



wwPDB EM Validation Summary Report ⓘ

Dec 12, 2022 – 12:55 PM EST

PDB ID : 3J2C
EMDB ID : EMD-5504
Title : Dissecting the in vivo assembly of the 30S ribosomal subunit reveals the role of RimM
Authors : Guo, Q.; Goto, S.; Chen, Y.; Muto, A.; Himeno, H.; Deng, H.; Lei, J.; Gao, N.
Deposited on : 2012-09-28
Resolution : 13.20 Å (reported)
Based on initial model : 3OFA

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

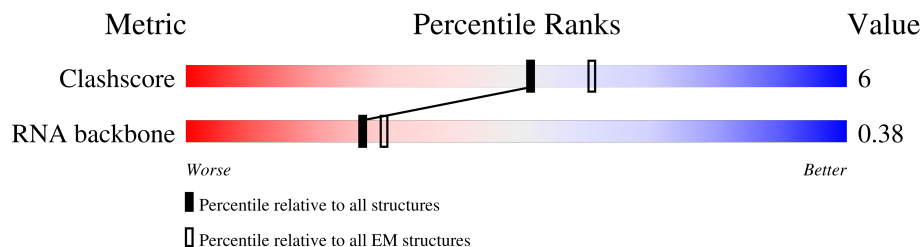
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

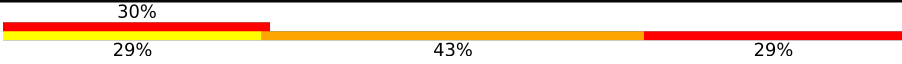
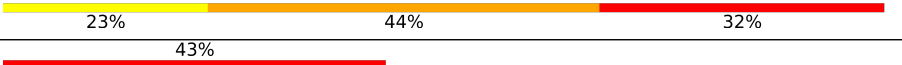
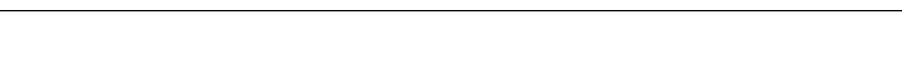
The reported resolution of this entry is 13.20 Å.

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
RNA backbone	4643	859

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	M	462	
2	N	927	
3	O	144	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 49444 atoms, of which 16558 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 RNA chain called 16S rRNA head domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	M	462	Total	C	H	N	O	P	0	0
			14865	4410	4987	1793	3214	461		

- Molecule 2 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	N	927	Total	C	H	N	O	P	0	0
			29941	8884	10017	3681	6433	926		

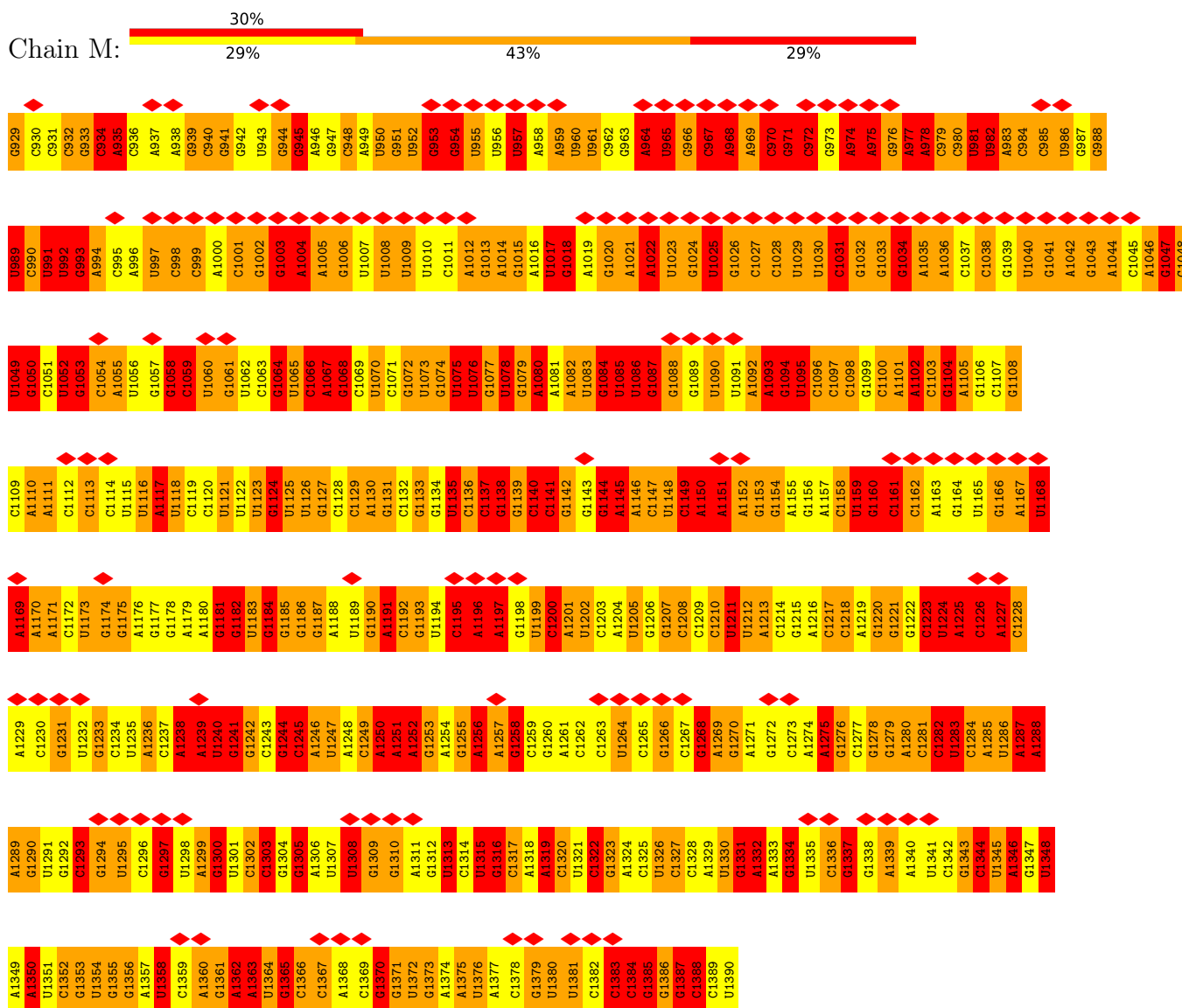
- Molecule 3 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	O	144	Total	C	H	N	O	P	0	0
			4638	1377	1554	562	1002	143		

