



## wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 02:01 AM EST

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

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We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev43  
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 : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

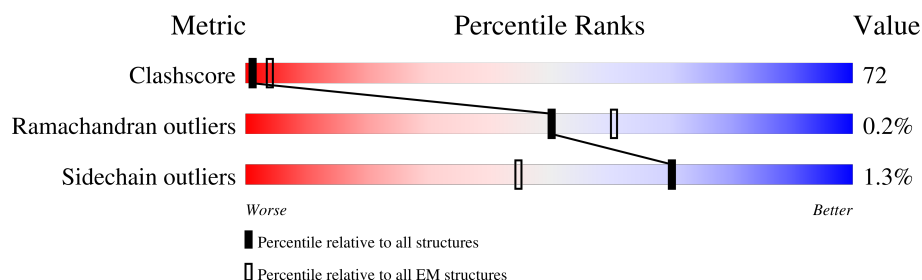
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 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.



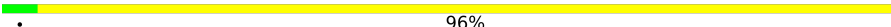
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	O	31	

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Mol	Chain	Length	Quality of chain
8	P	26	 96%

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		

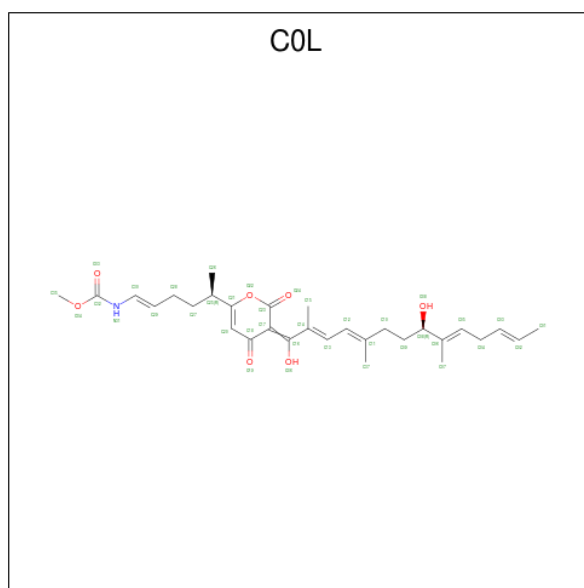
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: 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 (three-letter code: C0L) (formula: C<sub>30</sub>H<sub>41</sub>NO<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).

