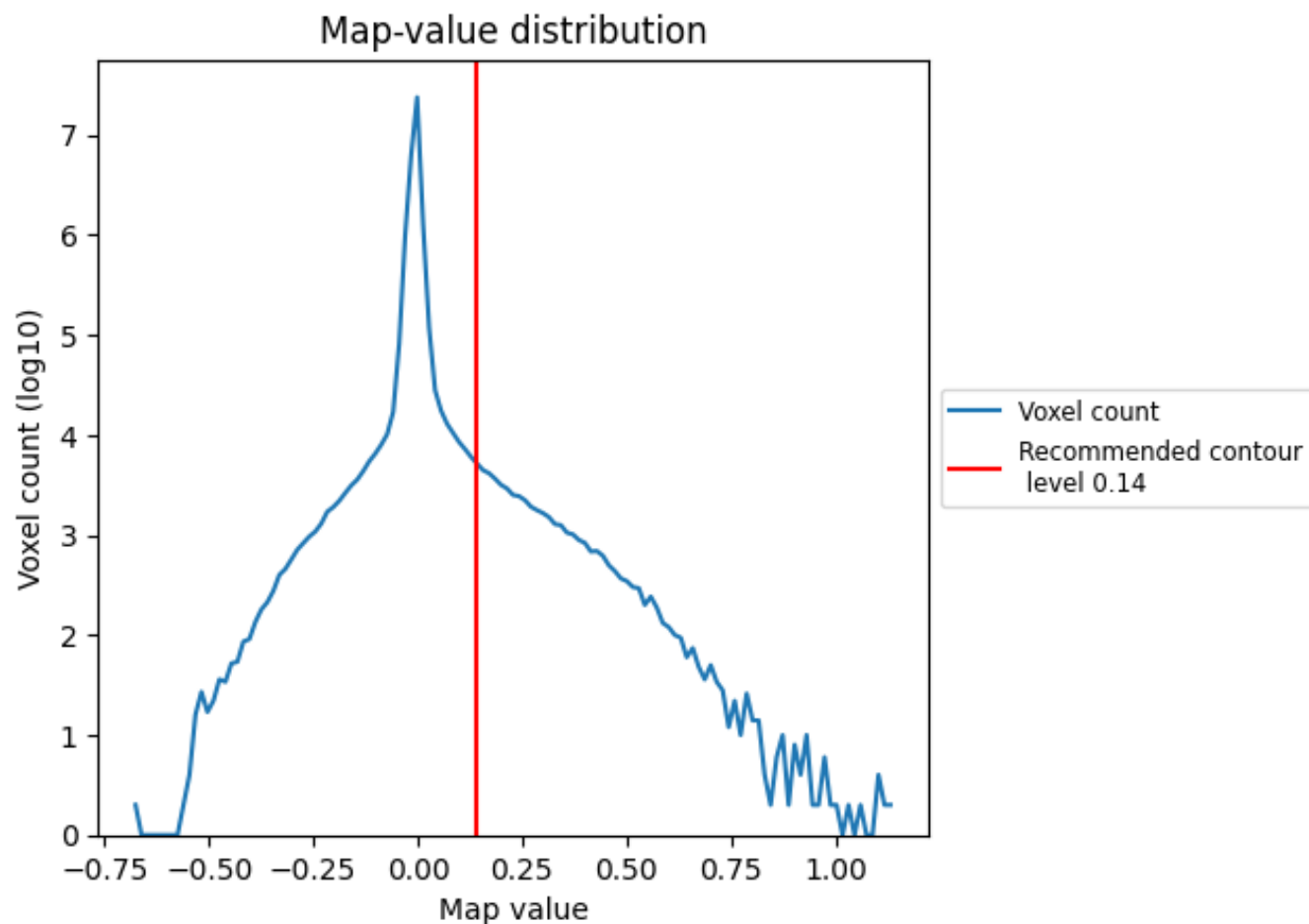
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