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: 16S rRNA head domain



• Molecule 2: 16S rRNA body domain



G902	U842	A782	G722	U662	A602	G542	A482	C422	G362	G302	G242	A182	G122	U62	A2
G903	U843	C783	U723	A663	U603	U543	C483	G423	A363	A303	A243	C183	U123	C63	A3
U904	G844	A784	G724	G664	G604	C544	U484	G424	A364	G304	U244	U184	U124	G64	U4
U905	A845	G785	G725	G665	U605	C545	U485	G425	U365	G305	U245	U185	U125	A65	U5
A906	G846	G786	G726	G666	G606	C546	U486	U426	A366	A306	U246	G186	G126	A66	U6
A907	G847	G787	G727	G667	A607	A547	A487	U427	U367	C307	G247	G187	G127	A67	A7
A908	C848	U788	A728	G668	A608	G548	C488	G428	U368	G308	C248	C188	G128	G68	A8
A909	U849	U789	A729	G669	A609	C549	C489	U429	G369	A309	U249	C189	A129	G69	A9
U910	U850	A790	G730	G670	U610	G550	C490	A430	C370	G310	U250	A190	U130	U70	A10
U911	G851	G791	G731	G671	C611	U551	G491	A431	A371	C311	U251	G191	A131	A71	G11
C912	U852	A792	G732	U672	C612	U552	C492	A432	C372	C312	U252	A192	C132	A72	G12
A913	C853	U793	G733	A673	C613	A553	A493	G433	A373	A313	U253	C193	U133	C73	U13
A914	U854	A794	G734	G674	C614	A554	G494	U434	A374	C314	U254	C194	G134	A74	U14
A915	U855	C795	C735	A675	G615	U555	A495	A435	U375	A315	G255	A195	C135	G75	U15
C856	C856	C796	C736	U676	G616	C556	A496	A436	G376	C316	U256	A196	G136	G76	A16
G917	C857	C797	C737	U677	G617	G557	A497	U437	G377	U317	G257	A197	U137	A77	A17
A918	U858	U798	C738	U678	C618	G558	A498	U438	G378	G318	U258	A198	G138	A78	U18
A919	G859	C799	C739	G679	U619	A559	A499	U439	C379	G319	U259	A199	A139	A79	U19
U920	A860	U800	U740	C680	C620	A560	G500	C440	G380	A320	G260	G200	U140	A80	A19
U921	C861	U801	G741	A681	A621	U561	C501	A441	C381	A321	U261	G201	G141	A81	U20
G922	C862	A802	G742	G682	A622	A562	A502	G442	C382	C322	G262	G202	G142	G82	G21
A923	U863	G803	A743	G683	C623	A563	C503	G443	A383	U323	A263	G203	A143	C83	C23
C924	A864	U804	C744	U684	C624	C564	C504	G444	G384	A324	G264	G204	G144	U84	U24
G925	A865	C805	G745	G685	U625	U565	G505	G445	C385	A325	G265	A205	G145	U85	U25
C866	C866	C806	A746	U686	G626	G566	G506	G446	C386	G326	G266	C206	G146	G86	C25
G927	C867	A807	A747	A687	G627	C567	C507	G447	U387	A327	G267	C207	G147	C87	A26
C868	C868	C808	G748	G688	G628	G568	U508	A448	G388	C328	U268	U208	G148	U88	G27
G869	G869	G809	A749	C689	A629	C569	A509	G449	U389	A329	G269	U209	G149	A28	A28
U870	C870	C810	C750	G690	A630	G570	A510	G450	U390	C330	A270	C210	U150	C90	U29
U871	C871	C811	U751	G691	C631	U571	C511	A451	U391	G331	C271	G211	U151	U91	U30
A872	U872	G812	G752	U692	U632	A572	U512	A452	C392	G332	C272	G212	A152	U92	G31
A873	C873	U813	A753	G693	G633	A573	C513	G453	A393	U333	U273	C213	C153	U93	A32
G874	A874	A814	C754	A694	C634	A574	G514	G454	C394	C334	A274	C214	U154	G94	A33
U875	A875	A815	G755	A695	A635	C575	G515	A455	C395	G335	G275	C215	A155	C95	A34
C876	C876	C816	C756	A696	U636	C576	U516	A456	C396	A336	G276	U216	C156	U96	C35
A877	C877	C817	U757	U697	C637	G577	G517	G457	C397	G337	C277	C217	U157	C97	C36
A878	G878	G818	C758	G698	U638	C578	C518	U458	U398	A338	G278	U218	G158	A98	U37
C879	C879	A819	A759	C699	G639	A579	C519	A459	G399	C339	A279	U219	G159	C99	G38
U880	U880	U820	G760	G700	A640	C580	A520	A460	C400	U340	C280	G220	A160	G100	G39
C881	C881	C821	G761	U701	U641	G581	G521	A461	C401	C341	G281	C221	A161	A101	C40
C882	C882	U822	U762	A702	A642	C582	C522	G462	G402	C342	A282	C222	A162	G41	G41
C883	C883	C823	G763	G703	C643	A583	A523	U463	C403	U343	U283	A223	C163	U103	G42
U884	G884	G824	C764	A704	U644	G584	G524	U464	G404	A344	C284	U224	G164	G104	C43
C885	C885	A825	G765	G705	G645	G585	C525	A465	U405	C345	G285	C225	G165	G105	A44
G886	G886	C826	A766	A706	G646	C586	C526	A466	G406	G346	C286	G226	U166	C106	A45
C887	C887	U827	A767	U707	C647	G587	G527	U467	U407	G347	U287	G227	A167	G107	G46
G888	G888	U828	A768	C708	A648	G588	C528	U468	A408	C348	A288	A228	G168	G108	C47
A889	G889	G829	G769	U709	A649	U589	G529	C469	U409	G349	G289	U229	C169	A109	C48
G890	G890	G830	G770	G710	G650	U590	G530	C470	G410	G350	C290	G230	U170	G110	U49
U891	C891	A831	G771	G711	C651	U591	U531	U471	A411	G351	U291	U231	A171	G111	A50
A892	C892	G832	U772	A712	U652	G592	A532	U472	A412	C352	G292	G232	A172	G112	A51
C893	C893	G833	G773	G713	U653	U593	A533	U473	G413	C353	G293	C233	U173	G113	C52
G894	G894	U834	G774	G714	C654	U594	U534	A474	A414	G354	U294	C234	A174	U114	A53
C895	C895	U835	G775	A715	A655	A595	A535	G475	A415	C355	C295	C235	C175	G115	C54
C896	C896	G836	G776	A716	G656	G596	C536	U476	G416	A356	U296	G236	C176	A116	U55
C897	C897	U837	A777	U717	U657	G597	G537	C477	G417	G357	G297	G237	G177	G117	U56
G898	G898	C838	G778	A718	C658	U598	G538	A478	C418	U358	A298	A238	C178	U118	C57
C899	C899	C839	C779	A719	U659	C599	A539	U479	C419	G359	G299	U239	A179	A119	C58
A900	A900	C720	A780	C720	G660	A600	G540	U480	U420	G360	A300	G240	U180	A120	A59
G928	A901	C841	A781	G721	G661	G501	G541	G481	U421	G361	C301	G241	A181	U121	G61

