



wwPDB EM Validation Summary Report ⓘ

Mar 13, 2024 – 12:42 PM JST

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

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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:

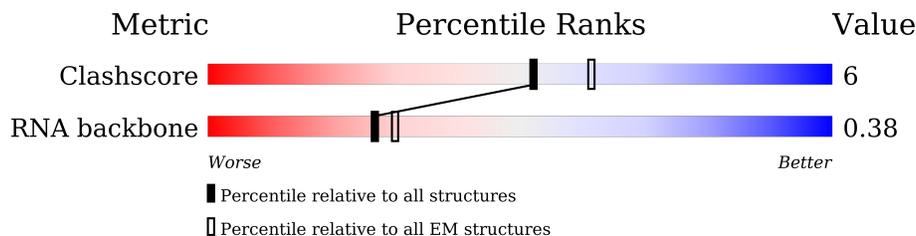
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

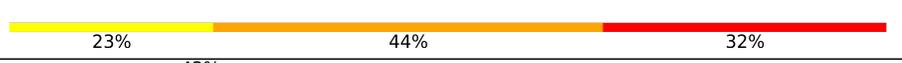
The reported resolution of this entry is 13.20 Å.

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
			Total	C	H	N	O	P		
1	M	462	14865	4410	4987	1793	3214	461	0	0

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

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

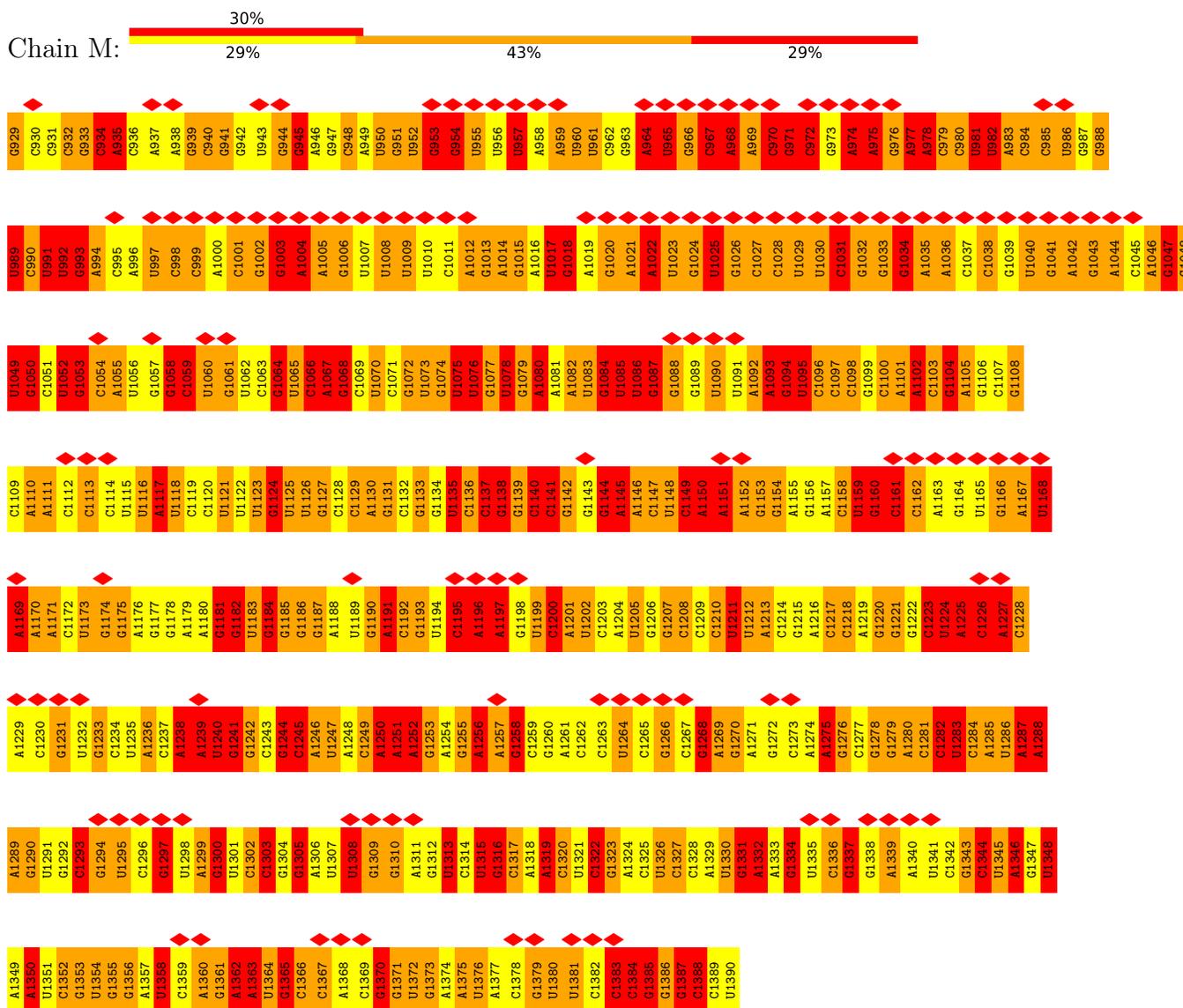
- Molecule 3 is a RNA chain called 16S rRNA body domain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
3	O	144	4638	1377	1554	562	1002	143	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: 16S rRNA head domain

