



wwPDB EM Validation Summary Report ⓘ

Mar 3, 2024 – 07:54 AM EST

PDB ID : 6C06
EMDB ID : EMD-7323
Title : Mycobacterium tuberculosis RNAP Holo/RbpA/Fidaxomicin
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.; Lilic, M.
Deposited on : 2017-12-27
Resolution : 5.15 Å (reported)

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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
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
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

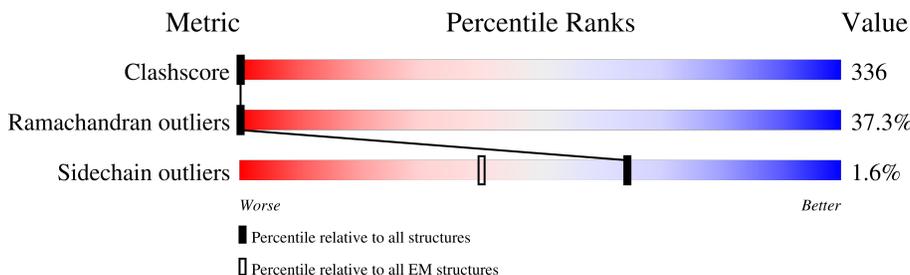
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.15 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	347	37% 28% 35%
1	B	347	48% 19% 32%
2	C	1181	58% 33% 6%
3	D	1324	54% 37% 5%
4	E	110	37% 35% 25%
5	F	531	39% 19% 39%
6	J	111	9% 63% 31%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	FI8	D	1404	X	-	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 26170 atoms, of which 74 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	1111	Total	C	N	O	S	0	0
			8556	5361	1504	1652	39		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879
C	1186	GLY	-	expression tag	UNP V9Z879
C	1187	ALA	-	expression tag	UNP V9Z879

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	1263	Total	C	N	O	S	0	0
			9857	6175	1791	1850	41		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	83	649	414	108	127	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	326	2588	1617	467	495	9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	107	872	539	162	168	3	0	0

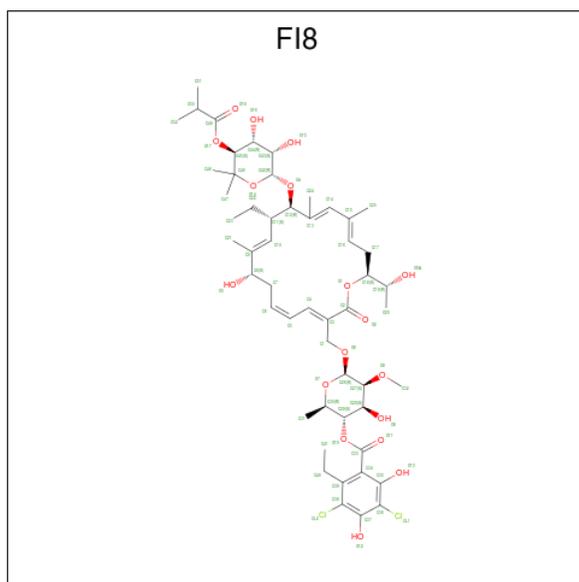
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Zn	0
			2	2	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

- Molecule 9 is Fidaxomicin (three-letter code: FI8) (formula: C₅₂H₇₄Cl₂O₁₈).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	H		O
9	D	1	146	52	2	74	18	0

HIS	GLN	LEU	GLY	LEU	SER	LEU	ARG	SER	LEU	LYS	ASP	PRO	PRO	PRO	PRO	GLU	VAL	ALA	GLY	TYR	ASP	ASN	VAL	VAL	ALA	ALA	THR	GLY	THR	TRP	SER	SER	THR	GLU	GLY	GLY	ALA	ALA	GLU	THR	GLU	GLN	LEU
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● Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 58% 33% 6%