● Molecule 3: 16S rRNA body domain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	44392	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	Weiner filter	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	80000	Depositor
Image detector	GATAN ULTRASCAN 4000 (4k x 4k)	Depositor
Maximum map value	4.325	Depositor
Minimum map value	-6.829	Depositor
Average map value	-4.406	Depositor
Map value standard deviation	0.508	Depositor
Recommended contour level	-3.2	Depositor
Map size (\AA)	345.0, 345.0, 345.0	wwPDB
Map dimensions	125, 125, 125	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	2.76, 2.76, 2.76	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	M	3.43	1534/11053 (13.9%)	3.80	2624/17234 (15.2%)
2	N	3.44	3141/22318 (14.1%)	3.88	5510/34825 (15.8%)
3	O	3.32	455/3452 (13.2%)	3.95	849/5383 (15.8%)
All	All	3.43	5130/36823 (13.9%)	3.86	8983/57442 (15.6%)

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	M	0	236
2	N	0	522
3	O	0	78
All	All	0	836

The worst 5 of 5130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	1502	A	N7-C5	-20.70	1.26	1.39
1	M	1251	A	N9-C4	18.33	1.48	1.37
2	N	124	C	N1-C6	-18.06	1.26	1.37
2	N	533	A	N7-C5	-17.64	1.28	1.39
2	N	350	G	C6-N1	17.60	1.51	1.39

The worst 5 of 8983 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	1253	G	N1-C6-O6	26.96	136.07	119.90
3	O	1455	G	N1-C6-O6	26.35	135.71	119.90
3	O	1458	G	N1-C6-O6	25.20	135.02	119.90
1	M	1362	A	P-O3'-C3'	24.79	149.44	119.70
3	O	1405	G	C5-C6-O6	-24.61	113.83	128.60

There are no chirality outliers.

5 of 836 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	929	G	Sidechain
1	M	933	G	Sidechain
1	M	934	C	Sidechain
1	M	935	A	Sidechain
1	M	939	G	Sidechain

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	M	9878	4987	4986	67	0
2	N	19924	10017	10006	206	0
3	O	3084	1554	1553	14	0
All	All	32886	16558	16545	281	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 6.

The worst 5 of 281 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:M:998:C:H42	1:M:1042:A:H61	1.38	0.71
2:N:50:A:H1'	2:N:52:C:C6	2.25	0.71
2:N:664:G:H22	2:N:741:G:H1	1.38	0.70
2:N:858:G:H1	2:N:869:G:H2'	1.55	0.70
2:N:411:A:H61	2:N:428:G:H1'	1.57	0.70

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	M	461/462 (99%)	152 (32%)	41 (8%)
2	N	926/927 (99%)	255 (27%)	84 (9%)
3	O	143/144 (99%)	31 (21%)	9 (6%)
All	All	1530/1533 (99%)	438 (28%)	134 (8%)

5 of 438 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	M	932	C
1	M	934	C
1	M	935	A
1	M	944	G
1	M	953	G

5 of 134 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	N	641	U
2	N	733	G
3	O	1513	A
2	N	65	A
2	N	60	A

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.