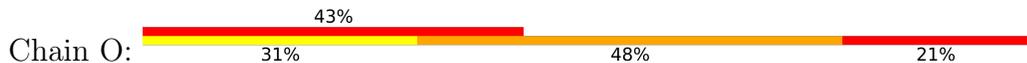


- Molecule 2: 16S rRNA body domain



A2	A3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15	U16	U17	U18	U19	U20	U21	U22	U23	U24	U25	U26	U27	U28	U29	U30	U31	U32	U33	U34	U35	U36	U37	U38	U39	U40	U41	U42	U43	U44	U45	U46	U47	U48	U49	U50	U51	U52	U53	U54	U55	U56	U57	U58	U59	U60	U61	U62	U63	U64	U65	U66	U67	U68	U69	U70	U71	U72	U73	U74	U75	U76	U77	U78	U79	U80	U81	U82	U83	U84	U85	U86	U87	U88	U89	U90	U91	U92	U93	U94	U95	U96	U97	U98	U99	U100	U101	U102	U103	U104	U105	U106	U107	U108	U109	U110	U111	U112	U113	U114	U115	U116	U117	U118	U119	U120	U121	U122	U123	U124	U125	U126	U127	U128	U129	U130	U131	U132	U133	U134	U135	U136	U137	U138	U139	U140	U141	U142	U143	U144	U145	U146	U147	U148	U149	U150	U151	U152	U153	U154	U155	U156	U157	U158	U159	U160	U161	U162	U163	U164	U165	U166	U167	U168	U169	U170	U171	U172	U173	U174	U175	U176	U177	U178	U179	U180	U181	U182	U183	U184	U185	U186	U187	U188	U189	U190	U191	U192	U193	U194	U195	U196	U197	U198	U199	U200	U201	U202	U203	U204	U205	U206	U207	U208	U209	U210	U211	U212	U213	U214	U215	U216	U217	U218	U219	U220	U221	U222	U223	U224	U225	U226	U227	U228	U229	U230	U231	U232	U233	U234	U235	U236	U237	U238	U239	U240	U241	U242	U243	U244	U245	U246	U247	U248	U249	U250	U251	U252	U253	U254	U255	U256	U257	U258	U259	U260	U261	U262	U263	U264	U265	U266	U267	U268	U269	U270	U271	U272	U273	U274	U275	U276	U277	U278	U279	U280	U281	U282	U283	U284	U285	U286	U287	U288	U289	U290	U291	U292	U293	U294	U295	U296	U297	U298	U299	U300	U301	U302	U303	U304	U305	U306	U307	U308	U309	U310	U311	U312	U313	U314	U315	U316	U317	U318	U319	U320	U321	U322	U323	U324	U325	U326	U327	U328	U329	U330	U331	U332	U333	U334	U335	U336	U337	U338	U339	U340	U341	U342	U343	U344	U345	U346	U347	U348	U349	U350	U351	U352	U353	U354	U355	U356	U357	U358	U359	U360	U361	U362	U363	U364	U365	U366	U367	U368	U369	U370	U371	U372	U373	U374	U375	U376	U377	U378	U379	U380	U381	U382	U383	U384	U385	U386	U387	U388	U389	U390	U391	U392	U393	U394	U395	U396	U397	U398	U399	U400	U401	U402	U403	U404	U405	U406	U407	U408	U409	U410	U411	U412	U413	U414	U415	U416	U417	U418	U419	U420	U421	U422	U423	U424	U425	U426	U427	U428	U429	U430	U431	U432	U433	U434	U435	U436	U437	U438	U439	U440	U441	U442	U443	U444	U445	U446	U447	U448	U449	U450	U451	U452	U453	U454	U455	U456	U457	U458	U459	U460	U461	U462	U463	U464	U465	U466	U467	U468	U469	U470	U471	U472	U473	U474	U475	U476	U477	U478	U479	U480	U481	U482	U483	U484	U485	U486	U487	U488	U489	U490	U491	U492	U493	U494	U495	U496	U497	U498	U499	U500	U501	U502	U503	U504	U505	U506	U507	U508	U509	U510	U511	U512	U513	U514	U515	U516	U517	U518	U519	U520	U521	U522	U523	U524	U525	U526	U527	U528	U529	U530	U531	U532	U533	U534	U535	U536	U537	U538	U539	U540	U541	U542	U543	U544	U545	U546	U547	U548	U549	U550	U551	U552	U553	U554	U555	U556	U557	U558	U559	U560	U561	U562	U563	U564	U565	U566	U567	U568	U569	U570	U571	U572	U573	U574	U575	U576	U577	U578	U579	U580	U581	U582	U583	U584	U585	U586	U587	U588	U589	U590	U591	U592	U593	U594	U595	U596	U597	U598	U599	U600	U601	U602	U603	U604	U605	U606	U607	U608	U609	U610	U611	U612	U613	U614	U615	U616	U617	U618	U619	U620	U621	U622	U623	U624	U625	U626	U627	U628	U629	U630	U631	U632	U633	U634	U635	U636	U637	U638	U639	U640	U641	U642	U643	U644	U645	U646	U647	U648	U649	U650	U651	U652	U653	U654	U655	U656	U657	U658	U659	U660	U661	U662	U663	U664	U665	U666	U667	U668	U669	U670	U671	U672	U673	U674	U675	U676	U677	U678	U679	U680	U681	U682	U683	U684	U685	U686	U687	U688	U689	U690	U691	U692	U693	U694	U695	U696	U697	U698	U699	U700	U701	U702	U703	U704	U705	U706	U707	U708	U709	U710	U711	U712	U713	U714	U715	U716	U717	U718	U719	U720	U721	U722	U723	U724	U725	U726	U727	U728	U729	U730	U731	U732	U733	U734	U735	U736	U737	U738	U739	U740	U741	U742	U743	U744	U745	U746	U747	U748	U749	U750	U751	U752	U753	U754	U755	U756	U757	U758	U759	U760	U761	U762	U763	U764	U765	U766	U767	U768	U769	U770	U771	U772	U773	U774	U775	U776	U777	U778	U779	U780	U781	U782	U783	U784	U785	U786	U787	U788	U789	U790	U791	U792	U793	U794	U795	U796	U797	U798	U799	U800	U801	U802	U803	U804	U805	U806	U807	U808	U809	U810	U811	U812	U813	U814	U815	U816	U817	U818	U819	U820	U821	U822	U823	U824	U825	U826	U827	U828	U829	U830	U831	U832	U833	U834	U835	U836	U837	U838	U839	U840	U841	U842	U843	U844	U845	U846	U847	U848	U849	U850	U851	U852	U853	U854	U855	U856	U857	U858	U859	U860	U861	U862	U863	U864	U865	U866	U867	U868	U869	U870	U871	U872	U873	U874	U875	U876	U877	U878	U879	U880	U881	U882	U883	U884	U885	U886	U887	U888	U889	U890	U891	U892	U893	U894	U895	U896	U897	U898	U899	U900	U901	U902	U903	U904	U905	U906	U907	U908	U909	U910	U911	U912	U913	U914	U915	U916	U917	U918	U919	U920	U921	U922	U923	U924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	U935	U936	U937	U938	U939	U940	U941	U942	U943	U944	U945	U946	U947	U948	U949	U950	U951	U952	U953	U954	U955	U956	U957	U958	U959	U960	U961	U962	U963	U964	U965	U966	U967	U968	U969	U970	U971	U972	U973	U974	U975	U976	U977	U978	U979	U980	U981	U982	U983	U984	U985	U986	U987	U988	U989	U990	U991	U992	U993	U994	U995	U996	U997	U998	U999	U1000
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● Molecule 3: 16S rRNA body domain



