



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:04 AM UTC

PDB ID : 6C06 / pdb_00006c06
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)

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:

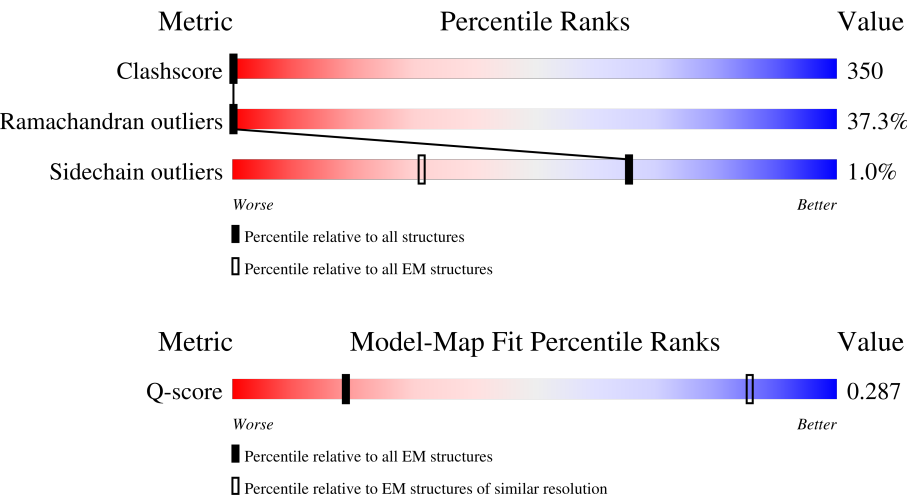
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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.



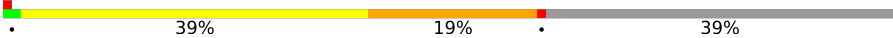
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	694 (4.65 - 5.65)

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%27%•35%
1	B	347	•48%19%•32%
2	C	1181	•58%33%•6%
3	D	1324	•54%38%•5%

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	531	
6	J	111	

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

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
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
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
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
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

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
5	F	326	Total	C	N	O	S	0	0
			2588	1617	467	495	9		

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
6	J	107	Total	C	N	O	S	0	0
			872	539	162	168	3		

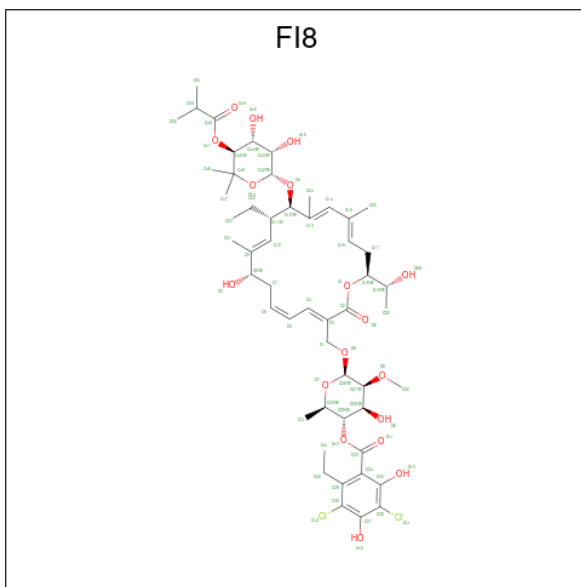
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 9 is Fidaxomicin (CCD ID: FI8) (formula: C₅₂H₇₄Cl₂O₁₈).

