



Full wwPDB EM Validation Report ⓘ

Aug 10, 2026 – 03:26 PM EDT

PDB ID : 35ZV / pdb_000035zv
EMDB ID : EMD-77307
Title : yeast 26S proteasome base assembly intermediate, Rpn14-Rpt6
Authors : Hsieh, H.H.; Martin, A.
Deposited on : 2026-05-26
Resolution : 3.11 Å(reported)

This is a Full wwPDB EM Validation 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.dev133
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 EMD 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) : 2.50

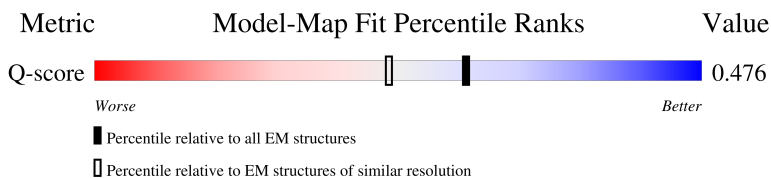
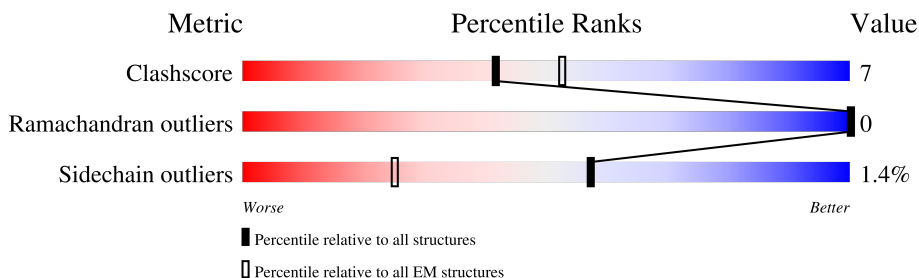
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.11 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	14465 (2.61 - 3.61)

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	993	
2	I	405	
3	J	428	
4	M	417	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6397 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 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	166	Total	C	N	O	S	0	0
			1355	864	215	273	3		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	240	Total	C	N	O	S	0	0
			1875	1179	337	345	14		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	6	Total	C	N	O	S	0	0
			46	29	6	10	1		

- Molecule 4 is a protein called 26S proteasome regulatory subunit RPN14.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	395	Total	C	N	O	S	0	0
			3090	1947	522	610	11		

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
5	I	1	Total	C	N	O	P	0
			31	10	5	13	3	

Lys	Lys	Lys	Met	Asp
Asn	Val	Asn	Val	Leu
Pro	Val	Asn	Phe	Glu
Asp	Val	Arg	Asn	Val
Thr	Val	Val	Asp	Ser
Arg	Gly	Gly	Ala	Asn
Glu	Gln	Gln	His	Ser
Glu	Val	Ala	Val	Ile
Glu	Val	Val	Leu	Phe
	Glu	Glu	Asn	Ala
	Thr	Thr	Lys	Met
	Val	Val	Val	Gly
	Gly	Gly	Thr	Gly
	Gln	Gln	Leu	Cys
	Ala	Ala	Ala	Gly
	Ala	Ala	Ser	Ala
	Gly	Arg	Ile	Gly
	Pro	Pro	Leu	Thr
	Lys	Lys	Thr	Asn
	Ile	Ile	Ala	Asn
	Thr	Thr	Val	Arg
	Gly	Gly	Gly	Arg
	Trp	Leu	Leu	Leu
	Ile	Ile	Val	Ala
	Thr	Thr	Val	Gln
	Gln	Gln	Pro	Leu
	Ser	Ser	Ser	Leu
	Thr	Thr	Phe	Arg
	Pro	Pro	Met	Gln
	Val	Val	Leu	Leu
	Leu	Leu	Lys	Ser
	Leu	Leu	His	Ser
	Asn	Asn	His	Thr
	His	His	Gln	Ser
	Gly	Gly	Leu	Arg
	Glu	Glu	Phe	Glu
	Ala	Ala	Thr	Gln
	Glu	Glu	Met	Asp
	Leu	Leu	Leu	Ala
	Glu	Glu	Asn	Leu
	Thr	Thr	Ala	Phe
	Thr	Thr	Gly	Ile
	Asp	Asp	Ile	Thr
	Glu	Glu	Arg	Arg
	Thr	Thr	Pro	Leu
	Ser	Ser	Lys	Ala
	His	His	Phe	Gln
	Ile	Ile	Ile	Leu
	Glu	Glu	Leu	Gly
	Val	Val	Ala	Leu
	Thr	Thr	Ala	Leu
	Ile	Ile	Lys	His
	Leu	Leu	Asn	Leu
	Thr	Thr	Asp	Gly
	Val	Val	Gly	Lys
	Thr	Thr	Glu	Thr
	Met	Met	Pro	Gly
	Thr	Thr	Ile	Thr

- Molecule 2: 26S proteasome regulatory subunit 8 homolog

[illegible]

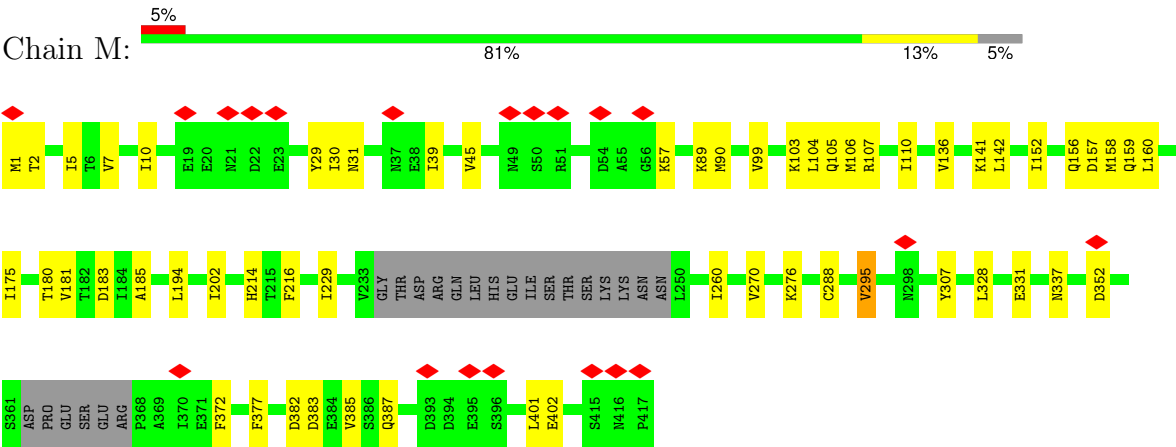
- Molecule 3: 26S proteasome regulatory subunit 6B homolog