U1391	G1392	U1393	A1394	C1395	A1396	C1397	A1398	C1399	C1400	C1401	C1402	C1403	C1404	G1405	U1406	C1407	A1408	C1409	A1410	C1411	C1412	A1413	U1414	G1415	G1416	G1417	A1418	G1419	U1420	G1421	G1422	G1423	U1424	U1425	G1426	C1427	A1428	A1429	A1430	A1431	G1432	A1433	A1434	G1435	U1436	A1437	G1438	G1439	U1440	A1441	G1442	C1443	U1444	U1445	A1446	A1447	C1448	C1449	U1450
U1451	C1452	G1453	G1454	G1455	A1456	G1457	G1458	G1459	C1460	G1461	C1462	U1463	U1464	A1465	C1466	A1468	C1469	U1470	U1471	U1472	G1473	U1474	G1475	A1476	U1477	U1478	C1479	A1480	U1481	G1482	A1483	C1484	U1485	G1486	G1487	G1488	G1489	U1490	G1491	A1492	A1493	G1494	U1495	C1496	G1497	U1498	A1499	A1500	C1501	A1502	A1503	G1504	G1505	U1506	A1507	A1508	C1509	C1510	
G1511	U1512	A1513	G1514	G1515	G1516	G1517	A1518	A1519	C1520	C1521	U1522	G1523	C1524	G1525	G1526	U1527	U1528	G1529	G1530	A1531	U1532	C1533	A1534																																				

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 [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	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 [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	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.

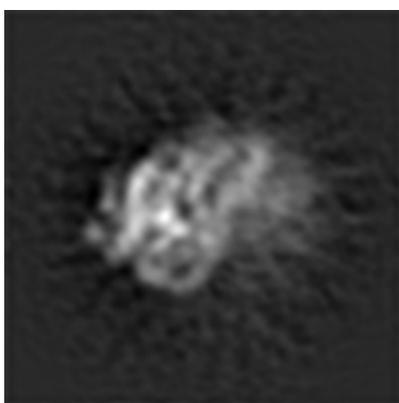
6 Map visualisation [i](#)

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.

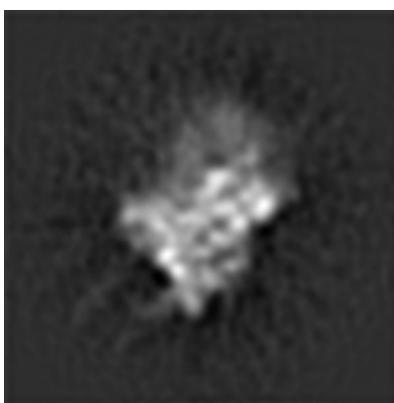
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

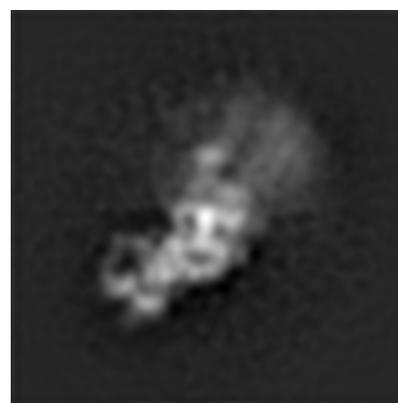
6.1.1 Primary map



X



Y

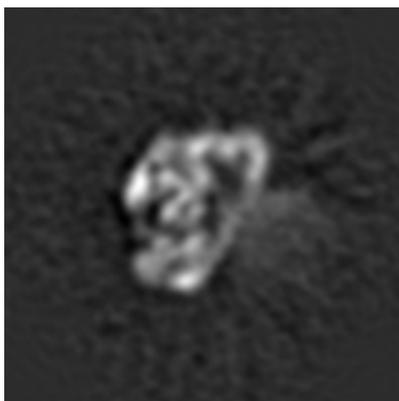


Z

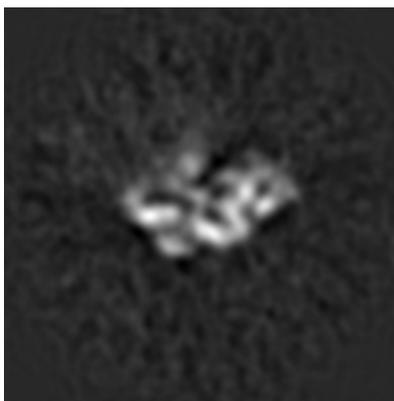
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