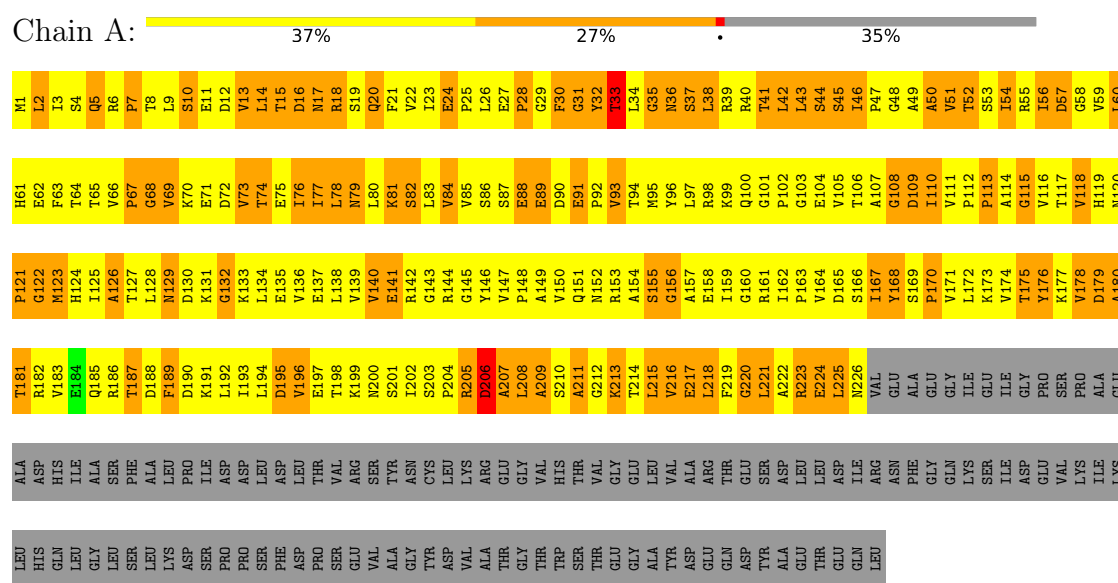


Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	Cl	H	O	0
			146	52	2	74	18	

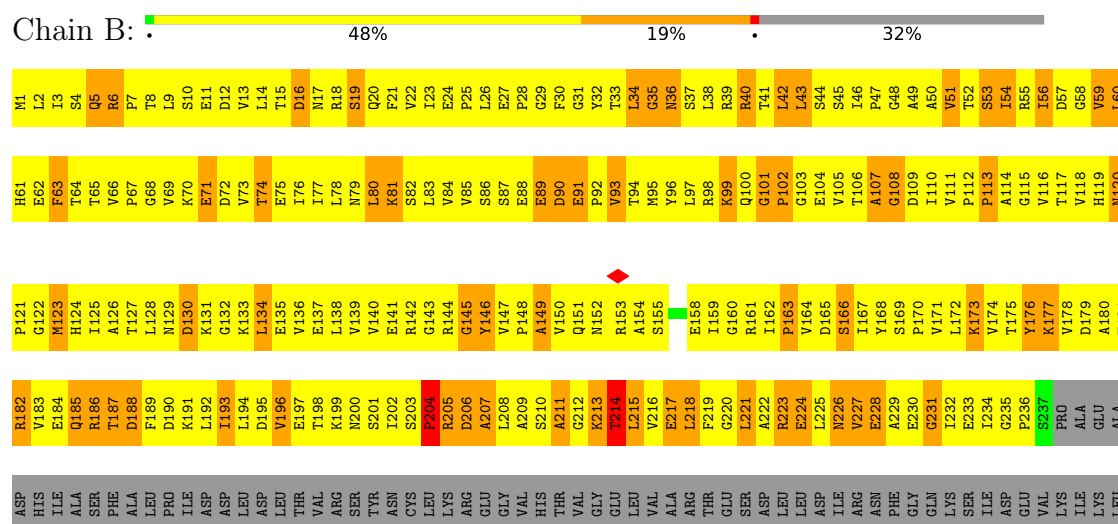
3 Residue-property plots

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: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



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

Chain C:  58% 33% 6%

L907	A908	D909	G910	T911	P912	V913	D914	L915	L916	L917	N918	T919	H920	G921	V922	P923	R924	R925	N926	N927	I928	G929	Q930	I931	L932	E933	T934	H935	L936	G937	V938	C939	A940	H941	S942	G943	D944	K945	V946	D947	A948	I949	K950	G951	V952	P953	D954	V955	A956	A957	L958	L959	P960	D961	E962	L963	L964	E965	A966																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
R847	G848	D849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849	R849	G849

Y1027	E1087	LEU
M1028	L1088	ARG
Y1029	L1089	GLU
I1030	D124	ASP
N1031	N5	V4
Y1032	N6	F6
L1033	F7	F7
S1034	D8	D8
H1035	E9	E9
L1036	L10	L10
V1037	R11	R11
F1037	G12	G12
F977	G13	G13
D978	L14	L14
G979	A15	A15
A980	T16	T16
Q981	A17	A17
E982	E18	E18
A983	E19	E19
E984	E20	E20
L985	E21	E21
S1045	E22	E22
T1046	E23	E23
T1046	E24	E24
G1047	E25	E25
G987	E26	E26
L988	E27	E27
Y1048	E28	E28
Y1049	E29	E29
S1050	E30	E30
M1051	E31	E31
L1052	E32	E32
L1052	E33	E33
T1053	E34	E34
Q1054	E35	E35
Q1055	E36	E36
Q1056	E37	E37
L1057	E38	E38
G1058	E39	E39
G1059	E40	E40
A1061	E41	E41
Q1062	E42	E42
F1063	E43	E43
G1064	E44	E44
G1065	E45	E45
G1066	E46	E46
R1067	E47	E47
F1068	E48	E48
M1069	E49	E49
E1070	E50	E50
F1071	E51	E51
D1072	E52	E52
G1073	E53	E53
W1074	E54	E54
A1075	E55	E55
M1076	E56	E56
Q1077	E57	E57
P1078	E58	E58
Y1079	E59	E59
G1080	E60	E60
P1081	E61	E61
Y1082	E62	E62
P1083	E63	E63
T1084	E64	E64
L1085	E65	E65
Q1086	E66	E66

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



Y61	A121	L181	Y241	A301	A362	V422	Q482	A542	A602	V662
C62	P122	A182	R242	F302	P363	D423	V483	V543	S603	M663
G63	E243	E183	L244	Q303	P364	Y424	W484	H544	G604	A664
K64	D124	E184	V245	Q304	I365	S425	D485	L545	D605	E665
Y65	L184	E185	D246	N307	I366	G426	W486	P546	H606	T666
K66	E126	E186	R247	S308	V367	R427	L487	L547	P607	T667
R67	K127	E187	Y248	P309	N368	S428	E488	S548	E608	L668
V68	I128	E188	G249	M310	N369	Y429	E489	A549	T609	R669
R69	L129	E189	E250	G311	E370	L430	W490	E550	G610	G670
F70	G130	E190	Y251	G312	K371	V431	A491	A551	V611	V671
K71	F131	A191	F252	N313	R372	W432	A492	Q552	Y612	M672
G72	A132	K190	G253	V314	M373	G433	E493	A553	S613	F673
I73	E133	K191	L254	L314	L374	P434	H494	E554	S614	M674
I74	Y134	A191	G254	D315	Q375	Q435	P495	A555	P615	E675
C75	V135	D192	A255	A316	E376	L436	V496	R556	A616	L676
E76	T136	E193	M256	V317	S377	K437	L497	T557	E617	L677
R77	T137	A194	G257	P318	F378	L438	L498	L558	A618	F678
C78	E138	R194	A258	V319	D379	H439	M499	M559	L619	L679
S24	Y139	E195	E259	I320	A380	Q440	R500	L560	M620	G680
A85	H145	G201	I260	P321	L381	C441	A501	S561	A621	P681
K86	D140	K196	S260	F322	F382	G442	P502	S562	A622	P682
V87	E141	E197	Q262	E323	D383	L443	T503	M563	D623	F683
R89	E142	R198	K263	L330	N384	P444	L504	M564	R624	V684
Y90	M143	D199	L264	M205	G385	K445	H505	I565	G625	M685
E96	T150	G200	L265	D201	R386	L446	R506	L566	V626	K686
A156	E151	G201	E266	M202	K387	M447	L507	S567	L627	Q687
R206	E152	E202	N267	V328	G388	A448	G508	P568	S628	M688
Q207	E153	E203	E273	Q329	R389	L449	T509	A569	V629	H689
E154	E154	R209	A274	F335	P390	E450	Q510	S570	R630	K690
D210	M155	E204	E275	A336	N391	L451	A511	Q571	A631	K691
E276	R211	M205	S276	T337	F392	F452	F512	F572	K632	V692
L277	E157	R206	L277	S338	T392	F453	E513	P573	L633	Q693
V157	E158	Q213	R278	D339	G393	K453	G519	L579	K634	A694
E158	E159	E214	D279	L340	P394	P454	K520	D580	L640	L700
R159	K160	R215	E280	N341	S401	V461	A521	M581	R641	A701
E161	E161	L216	I281	D342	L402	D462	I522	V582	P642	E702
V162	E162	D217	R282	L343	S403	L463	Q523	T583	P643	R703
E163	E163	R218	N283	Y344	D404	N464	L524	G584	V644	Y704
D164	E164	L219	G284	R345	L405	H465	H525	L585	E645	P705
Q165	E165	E220	K285	R346	L406	A466	P526	Y586	L646	K706
Y106	E166	D221	G286	V347	G407	Q467	L527	Y587	E647	T707
F107	D167	I222	Q287	N348	K408	N468	V528	L588	A648	V708
C48	E168	K223	K288	K409	N349	I469	C529	T589	E649	V709
E169	E169	S224	K289	R350	Q410	K470	E530	T590	L650	A710
K50	V110	T225	L290	N351	G411	S471	A531	E591	F651	Q711
I51	P111	F226	R291	N352	R412	K472	F532	V592	T712	T712
F52	S112	T227	A292	R353	F413	K473	N533	P593	H653	G713
G53	R113	K228	L293	L354	R414	A474	A534	G594	V714	S714
E64	E173	K294	K294	R355	Q415	M475	D535	D595	G655	K715
L114	A174	R229	R295	R356	L416	V476	F536	T596	L716	V656
G115	Q175	A230	R296	R357	L417	E477	D537	G597	K657	K717
R56	K176	P231	L296	L357	L418	R478	Q538	E598	P658	D718
D57	L177	K232	K297	R358	G419	Q479	D539	Y599	A659	A719
W58	E178	Q233	V298	D359	K420	R480	Q540	G600	D660	G720
E59	A179	E179	V299	L360	R421	P481	M541	P601	A661	F721
L120	D180	E237	V236	V236	A300					
		E238	N239	L240						