E1	E2	E3	E4	E5	E6	E7	E8	E9	E10	E11	E12	E13	E14	E15	E16	E17	E18	E19	E20	E21	E22	E23	E24	E25	E26	E27	E28	E29	E30	E31	E32	E33	E34	E35	E36	E37	E38	E39	E40	E41	E42	E43	E44	E45	E46	E47	E48	E49	E50	E51	E52	E53	E54	E55	E56	E57	E58	E59	E60	E61	E62	E63	E64	E65	E66	E67	E68	E69	E70	E71	E72	E73	E74	E75	E76	E77	E78	E79	E80	E81	E82	E83	E84	E85	E86	E87	E88	E89	E90	E91	E92	E93	E94	E95	E96	E97	E98	E99	E100	E101	E102	E103	E104	E105	E106	E107	E108	E109	E110	E111	E112	E113	E114	E115	E116	E117	E118	E119	E120	E121	E122	E123	E124	E125	E126	E127	E128	E129	E130	E131	E132	E133	E134	E135	E136	E137	E138	E139	E140	E141	E142	E143	E144	E145	E146	E147	E148	E149	E150	E151	E152	E153	E154	E155	E156	E157	E158	E159	E160	E161	E162	E163	E164	E165	E166	E167	E168	E169	E170	E171	E172	E173	E174	E175	E176	E177	E178	E179	E180	E181	E182	E183	E184	E185	E186	E187	E188	E189	E190	E191	E192	E193	E194	E195	E196	E197	E198	E199	E200	E201	E202	E203	E204	E205	E206	E207	E208	E209	E210	E211	E212	E213	E214	E215	E216	E217	E218	E219	E220	E221	E222	E223	E224	E225	E226	E227	E228	E229	E230	E231	E232	E233	E234	E235	E236	E237	E238	E239	E240	E241	E242	E243	E244	E245	E246	E247	E248	E249	E250	E251	E252	E253	E254	E255	E256	E257	E258	E259	E260	E261	E262	E263	E264	E265	E266	E267	E268	E269	E270	E271	E272	E273	E274	E275	E276	E277	E278	E279	E280	E281	E282	E283	E284	E285	E286	E287	E288	E289	E290	E291	E292	E293	E294	E295	E296	E297	E298	E299	E300	E301	E302	E303	E304	E305	E306	E307	E308	E309	E310	E311	E312	E313	E314	E315	E316	E317	E318	E319	E320	E321	E322	E323	E324	E325	E326	E327	E328	E329	E330	E331	E332	E333	E334	E335	E336	E337	E338	E339	E340	E341	E342	E343	E344	E345	E346	E347	E348	E349	E350	E351	E352	E353	E354	E355	E356	E357	E358	E359	E360	E361	E362	E363	E364	E365	E366	E367	E368	E369	E370	E371	E372	E373	E374	E375	E376	E377	E378	E379	E380	E381	E382	E383	E384	E385	E386	E387	E388	E389	E390	E391	E392	E393	E394	E395	E396	E397	E398	E399	E400	E401	E402	E403	E404	E405	E406	E407	E408	E409	E410	E411	E412	E413	E414	E415	E416	E417	E418	E419	E420	E421	E422	E423	E424	E425	E426	E427	E428	E429	E430	E431	E432	E433	E434	E435	E436	E437	E438	E439	E440	E441	E442	E443	E444	E445	E446	E447	E448	E449	E450	E451	E452	E453	E454	E455	E456	E457	E458	E459	E460	E461	E462	E463	E464	E465	E466	E467	E468	E469	E470	E471	E472	E473	E474	E475	E476	E477	E478	E479	E480	E481	E482	E483	E484	E485	E486	E487	E488	E489	E490	E491	E492	E493	E494	E495	E496	E497	E498	E499	E500	E501	E502	E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552	E553	E554	E555	E556	E557	E558	E559	E560	E561	E562	E563	E564	E565	E566	E567	E568	E569	E570	E571	E572	E573	E574	E575	E576	E577	E578	E579	E580	E581	E582	E583	E584	E585	E586	E587	E588	E589	E590	E591	E592	E593	E594	E595	E596	E597	E598	E599	E600	E601	E602	E603	E604	E605	E606	E607	E608	E609	E610	E611	E612	E613	E614	E615	E616	E617	E618	E619	E620	E621	E622	E623	E624	E625	E626	E627	E628	E629	E630	E631	E632	E633	E634	E635	E636	E637	E638	E639	E640	E641	E642	E643	E644	E645	E646	E647	E648	E649	E650	E651	E652	E653	E654	E655	E656	E657	E658	E659	E660	E661	E662	E663	E664	E665	E666	E667	E668	E669	E670	E671	E672	E673	E674	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E694	E695	E696	E697	E698	E699	E700	E701	E702	E703	E704	E705	E706	E707	E708	E709	E710	E711	E712	E713	E714	E715	E716	E717	E718	E719	E720	E721	E722	E723	E724	E725	E726	E727	E728	E729	E730	E731	E732	E733	E734	E735	E736	E737	E738	E739	E740	E741	E742	E743	E744	E745	E746	E747	E748	E749	E750	E751	E752	E753	E754	E755	E756	E757	E758	E759	E760	E761	E762	E763	E764	E765	E766	E767	E768	E769	E770	E771	E772	E773	E774	E775	E776	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786	E787	E788	E789	E790	E791	E792	E793	E794	E795	E796	E797	E798	E799	E800	E801	E802	E803	E804	E805	E806	E807	E808	E809	E810	E811	E812	E813	E814	E815	E816	E817	E818	E819	E820	E821	E822	E823	E824	E825	E826	E827	E828	E829	E830	E831	E832	E833	E834	E835	E836	E837	E838	E839	E840	E841	E842	E843	E844	E845	E846	E847	E848	E849	E850	E851	E852	E853	E854	E855	E856	E857	E858	E859	E860	E861	E862	E863	E864	E865	E866	E867	E868	E869	E870	E871	E872	E873	E874	E875	E876	E877	E878	E879	E880	E881	E882	E883	E884	E885	E886	E887	E888	E889	E890	E891	E892	E893	E894	E895	E896	E897	E898	E899	E900	E901	E902	E903	E904	E905	E906	E907	E908	E909	E910	E911	E912	E913	E914	E915	E916	E917	E918	E919	E920	E921	E922	E923	E924	E925	E926	E927	E928	E929	E930	E931	E932	E933	E934	E935	E936	E937	E938	E939	E940	E941	E942	E943	E944	E945	E946	E947	E948	E949	E950	E951	E952	E953	E954	E955	E956	E957	E958	E959	E960	E961	E962	E963	E964	E965	E966	E967	E968	E969	E970	E971	E972	E973	E974	E975	E976	E977	E978	E979	E980	E981	E982	E983	E984	E985	E986	E987	E988	E989	E990	E991	E992	E993	E994	E995	E996	E997	E998	E999	E1000	E1001	E1002	E1003	E1004	E1005	E1006	E1007	E1008	E1009	E1010	E1011	E1012	E1013	E1014	E1015	E1016	E1017	E1018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● Molecule 4: 26S proteasome regulatory subunit RPN14



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208110	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.706	Depositor
Minimum map value	-0.400	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	536.576, 536.576, 536.576	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.048, 1.048, 1.048	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: ATP

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	0.13	0/1379	0.34	0/1863
2	I	0.15	0/1900	0.40	0/2552
3	J	0.08	0/45	0.31	0/58
4	M	0.12	0/3147	0.36	0/4258
All	All	0.13	0/6471	0.37	0/8731

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1355	0	1327	23	0
2	I	1875	0	1944	29	0
3	J	46	0	48	0	0
4	M	3090	0	3008	38	0
5	I	31	0	12	1	0
All	All	6397	0	6339	87	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 7.

