



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 05:08 AM UTC

PDB ID : 6M7J / pdb_00006m7j
EMDB ID : EMD-9047
Title : Mycobacterium tuberculosis RNAP with RbpA/us fork and Corallopynonin
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.
Deposited on : 2018-08-20
Resolution : 4.40 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:

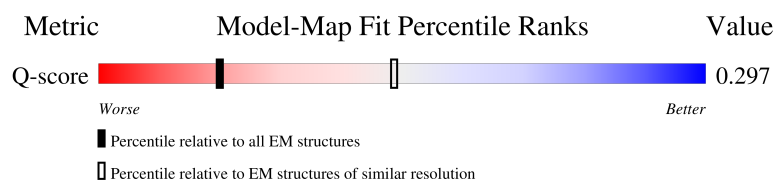
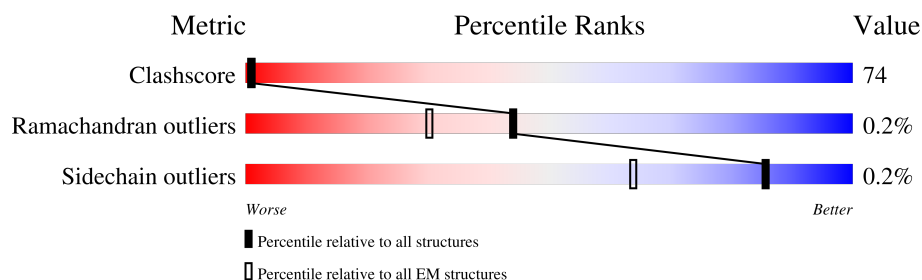
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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

The reported resolution of this entry is 4.40 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.



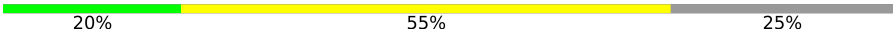
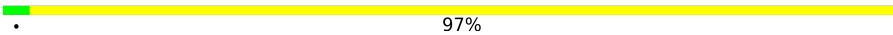
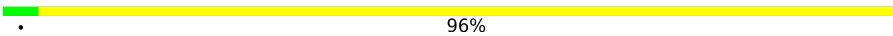
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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	12% 52% 35%
1	B	347	14% 54% 32%
2	C	1179	21% 72% 6%
3	D	1326	24% 72% 5%

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	531	
6	J	111	
7	O	31	
8	P	26	

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
11	C0L	D	1404	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27223 atoms, of which 40 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	225	Total	C	N	O	S	0	0
			1716	1080	296	338	2		
1	B	237	Total	C	N	O	S	0	0
			1759	1112	298	346	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
			8586	5378	1507	1662	39		

There are 7 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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1266	Total	C	N	O	S	0	0
			9873	6184	1794	1853	42		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP A5U053
D	0	ALA	-	expression tag	UNP A5U053

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A5U053
D	1318	HIS	-	expression tag	UNP A5U053
D	1319	HIS	-	expression tag	UNP A5U053
D	1320	HIS	-	expression tag	UNP A5U053
D	1321	HIS	-	expression tag	UNP A5U053
D	1322	HIS	-	expression tag	UNP A5U053
D	1323	HIS	-	expression tag	UNP A5U053
D	1324	HIS	-	expression tag	UNP A5U053

- 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	319	Total	C	N	O	S	0	0
			2518	1571	456	482	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP P9WGI0
F	-1	PRO	-	expression tag	UNP P9WGI0
F	0	HIS	-	expression tag	UNP P9WGI0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	108	Total	C	N	O	S	0	0
			881	543	168	167	3		

- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	31	Total	C	N	O	P	0	0
			634	305	114	185	30		

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	26	Total	C	N	O	P	0	0
			526	254	94	153	25		

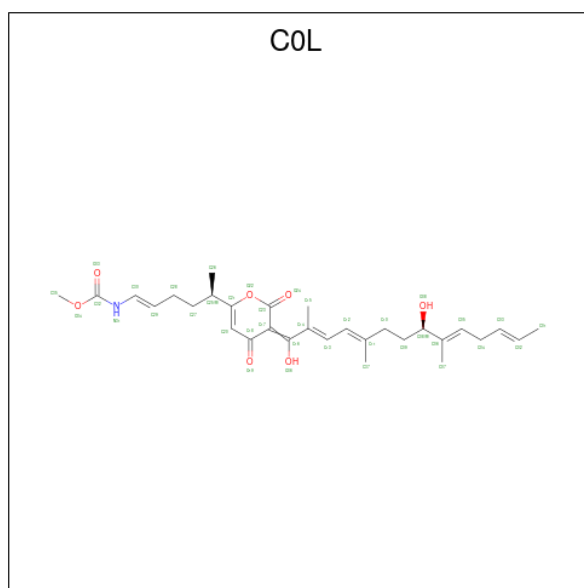
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

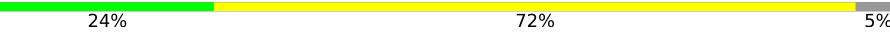
- Molecule 11 is methyl [(1E,5R)-5-{(3E)-3-[(2E,4E,8R,9E,12E)-1,8-dihydroxy-2,5,9-trimethyltetradeca-2,4,9,12-tetraen-1-ylidene]-2,4-dioxo-3,4-dihydro-2H-pyran-6-yl}hex-1-en-1-yl]carbamate (CCD ID: C0L) (formula: C₃₀H₄₁NO₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	H	N	O	0
			78	30	40	1	7	

