



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:59 AM UTC

PDB ID : 8XKR / pdb_00008xkr
EMDB ID : EMD-38423
Title : Cryo-EM structure of human insulin receptor bound to 4 IGF-I, conformation 2
Authors : Xi, Z.
Deposited on : 2023-12-24
Resolution : 3.53 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

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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
MolProbity : 4-5-2 with Phenix2.0
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

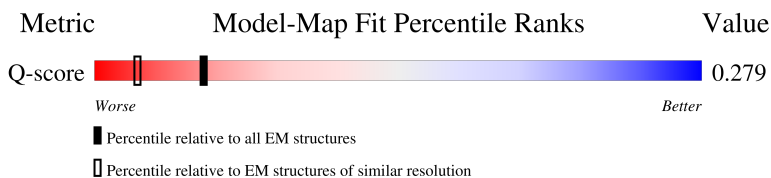
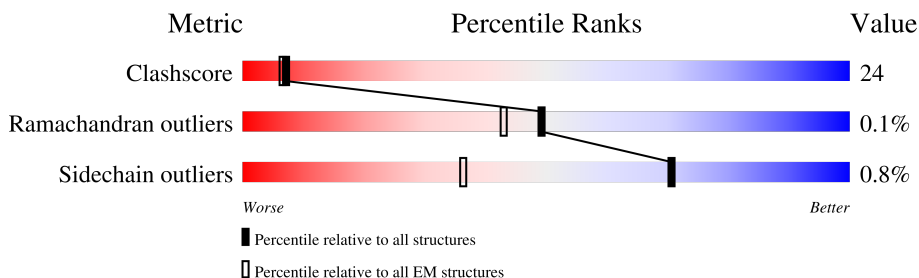
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	C	195	12% 10% 77%
1	D	195	10% 8% 9% 83%
1	E	195	6% 10% .. 82%
1	F	195	8% 9% 12% . 79%

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Mol	Chain	Length	Quality of chain
2	A	1370	9% 34% 25% 41%
2	B	1370	8% 33% 25% 42%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14118 atoms, of which 0 are hydrogens and 0 are deuteriums.

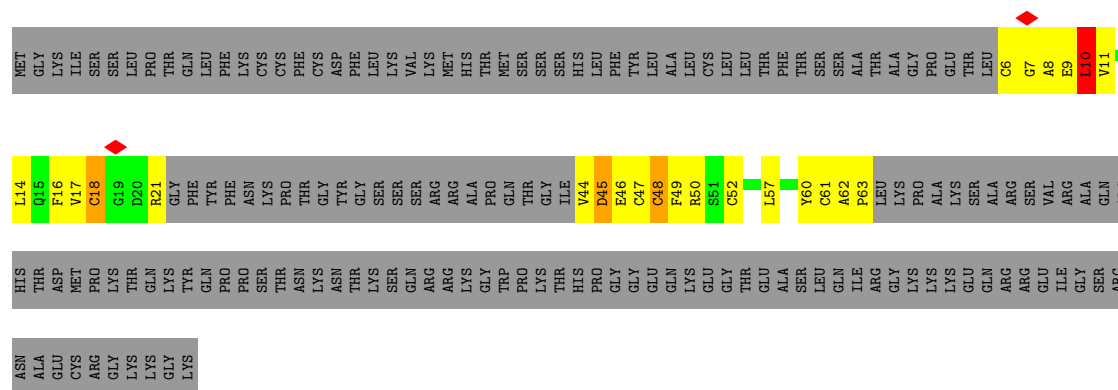
In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Insulin-like growth factor I.

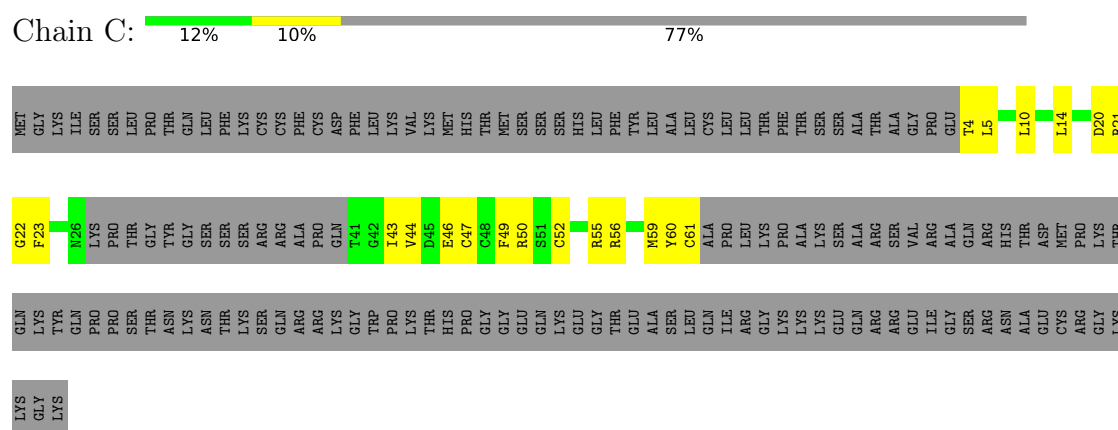
Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	41	Total	C	N	O	S	0	0
			311	191	52	61	7		
1	D	33	Total	C	N	O	S	0	0
			254	157	43	49	5		
1	E	36	Total	C	N	O	S	0	0
			279	170	49	53	7		
1	C	44	Total	C	N	O	S	0	0
			347	217	58	65	7		

- Molecule 2 is a protein called Isoform Short of Insulin receptor.

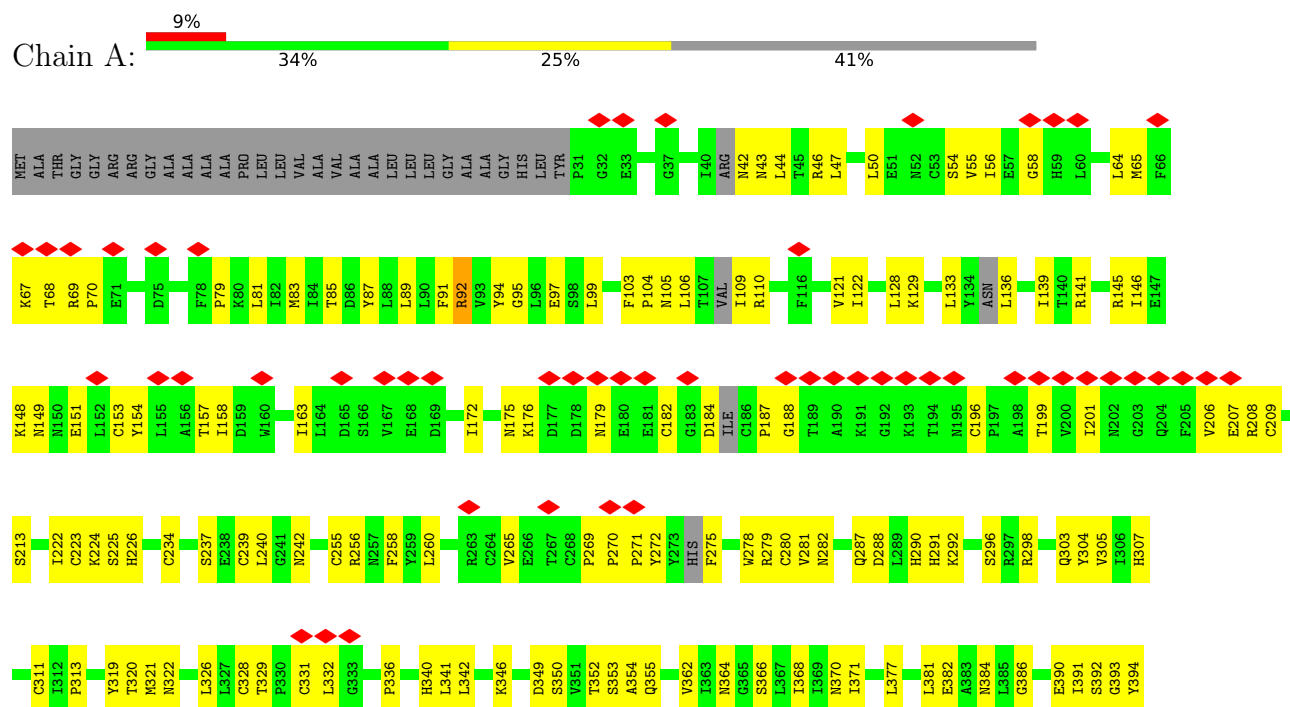
Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	813	Total	C	N	O	S	0	0
			6544	4148	1123	1224	49		
2	B	795	Total	C	N	O	S	0	0
			6383	4041	1102	1191	49		