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 ($\text{\AA}$)	330.0, 330.0, 330.0	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, FI8

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	0.78	1/2380 (0.0%)
1	B	0.50	0/1802	0.82	0/2454
2	C	0.57	2/8714 (0.0%)	0.86	13/11824 (0.1%)
3	D	0.57	2/10021 (0.0%)	0.86	16/13549 (0.1%)
4	E	0.54	0/662	0.81	0/901
5	F	0.44	0/2622	0.69	0/3538
6	J	0.45	0/888	0.75	0/1199
All	All	0.54	4/26459 (0.0%)	0.83	30/35845 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	613	ARG	CA-C	-7.37	1.43	1.52
3	D	88	ARG	CA-C	-6.86	1.43	1.52
3	D	564	ASN	CA-CB	-6.13	1.44	1.53
2	C	723	ILE	C-N	-5.82	1.21	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	500	ARG	CA-C-N	-10.42	104.69	121.57
3	D	500	ARG	C-N-CA	-10.42	104.69	121.57
2	C	53	LEU	CB-CA-C	-8.72	106.51	116.63
2	C	156	ASP	CA-C-N	-7.43	107.51	122.90
2	C	156	ASP	C-N-CA	-7.43	107.51	122.90

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	1376	0
1	B	1775	0	1809	1437	0
2	C	8556	0	8459	6235	0
3	D	9857	0	9923	7323	0
4	E	649	0	645	440	0
5	F	2588	0	2602	1633	0
6	J	872	0	852	574	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	18228	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 350.

The worst 5 of 18228 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 ⓘ

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%)	193 (99%)	2 (1%)	68	77
1	B	197/297 (66%)	196 (100%)	1 (0%)	81	82
2	C	924/997 (93%)	916 (99%)	8 (1%)	70	77
3	D	1041/1103 (94%)	1028 (99%)	13 (1%)	63	74
4	E	69/89 (78%)	68 (99%)	1 (1%)	59	72
5	F	272/429 (63%)	271 (100%)	1 (0%)	84	83
6	J	93/97 (96%)	92 (99%)	1 (1%)	65	75
All	All	2791/3309 (84%)	2764 (99%)	27 (1%)	65	77

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	228	LYS
3	D	355	LYS
4	E	36	THR
3	D	325	ARG
3	D	359	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	930	GLN
5	F	299	ASN
3	D	207	GLN
5	F	234	GLN
5	F	459	GLN

5.3.3 RNA ⓘ

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](#)

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	1.93	20 (27%)	96,109,109	2.10	29 (30%)

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 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1404	FI8	C1-C3	5.77	1.57	1.50
9	D	1404	FI8	C14-C15	4.69	1.54	1.45
9	D	1404	FI8	C14-C13	4.16	1.39	1.33
9	D	1404	FI8	O1-C18	-3.92	1.39	1.46
9	D	1404	FI8	O17-C49	3.90	1.43	1.34

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1404	FI8	C5-C4-C3	-7.48	117.97	126.92
9	D	1404	FI8	C29-O10-C33	-5.41	108.61	117.24
9	D	1404	FI8	C26-C27-C28	5.18	118.83	110.37
9	D	1404	FI8	C7-C6-C5	-4.70	119.45	125.44
9	D	1404	FI8	C31-C30-C29	-4.68	106.42	113.39

All (2) chirality outliers are listed below:

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

5 of 34 torsion outliers are listed below:

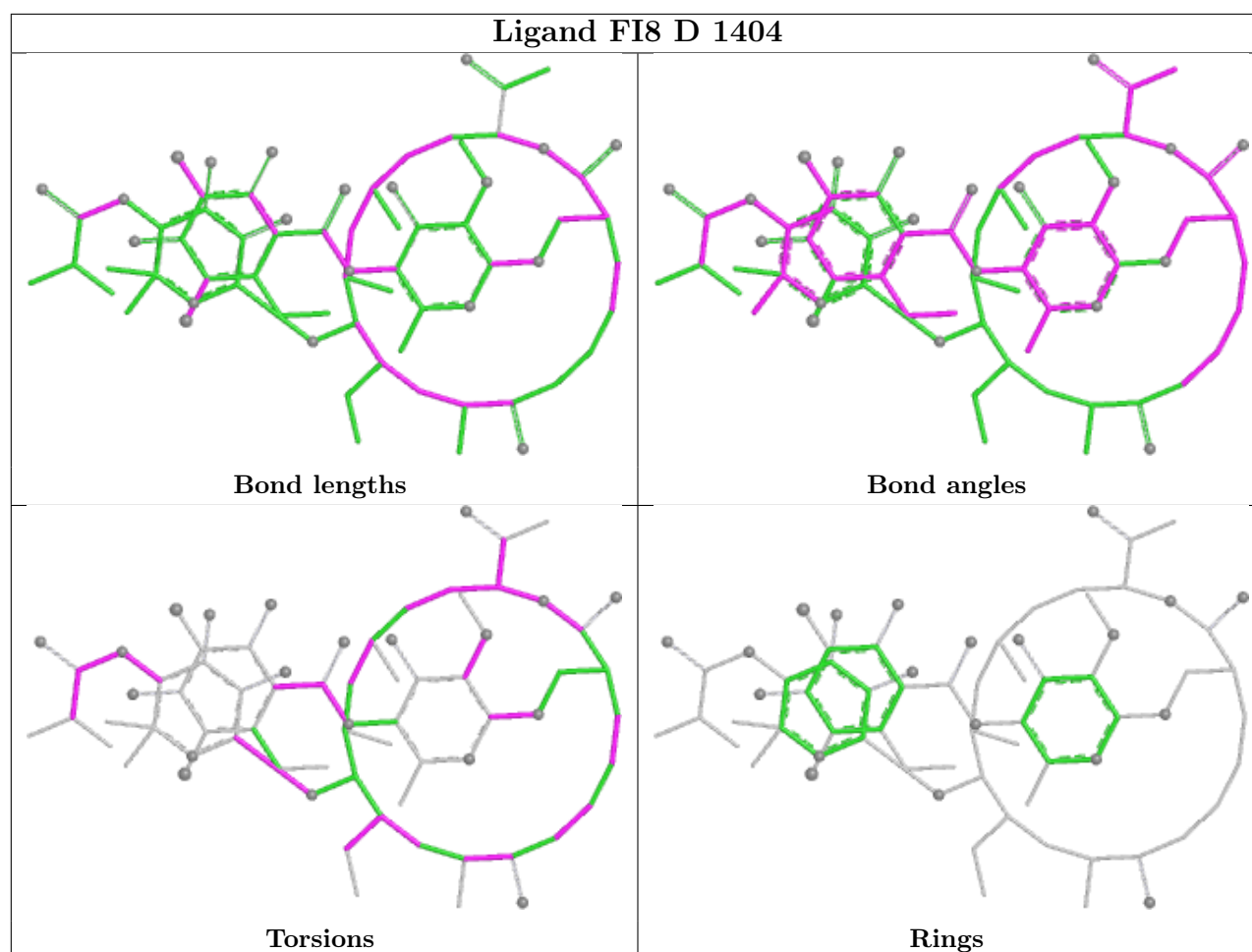
Mol	Chain	Res	Type	Atoms
9	D	1404	FI8	C9-C10-C11-C12
9	D	1404	FI8	C10-C11-C22-C23
9	D	1404	FI8	C12-C11-C22-C23
9	D	1404	FI8	C15-C16-C17-C18
9	D	1404	FI8	C16-C17-C18-C19

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.

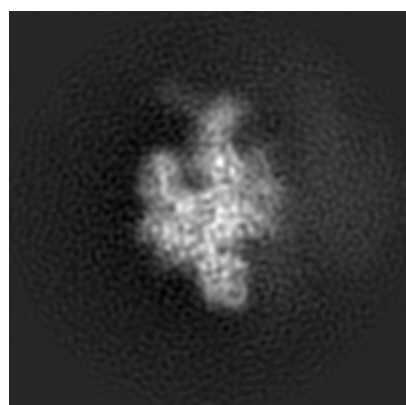
6 Map visualisation [i](#)

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.

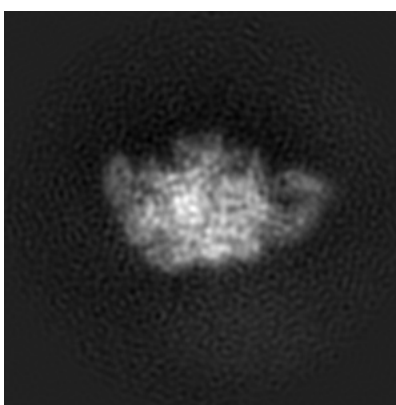
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

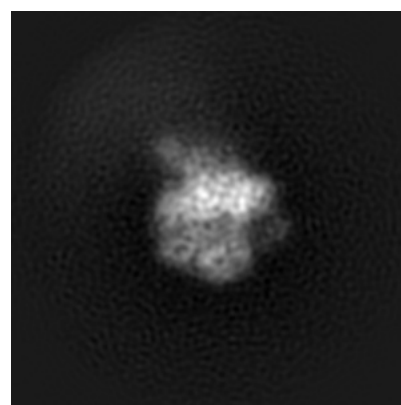
6.1.1 Primary map



X



Y

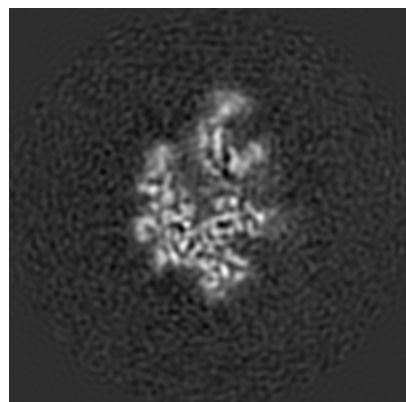


Z

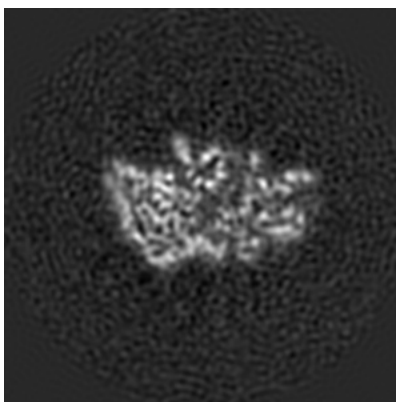
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