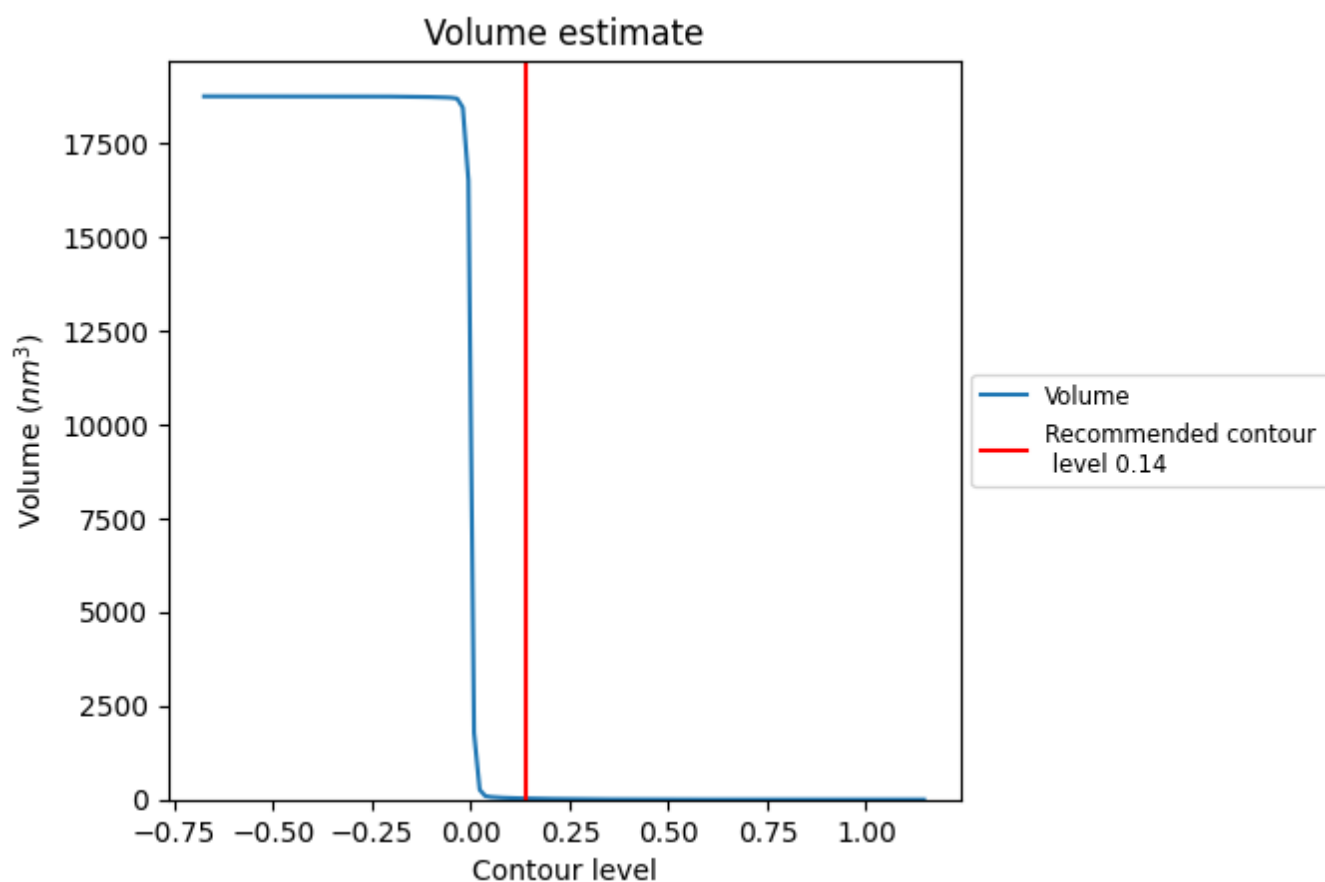
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

