



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 12:36 AM EST

PDB ID : 6W4O
EMDB ID : EMD-21535
Title : CaMKII alpha-30 Cryo-EM reconstruction
Authors : Chao, L.H.; Stratton, M.M.
Deposited on : 2020-03-11
Resolution : 4.80 Å(reported)
Based on initial models : 5IG3, 3SOA

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

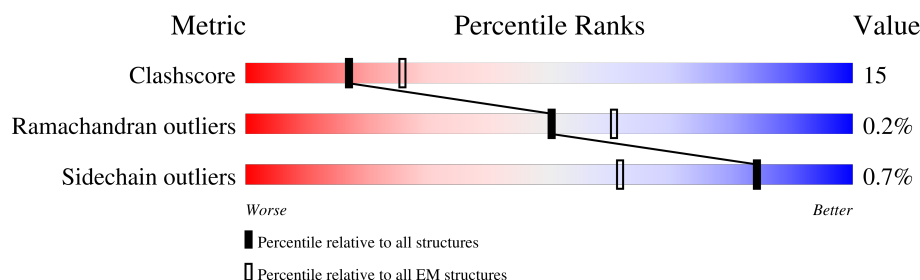
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	473	
1	B	473	
1	C	473	
1	D	473	
1	E	473	
1	F	473	
1	G	473	
1	I	473	

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Mol	Chain	Length	Quality of chain
1	J	473	<div><div></div><div>21%5%73%</div></div>
1	K	473	<div><div></div><div>22%.74%</div></div>
1	L	473	<div><div></div><div>22%.74%</div></div>
1	M	473	<div><div></div><div>22%.74%</div></div>
2	O	473	<div><div></div><div>26%34%.38%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14475 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 Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	128	Total	C	N	O	S	0	0
			1040	658	186	191	5		
1	B	126	Total	C	N	O	S	0	0
			1023	650	181	187	5		
1	C	126	Total	C	N	O	S	0	0
			1022	648	181	188	5		
1	D	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	E	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	F	122	Total	C	N	O	S	0	0
			988	625	176	182	5		
1	G	128	Total	C	N	O	S	0	0
			1041	658	187	191	5		
1	I	126	Total	C	N	O	S	0	0
			1023	650	181	187	5		
1	J	126	Total	C	N	O	S	0	0
			1022	648	181	188	5		
1	K	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	L	123	Total	C	N	O	S	0	0
			994	630	176	183	5		
1	M	122	Total	C	N	O	S	0	0
			988	625	176	182	5		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-322	SER	-	expression tag	UNP Q9UQM7
B	-337	SER	-	expression tag	UNP Q9UQM7
C	-332	SER	-	expression tag	UNP Q9UQM7
D	-334	SER	-	expression tag	UNP Q9UQM7
E	-336	SER	-	expression tag	UNP Q9UQM7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-337	SER	-	expression tag	UNP Q9UQM7
G	-322	SER	-	expression tag	UNP Q9UQM7
I	-337	SER	-	expression tag	UNP Q9UQM7
J	-332	SER	-	expression tag	UNP Q9UQM7
K	-334	SER	-	expression tag	UNP Q9UQM7
L	-336	SER	-	expression tag	UNP Q9UQM7
M	-337	SER	-	expression tag	UNP Q9UQM7

- Molecule 2 is a protein called Calcium/calmodulin-dependent protein kinase type II subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	293	Total	C	N	O	S	0	0
			2352	1503	415	423	11		

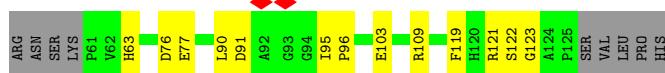
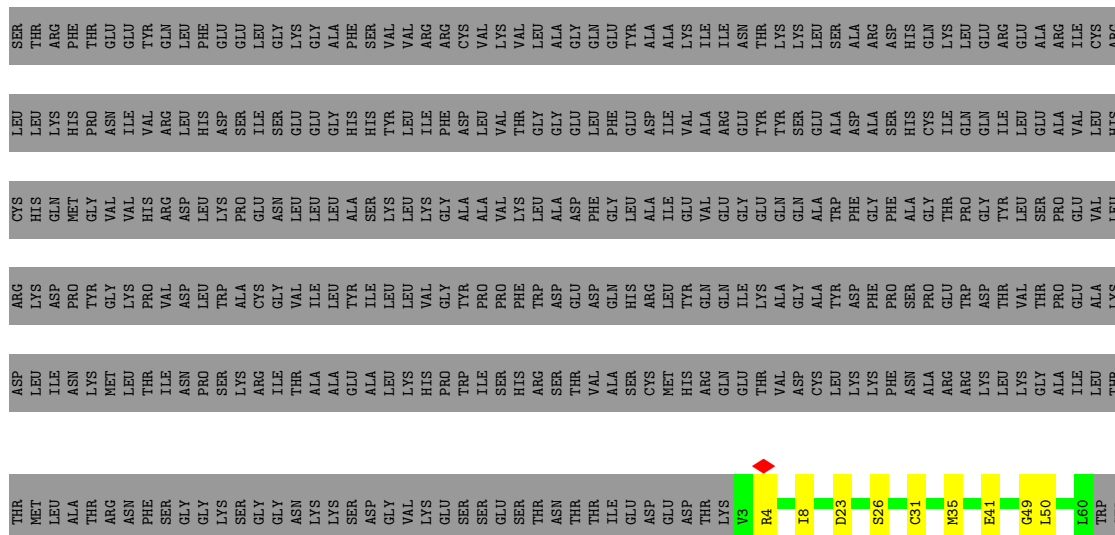
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	0	SER	-	expression tag	UNP Q9UQM7
O	34	MET	LYS	engineered mutation	UNP Q9UQM7
O	127	ASN	ASP	conflict	UNP Q9UQM7



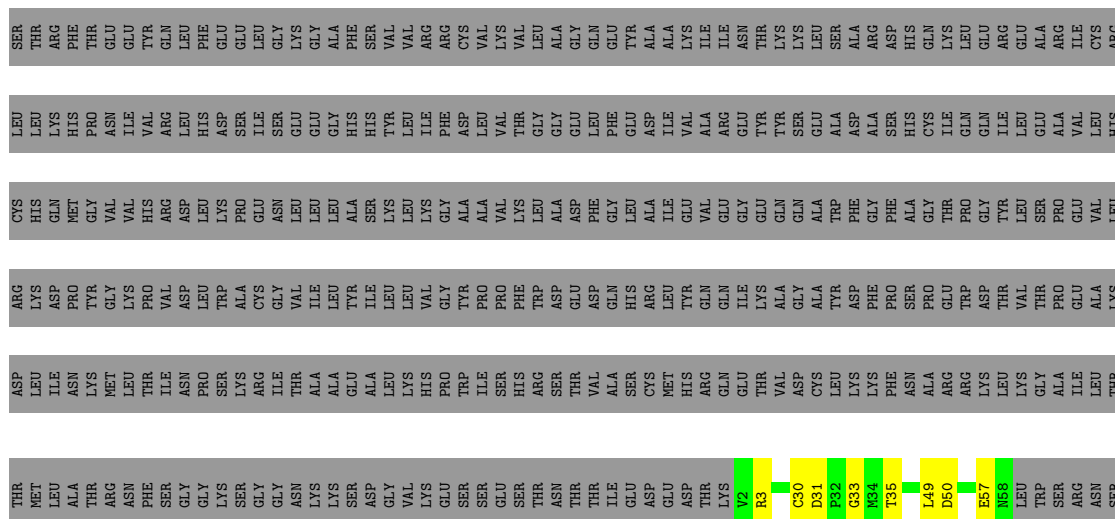
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