All (87) 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:I:181:GLN:HB2	2:I:284:THR:HB	1.61	0.80
4:M:141:LYS:HG3	4:M:183:ASP:HA	1.74	0.69
4:M:260:ILE:HG22	4:M:270:VAL:HG22	1.75	0.67
1:C:53:VAL:HG12	1:C:57:LYS:HZ2	1.60	0.66
2:I:248:ASP:HA	2:I:293:ALA:HB3	1.76	0.66
1:C:87:LYS:HG2	1:C:88:PRO:HD3	1.78	0.65
4:M:110:ILE:HD12	4:M:142:LEU:HD22	1.78	0.65
2:I:296:ARG:HA	2:I:296:ARG:NH1	2.11	0.64
4:M:152:ILE:HD11	4:M:160:LEU:HD23	1.81	0.62
4:M:337:ASN:HD22	4:M:387:GLN:HA	1.64	0.62
4:M:104:LEU:HG	4:M:105:GLN:H	1.65	0.62
4:M:385:VAL:HG21	4:M:402:GLU:OE2	2.01	0.61
2:I:170:HIS:CE1	4:M:136:VAL:HG13	2.37	0.60
4:M:1:MET:HE3	4:M:2:THR:N	2.16	0.59
4:M:103:LYS:HA	4:M:107:ARG:HA	1.83	0.59
4:M:156:GLN:HA	4:M:180:THR:HG23	1.85	0.59
4:M:10:ILE:HG13	4:M:30:ILE:HG12	1.83	0.59
4:M:183:ASP:HB3	4:M:229:ILE:HG12	1.85	0.59
1:C:93:ARG:HH11	1:C:93:ARG:HG3	1.67	0.59
1:C:165:TYR:CD1	1:C:227:ILE:HA	2.38	0.58
1:C:224:LEU:HD23	1:C:227:ILE:HD11	1.86	0.57
4:M:1:MET:HE3	4:M:2:THR:H	1.67	0.57
2:I:167:PRO:HB2	2:I:289:LYS:HE3	1.86	0.56
4:M:136:VAL:HB	4:M:157:ASP:HB3	1.88	0.56
4:M:160:LEU:HD11	4:M:181:VAL:HG11	1.88	0.55
4:M:328:LEU:HD21	4:M:331:GLU:HB2	1.89	0.55
4:M:99:VAL:HG21	4:M:401:LEU:HD23	1.88	0.54
4:M:89:LYS:HG3	4:M:90:MET:HG3	1.90	0.53
2:I:283:GLU:HG2	2:I:286:LYS:HG3	1.91	0.53
1:C:222:ASP:O	1:C:226:GLU:HG3	2.09	0.52
1:C:208:VAL:HG23	1:C:209:PRO:HD3	1.91	0.52
1:C:224:LEU:HA	1:C:227:ILE:HG12	1.92	0.51
1:C:50:GLU:O	1:C:54:GLU:HG2	2.12	0.50
4:M:352:ASP:HB2	4:M:382:ASP:HB2	1.92	0.50
2:I:332:SER:HB2	2:I:337:LEU:HD11	1.93	0.50
2:I:386:VAL:O	2:I:390:MET:HG2	2.11	0.49
1:C:210:TYR:HE1	1:C:214:HIS:CE1	2.31	0.49
4:M:214:HIS:CD2	4:M:276:LYS:HD2	2.48	0.49
2:I:276:LEU:HB3	2:I:309:ARG:NH2	2.28	0.48
1:C:154:ILE:HG13	1:C:210:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:5:ILE:HG12	4:M:372:PHE:HB2	1.95	0.48
4:M:57:LYS:H	4:M:57:LYS:HD2	1.77	0.48
4:M:260:ILE:HD11	4:M:295:VAL:HG23	1.95	0.48
2:I:359:LYS:HE3	2:I:359:LYS:HB2	1.68	0.47
2:I:342:ASN:HB2	4:M:29:TYR:CD2	2.50	0.47
2:I:146:THR:OG1	2:I:149:MET:HE3	2.15	0.47
4:M:185:ALA:HB3	4:M:194:LEU:HB2	1.95	0.47
2:I:163:VAL:HG11	2:I:185:VAL:HB	1.97	0.47
2:I:235:VAL:O	2:I:239:GLU:HG3	2.14	0.47
2:I:326:GLU:HG3	2:I:329:ARG:NH1	2.30	0.46
4:M:288:CYS:SG	4:M:307:TYR:HB3	2.56	0.46
4:M:99:VAL:HG12	4:M:387:GLN:HG2	1.97	0.46
2:I:187:LEU:HB3	2:I:316:PHE:HE2	1.82	0.45
4:M:105:GLN:NE2	4:M:106:MET:HB2	2.31	0.45
1:C:49:LEU:HD23	1:C:92:LEU:HG	1.98	0.45
1:C:43:ALA:O	1:C:47:THR:HG23	2.16	0.45
1:C:71:LEU:O	1:C:75:ILE:HG13	2.16	0.45
1:C:209:PRO:HG3	1:C:236:PHE:CD1	2.52	0.44
2:I:297:LEU:HD12	2:I:300:LEU:HD12	2.00	0.44
4:M:158:MET:HE3	4:M:158:MET:HB2	1.82	0.44
2:I:335:MET:HE1	2:I:362:CYS:O	2.17	0.44
4:M:31:ASN:HD22	4:M:39:ILE:HG21	1.83	0.44
1:C:49:LEU:HD21	1:C:88:PRO:HB3	2.00	0.43
2:I:226:GLY:HA2	2:I:229:MET:HE3	1.99	0.43
2:I:187:LEU:HB3	2:I:316:PHE:CE2	2.53	0.43
1:C:108:ASP:HB3	1:C:111:LEU:HB2	1.99	0.43
2:I:153:LEU:HD13	2:I:316:PHE:HE1	1.83	0.43
2:I:359:LYS:HD2	5:I:501:ATP:O3'	2.19	0.43
1:C:197:LYS:HB2	1:C:197:LYS:HE2	1.75	0.42
2:I:186:ILE:HA	2:I:292:MET:HB2	2.01	0.42
2:I:190:PRO:HD2	2:I:316:PHE:O	2.20	0.42
4:M:7:VAL:HA	4:M:377:PHE:CZ	2.55	0.42
4:M:372:PHE:HD2	4:M:372:PHE:H	1.66	0.42
2:I:171:PRO:HB3	2:I:181:GLN:HE22	1.83	0.42
4:M:99:VAL:HA	4:M:110:ILE:O	2.19	0.42
2:I:139:VAL:HG23	2:I:211:ILE:HG12	2.01	0.42
4:M:337:ASN:ND2	4:M:387:GLN:HA	2.32	0.42
1:C:154:ILE:HG13	1:C:210:TYR:CE2	2.55	0.42
1:C:203:LEU:O	1:C:207:ILE:HG13	2.20	0.42
1:C:204:CYS:O	1:C:208:VAL:HG22	2.19	0.42
2:I:173:LEU:HD21	4:M:159:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:269:GLN:H	2:I:269:GLN:CD	2.28	0.41
4:M:202:ILE:HB	4:M:216:PHE:HB2	2.03	0.41
2:I:359:LYS:HG3	2:I:360:GLY:N	2.37	0.40
1:C:210:TYR:HE1	1:C:214:HIS:ND1	2.19	0.40
4:M:385:VAL:HG11	4:M:402:GLU:HG2	2.03	0.40
1:C:46:LYS:HB2	1:C:46:LYS:HE3	1.77	0.40

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	160/993 (16%)	158 (99%)	2 (1%)	0	100	100
2	I	234/405 (58%)	229 (98%)	5 (2%)	0	100	100
3	J	4/428 (1%)	4 (100%)	0	0	100	100
4	M	389/417 (93%)	379 (97%)	10 (3%)	0	100	100
All	All	787/2243 (35%)	770 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	154/850 (18%)	152 (99%)	2 (1%)	61	75
2	I	206/352 (58%)	203 (98%)	3 (2%)	57	73
3	J	5/374 (1%)	4 (80%)	1 (20%)	1	6
4	M	343/364 (94%)	339 (99%)	4 (1%)	63	76
All	All	708/1940 (36%)	698 (99%)	10 (1%)	57	74

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	51	LEU
1	C	107	THR
2	I	359	LYS
2	I	377	VAL
2	I	394	GLN
3	J	3	GLU
4	M	45	VAL
4	M	175	ILE
4	M	295	VAL
4	M	383	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	129	ASN
1	C	132	HIS
1	C	214	HIS
4	M	128	GLN
4	M	170	ASN
4	M	192	ASN
4	M	214	HIS
4	M	281	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is 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	$\# Z > 2$
5	ATP	I	501	-	32,33,33	0.28	0	48,52,52	0.37	0

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
5	ATP	I	501	-	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