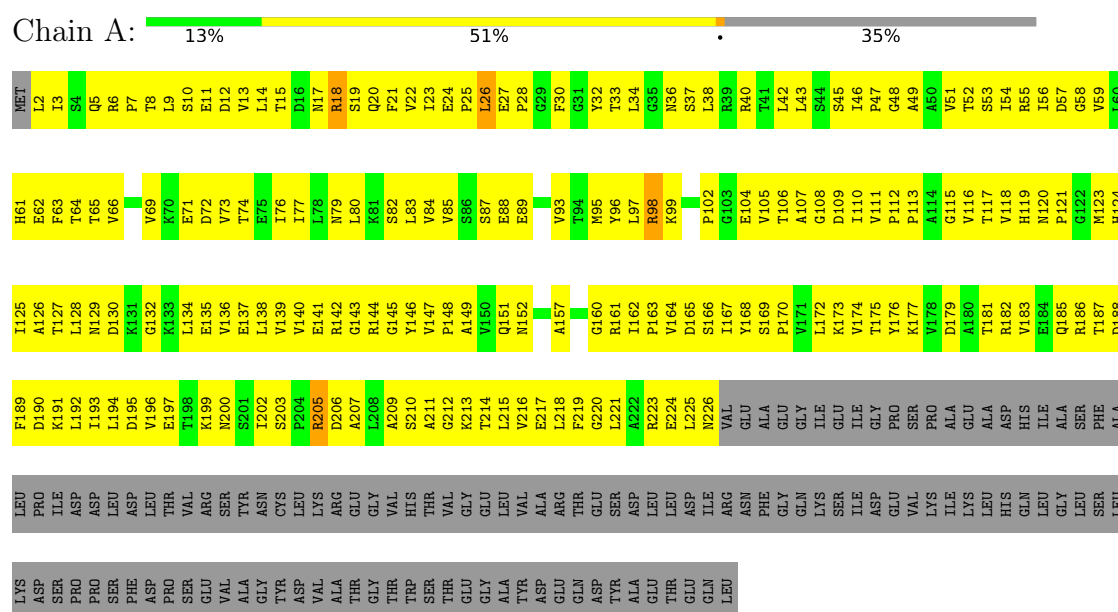


Mol	Chain	Residues	Atoms					AltConf
11	D	1	Total	C	H	N	O	0
			78	30	40	1	7	

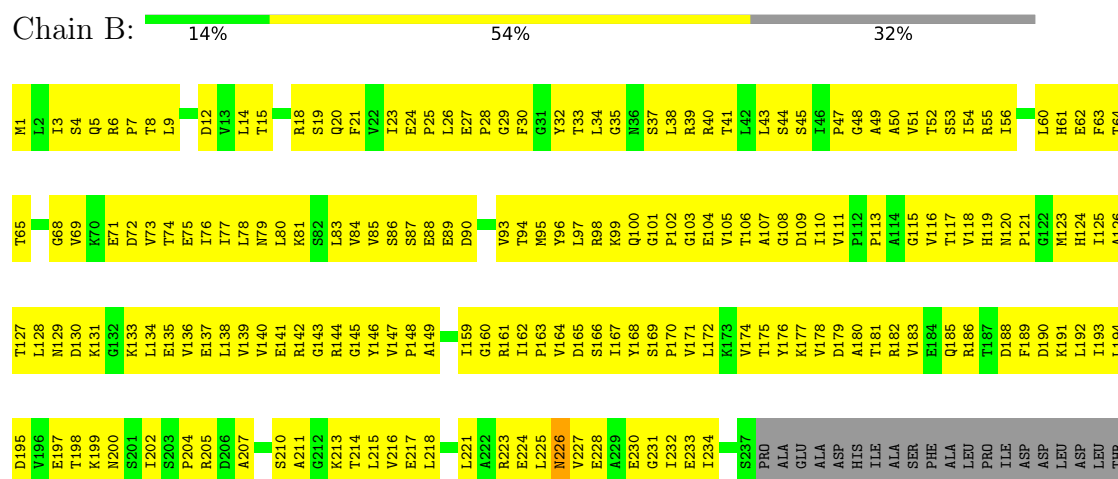
### 3 Residue-property plots

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





VAL	ARG	ASN	THR	TYR	GLY	CYS	LEU	LYS	LEU	ARG	GLU	GLY	VAL	HIS	THR	THR	GLY	GLU	LEU	VAL	ALA	ARG	THR	GLU	ASP	SER	ASP	LEU	LEU	ASP	ARG	ASN	PHE	GLY	GLN	LYS	SER	ILE	ASP	GLU	VAL	LYS	ILE	LYS	HIS	GLN	LEU	GLY	LEU	SER	LYS	LEU	SER	ASP	ASP	PRO	PRO	PHE	PHE	ASP	ASP
SER	GLU	VAL	ALA	GLY	THR	ASP	VAL	ALA	THR	GLY	THR	THR	THR	TRP	SER	THR	GLU	GLY	ALA	THR	ASP	GLU	GLN	ASP	THR	ALA	GLU	THR	GLU	GLN	LEU																														

- Molecule 2: DNA-directed RNA polymerase subunit beta

[illegible]