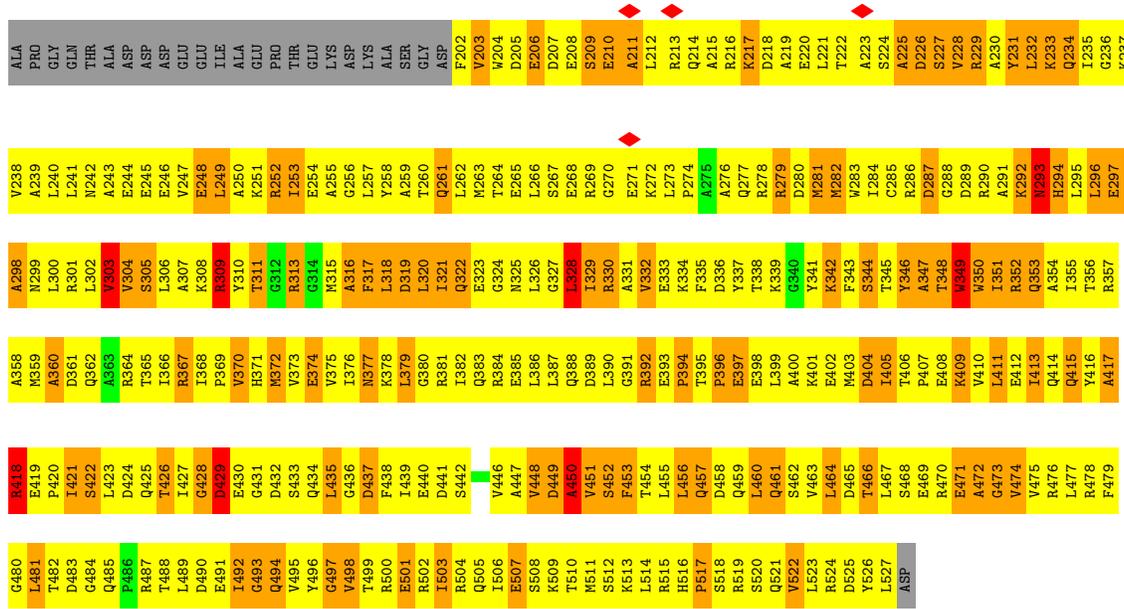
MET	ALA	ASP	SER	GLN	SER	LEU	ARG	SER	LEU	LYS	THR	PRO	PRO	PRO	PRO	ARG	PRO	GLN	SER	SER	SER	ASN	VAL	VAL	ALA	ALA	THR	GLY	THR	TRP	SER	SER	THR	GLU	GLY	GLY	ALA	ALA	GLU	THR	GLU	GLN	LEU																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
S67	P68	R69	W70	R71	E72	S73	A74	A75	A76	A77	E78	N81	N82	N83	N84	N85	N86	N87	N88	N89	N90	N91	N92	N93	N94	N95	N96	N97	N98	N99	S100	S101	S102	S103	S104	S105	S106	S107	S108	S109	S110	S111	S112	S113	S114	S115	S116	S117	S118	S119	S120	S121	S122	S123	S124	S125	S126	S127	S128	S129	S130	S131	S132	S133	S134	S135	S136	S137	S138	S139	S140	S141	S142	S143	S144	S145	S146	S147	S148	S149	S150	S151	S152	S153	S154	S155	S156	S157	S158	S159	S160	S161	S162	S163	S164	S165	S166	S167	S168	S169	S170	S171	S172	S173	S174	S175	S176	S177	S178	S179	S180	S181	S182	S183	S184	S185	S186	S187	S188	S189	S190	S191	S192	S193	S194	S195	S196	S197	S198	S199	S200	S201	S202	S203	S204	S205	S206	S207	S208	S209	S210	S211	S212	S213	S214	S215	S216	S217	S218	S219	S220	S221	S222	S223	S224	S225	S226	S227	S228	S229	S230	S231	S232	S233	S234	S235	S236	S237	S238	S239	S240	S241	S242	S243	S244	S245	S246	S247	S248	S249	S250	S251	S252	S253	S254	S255	S256	S257	S258	S259	S260	S261	S262	S263	S264	S265	S266	S267	S268	S269	S270	S271	S272	S273	S274	S275	S276	S277	S278	S279	S280	S281	S282	S283	S284	S285	S286	S287	S288	S289	S290	S291	S292	S293	S294	S295	S296	S297	S298	S299	S300	S301	S302	S303	S304	S305	S306	S307	S308	S309	S310	S311	S312	S313	S314	S315	S316	S317	S318	S319	S320	S321	S322	S323	S324	S325	S326	S327	S328	S329	S330	S331	S332	S333	S334	S335	S336	S337	S338	S339	S340	S341	S342	S343	S344	S345	S346	S347	S348	S349	S350	S351	S352	S353	S354	S355	S356	S357	S358	S359	S360	S361	S362	S363	S364	S365	S366	S367	S368	S369	S370	S371	S372	S373	S374	S375	S376	S377	S378	S379	S380	S381	S382	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S397	S398	S399	S400	S401	S402	S403	S404	S405	S406	S407	S408	S409	S410	S411	S412	S413	S414	S415	S416	S417	S418	S419	S420	S421	S422	S423	S424	S425	S426	S427	S428	S429	S430	S431	S432	S433	S434	S435	S436	S437	S438	S439	S440	S441	S442	S443	S444	S445	S446	S447	S448	S449	S450	S451	S452	S453	S454	S455	S456	S457	S458	S459	S460	S461	S462	S463	S464	S465	S466	S467	S468	S469	S470	S471	S472	S473	S474	S475	S476	S477	S478	S479	S480	S481	S482	S483	S484	S485	S486	S487	S488	S489	S490	S491	S492	S493	S494	S495	S496	S497	S498	S499	S500	S501	S502	S503	S504	S505	S506	S507	S508	S509	S510	S511	S512	S513	S514	S515	S516	S517	S518	S519	S520	S521	S522	S523	S524	S525	S526	S527	S528	S529	S530	S531	S532	S533	S534	S535	S536	S537	S538	S539	S540	S541	S542	S543	S544	S545	S546	S547	S548	S549	S550	S551	S552	S553	S554	S555	S556	S557	S558	S559	S560	S561	S562	S563	S564	S565	S566	S567	S568	S569	S570	S571	S572	S573	S574	S575	S576	S577	S578	S579	S580	S581	S582	S583	S584	S585	S586	S587	S588	S589	S590	S591	S592	S593	S594	S595	S596	S597	S598	S599	S600	S601	S602	S603	S604	S605	S606	S607	S608	S609	S610	S611	S612	S613	S614	S615	S616	S617	S618	S619	S620	S621	S622	S623	S624	S625	S626	S627	S628	S629	S630	S631	S632	S633	S634	S635	S636	S637	S638	S639	S640	S641	S642	S643	S644	S645	S646	S647	S648	S649	S650	S651	S652	S653	S654	S655	S656	S657	S658	S659	S660	S661	S662	S663	S664	S665	S666	S667	S668	S669	S670	S671	S672	S673	S674	S675	S676	S677	S678	S679	S680	S681	S682	S683	S684	S685	S686	S687	S688	S689	S690	S691	S692	S693	S694	S695	S696	S697	S698	S699	S700	S701	S702	S703	S704	S705	S706	S707	S708	S709	S710	S711	S712	S713	S714	S715	S716	S717	S718	S719	S720	S721	S722	S723	S724	S725	S726	S727	S728	S729	S730	S731	S732	S733	S734	S735	S736	S737	S738	S739	S740	S741	S742	S743	S744	S745	S746	S747	S748	S749	S750	S751	S752	S753	S754	S755	S756	S757	S758	S759	S760	S761	S762	S763	S764	S765	S766	S767	S768	S769	S770	S771	S772	S773	S774	S775	S776	S777	S778	S779	S780	S781	S782	S783	S784	S785	S786	S787	S788	S789	S790	S791	S792	S793	S794	S795	S796	S797	S798	S799	S800	S801	S802	S803	S804	S805	S806	S807	S808	S809	S810	S811	S812	S813	S814	S815	S816	S817	S818	S819	S820	S821	S822	S823	S824	S825	S826	S827	S828	S829	S830	S831	S832	S833	S834	S835	S836	S837	S838	S839	S840	S841	S842	S843	S844	S845	S846	S847	S848	S849	S850	S851	S852	S853	S854	S855	S856	S857	S858	S859	S860	S861	S862	S863	S864	S865	S866	S867	S868	S869	S870	S871	S872	S873	S874	S875	S876	S877	S878	S879	S880	S881	S882	S883	S884	S885	S886	S887	S888	S889	S890	S891	S892	S893	S894	S895	S896	S897	S898	S899	S900	S901	S902	S903	S904	S905	S906	S907	S908	S909	S910	S911	S912	S913	S914	S915	S916	S917	S918	S919	S920	S921	S922	S923	S924	S925	S926	S927	S928	S929	S930	S931	S932	S933	S934	S935	S936	S937	S938	S939	S940	S941	S942	S943	S944	S945	S946	S947	S948	S949	S950	S951	S952	S953	S954	S955	S956	S957	S958	S959	S960	S961	S962	S963	S964	S965	S966	S967	S968	S969	S970	S971	S972	S973	S974	S975	S976	S977	S978	S979	S980	S981	S982	S983	S984	S985	S986	S987	S988	S989	S990	S991	S992	S993	S994	S995	S996	S997	S998	S999	S1000	S1001	S1002	S1003	S1004	S1005	S1006	S1007	S1008	S1009	S1010	S1011	S1012	S1013	S1014	S1015	S1016	S1017	S1018	S1019	S1020	S1021	S1022	S1023	S1024	S1025	S1026	S1027	S1028	S1029	S1030	S1031	S1032	S1033	S1034	S1035	S1036	S1037	S1038	S1039	S1040	S1041	S1042	S1043	S1044	S1045	S1046	S1047	S1048	S1049	S1050	S1051	S1052	S1053	S1054	S1055	S1056	S1057	S1058	S1059	S1060	S1061	S106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Q967	Y1027	E1087	LEU
P968	M1028	L1088	ARG
A969	Y1029	L1089	GLU
A970	I1030	L1090	GLY
Y971	M1031	I1091	GLU
Y972	K1032	K1092	ASP
S973	L1033	S1093	GLU
F974	H1034	D1094	ASP
F975	H1035	D1095	LEU
Y976	L1036	L1096	GLU
F977	V1037	V1097	ARG
D978	D1038	D1098	ALA
G979	D1039	R1099	ALA
A980	K1040	V1100	ALA
Q981	I1041	K1101	ASN
E982	H1042	V1102	LEU
A983	A1043	Y1103	GLY
E984	R1044	E1104	ILE
L985	S1045	A1105	ASN
Q986	T1046	I1106	LEU
G987	G1047	V1107	SER
L988	P1048	K1108	ARG
L989	Y1049	G1109	ASN
S990	S1050	R1110	GLU
C991	M1051	N1111	SER
T992	L1052	I1112	ALA
L993	T1053	P1113	SER
P994	Q1054	Q1114	VAL
A995	Q1055	P1115	GLU
R996	P1056	A1116	ASP
D997	L1057	I1117	LEU
G998	G1058	P1118	ALA
D999	G1059	E1119	LEU
V1000	K1060	S1120	ALA
L1001	A1061	F1121	ARG
V1002	Q1062	H1122	HIS
D1003	F1063	V1123	GLY
A1004	G1064	L1124	GLY
D1005	G1065	L1125	SER
G1006	Q1066	K1126	GLY
K1007	R1067	E1127	ALA
A1008	F1068	L1128	F107
M1009	G1069	K1129	C48
L1010	E1070	S1130	E49
F1011	M1071	L1131	K60
D1012	E1072	C1132	G45
G1013	C1073	L1133	F47
R1014	W1074	M1134	K108
S1015	A1075	V1135	G109
K1016	M1076	E1136	E109
E1017	Q1077	V1137	V110
P1018	A1078	L1138	P111
F1019	Y1079	S1139	S112
P1020	G1080	L1140	R113
Y1021	A1081	GLY	G53
P1022	A1082	ALA	P84
V1023	X1083	ALA	T55
V1024	T1084	ILE	D57
V1025	L1085	ALA	M68
G1026	Q1086	GLU	L118
			L119
			L120