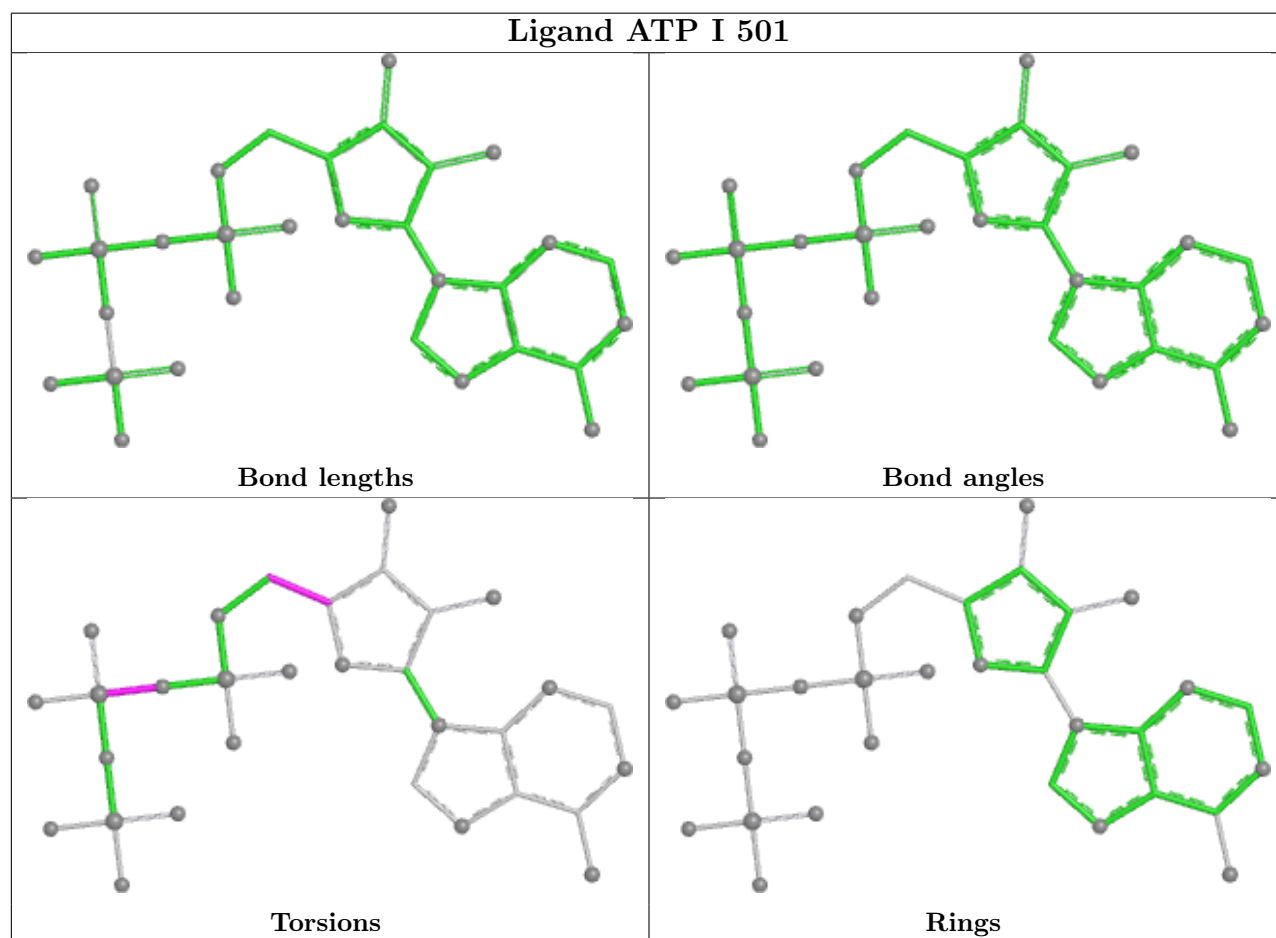
Mol	Chain	Res	Type	Atoms
5	I	501	ATP	O4'-C4'-C5'-O5'
5	I	501	ATP	C3'-C4'-C5'-O5'
5	I	501	ATP	PA-O3A-PB-O1B
5	I	501	ATP	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	501	ATP	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

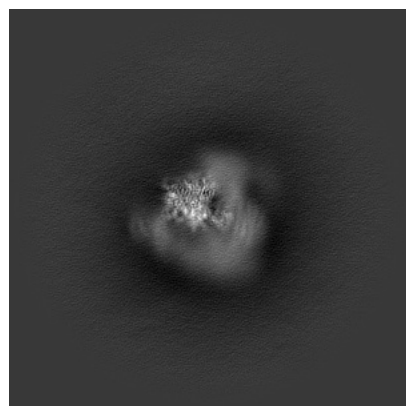
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-77307. These allow visual inspection of the internal detail of the map and identification of artifacts.

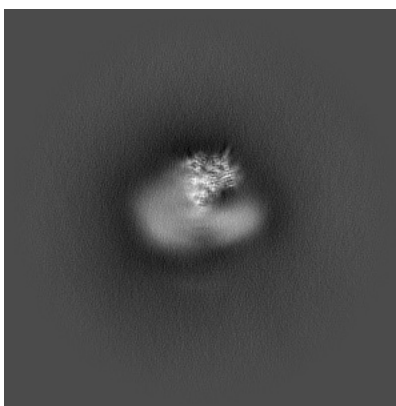
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

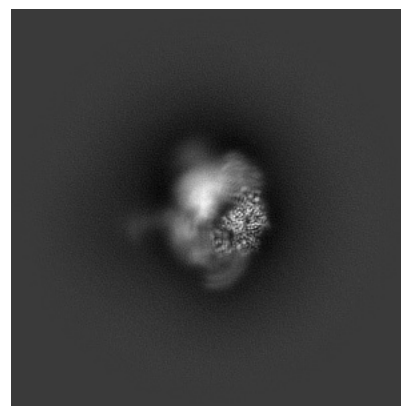
6.1.1 Primary map



X

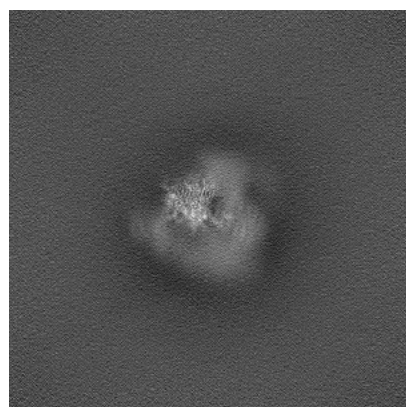


Y

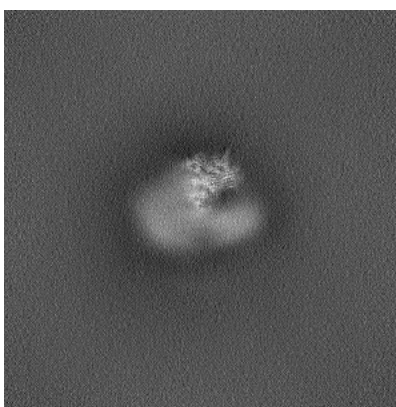


Z

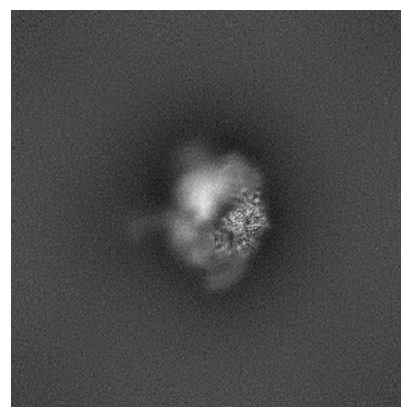
6.1.2 Raw map



X



Y

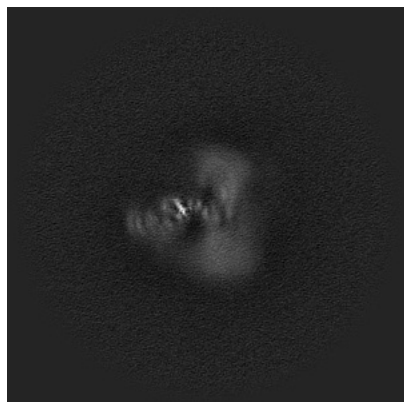


Z

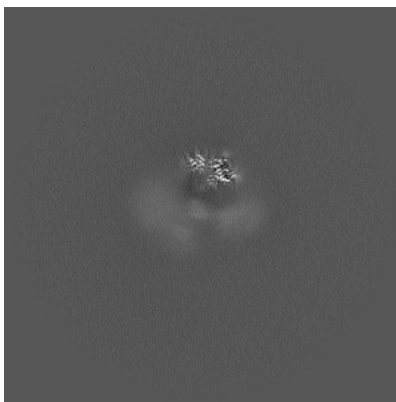
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

