



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:13 PM UTC

PDB ID : 8WUI / pdb_00008wui
EMDB ID : EMD-37855
Title : SKOR D312N L271P double mutation
Authors : Gao, X.; Sun, T.; Lu, Y.; Jia, Y.; Xu, X.; Zhang, Y.; Fu, P.; Yang, G.
Deposited on : 2023-10-20
Resolution : 3.40 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

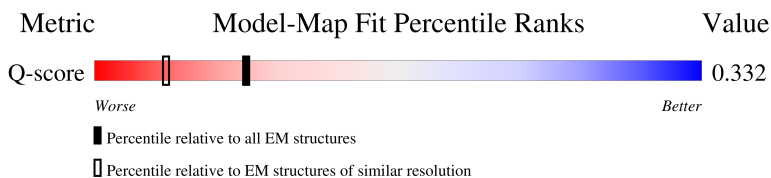
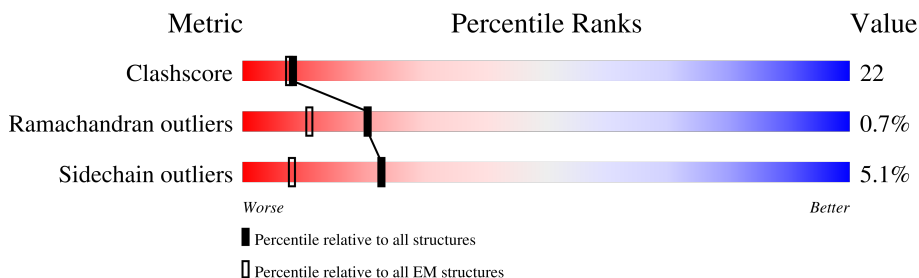
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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	14717 (2.90 - 3.90)

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	838	26% 34% 19% 45%
1	B	838	27% 34% 19% 46%
1	C	838	27% 34% 19% 45%
1	D	838	27% 33% 19% 46%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15340 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 Potassium channel SKOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	449	Total	C	N	O	S	0	0
			3706	2432	612	639	23		
1	A	464	Total	C	N	O	S	0	0
			3832	2510	637	662	23		
1	D	449	Total	C	N	O	S	0	0
			3706	2432	612	639	23		
1	C	464	Total	C	N	O	S	0	0
			3832	2510	637	662	23		

There are 48 discrepancies between the modelled and reference sequences:

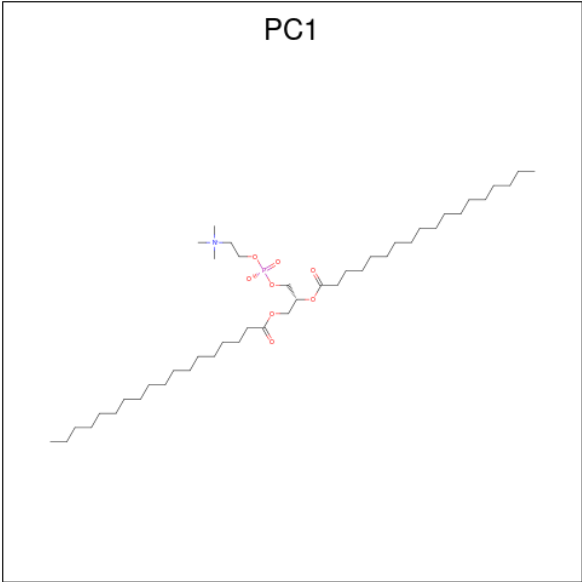
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP Q9M8S6
B	-8	ASP	-	expression tag	UNP Q9M8S6
B	-7	TYR	-	expression tag	UNP Q9M8S6
B	-6	LYS	-	expression tag	UNP Q9M8S6
B	-5	ASP	-	expression tag	UNP Q9M8S6
B	-4	ASP	-	expression tag	UNP Q9M8S6
B	-3	ASP	-	expression tag	UNP Q9M8S6
B	-2	ASP	-	expression tag	UNP Q9M8S6
B	-1	LYS	-	expression tag	UNP Q9M8S6
B	0	HIS	-	expression tag	UNP Q9M8S6
B	271	PRO	LEU	engineered mutation	UNP Q9M8S6
B	312	ASN	ASP	engineered mutation	UNP Q9M8S6
A	-9	MET	-	initiating methionine	UNP Q9M8S6
A	-8	ASP	-	expression tag	UNP Q9M8S6
A	-7	TYR	-	expression tag	UNP Q9M8S6
A	-6	LYS	-	expression tag	UNP Q9M8S6
A	-5	ASP	-	expression tag	UNP Q9M8S6
A	-4	ASP	-	expression tag	UNP Q9M8S6
A	-3	ASP	-	expression tag	UNP Q9M8S6
A	-2	ASP	-	expression tag	UNP Q9M8S6
A	-1	LYS	-	expression tag	UNP Q9M8S6
A	0	HIS	-	expression tag	UNP Q9M8S6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	271	PRO	LEU	engineered mutation	UNP Q9M8S6
A	312	ASN	ASP	engineered mutation	UNP Q9M8S6
D	-9	MET	-	initiating methionine	UNP Q9M8S6
D	-8	ASP	-	expression tag	UNP Q9M8S6
D	-7	TYR	-	expression tag	UNP Q9M8S6
D	-6	LYS	-	expression tag	UNP Q9M8S6
D	-5	ASP	-	expression tag	UNP Q9M8S6
D	-4	ASP	-	expression tag	UNP Q9M8S6
D	-3	ASP	-	expression tag	UNP Q9M8S6
D	-2	ASP	-	expression tag	UNP Q9M8S6
D	-1	LYS	-	expression tag	UNP Q9M8S6
D	0	HIS	-	expression tag	UNP Q9M8S6
D	271	PRO	LEU	engineered mutation	UNP Q9M8S6
D	312	ASN	ASP	engineered mutation	UNP Q9M8S6
C	-9	MET	-	initiating methionine	UNP Q9M8S6
C	-8	ASP	-	expression tag	UNP Q9M8S6
C	-7	TYR	-	expression tag	UNP Q9M8S6
C	-6	LYS	-	expression tag	UNP Q9M8S6
C	-5	ASP	-	expression tag	UNP Q9M8S6
C	-4	ASP	-	expression tag	UNP Q9M8S6
C	-3	ASP	-	expression tag	UNP Q9M8S6
C	-2	ASP	-	expression tag	UNP Q9M8S6
C	-1	LYS	-	expression tag	UNP Q9M8S6
C	0	HIS	-	expression tag	UNP Q9M8S6
C	271	PRO	LEU	engineered mutation	UNP Q9M8S6
C	312	ASN	ASP	engineered mutation	UNP Q9M8S6

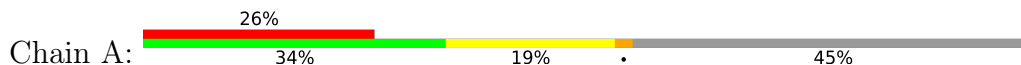
- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C			0
			17	17			
2	B	1	Total	C			0
			17	17			
2	B	1	Total	C			0
			17	17			
2	A	1	Total	C			0
			17	17			
2	A	1	Total	C			0
			17	17			
2	A	1	Total	C	O	P	0
			30	21	8	1	
2	A	1	Total	C			0
			17	17			
2	D	1	Total	C			0
			17	17			
2	D	1	Total	C			0
			17	17			
2	D	1	Total	C			0
			17	17			
2	C	1	Total	C	O	P	0
			30	21	8	1	
2	C	1	Total	C			0
			17	17			
2	C	1	Total	C			0
			17	17			
2	C	1	Total	C			0
			17	17			

THR	ALA	LYS	GLU	GLN	LEU	ASN	VAL	PRO	GLU	ALA	SER	CYS	VAL	LEU	SER	GLU	ASP	GLU	ALA	LYS	ILE	ILE	ASP	VAL	ASP	LEU	ILE	SER	ASP	GLY	GLN	LYS	LEU	TYR	LEU	ALA	VAL	GLU	THR
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- Molecule 1: Potassium channel SKOR