T835	L899	1971	M1031	I1091	GLU
S836	P900	V972	K1032	K1092	ASP
L837	P901	V973	K1033	S1093	GLU
K838	V901	T974	H1034	T1094	ASP
E902	E902	P975	L1035	D1095	LEU
P840	D903	V976	L1036	T1096	GLU
H841	M904	F977	V1037	V1097	ARG
G842	P905	G978	D1038	G1098	ALA
E843	P906	D979	D1039	G1099	ALA
S844	L907	A980	K1040	K1100	ALA
G845	A908	Q981	I1041	V1101	ASN
K846	D909	E982	H1042	V1102	LEU
V847	G910	A983	A1043	V1103	GLY
	T911	E984	R1044	E1104	ILE
I850	P912	L985	S1045	A1105	ASN
R851	V913	Q986	T1046	I1106	LEU
V852	D914	G987	G1047	V1107	SER
F853	I915	L988	P1048	K1108	ARG
S854	I916	L989	V1049	G1109	ASN
R855		S990	S1050	E1110	GLU
E856	V922	C991	M1051	N1111	SER
D857	P923	T992	I1052	I1112	ALA
E858	R924	L993	T1053	P1113	ALA
D859	R925	P994	Q1054	E1114	VAL
E860	M926	N995	Q1055	P1115	GLU
L861	N927	R996	P1056	G1116	ASP
P862	I928	D997	L1057	I1117	LEU
A863	G929	G998	G1058	P1118	ALA
G864	Q930	D999	G1059	G1119	LEU
V865	I931	V1000	K1060	S1120	ALA
N866	L932	L1001	A1061	F1121	ARG
E867	E933	V1002	Q1062	K1122	HIS
L868	T934	D1003	F1063	L1123	GLY
V869		A1004	G1064	L1124	GLY
R870	H941	D1005	G1065	L1125	SER
V871	S942	K1006	Q1066	K1126	
V872	G943	K1007	K1067	L1127	
V873	W944	A1008	F1068	L1128	
A874	K945	M1009	G1069	Q1129	
Q875	V946	L1010	E1070	S1130	
K876		F1011	M1071	L1131	
R877	V952	D1012	E1072	G1132	
K878	D953	G1013	G1073	L1133	
L879	D954	R1014	K1074	N1134	
S880	W955	A1015	A1075	V1135	
D881	A956	G1016	M1076	V1136	
G882	A957	E1017	Q1077	V1137	
D883	R958	P1018	A1078	L1138	
K884	L959	F1019	Y1079	S1139	
L885	P960	P1020	G1080	S1140	
A886	D961	Y1021	A1081	ASP	
G887	E962	P1022	A1082	GLY	
L888	L963	V1023	Y1083	ALA	
H889	L964	T1024	T1084	ALA	
G890	E965	V1025	L1085	ILE	
N891	A966	G1026	Q1086	GLU	
K892	Q967	Y1027	E1087	LEU	
	P968	M1028	L1088	ARG	
I895	N969	Y1029	L1089	GLU	
G896	A970	T1030	T1090	GLY	

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

Chain D:  24% 72% 5%

G-1	G43	I128	R194	G257	V391	R459	A521
N5	K64	I129	R195	G258	R325	L460	I522
F6	Y65	F130	K196	S260	P326	V461	Q523
F7	K66	Y131	V197	L261	N327	D462	L524
D8	V67	A132	R198	Q262	V328		H525
E9	K68	A133	D199	K263	Q329		P526
L10	R69	Y134	G200	L264		A466	L527
R11	F70	V135	G201	L265	R334	Q467	V528
I12	K71	I136	E202	E266	F335	M468	C529
G13	G72	T137	R203	N267	A336	T469	C530
L14	I73	S138	E204	F268	L405	K470	A531
A15	T74	V139	R205	D269	D406	S471	E532
V16	C75	D140	R206	L270	L340	A472	F533
E17	E76	E141	Q207		N341	R473	N533
A18	R77	E142	I208	A274	D342	M474	A534
D19	C78	M143	R209	E275	L343	M475	D535
I20	G79	R144	D210	S276	Y344	E477	M541
R21	V80	H145	R211	L277	R345	R478	A542
Q22	E81	N146	A212	R278	R346	Q479	V543
W23	V82	E147	Q213	D279	V347	R480	H544
S24	T83	L148	R214	V280	L348	P481	L545
Y25	R84	E149	E215	L281	N349	Q482	P546
G26	A85	T150	L216	R282	R350	L547	L547
E27	K86	D217	D218	N283	N351	V484	S548
V28	V87	L151	R218	G284	G352	D485	A549
K29	R88	A153	L219	K285	R353	V486	E550
E30	E90	M155	E220	G286	L354	L487	A551
P31	R91	A156	D221	Q287	K355	E488	Q552
E32	N92	V157	W223	K288	R356	E489	A553
T33	Q93	E158		L290	L357	V490	E554
L34	H94	R159	F226		T358	L491	A555
N35	E96	V162	T227	L293	D359	A492	R556
Y36		E163	K228	K294	L360	E493	I557
T38	P100	D164	L229	R295	G361	H494	L558
L39	V101	Q165	A230	L296	A362	P495	M559
K40	L102	R166	P231	K297	P363	V496	L560
P41	H103		K232	V298	E364	L497	S561
E42	I104		Q233	V299	T365	L498	S562
D43	Y105		L234		I366	M499	N563
G45	F107		T235	F302	V367	R500	N564
L46	K108		D237	Q303	N368	P502	L566
F47	G109		E238	Q304	E370	T503	S567
C48	V110		L240	S305	R372	L504	
E49	P111		Y241	G306	K373	H505	S570
X50	S112		R242	N307	L374	L507	G571
J51	R113		E243	K310	Q375	G508	R572
F52	L114		L244	G311	E376	L573	P573
G53	L118		V245	S312	S377	L574	L574
P54	D119		D246	V313	V378	Q510	A575
T55	L120		R247	L314	D379	A511	M576
R56	A121		Y248	D315	A380	F512	P577
D57				L381	L451	E513	R578
V58	D124		Y251	P318	F452	P514	L579
E59	L125		F252	V319	F382	N515	D580
C60	E126		T253	P321	D383	L516	N581
Y61	A191		G385	G386	N384	V517	V582
C62	K127		N256		G386	E518	G584
						G519	L585
						K520	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	223000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69.9	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	1.726	Depositor
Minimum map value	-0.457	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.082	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	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, C0L, 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	0.39	0/1742	0.58	0/2370
1	B	0.39	0/1786	0.60	0/2435
2	C	0.43	3/8744 (0.0%)	0.66	7/11860 (0.1%)
3	D	0.39	0/10037	0.63	4/13570 (0.0%)
4	E	0.38	0/662	0.54	0/901
5	F	0.38	0/2549	0.68	5/3438 (0.1%)
6	J	0.31	0/897	0.65	0/1210
7	O	0.41	0/710	0.45	0/1095
8	P	0.42	0/589	0.47	0/906
All	All	0.40	3/27716 (0.0%)	0.63	16/37785 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1068	PHE	C-N	8.16	1.45	1.33
2	C	1068	PHE	CA-C	7.10	1.62	1.52
2	C	1074	TRP	CA-CB	6.59	1.64	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	447	ALA	CA-C-N	-11.04	103.02	120.47
5	F	447	ALA	C-N-CA	-11.04	103.02	120.47
2	C	1074	TRP	CA-CB-CG	10.67	133.87	113.60
2	C	282	ARG	CA-C-N	-10.21	108.80	119.83
2	C	282	ARG	C-N-CA	-10.21	108.80	119.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1716	0	1756	299	0
1	B	1759	0	1783	335	0
2	C	8586	0	8511	1388	0
3	D	9873	0	9941	1494	0
4	E	649	0	645	94	0
5	F	2518	0	2540	425	0
6	J	881	0	861	161	0
7	O	634	0	350	75	0
8	P	526	0	296	65	0
9	D	2	0	0	0	0
10	D	1	0	0	0	0
11	D	38	40	0	22	0
All	All	27183	40	26683	3958	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 74.