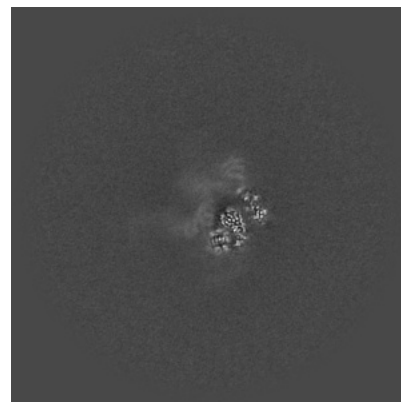
6.2.1 Primary map



X Index: 256

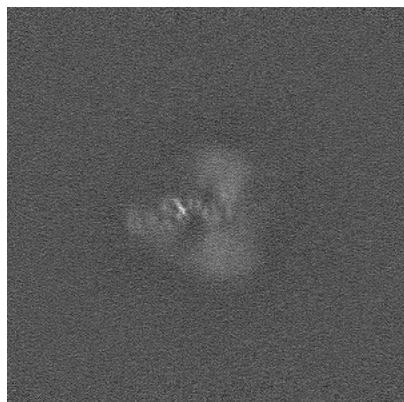


Y Index: 256



Z Index: 256

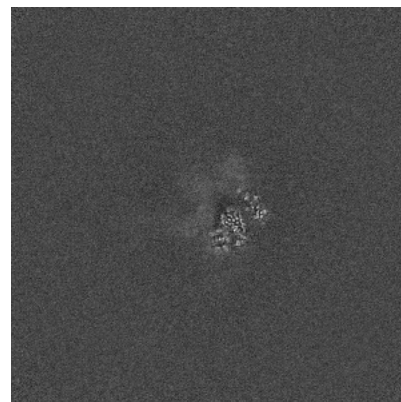
6.2.2 Raw map



X Index: 256



Y Index: 256

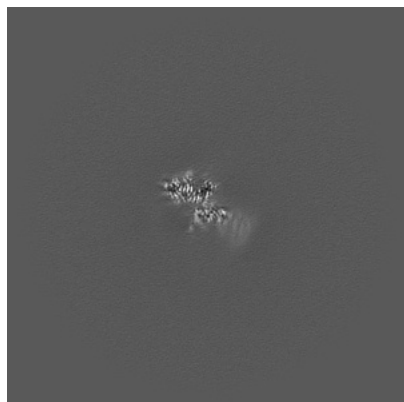


Z Index: 256

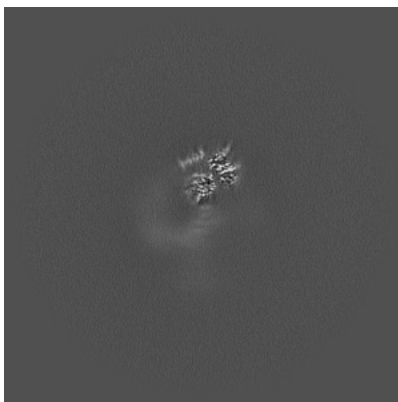
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 308

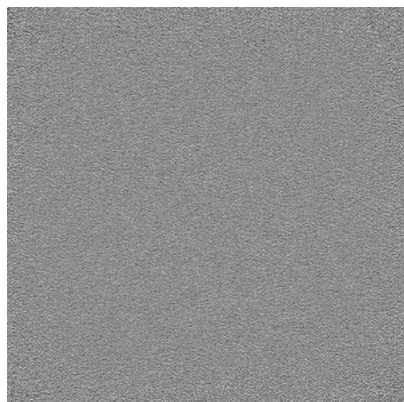


Y Index: 235

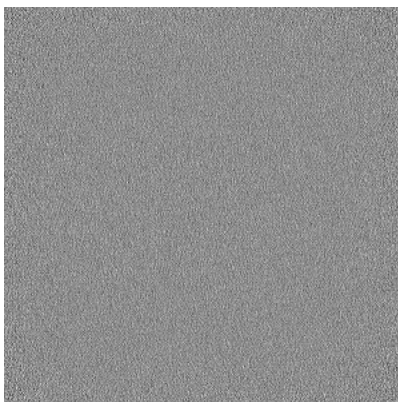


Z Index: 283

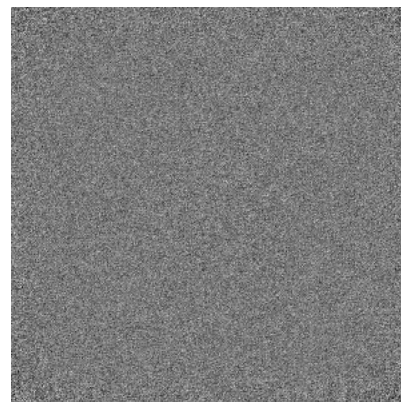
6.3.2 Raw map



X Index: 0



Y Index: 0

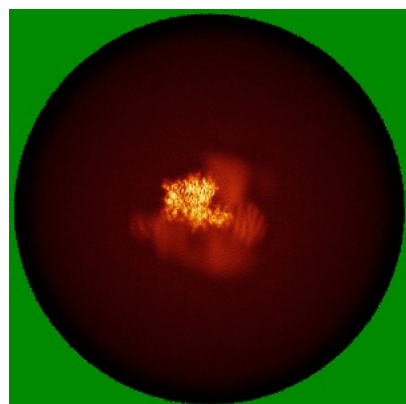


Z Index: 511

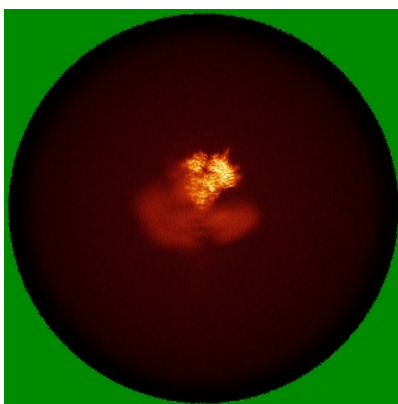
The images above show the largest variance slices of the map in three orthogonal directions.

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

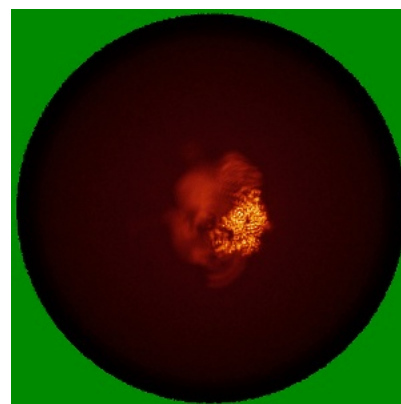
6.4.1 Primary map



X

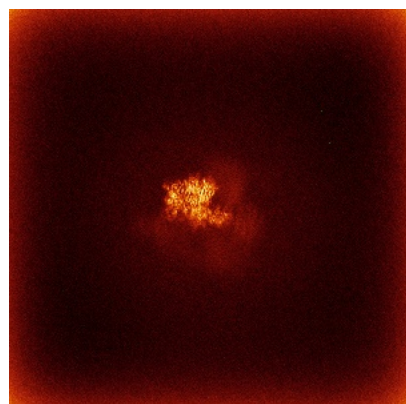


Y

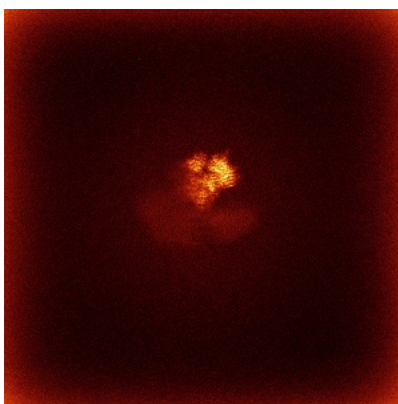


Z

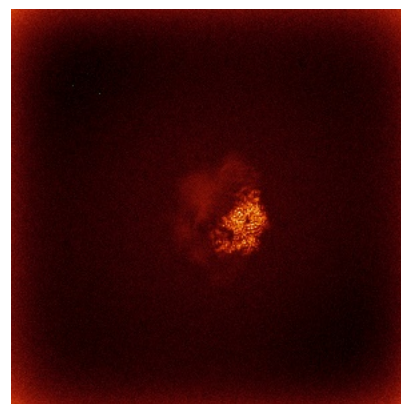
6.4.2 Raw map



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.

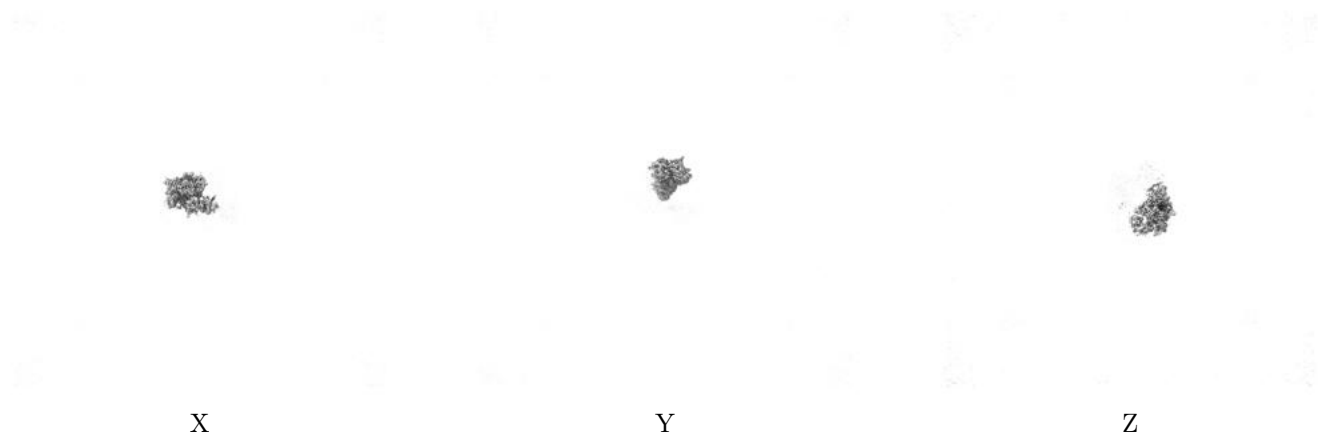
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