• Molecule 1: Insulin-like growth factor I



• Molecule 2: Isoform Short of Insulin receptor



L396	K396	L397	K397	L398	K398	L399	K399	L400	K400	L401	K401	L402	K402	L403	K403	L404	K404	L405	K405	L406	K406	L407	K407	L408	K408	L409	K409	L410	K410	L411	K411	L412	K412	L413	K413	L414	K414	L415	K415	L416	K416	L417	K417	L418	K418	L419	K419	L420	K420	L421	K421	L422	K422	L423	K423	L424	K424	L425	K425	L426	K426	L427	K427	L428	K428	L429	K429	L430	K430	L431	K431	L432	K432	L433	K433	L434	K434	L435	K435	L436	K436	L437	K437	L438	K438	L439	K439	L440	K440	L441	K441	L442	K442	L443	K443	L444	K444	L445	K445	L446	K446	L447	K447	L448	K448	L449	K449	L450	K450	L451	K451	L452	K452	L453	K453	L454	K454	L455	K455	L456	K456	L457	K457	L458	K458	L459	K459	L460	K460	L461	K461	L462	K462	L463	K463	L464	K464	L465	K465	L466	K466	L467	K467	L468	K468	L469	K469	L470	K470	L471	K471	L472	K472	L473	K473	L474	K474	L475	K475	L476	K476	L477	K477	L478	K478	L479	K479	L480	K480	L481	K481	L482	K482	L483	K483	L484	K484	L485	K485	L486	K486	L487	K487	L488	K488	L489	K489	L490	K490	L491	K491	L492	K492	L493	K493	L494	K494	L495	K495	L496	K496	L497	K497	L498	K498	L499	K499	L500	K500	L501	K501	L502	K502	L503	K503	L504	K504	L505	K505	L506	K506	L507	K507	L508	K508	L509	K509	L510	K510	L511	K511	L512	K512	L513	K513	L514	K514	L515	K515	L516	K516	L517	K517	L518	K518	L519	K519	L520	K520	L521	K521	L522	K522	L523	K523	L524	K524	L525	K525	L526	K526	L527	K527	L528	K528	L529	K529	L530	K530	L531	K531	L532	K532	L533	K533	L534	K534	L535	K535	L536	K536	L537	K537	L538	K538	L539	K539	L540	K540	L541	K541	L542	K542	L543	K543	L544	K544	L545	K545	L546	K546	L547	K547	L548	K548	L549	K549	L550	K550	L551	K551	L552	K552	L553	K553	L554	K554	L555	K555	L556	K556	L557	K557	L558	K558	L559	K559	L560	K560	L561	K561	L562	K562	L563	K563	L564	K564	L565	K565	L566	K566	L567	K567	L568	K568	L569	K569	L570	K570	L571	K571	L572	K572	L573	K573	L574	K574	L575	K575	L576	K576	L577	K577	L578	K578	L579	K579	L580	K580	L581	K581	L582	K582	L583	K583	L584	K584	L585	K585	L586	K586	L587	K587	L588	K588	L589	K589	L590	K590	L591	K591	L592	K592	L593	K593	L594	K594	L595	K595	L596	K596	L597	K597	L598	K598	L599	K599	L600	K600	L601	K601	L602	K602	L603	K603	L604	K604	L605	K605	L606	K606	L607	K607	L608	K608	L609	K609	L610	K610	L611	K611	L612	K612	L613	K613	L614	K614	L615	K615	L616	K616	L617	K617	L618	K618	L619	K619	L620	K620	L621	K621	L622	K622	L623	K623	L624	K624	L625	K625	L626	K626	L627	K627	L628	K628	L629	K629	L630	K630	L631	K631	L632	K632	L633	K633	L634	K634	L635	K635	L636	K636	L637	K637	L638	K638	L639	K639	L640	K640	L641	K641	L642	K642	L643	K643	L644	K644	L645	K645	L646	K646	L647	K647	L648	K648	L649	K649	L650	K650	L651	K651	L652	K652	L653	K653	L654	K654	L655	K655	L656	K656	L657	K657	L658	K658	L659	K659	L660	K660	L661	K661	L662	K662	L663	K663	L664	K664	L665	K665	L666	K666	L667	K667	L668	K668	L669	K669	L670	K670	L671	K671	L672	K672	L673	K673	L674	K674	L675	K675	L676	K676	L677	K677	L678	K678	L679	K679	L680	K680	L681	K681	L682	K682	L683	K683	L684	K684	L685	K685	L686	K686	L687	K687	L688	K688	L689	K689	L690	K690	L691	K691	L692	K692	L693	K693	L694	K694	L695	K695	L696	K696	L697	K697	L698	K698	L699	K699	L700	K700	L701	K701	L702	K702	L703	K703	L704	K704	L705	K705	L706	K706	L707	K707	L708	K708	L709	K709	L710	K710	L711	K711	L712	K712	L713	K713	L714	K714	L715	K715	L716	K716	L717	K717	L718	K718	L719	K719	L720	K720	L721	K721	L722	K722	L723	K723	L724	K724	L725	K725	L726	K726	L727	K727	L728	K728	L729	K729	L730	K730	L731	K731	L732	K732	L733	K733	L734	K734	L735	K735	L736	K736	L737	K737	L738	K738	L739	K739	L740	K740	L741	K741	L742	K742	L743	K743	L744	K744	L745	K745	L746	K746	L747	K747	L748	K748	L749	K749	L750	K750	L751	K751	L752	K752	L753	K753	L754	K754	L755	K755	L756	K756	L757	K757	L758	K758	L759	K759	L760	K760	L761	K761	L762	K762	L763	K763	L764	K764	L765	K765	L766	K766	L767	K767	L768	K768	L769	K769	L770	K770	L771	K771	L772	K772	L773	K773	L774	K774	L775	K775	L776	K776	L777	K777	L778	K778	L779	K779	L780	K780	L781	K781	L782	K782	L783	K783	L784	K784	L785	K785	L786	K786	L787	K787	L788	K788	L789	K789	L790	K790	L791	K791	L792	K792	L793	K793	L794	K794	L795	K795	L796	K796	L797	K797	L798	K798	L799	K799	L800	K800	L801	K801	L802	K802	L803	K803	L804	K804	L805	K805	L806	K806	L807	K807	L808	K808	L809	K809	L810	K810	L811	K811	L812	K812	L813	K813	L814	K814	L815	K815	L816	K816	L817	K817	L818	K818	L819	K819	L820	K820	L821	K821	L822	K822	L823	K823	L824	K824	L825	K825	L826	K826	L827	K827	L828	K828	L829	K829	L830	K830	L831	K831	L832	K832	L833	K833	L834	K834	L835	K835	L836	K836	L837	K837	L838	K838	L839	K839	L840	K840	L841	K841	L842	K842	L843	K843	L844	K844	L845	K845	L846	K846	L847	K847	L848	K848	L849	K849	L850	K850	L851	K851	L852	K852	L853	K853	L854	K854	L855	K855	L856	K856	L857	K857	L858	K858	L859	K859	L860	K860	L861	K861	L862	K862	L863	K863	L864	K864	L865	K865	L866	K866	L867	K867	L868	K868	L869	K869	L870	K870	L871	K871	L872	K872	L873	K873	L874	K874	L875	K875	L876	K876	L877	K877	L878	K878	L879	K879	L880	K880	L881	K881	L882	K882	L883	K883	L884	K884	L885	K885	L886	K886	L887	K887	L888	K888	L889	K889	L890	K890	L891	K891	L892	K892	L893	K893	L894	K894	L895	K895	L896	K896	L897	K897	L898	K898	L899	K899	L900	K900	L901	K901	L902	K902	L903	K903	L904	K904	L905	K905	L906	K906	L907	K907	L908	K908	L909	K909	L910	K910	L911	K911	L912	K912	L913	K913	L914	K914	L915	K915	L916	K916	L917	K917	L918	K918	L919	K919	L920	K920	L921	K921	L922	K922	L923	K923	L924	K924	L925	K925	L926	K926	L927	K927	L928	K928	L929	K929	L930	K930	L931	K931	L932	K932	L933	K933	L934	K934	L935	K935	L936	K936	L937	K937	L938	K938	L939	K939	L940	K940	L941	K941	L942	K942	L943	K943	L944	K944	L945	K945	L946	K946	L947	K947	L948	K948	L949	K949	L950	K950	L951	K951	L952	K952	L953	K953	L954	K954	L955	K955	L956	K956	L957	K957	L958	K958	L959	K959	L960	K960	L961	K961	L962	K962	L963	K963	L964	K964	L965	K965	L966	K966	L967	K967	L968	K968	L969	K969	L970	K970	L971	K971	L972	K972	L973	K973	L974	K974	L975	K975	L976	K976	L977	K977	L978	K978	L979	K979	L980	K980	L981	K981	L982	K982	L983	K983	L984	K984	L985	K985	L986	K986	L987	K987	L988	K988	L989	K989	L990	K990	L991	K991	L992	K992	L993	K993	L994	K994	L995	K995	L996	K996	L997	K997	L998	K998	L999	K999	L1000	K1000	L1001	K1001	L1002	K1002	L1003	K1003	L1004	K1004	L1005	K1005	L1006	K1006	L1007	K1007	L1008	K1008	L1009	K1009	L1010	K1010	L1011	K1011	L1012	