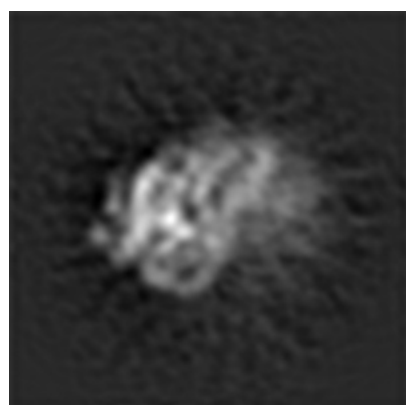
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-5504. These allow visual inspection of the internal detail of the map and identification of artifacts.

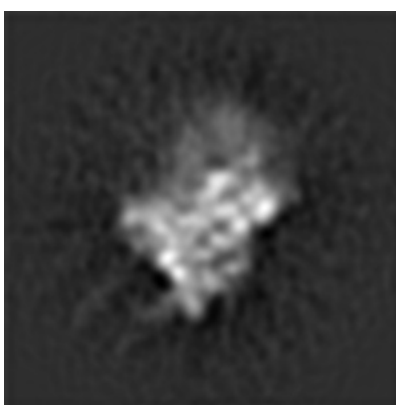
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

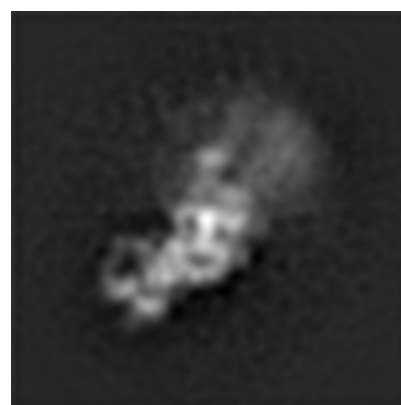
6.1.1 Primary map



X



Y

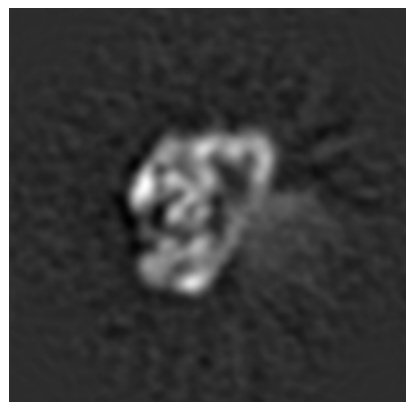


Z

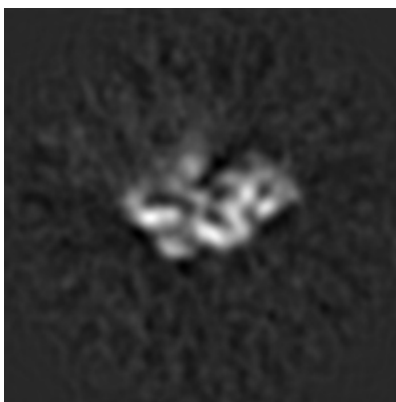
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

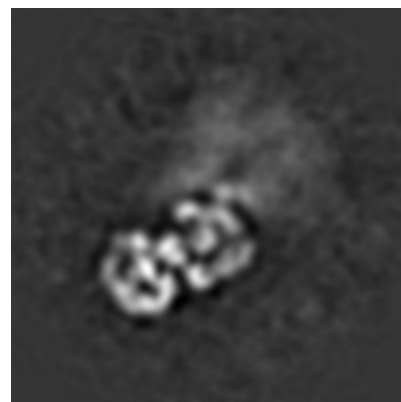
6.2.1 Primary map



X Index: 62



Y Index: 62

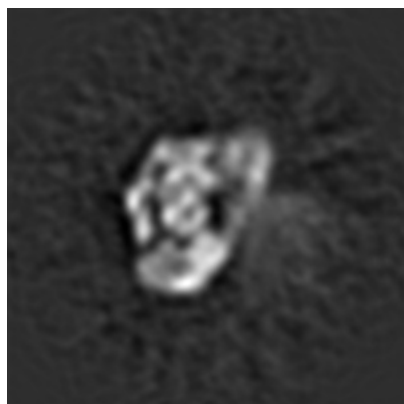


Z Index: 62

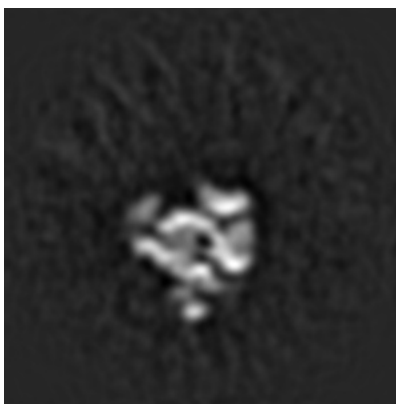
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