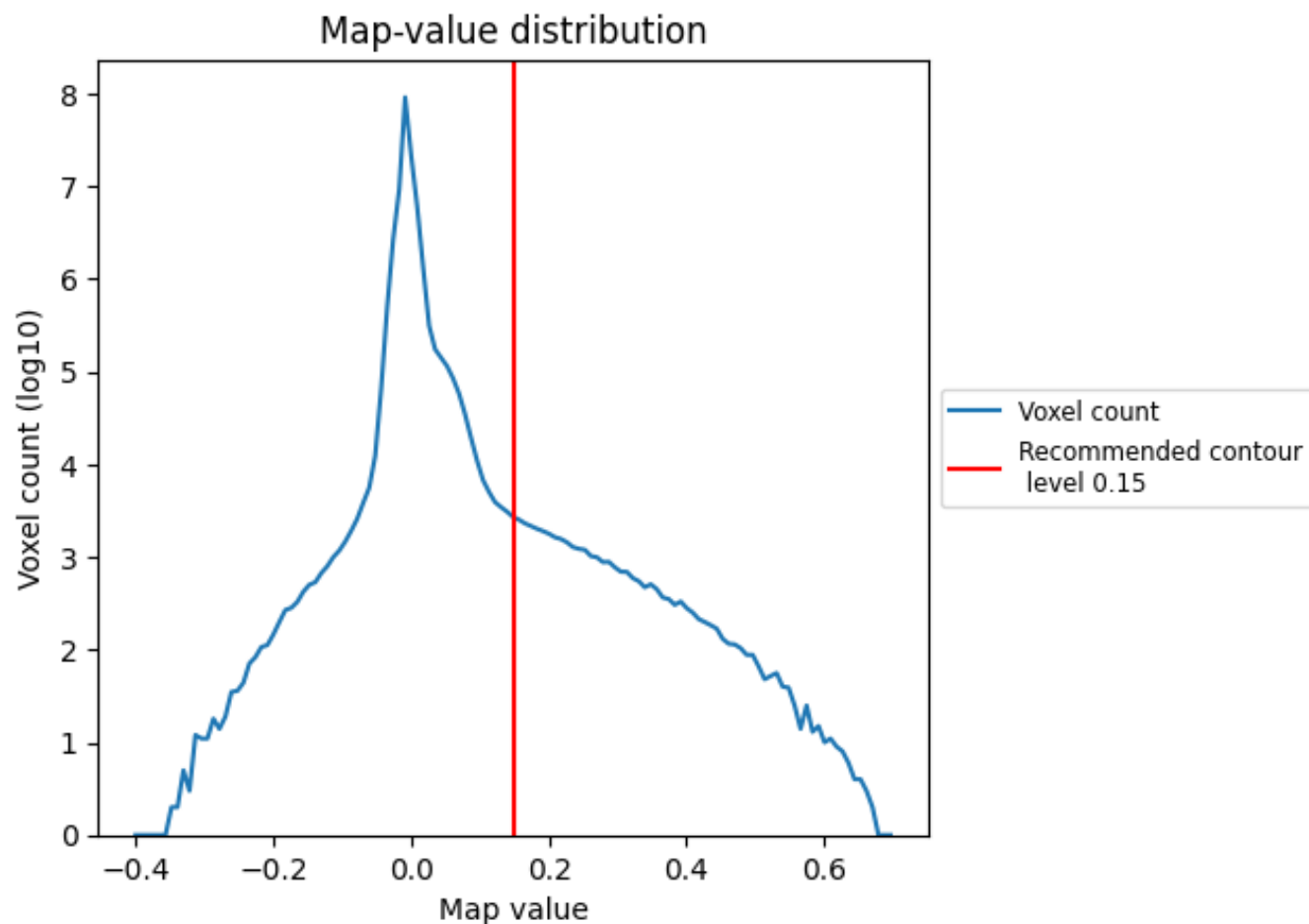
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

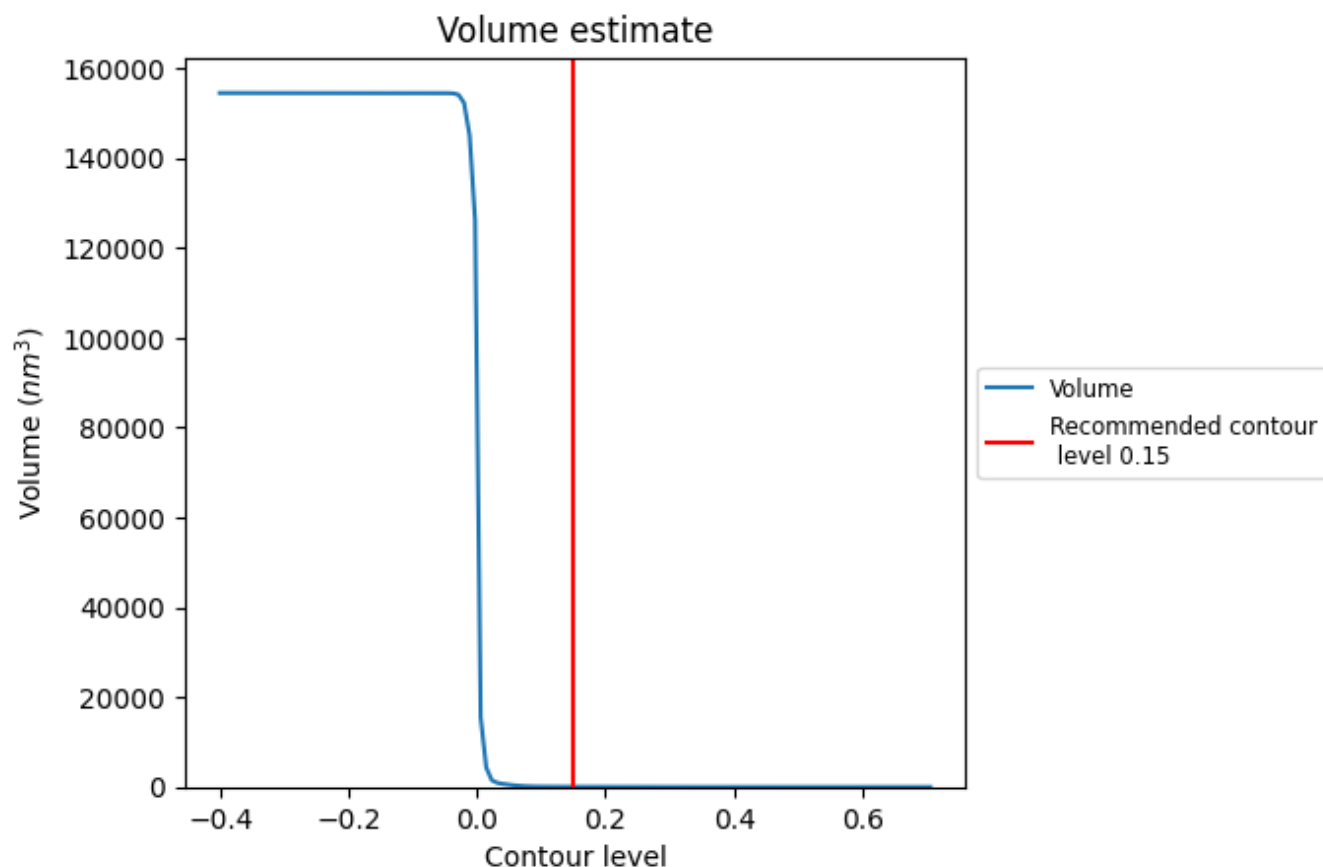
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