K1012	L1013	K1013	L1014	K1014	L1015	K1015	L1016	K1016	L1017	K1017	L1018	K1018	L1019	K1019	L1020	K1020	L1021	K1021	L1022	K1022	L1023	K1023	L1024	K1024	L1025	K1025	L1026	K1026	L1027	K1027	L1028	K1028	L1029	K1029	L1030	K1030	L1031	K1031	L1032	K1032	L1033	K1033	L1034	K1034	L1035	K1035	L1036	K1036	L1037	K1037	L1038	K1038	L1039	K1039	L1040	K1040	L1041	K1041	L1042	K1042	L1043	K1043	L1044	K1044	L1045	K1045	L1046	K1046	L1047	K1047	L1048	K1048	L1049	K1049	L1050	K1050	L1051	K1051	L1052	K1052	L1053	K1053	L1054	K1054	L1055	K1055	L1056	K1056	L1057	K1057	L1058	K1058	L1059	K1059	L1060	K1060	L1061	K1061	L1062	K1062	L1063	K1063	L1064	K1064	L1065	K1065	L1066	K1066	L1067	K1067	L1068	K1068	L1069	K1069	L1070	K1070	L1071	K1071	L1072	K1072	L1073	K1073	L1074	K1074	L1075	K1075	L1076	K1076	L1077	K1077	L1078	K1078	L1079	K1079	L1080	K1080	L1081	K1081	L1082	K1082	L1083	K1083	L1084	K1084	L1085	K1085	L1086	K1086	L1087	K1087	L1088	K1088	L1089	K1089	L1090	K1090	L1091	K1091	L1092	K1092	L1093	K1093	L1094	K1094	L1095	K1095	L1096	K1096	L1097	K1097	L1098	K1098	L1099	K1099	L1100	K1100	L1101	K1101	L1102	K1102	L1103	K1103	L1104	K1104	L1105	K1105	L1106	K1106	L1107	K1107	L1108	K1108	L1109	K1109	L1110	K1110	L1111	K1111	L1112	K1112	L1113	K1113	L1114	K1114	L1115	K1115	L1116	K1116	L1117	K1117	L1118	K1118	L1119	K1119	L1120	K1120	L1121	K1121	L1122	K1122	L1123	K1123	L1124	K1124	L1125	K1125	L1126	K1126	L1127	K1127	L1128	K1128	L1129	K1129	L1130	K1130	L1131	K1131	L1132	K1132	L1133	K1133	L1134	K1134	L1135	K1135	L1136	K1136	L1137	K1137	L1138	K1138	L1139	K1139	L1140	K1140	L1141	K1141	L1142	K1142	L11
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ASP	GLY	MET	SER	TRP	LYS	E883	D816	SER	SER	GLU	V815	V542	W469	V362	N257	I163	F73
PRO	LEU	ILE	VAL	GLU	ILE	E883	E820	LEU	GLU	ASP	Q816	D546	E470	I363	F258	L164	R74
ASN	PRO	GLN	MET	VAL	ILE	L884	R821	ASP	ASP	ASP	T620	D546	E471	N364	Y259	D165	S77
CYS	ARG	ALA	PHE	GLY	PRO	H885	A826	VAL	GLN	GLN	P625	D549	T475	S366	R263	S166	F78
PRO	TRP	ILE	THR	GLY	ILE	L886	V827	ASN	ASN	HIS	I629	A550	R478	L367	E266	D169	I82
ARG	ALA	PHE	CYS	THR	PHE	V888	W828	VAL	ASN	HIS	I629	C551	Q479	I369	T267	D177	M83
VAL	ASP	ALA	HIS	THR	THR	S899	R831	VAL	THR	ASN	I638	W556	E480	N370	E269	I172	M84
LEU	LEU	VAL	HIS	THR	THR	R890	T832	ALA	GLU	GLU	S632	T557	ARG	I371	C288	N175	D86
ASP	ASP	VAL	VAL	THR	THR	K891	M833	VAL	VAL	GLU	S634	V558	ASN	R372	P270	K176	T82
LEU	LEU	VAL	VAL	THR	THR	H892	P834	PRO	PRO	GLU	S635	V559	I484	N375	P271	D177	D85
MET	LYS	TYR	LEU	LEU	SER	F893	E835	THR	ASP	ASP	P648	P563	A485	I388	Y272	D177	L89
ASP	ASP	LEU	LEU	GLY	VAL	A894	A836	VAL	SER	SER	I638	P563	A485	I388	H274	C186	L90
MET	GLY	GLN	GLY	GLN	VAL	A894	A836	VAL	SER	SER	I638	P563	A485	I388	H274	C186	F91
CYS	PHE	VAL	VAL	VAL	ILE	L895	R837	ALA	ALA	ALA	I639	N568	T488	E389	W278	P187	R92
TRP	THR	THR	VAL	VAL	GLY	E896	A837	PHE	GLU	GLU	K641	D569	N489	E390	R279	A190	V93
PHE	THR	THR	VAL	VAL	GLY	E897	ASP	PRO	CYS	CYS	K642	P570	C495	S392	C280	A190	G95
ASN	THR	TYR	LYS	GLY	ILE	G898	D840	ASN	SER	SER	P648	K571	E496	G393	H290	A198	L96
SER	THR	TYR	LYS	GLY	ILE	C899	T841	THR	THR	THR	H651	S572	N497	C393	K291	T199	E97
PRO	VAL	THR	LEU	LEU	THR	R900	W842	SER	CYS	CYS	H651	S572	E498	K293	K291	V200	S98
MET	VAL	THR	LEU	LEU	THR	L901	G843	THR	LYS	LYS	T653	H575	L499	K294	H290	N202	L99
ARG	VAL	THR	LEU	LEU	THR	R902	P844	VAL	ASP	ASP	H654	P576	L500	K294	K290	N202	G95
PRO	THR	THR	VAL	VAL	ARG	G903	T846	PRO	PRO	SER	H654	G577	L500	S400	C280	N202	K100
THR	PHE	GLY	GLN	GLN	ARG	L904	H847	THR	SER	SER	T656	W578	L499	K396	K291	V200	T107
LEU	VAL	VAL	VAL	VAL	PRO	R905	H847	SER	ILE	ILE	L656	M580	L500	I397	K291	V200	V108
ILE	LEU	VAL	VAL	VAL	PRO	S906	E848	PRO	PRO	LEU	V658	R581	L500	R398	K291	V200	I109
VAL	TRP	VAL	ALA	ALA	GLY	P906	T849	GLU	GLU	GLU	V659	R581	L500	R398	K291	V200	R110
ASN	GLY	ALA	HIS	GLY	PRO	G907	F850	GLU	GLU	GLU	V660	R581	L500	R398	K291	V200	G111
LEU	ILE	ALA	HIS	GLY	PRO	R908	F850	HIS	GLU	GLU	V661	R581	L500	R398	K291	V200	V121
LEU	ILE	ALA	HIS	GLY	PRO	R909	E851	GLU	GLU	GLU	V662	R581	L500	R398	K291	V200	I122
ASP	LEU	VAL	VAL	VAL	TYR	S910	N852	SER	SER	SER	A663	R581	L500	R398	K291	V200	M125
ASP	LEU	VAL	VAL	VAL	TYR	V911	N853	SER	SER	SER	A663	R581	L500	R398	K291	V200	L128
LEU	GLY	VAL	TYR	VAL	ALA	R912	W854	PHE	PHE	PHE	S666	R581	L500	R398	K291	V200	K129
THR	GLY	VAL	TYR	VAL	ALA	R913	W855	ARG	ARG	ARG	F669	R581	L500	R398	K291	V200	E130
THR	GLY	VAL	TYR	VAL	ALA	R914	N856	THR	THR	THR	E670	R581	L500	R398	K291	V200	L131
PRO	GLY	VAL	TYR	VAL	ALA	S917	N858	THR	THR	THR	L671	R581	L500	R398	K291	V200	G132
GLU	LEU	VAL	TYR	VAL	ALA	L918	W859	THR	THR	THR	L672	R581	L500	R398	K291	V200	L136
VAL	GLY	VAL	TYR	VAL	ALA	R921	N860	THR	THR	THR	L673	R581	L500	R398	K291	V200	M137
THR	GLY	VAL	TYR	VAL	ALA	G922	P861	THR	THR	THR	L674	R581	L500	R398	K291	V200	N138
THR	GLY	VAL	TYR	VAL	ALA	G923	P862	THR	THR	THR	L675	R581	L500	R398	K291	V200	T140
VAL	GLY	VAL	TYR	VAL	ALA	W924	R863	THR	THR	THR	L676	R581	L500	R398	K291	V200	R141
GLY	LEU	VAL	TYR	VAL	ALA	G925	P864	THR	THR	THR	L677	R581	L500	R398	K291	V200	V144
GLY	LEU	VAL	TYR	VAL	ALA	T926	P865	THR	THR	THR	L678	R581	L500	R398	K291	V200	R145
GLY	LEU	VAL	TYR	VAL	ALA	E926	N866	THR	THR	THR	L679	R581	L500	R398	K291	V200	I146
GLY	LEU	VAL	TYR	VAL	ALA	P927	L868	THR	THR	THR	L679	R581	L500	R398	K291	V200	N150
GLY	LEU	VAL	TYR	VAL	ALA	T928	L869	THR	THR	THR	L679	R581	L500	R398	K291	V200	L155
GLY	LEU	VAL	TYR	VAL	ALA	G929	W870	THR	THR	THR	L679	R581	L500	R398	K291	V200	A156
GLY	LEU	VAL	TYR	VAL	ALA	F930	L871	THR	THR	THR	L679	R581	L500	R398	K291	V200	T157
GLY	LEU	VAL	TYR	VAL	ALA	G931	W872	THR	THR	THR	L679	R581	L500	R398	K291	V200	I157
GLY	LEU	VAL	TYR	VAL	ALA	V932	E873	THR	THR	THR	L679	R581	L500	R398	K291	V200	D159
GLY	LEU	VAL	TYR	VAL	ALA	T933	W874	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	D934	N875	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	Y935	W876	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	LEU	R877	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	ASP	N878	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	VAL	R878	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	PRO	W879	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	SER	N880	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	ASN	D881	THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	ILE		THR	THR	THR	L679	R581	L500	R398	K291	V200	
GLY	LEU	VAL	TYR	VAL	ALA	ALA		THR	THR	THR	L679	R581	L500	R398	K291	V200	