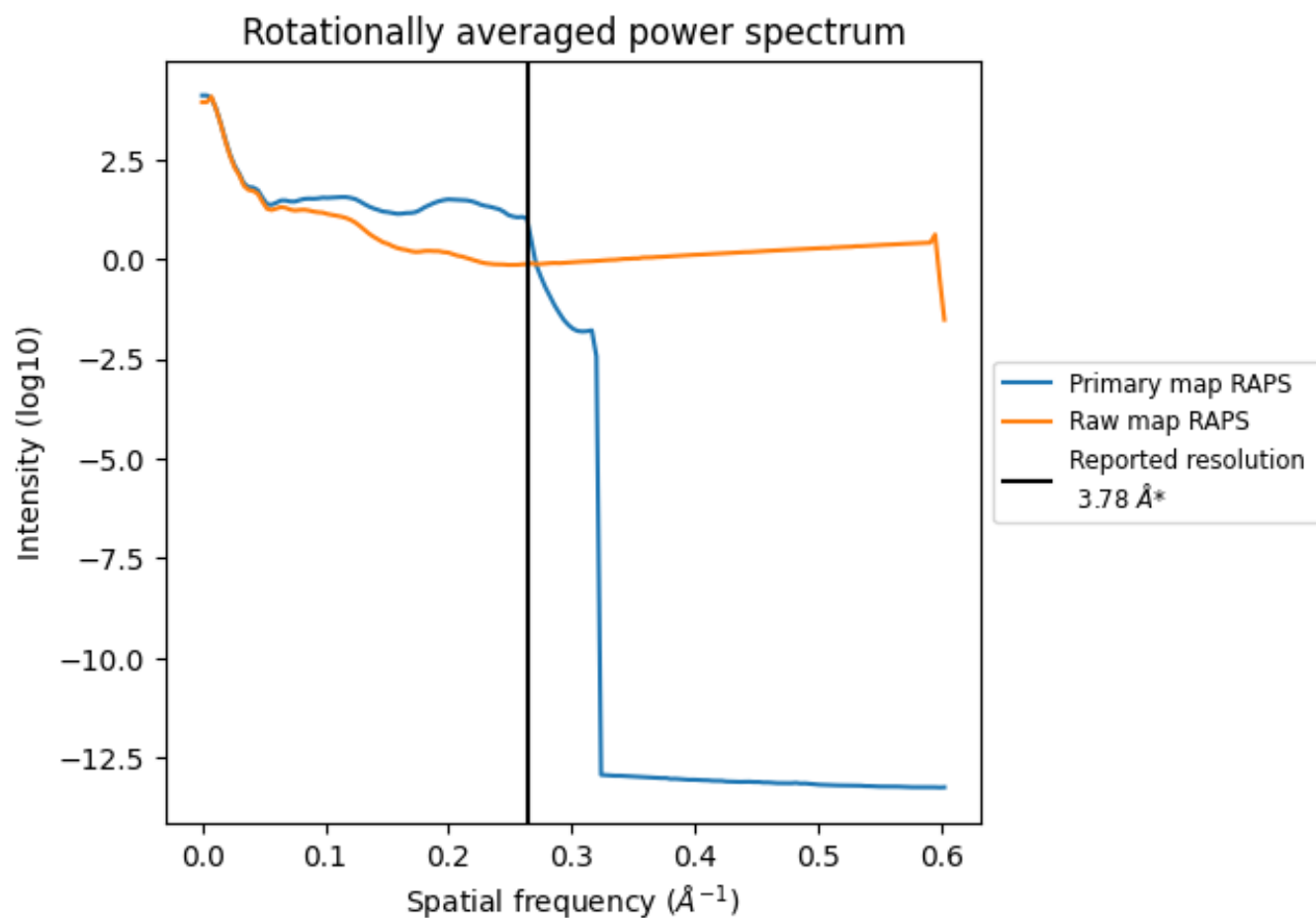
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29 nm³; this corresponds to an approximate mass of 26 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 ⓘ

