



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 12:21 pm GMT

PDB ID : 6ROW
EMDB ID : EMD-4975
Title : Haemonchus galactose containing glycoprotein complex
Authors : Scarff, C.A.; Thompson, R.F.; Newlands, G.F.J.; Jamson, H.; Kennaway, C.; da Silva, V.J.; Rabelo, E.M.; Song, C.F.; Trinick, J.; Smith, W.D.; Muench, S.P.
Deposited on : 2019-05-13
Resolution : 4.50 Å(reported)

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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.dev113
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

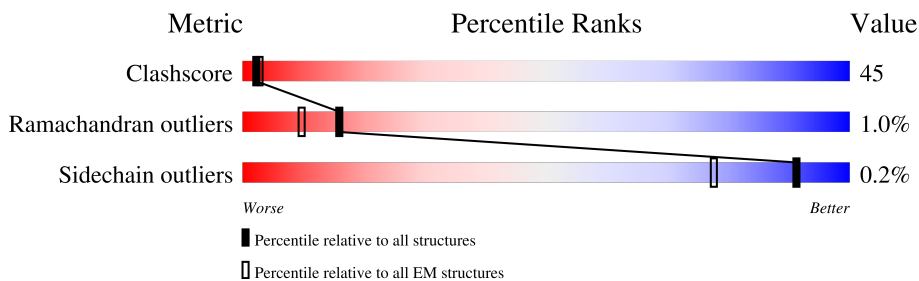
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	755	
1	B	755	
1	C	755	
1	D	755	
2	E	369	
2	F	369	
3	G	253	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 43049 atoms, of which 20156 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 Putative zinc metallopeptidase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	596	9475	3063	4638	824	919	31	0	0
1	B	619	9828	3187	4817	845	946	33	0	0
1	C	583	9290	3010	4556	801	893	30	0	0
1	D	566	8988	2910	4413	777	860	28	0	0

- Molecule 2 is a protein called Parasite pepsinogen.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
2	E	299	2133	860	676	299	298	0	0
2	F	293	2093	844	664	293	292	0	0

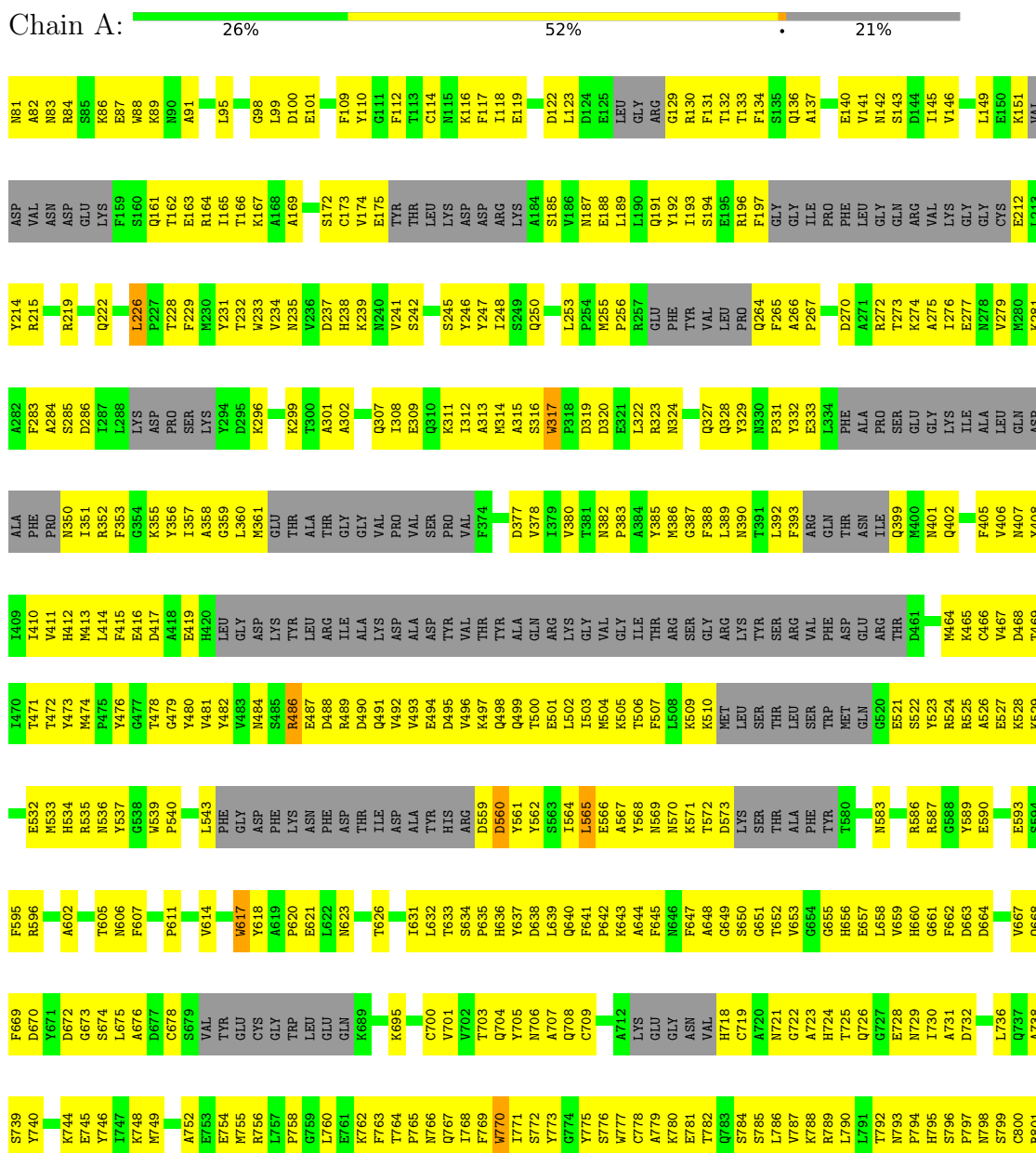
- Molecule 3 is a protein called Cysteine Protease.

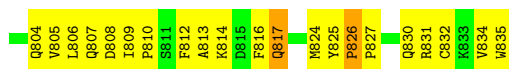
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	H	N	O		
3	G	173	1242	504	392	173	173	0	0