The worst 5 of 3958 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:415:GLN:HA	5:F:418:ARG:CD	1.03	1.48
3:D:1249:LYS:HE3	11:D:1404:C0L:N31	1.28	1.46
5:F:415:GLN:CA	5:F:418:ARG:CD	1.97	1.39
5:F:439:ILE:CA	6:J:6:LEU:HD12	1.53	1.37
3:D:641:ARG:N	3:D:657:GLN:HG2	1.40	1.35

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	223/347 (64%)	192 (86%)	31 (14%)	0	100	100
1	B	235/347 (68%)	199 (85%)	36 (15%)	0	100	100
2	C	1109/1179 (94%)	959 (86%)	146 (13%)	4 (0%)	30	66
3	D	1260/1326 (95%)	1109 (88%)	150 (12%)	1 (0%)	48	83
4	E	81/110 (74%)	72 (89%)	9 (11%)	0	100	100
5	F	317/531 (60%)	291 (92%)	24 (8%)	2 (1%)	21	58
6	J	106/111 (96%)	91 (86%)	14 (13%)	1 (1%)	14	49
All	All	3331/3951 (84%)	2913 (88%)	410 (12%)	8 (0%)	44	77

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	231	ARG
2	C	1074	TRP
3	D	422	VAL
5	F	224	SER
5	F	447	ALA

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	194/297 (65%)	194 (100%)	0	100	100
1	B	194/297 (65%)	194 (100%)	0	100	100
2	C	933/997 (94%)	930 (100%)	3 (0%)	86	84
3	D	1042/1103 (94%)	1039 (100%)	3 (0%)	86	84
4	E	69/89 (78%)	69 (100%)	0	100	100
5	F	264/429 (62%)	264 (100%)	0	100	100
6	J	93/97 (96%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2789/3309 (84%)	2783 (100%)	6 (0%)	85	85

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	417	LEU
3	D	422	VAL
3	D	657	GLN
2	C	231	ARG
2	C	229	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1054	GLN
3	D	352	ASN
5	F	325	ASN
2	C	1055	GLN
3	D	207	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
11	C0L	D	1404	-	37,38,38	2.65	13 (35%)	37,49,49	2.80	12 (32%)

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
11	C0L	D	1404	-	-	20/38/57/57	0/1/1/1

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	1404	C0L	O24-C23	8.84	1.39	1.21
11	D	1404	C0L	O19-C18	5.67	1.39	1.24
11	D	1404	C0L	C17-C16	4.85	1.50	1.39
11	D	1404	C0L	O36-C16	-4.55	1.18	1.33
11	D	1404	C0L	C17-C18	-4.20	1.35	1.45

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	1404	C0L	O34-C32-N31	9.70	120.31	109.15
11	D	1404	C0L	C35-O34-C32	-6.28	108.37	115.63
11	D	1404	C0L	O22-C21-C25	5.51	116.19	111.35
11	D	1404	C0L	O36-C16-C17	4.93	128.88	120.03
11	D	1404	C0L	C23-C17-C18	4.44	121.99	119.41

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1404	C0L	C13-C14-C16-O36
11	D	1404	C0L	C15-C14-C16-O36
11	D	1404	C0L	C14-C16-C17-C18
11	D	1404	C0L	C14-C16-C17-C23

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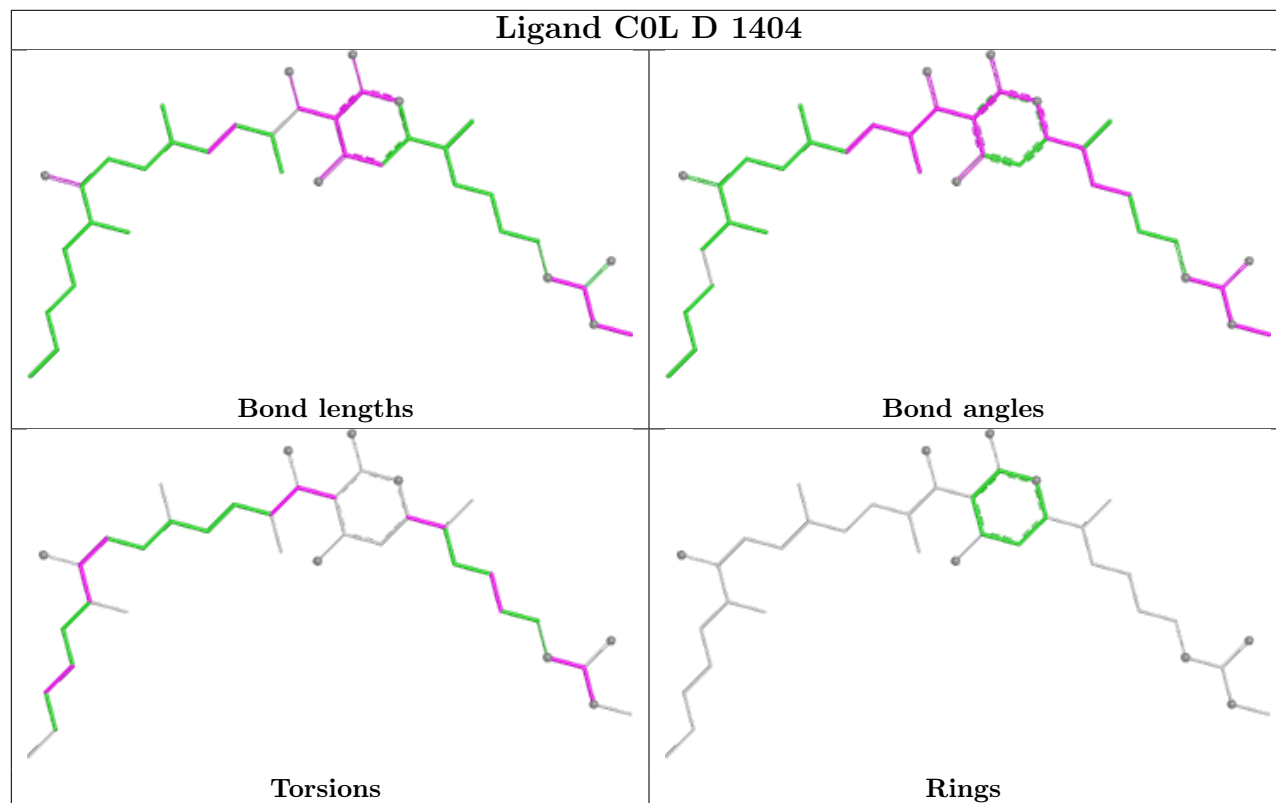
Mol	Chain	Res	Type	Atoms
11	D	1404	C0L	O36-C16-C17-C18