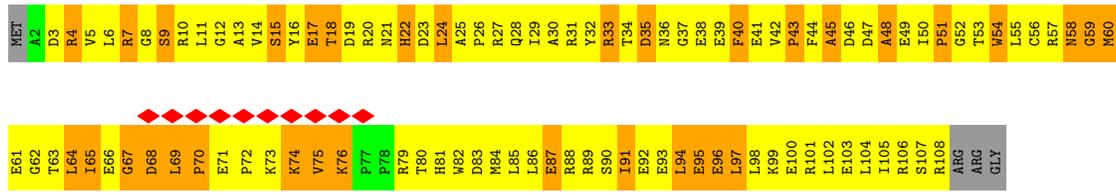
• Molecule 3: DNA-directed RNA polymerase subunit beta'



MET	Y61	A121	L181	Y241	A301	A362	V422	Q482	A542	A602	H662
LEU	C62	P122	A182	R242	F302	P363	D423	V483	V543	S603	M663
ASP	G63	K123	E183	L244	Q303	I364	Y424	W484	H544	G604	A664
V4	K64	D124	L184	V245	Q304	L365	S425	D485	L545	D605	E665
N5	K65	L125	E185	D246	N307	V367	R426	W486	P546	H606	T666
F6	G66	E126	L186	R247	S308	M368	S428	E488	S548	P607	T667
F7	R67	K127	E187	Y248	P309	N369	Y429	E489	A549	E608	L668
D8	V68	I128	E188	G249	M310	E370	L430	V490	E550	T609	G689
E9	R69	L129	E189	E250	G311	K371	V431	I491	A551	G610	R670
L10	F70	G130	A190	F251	M312	R372	Y432	W492	Q552	V611	M671
R11	K71	F131	A191	F252	K313	K373	G433	A493	Q553	Y612	M672
I12	G72	A132	K190	T253	L314	L374	P434	H494	E554	S613	F673
G13	I73	A133	A191	G254	D315	Q375	Q435	P495	A555	M614	M674
L14	I74	Y134	D192	A255	A316	E376	L436	V496	R556	P615	E675
A15	C75	V135	D193	E256	V317	S377	K437	L497	L557	A616	L676
T16	E76	T136	A193	M256	P318	E378	L438	L498	L558	A617	L677
A17	R77	T137	R194	A258	V319	R379	H439	M499	M559	A618	F678
E18	C78	S138	R194	E259	I320	A380	Q440	A501	L560	L619	L679
D19	G79	V139	R195	E260	I321	L381	C441	A501	S561	M620	G680
I20	V80	D140	K196	S260	P322	F382	G442	A501	S562	A621	F681
R21	E81	E141	V197	L261	P323	D383	L443	T503	S563	A622	F682
Q22	R82	E142	R198	Q262	E323	D384	L443	T503	M563	D623	F683
K29	S83	E143	R198	K263	L324	N384	P444	L504	M564	R624	V684
S24	R84	R144	D199	L264	K325	G385	K445	H505	I565	G625	N685
S24	S24	R144	G200	L265	P326	R386	L446	R506	L566	V626	K686
Y25	A85	H145	G201	E266	M327	R387	M447	L507	S567	L627	Q687
G26	K86	M146	E202	E266	V328	G388	A448	G508	P568	S628	H688
E27	V87	E147	R203	N267	Q329	R389	L449	T509	A569	V629	H689
E28	R88	L148	R204	F268	E330	R390	L449	T509	S570	R630	K690
Q28	R89	E149	E204	D269	L330	P391	E450	Q510	K571	A631	K691
K29	E90	A150	M205	E270	D331	V392	L451	A511	C571	A631	K691
K30	E90	A156	M205	L271	G332	T392	F452	F512	R572	K632	K692
A156	R91	L151	R206	D271	G333	C393	F452	F512	R573	K633	V693
P31	M92	E152	Q207	A272	G334	C394	K453	E513	P573	L634	Q693
E32	E92	E153	Q207	E273	R335	G395	P454	P514	L574	A634	A694
E33	I93	A154	I208	E273	F336	N396	F455	M515	A575	V635	A695
I34	H94	E154	R209	A274	A337	E397	V456	L516	M576	R636	T696
N35	N95	M155	R210	E275	L338	R397	V457	V517	P577	L637	L697
Y36	E96	A156	R211	S276	T337	P398	K458	K458	P398	T638	N698
Y36	L97	A156	R212	L277	S338	S398	K458	K458	L399	Q639	D699
R37	L97	V157	A212	L277	S338	L399	L459	G519	L460	L640	L700
R37	A98	E158	Q213	R278	D339	L399	L460	K520	V461	R641	A701
T38	A99	R159	Q214	D279	L340	S401	L461	K521	D462	E702	E702
L39	P100	K160	R215	V280	N341	S401	L462	A521	D462	P642	E703
L46	K40	E161	L216	I281	L342	L402	L463	I522	L463	P643	R703
P41	P101	A162	D217	R282	L343	S403	L464	Q523	L464	P644	Y704
E42	E102	V162	D217	N283	Y344	D404	H465	L524	H465	E645	P705
K43	K43	E163	R218	G284	R345	L405	H465	H525	L406	E646	K706
G109	M104	D164	L219	K285	R346	L406	A466	P526	K407	L646	V706
G45	W106	Q165	E220	G286	V347	K407	Q467	V527	G408	E647	T707
F47	F107	D167	D221	Q287	I348	G408	Q468	V528	L588	A648	V708
C48	K108	G168	R222	R288	K349	K409	K409	C529	T589	E649	V709
E49	E109	E169	S224	K289	R350	Q410	K470	E530	T590	L650	A710
K60	K60	E170	T225	L290	N351	G411	S471	A531	E591	F651	Q711
I51	P110	L170	T226	R291	M352	R412	A472	F532	V592	T712	T712
S112	S112	A172	I227	A292	R353	F413	K473	M533	P593	H652	G652
G53	R113	R173	K228	L293	L354	R414	R474	A534	A534	T713	H653
P84	L114	A174	L229	K294	K355	Q415	M475	D535	D595	D714	D714
T55	G115	Q175	A230	R295	R356	N416	V476	F536	D596	K715	K715
D57	L116	K176	P231	L296	L357	L417	E477	D537	T596	L716	L716
L117	L117	L177	K232	K297	I358	L418	R478	G538	G597	K717	K717
M68	L118	E178	Q233	V298	D359	G419	Q479	D539	E598	D718	D718
E59	L119	A179	L234	V299	L360	K420	R480	Q540	F600	A719	A719
C60	L120	A180	V236	A300	G361	R421	P481	M541	P601	G720	G720
			D237	E238	N239	L240				F721	F721



• Molecule 6: RNA polymerase-binding protein RbpA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	6.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.069	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0201	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	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: MG, FI8, ZN