3 Residue-property plots

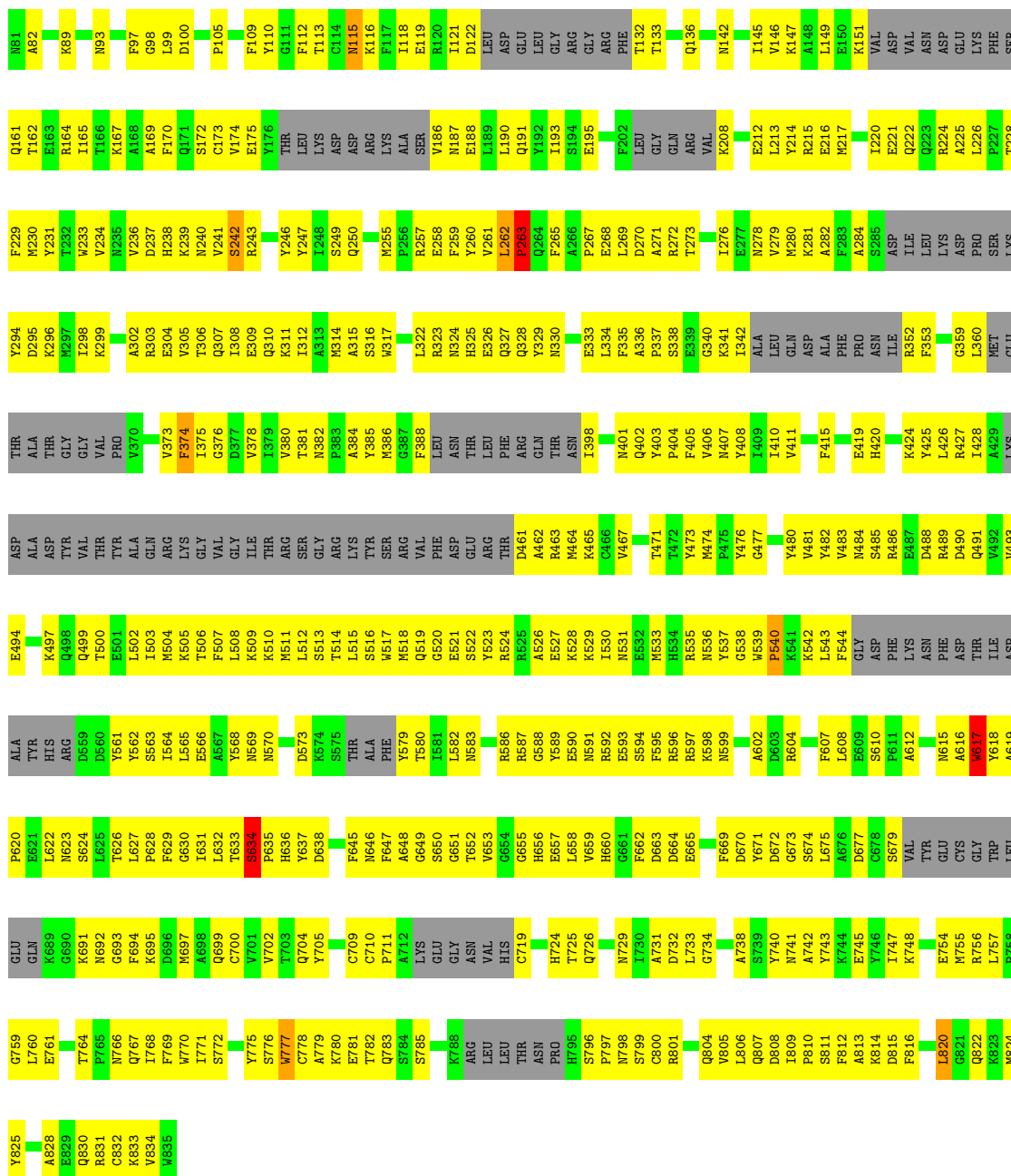
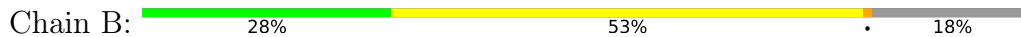
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Putative zinc metallopeptidase

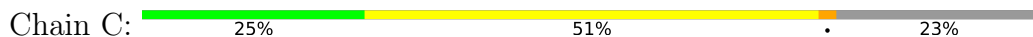




● Molecule 1: Putative zinc metallopeptidase

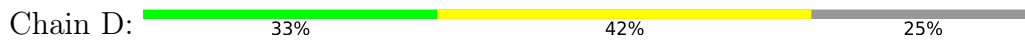


● Molecule 1: Putative zinc metallopeptidase



N81	VAL	ASN	ASP	S85	GLU	K86	LYS	E87	PHE	K89	S160	Q161	T162	E163	N93	A92	T94	L95	L96	F97	A168	G98	F170	D100	E101	S102	V103	D104	P105	C106	E107	D108	F109	D180	D181	G111	G114	N115	S185	A186	N187	E188	L189	ASP	GLU	LEU	LEU	GLY	ARG	ARG	GLY	ARG	F197	F131	T132	G198	G199	T200	F134	A137	Q138	S143	D144	I145	V146	L149	E150	K151	VAL	ASP																																																																																																																																																																																																																																																																																														
E216	M217	G218	R219	L220	E221	Q222	Q223	R224	A225	L226	L226	P227	T228	T228	F229	M230	Y231	K299	T232	W233	V234	M235	V236	D237	H238	K239	N240	V241	S242	R243	N244	S245	Y246	Y247	I248	S249	Q250	P251	L253	F254	M255	P256	R257	E258	F259	Y260	V261	L262	P263	Q264	F265	A266	P267	E268	L269	D270	A271	R272	T273	K274	R215																																																																																																																																																																																																																																																																																																							
E277	M280	A284	K289	ASP	PRD	F353	G354	K355	Y356	D395	K296	M297	I298	K299	T300	A301	A302	E304	V305	H238	T306	Q307	L308	E309	Q310	K311	I312	A313	M314	A315	S316	W317	P318	S316	D319	L322	R323	N324	H325	E326	Q327	Q328	Y329	N330	P331	Y332	L333	L334	F335	A336	P337	G340	LYS	ILE	ALA	LEU	V467																																																																																																																																																																																																																																																																																																											
N407	Y408	I409	V411	H412	M413	L414	F415	G416	D417	A418	GLU	HIS	LEU	LEU	ASP	ASP	LYS	TYR	ALA	THR	GLY	ARG	ILE	ALA	VAL	LYS	ASP	ALA	ASP	Q310	T312	G376	D377	V378	I379	V380	N382	P383	A384	Y385	N386	G387	F388	LEU	ASN	THR	LEU	TYR	SER	ARG	VAL	ILE	THR	ARG	SER	GLY	ASP	ASN	GLN	TYR	PRO	PHE	VAL	V467																																																																																																																																																																																																																																																																																																				
I470	T471	T472	Y473	M474	P475	Y476	G477	K478	C479	Y480	V481	Y482	M484	S485	R486	E487	R488	V493	E494	D495	V496	K497	Q498	Q499	T500	E501	L502	L503	M504	T506	K510	M511	L512	S513	T514	L515	S516	M517	M518	Q519	S520	E521	E522	Y523	R524	R525	S526	E527	C528	K529	L530	M531	E532	M533	H534	R535	L536	E537	L538	H539	H540	H541	H542	H543	H544	H545	H546	H547	H548	H549	H550	H551	H552	H553	H554	H555	H556	H557	H558	H559	H560	H561	H562	H563	H564	H565	H566	H567	H568	H569	H570	H571	H572	H573	H574	H575	H576	H577	H578	H579	H580	H581	H582	H583	H584	H585	H586	H587	H588	H589	H590	H591	H592	H593	H594	H595	H596	H597	H598	H599	H600	H601	H602	H603	H604	H605	H606	H607	H608	H609	H610	H611	H612	H613	H614	H615	H616	H617	H618	H619	H620	H621	H622	H623	H624	H625	H626	H627	H628	H629	H630	H631	H632	H633	H634	H635	H636	H637	H638	H639	H640	H641	H642	H643	H644	H645	H646	H647	H648	H649	H650	H651	H652	H653	H654	H655	H656	H657	H658	H659	H660	H661	H662	H663	H664	H665	H666	H667	H668	H669	H670	H671	H672	H673	H674	H675	H676	H677	H678	H679	H680	H681	H682	H683	H684	H685	H686	H687	H688	H689	H690	H691	H692	H693	H694	H695	H696	H697	H698	H699	H700	H701	H702	H703	H704	H705	H706	H707	H708	H709	H710	H711	H712	H713	H714	H715	H716	H717	H718	H719	H720	H721	H722	H723	H724	H725	H726	H727	H728	H729	H730	H731	H732	H733	H734	H735	H736	H737	H738	H739	H740	H741	H742	H743	H744	H745	H746	H747	H748	H749	H750	H751	H752	H753	H754	H755	H756	H757	H758	H759	H760	H761	H762	H763	H764	H765	H766	H767	H768	H769	H770	H771	H772	H773	H774	H775	H776	H777	H778	H779	H780	H781	H782	H783	H784	H785	H786	H787	H788	H789	H790	H791	H792	H793	H794	H795	H796	H797	H798	H799	H800	H801	H802	H803	H804	H805	H806	H807	H808	H809	H810	H811	H812	H813	H814	H815	H816	H817	H818	H819	H820	H821	H822	H823	H824	H825	H826	H827	H828	H829	H830	H831	H832	H833	H834	H835
M533	H534	R535	N536	R537	G538	M539	F540	K541	L542	L543	F544	G545	ASP	PHE	LYS	ASN	PHE	ASP	THR	ILE	ASP	ALA	ALA	TYR	HIS	ARG	D569	Y562	S563	I564	L565	E566	A567	Y568	N569	N570	K571	T572	D573	K574	S575	THR	ALA	PHE	Y579	T580	L581	L582	M583	L584	L585	R586	R587	C588	Y589	K590	E591	D592	M593	E593																																																																																																																																																																																																																																																																																																								
S594	F595	R596	R597	K598	N599	E600	F607	L608	E609	S610	F611	A612	V613	V614	W617	V618	A619	P620	E621	L622	ALA	ALA	GLN	K689	S690	K691	F694	R695	D696	M697	A698	Q699	Y705	N706	A707	Q708	C710	G711	H718	ASP	VAL	M646	F647	A648	T652	E657	L658	V659	H660	C588	G661	F662	D663	D664	D665	E665																																																																																																																																																																																																																																																																																																												
G666	V667	Q668	F669	ASP	TYR	ASP	GLY	SER	LEU	ALA	ASP	CYS	SER	VAL	LYS	TYR	GLU	GLY	TRP	LEU	LEU	K689	S690	K691	F694	R695	D696	M697	A698	Q699	Y705	N706	A707	Q708	C710	G711	H718	ASP	VAL	M646	F647	A648	T652	E657	L658	V659	H660	C588	G661	F662	D663	D664	D665	E665																																																																																																																																																																																																																																																																																																														
L733	L736	Q737	A738	S739	Y740	H741	L742	L743	K744	E745	Y746	L747	LYS	MET	LYS	CYS	GLY	ALA	GLU	E754	M755	R756	L757	P758	G759	L760	E761	K762	F763	T764	F765	N766	Q767	F769	W770	I771	G774	Y775	S776	W777	C778	A779	T782	Q783	S784	L786	L790	H724	T725	T792	N793	F794	H795	I730																																																																																																																																																																																																																																																																																																														
N798	S799	C800	R801	W802	N803	O804	W805	L806	A807	D808	L809	P810	S811	F812	A813	K814	S815	R816	Q817	C818	L820	E821	O822	K823	H824	Y825	PRO	PRO	ALA	ALA	GLU	GLN	ARG	C832	H834	H835	G774	Y775	S776	W777	C778	A779	T782	Q783	S784	L786	L790	H724	T725	T792	N793	F794	H795	I730																																																																																																																																																																																																																																																																																																														