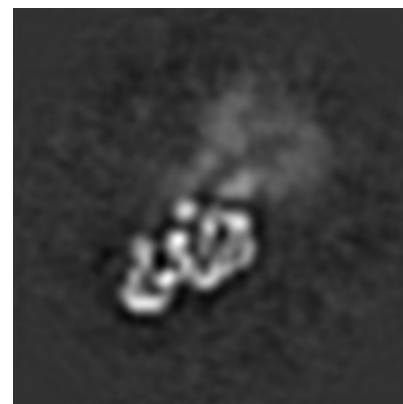
6.3.1 Primary map



X Index: 60



Y Index: 42

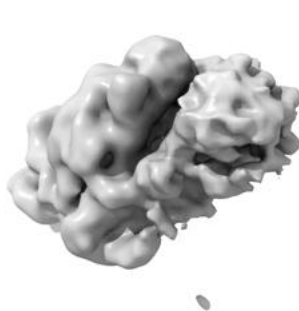


Z Index: 65

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

6.4 Orthogonal surface views [i](#)

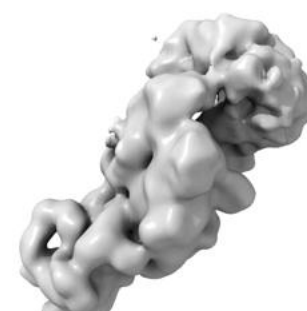
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level - 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