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	0.51	0/1750	0.70	1/2380 (0.0%)
1	B	0.49	0/1802	0.69	0/2454
2	C	0.56	1/8714 (0.0%)	0.73	12/11824 (0.1%)
3	D	0.55	0/10021	0.73	11/13549 (0.1%)
4	E	0.53	0/662	0.71	0/901
5	F	0.46	0/2622	0.62	1/3538 (0.0%)
6	J	0.48	0/888	0.63	0/1199
All	All	0.54	1/26459 (0.0%)	0.71	25/35845 (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	3
1	B	0	2
2	C	0	32
3	D	0	36
4	E	0	4
5	F	0	5
6	J	0	1
All	All	0	83

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	723	ILE	C-N	-5.45	1.21	1.34

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	723	ILE	C-N-CA	-11.72	92.40	121.70
3	D	114	LEU	CA-CB-CG	-7.88	97.17	115.30
2	C	237	LEU	CA-CB-CG	-7.35	98.40	115.30
3	D	374	LEU	CA-CB-CG	-7.30	98.52	115.30
1	A	78	LEU	CA-CB-CG	-7.17	98.81	115.30

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	GLY	Peptide
1	A	42	LEU	Peptide
1	A	69	VAL	Peptide
1	B	204	PRO	Peptide
1	B	214	THR	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	1724	0	1768	1333	0
1	B	1775	0	1809	1380	0
2	C	8556	0	8459	5988	0
3	D	9857	0	9923	7031	0
4	E	649	0	645	424	0
5	F	2588	0	2602	1573	0
6	J	872	0	852	560	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
9	D	72	74	0	16	0
All	All	26096	74	26058	17506	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 336.

The worst 5 of 17506 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)
5:F:279:ARG:O	5:F:283:TRP:HB3	1.25	1.34
1:B:39:ARG:O	1:B:43:LEU:HB3	1.26	1.33
2:C:1099:ARG:O	2:C:1103:TYR:HB2	1.25	1.32
3:D:162:VAL:O	3:D:166:ARG:HB2	1.28	1.31
2:C:424:VAL:O	2:C:428:LYS:HB3	1.30	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	224/347 (65%)	80 (36%)	52 (23%)	92 (41%)	0	0
1	B	235/347 (68%)	98 (42%)	68 (29%)	69 (29%)	0	0
2	C	1109/1181 (94%)	394 (36%)	323 (29%)	392 (35%)	0	0
3	D	1257/1324 (95%)	396 (32%)	355 (28%)	506 (40%)	0	0
4	E	81/110 (74%)	14 (17%)	25 (31%)	42 (52%)	0	0
5	F	324/531 (61%)	109 (34%)	104 (32%)	111 (34%)	0	0
6	J	105/111 (95%)	45 (43%)	29 (28%)	31 (30%)	0	0
All	All	3335/3951 (84%)	1136 (34%)	956 (29%)	1243 (37%)	0	0

5 of 1243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	5	GLN
1	A	16	ASP
1	A	17	ASN
1	A	20	GLN

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	195/297 (66%)	190 (97%)	5 (3%)	46	66
1	B	197/297 (66%)	195 (99%)	2 (1%)	76	86
2	C	924/997 (93%)	910 (98%)	14 (2%)	65	80
3	D	1041/1103 (94%)	1026 (99%)	15 (1%)	67	80
4	E	69/89 (78%)	67 (97%)	2 (3%)	42	64
5	F	272/429 (63%)	269 (99%)	3 (1%)	73	84
6	J	93/97 (96%)	90 (97%)	3 (3%)	39	61
All	All	2791/3309 (84%)	2747 (98%)	44 (2%)	64	79

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	500	ARG
3	D	1268	ARG
3	D	733	MET
3	D	1085	ARG
4	E	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	234	GLN
5	F	325	ASN
2	C	751	HIS
2	C	729	HIS
5	F	353	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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
9	FI8	D	1404	-	74,75,75	1.90	19 (25%)	88,109,109	2.08	24 (27%)

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
9	FI8	D	1404	-	2/2/29/29	34/75/118/118	0/3/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1404	FI8	C1-C3	5.59	1.57	1.50
9	D	1404	FI8	C14-C15	4.48	1.54	1.45
9	D	1404	FI8	O1-C18	-3.96	1.39	1.46
9	D	1404	FI8	C14-C13	3.88	1.39	1.33
9	D	1404	FI8	O17-C49	3.83	1.43	1.34

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1404	FI8	C5-C4-C3	-7.51	117.97	127.00
9	D	1404	FI8	C29-O10-C33	-5.38	108.61	117.21
9	D	1404	FI8	C26-C27-C28	4.91	118.83	110.38
9	D	1404	FI8	C7-C6-C5	-4.62	119.45	125.41
9	D	1404	FI8	C31-C30-C29	-4.58	106.42	113.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	D	1404	FI8	C19
9	D	1404	FI8	C27

5 of 34 torsion outliers are listed below:

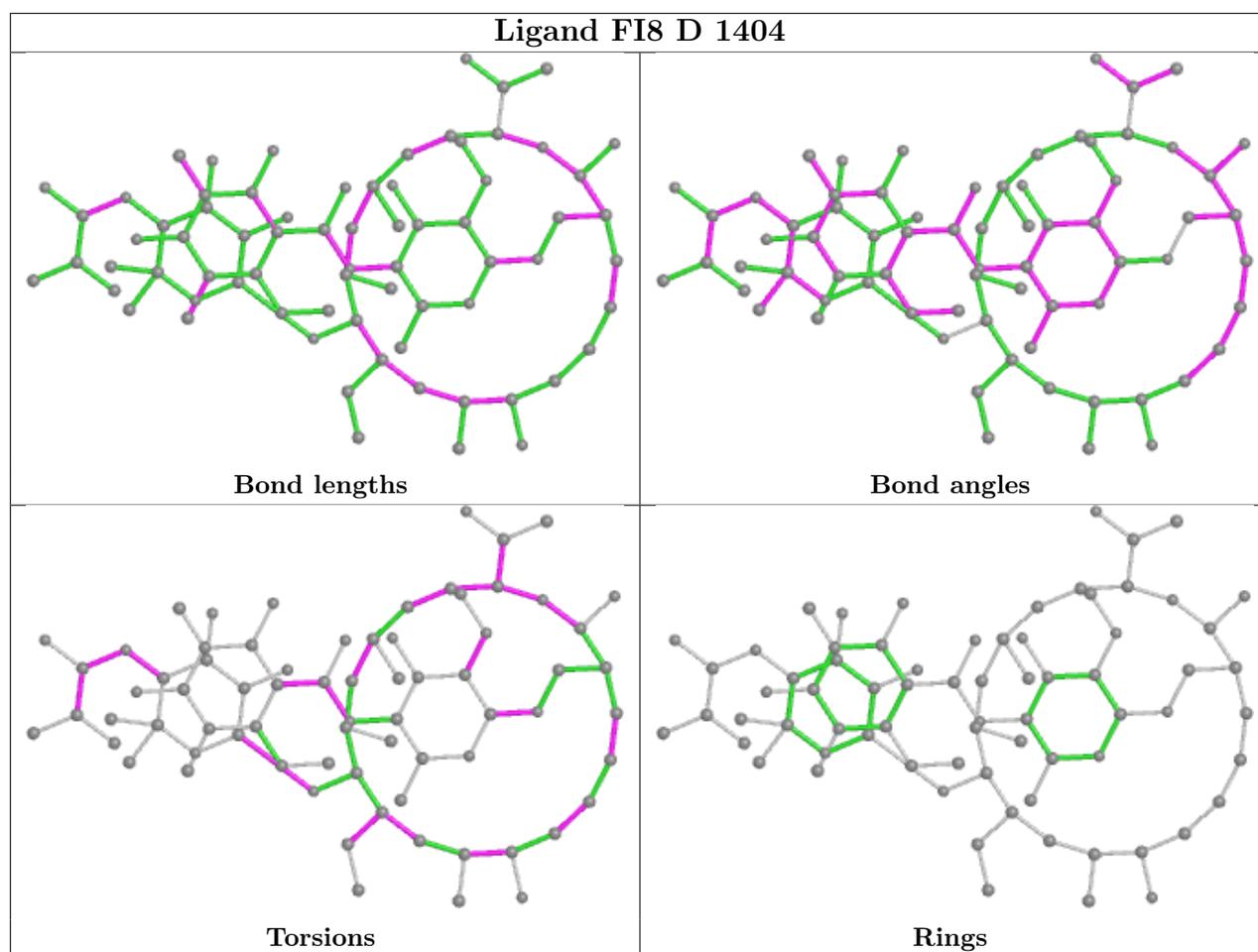
Mol	Chain	Res	Type	Atoms
9	D	1404	FI8	C9-C10-C11-C12
9	D	1404	FI8	C9-C10-C11-C22
9	D	1404	FI8	C15-C16-C17-C18
9	D	1404	FI8	C16-C17-C18-C19
9	D	1404	FI8	C17-C18-C19-O5A