● Molecule 1: Putative zinc metallopeptidase



W81	A82	N83	R84	S85	W88	F97	L806	G98	L99	D100	E101	F109	F112	T113	C114	M115	K116	I117	I118	E119	R120	I121	D122	L123	ASP	GLU	LEU	L123	GLN	TYR	D696	L269	D270	A271	R272	G219	T132	T133	F134	S135	Q136	A137	Q138	L139	E140	V141	S142	S143	D144	I145	V146	K147	L149	V154	ASN	ASP	G218	R219	I220	E221	Q222	Q223					
S160	Q161	T162	R163	R164	S165	T166	K167	Q171	V174	E175	THR	THR	LEU	LYS	ASP	ASP	ARG	LYS	ALA	SER	VAL	ASN	GLU	LEU	LEU	L226	L262	Q264	P267	E268	L269	D270	A271	R272	PHE	GLY	ILE	PRO	PHE	GLY	LEU	GLN	ARG	VAL	LYS	GLY	LYS	CYS	GLU	LEU	VAL	LYS	S143	D144	I145	V146	K147	L149	V154	ASN	ASP	G218	R219	I220	E221	Q222	Q223
R224	A225	L226	P227	T228	F229	M230	T231	T232	V236	D237	H238	V241	Y246	Y247	Q250	E258	V261	L262	P263	Q264	P267	E268	L269	D270	A271	R272	T273	I276	E277	R278	V279	M280	F283	A284	SER	ASP	ILE	LEU	LYS	ASP	PRO	SER	LYS	TYR	D295	K296	M297	I298	K299	T300																	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110863	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 ($e^-/\text{\AA}^2$)	62.5	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.303	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	387.66003, 387.66003, 387.66003	wwPDB
Map dimensions	364, 364, 364	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	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	A	0.91	3/4938 (0.1%)	0.76	4/6653 (0.1%)
1	B	0.88	7/5122 (0.1%)	0.77	3/6903 (0.0%)
1	C	0.82	5/4835 (0.1%)	0.73	2/6513 (0.0%)
1	D	0.78	2/4674 (0.0%)	0.71	2/6304 (0.0%)
2	E	0.32	0/1452	0.52	0/2003
2	F	0.39	0/1424	0.56	0/1965
3	G	0.80	0/841	0.91	5/1154 (0.4%)
All	All	0.81	17/23286 (0.1%)	0.73	16/31495 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
1	C	0	6
1	D	0	1
All	All	0	16

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	263	PRO	N-CD	-13.97	1.28	1.47
1	B	540	PRO	N-CD	8.81	1.60	1.47
1	C	816	PHE	CA-CB	-7.78	1.36	1.53
1	B	617	TRP	CB-CG	-7.30	1.37	1.50
1	A	617	TRP	CB-CG	-7.19	1.37	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	LEU	C-N-CD	-8.98	100.84	120.60
1	A	565	LEU	CA-CB-CG	-7.90	97.13	115.30
1	C	253	LEU	CA-CB-CG	-7.60	97.83	115.30
1	B	262	LEU	N-CA-C	7.23	130.52	111.00
1	A	129	GLY	N-CA-C	7.07	130.77	113.10

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	VAL	Peptide
1	A	486	ARG	Peptide
1	A	560	ASP	Peptide
1	A	676	ALA	Peptide
1	A	826	PRO	Peptide

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	A	4837	4638	4636	503	0
1	B	5011	4817	4815	524	0
1	C	4734	4556	4555	455	0
1	D	4575	4413	4413	355	0
2	E	1457	676	676	60	0
2	F	1429	664	663	41	0
3	G	850	392	389	2	0
All	All	22893	20156	20147	1925	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 45.

The worst 5 of 1925 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:PRO:HA	1:B:607:PHE:CZ	1.47	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:HD3	1:A:329:TYR:CE2	1.64	1.33
1:A:234:VAL:HG23	1:A:245:SER:O	1.20	1.29
1:D:760:LEU:HD11	1:D:763:PHE:CE2	1.67	1.29
1:A:474:MET:CE	1:A:586:ARG:HD2	1.64	1.27

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	564/755 (75%)	375 (66%)	188 (33%)	1 (0%)	44	78
1	B	589/755 (78%)	385 (65%)	196 (33%)	8 (1%)	9	40
1	C	551/755 (73%)	364 (66%)	181 (33%)	6 (1%)	12	46
1	D	536/755 (71%)	378 (70%)	153 (28%)	5 (1%)	14	51
2	E	289/369 (78%)	217 (75%)	72 (25%)	0	100	100
2	F	283/369 (77%)	198 (70%)	81 (29%)	4 (1%)	9	40
3	G	155/253 (61%)	121 (78%)	29 (19%)	5 (3%)	3	21
All	All	2967/4011 (74%)	2038 (69%)	900 (30%)	29 (1%)	16	49

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	817	GLN
1	C	820	LEU
2	F	168	PHE
3	G	104	PRO
1	C	107	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	521/655 (80%)	521 (100%)	0	100	100
1	B	538/655 (82%)	536 (100%)	2 (0%)	89	90
1	C	510/655 (78%)	510 (100%)	0	100	100
1	D	492/655 (75%)	490 (100%)	2 (0%)	89	90
All	All	2061/2620 (79%)	2057 (100%)	4 (0%)	91	93

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	617	TRP
1	B	724	HIS
1	D	388	PHE
1	D	607	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	382	ASN
1	C	536	ASN
1	C	795	HIS
1	C	583	ASN
1	A	704	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.

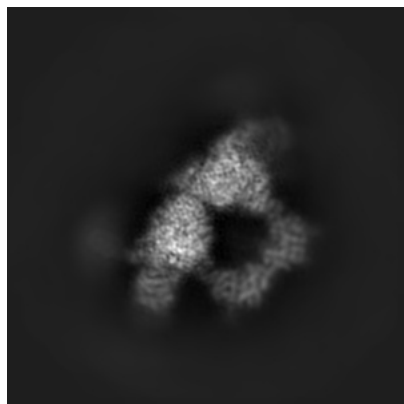
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4975. These allow visual inspection of the internal detail of the map and identification of artifacts.