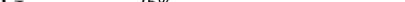
Chain E: 21% 5% 74%



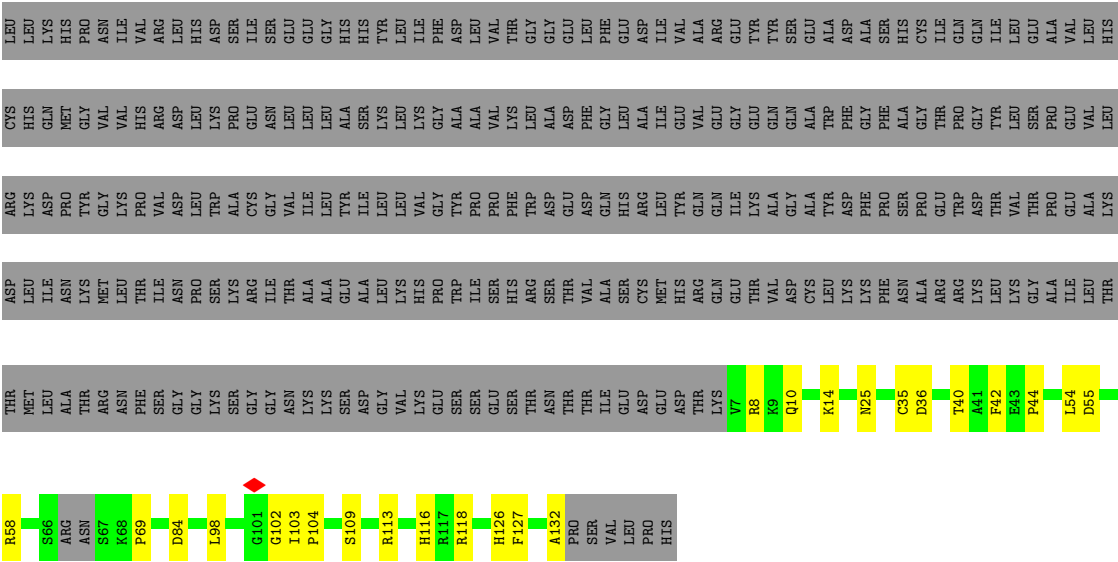
- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha

Chain F: 22% 0% 74%

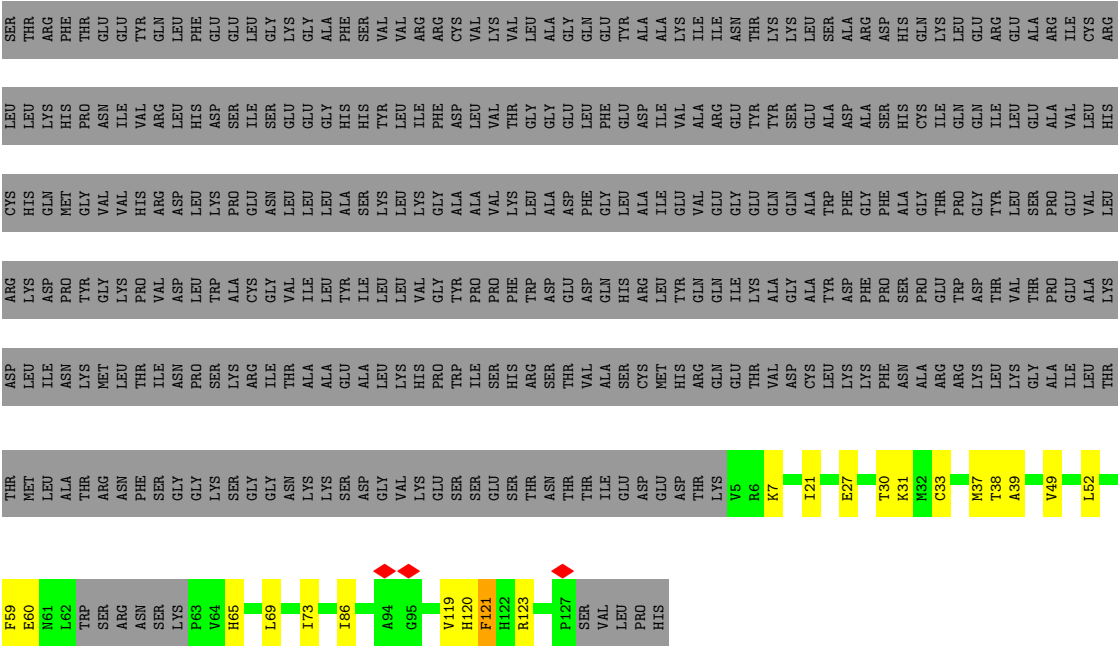


Chain G:  25% 73%

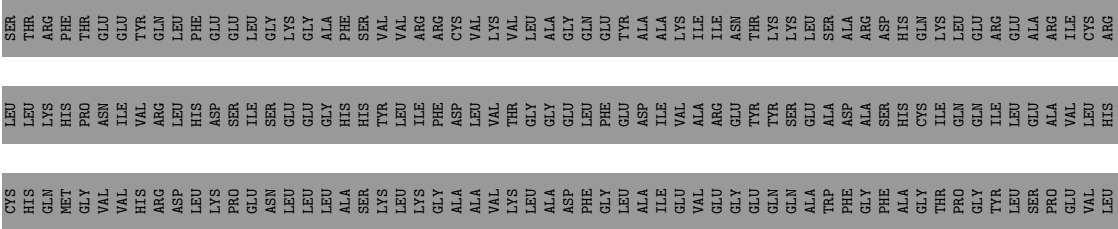




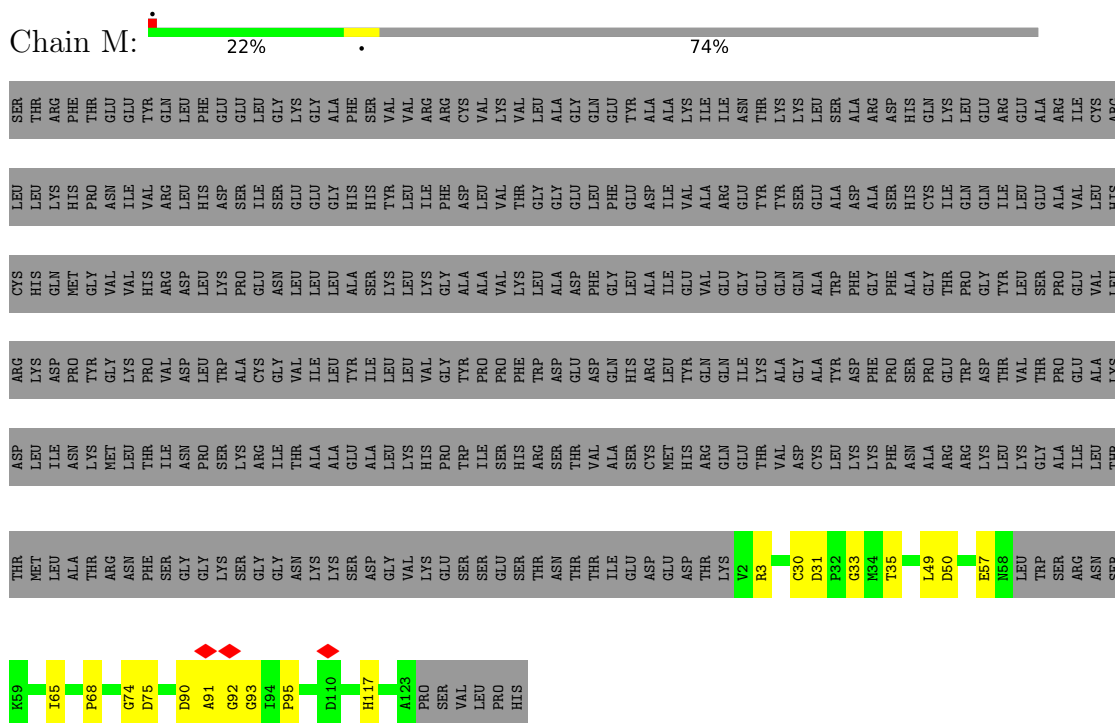
● Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