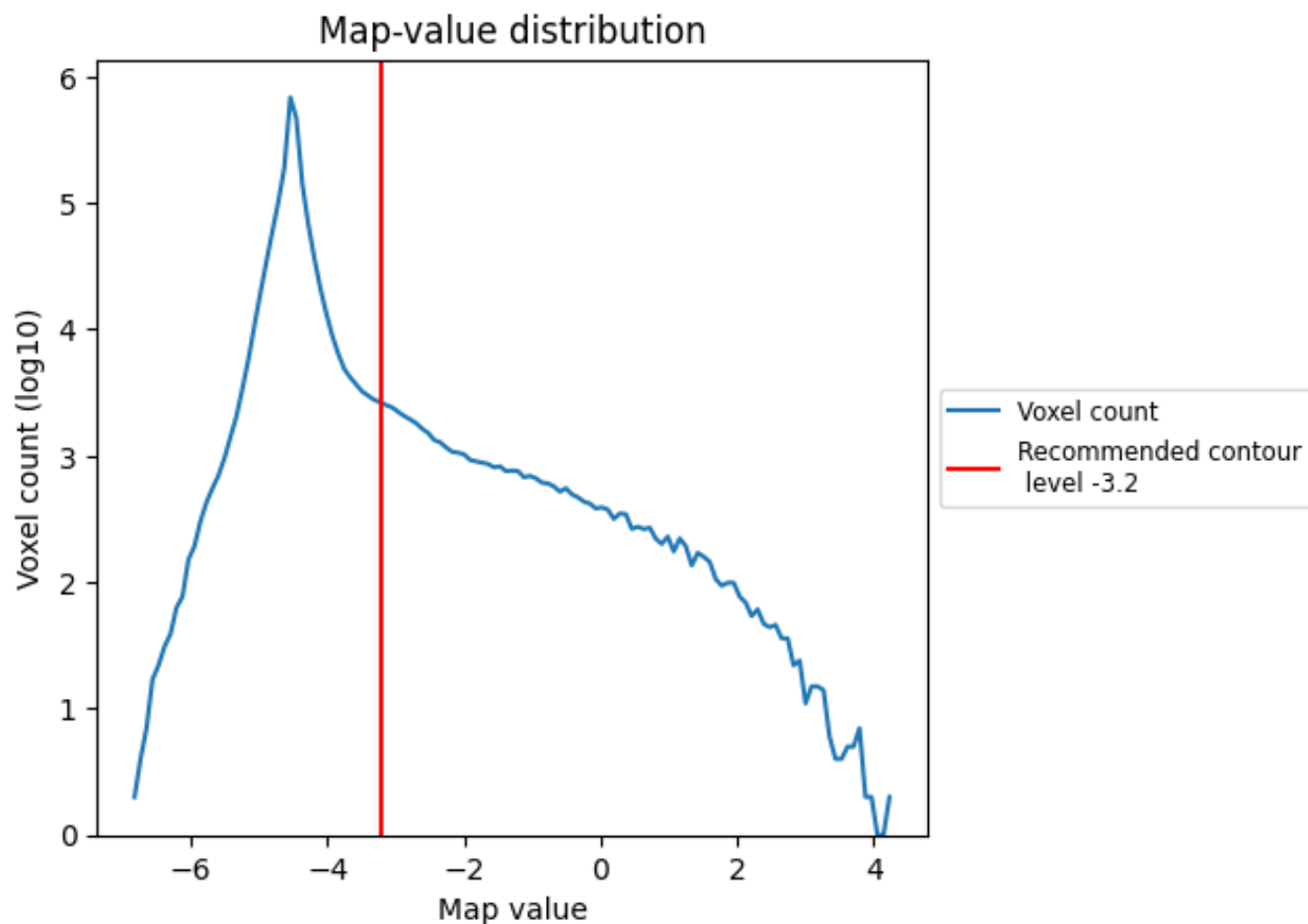
6.5 Mask visualisation

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

7 Map analysis [i](#)

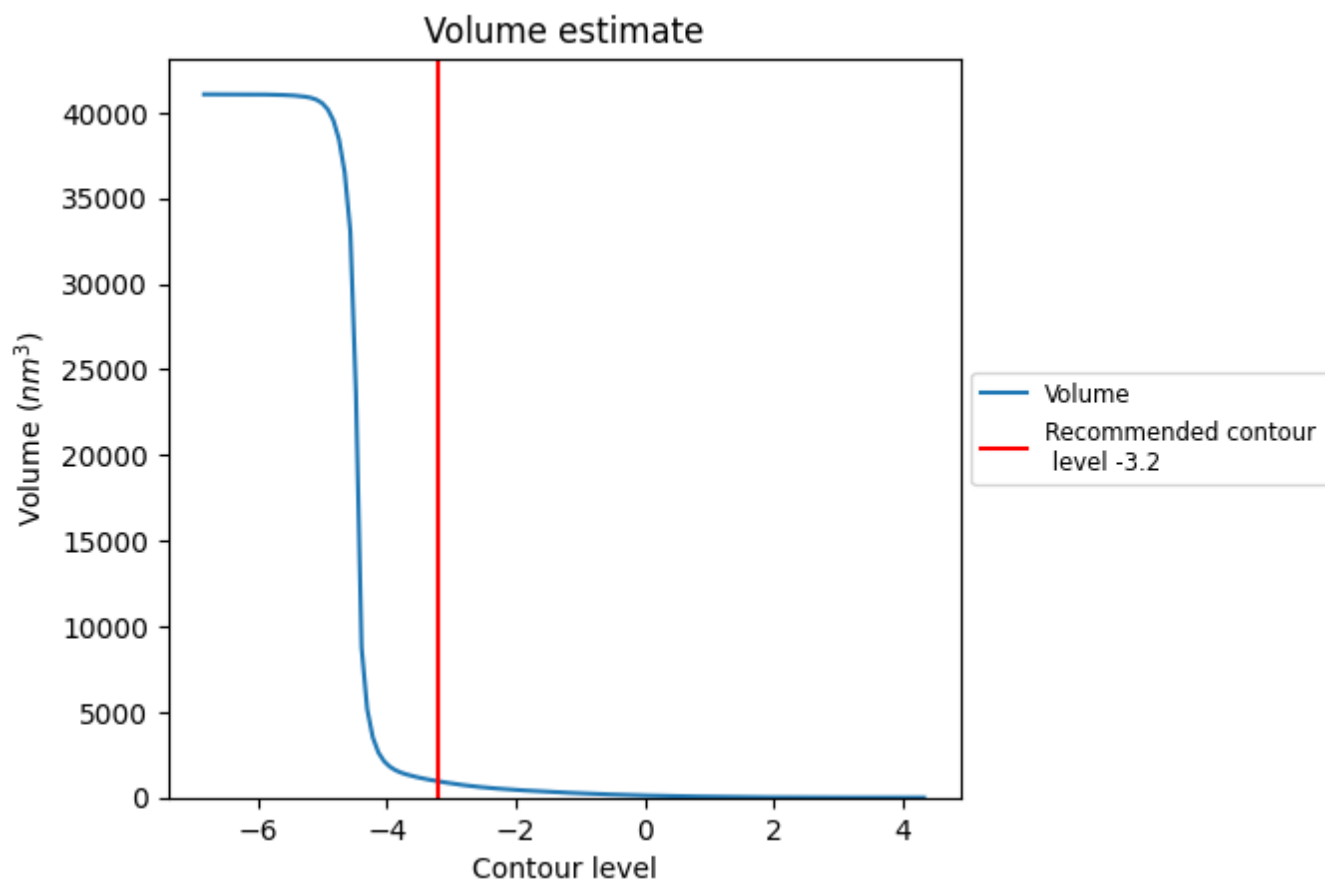
This section contains the results of statistical analysis of the map.

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.

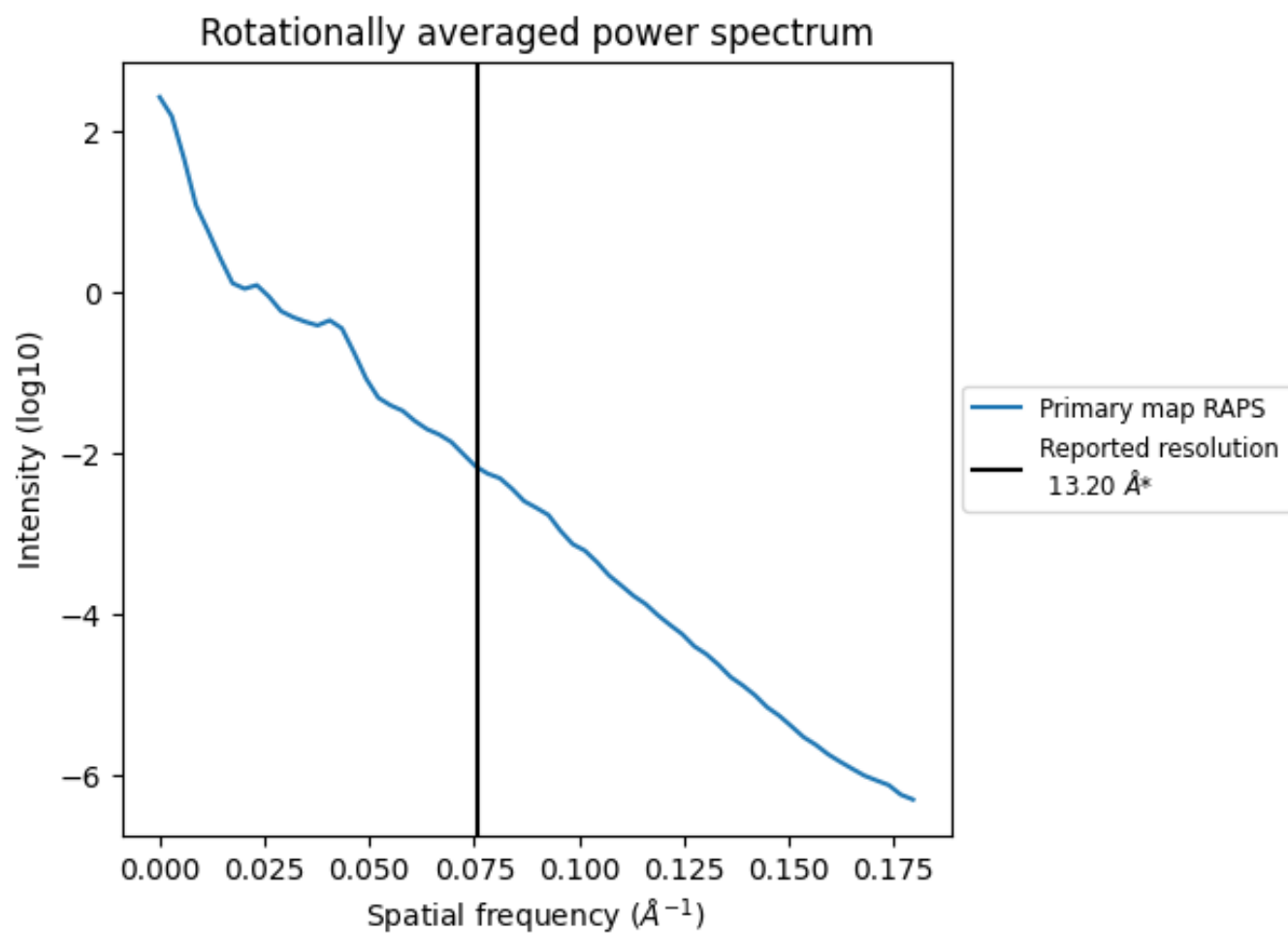
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 949 nm³; this corresponds to an approximate mass of 858 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 0.076 \AA^{-1}