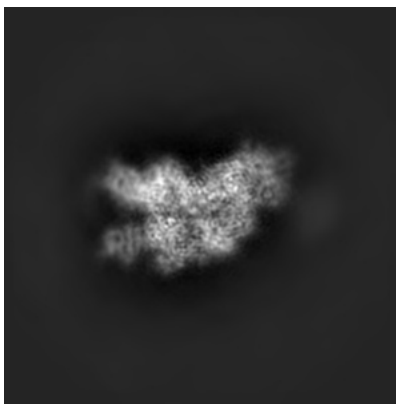
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

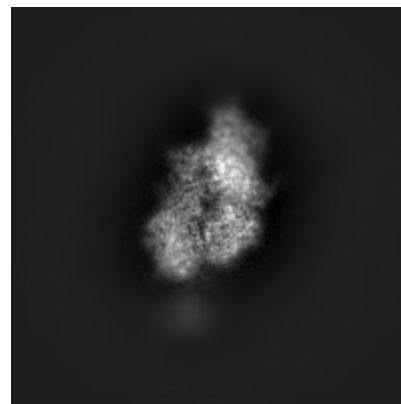
6.1.1 Primary map



X

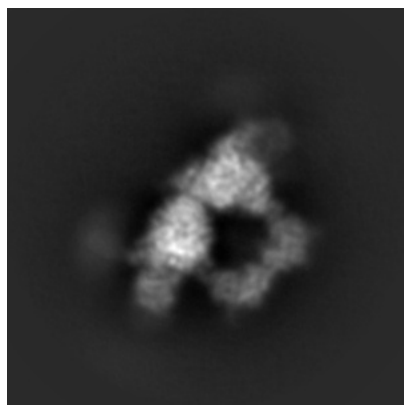


Y

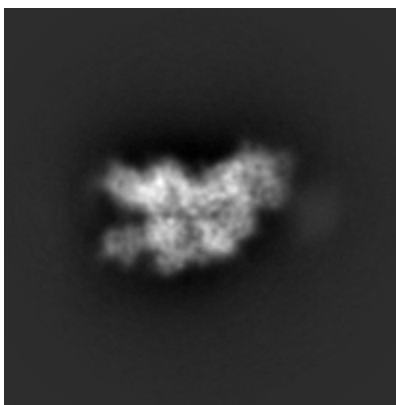


Z

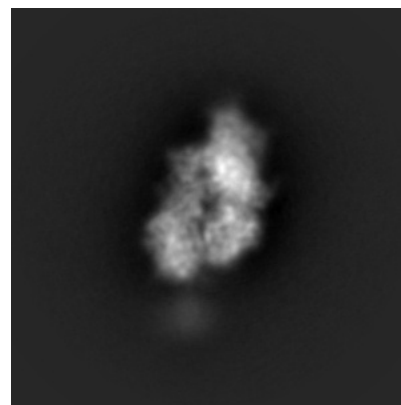
6.1.2 Raw map



X



Y

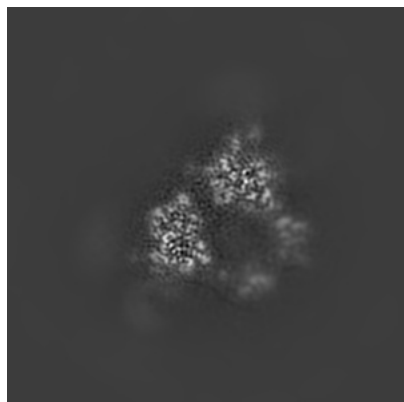


Z

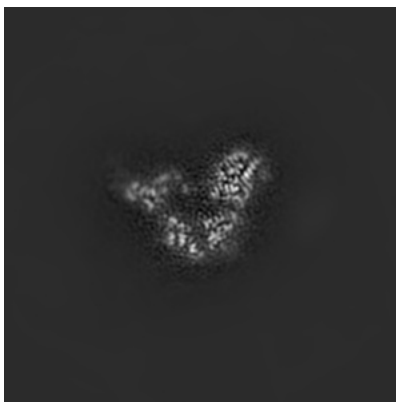
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

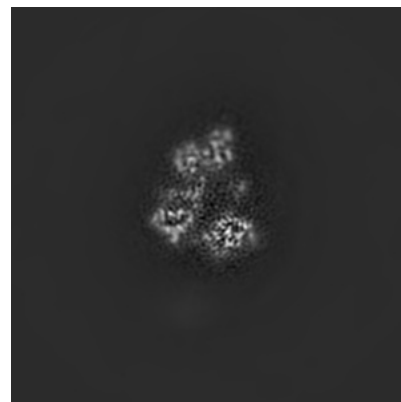
6.2.1 Primary map



X Index: 182

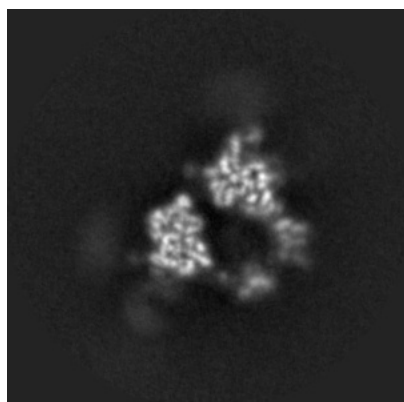


Y Index: 182

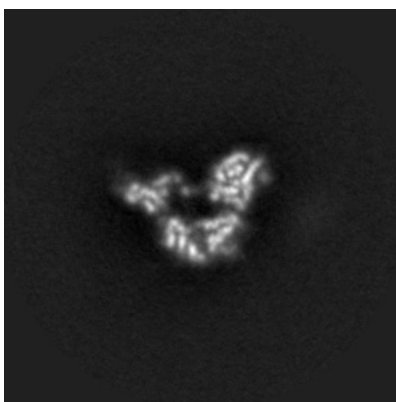


Z Index: 182

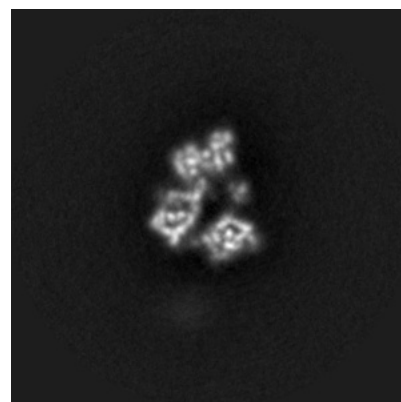
6.2.2 Raw map



X Index: 182



Y Index: 182

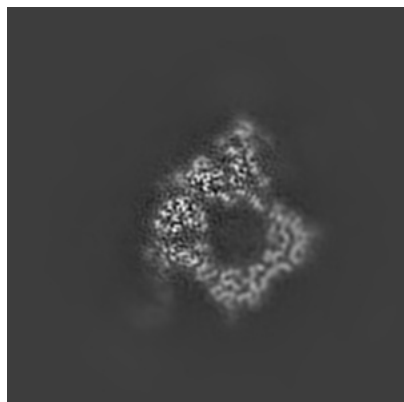


Z Index: 182

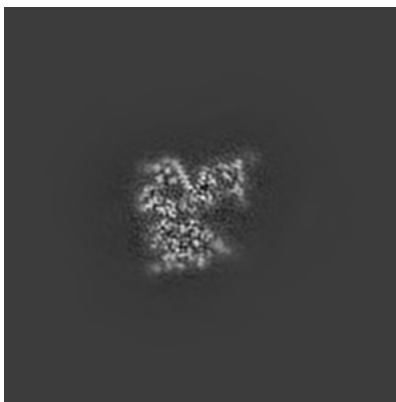
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