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	1404	C0L	22	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.

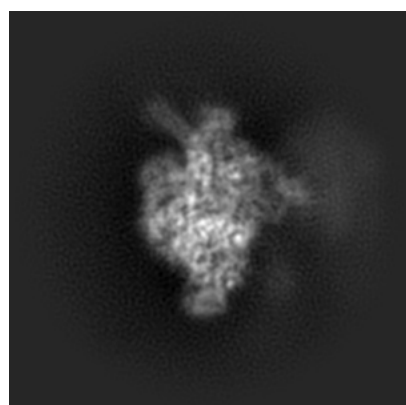
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9047. These allow visual inspection of the internal detail of the map and identification of artifacts.

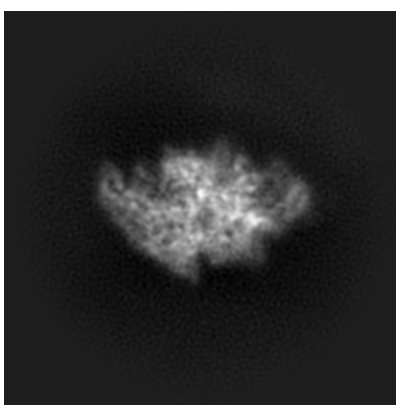
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

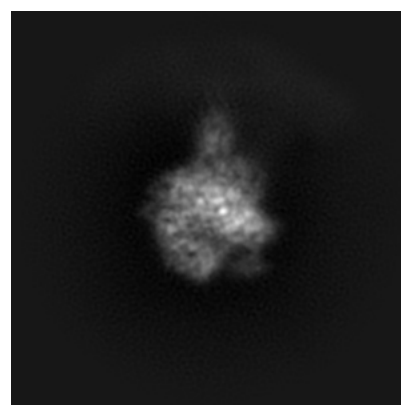
6.1.1 Primary map



X



Y

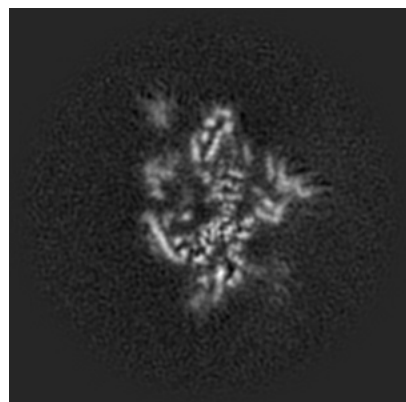


Z

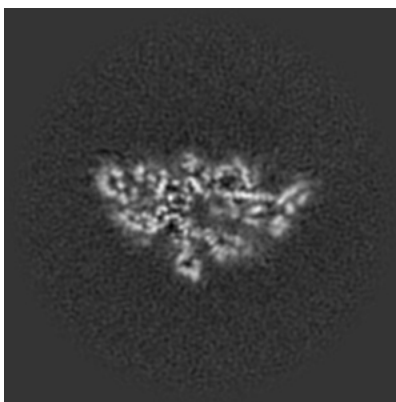
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

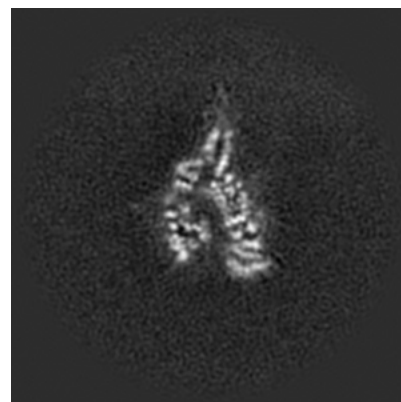
6.2.1 Primary map



X Index: 128



Y Index: 128

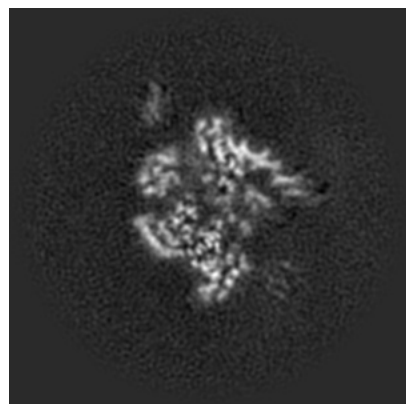


Z Index: 128

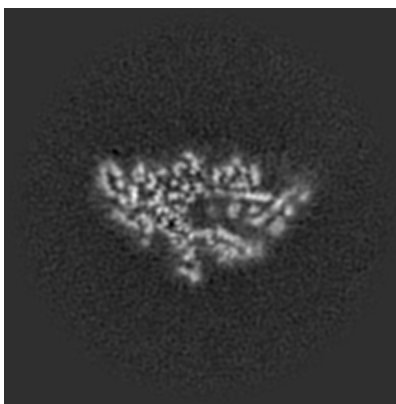
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