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1404	FI8	16	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 [i](#)

There are no chain breaks in this entry.

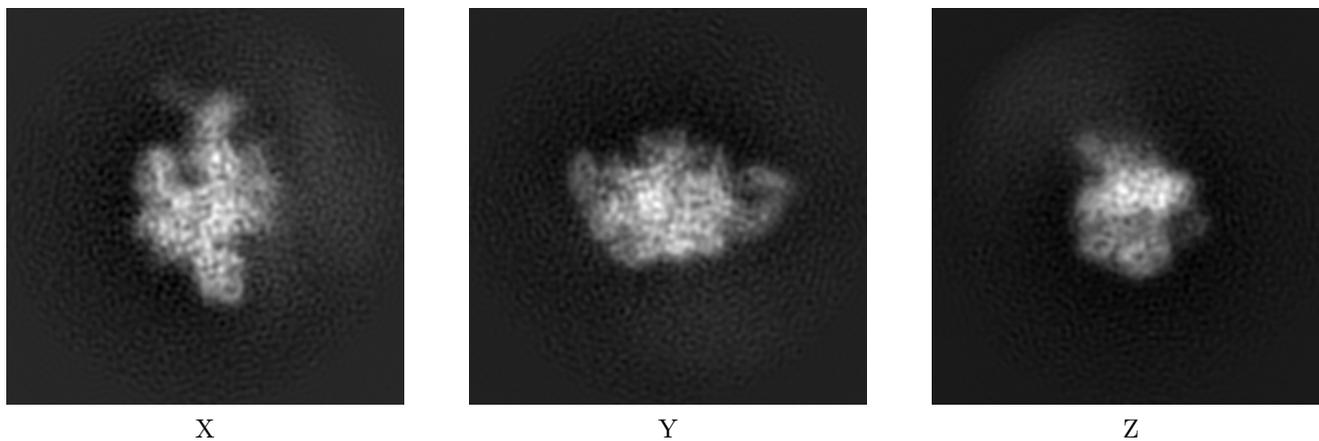
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-7323. 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](#)

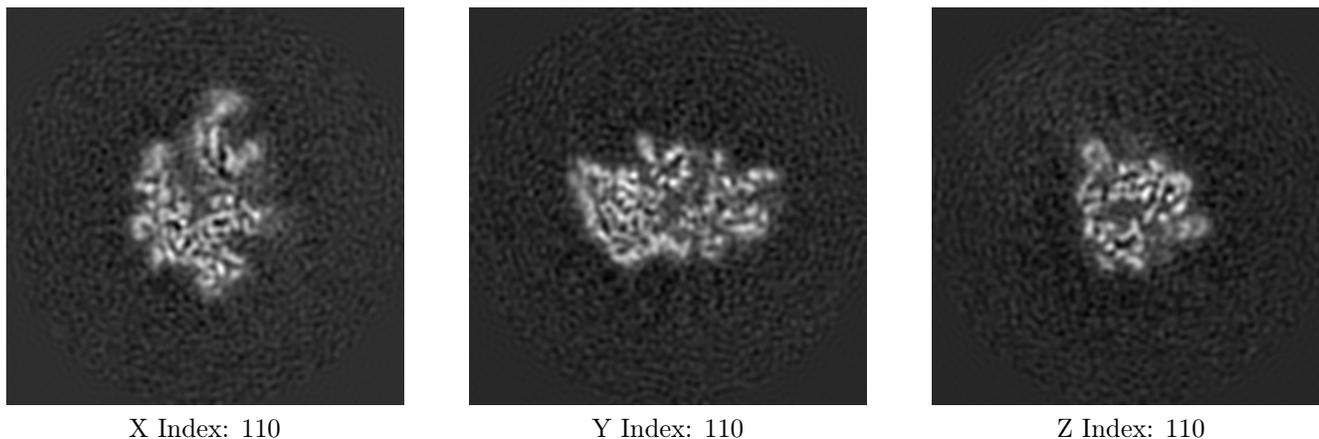
6.1.1 Primary map



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

6.2 Central slices [i](#)

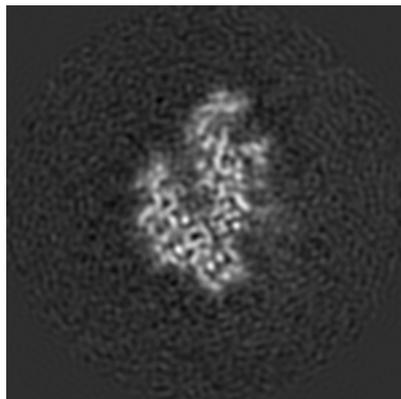
6.2.1 Primary map



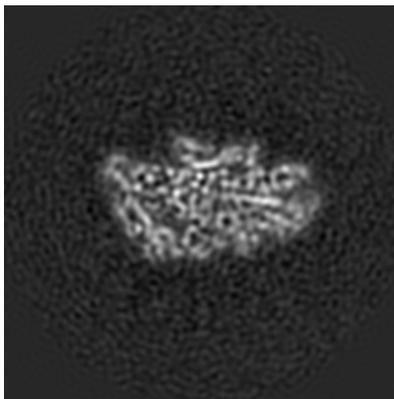
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

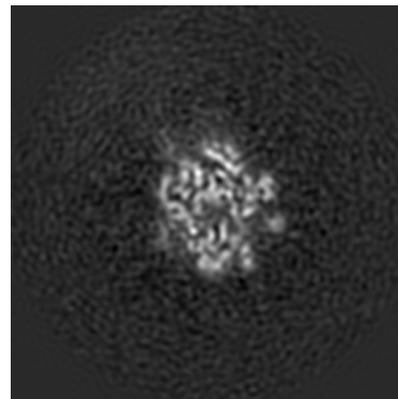
6.3.1 Primary map



X Index: 105



Y Index: 114

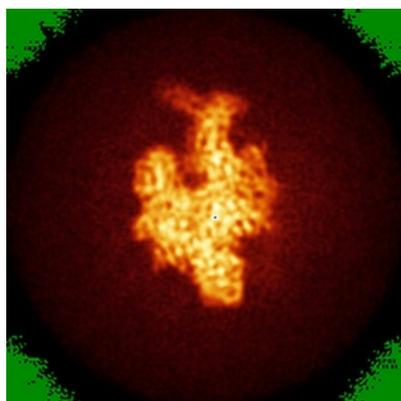


Z Index: 104

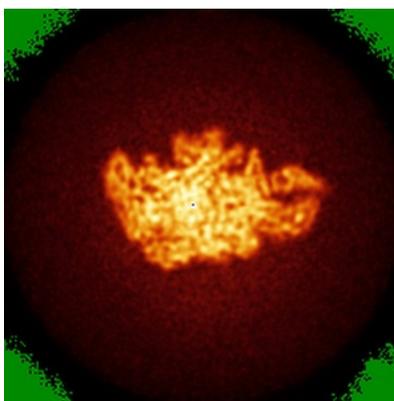
The images above show the largest variance slices of the map in three orthogonal directions.