D834	G886	A970	M1031	I1091	GLU
T835	L889	Y971	K1032	K1092	ASP
S836	P900	Y972	H1033	S1093	GLU
L837	V901	V973	H1035	D1094	ASP
K838	E902	P974	L1036	T1095	LEU
V839	D903	P975	V1037	D1096	GLU
P840	M904	V976	V1037	V1097	ARG
H841	P905	P977	D1038	G1098	ALA
G842	P906	D978	K1040	R1099	ALA
E843	F907	G979	K1041	V1100	ALA
S844	L907	A980	H1042	K1101	ASN
K845	A908	Q981	A1043	V1102	LEU
G846	D909	Q982	A1044	V1103	GLY
V847	G910	E982	R1044	E1104	ILE
I850	P911	L985	S1045	A1105	ASN
R851	P912	Q986	T1046	I1106	LEU
V852	V913	G987	G1047	V1107	SER
S853	D914	L988	P1048	K1108	ARG
R854	I915	L989	Y1049	G1109	ASN
R855	I916	S990	S1050	E1110	GLU
E856	V922	C991	M1051	N1111	SER
D857	P923	L993	T1052	I1112	ALA
R858	R924	P994	Q1054	P1113	ALA
E859	R925	N995	Q1055	E1114	VAL
E860	M926	R996	P1056	G1116	ASP
L861	N927	D997	L1057	I1117	LEU
P862	L928	D999	G1058	P1118	ALA
A863	G929	V999	G1059	E1119	LEU
G864	Q930	A1000	K1060	S1120	ALA
V865	L931	L1001	A1061	F1121	ARG
N866	L932	V1002	Q1062	K1122	HIS
E867	E933	D1003	F1063	V1123	GLY
L868	T934	A1004	L1124	L1124	GLY
R869	H941	D1005	Q1066	K1126	SER
R870	S942	G1006	K1067	E1127	
V871	G943	A1008	P1067	L1128	
Y872	W944	M1009	F1068	Q1129	
V873	K945	L1010	G1069	S1130	
A874	V946	F1011	E1070	L1131	
Q875	V952	D1012	M1071	G1132	
K876	P953	G1013	E1072	L1133	
R877	D954	R1014	G1073	N1134	
K878	W955	S1015	S1074	V1135	
I879	A956	G1016	A1075	E1136	
S880	G881	E1017	M1076	V1137	
D881	G882	P1018	Q1077	L1138	
D883	R958	F1019	A1078	S1139	
K884	L959	P1020	Y1079	A1140	
L885	P960	Y1021	G1080	ASP	
A886	D961	P1022	A1081	GLY	
G887	E962	V1023	Y1082	ALA	
R888	L963	T1024	A1083	ALA	
H889	L964	V1025	T1084	ALA	
G890	E965	G1026	I1085	ILE	
N891	A966	Y1027	Q1086	GLU	
K892	Q967	M1028	E1087	LEU	
I895	P968	Y1029	L1088	ARG	
	N969	T1030	L1089	GLU	
			T1090	GLY	