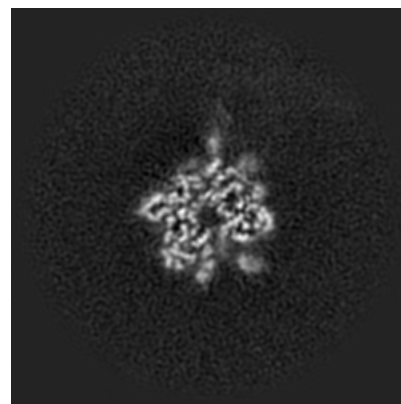
6.3.1 Primary map



X Index: 122



Y Index: 126

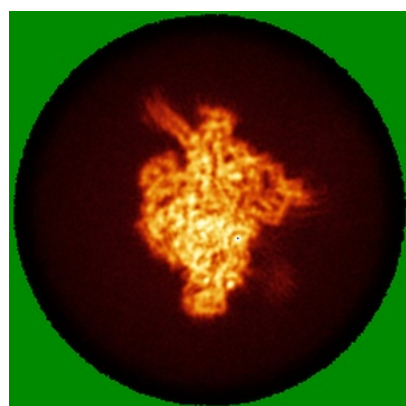


Z Index: 119

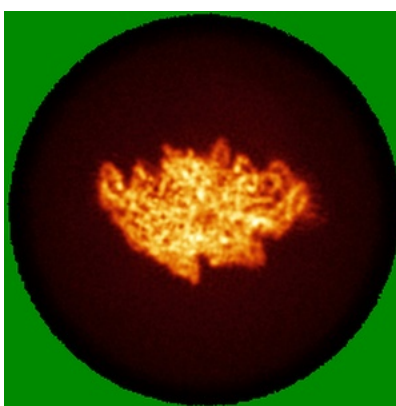
The images above show the largest variance slices of the map in three orthogonal directions.

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

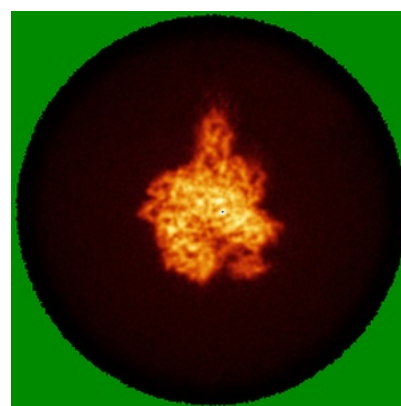
6.4.1 Primary map



X



Y

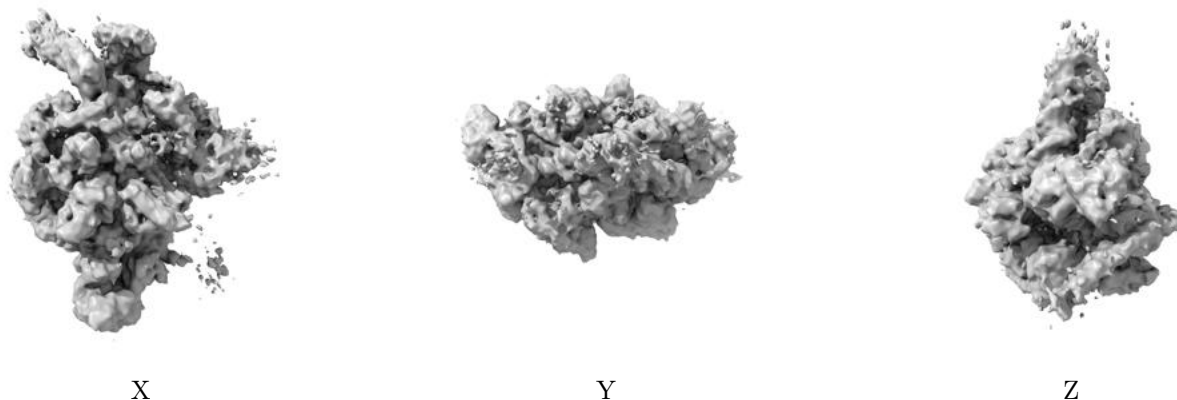


Z

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

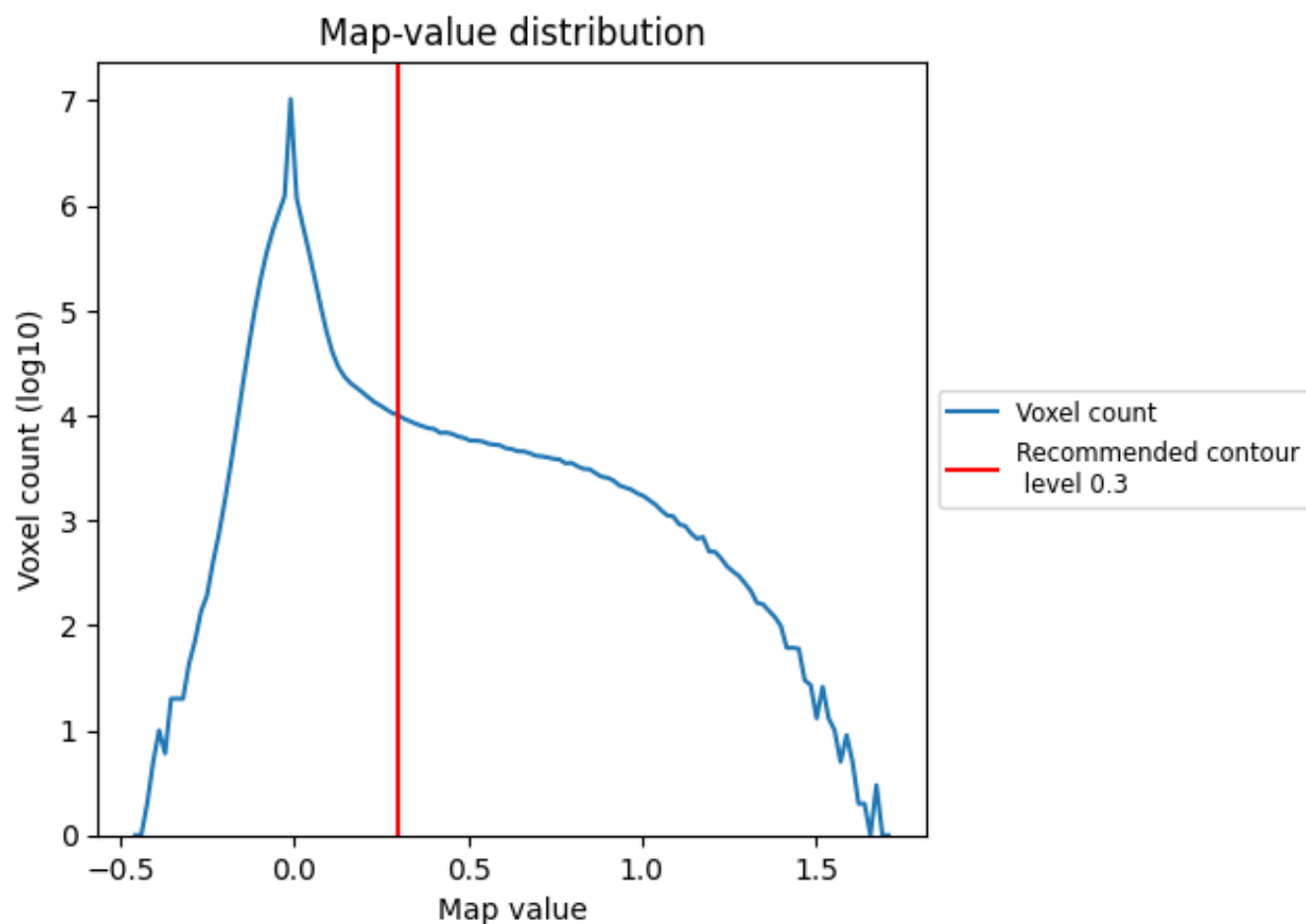
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