NET	ASP	TYR	LYS	ASP	ASP	ASP	ASP	HIS	MET	GLY	GLY	SER	SER	GLY	GLY	VAL	SER	TYR	ARG	SER	GLY	GLY	GLU	GLU	LEU	GLU	ASP	ASP	PHE	ARG	ASP	GLY	ILE	VAL	GLU	SER	SER	ASN	PRO	LEU	THR	LEU	GLY	LEU
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ASP	PHE	ALA	GLY	GLY	SER	GLY	GLY	LYS	PHE	THR	VAL	ILE	ASN	GLY	ILE	ARG	ASP	ILE	SER	ARG	GLY	S73	P77	R60	W92	A93	S97	P98	P99	F104	G105	F106	F107	P111	A120	G121	I122	I123	A124	F125	L126	I129	L130	L131	T132	F133	A136	F137	R138	N140
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S140	R141	T142	R144	M145	Y147	R148	R149	S150	S151	I152	A153	L154	R155	Y156	L157	F161	L165	L166	A167	W171	D172	I173	I174	L187	L188	L189	I190	R191	R194	L200	M205	E206	I209	R210	T211	N212	T216	L221	V224	E225	F236	L256	K257	L258
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G259	G260	G261	G271	G272	G273	G274	G279	G280	G281	G282	G283	G284	G285	G293	G294	I303	F304	A305	M306	M313	I320	T324	K329	G330	S331	K332	T333	E334	R335	F336	R337	D338	K339	M340	A341	D342	T343	M344	R345	Y346	M347	M348	R349	K350	K351	L352	G353	R354	K355	L356	L357	L358	L359	L360	L361	L362	L363	L364	L365	L366	L367	L368	L369	L370	L371	L372	L373	L374	L375	L376	L377	L378	L379	L380	L381	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L396	L397	L398	L399	L400	L401	L402	L403	L404	L405	L406	L407	L408	L409	L410	L411	L412	L413	L414	L415	L416	L417	L418	L419	L420	L421	L422	L423	L424	L425	L426	L427	L428	L429	L430	L431	L432	L433	L434	L435	L436	L437	L438	L439	L440	L441	L442	L443	L444	L445	L446	L447	L448	L449	L450	L451	L452	L453	L454	L455	L456	L457	L458	L459	L460	L461	L462	L463	L464	L465	L466	L467	L468	L469	L470	L471	L472	L473	L474	L475	L476	L477	L478	L479	L480	L481	L482	L483	L484	L485	L486	L487	L488	L489	L490	L491	L492	L493	L494	L495	L496	L497	L498	L499	L500	L501	L502	L503	L504	L505	L506	L507	L508	L509	L510	L511	L512	L513	L514	L515	L516	L517	L518	L519	L520	L521	L522	L523	L524	L525	L526	L527	L528	L529	L530	L531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	L1000
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Q358	Q359	T360	T361	T362	T363	T364	T365	T366	Q367	T368	E369	Q370	Q371	Q372	T373	E374	A375	A376	V377	L378	Q379	D380	T381	P382	V383	S384	T385	R386	A387	R388	T389	A390	Q391	T392	L393	T394	L395	P396	Y397	T398	E399	K400	V401	P402	L403	F404	R405	G406	C407	S408	S409	E410	F411	T412	H413	Q414	T415	V416
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R418	L419	H420	E421	E422	F423	F424	L425	P426	G427	E428	V429	I430	M431	E432	G433	G434	S435	V436	V437	D438	Q439	L440	L441	F442	V443	C444	H445	G446	V447	L448	E449	E450	I451	G452	I453	THR	LYS	ASP	GLY	GLY	SER	GLU	GLU	I455	V462	A463	V464	L465	G466	P467	D468	H469	S470	F471	G472	E473	I474	S475	I476	I477
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C478	M479	L480	P481	Q482	P483	Y484	Y485	T486	R487	V488	A489	E490	L491	C492	R493	L494	L495	R496	L497	D498	K499	Q500	S501	F502	M503	M504	F505	E506	E507	F508	F509	F510	H511	D512	G513	G514	R515	F516	L517	M518	N519	L520	L521	E522	G523	K524	E525	S526	N527	V528	R529	F530	K531	Q532	L533	E534	S535	D536	F537
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[illegible]

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

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

TRP	VAL	PRO	ARG	SER	ILE	GLU	GLU	LEU	ILE	ARG	THR	ALA	LYS	GLU	GLN	LEU	ASN	VAL	PRO	GLU	ALA	CYS	VAL	LEU	SER	GLU	ASP	GLU	ALA	LYS	ILE	ILE	ASP	VAL	ASP	LEU	ILE	SER	ASP	GLY	GLN	LYS	LEU	TYR	LEU	LEU	ALA	VAL	GLU	THR
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- Molecule 1: Potassium channel SKOR



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97040	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.795	Depositor
Minimum map value	-1.079	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.184	Depositor
Map size (Å)	291.19998, 291.19998, 291.19998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: PC1

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	0.42	1/3925 (0.0%)	0.62	7/5307 (0.1%)
1	B	0.27	0/3797	0.45	1/5136 (0.0%)
1	C	0.42	1/3925 (0.0%)	0.62	6/5307 (0.1%)
1	D	0.26	0/3797	0.48	4/5136 (0.1%)
All	All	0.35	2/15444 (0.0%)	0.55	18/20886 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	ASN	C-O	5.93	1.31	1.24
1	C	355	ASN	C-O	5.87	1.31	1.24

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	ASN	N-CA-C	-8.17	101.94	112.23
1	C	348	ASN	N-CA-C	-8.15	101.96	112.23
1	D	226	LEU	N-CA-C	-7.48	104.00	113.72
1	C	332	LYS	N-CA-C	-7.47	103.08	111.14
1	A	332	LYS	N-CA-C	-7.44	103.11	111.14

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	380	ASP	Mainchain
1	C	380	ASP	Mainchain

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	3832	0	3881	230	0
1	B	3706	0	3754	189	0
1	C	3832	0	3881	210	0
1	D	3706	0	3754	195	0
2	A	81	0	123	34	0
2	B	51	0	90	24	0
2	C	81	0	123	36	0
2	D	51	0	90	20	0
All	All	15340	0	15696	672	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 22.

The worst 5 of 672 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:304:PHE:CD1	2:B:901:PC1:H2E1	1.15	1.66
1:C:272:TRP:HD1	2:C:902:PC1:C21	1.00	1.65
1:C:107:PHE:CE1	2:C:901:PC1:H11	1.16	1.62
1:A:346:TYR:CE2	1:D:378:LEU:HD22	1.33	1.57
1:C:107:PHE:CZ	2:C:901:PC1:H11	1.38	1.55

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/838 (55%)	422 (92%)	35 (8%)	3 (1%)	18	47
1	B	445/838 (53%)	418 (94%)	23 (5%)	4 (1%)	14	42
1	C	460/838 (55%)	425 (92%)	32 (7%)	3 (1%)	18	47
1	D	445/838 (53%)	419 (94%)	23 (5%)	3 (1%)	18	47
All	All	1810/3352 (54%)	1684 (93%)	113 (6%)	13 (1%)	20	47

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	PHE
1	D	161	PHE
1	B	210	ARG
1	A	355	ASN
1	D	210	ARG

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	415/727 (57%)	385 (93%)	30 (7%)	13	39
1	B	400/727 (55%)	389 (97%)	11 (3%)	38	60
1	C	415/727 (57%)	384 (92%)	31 (8%)	12	38
1	D	400/727 (55%)	389 (97%)	11 (3%)	38	60
All	All	1630/2908 (56%)	1547 (95%)	83 (5%)	23	48

5 of 83 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	336	PHE
1	C	355	ASN
1	C	339	LYS
1	C	346	TYR
1	C	364	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	367	GLN
1	D	439	GLN
1	D	413	ASN
1	C	359	GLN
1	A	359	GLN

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](#)

14 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	PC1	D	901	-	16,16,53	0.17	0	15,15,61	0.09	0
2	PC1	B	903	-	16,16,53	0.17	0	15,15,61	0.08	0
2	PC1	C	902	-	16,16,53	0.16	0	15,15,61	0.09	0
2	PC1	C	903	-	16,16,53	0.17	0	15,15,61	0.11	0
2	PC1	B	901	-	16,16,53	0.15	0	15,15,61	0.08	0
2	PC1	C	904	-	16,16,53	0.15	0	15,15,61	0.07	0
2	PC1	A	903	-	29,29,53	0.46	0	32,34,61	0.57	1 (3%)
2	PC1	A	904	-	16,16,53	0.16	0	15,15,61	0.09	0
2	PC1	D	903	-	16,16,53	0.15	0	15,15,61	0.08	0
2	PC1	B	902	-	16,16,53	0.15	0	15,15,61	0.09	0
2	PC1	A	901	-	16,16,53	0.12	0	15,15,61	0.06	0
2	PC1	A	902	-	16,16,53	0.15	0	15,15,61	0.07	0
2	PC1	D	902	-	16,16,53	0.15	0	15,15,61	0.07	0
2	PC1	C	901	-	29,29,53	0.47	0	32,34,61	0.70	1 (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	PC1	D	901	-	-	8/14/14/57	-
2	PC1	B	903	-	-	9/14/14/57	-
2	PC1	C	902	-	-	7/14/14/57	-
2	PC1	C	903	-	-	11/14/14/57	-
2	PC1	B	901	-	-	9/14/14/57	-
2	PC1	C	904	-	-	10/14/14/57	-
2	PC1	A	903	-	-	14/31/31/57	-
2	PC1	A	904	-	-	6/14/14/57	-
2	PC1	D	903	-	-	8/14/14/57	-
2	PC1	B	902	-	-	11/14/14/57	-
2	PC1	A	901	-	-	6/14/14/57	-
2	PC1	A	902	-	-	10/14/14/57	-
2	PC1	D	902	-	-	8/14/14/57	-
2	PC1	C	901	-	-	14/31/31/57	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	903	PC1	O12-P-O14	2.43	120.31	110.83
2	C	901	PC1	O12-P-O14	2.22	119.48	110.83

There are no chirality outliers.