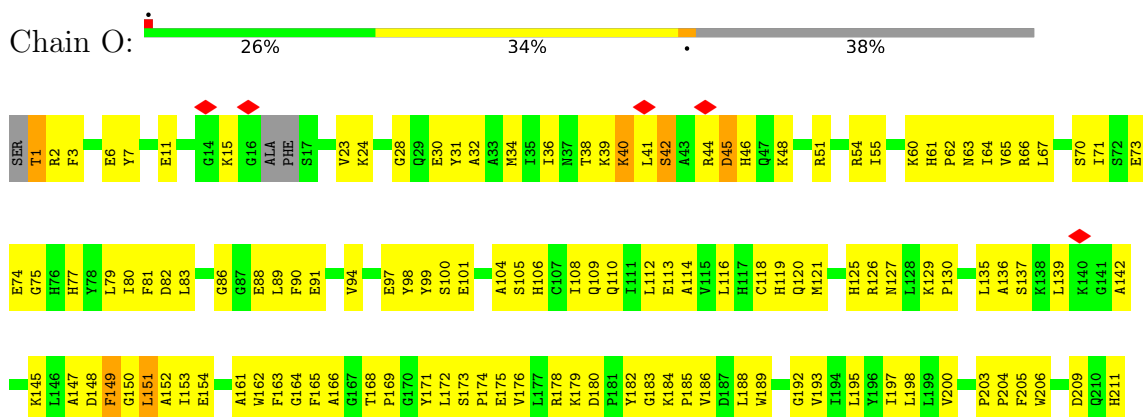
● Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



- Molecule 1: Calcium/calmodulin-dependent protein kinase type II subunit alpha



- Molecule 2: Calcium/calmodulin-dependent protein kinase type II subunit alpha



R212	R213	R214	R215	R216	R217	R218	R219	R220	R221	R222	R223	R224	R225	R226	R227	R228	R229	R230	R231	R232	R233	R234	R235	R236	R237	R238	R239	R240	R241	R242	R243	R244	R245	R246	R247	R248	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260	R261	R262	R263	R264	R265	R266	R267	R268	R269	R270	R271	R272	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000
K292	C293	ALA	ILE	LEU	THR	THR	MET	LEU	ALA	THR	THR	ARG	ASN	PHE	SER	GLY	GLY	LYS	SER	GLY	ASN	LYS	LYS	SER	ASP	GLY	GLY	ASN	LYS	LYS	GLY	GLY	VAL	LYS	GLU	GLU	GLU	SER	SER	SER	THR	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR																																																																																																																																																																																																																																																													

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	160211	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)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.011	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0072	Depositor
Map size (Å)	364.0, 364.0, 364.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/1067	0.42	0/1443
1	B	0.26	0/1050	0.42	0/1421
1	C	0.25	0/1048	0.42	0/1417
1	D	0.25	0/1019	0.41	0/1378
1	E	0.26	0/1019	0.42	0/1378
1	F	0.25	0/1012	0.41	0/1367
1	G	0.25	0/1068	0.42	0/1445
1	I	0.26	0/1050	0.41	0/1421
1	J	0.25	0/1048	0.42	0/1417
1	K	0.25	0/1019	0.42	0/1378
1	L	0.26	0/1019	0.42	0/1378
1	M	0.25	0/1012	0.41	0/1367
2	O	0.37	0/2407	0.65	2/3254 (0.1%)
All	All	0.28	0/14838	0.46	2/20064 (0.0%)

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
2	O	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	269	VAL	N-CA-C	5.71	126.42	111.00
2	O	151	LEU	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	O	149	PHE	Peptide
2	O	150	GLY	Peptide
2	O	40	LYS	Peptide

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	1040	0	1002	9	0
1	B	1023	0	985	12	0
1	C	1022	0	983	12	0
1	D	994	0	958	10	0
1	E	994	0	958	16	0
1	F	988	0	952	11	0
1	G	1041	0	1003	7	0
1	I	1023	0	985	13	0
1	J	1022	0	982	77	0
1	K	994	0	957	51	0
1	L	994	0	958	16	0
1	M	988	0	952	11	0
2	O	2352	0	2355	319	0
All	All	14475	0	14030	440	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 15.

The worst 5 of 440 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:J:14:LYS:HD3	2:O:291:LEU:CB	1.31	1.57
1:J:14:LYS:HB2	2:O:291:LEU:CG	1.29	1.53
1:K:27:GLU:CG	2:O:164:GLY:HA2	1.17	1.50
1:J:14:LYS:CB	2:O:291:LEU:CD1	1.95	1.42
1:K:27:GLU:HG2	2:O:162:TRP:NE1	1.35	1.42

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	126/473 (27%)	123 (98%)	3 (2%)	0	100	100
1	B	122/473 (26%)	119 (98%)	3 (2%)	0	100	100
1	C	122/473 (26%)	116 (95%)	6 (5%)	0	100	100
1	D	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	E	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	F	118/473 (25%)	117 (99%)	0	1 (1%)	19	59
1	G	126/473 (27%)	123 (98%)	3 (2%)	0	100	100
1	I	122/473 (26%)	119 (98%)	3 (2%)	0	100	100
1	J	122/473 (26%)	116 (95%)	6 (5%)	0	100	100
1	K	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	L	119/473 (25%)	116 (98%)	3 (2%)	0	100	100
1	M	118/473 (25%)	117 (99%)	0	1 (1%)	19	59
2	O	289/473 (61%)	270 (93%)	17 (6%)	2 (1%)	22	62
All	All	1741/6149 (28%)	1684 (97%)	53 (3%)	4 (0%)	50	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	91	ALA
1	M	91	ALA
2	O	42	SER
2	O	261	PRO

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	110/405 (27%)	109 (99%)	1 (1%)	78	87
1	B	109/405 (27%)	109 (100%)	0	100	100
1	C	109/405 (27%)	108 (99%)	1 (1%)	78	87
1	D	106/405 (26%)	105 (99%)	1 (1%)	78	87
1	E	106/405 (26%)	105 (99%)	1 (1%)	78	87
1	F	105/405 (26%)	105 (100%)	0	100	100
1	G	111/405 (27%)	110 (99%)	1 (1%)	78	87
1	I	109/405 (27%)	109 (100%)	0	100	100
1	J	109/405 (27%)	108 (99%)	1 (1%)	78	87
1	K	106/405 (26%)	105 (99%)	1 (1%)	78	87
1	L	106/405 (26%)	105 (99%)	1 (1%)	78	87
1	M	105/405 (26%)	105 (100%)	0	100	100
2	O	250/405 (62%)	247 (99%)	3 (1%)	71	84
All	All	1541/5265 (29%)	1530 (99%)	11 (1%)	84	90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	76	ASP
2	O	1	THR
2	O	260	HIS
2	O	45	ASP
1	G	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	120	HIS
2	O	286	ASN
1	G	73	ASN
1	G	140	HIS
1	I	72	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 monosaccharides 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.

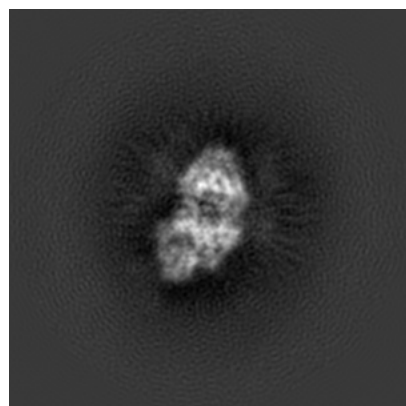
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21535. These allow visual inspection of the internal detail of the map and identification of artifacts.