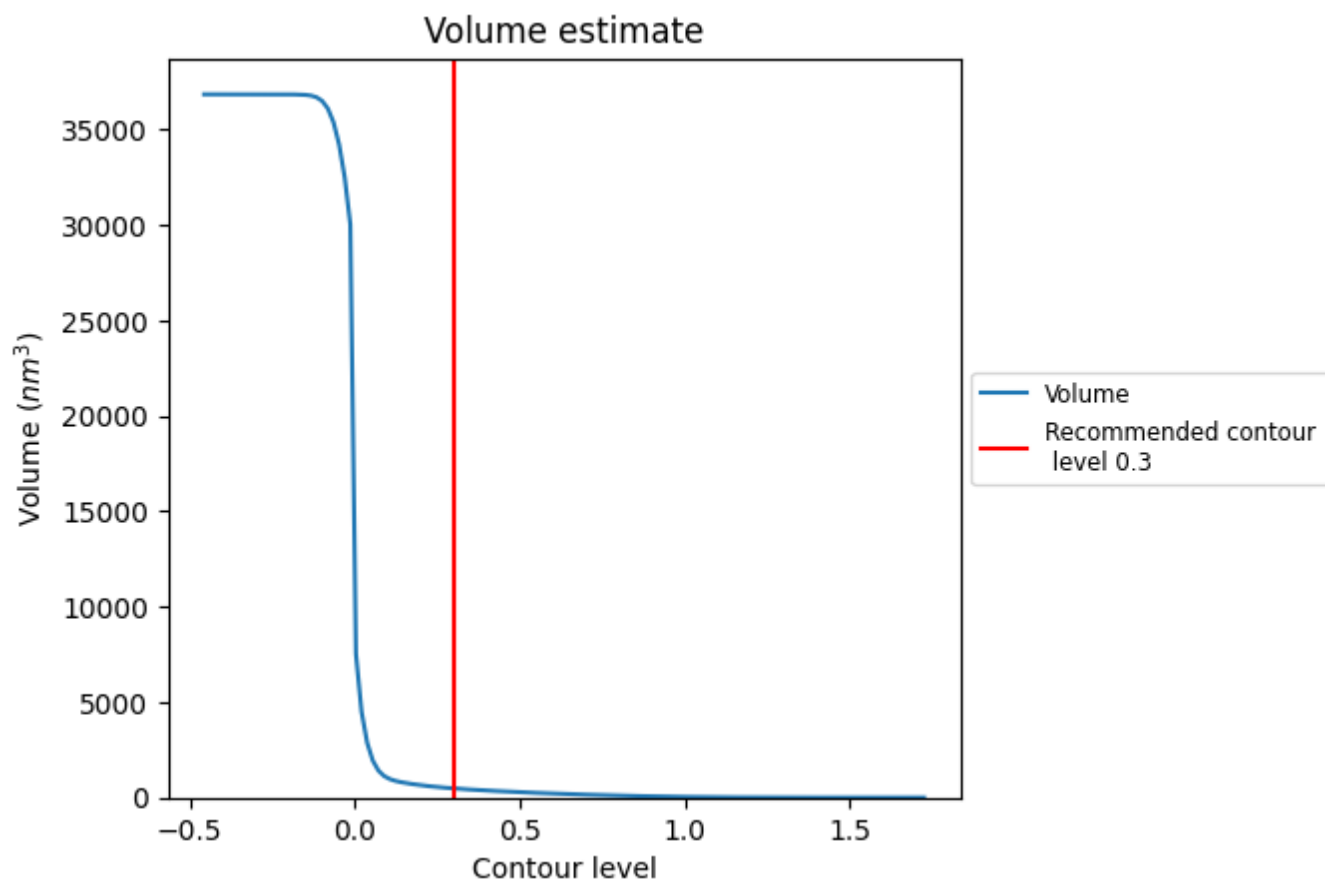
This section contains the results of statistical analysis of the map.

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.