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

Chain D:  24% 70% 5%

G-1	G43	I128	R194	G257	R325	V391	R459
N5	K64	I129	R195	S260	R326	R397	L460
F6	Y65	Y130	K196	I261	G258	P398	V461
D7	K66	F131	V197	K262	R327	L399	D462
F8	R67	A132	D198	K263	Q329	K400	A466
E9	V68	I133	G200	L264	Q329	S401	Q467
L10	R69	Y134	G201	L265	R334	L402	M468
R11	F70	V135	E202	E266	F335	S403	I469
I12	K71	I136	R203	N267	A336	D404	E530
G13	I73	S138	E204	F268	L405	G471	K470
L14	I74	V139	M205	D269	L406	A472	A472
A15	C75	D140	R206	I270	L340	K473	K473
T16	E76	E141	Q207		N341	K409	R474
A17	R77	E142	I208	A274	D342	Q410	M475
E18	C78	M143	R209	E275	L343	G411	V476
D19	G79	H144	D210	S276	Y344	R412	E477
I20	V80	R145	R211	L277	R345	M416	R478
R21	E81	N146	A212	R278	R346	L417	Q479
Q22	V82	E147	Q213	D279	V347	L418	R480
W23	T83	L148	R214	V280	L348	G419	L545
S24	R84	S149	L216	R282	R350	K420	Q482
Y25	A85	T150	L216	R282	R350	L547	V483
G26	K86	L151	D217	N283	N351	R421	V484
E27	V87	E152	R218	G284	N352	Y422	D485
V28	R88	A153	L219	K285	R353	D423	V486
R29	R89	E154	E220	G286	L354	Y424	L487
E30	E90	M155	D221	Q287	K355	A551	A551
P31	R91	A156	L222	K288	R356	G426	A552
E32	N92	V157	W223	R289	L357	R427	V489
T33	G93	E158	F226	L290	L358	S428	E554
I34	H94	R159	T227	L293	D359	A492	I491
N35	E96	V162	K228	G361	L360	L493	R556
Y36	P100	E163	L229	R294	G362	V431	I557
R37	T38	D164	A230	K295	P363	G432	L558
L39	V101	Q165	P231	L296	P364	K433	M559
K40	T102	R166	K232	K297	E364	Q435	L560
P41	H103	E169	Q233	V298	L365	L436	S561
E42	I104	L234	D237	V299	L366	K437	S562
D43	Y105	L235	L236	F302	V367	L438	N563
G45	F107	R173	D237	Q303	N368	H439	N564
L46	K108	A174	E238	Q304	E370	C441	L565
F47	G109	L177	E239	N307	K371	G442	L566
C48	V110	E178	L240	G306	R372	L443	S567
E49	P111	A179	Y241	K307	M373	P444	S570
X50	S112	D180	R242	K310	L374	K445	G571
I51	R113	L181	E243	G311	Q375	L446	P573
F52	L114	A182	L244	S377	E376	M447	L574
G53	L118	E183	V245	V312	S377	A448	A575
P54	D119	L184	D246	V313	V378	L449	M576
T55	L120	E185	R247	L314	A380	E450	P577
R56	L120	E185	Y248	D315	L381	L451	R578
D57	A121	G188	Y251	A316	F452	P514	L579
E58	D124	A189	F252	V317	R383	K453	M580
C60	E126	K190	T253	V318	N384	P454	M581
Y61	A191	A191	R386	V319	R386	F455	V517
C62	K127	A193	P322	P321	G519	V456	S583
					L585	G584	G584



WORLD WIDE  
PDB  
PROTEIN DATA BANK



A1	G2	C3	A4	C5	A6	A7	T8	T9	T10	A11	A12	C13	A14	C15	T16	T17	T18	T19	G20	T21	C22	A23	A24	G25	C26
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## 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: C0L, ZN, MG

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	0.40	0/1742	0.56	1/2370 (0.0%)
1	B	0.41	0/1786	0.57	0/2435
2	C	0.44	2/8744 (0.0%)	0.59	6/11860 (0.1%)
3	D	0.41	0/10037	0.55	2/13570 (0.0%)
4	E	0.41	0/662	0.53	0/901
5	F	0.39	0/2549	0.55	2/3438 (0.1%)
6	J	0.36	0/897	0.55	0/1210
7	O	0.90	0/710	1.01	0/1095
8	P	0.94	0/589	0.99	0/906
All	All	0.45	2/27716 (0.0%)	0.60	11/37785 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1068	PHE	C-N	6.87	1.45	1.33
2	C	1074	TRP	CB-CG	5.99	1.61	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1074	TRP	CA-CB-CG	10.61	133.87	113.70
2	C	1074	TRP	N-CA-CB	9.36	127.45	110.60
5	F	447	ALA	C-N-CA	-7.47	103.02	121.70
2	C	686	GLN	C-N-CA	-7.12	103.89	121.70
1	A	26	LEU	C-N-CA	-6.78	104.74	121.70

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	294	0
1	B	1759	0	1783	325	0
2	C	8586	0	8511	1348	0
3	D	9873	0	9941	1452	0
4	E	649	0	645	91	0
5	F	2518	0	2540	417	0
6	J	881	0	861	159	0
7	O	634	0	350	78	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	3865	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 72.