5 of 131 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	903	PC1	C1-O11-P-O12
2	A	903	PC1	C1-O11-P-O14
2	A	903	PC1	C1-O11-P-O13
2	C	901	PC1	C1-O11-P-O14
2	C	901	PC1	C22-C21-O21-C2

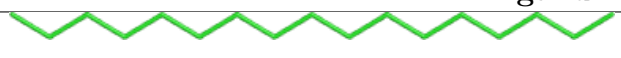
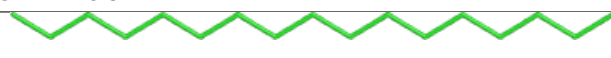
There are no ring outliers.

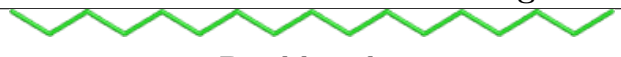
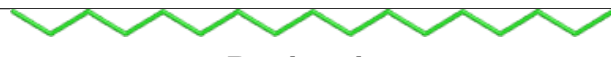
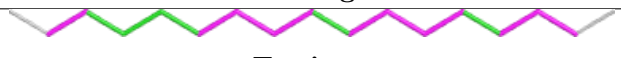
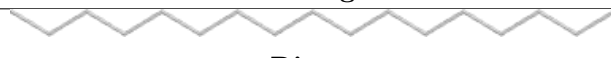
14 monomers are involved in 114 short contacts:

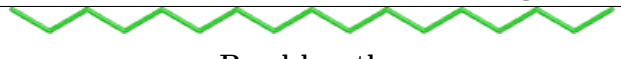
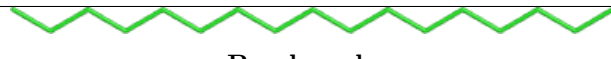
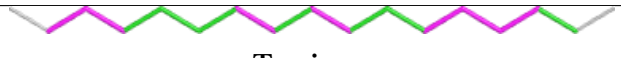
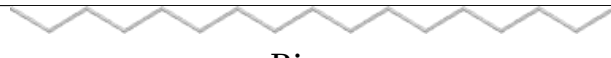
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	PC1	5	0
2	B	903	PC1	2	0
2	C	902	PC1	5	0
2	C	903	PC1	10	0
2	B	901	PC1	13	0
2	C	904	PC1	4	0
2	A	903	PC1	16	0
2	A	904	PC1	3	0
2	D	903	PC1	6	0
2	B	902	PC1	12	0
2	A	901	PC1	3	0
2	A	902	PC1	12	0
2	D	902	PC1	9	0
2	C	901	PC1	17	0

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

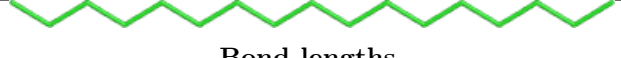
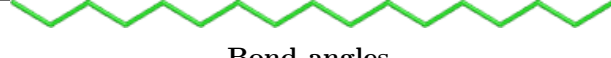
equivalents in the CSD to analyse the geometry.

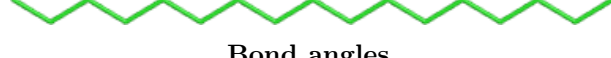
Ligand PC1 D 901			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

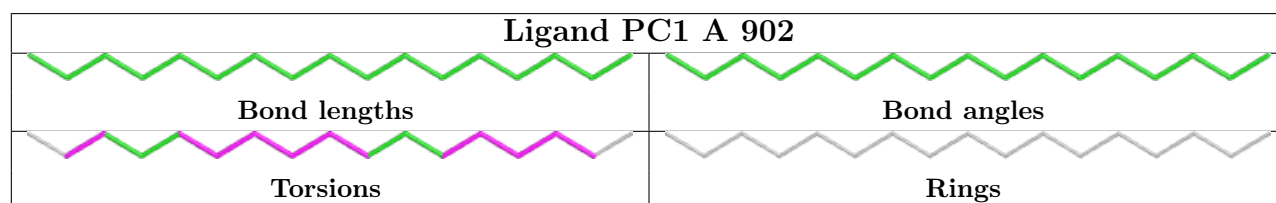
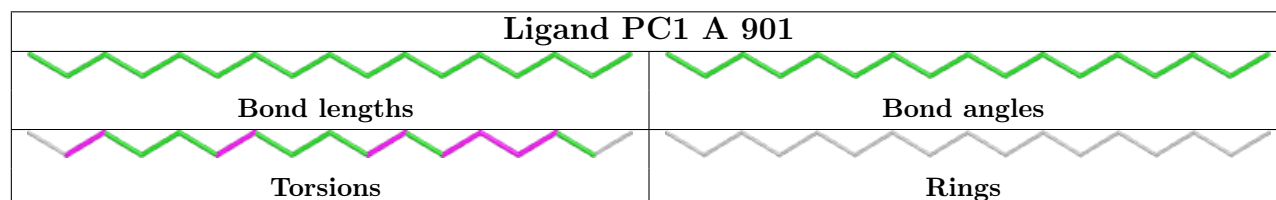
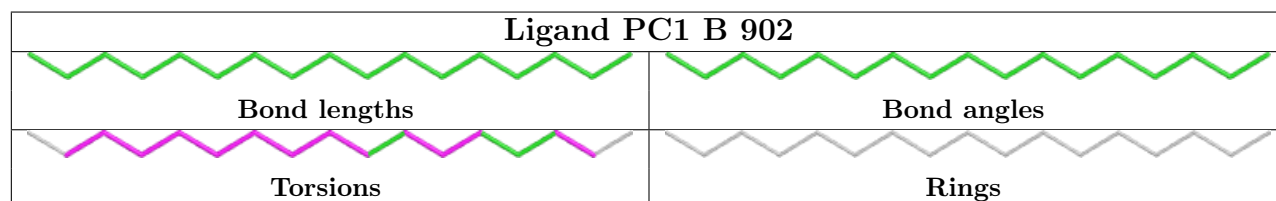
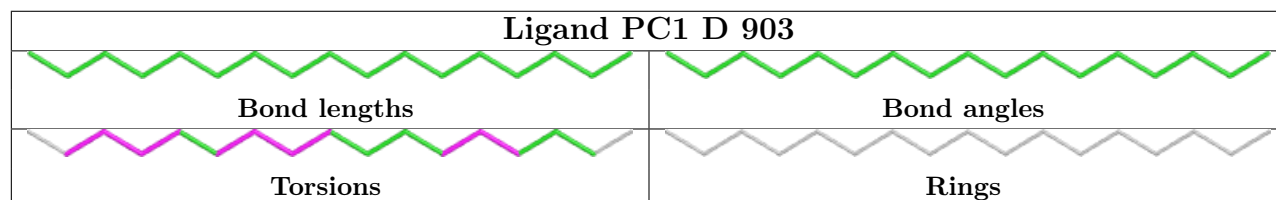
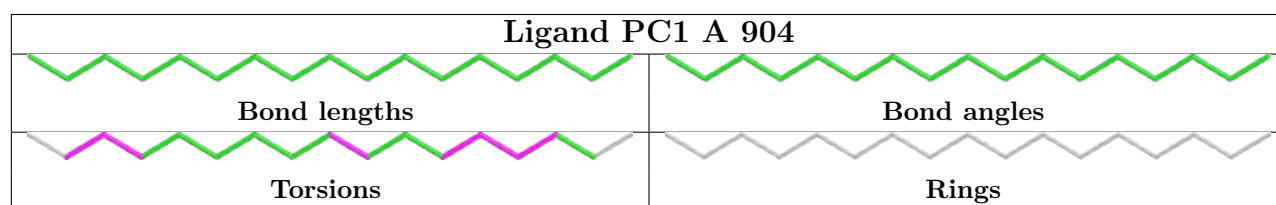
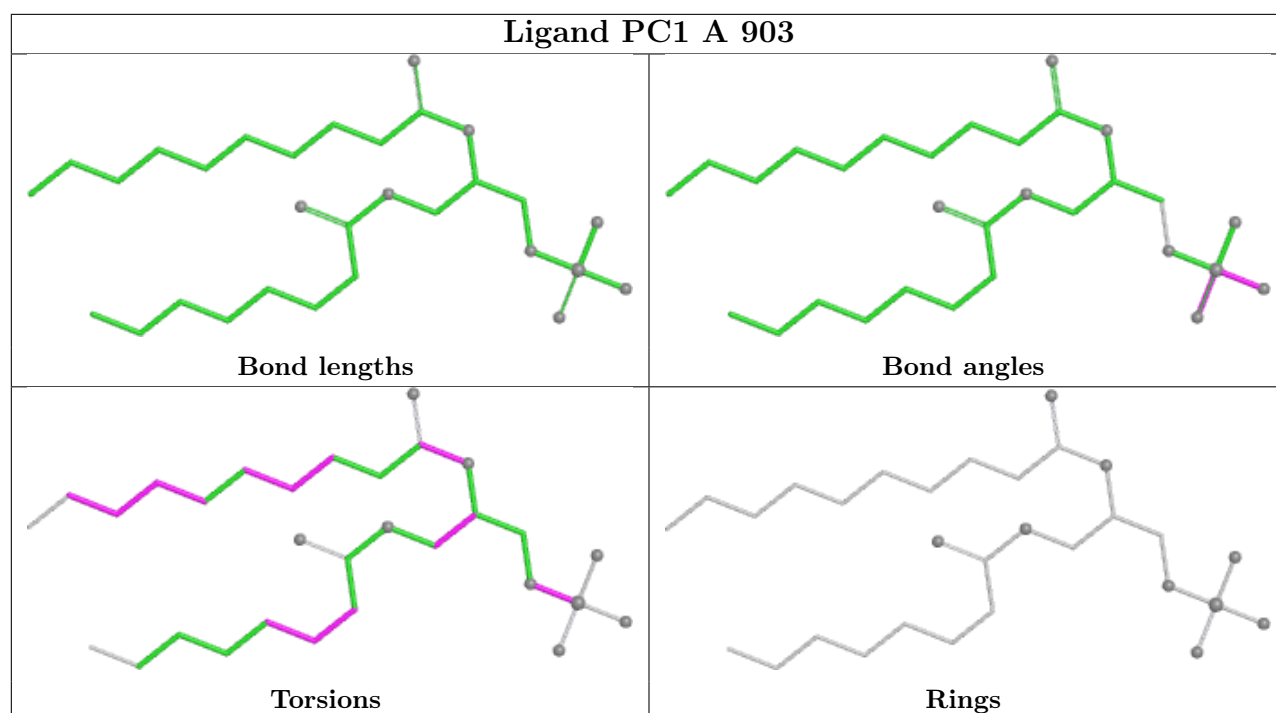
Ligand PC1 B 903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