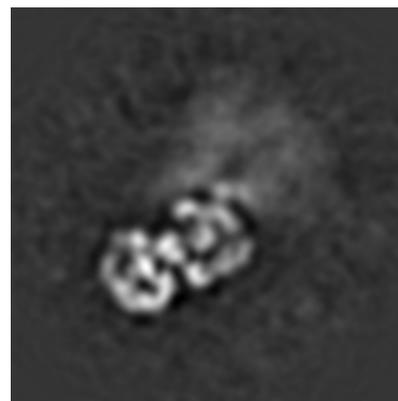
6.2.1 Primary map



X Index: 62



Y Index: 62

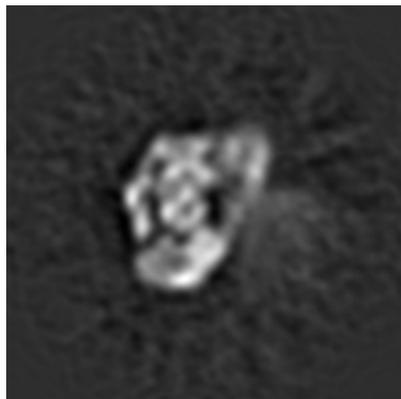


Z Index: 62

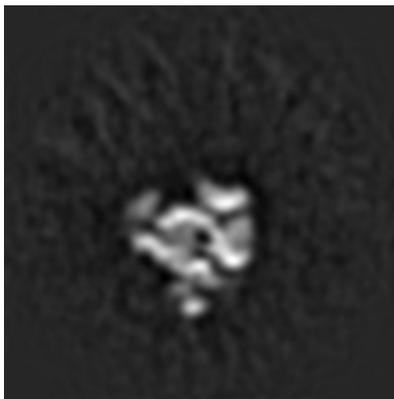
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

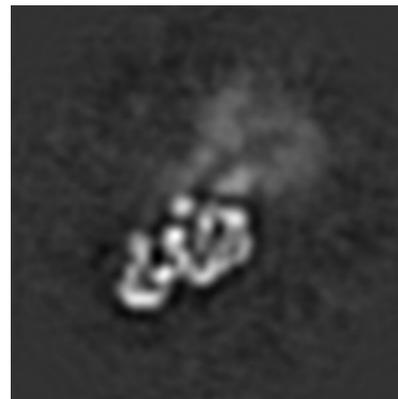
6.3.1 Primary map



X Index: 60



Y Index: 42

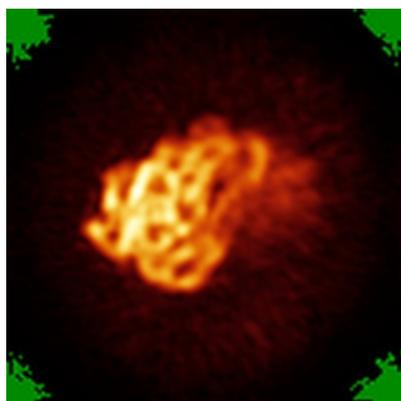


Z Index: 65

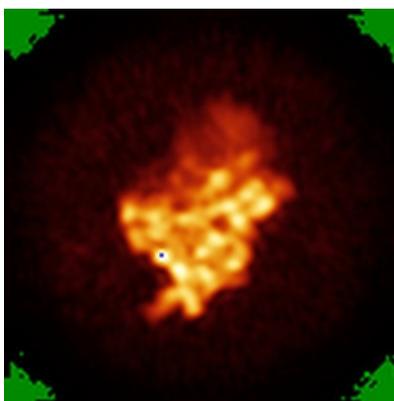
The images above show the largest variance slices of the map in three orthogonal directions.