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PRO
TYR
THR
HIS
MET
ASN
GLY
GLY
LYS
LYS
ASN
GLY
ARG
ILE
LEU
THR

LEU
PRO
ARG
SER
PRO
SER

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	85221	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)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.282	Depositor
Minimum map value	-0.123	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	337.92, 337.92, 337.92	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.66, 0.66, 0.66	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.19	0/351	0.51	0/469
1	D	0.17	0/254	0.48	0/339
1	E	0.46	0/281	1.00	1/375 (0.3%)
1	F	0.19	0/313	0.53	0/420
2	A	0.15	0/6694	0.34	0/9057
2	B	0.18	0/6535	0.37	0/8854
All	All	0.18	0/14428	0.39	1/19514 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	10	LEU	N-CA-C	-8.56	101.89	111.14

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	C	347	0	319	22	0
1	D	254	0	246	14	0
1	E	279	0	256	45	0
1	F	311	0	290	30	0
2	A	6544	0	6341	276	0
2	B	6383	0	6196	297	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14118	0	13648	658	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 24.

The worst 5 of 658 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:TYR:N	2:B:259:TYR:HH	1.57	1.03
1:E:14:LEU:HD11	1:E:57:LEU:O	1.60	1.01
2:B:157:THR:HB	2:B:209:CYS:H	1.22	1.00
1:E:18:CYS:SG	1:E:21:ARG:HG3	2.04	0.97
1:F:53:ASP:HB3	2:B:581:ARG:HG3	1.45	0.96

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	C	40/195 (20%)	30 (75%)	10 (25%)	0	100	100
1	D	29/195 (15%)	27 (93%)	2 (7%)	0	100	100
1	E	32/195 (16%)	24 (75%)	7 (22%)	1 (3%)	3	24
1	F	37/195 (19%)	34 (92%)	3 (8%)	0	100	100
2	A	785/1370 (57%)	713 (91%)	71 (9%)	1 (0%)	48	79
2	B	781/1370 (57%)	699 (90%)	82 (10%)	0	100	100
All	All	1704/3520 (48%)	1527 (90%)	175 (10%)	2 (0%)	49	79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	514	LEU
1	E	45	ASP

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	C	38/167 (23%)	38 (100%)	0	100	100
1	D	29/167 (17%)	28 (97%)	1 (3%)	32	58
1	E	31/167 (19%)	28 (90%)	3 (10%)	8	31
1	F	35/167 (21%)	34 (97%)	1 (3%)	37	60
2	A	736/1215 (61%)	732 (100%)	4 (0%)	81	81
2	B	717/1215 (59%)	713 (99%)	4 (1%)	78	80
All	All	1586/3098 (51%)	1573 (99%)	13 (1%)	70	77

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	512	ILE
2	A	513	LEU
2	B	580	MET
2	B	77	SER
2	B	89	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	245	GLN
2	B	811	GLN
2	B	432	ASN
2	B	853	ASN
2	B	588	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](#)

There are no ligands in this entry.

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.

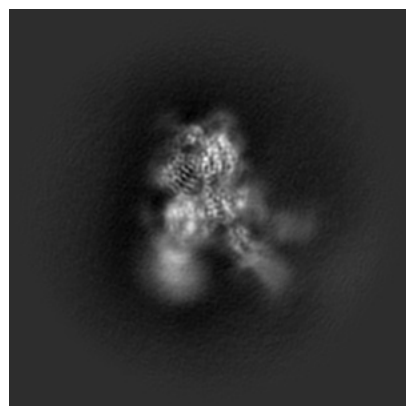
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38423. These allow visual inspection of the internal detail of the map and identification of artifacts.

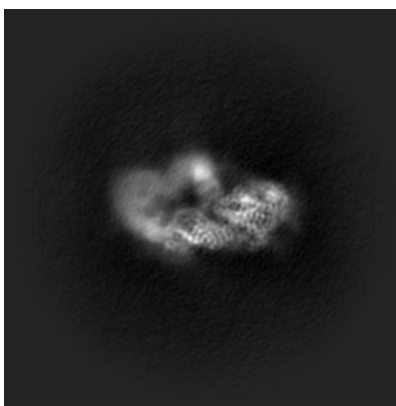
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

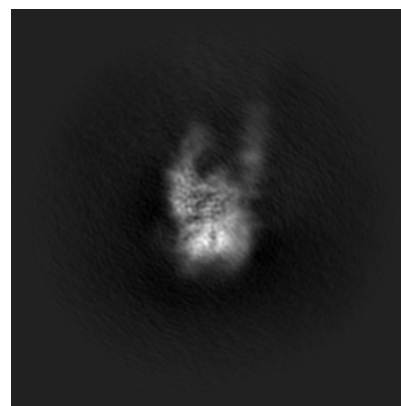
6.1.1 Primary map



X

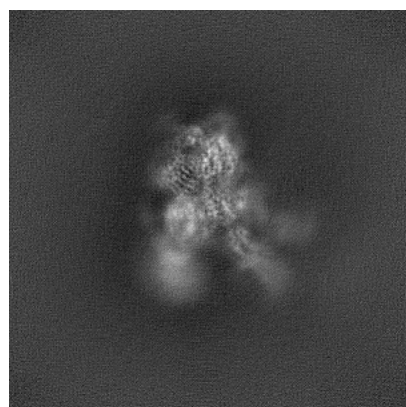


Y

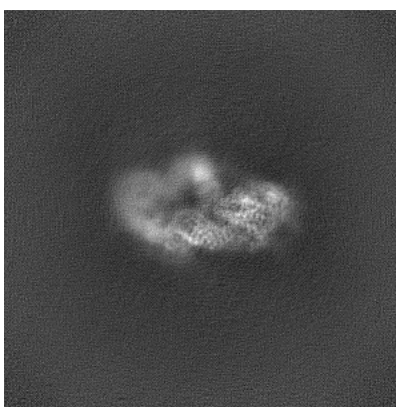


Z

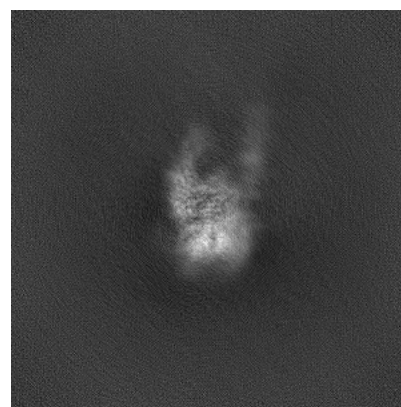
6.1.2 Raw map



X



Y

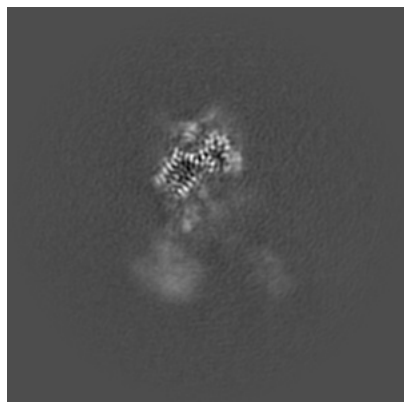


Z

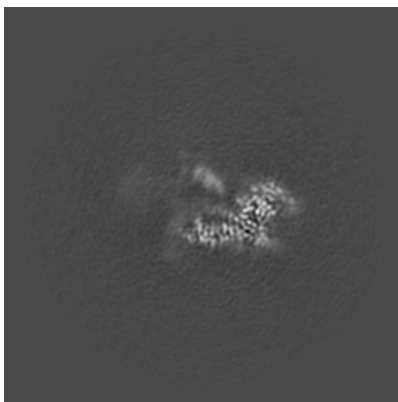
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