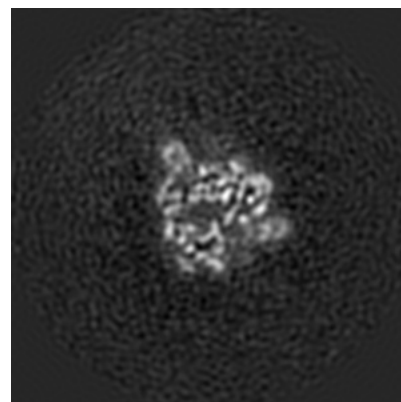
6.2.1 Primary map



X Index: 110



Y Index: 110

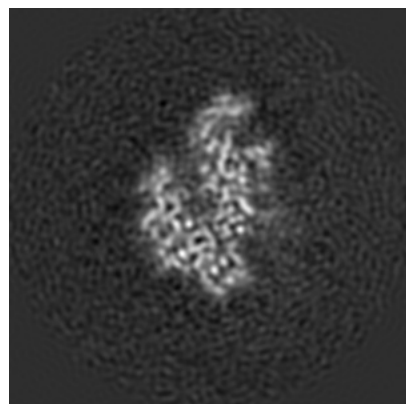


Z Index: 110

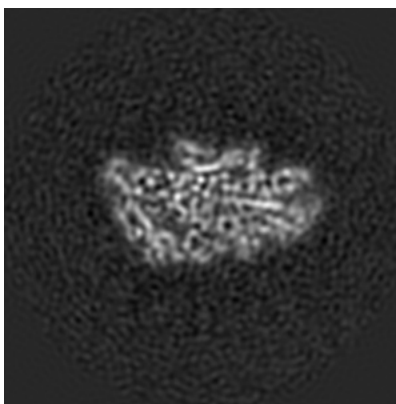
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

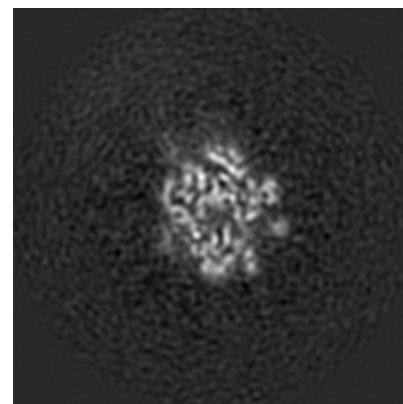
6.3.1 Primary map



X Index: 105



Y Index: 114

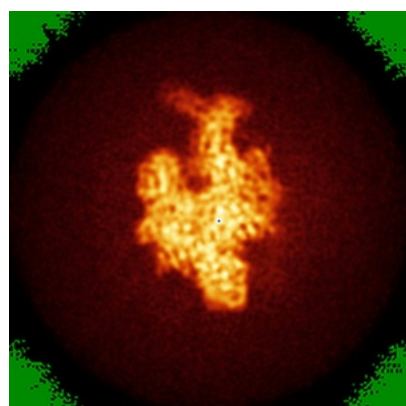


Z Index: 104

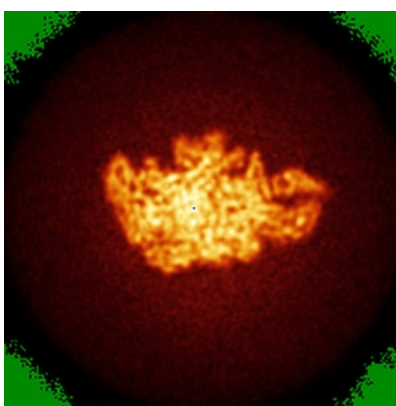
The images above show the largest variance slices of the map in three orthogonal directions.

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

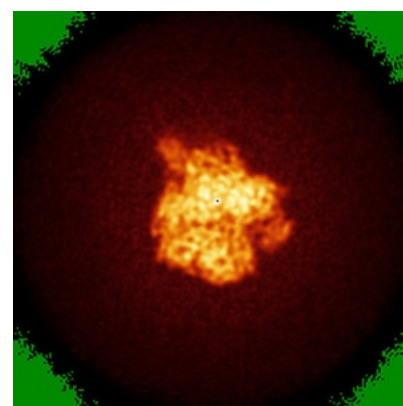
6.4.1 Primary map



X



Y



Z

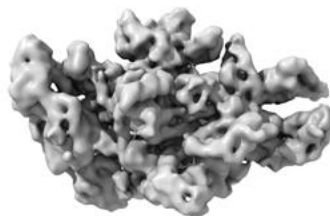
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

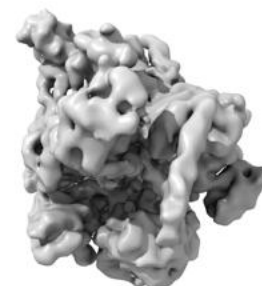
6.5.1 Primary map



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.