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

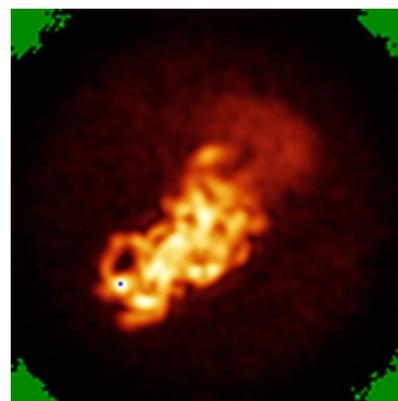
6.4.1 Primary map



X



Y

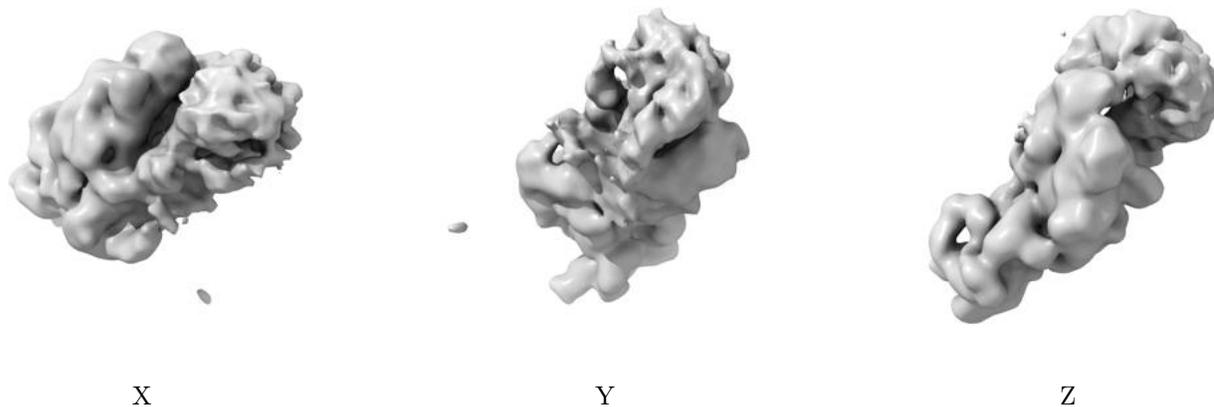


Z

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 - 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

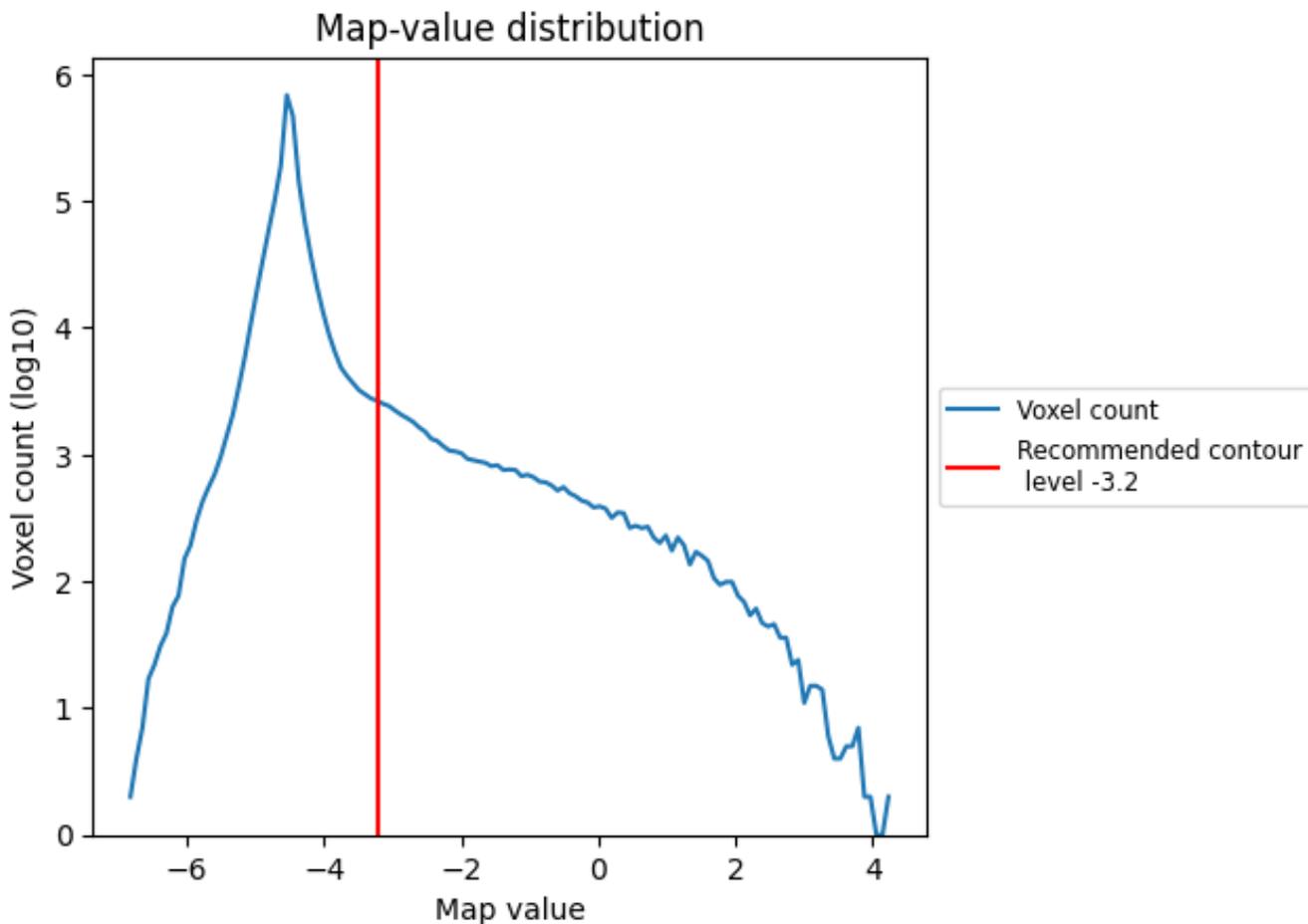
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