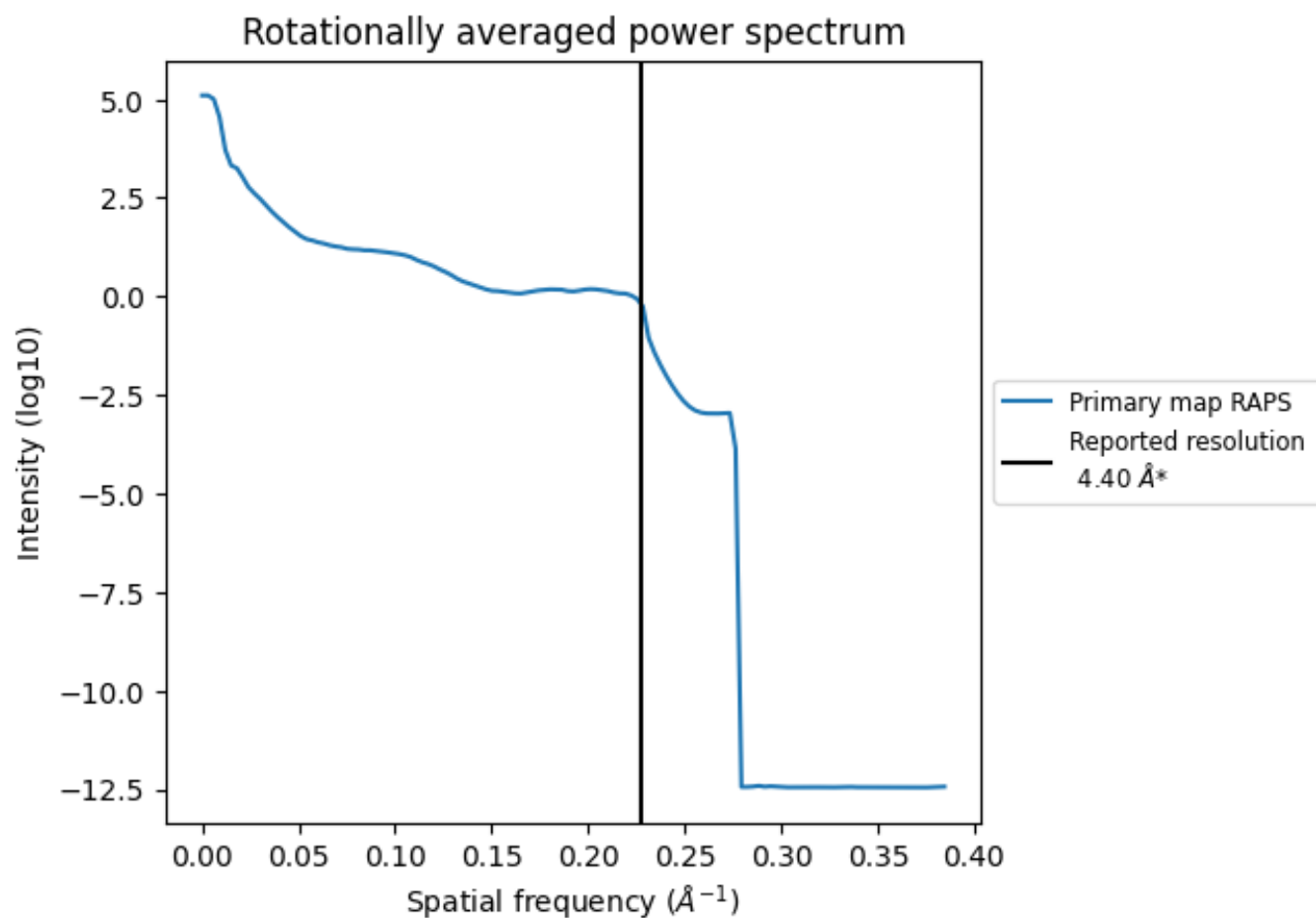
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm³; this corresponds to an approximate mass of 434 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 0.227 Å⁻¹

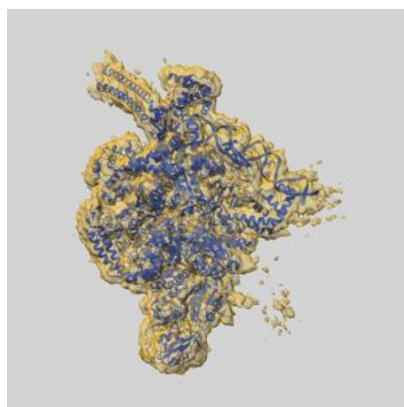
8 Fourier-Shell correlation

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

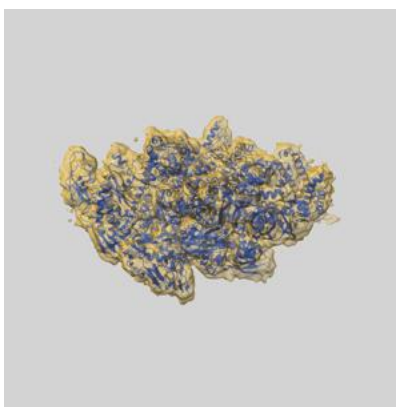
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9047 and PDB model 6M7J. Per-residue inclusion information can be found in section [3](#) on page [8](#).

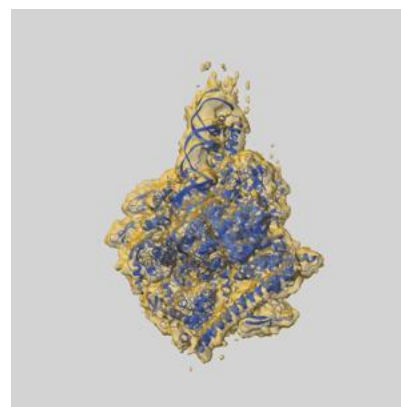
9.1 Map-model overlay [i](#)