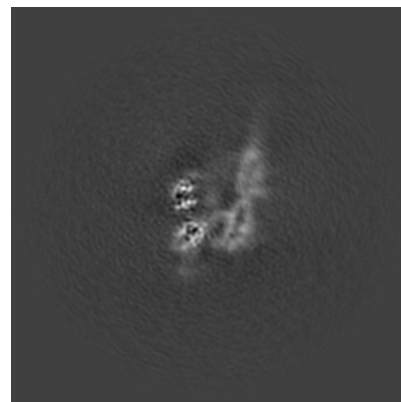
6.2.1 Primary map



X Index: 256

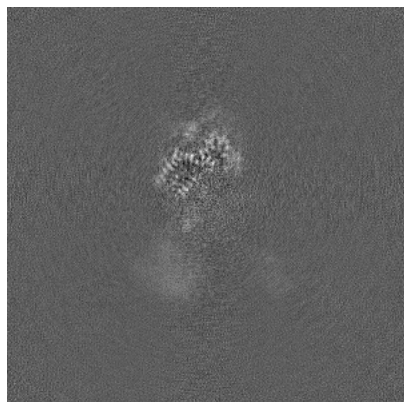


Y Index: 256

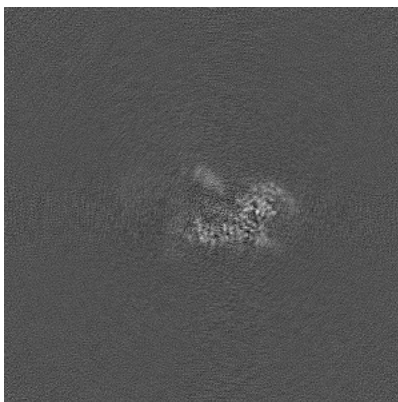


Z Index: 256

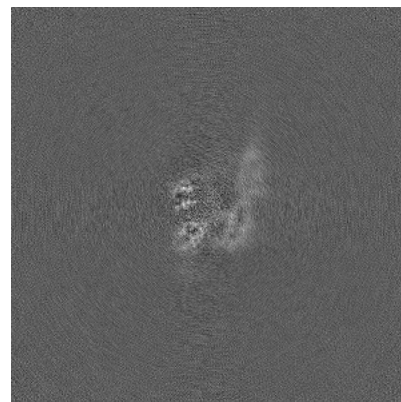
6.2.2 Raw map



X Index: 256



Y Index: 256

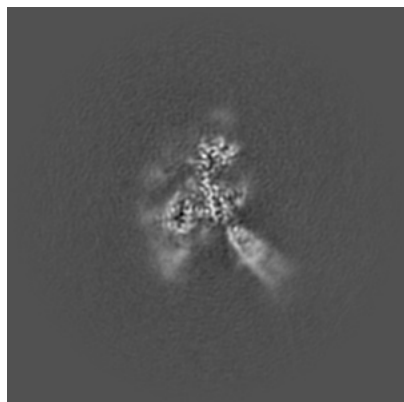


Z Index: 256

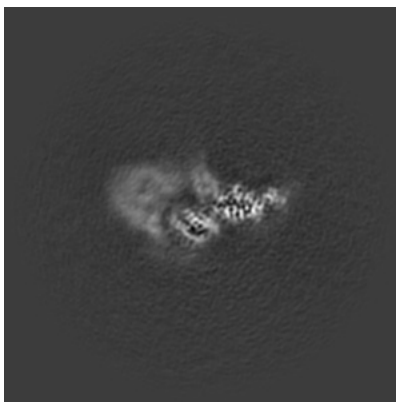
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

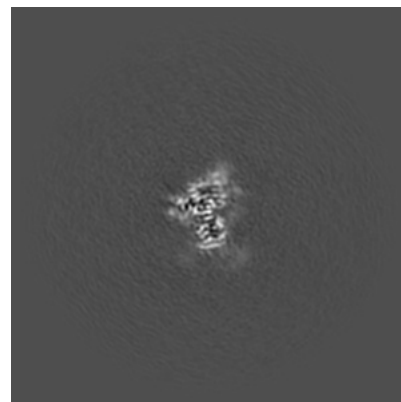
6.3.1 Primary map



X Index: 228

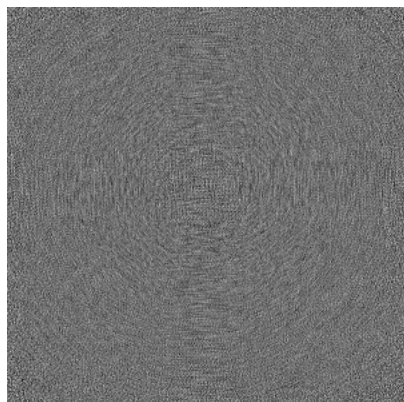


Y Index: 216

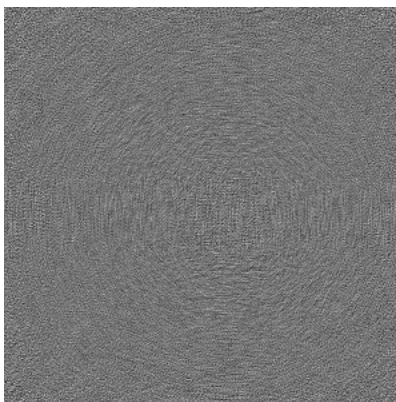


Z Index: 311

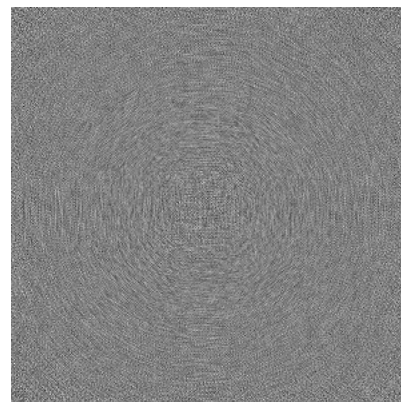
6.3.2 Raw map



X Index: 0



Y Index: 0

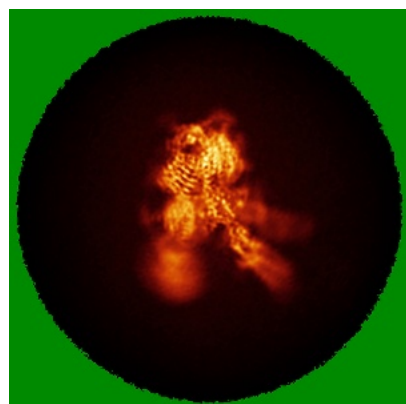


Z Index: 511

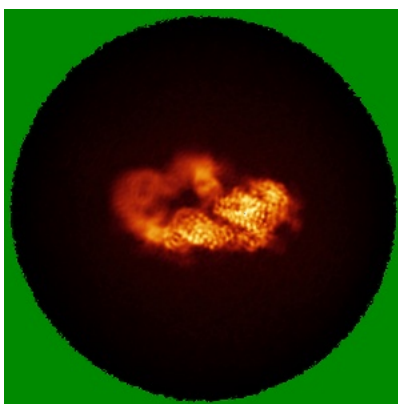
The images above show the largest variance slices of the map in three orthogonal directions.

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

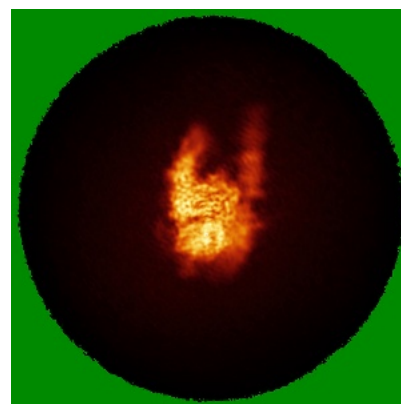
6.4.1 Primary map



X

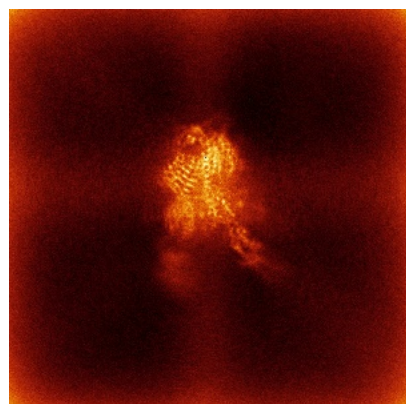


Y

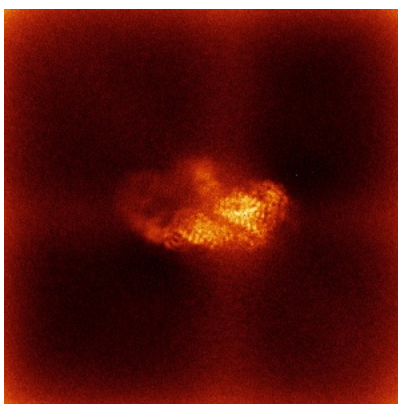


Z

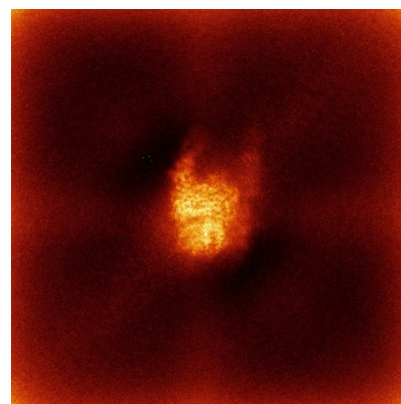
6.4.2 Raw map



X



Y

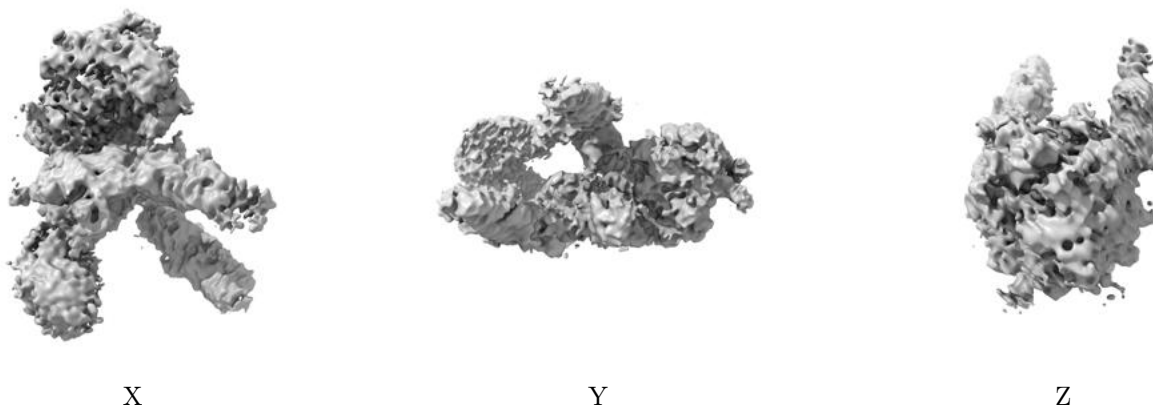


Z

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.