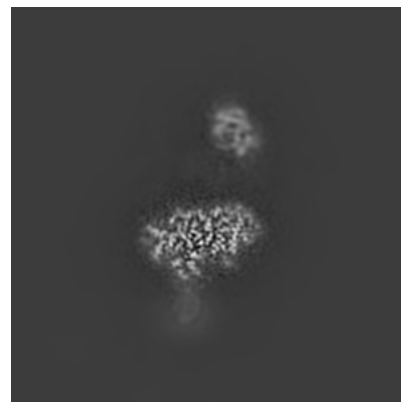
6.3.1 Primary map



X Index: 199

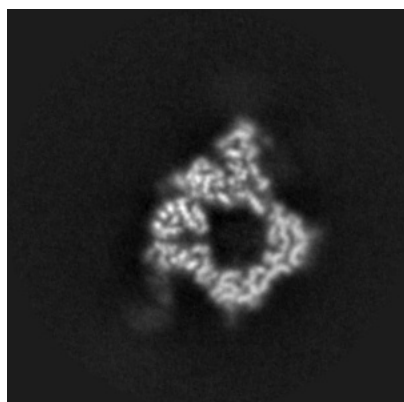


Y Index: 166

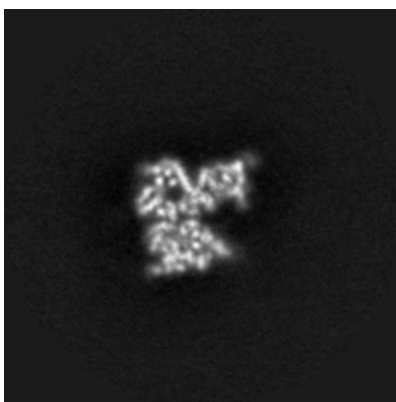


Z Index: 143

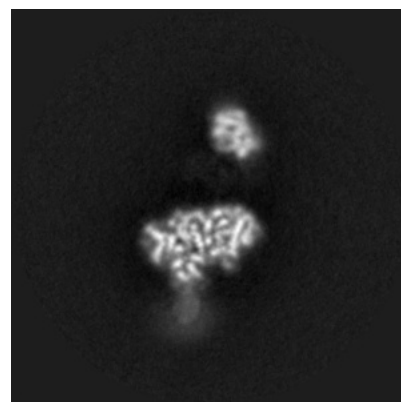
6.3.2 Raw map



X Index: 198



Y Index: 166

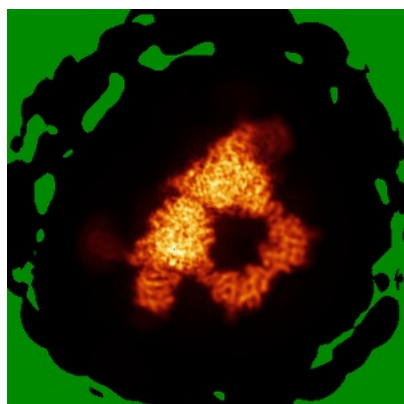


Z Index: 142

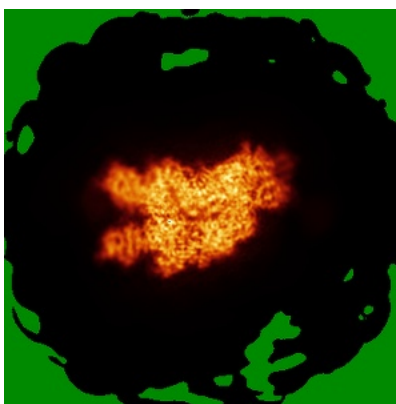
The images above show the largest variance slices of the map in three orthogonal directions.

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

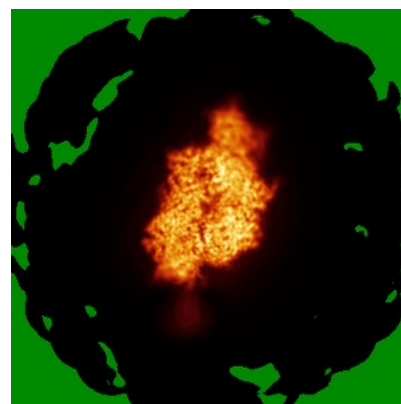
6.4.1 Primary map



X



Y

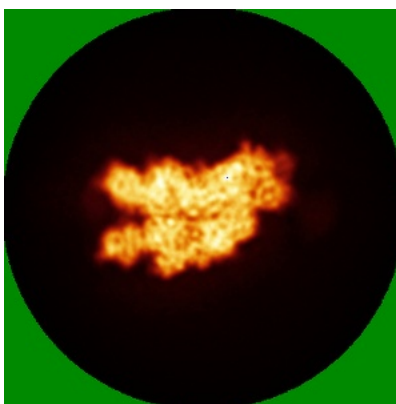


Z

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.

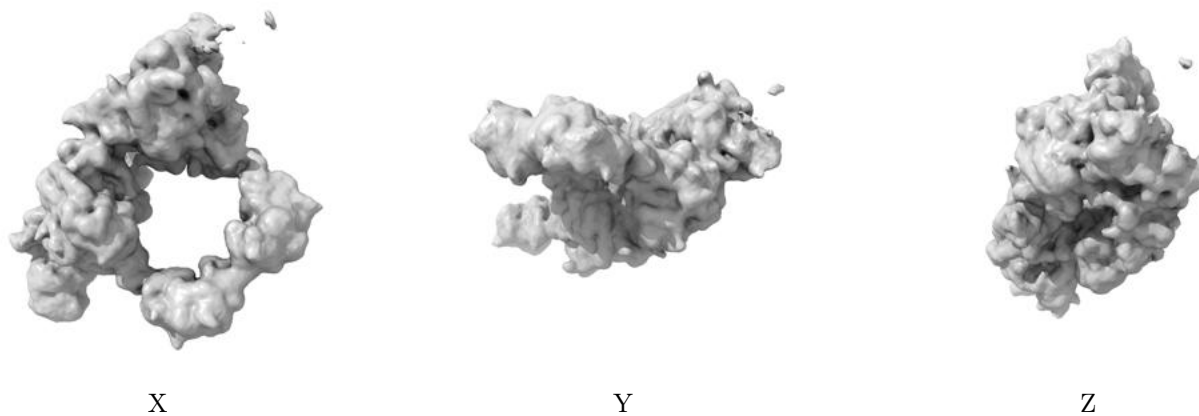
6.5 Orthogonal surface views [i](#)

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.

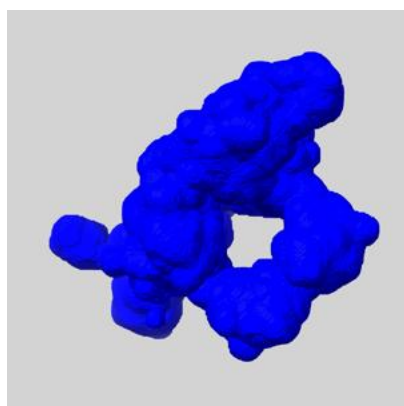
6.6 Mask visualisation [i](#)

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

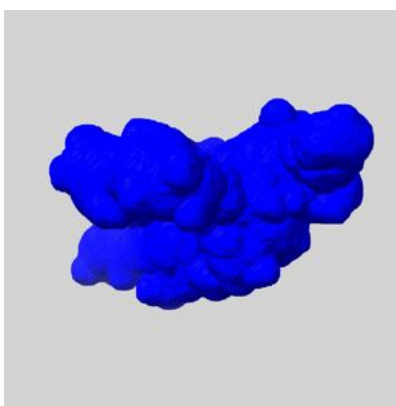
A mask typically either:

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

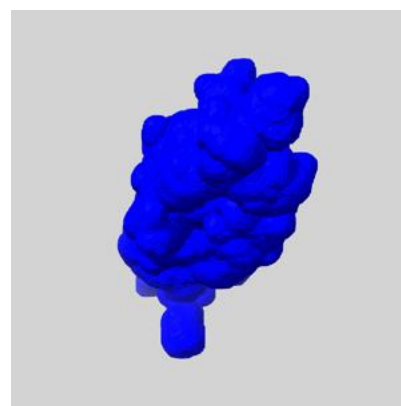
6.6.1 emd_4975_msk_1.map [i](#)