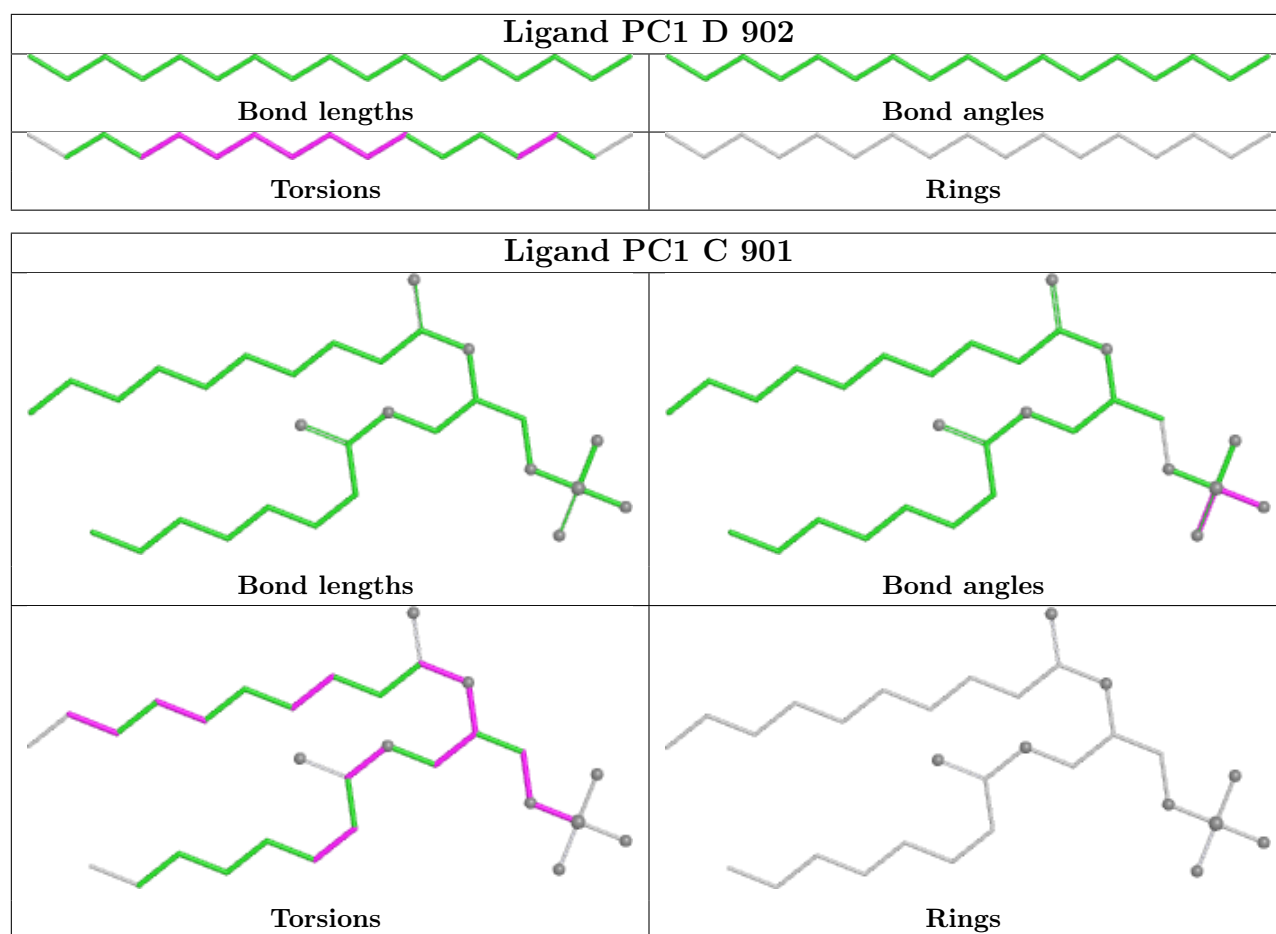
Ligand PC1 C 902			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 C 903			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 B 901			
 Bond lengths		 Bond angles	
 Torsions		 Rings	

Ligand PC1 C 904			
 Bond lengths		 Bond angles	
 Torsions		 Rings	





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.

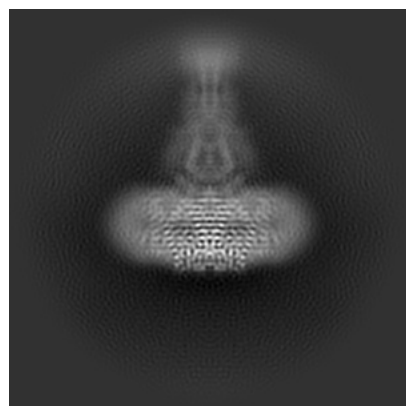
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-37855. These allow visual inspection of the internal detail of the map and identification of artifacts.

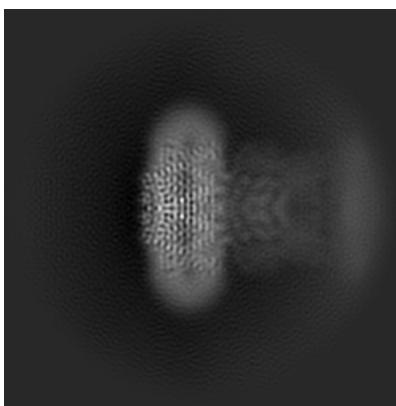
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