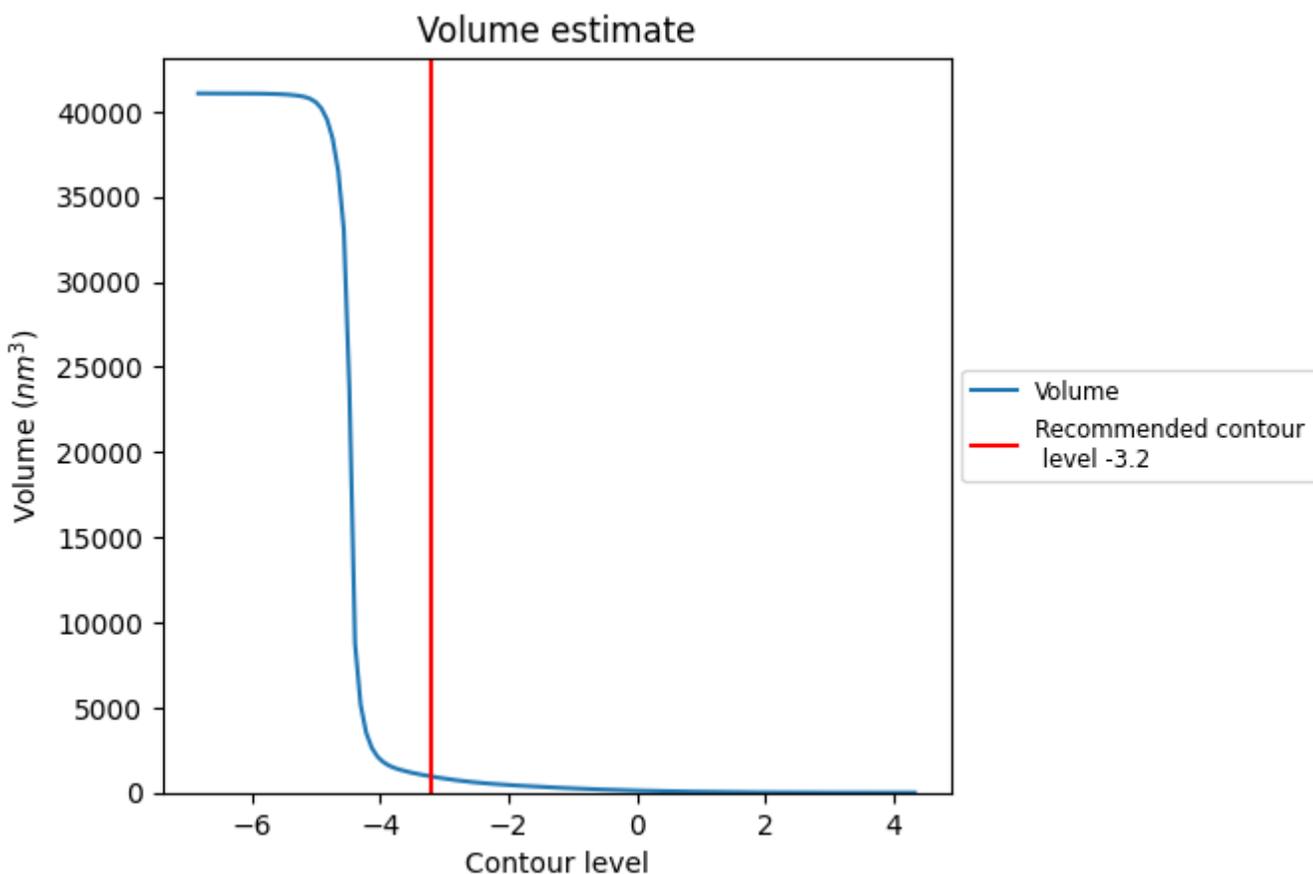
This section contains the results of statistical analysis of the map.

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.

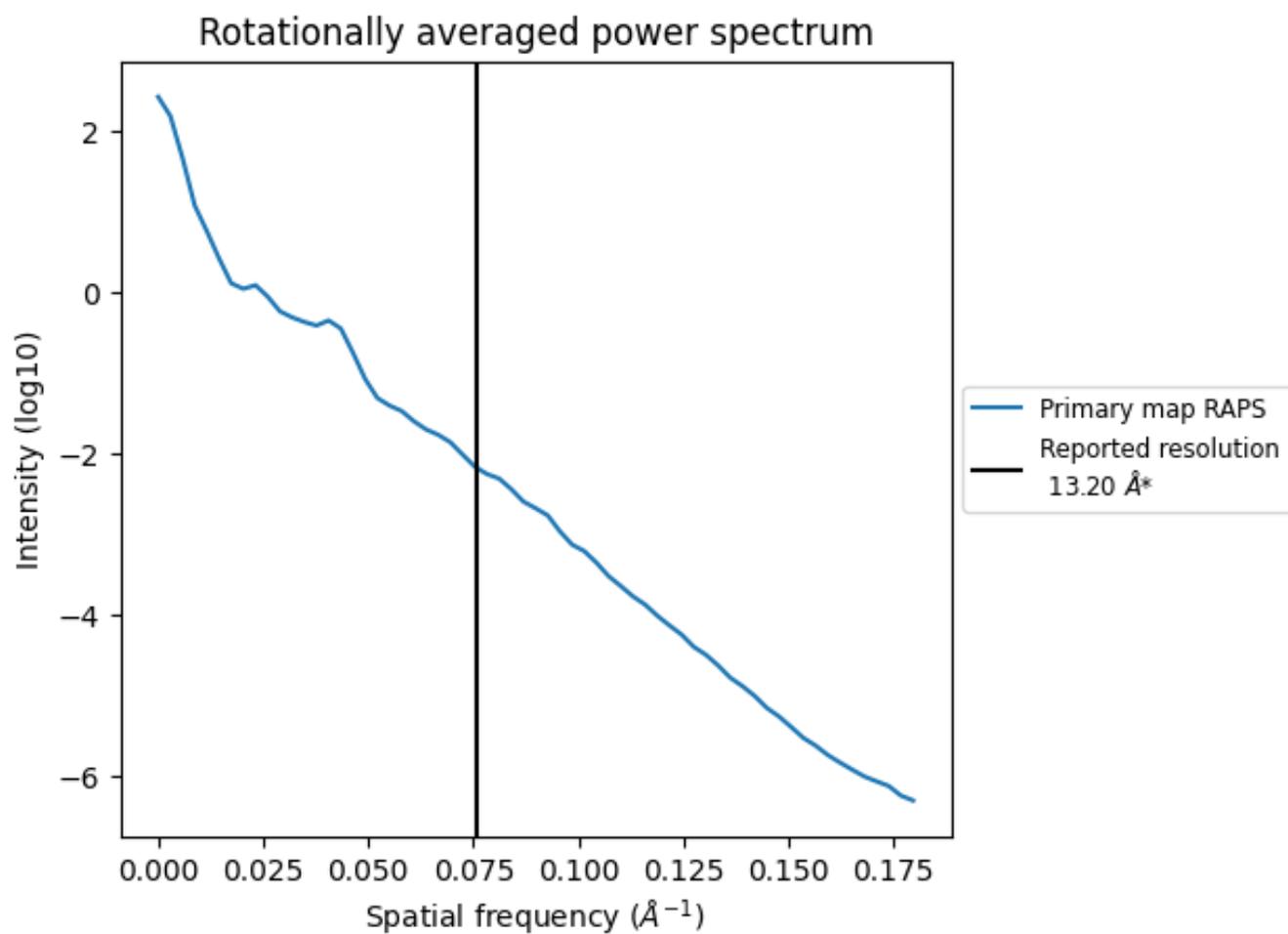
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.076 Å⁻¹