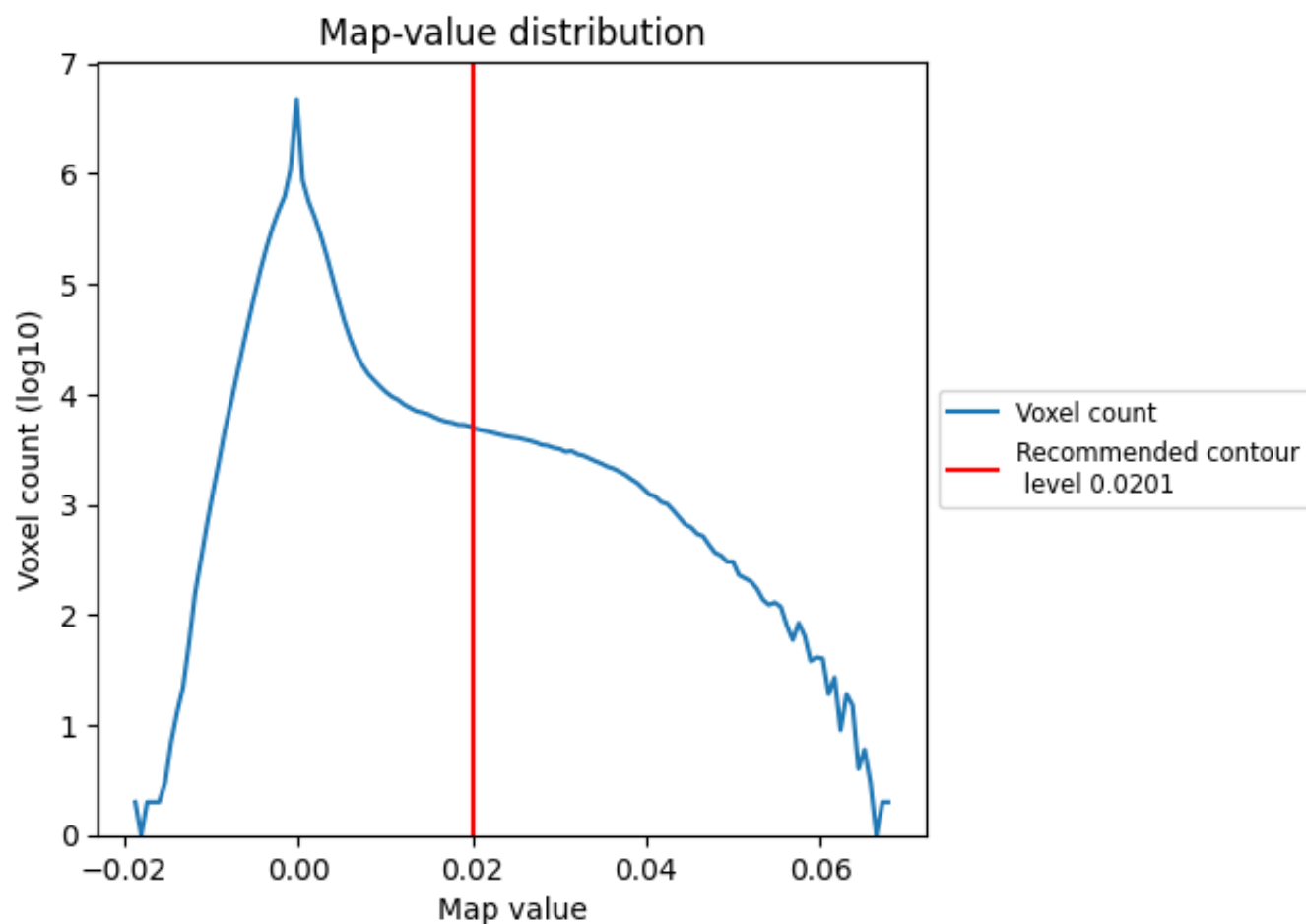
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

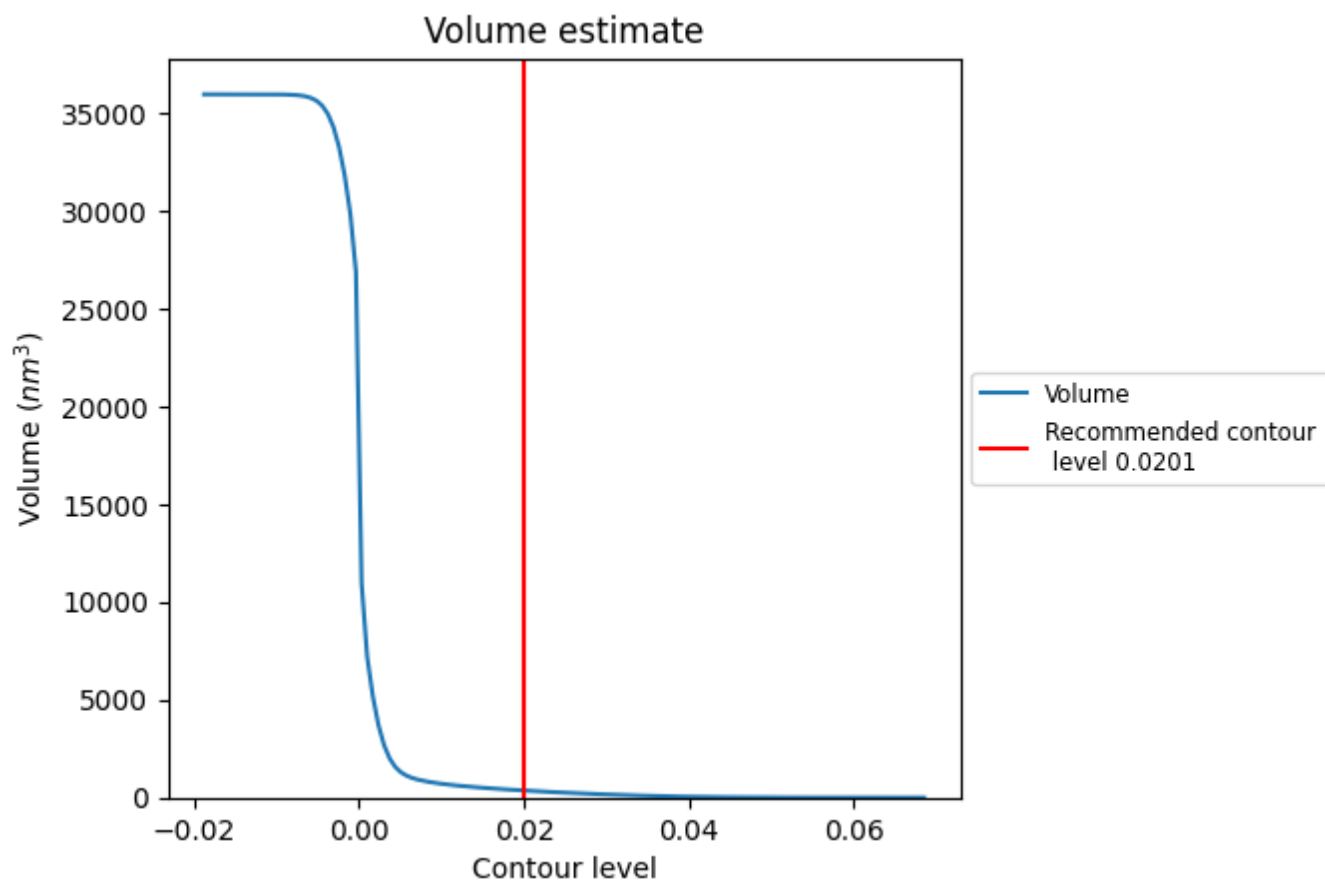
This section contains the results of statistical analysis of the map.

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.