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

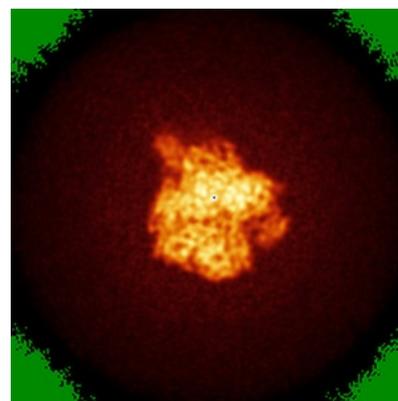
6.4.1 Primary map



X



Y

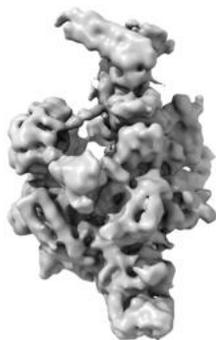


Z

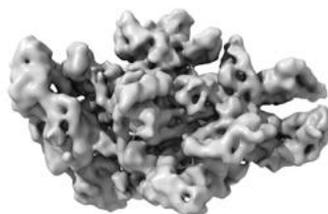
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

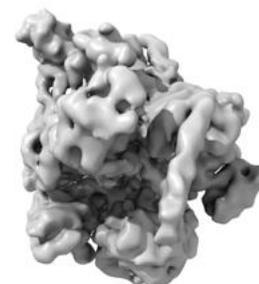
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0201. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

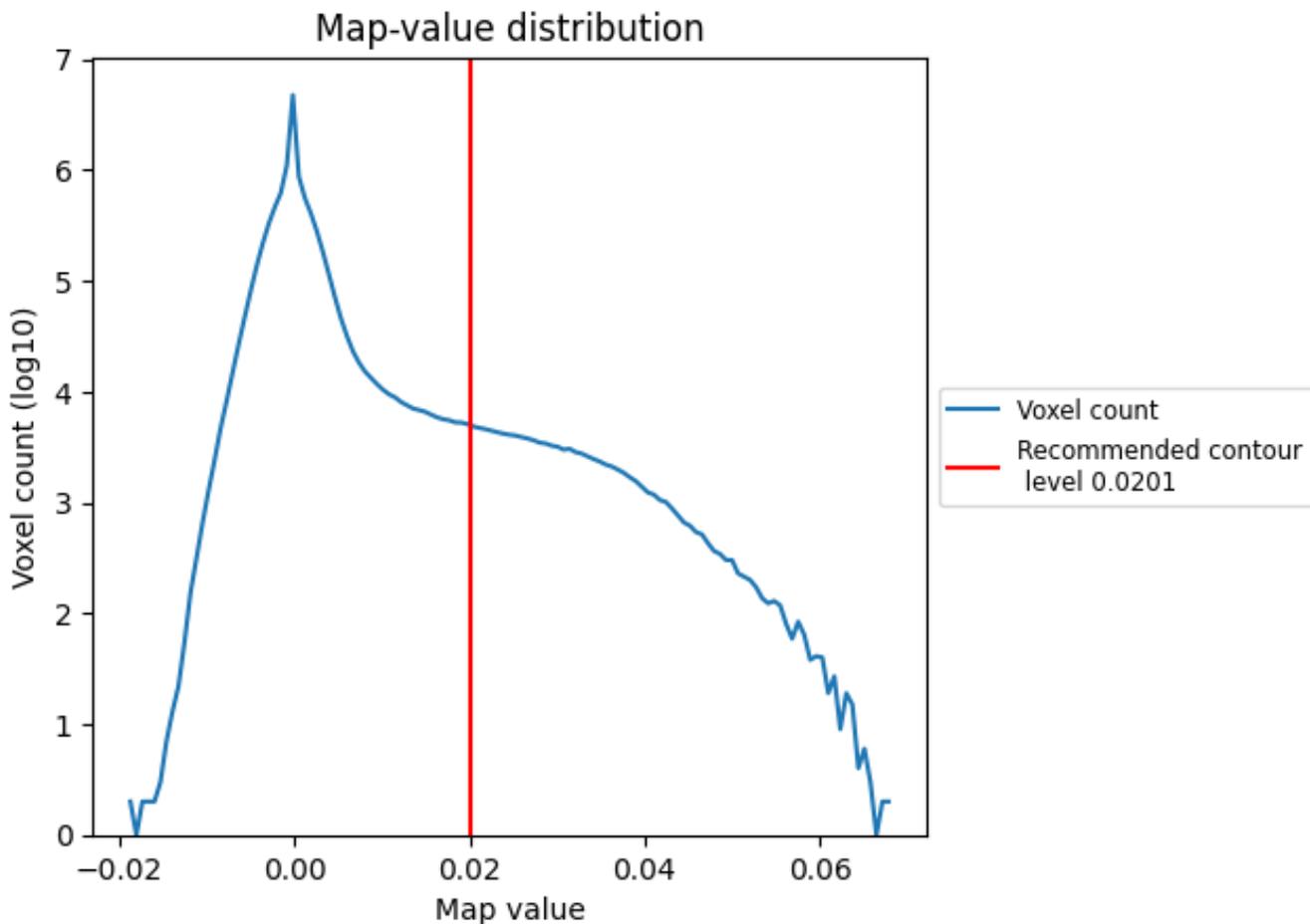
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

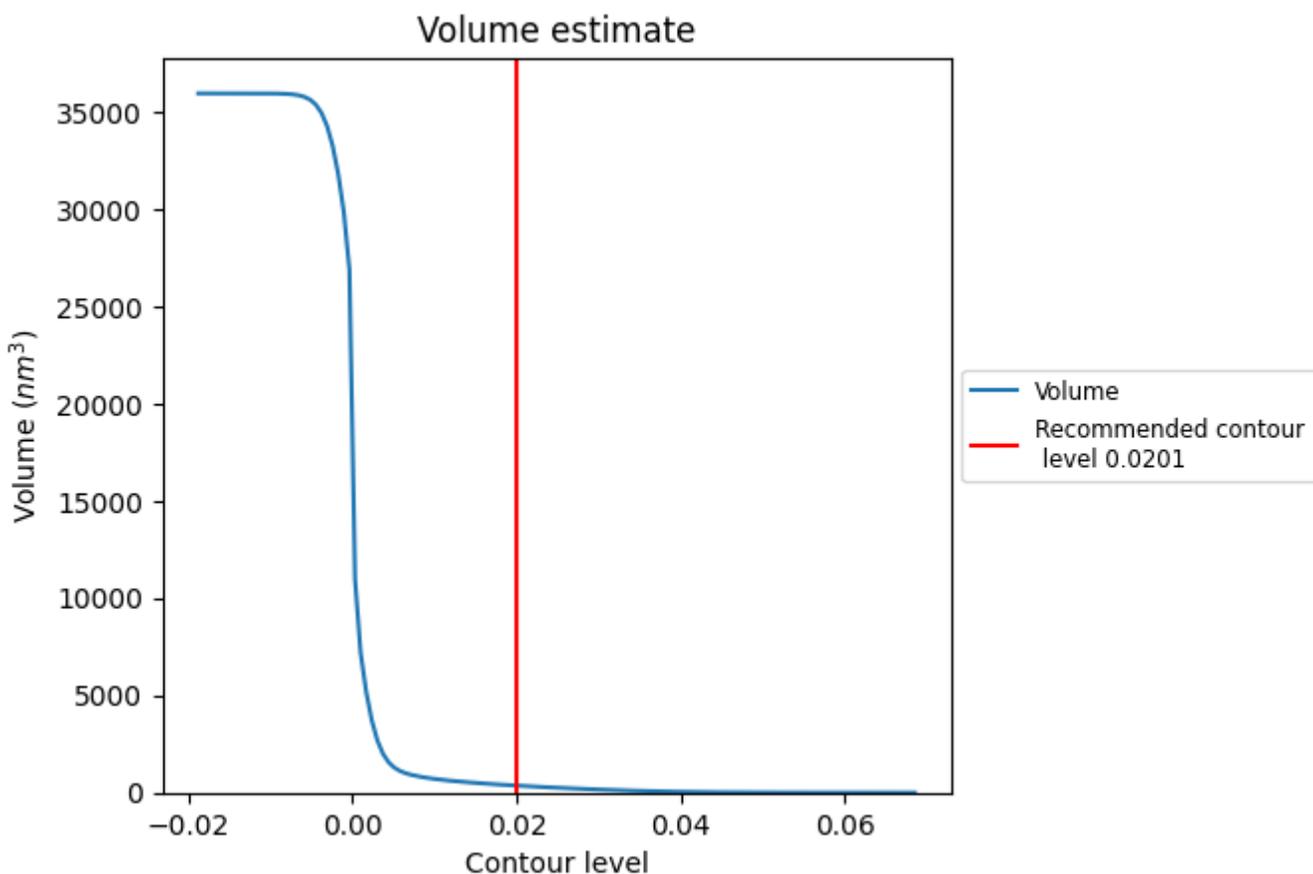
This section contains the results of statistical analysis of the map.