X



Y

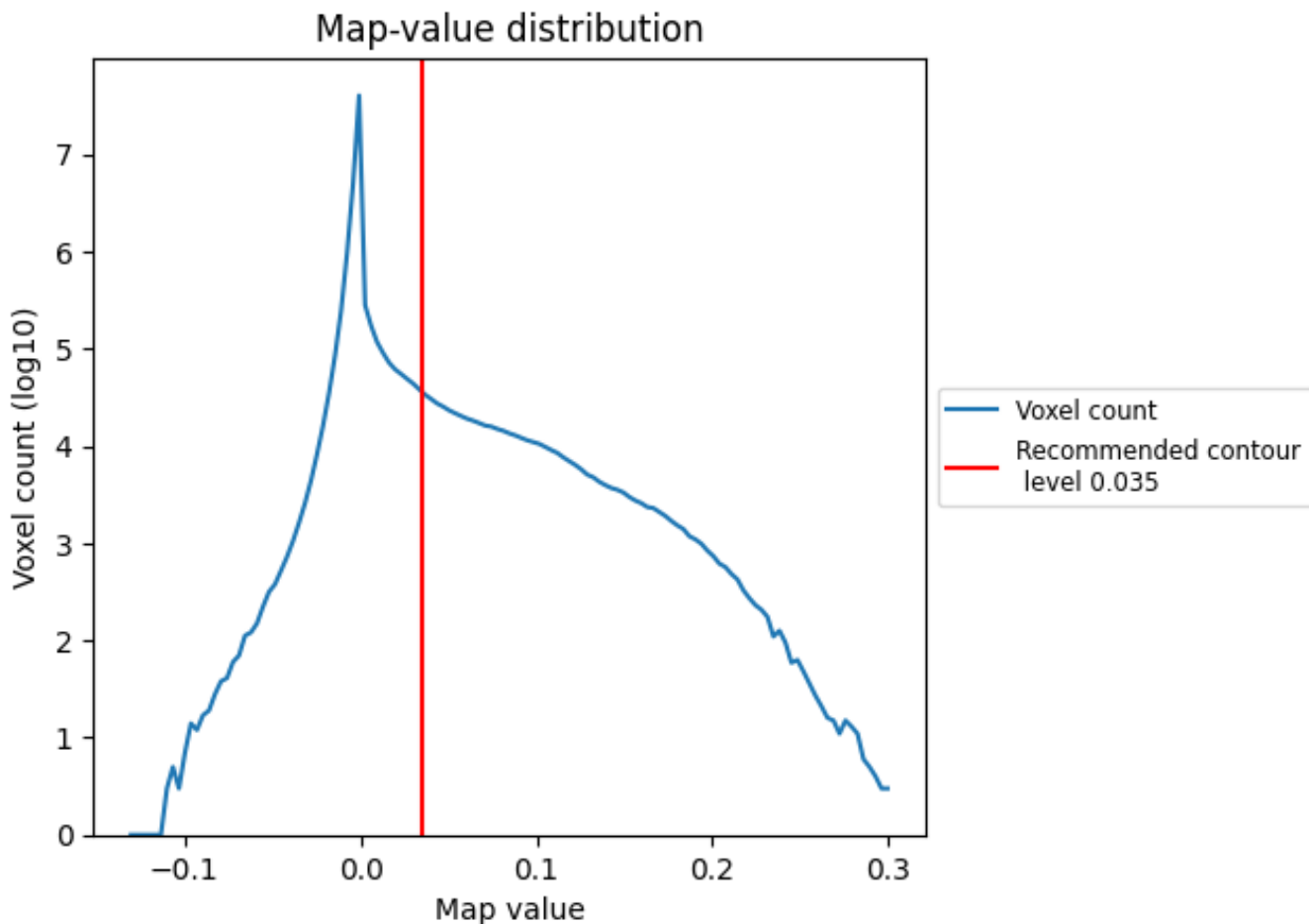


Z

7 Map analysis [i](#)

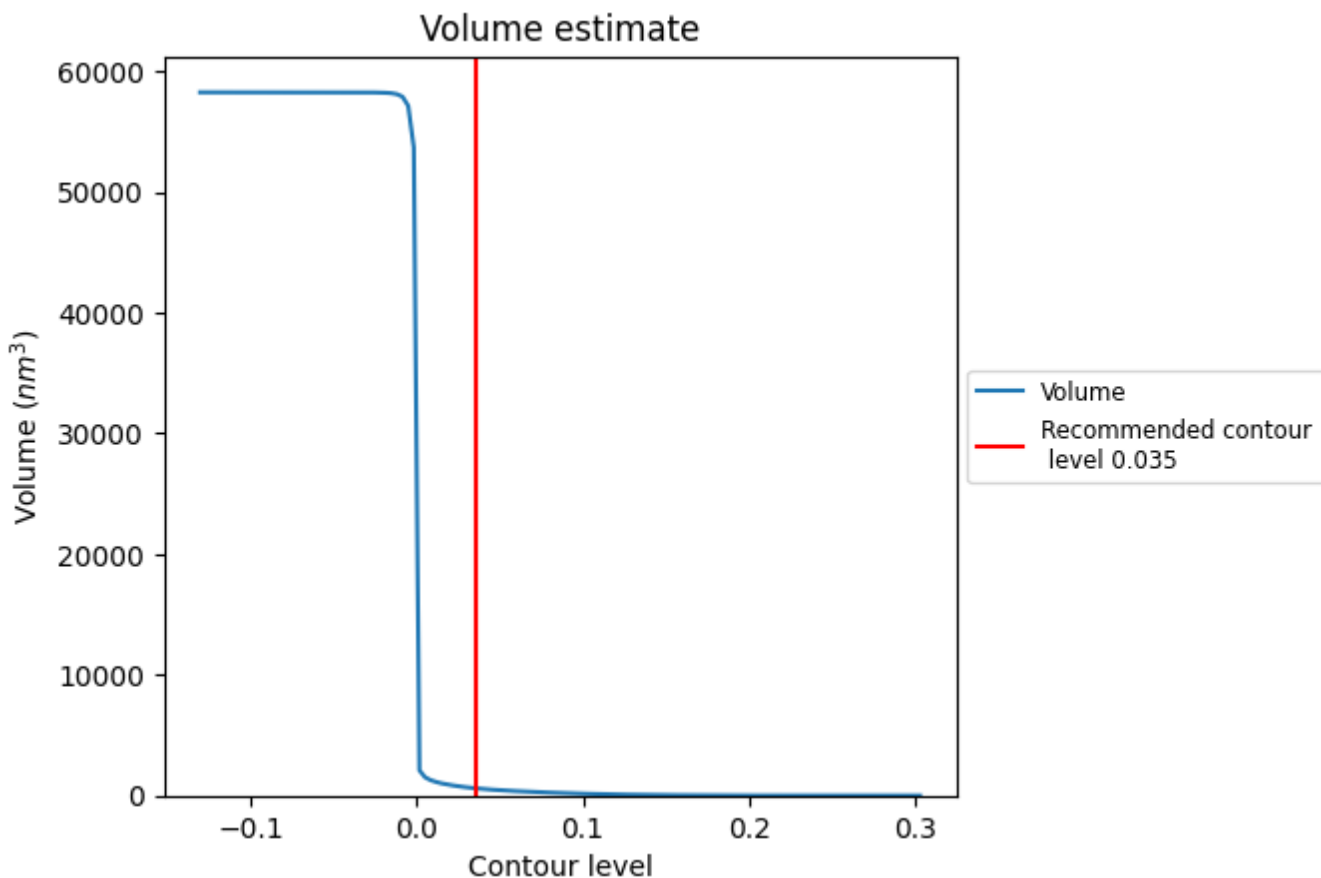
This section contains the results of statistical analysis of the map.

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.