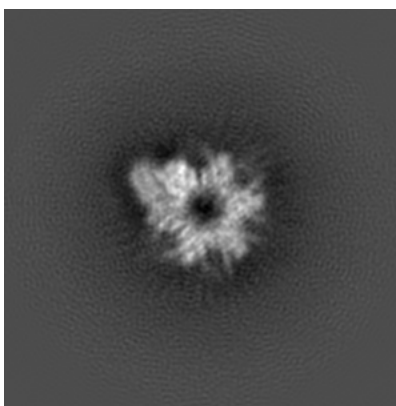
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

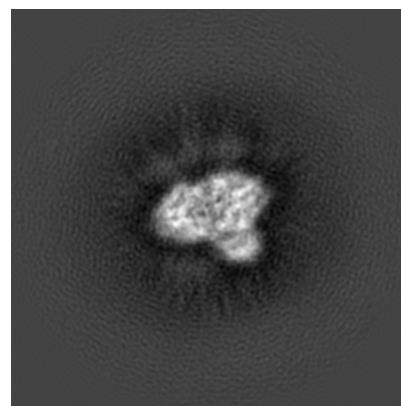
6.1.1 Primary map



X

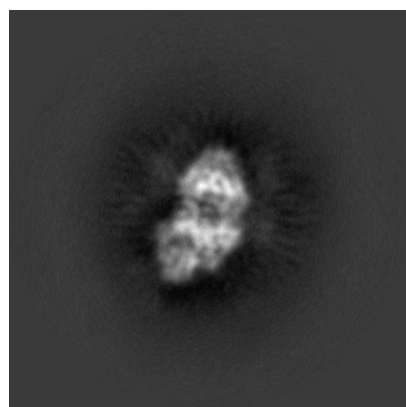


Y

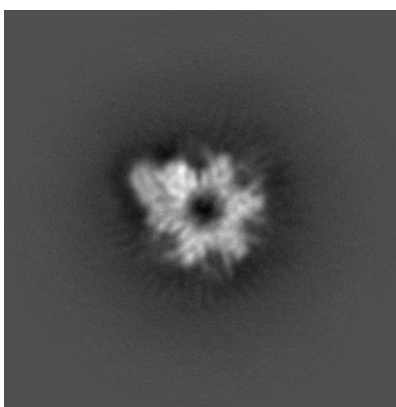


Z

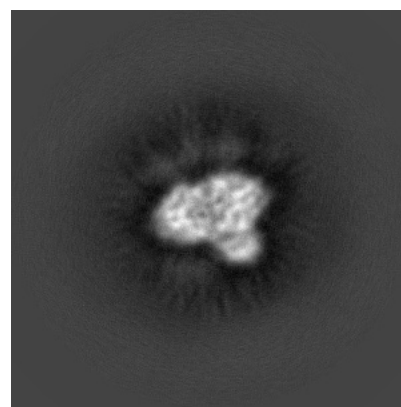
6.1.2 Raw map



X



Y

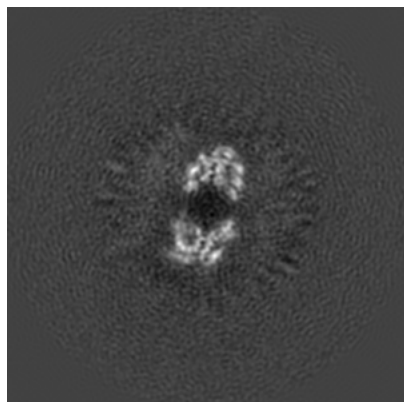


Z

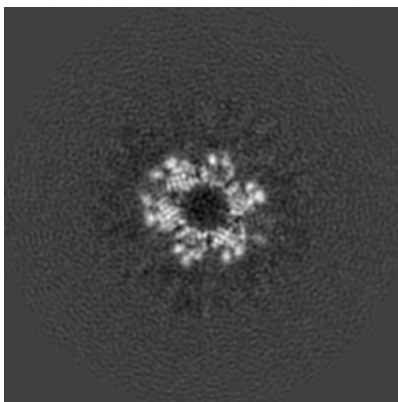
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

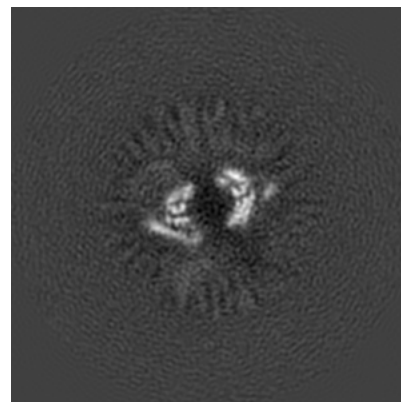
6.2.1 Primary map



X Index: 200

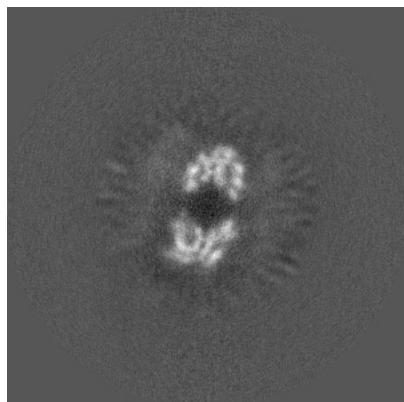


Y Index: 200

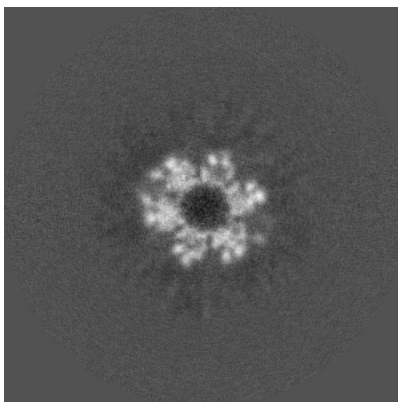


Z Index: 200

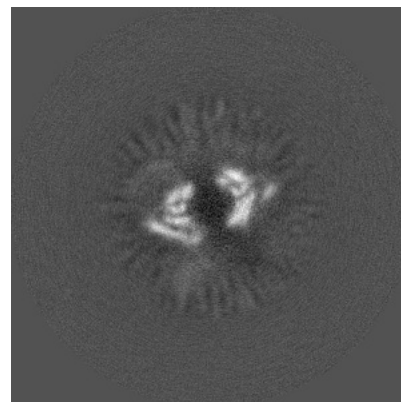
6.2.2 Raw map



X Index: 200



Y Index: 200

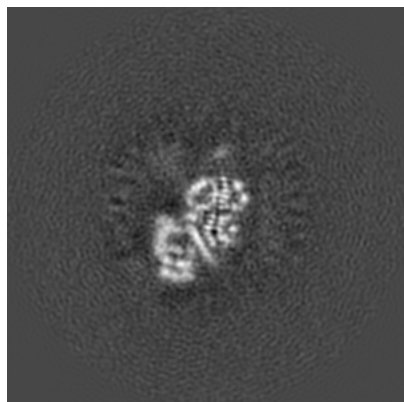


Z Index: 200

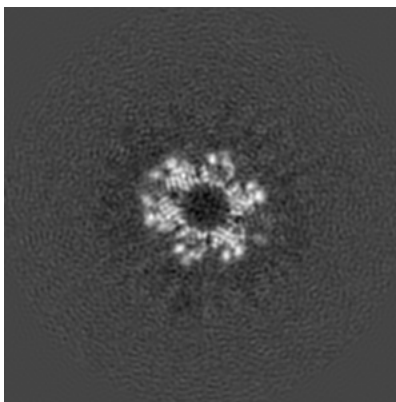
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