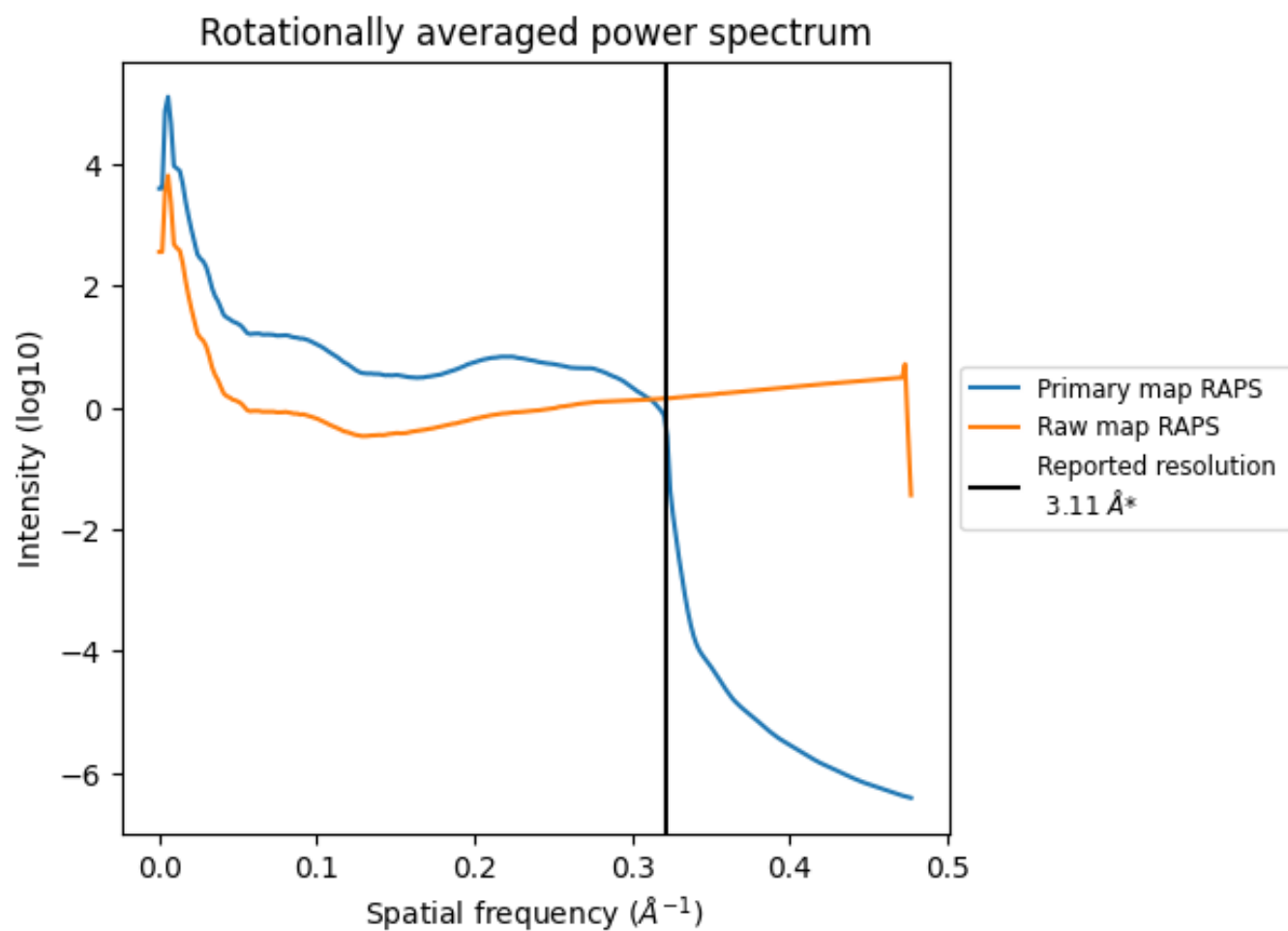
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41 nm^3 ; this corresponds to an approximate mass of 37 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 ⓘ

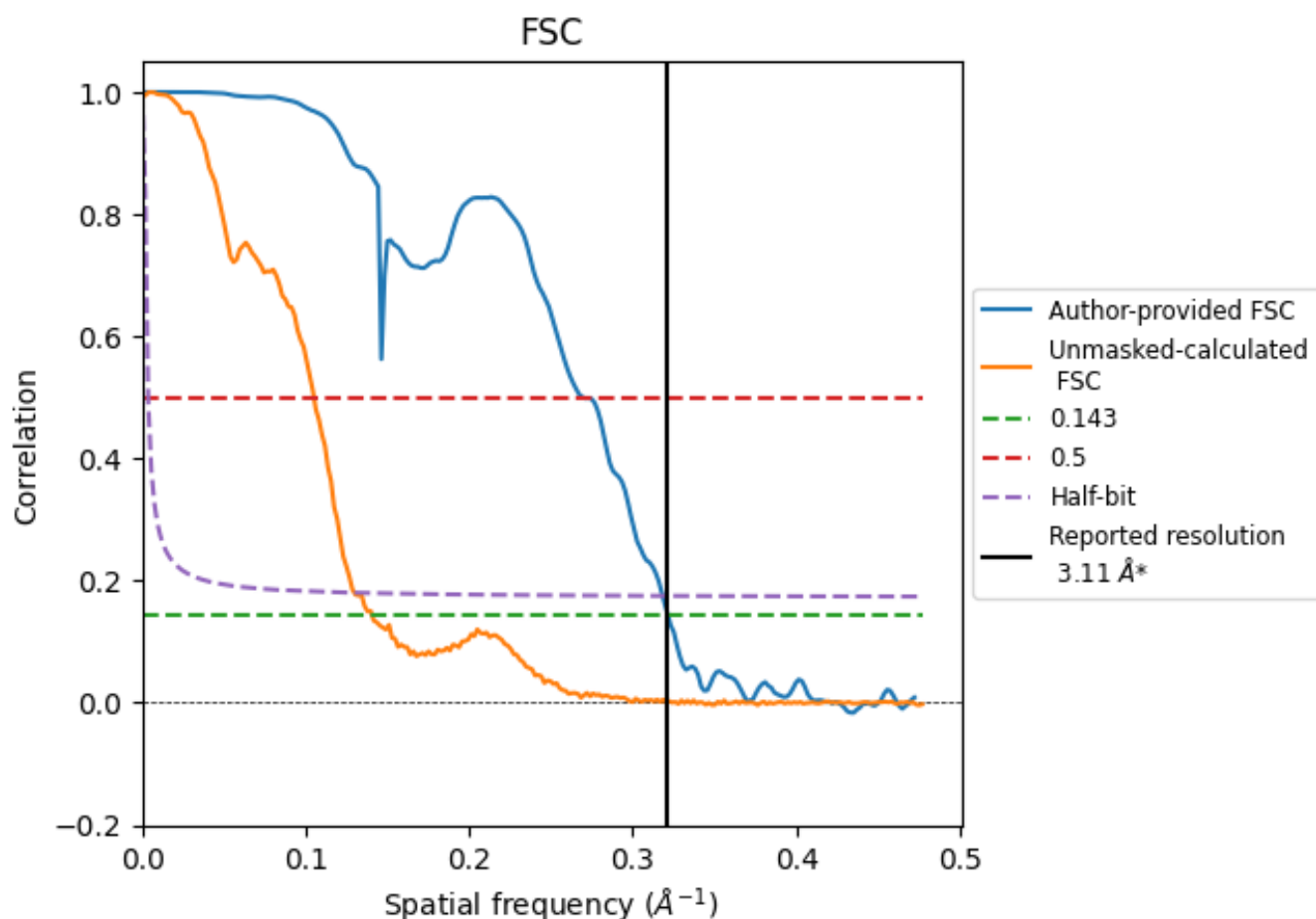


*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.322 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

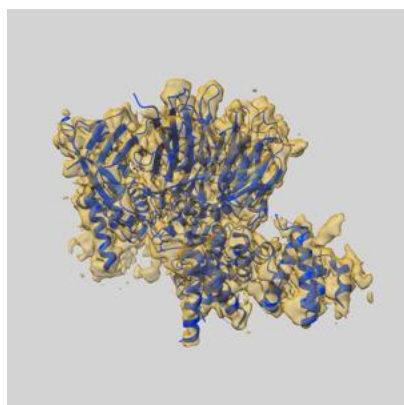
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.11	-	-
Author-provided FSC curve	3.11	3.71	3.14
Unmasked-calculated*	7.11	9.52	7.70

*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 7.11 differs from the reported value 3.11 by more than 10 %

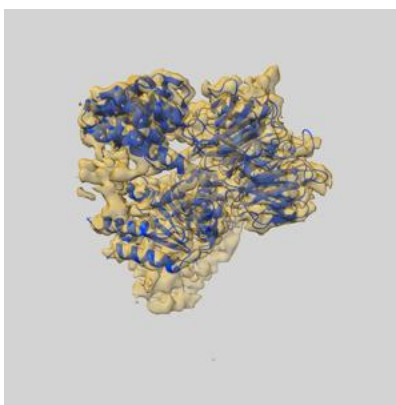
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-77307 and PDB model 35ZV. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