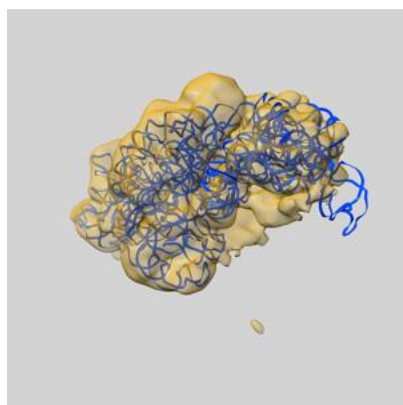
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

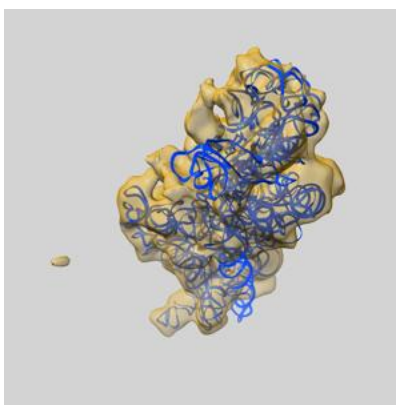
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-5504 and PDB model 3J2C. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

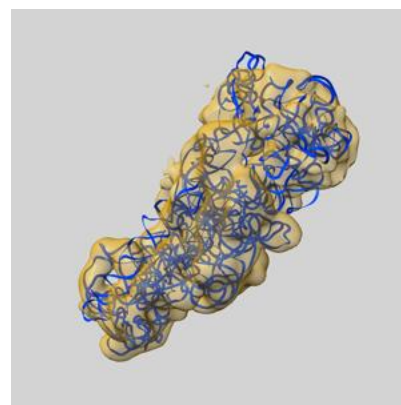
9.1 Map-model overlay [i](#)