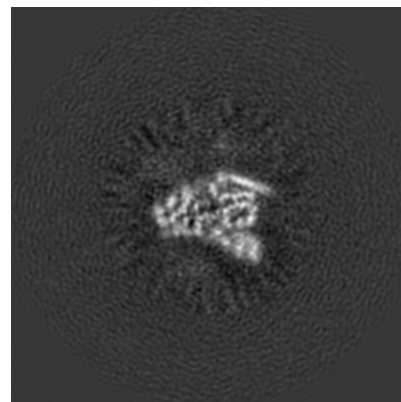
6.3.1 Primary map



X Index: 230

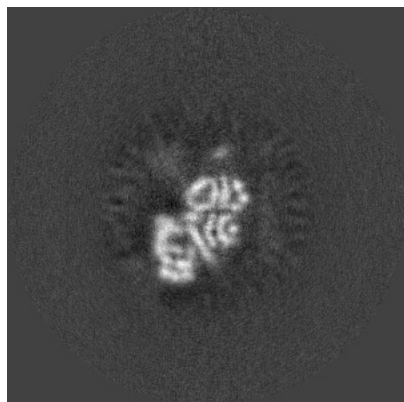


Y Index: 201

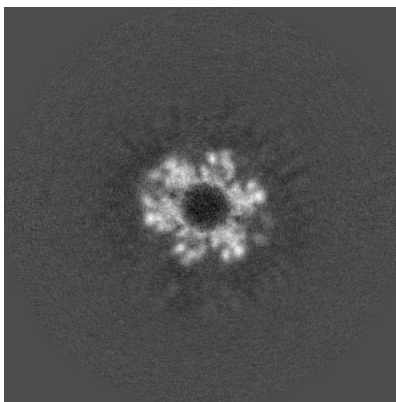


Z Index: 178

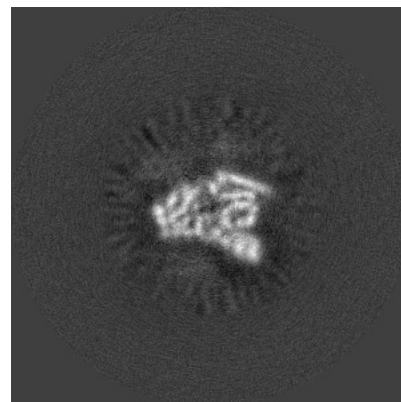
6.3.2 Raw map



X Index: 230



Y Index: 202

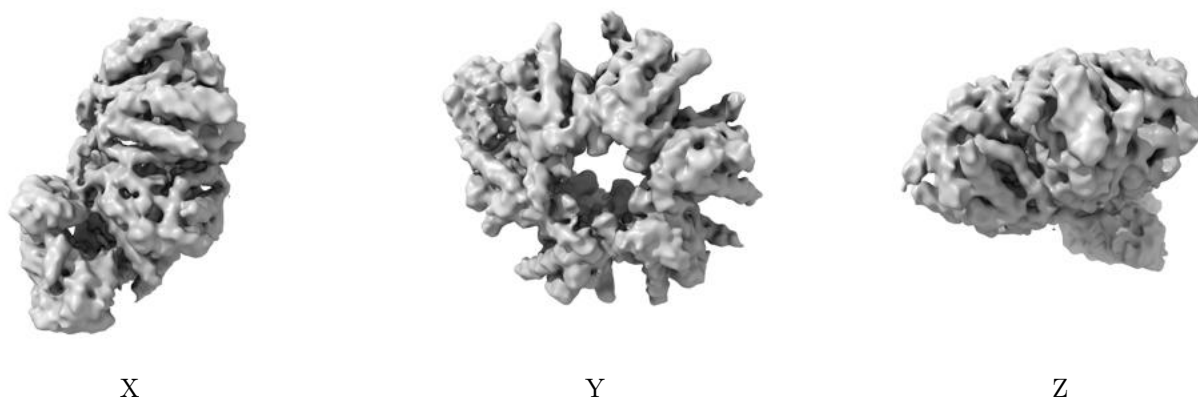


Z Index: 179

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

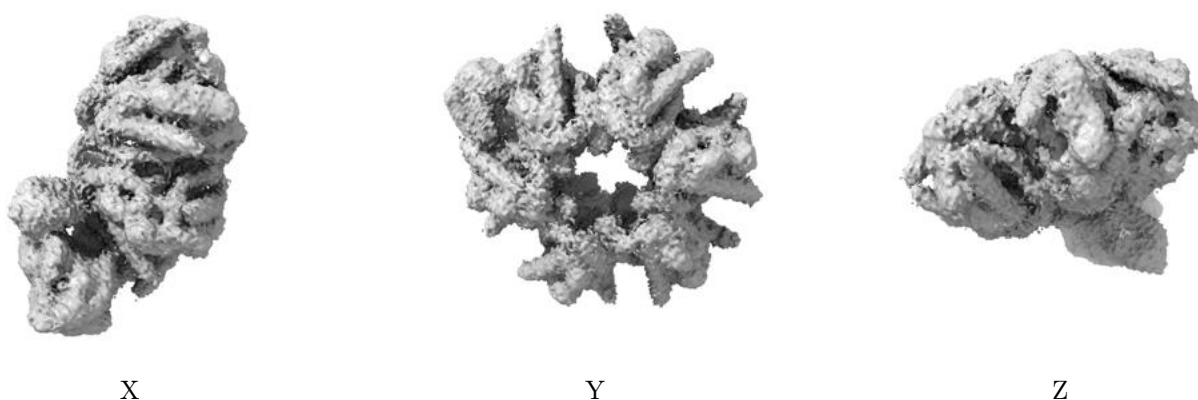
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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

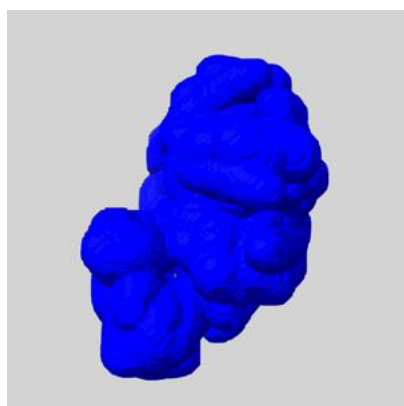
6.5 Mask visualisation [i](#)

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

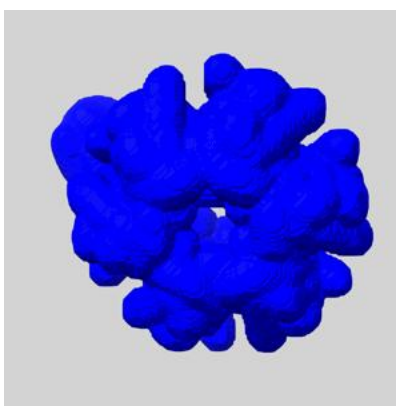
A mask typically either:

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

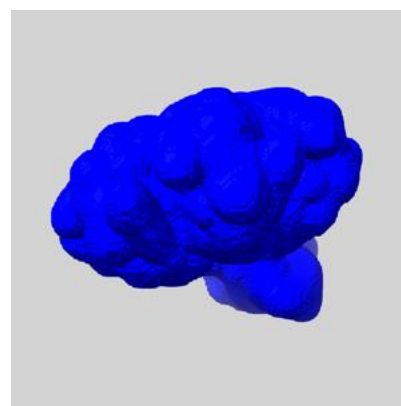
6.5.1 emd_21535_msk_1.map [i](#)