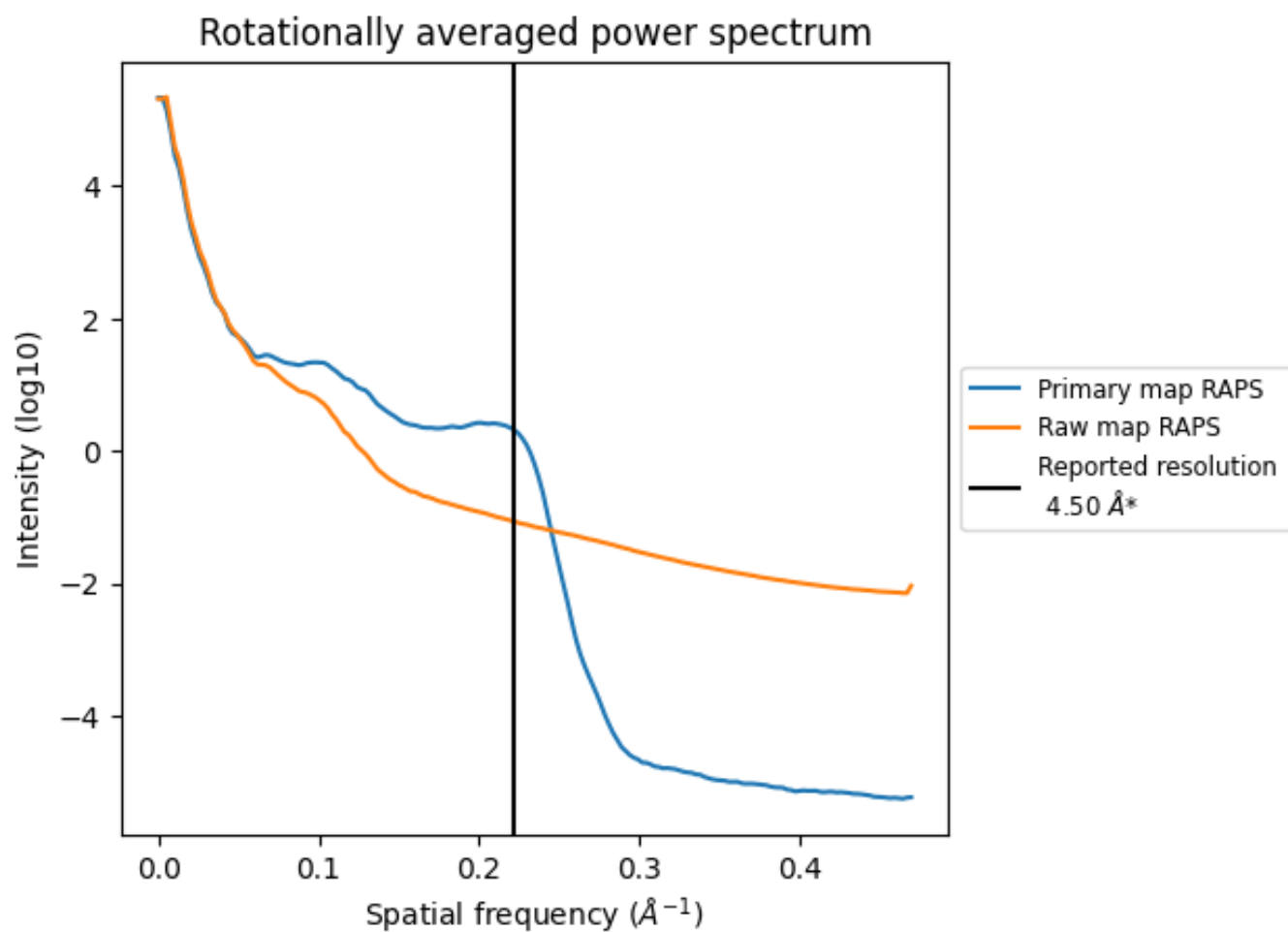
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 607 nm³; this corresponds to an approximate mass of 548 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 i

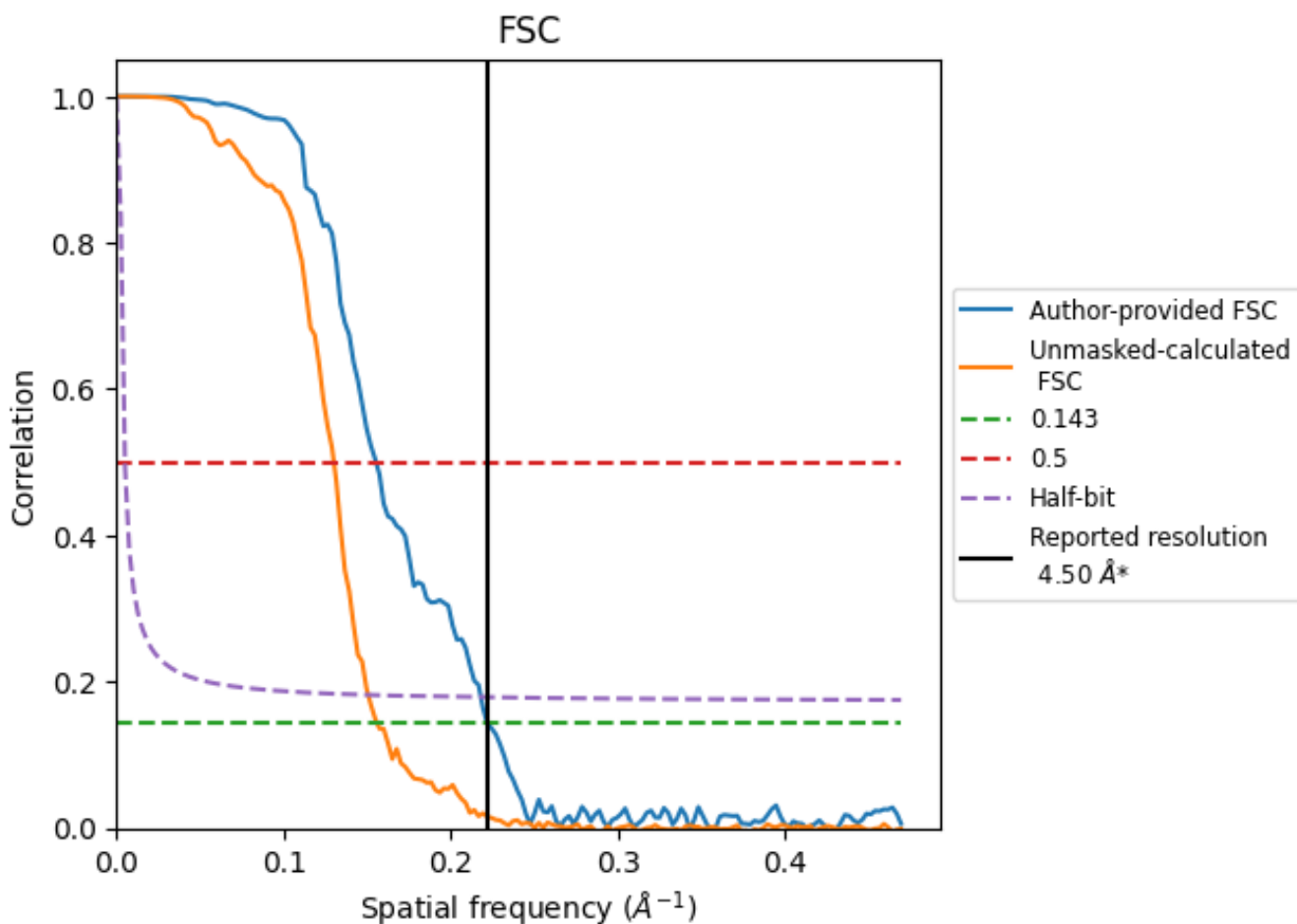


*Reported resolution corresponds to spatial frequency of 0.222 \AA^{-1}

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

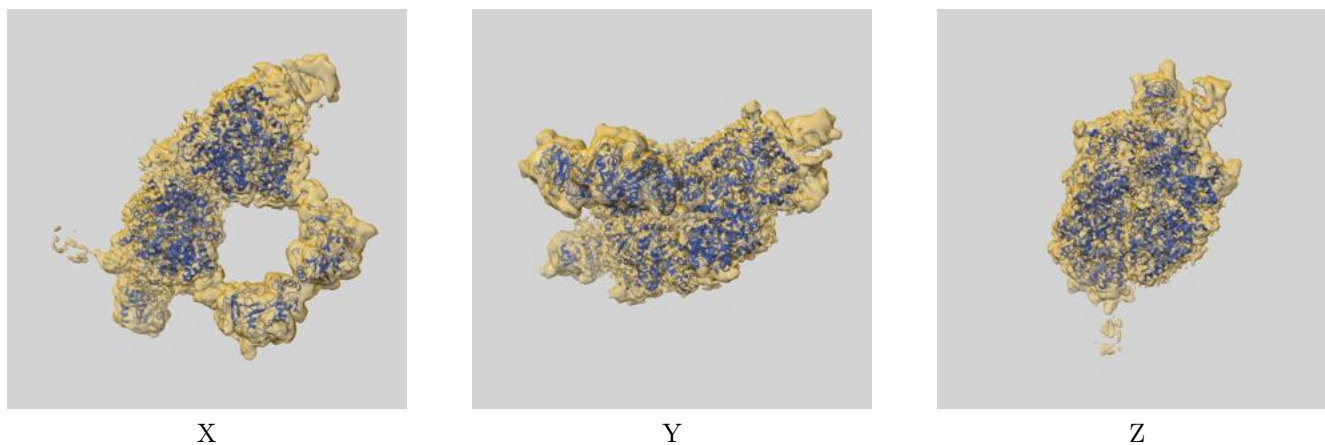
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.50	6.44	4.59
Unmasked-calculated*	6.41	7.69	6.64