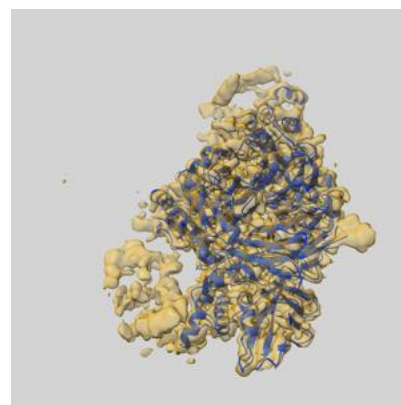
9.1 Map-model overlay [i](#)



X



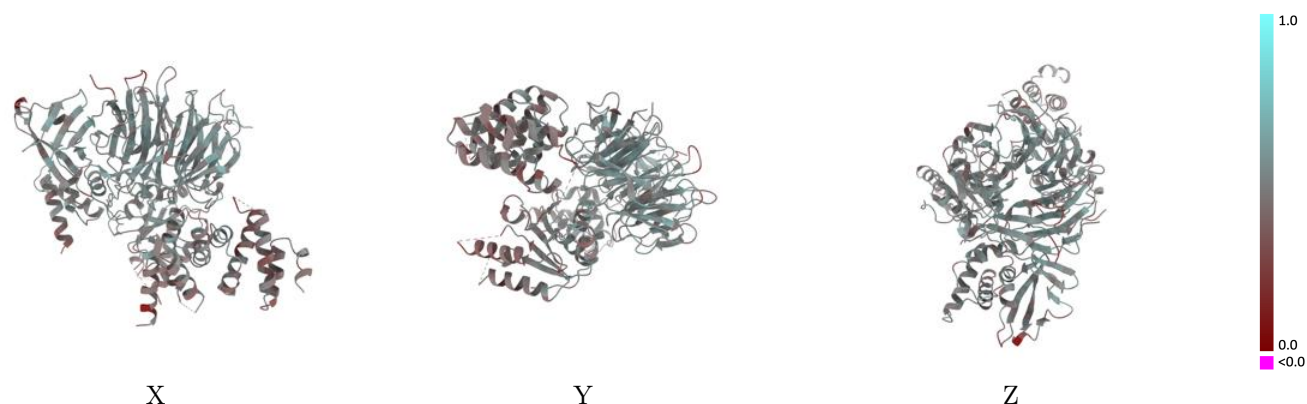
Y



Z

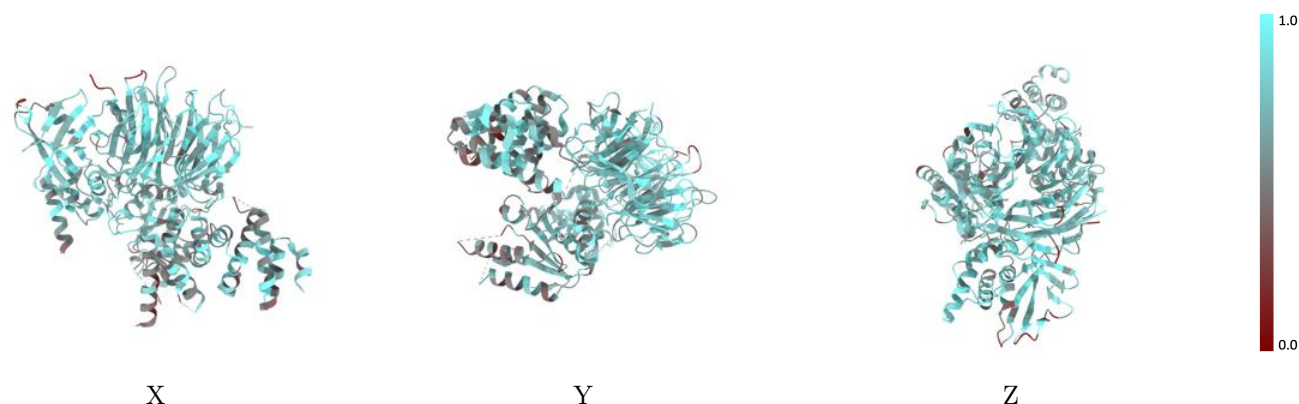
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



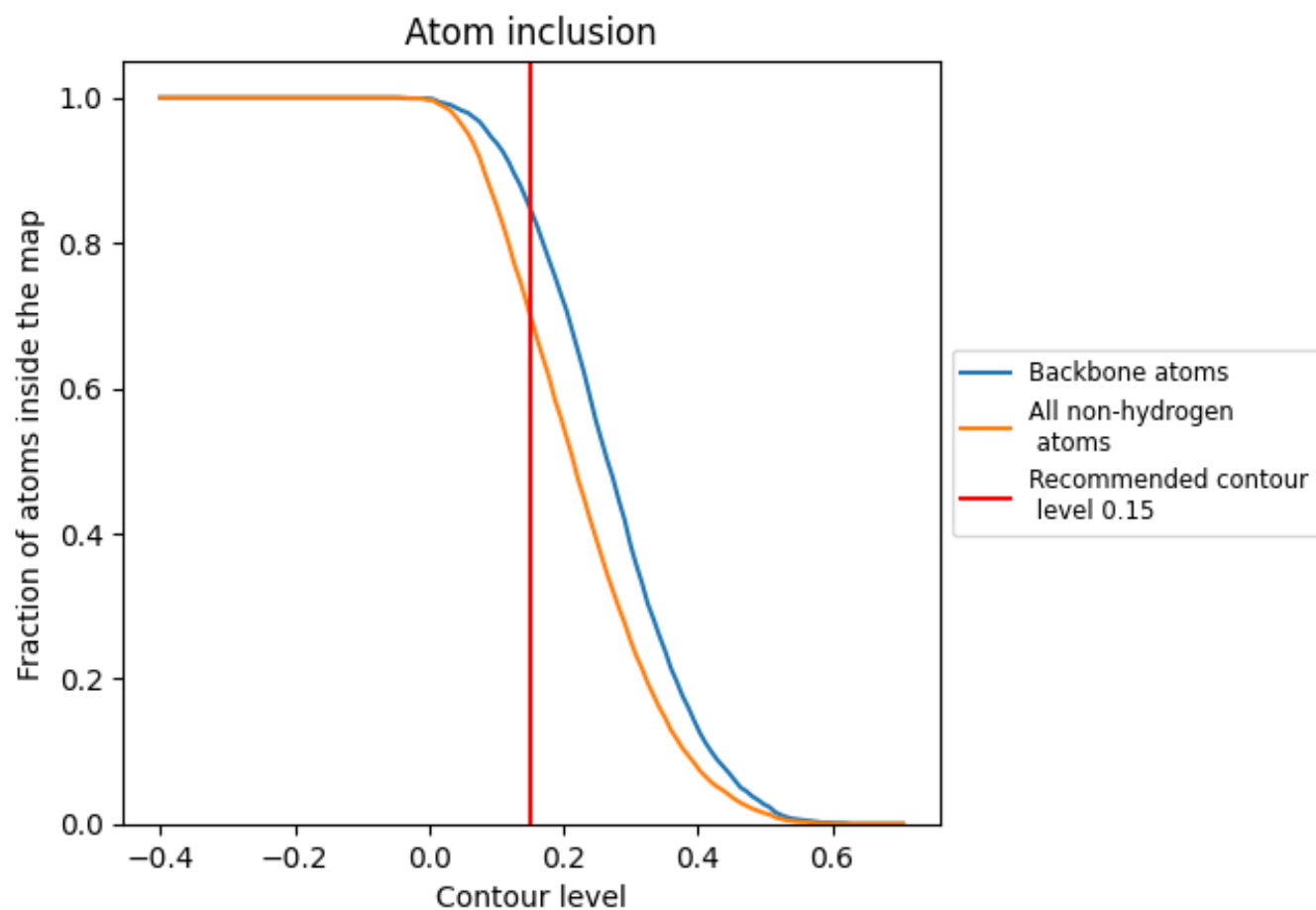
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 70% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7010	0.4760
C	0.6380	0.4400
I	0.6850	0.4590
J	0.7390	0.4680
M	0.7380	0.5030