X



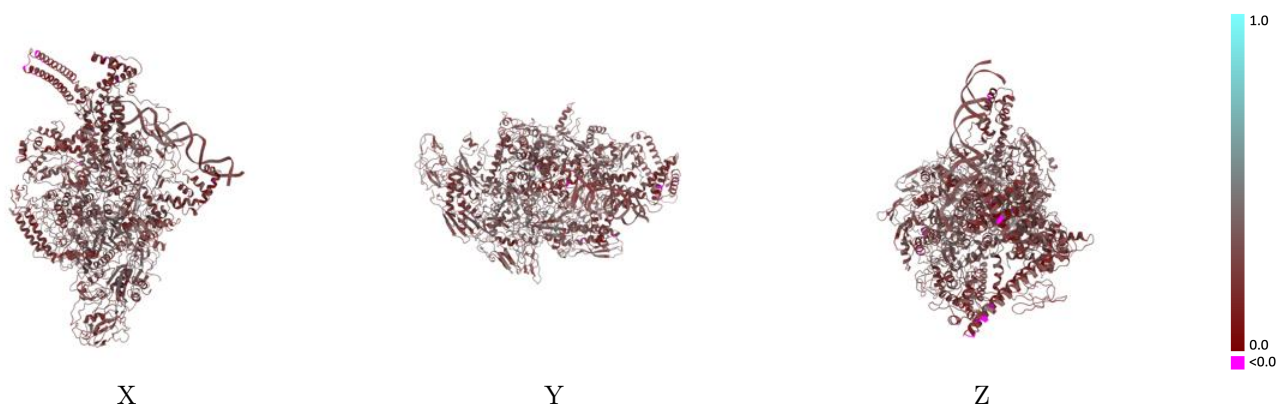
Y



Z

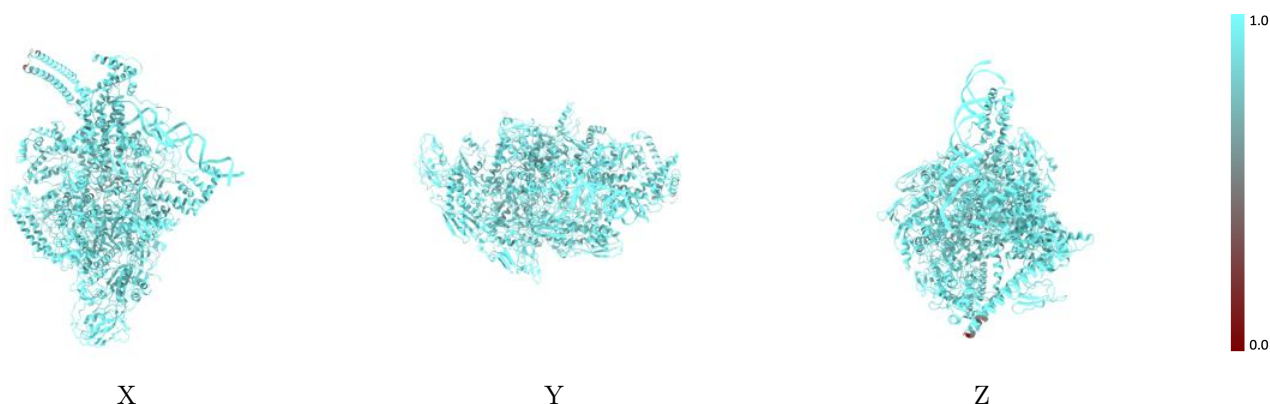
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



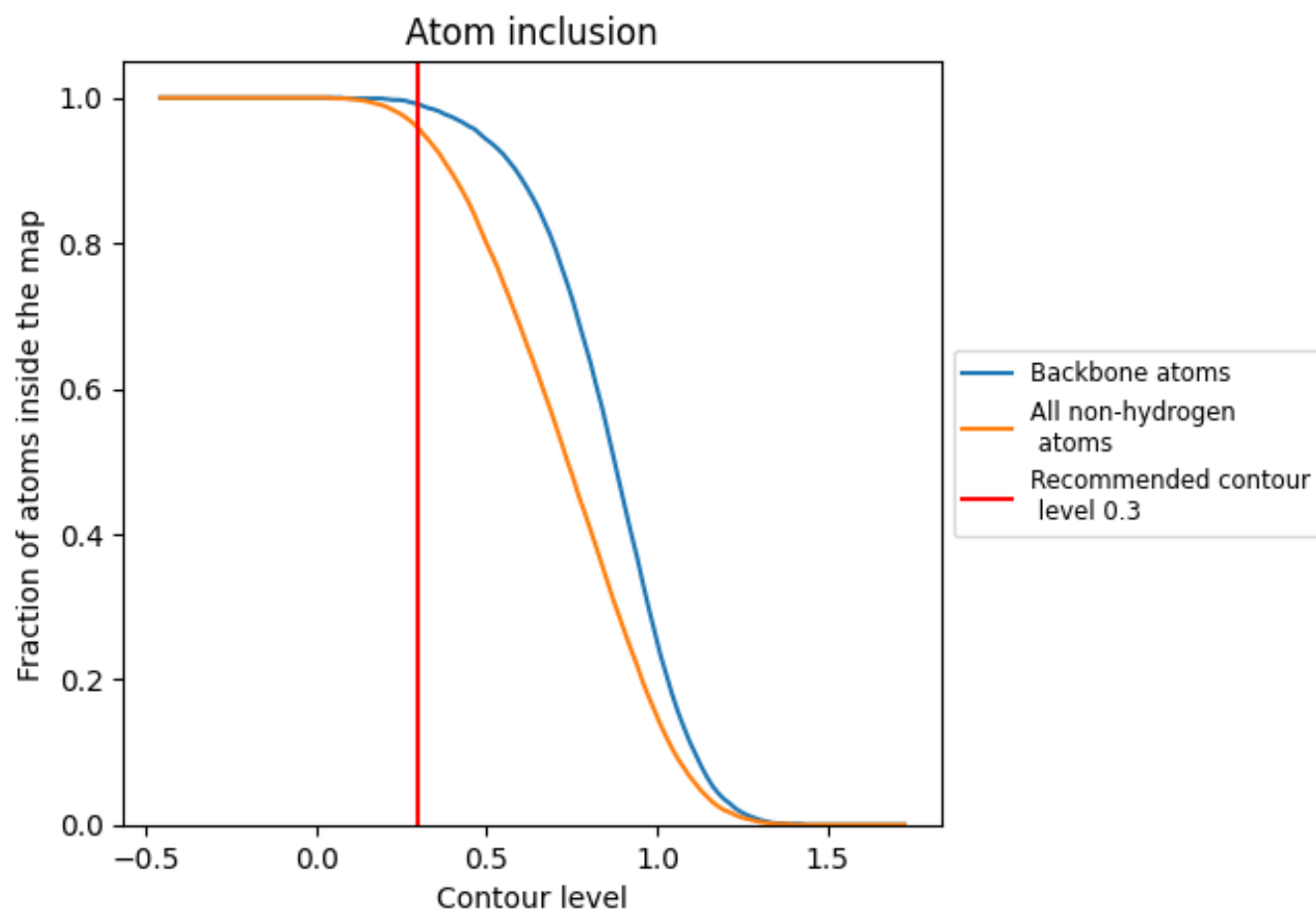
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 96% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.2970
A	0.9670	0.3200
B	0.9710	0.3000
C	0.9580	0.3070
D	0.9540	0.2960
E	0.9640	0.3080
F	0.9460	0.2500
J	0.9540	0.2830
O	0.9950	0.3060
P	0.9980	0.2990

1.0

0.0

<0.0