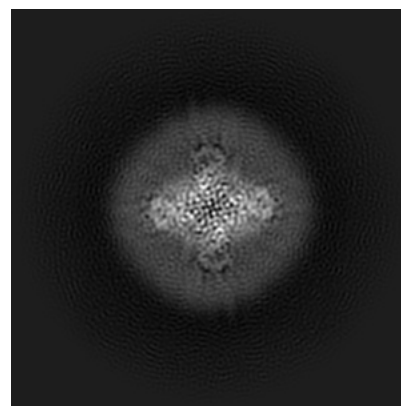
6.1.1 Primary map



X

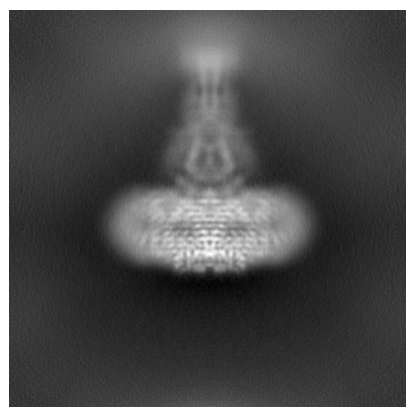


Y

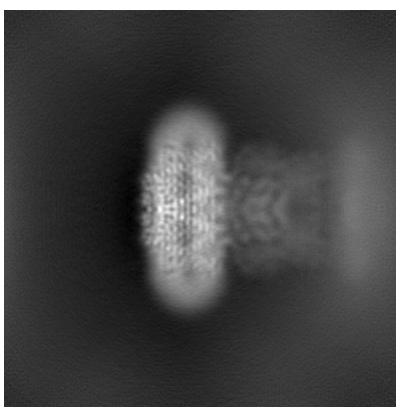


Z

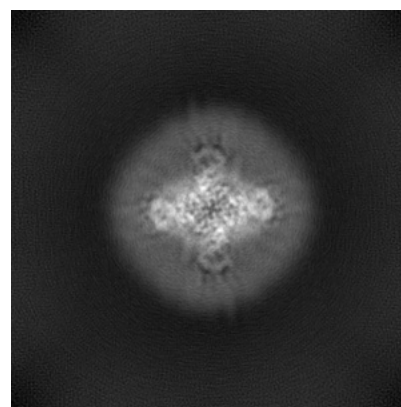
6.1.2 Raw map



X



Y

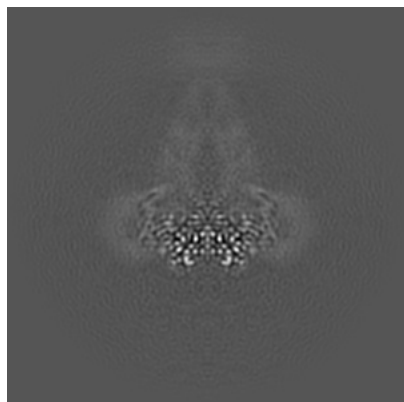


Z

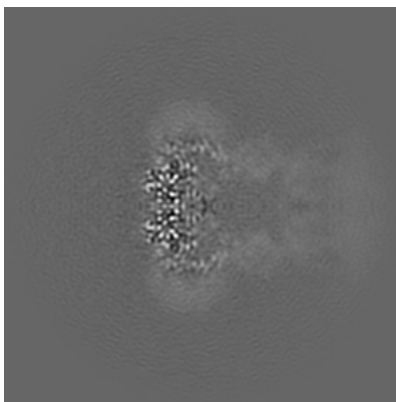
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

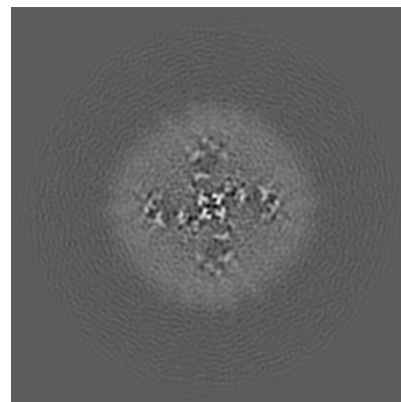
6.2.1 Primary map



X Index: 140

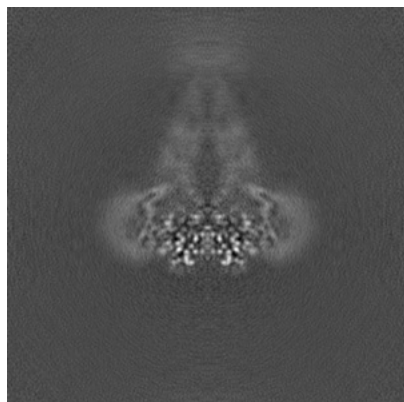


Y Index: 140

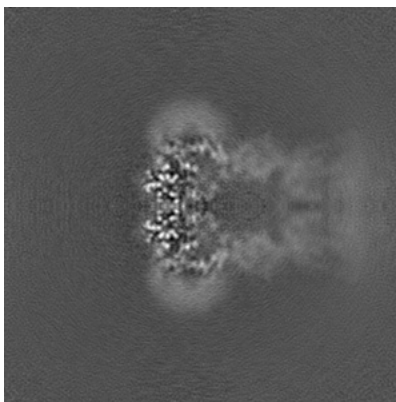


Z Index: 140

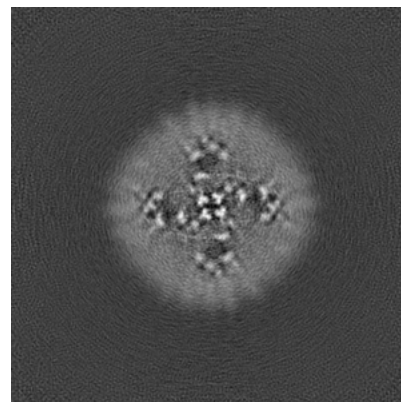
6.2.2 Raw map



X Index: 140



Y Index: 140

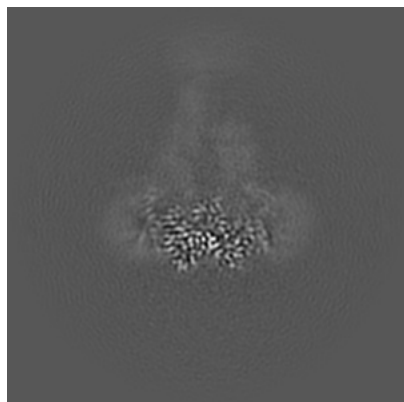


Z Index: 140

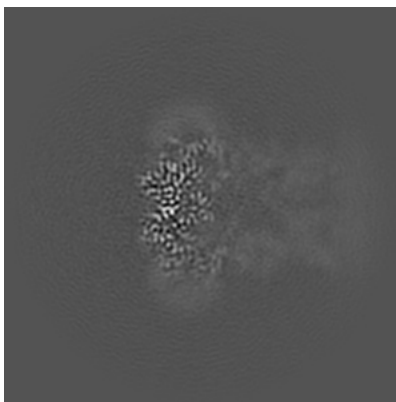
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

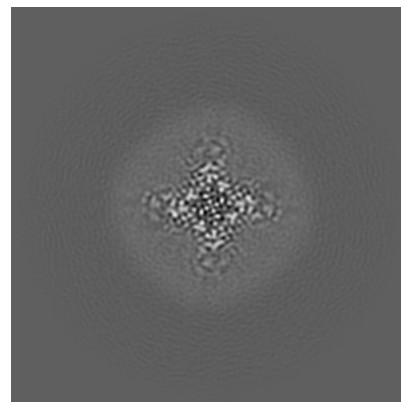
6.3.1 Primary map



X Index: 143

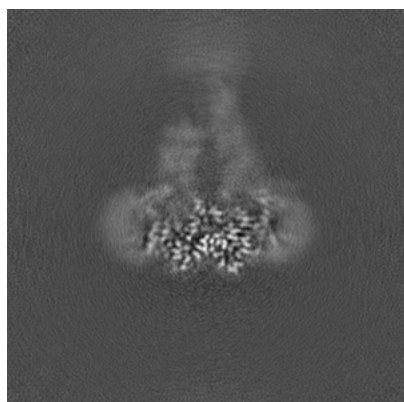


Y Index: 143

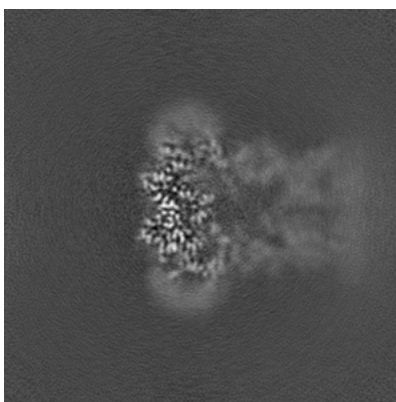


Z Index: 115

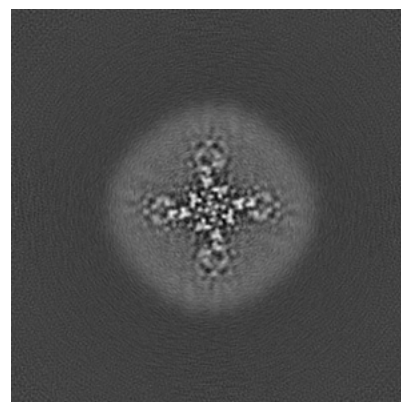
6.3.2 Raw map



X Index: 137



Y Index: 137

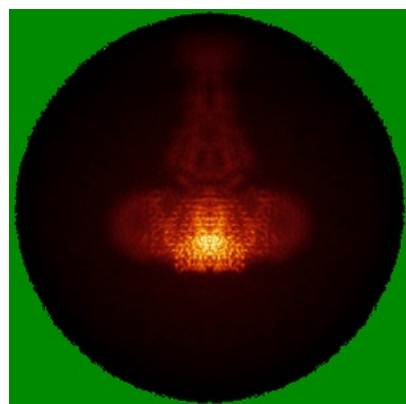


Z Index: 119

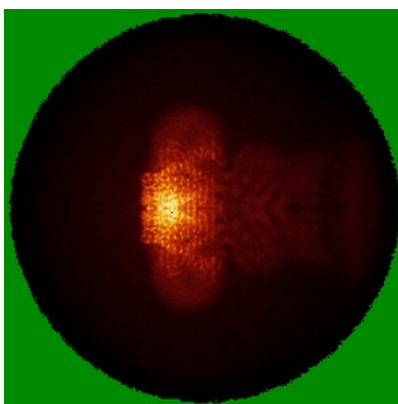
The images above show the largest variance slices of the map in three orthogonal directions.