X



Y

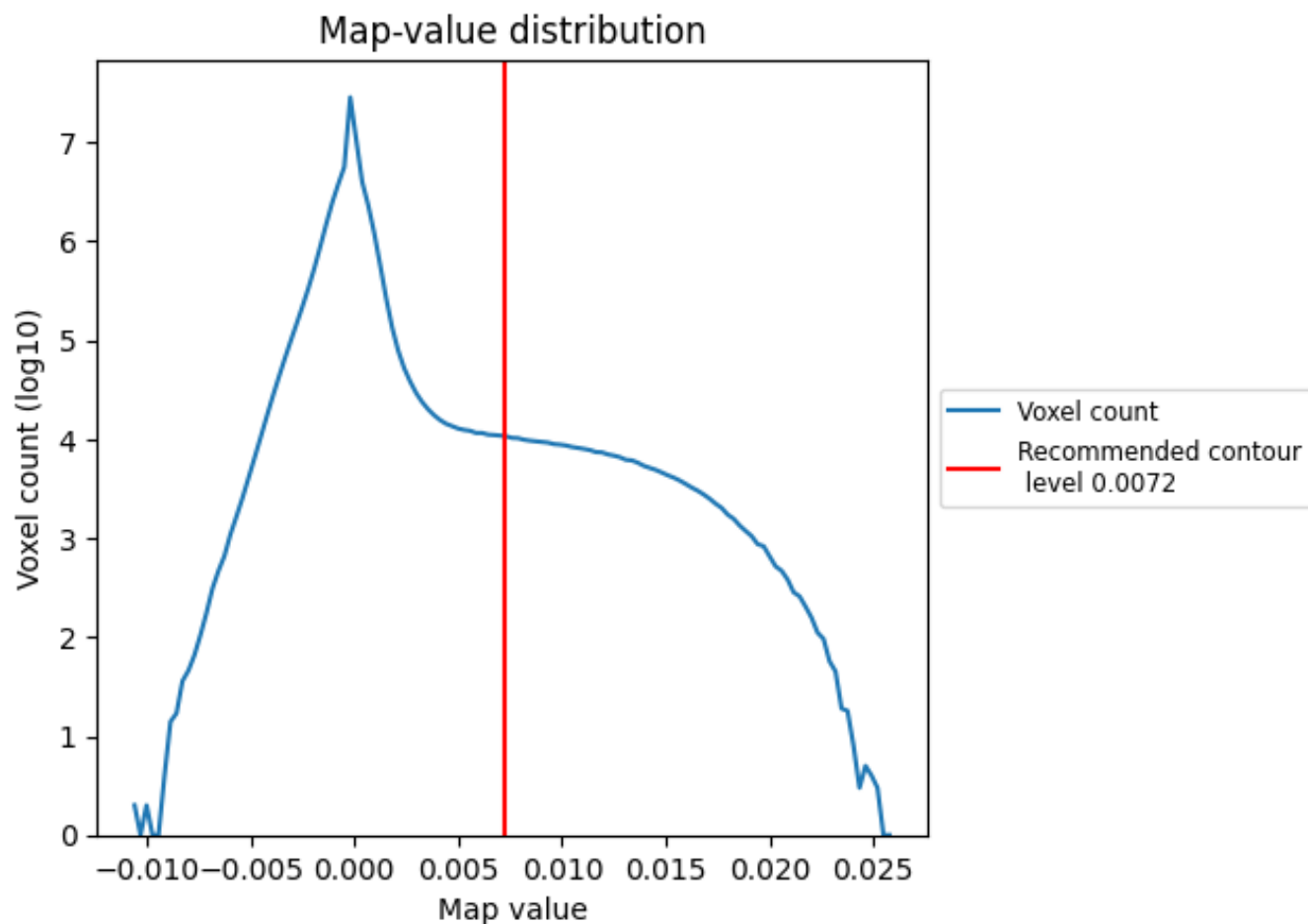


Z

7 Map analysis [i](#)

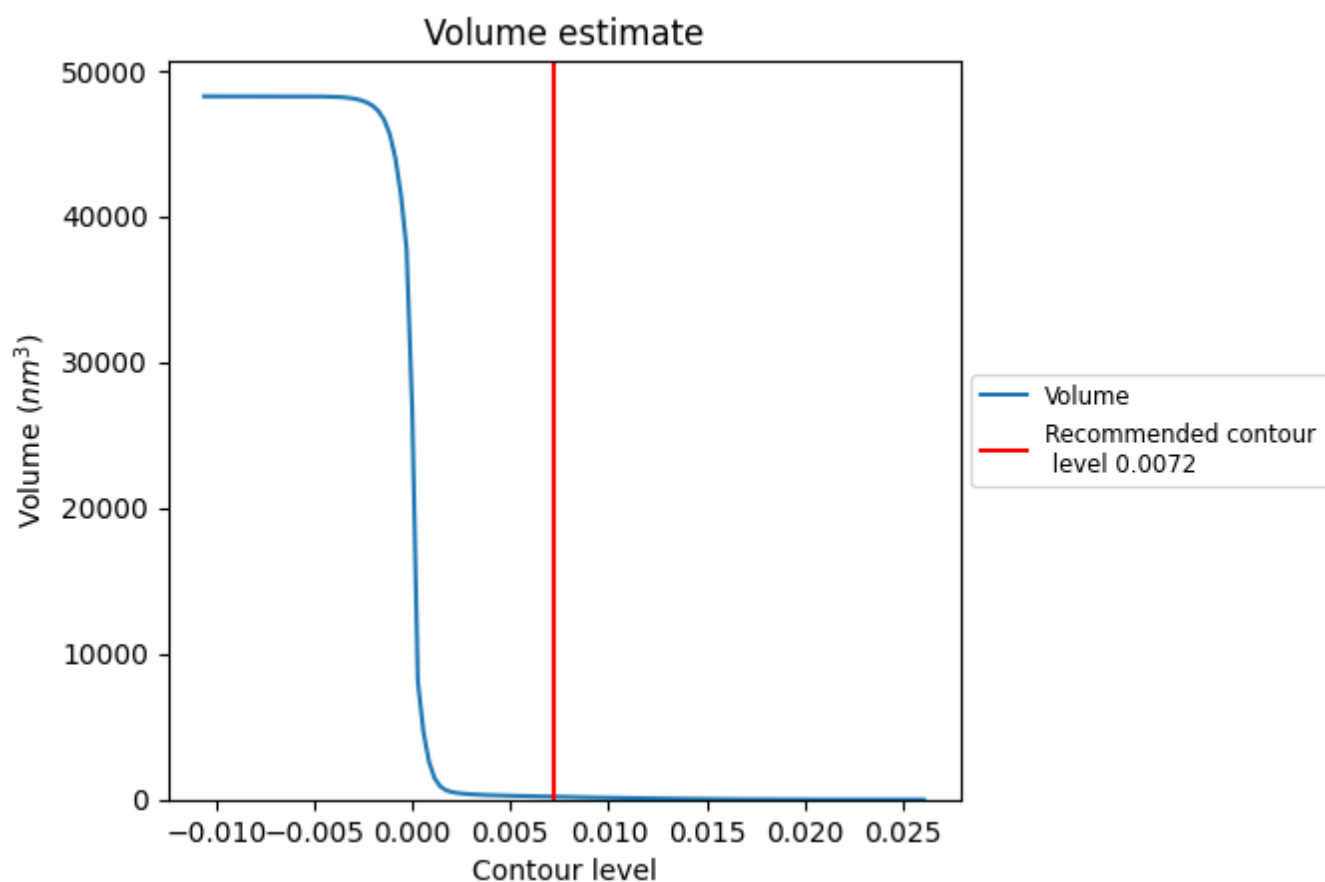
This section contains the results of statistical analysis of the map.

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.

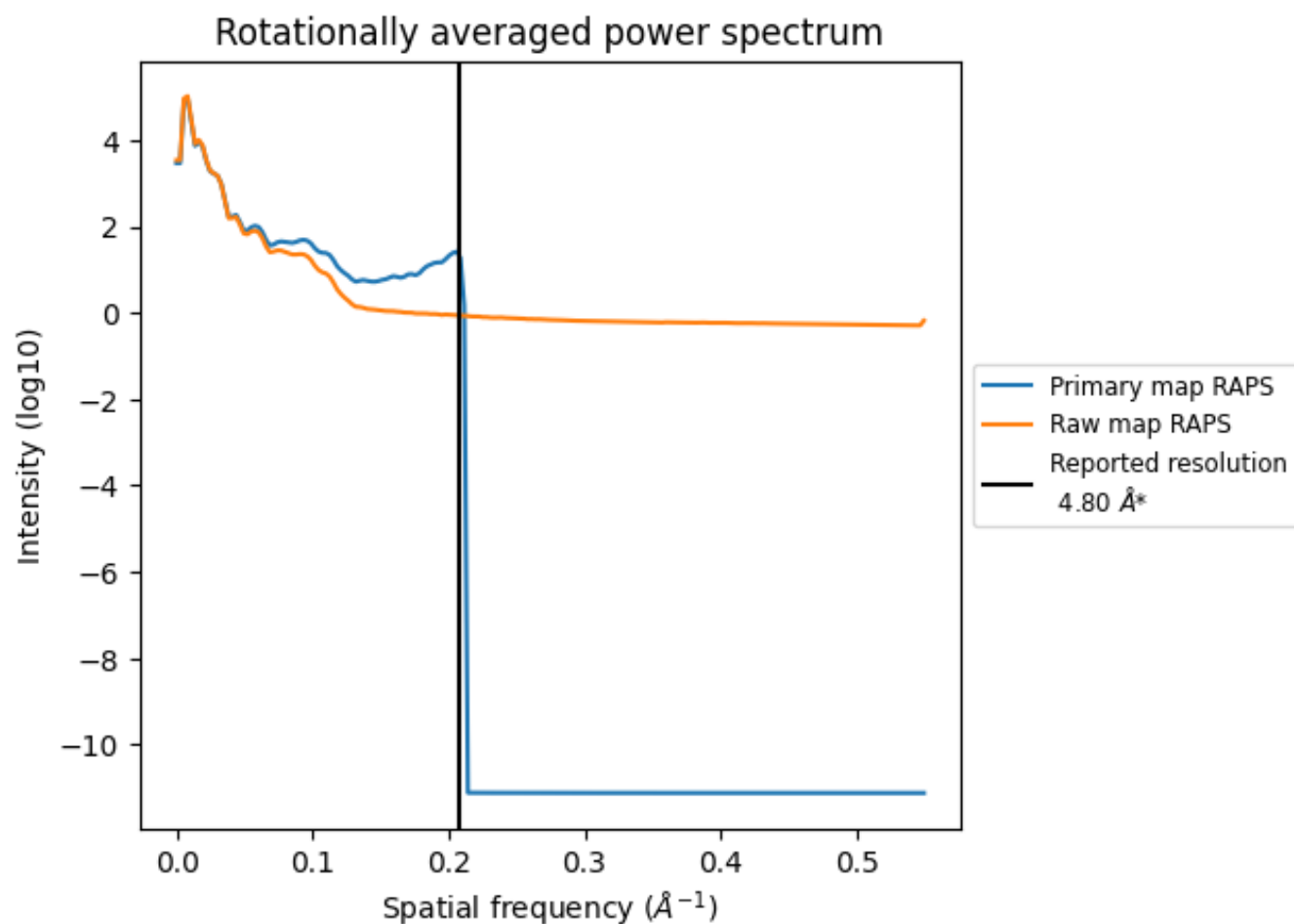
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 194 nm³; this corresponds to an approximate mass of 176 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 ⓘ