The worst 5 of 3865 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%)	34	72
3	D	1260/1326 (95%)	1109 (88%)	150 (12%)	1 (0%)	51	85
4	E	81/110 (74%)	72 (89%)	9 (11%)	0	100	100
5	F	317/531 (60%)	291 (92%)	24 (8%)	2 (1%)	25	65
6	J	106/111 (96%)	91 (86%)	14 (13%)	1 (1%)	17	56
All	All	3331/3951 (84%)	2913 (88%)	410 (12%)	8 (0%)	50	81

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%)	191 (98%)	3 (2%)	65	80
1	B	194/297 (65%)	193 (100%)	1 (0%)	88	93
2	C	933/997 (94%)	920 (99%)	13 (1%)	67	81
3	D	1042/1103 (94%)	1030 (99%)	12 (1%)	71	84
4	E	69/89 (78%)	68 (99%)	1 (1%)	67	81
5	F	264/429 (62%)	262 (99%)	2 (1%)	81	89
6	J	93/97 (96%)	89 (96%)	4 (4%)	29	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2789/3309 (84%)	2753 (99%)	36 (1%)	70 82

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1159	ARG
6	J	110	ARG
4	E	65	ASN
6	J	4	ARG
2	C	282	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	1062	GLN
3	D	465	HIS
5	F	325	ASN
3	D	5	ASN
3	D	307	ASN

### 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
11	C0L	D	1404	-	36,38,38	2.64	13 (36%)	38,49,49	2.97	12 (31%)

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	8.59	1.39	1.21
11	D	1404	C0L	O19-C18	5.65	1.39	1.24
11	D	1404	C0L	C17-C16	4.63	1.50	1.39
11	D	1404	C0L	O36-C16	-4.53	1.18	1.33
11	D	1404	C0L	C17-C18	-4.05	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	10.52	120.31	109.16
11	D	1404	C0L	C23-O22-C21	-6.85	118.02	122.22
11	D	1404	C0L	C35-O34-C32	-6.18	108.37	115.66
11	D	1404	C0L	O36-C16-C17	4.89	128.88	119.87
11	D	1404	C0L	C13-C12-C11	-4.75	120.00	127.30

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	1404	C0L	C05-C06-C08-C09
11	D	1404	C0L	C07-C06-C08-C09
11	D	1404	C0L	C13-C14-C16-O36
11	D	1404	C0L	C15-C14-C16-O36