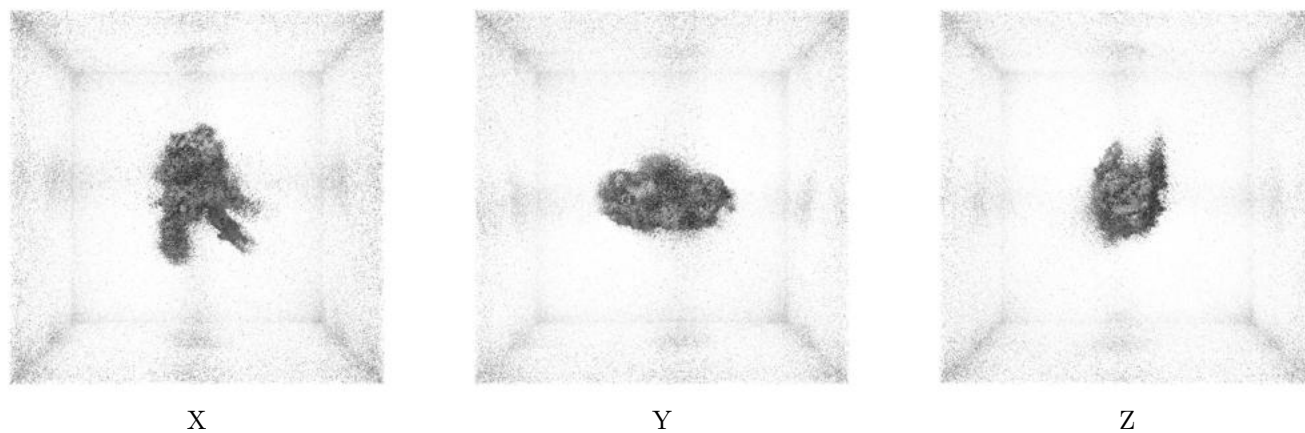
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. 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.

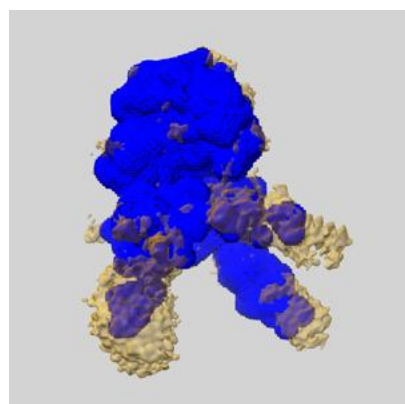
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

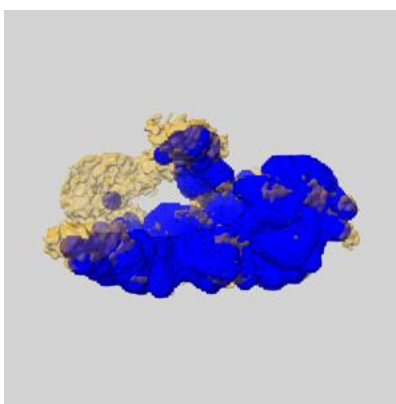
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

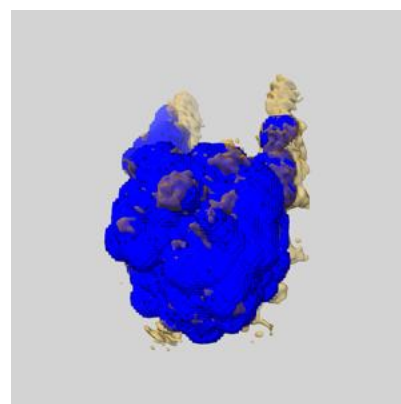
6.6.1 emd_38423_msk_1.map [i](#)



X



Y

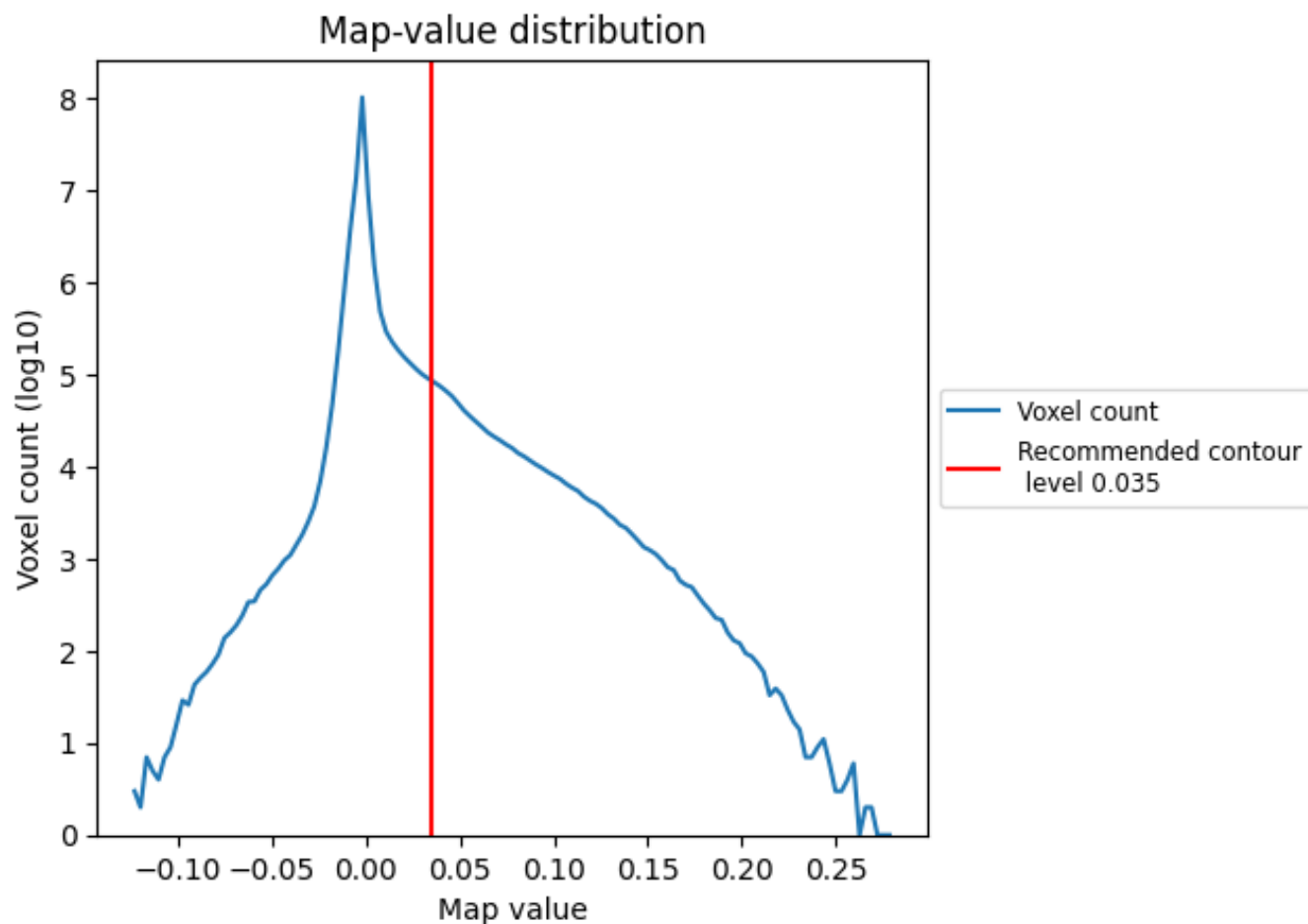


Z

7 Map analysis [i](#)

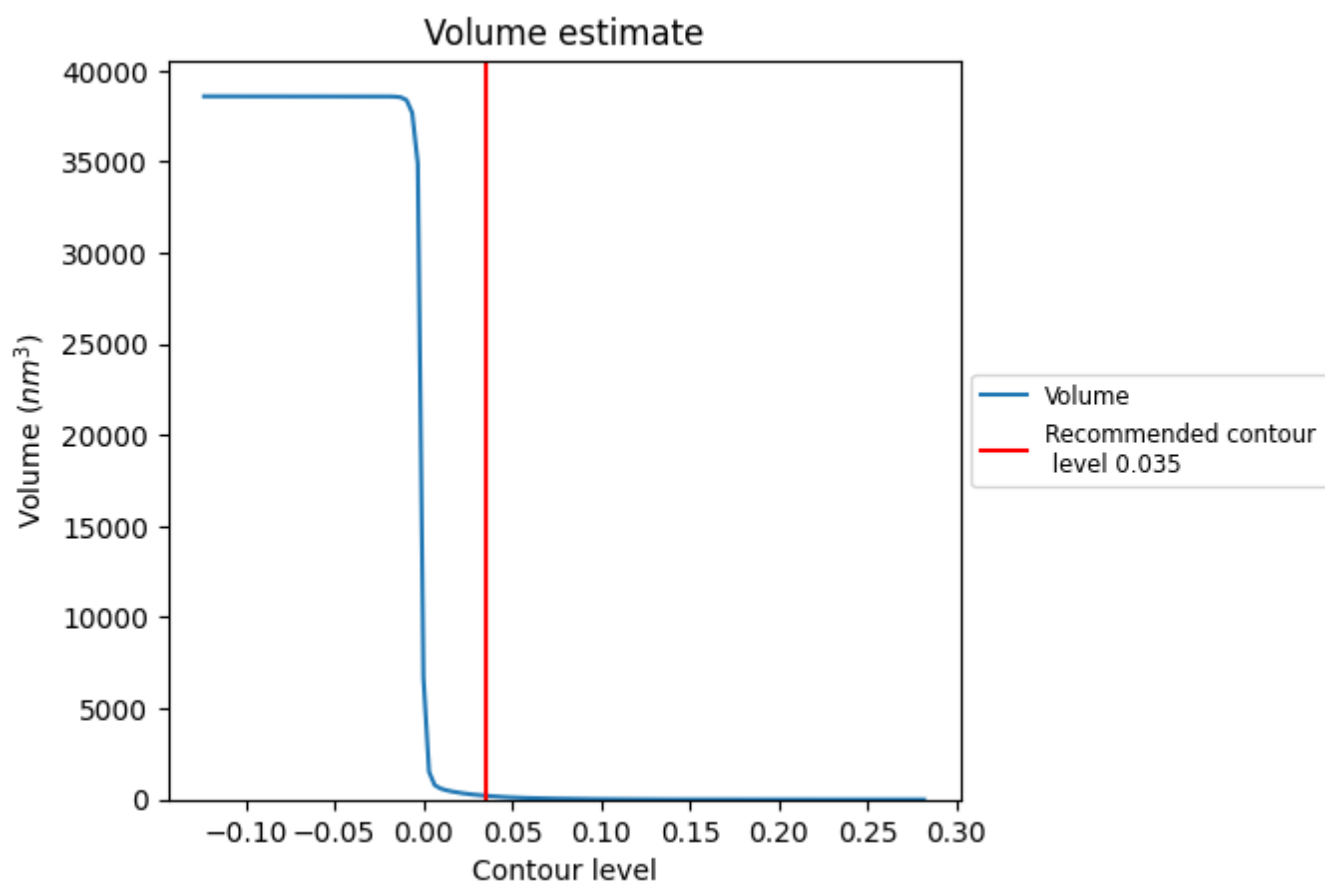
This section contains the results of statistical analysis of the map.