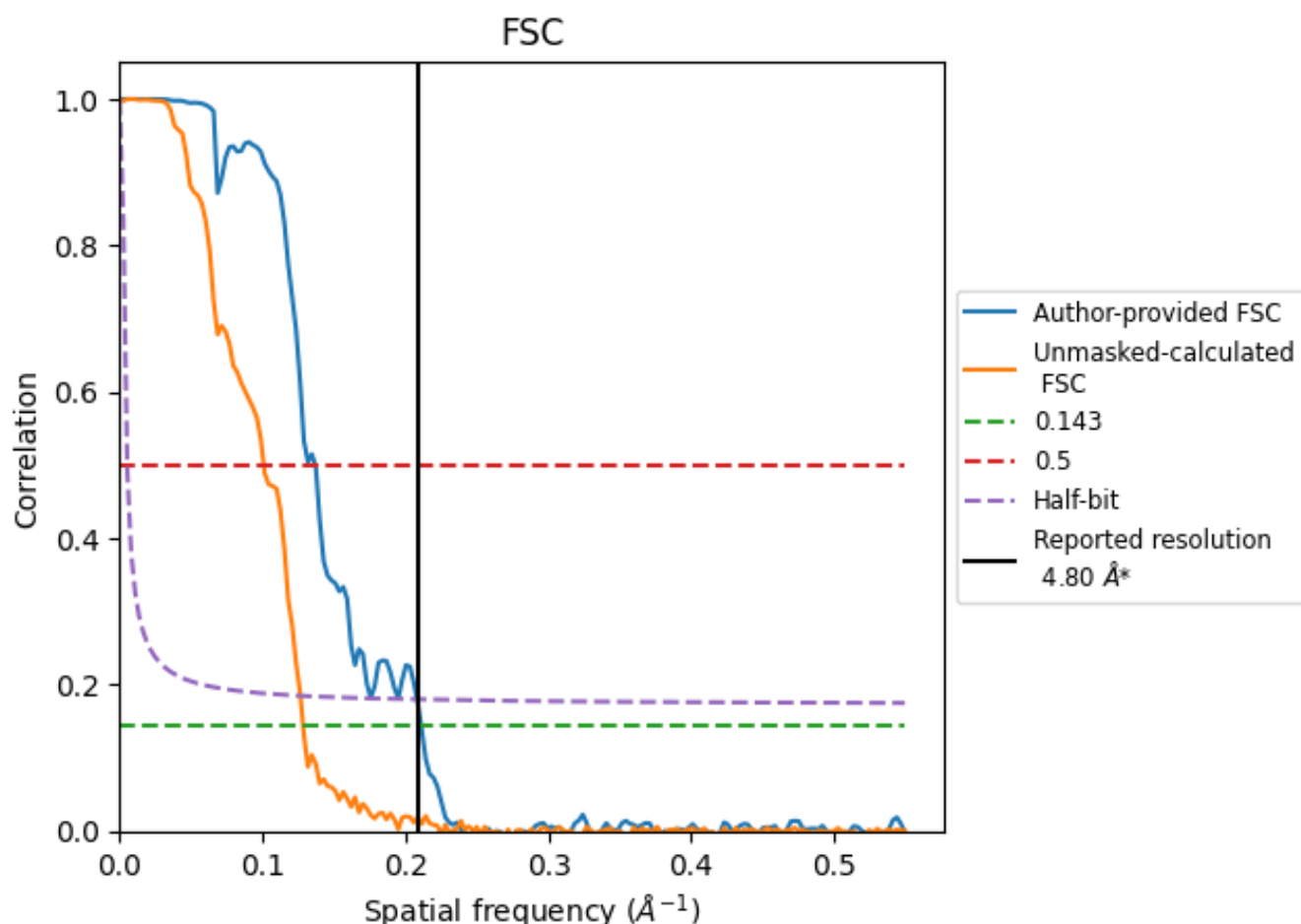


*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

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 0.208 Å⁻¹

8.2 Resolution estimates [i](#)

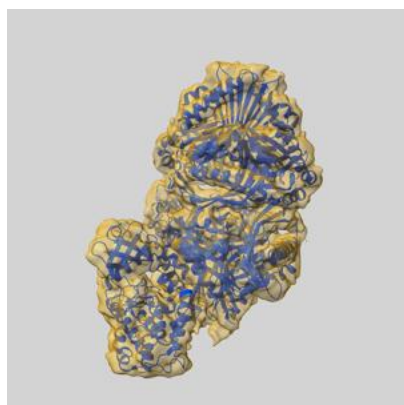
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	4.73	7.30	4.80
Unmasked-calculated*	7.78	9.90	7.90

*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 7.78 differs from the reported value 4.8 by more than 10 %

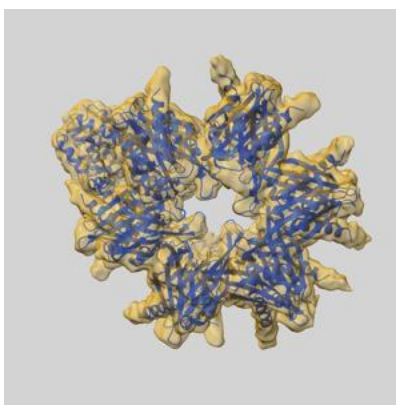
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21535 and PDB model 6W4O. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

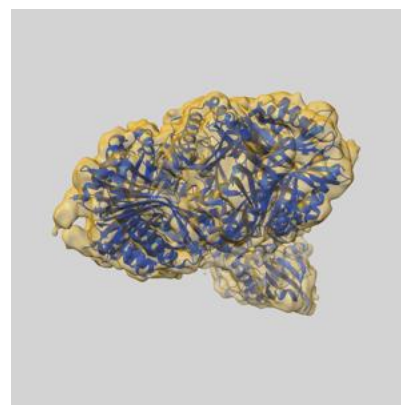
9.1 Map-model overlay [i](#)