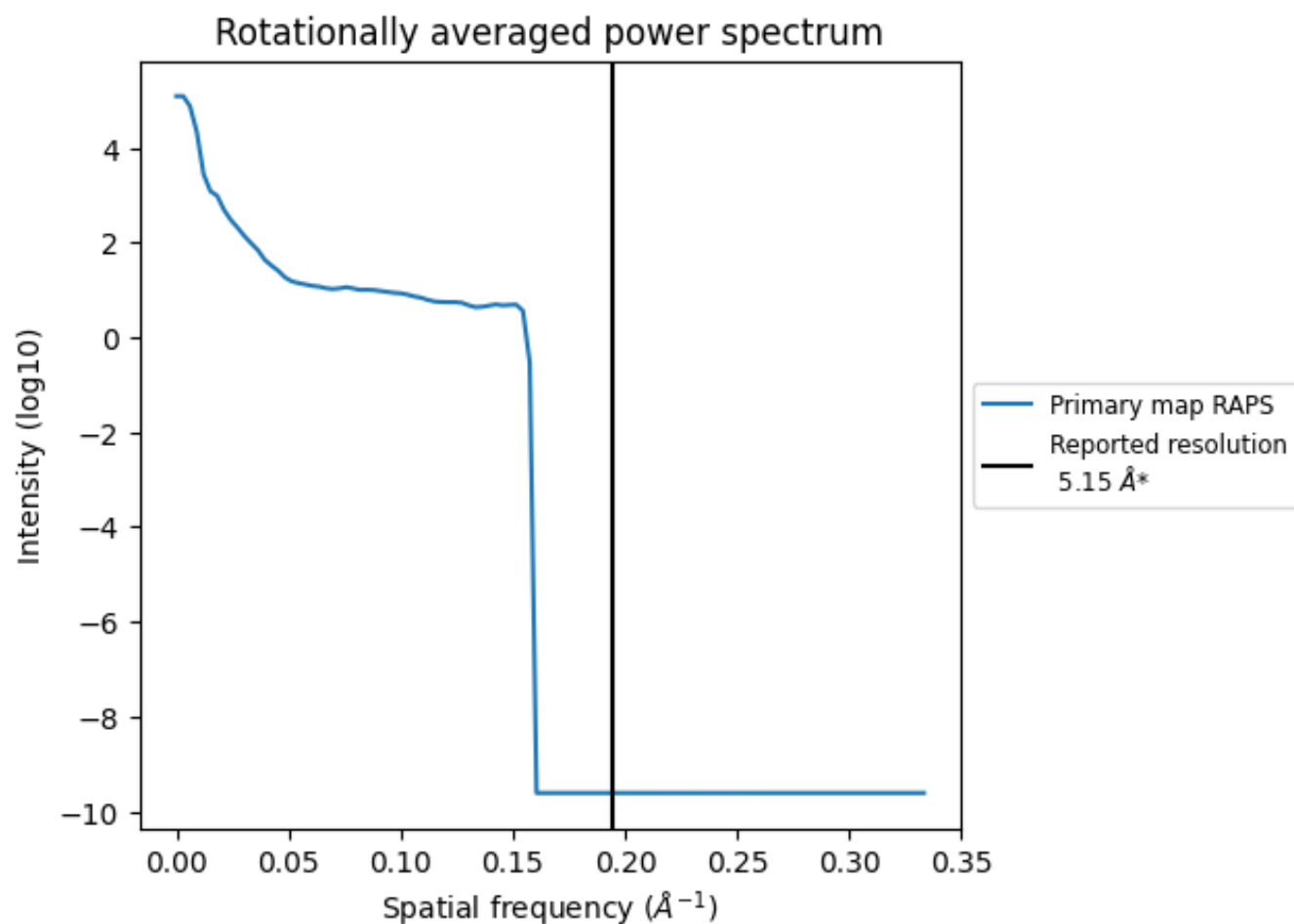
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 358 nm³; 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.194 $\text{\AA}^{-1}$

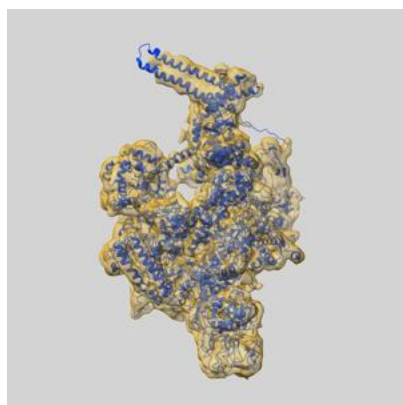
8 Fourier-Shell correlation

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

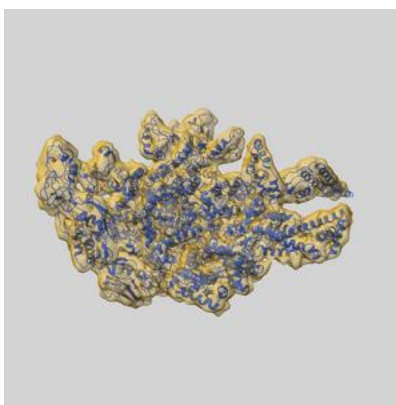
9 Map-model fit [i](#)

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](#).

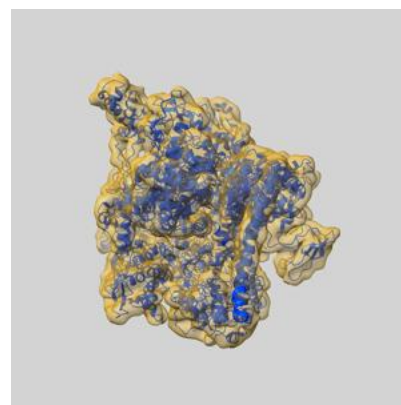
9.1 Map-model overlay [i](#)