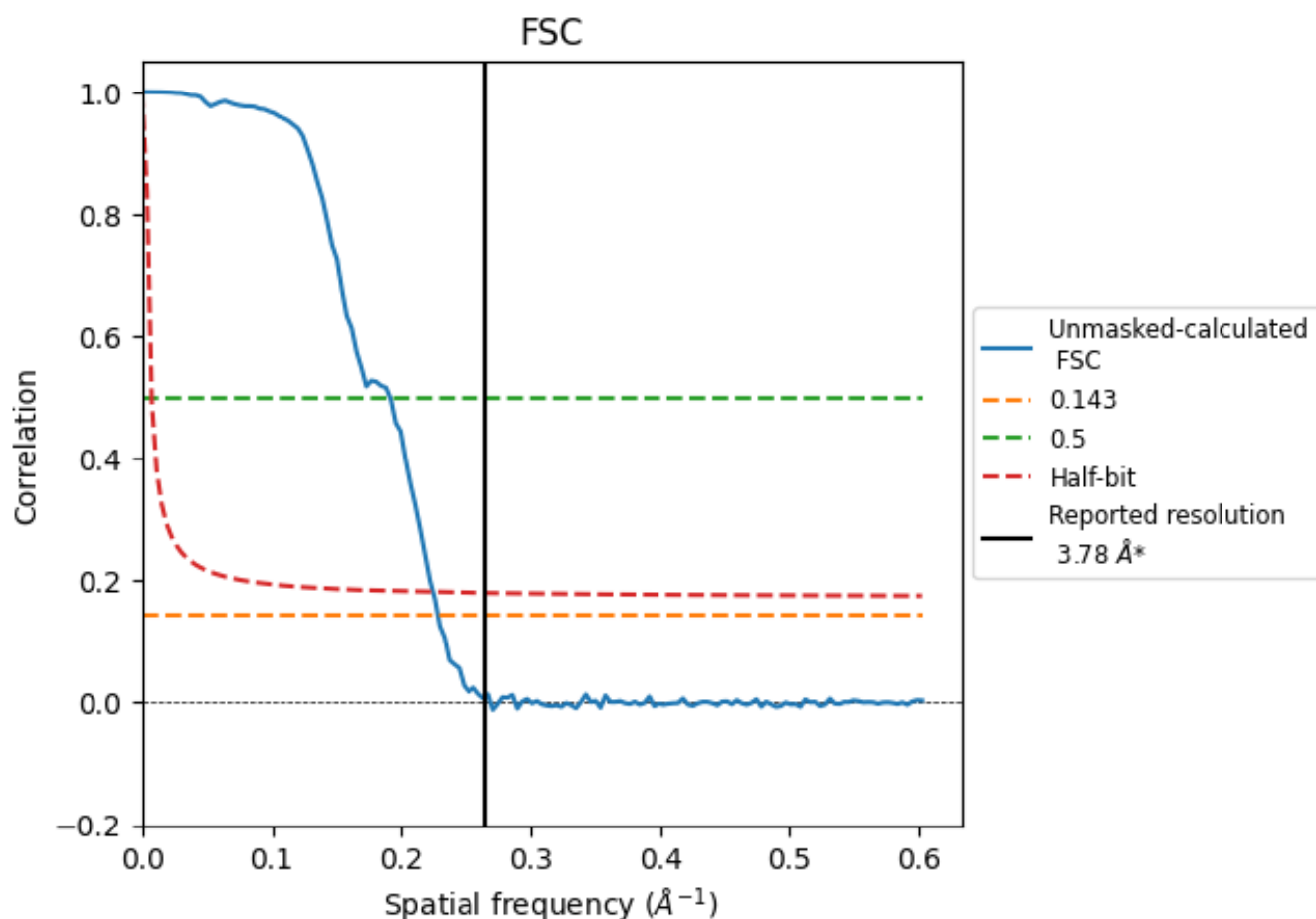


*Reported resolution corresponds to spatial frequency of 0.265 Å⁻¹

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 0.265 Å⁻¹

8.2 Resolution estimates [i](#)

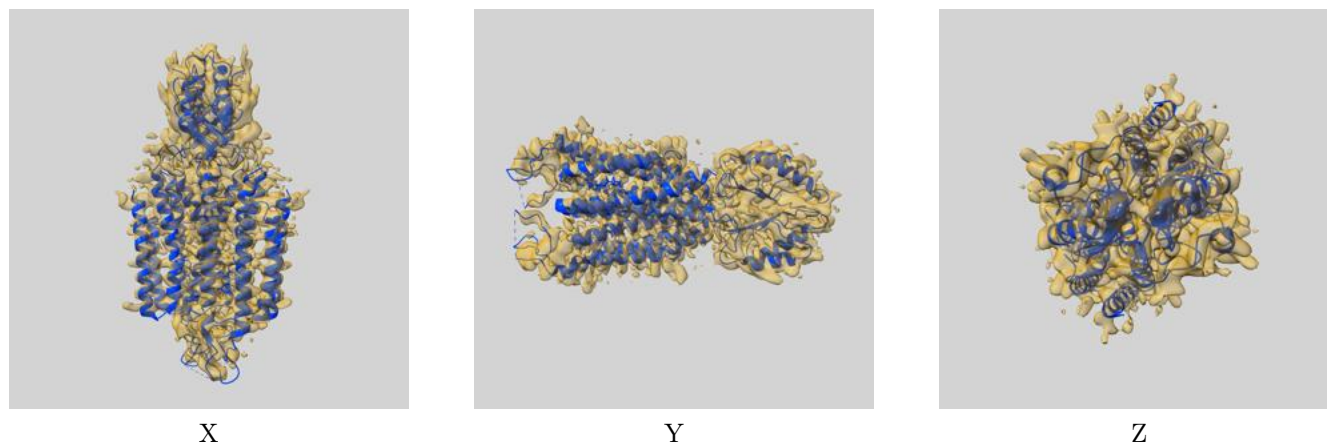
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.38	5.22	4.46