X



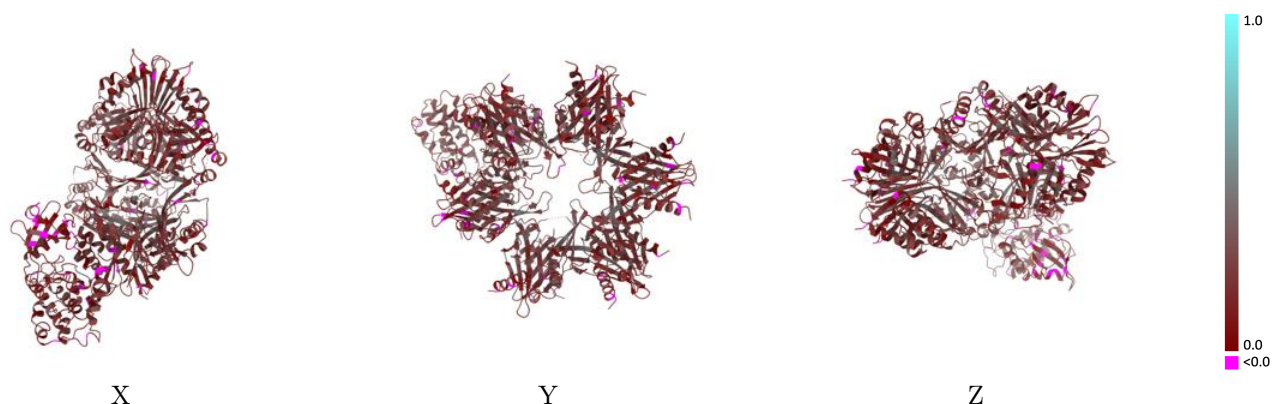
Y



Z

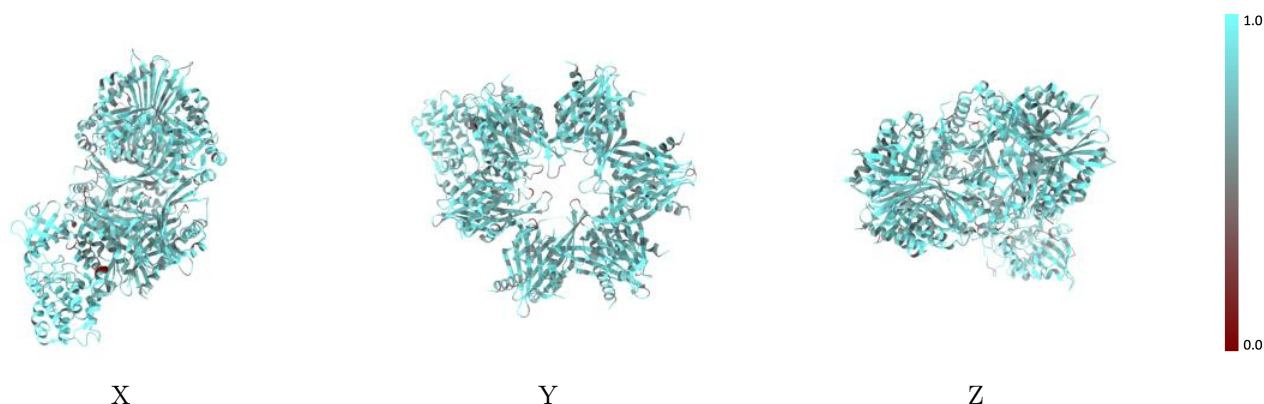
The images above show the 3D surface view of the map at the recommended contour level 0.0072 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



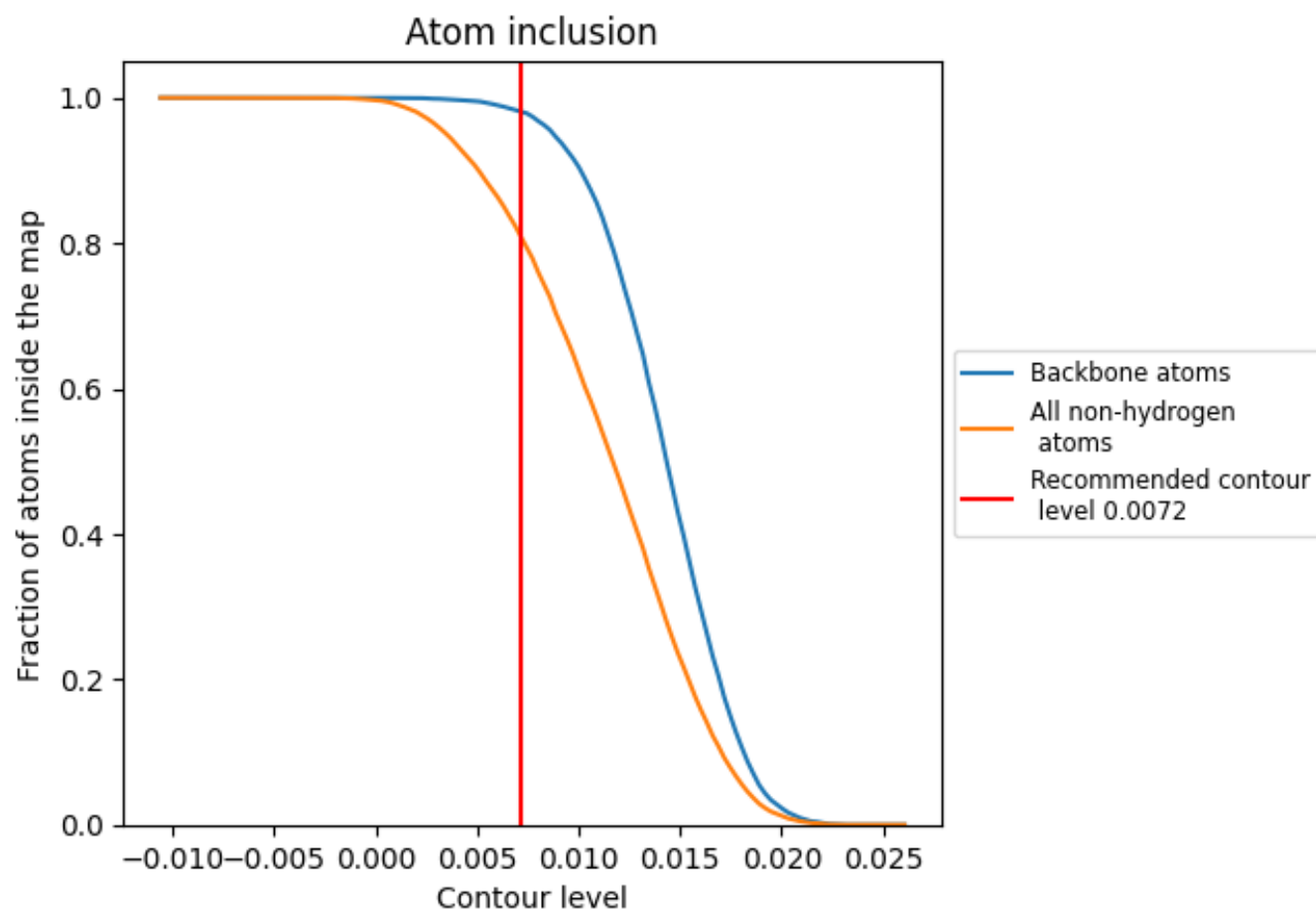
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0072).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.0072) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.8068</div>	<div><div></div>0.2130</div>
A	<div><div></div>0.7941</div>	<div><div></div>0.2140</div>
B	<div><div></div>0.7890</div>	<div><div></div>0.2160</div>
C	<div><div></div>0.7998</div>	<div><div></div>0.2260</div>
D	<div><div></div>0.8117</div>	<div><div></div>0.2150</div>
E	<div><div></div>0.7912</div>	<div><div></div>0.2130</div>
F	<div><div></div>0.8126</div>	<div><div></div>0.2290</div>
G	<div><div></div>0.7894</div>	<div><div></div>0.2170</div>
I	<div><div></div>0.7880</div>	<div><div></div>0.2110</div>
J	<div><div></div>0.7838</div>	<div><div></div>0.2360</div>
K	<div><div></div>0.7963</div>	<div><div></div>0.2270</div>
L	<div><div></div>0.8056</div>	<div><div></div>0.2180</div>
M	<div><div></div>0.7909</div>	<div><div></div>0.2270</div>
O	<div><div></div>0.8627</div>	<div><div></div>0.1750</div>

1.0

0.0

<0.0