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.

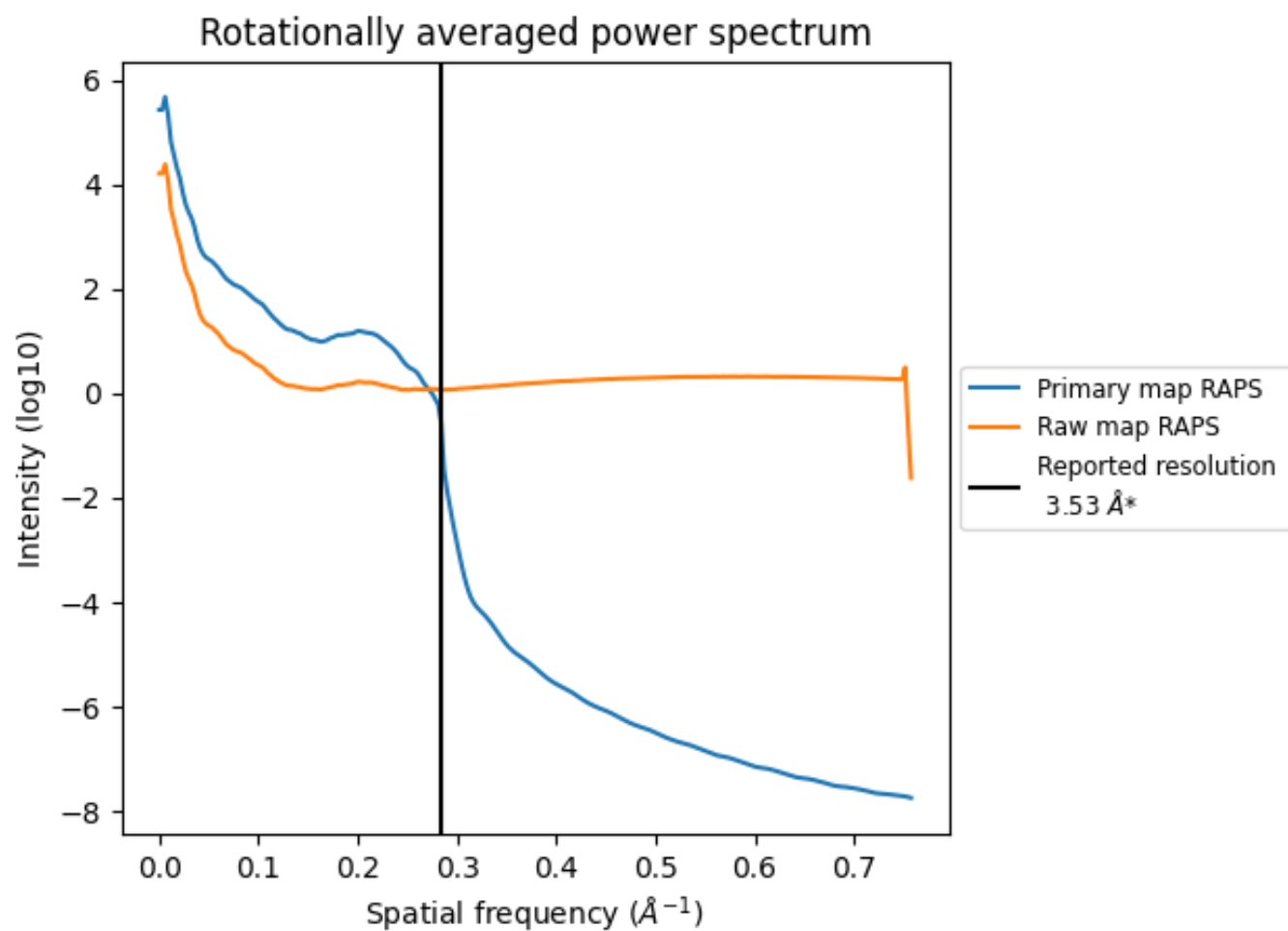
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 211 nm³; this corresponds to an approximate mass of 191 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 ⓘ

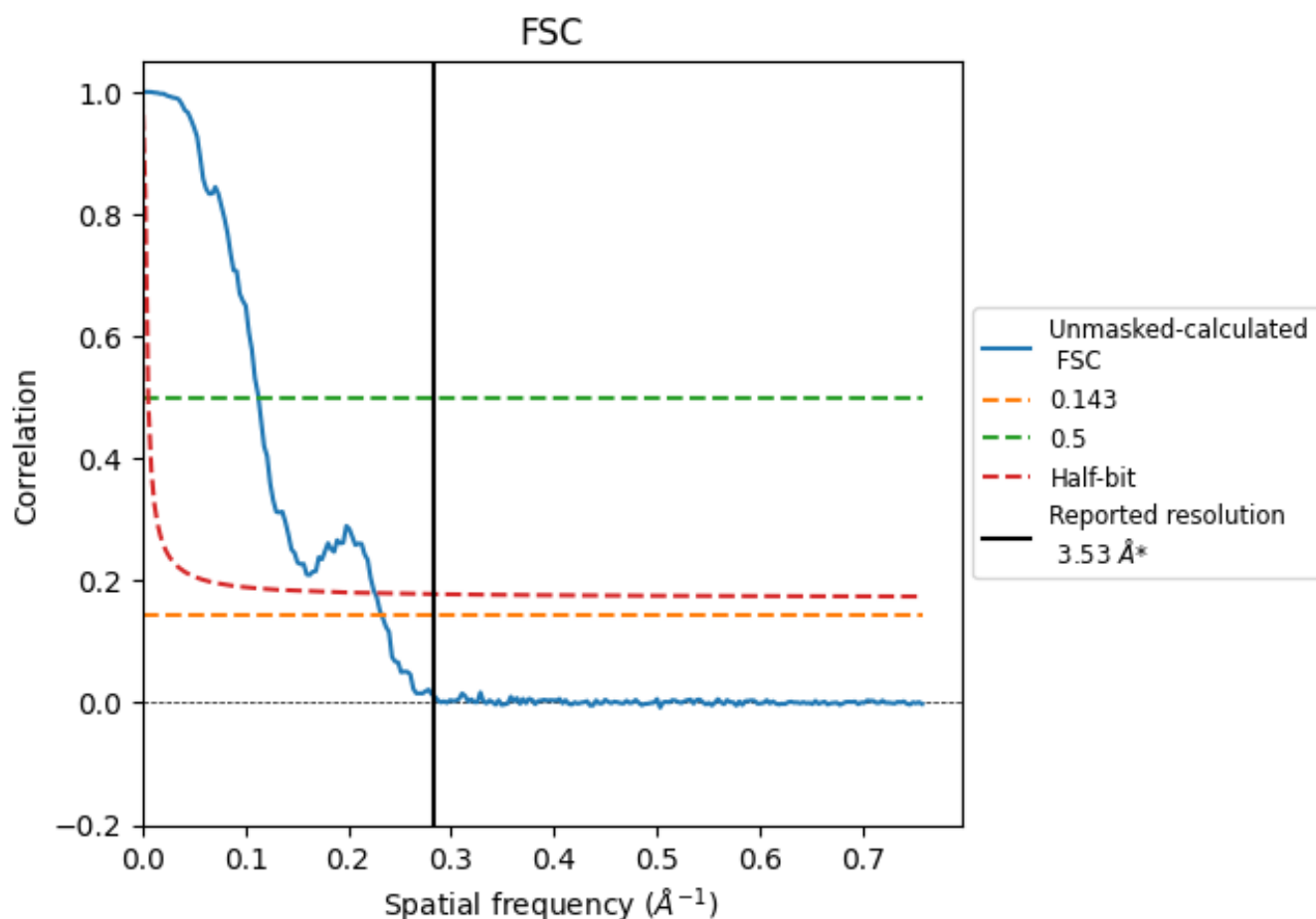


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

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 0.283 Å⁻¹

8.2 Resolution estimates [i](#)

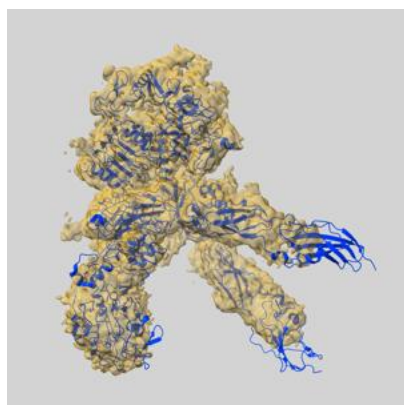
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	8.87	4.42