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.

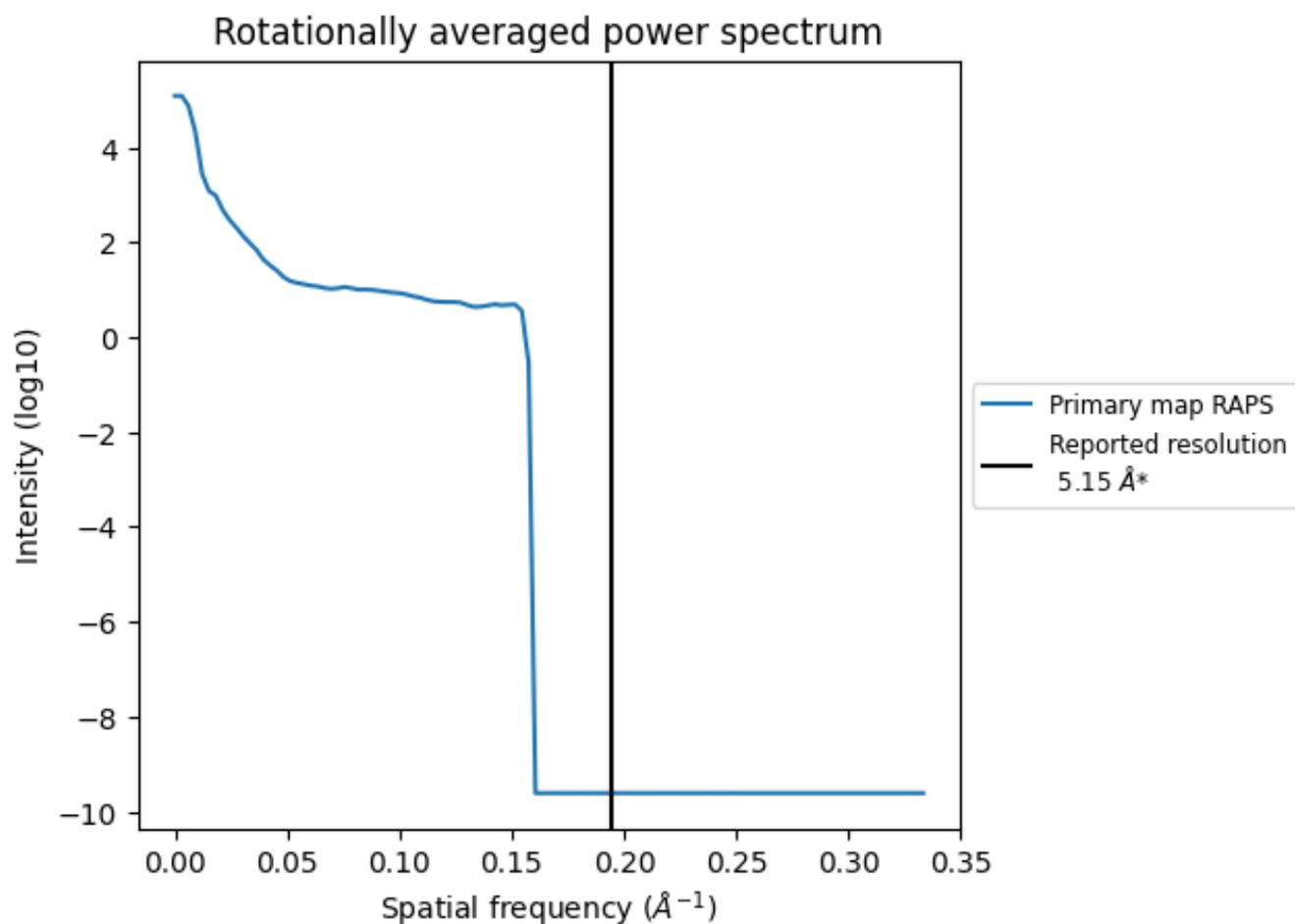
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm^3 ; this corresponds to an approximate mass of 323 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 0.194\AA^{-1}

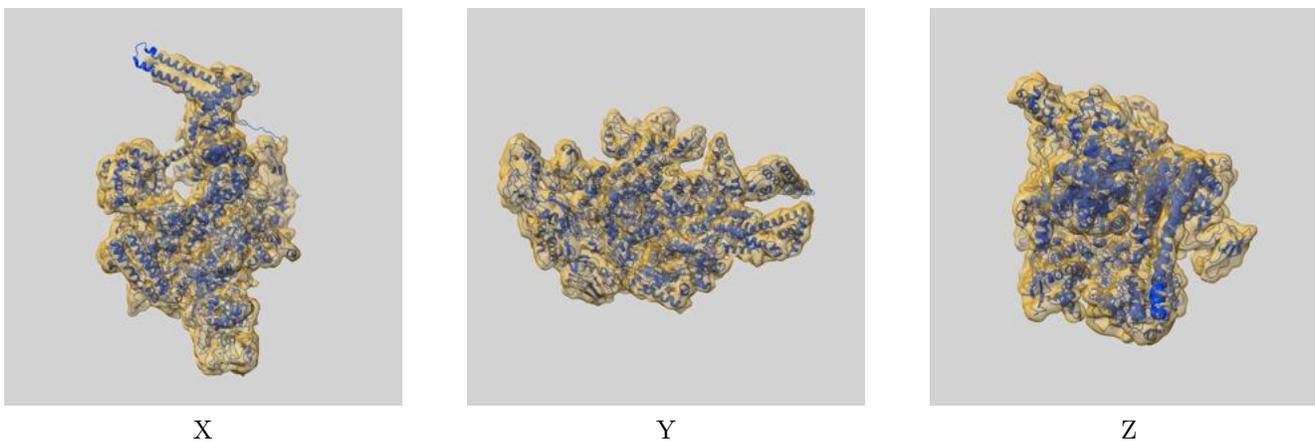
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