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

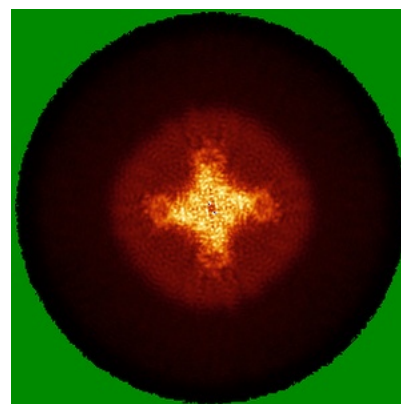
6.4.1 Primary map



X

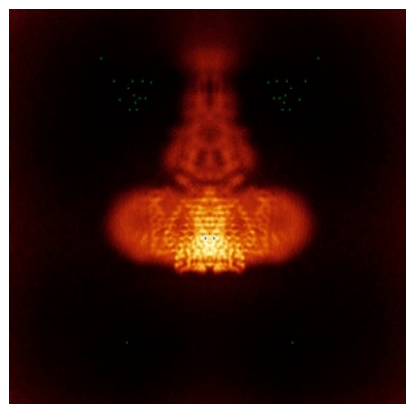


Y

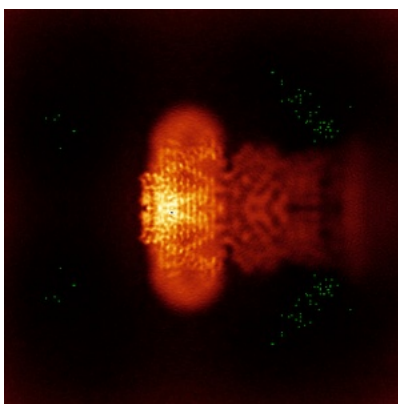


Z

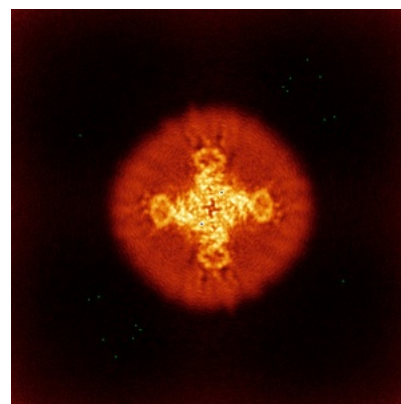
6.4.2 Raw map



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 0.184. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

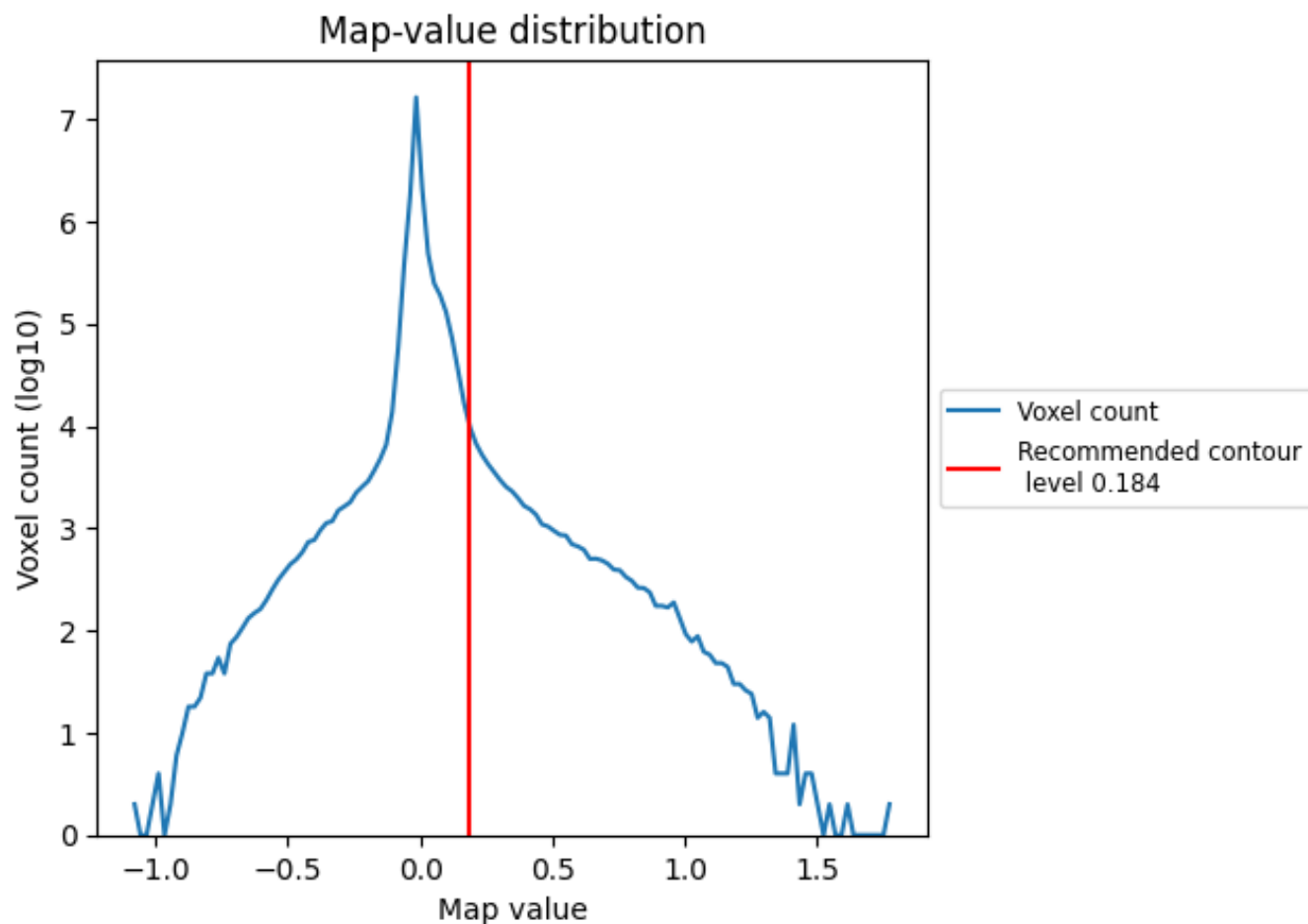
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

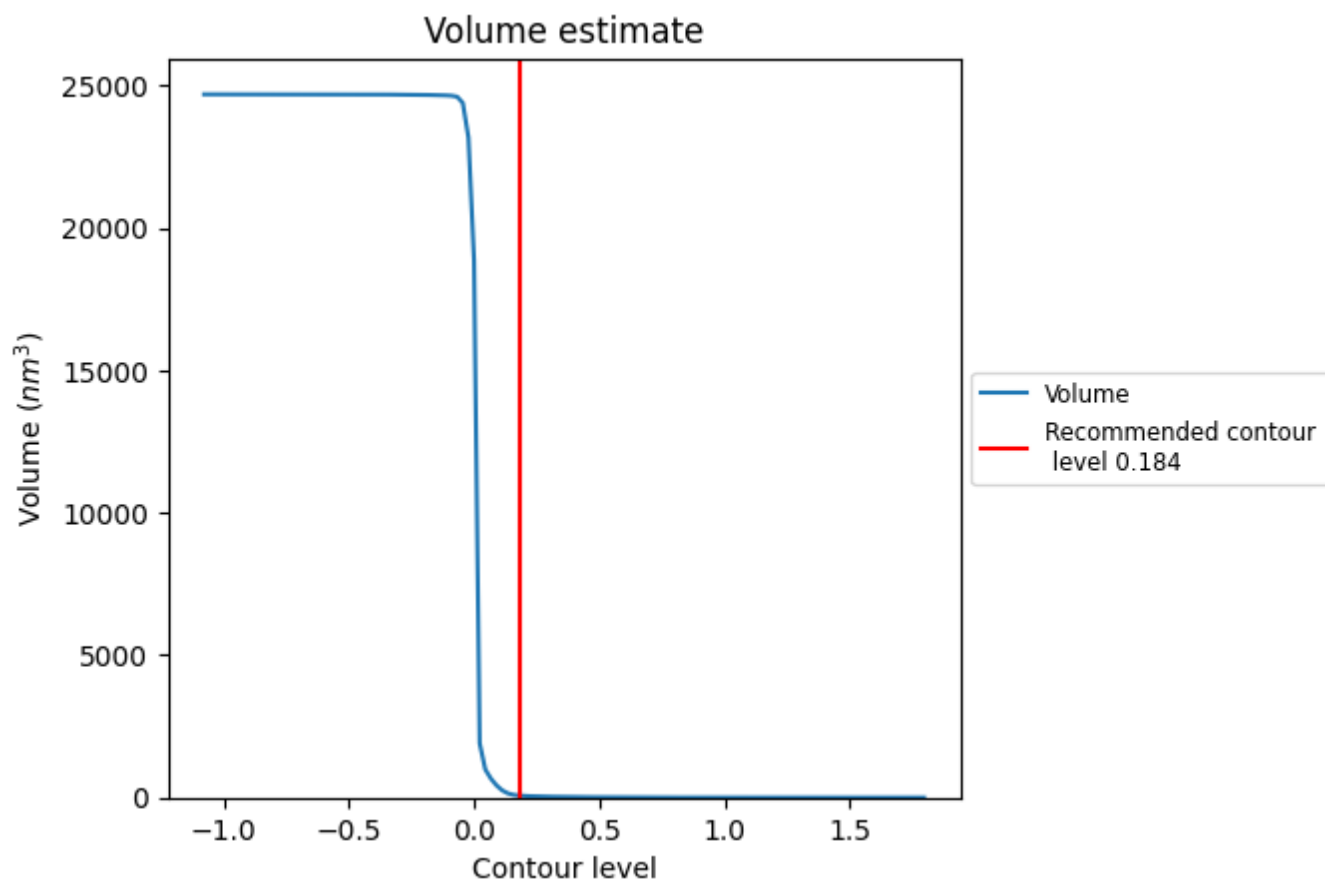
This section contains the results of statistical analysis of the map.