*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 4.30 differs from the reported value 3.53 by more than 10 %

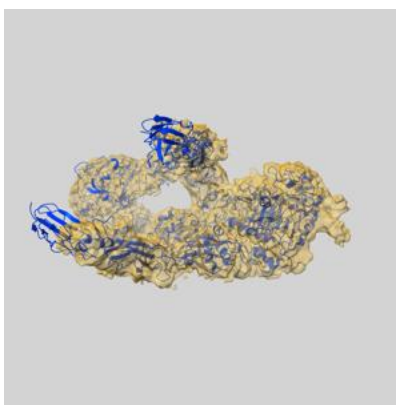
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38423 and PDB model 8XKR. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

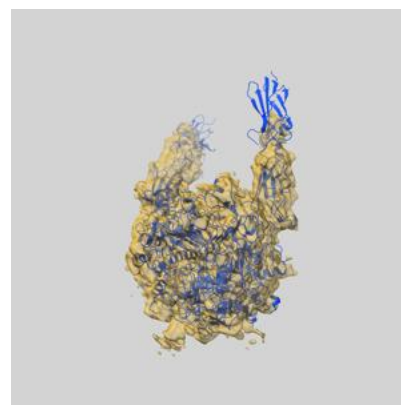
9.1 Map-model overlay [i](#)



X



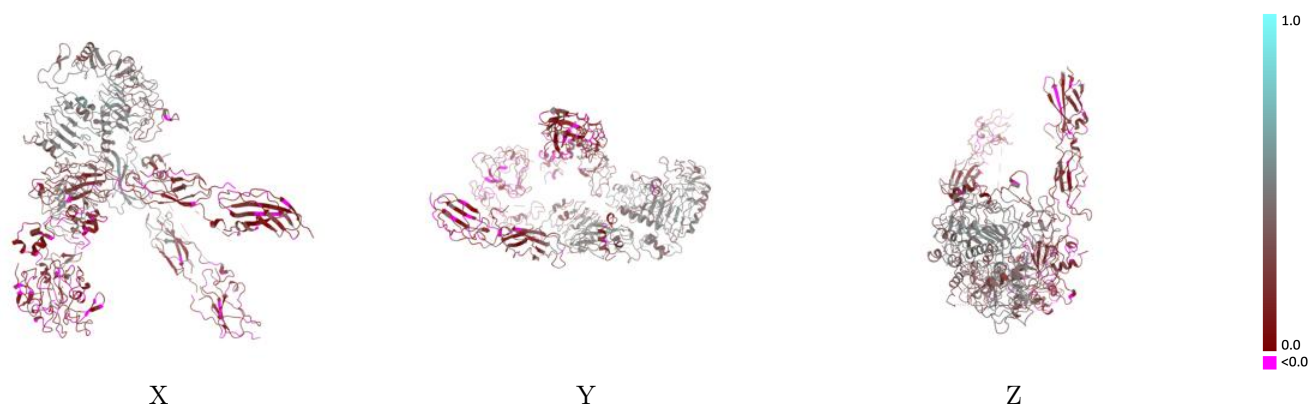
Y



Z

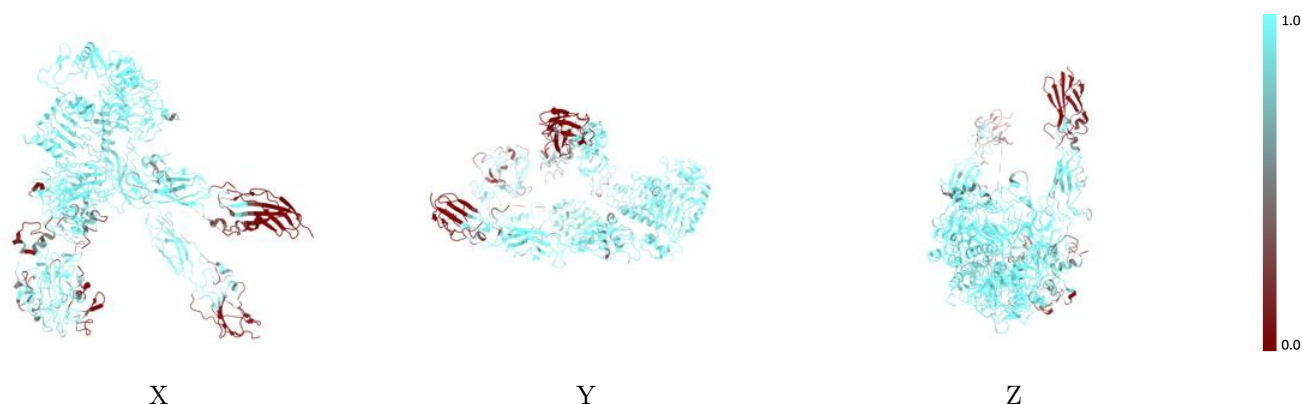
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



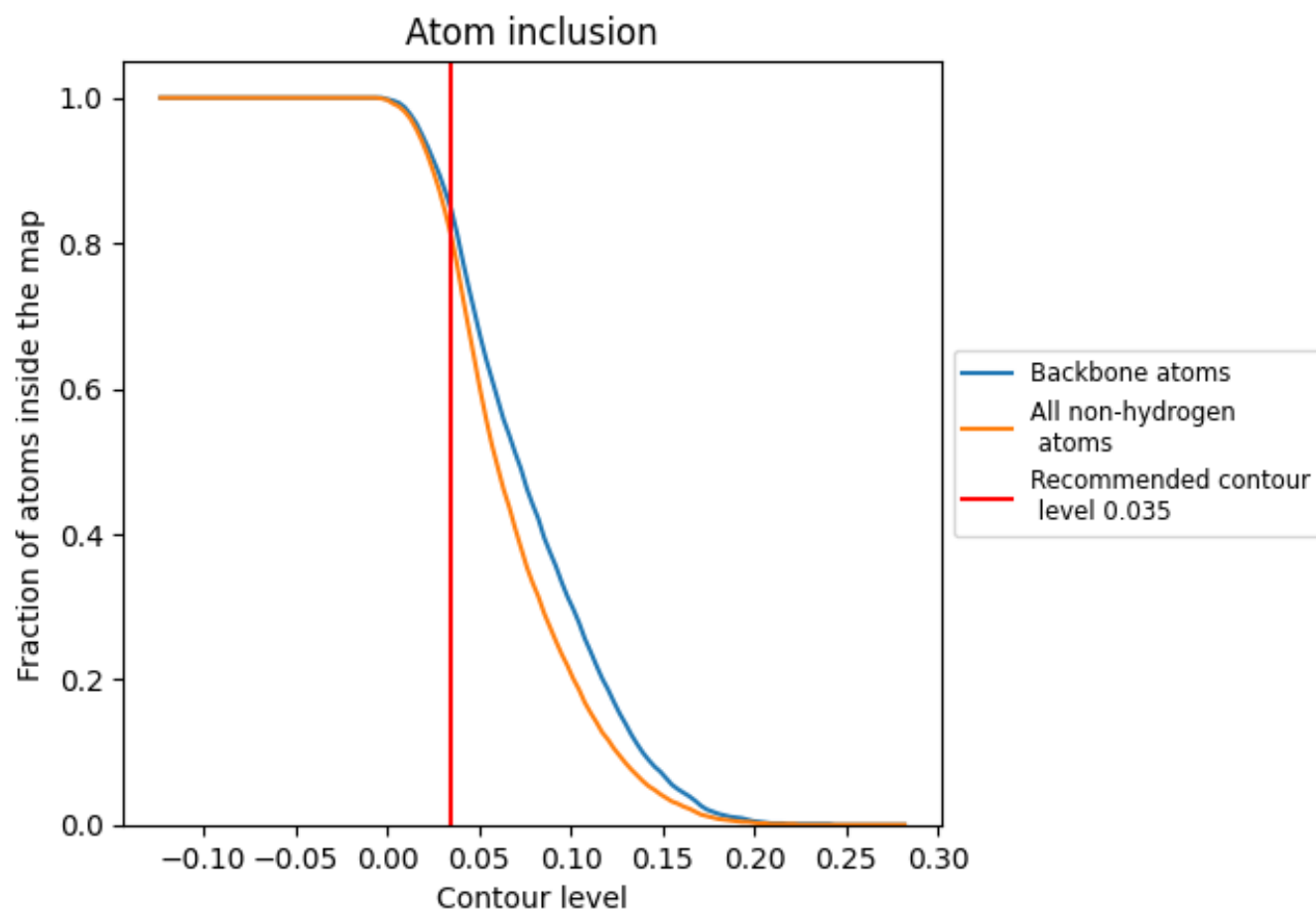
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.2790
A	0.8060	0.2480
B	0.8350	0.3250
C	0.9850	0.3980
D	0.3190	0.0730
E	0.8190	0.2570
F	0.5530	0.0540

1.0

0.0

<0.0