*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 4.38 differs from the reported value 3.78 by more than 10 %

9 Map-model fit [i](#)

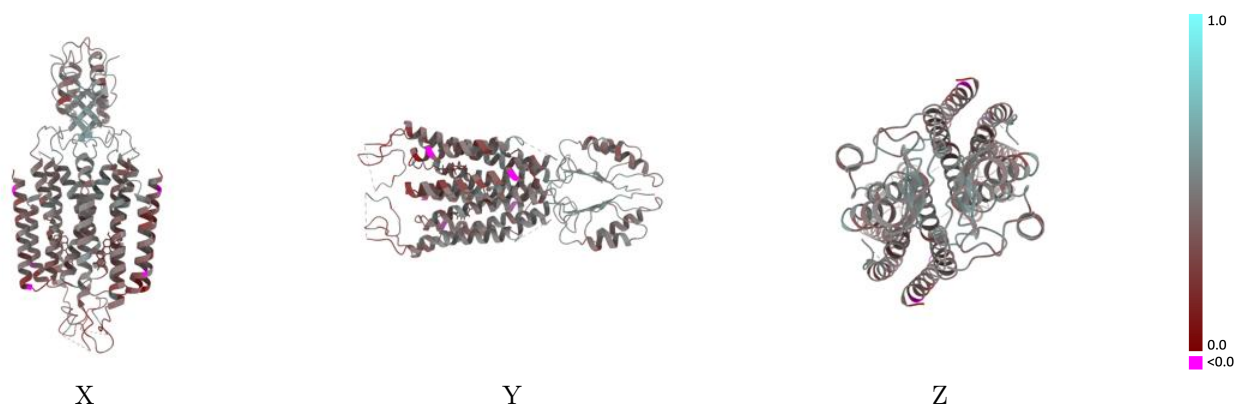
This section contains information regarding the fit between EMDB map EMD-62681 and PDB model 9L00. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



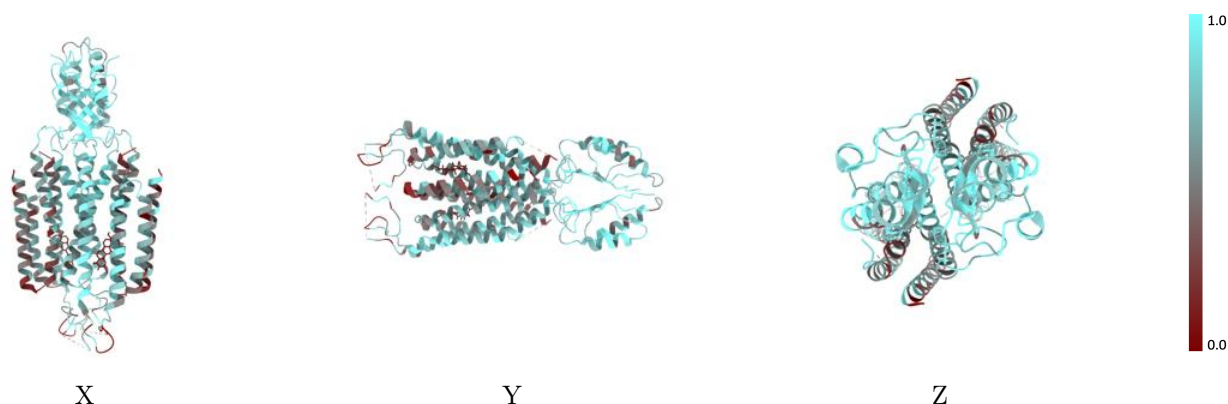
The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