X



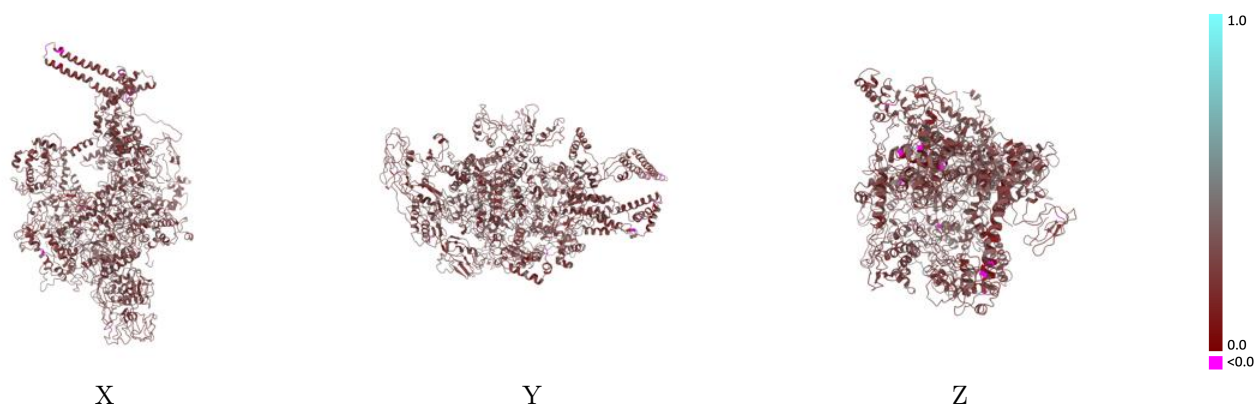
Y



Z

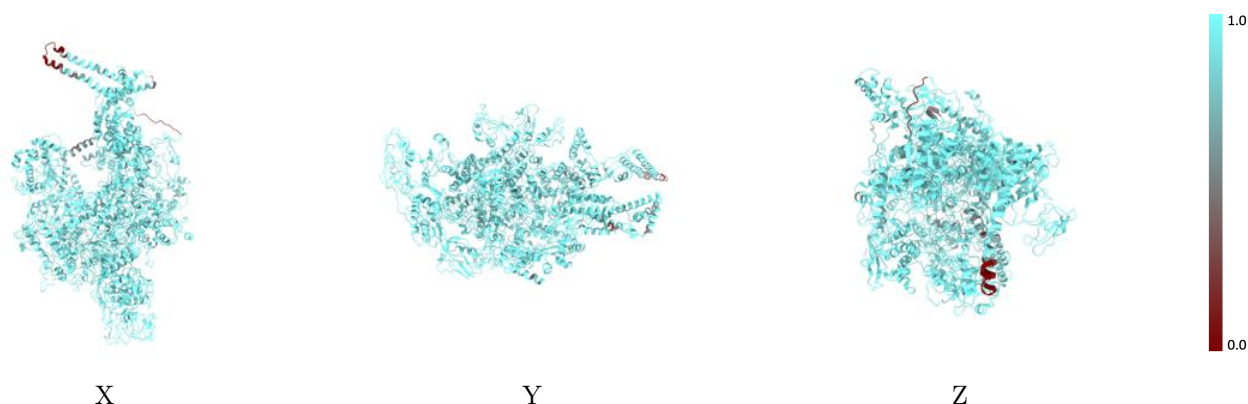
The images above show the 3D surface view of the map at the recommended contour level 0.0201 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



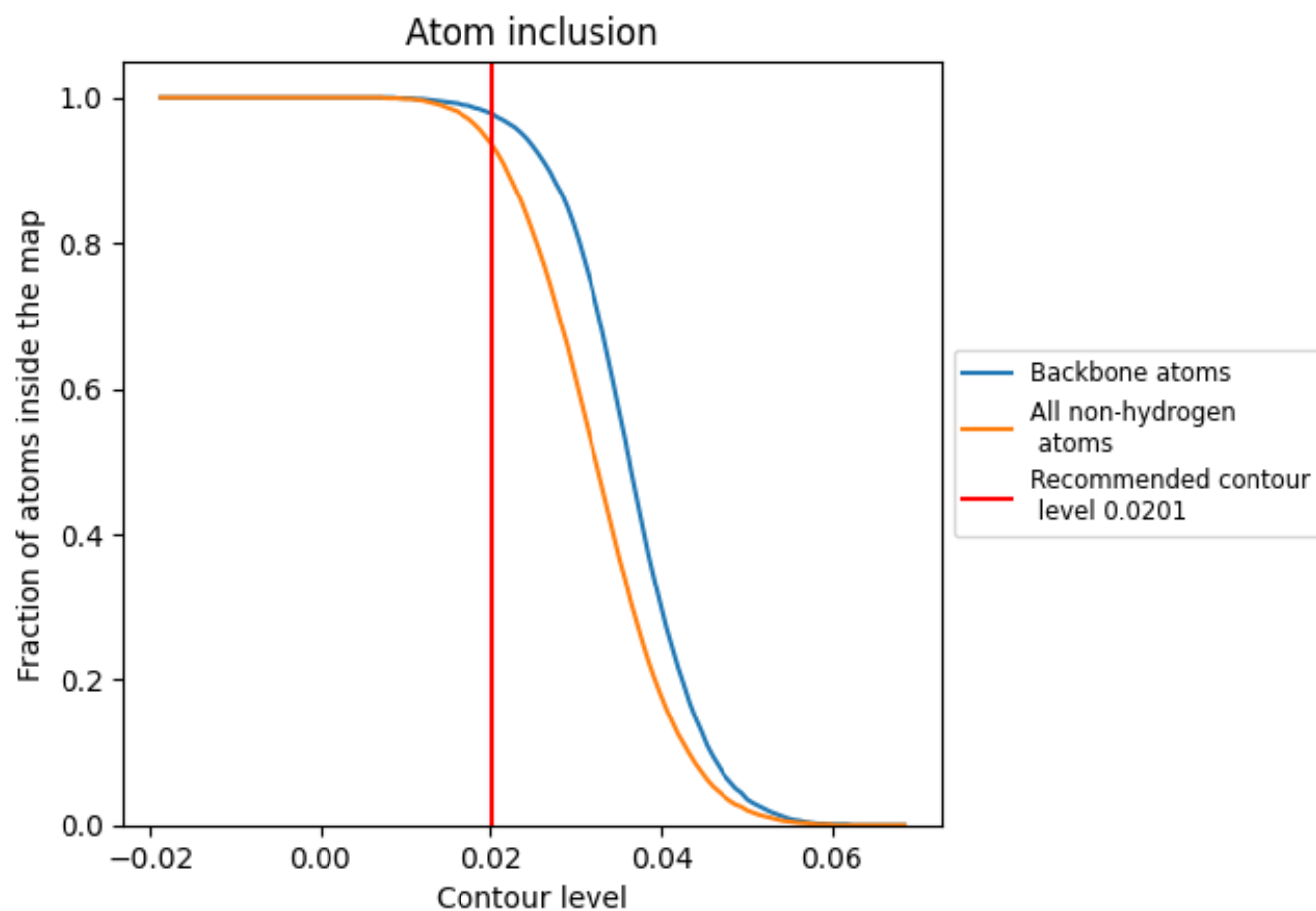
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0