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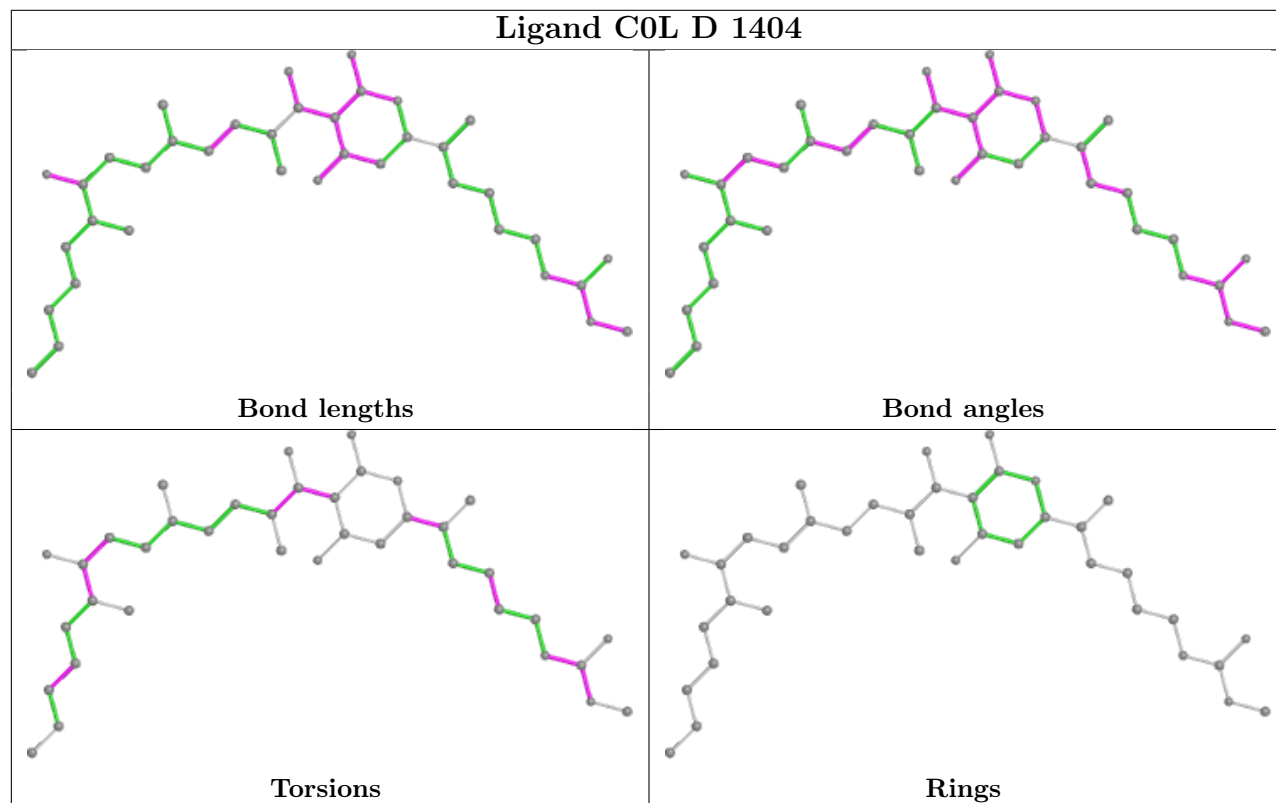
Mol	Chain	Res	Type	Atoms
11	D	1404	C0L	C14-C16-C17-C18

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.

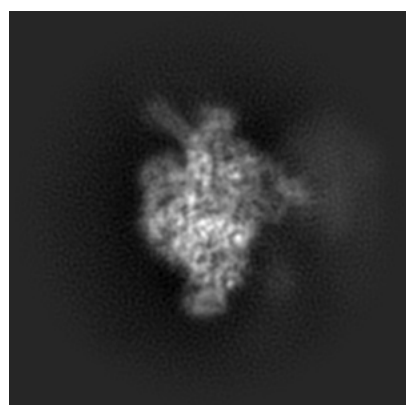
## 6 Map visualisation [i](#)

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.

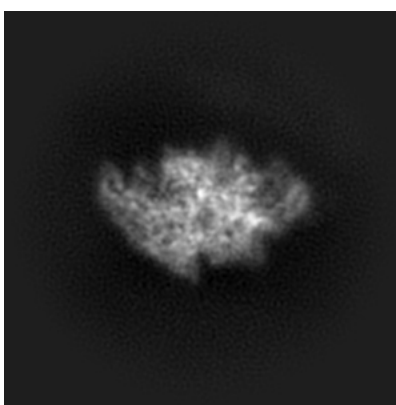
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