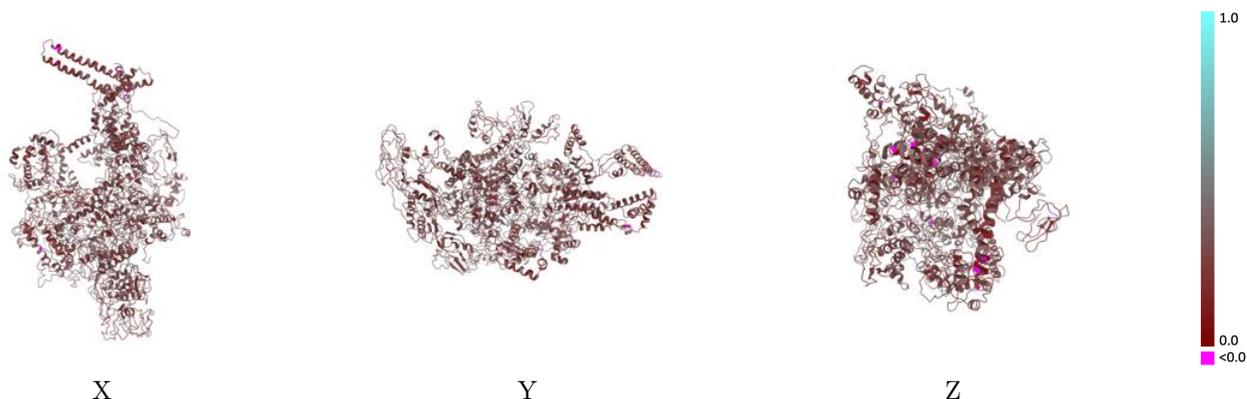
This section contains information regarding the fit between EMDB map EMD-7323 and PDB model 6C06. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



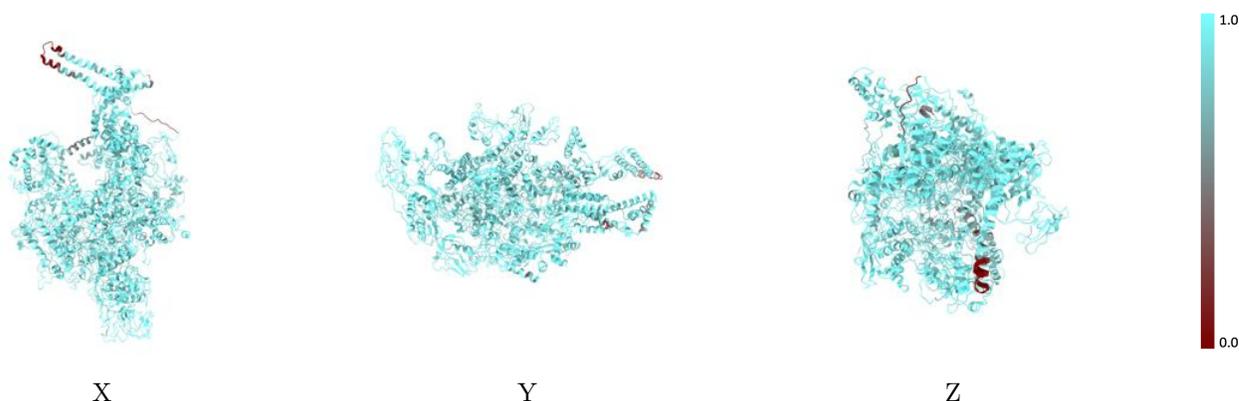
The images above show the 3D surface view of the map at the recommended contour level 0.0201 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



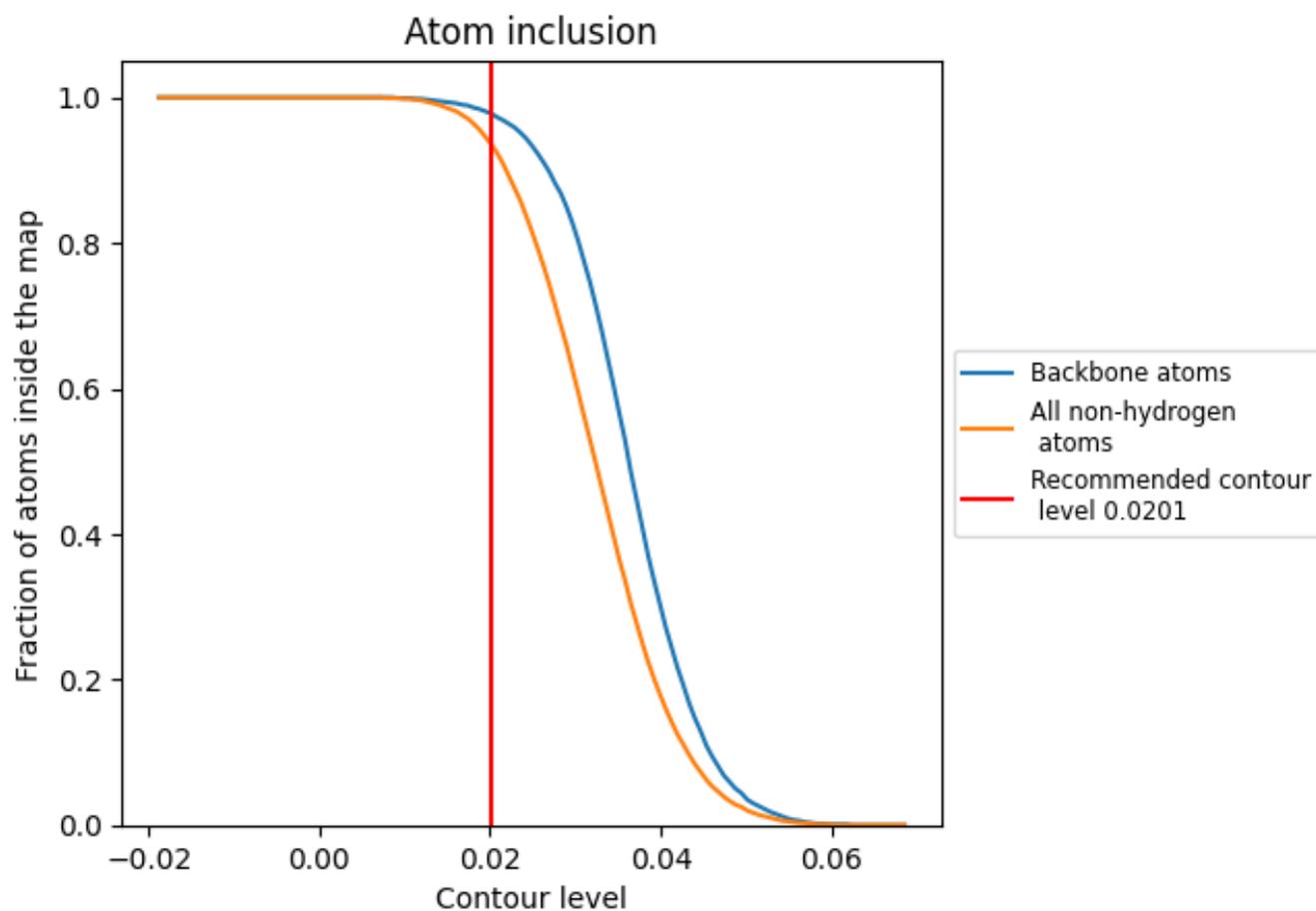
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0201).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% 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 (0.0201) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9360	 0.2870
A	 0.9610	 0.2950
B	 0.9660	 0.2850
C	 0.9500	 0.2920
D	 0.9300	 0.2860
E	 0.9430	 0.2960
F	 0.9060	 0.2730
J	 0.8620	 0.2810