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.

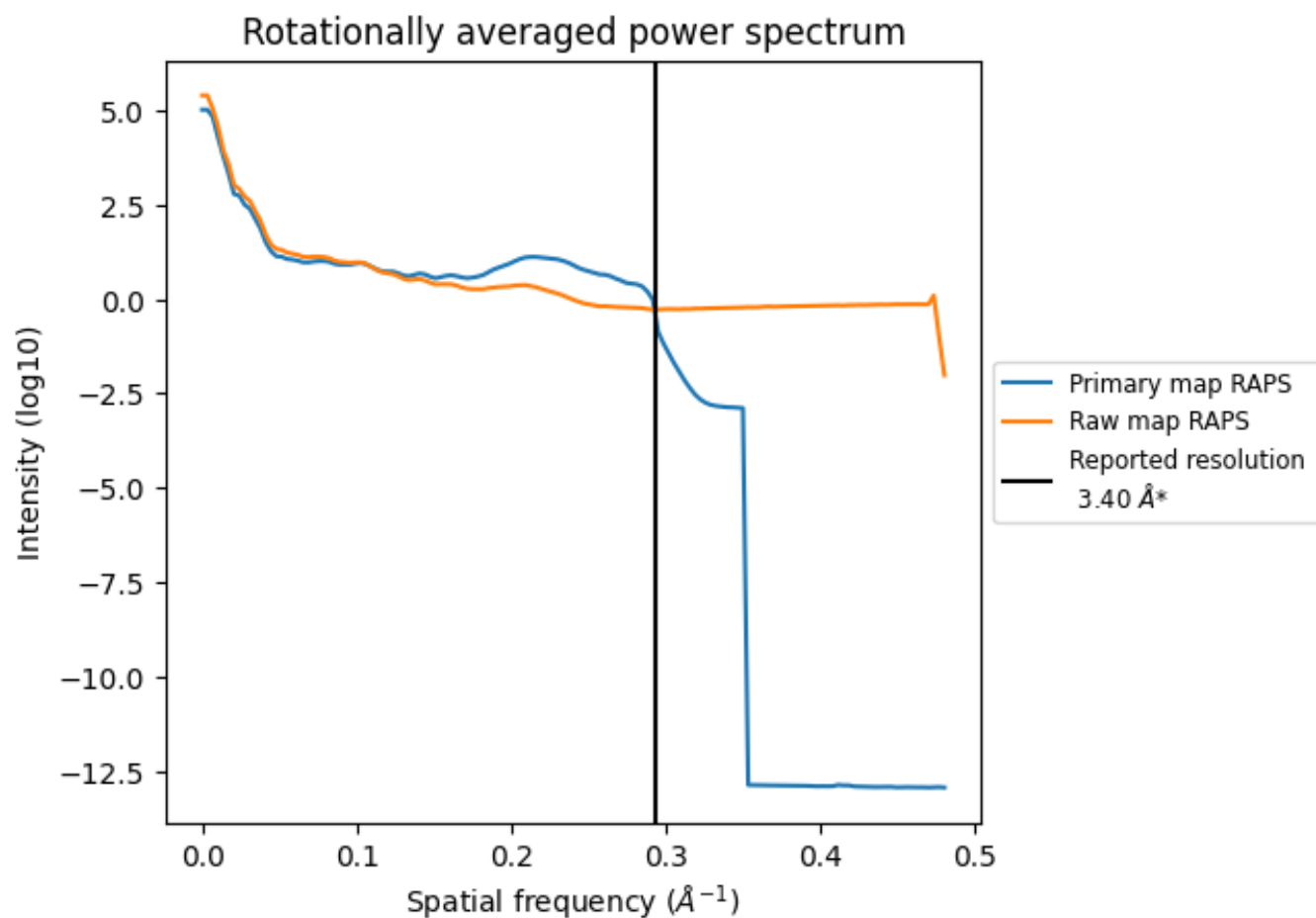
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 67 nm³; this corresponds to an approximate mass of 60 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 ⓘ

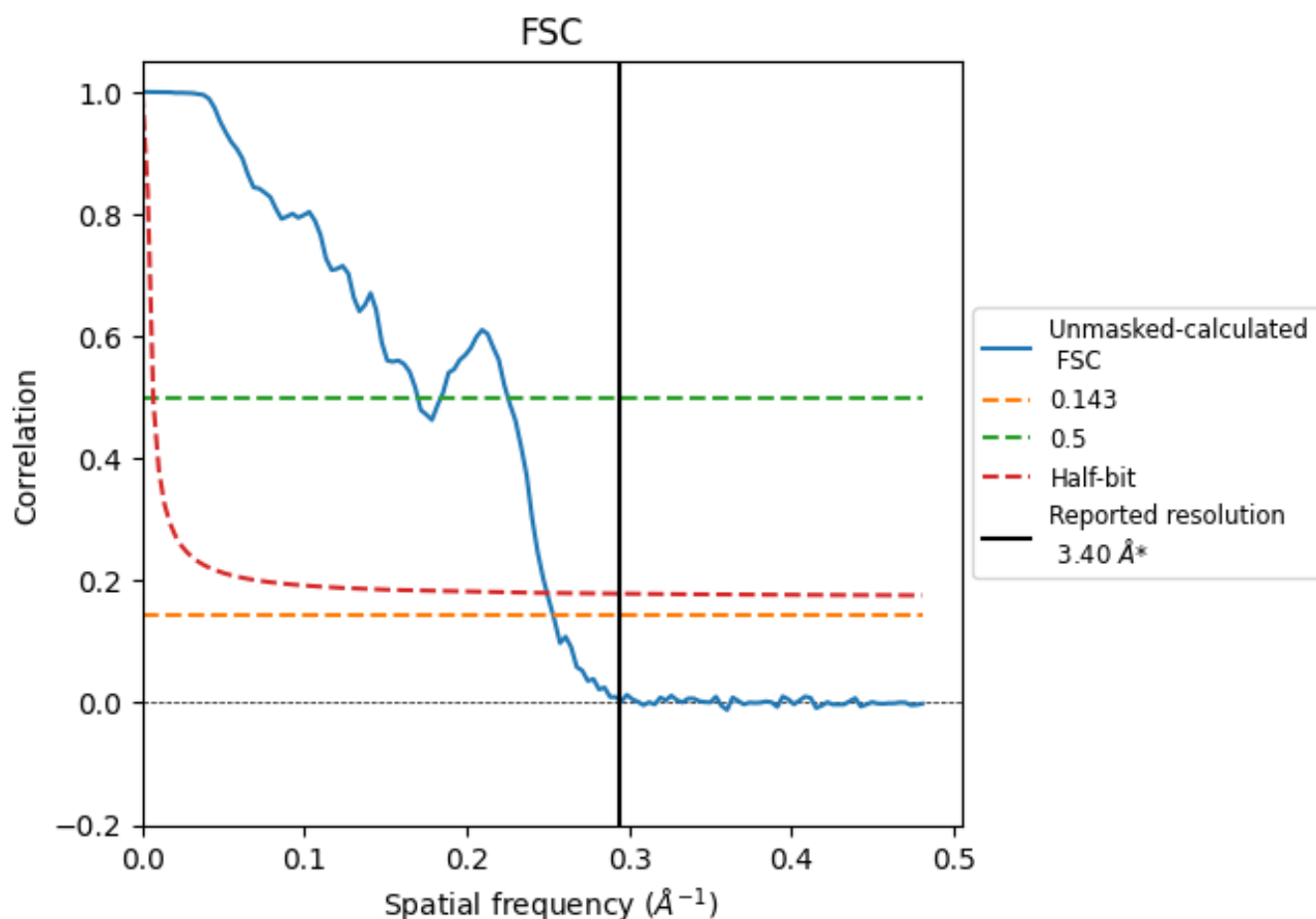


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

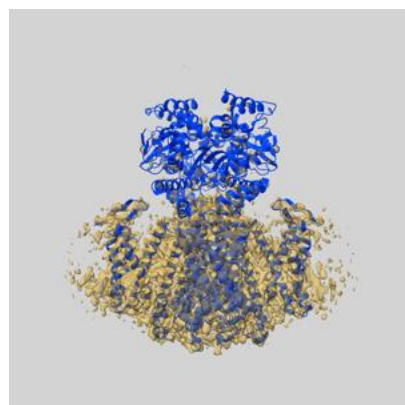
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	5.89	4.01

*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 3.95 differs from the reported value 3.4 by more than 10 %

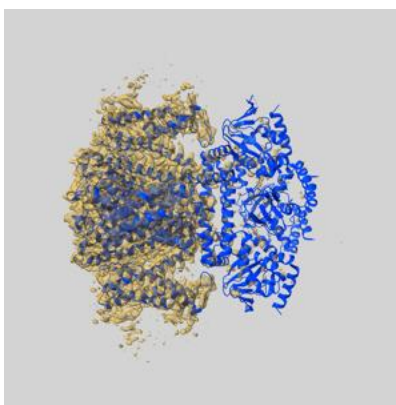
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-37855 and PDB model 8WUI. Per-residue inclusion information can be found in section 3 on page 6.