X



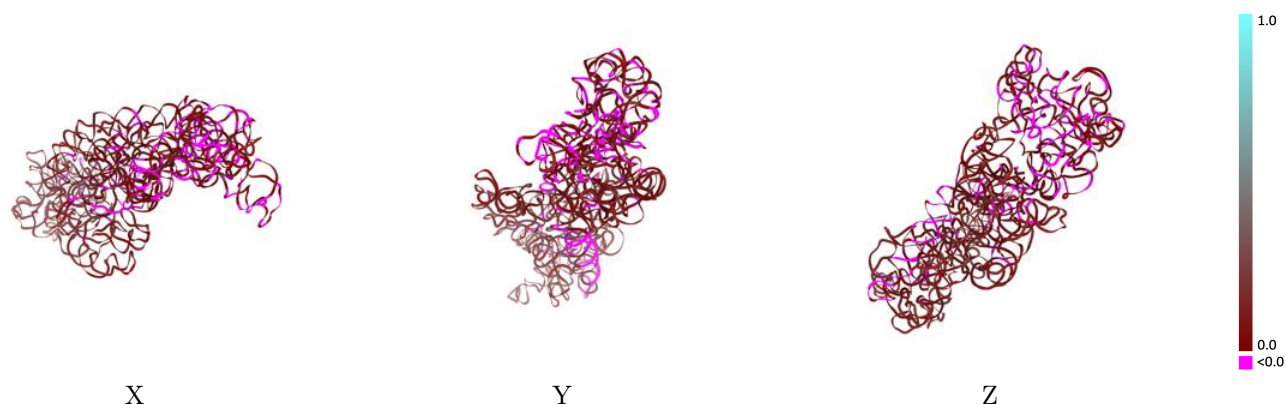
Y



Z

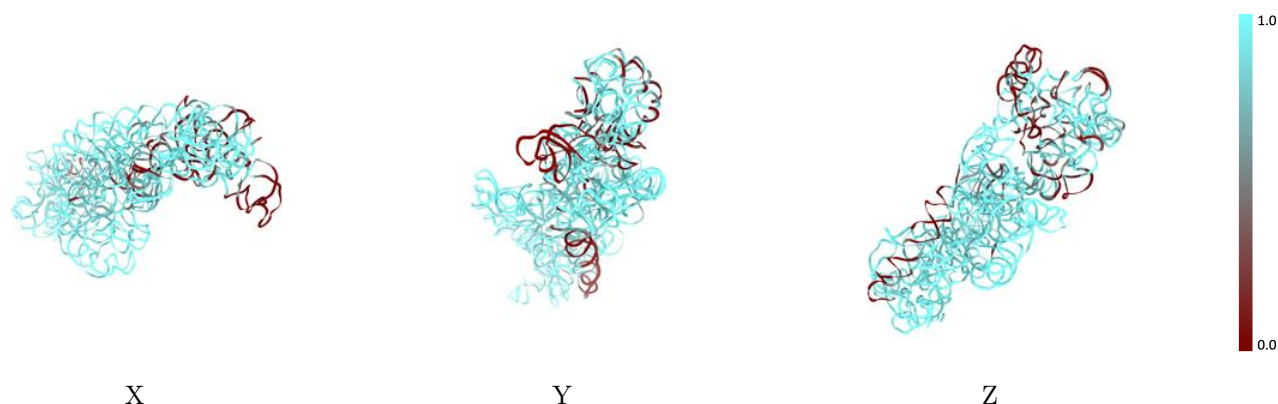
The images above show the 3D surface view of the map at the recommended contour level -3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



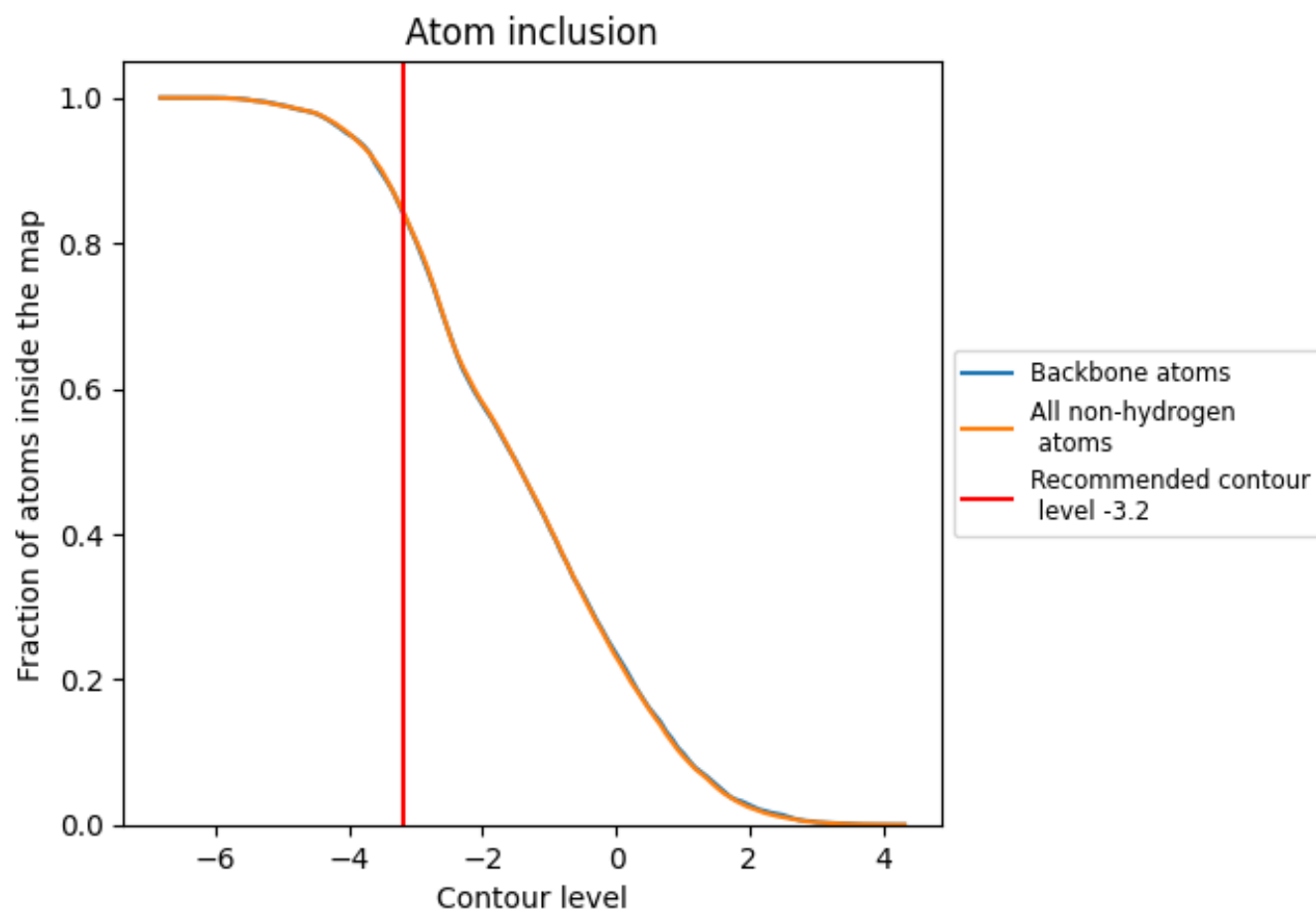
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (-3.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (-3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8448	<div></div> 0.0760
M	<div></div> 0.6651	<div></div> 0.0380
N	<div></div> 0.9862	<div></div> 0.1040
O	<div></div> 0.5347	<div></div> 0.0120