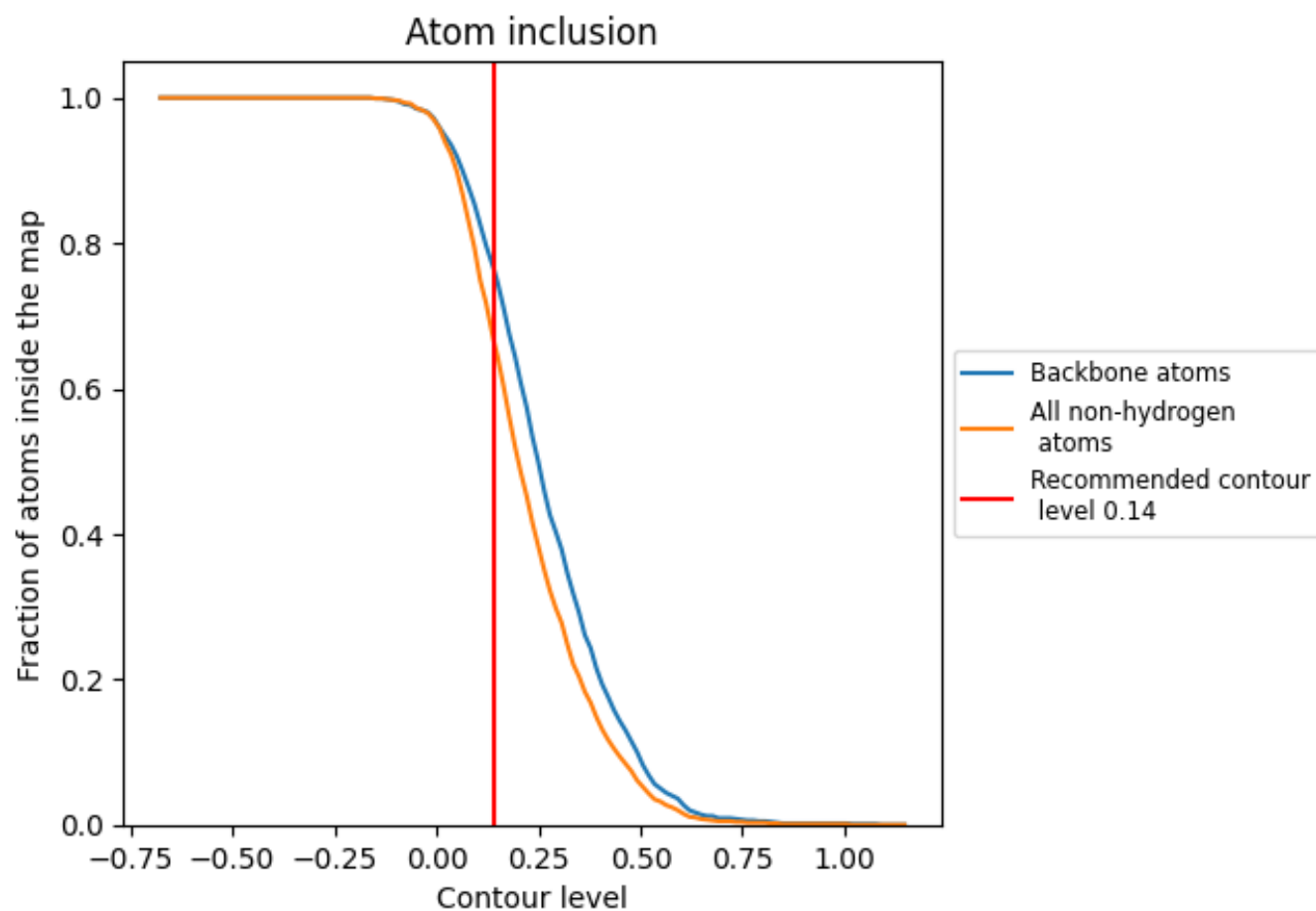
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.14).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6670	0.4120
A	0.6670	0.4110
B	0.6660	0.4130