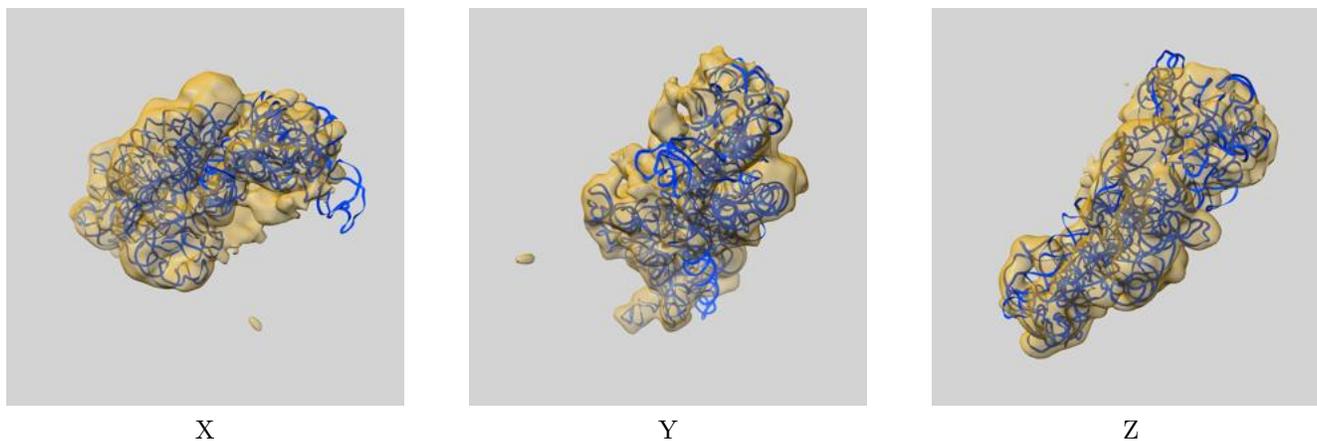
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

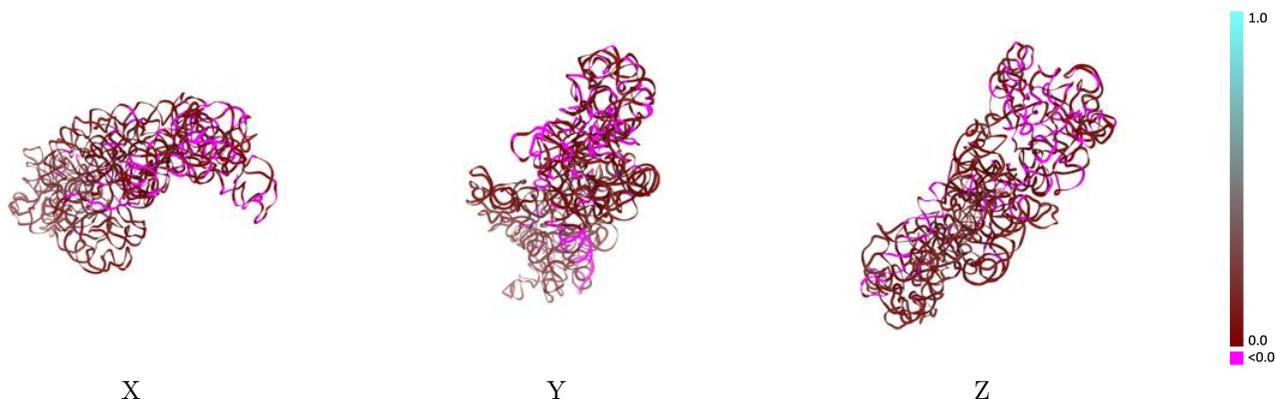
This section contains information regarding the fit between EMDB map EMD-5504 and PDB model 3J2C. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