*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 6.41 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

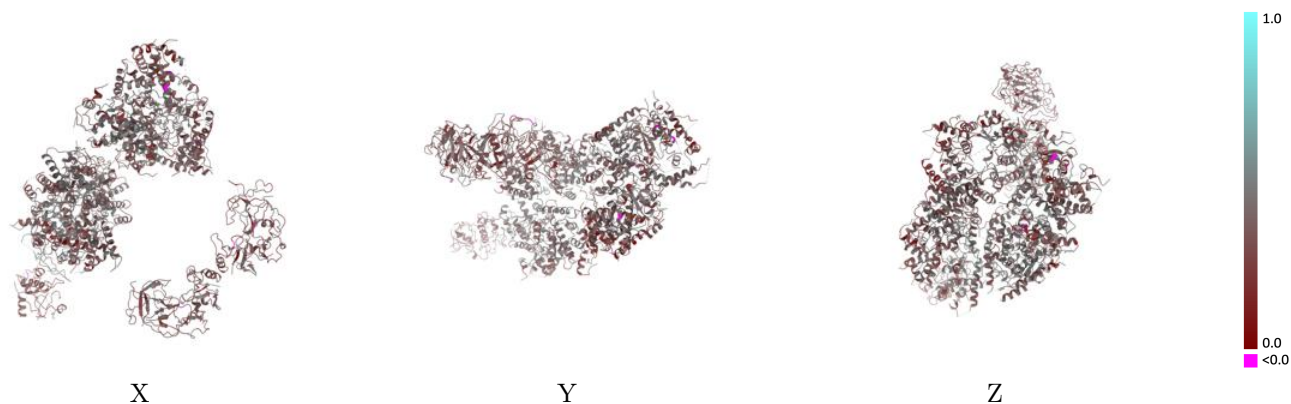
This section contains information regarding the fit between EMDB map EMD-4975 and PDB model 6ROW. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



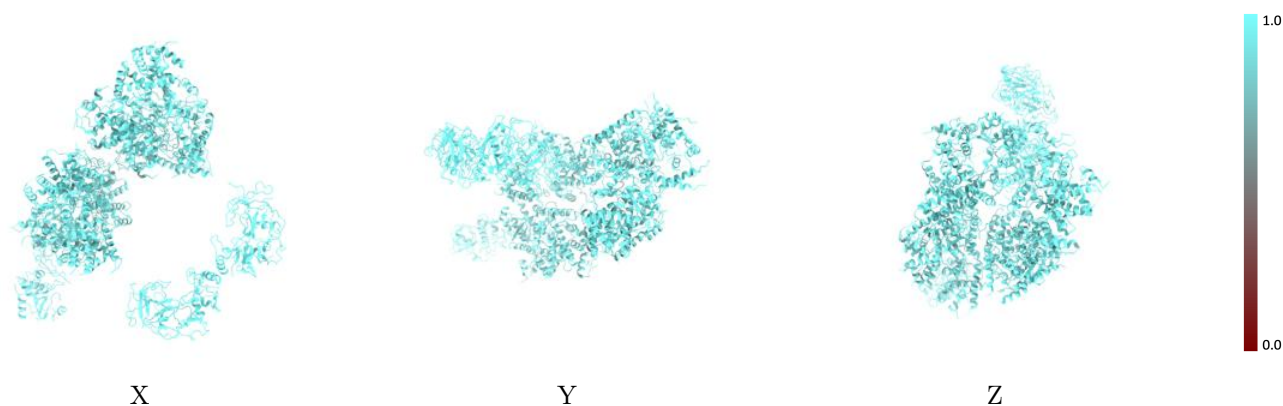
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



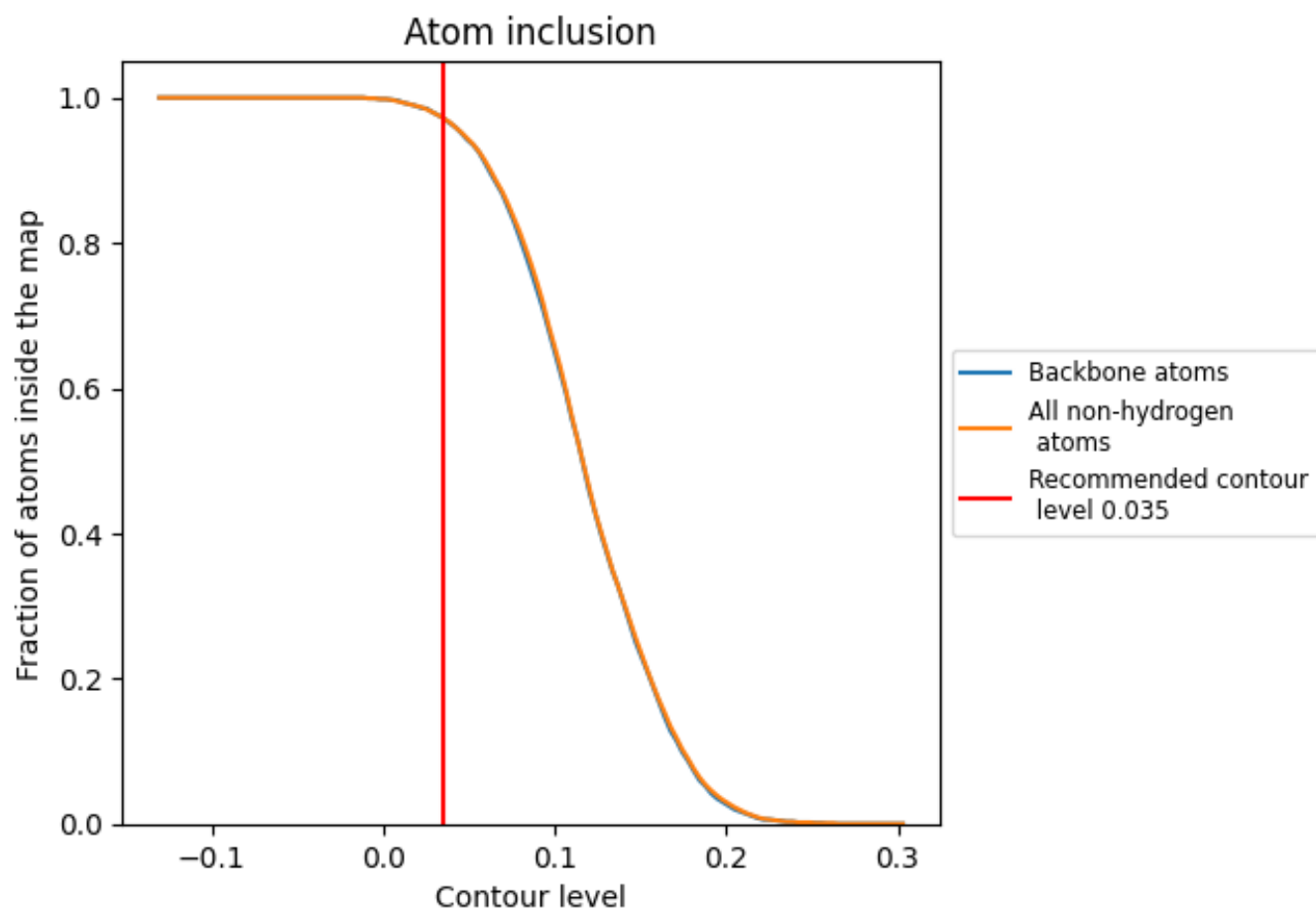
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 97% of all backbone atoms, 97% 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	 0.9720	 0.3790
A	 0.9760	 0.4040
B	 0.9660	 0.3870
C	 0.9730	 0.3890
D	 0.9620	 0.3650
E	 1.0000	 0.3610
F	 1.0000	 0.3400
G	 0.9980	 0.2980