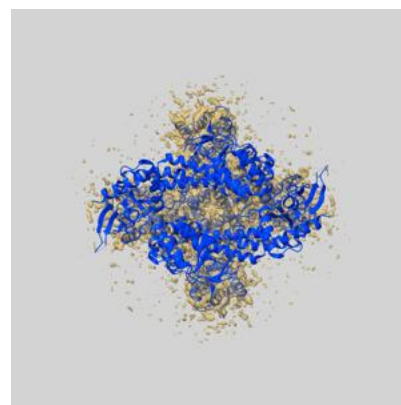
9.1 Map-model overlay [i](#)



X



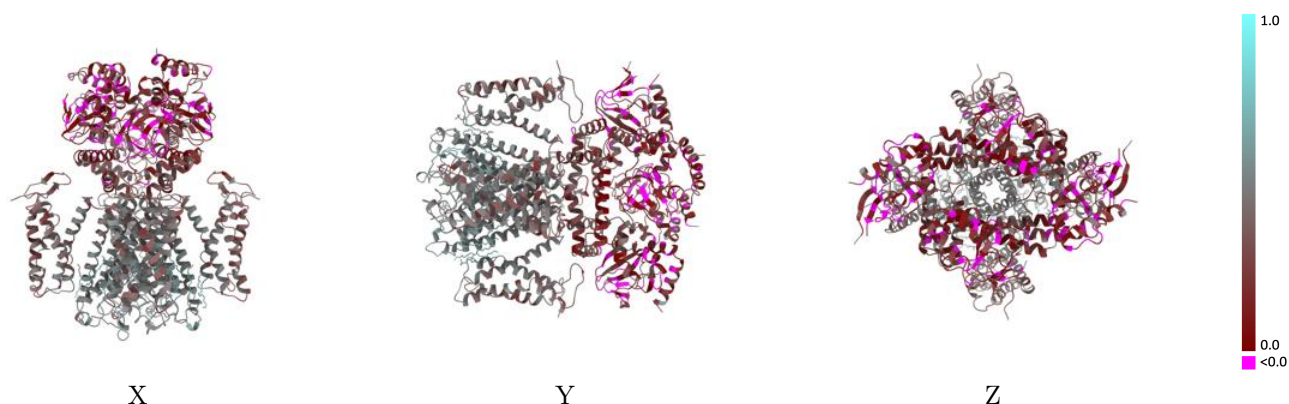
Y



Z

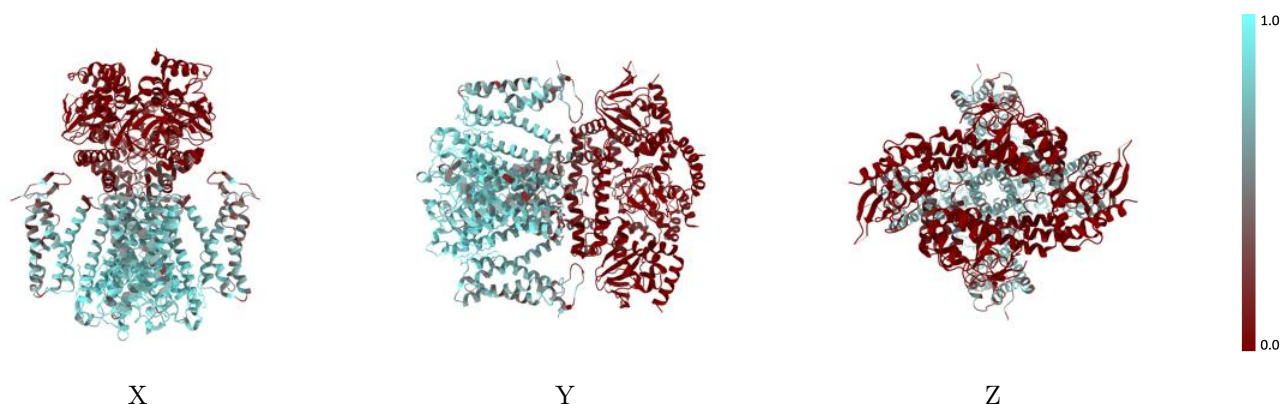
The images above show the 3D surface view of the map at the recommended contour level 0.184 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



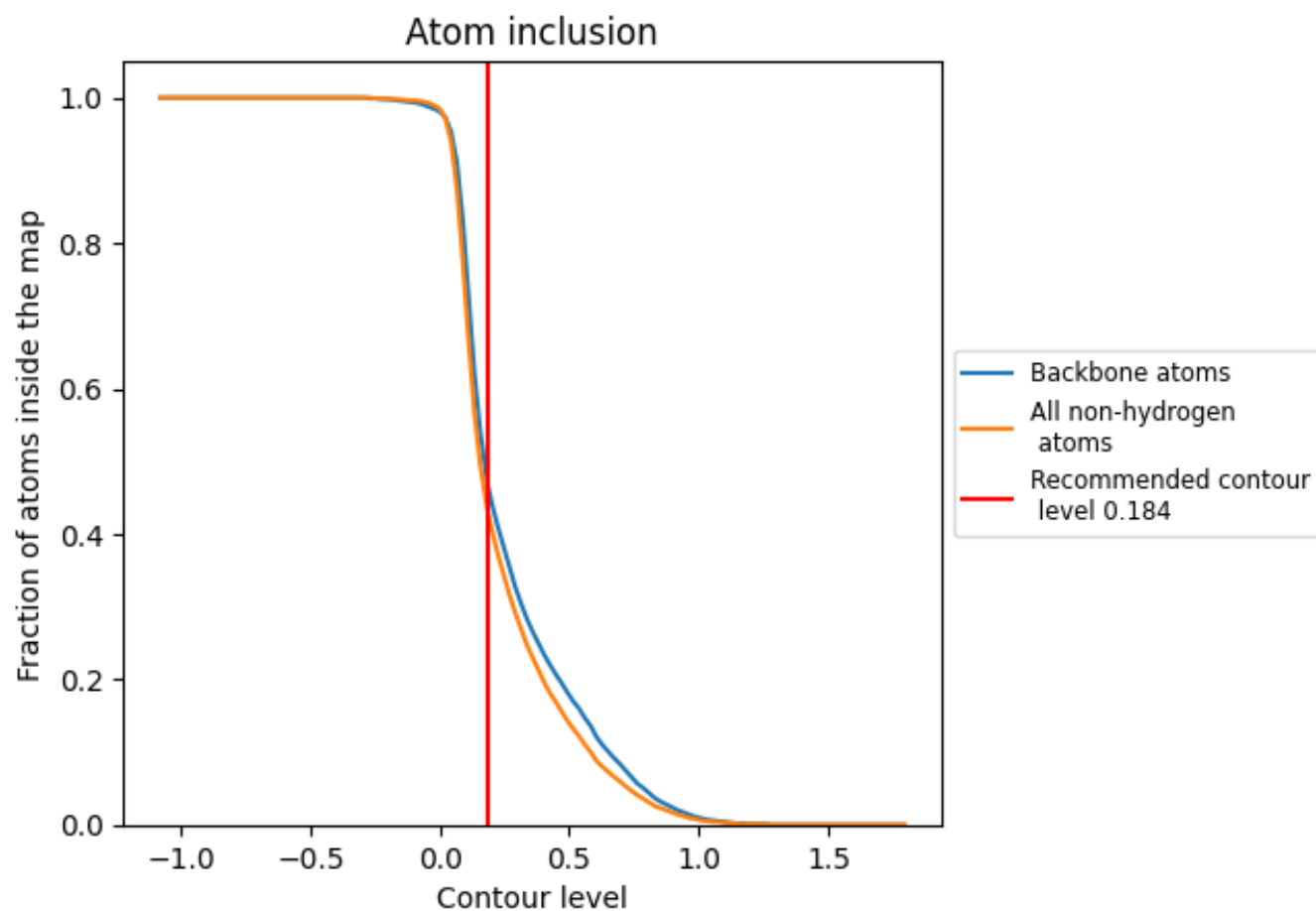
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.184).

9.4 Atom inclusion [i](#)



At the recommended contour level, 47% of all backbone atoms, 43% 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 (0.184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4320	0.3320
A	0.4370	0.3420
B	0.4290	0.3350
C	0.4310	0.3280
D	0.4290	0.3220