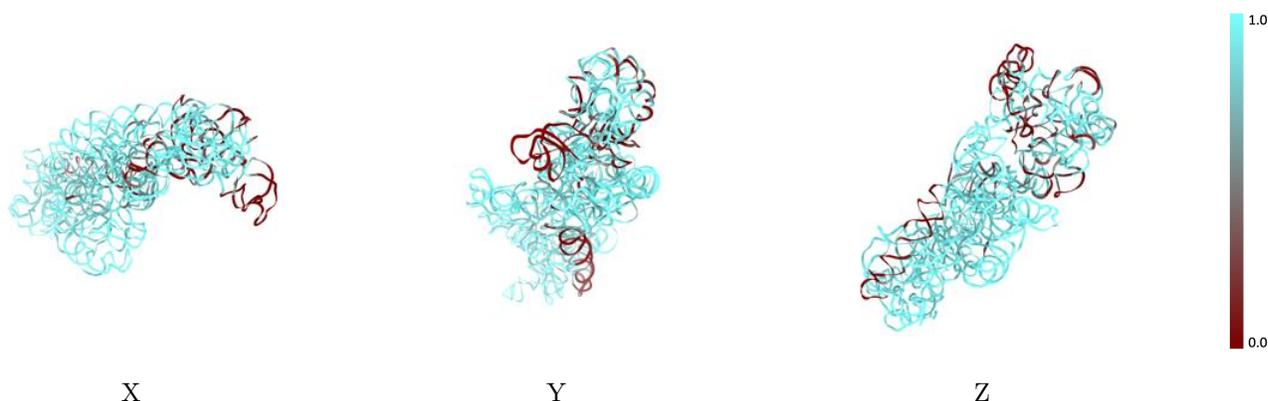
The images above show the 3D surface view of the map at the recommended contour level -3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



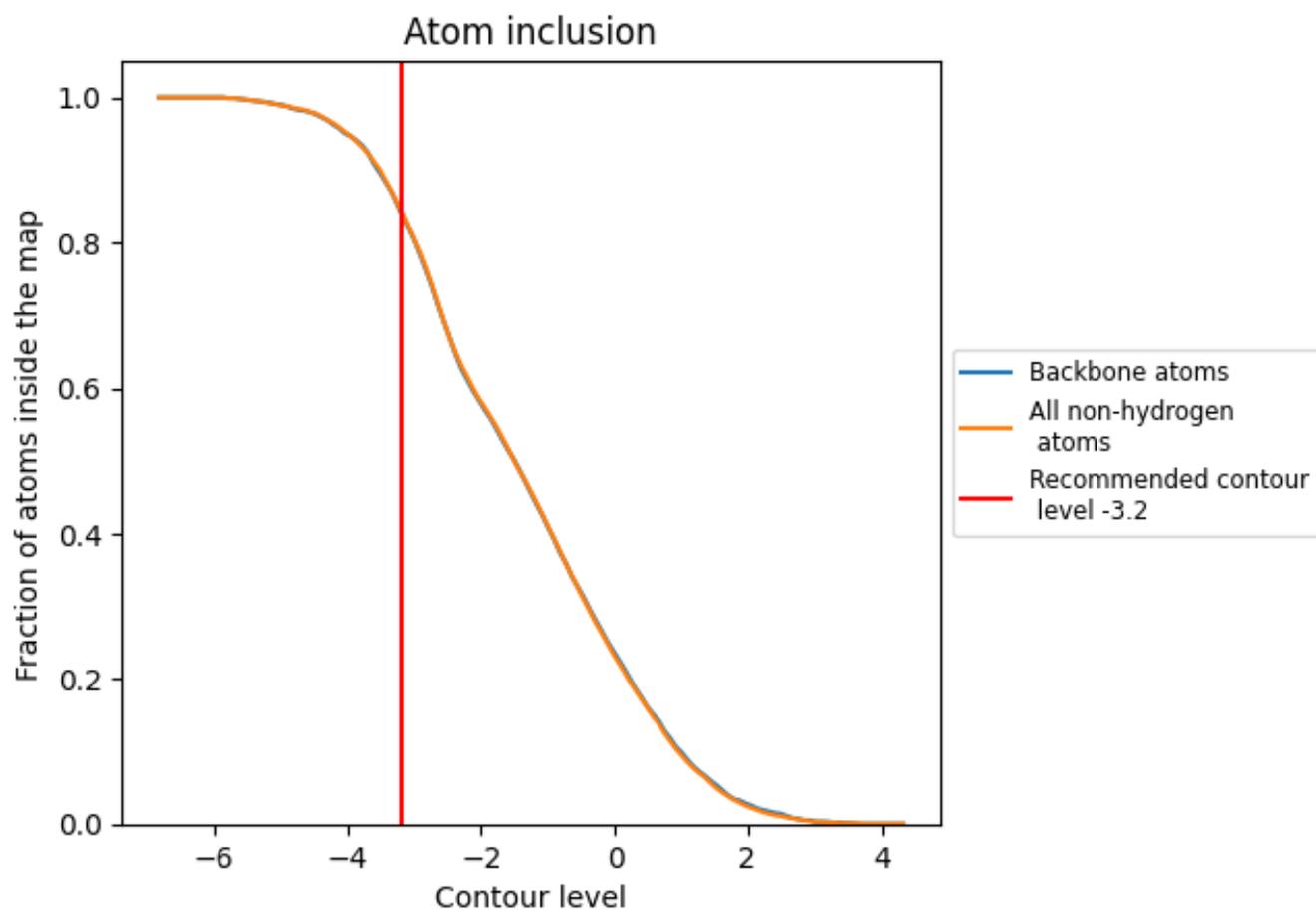
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.8450	 0.0760
M	 0.6650	 0.0380
N	 0.9860	 0.1040
O	 0.5350	 0.0120