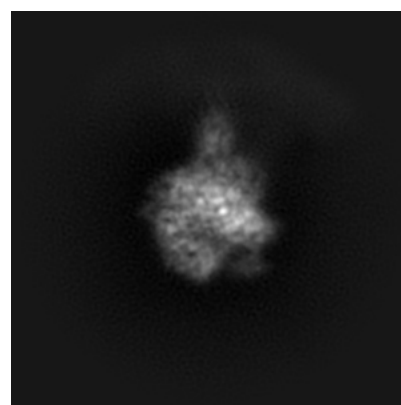
#### 6.1.1 Primary map



X



Y

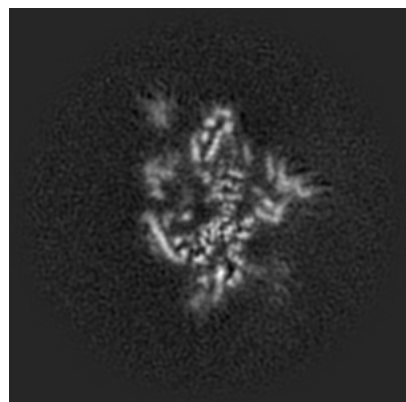


Z

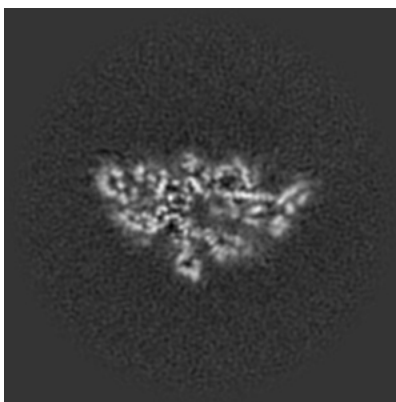
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

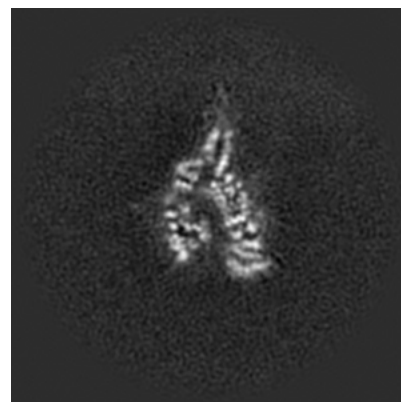
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

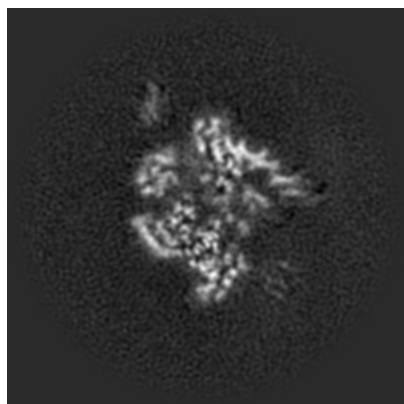


Z Index: 128

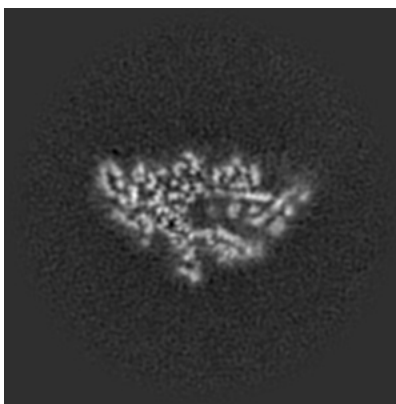
The images above show central slices of the map in three orthogonal directions.

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

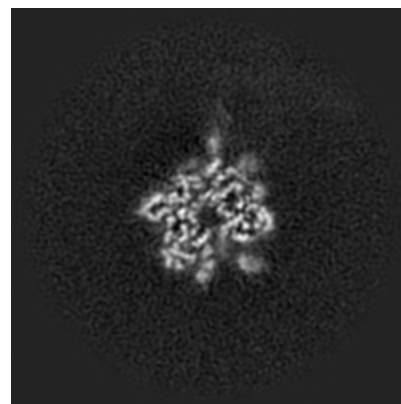
### 6.3.1 Primary map



X Index: 122



Y Index: 126



Z Index: 119

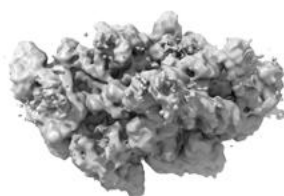
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.5 Mask visualisation

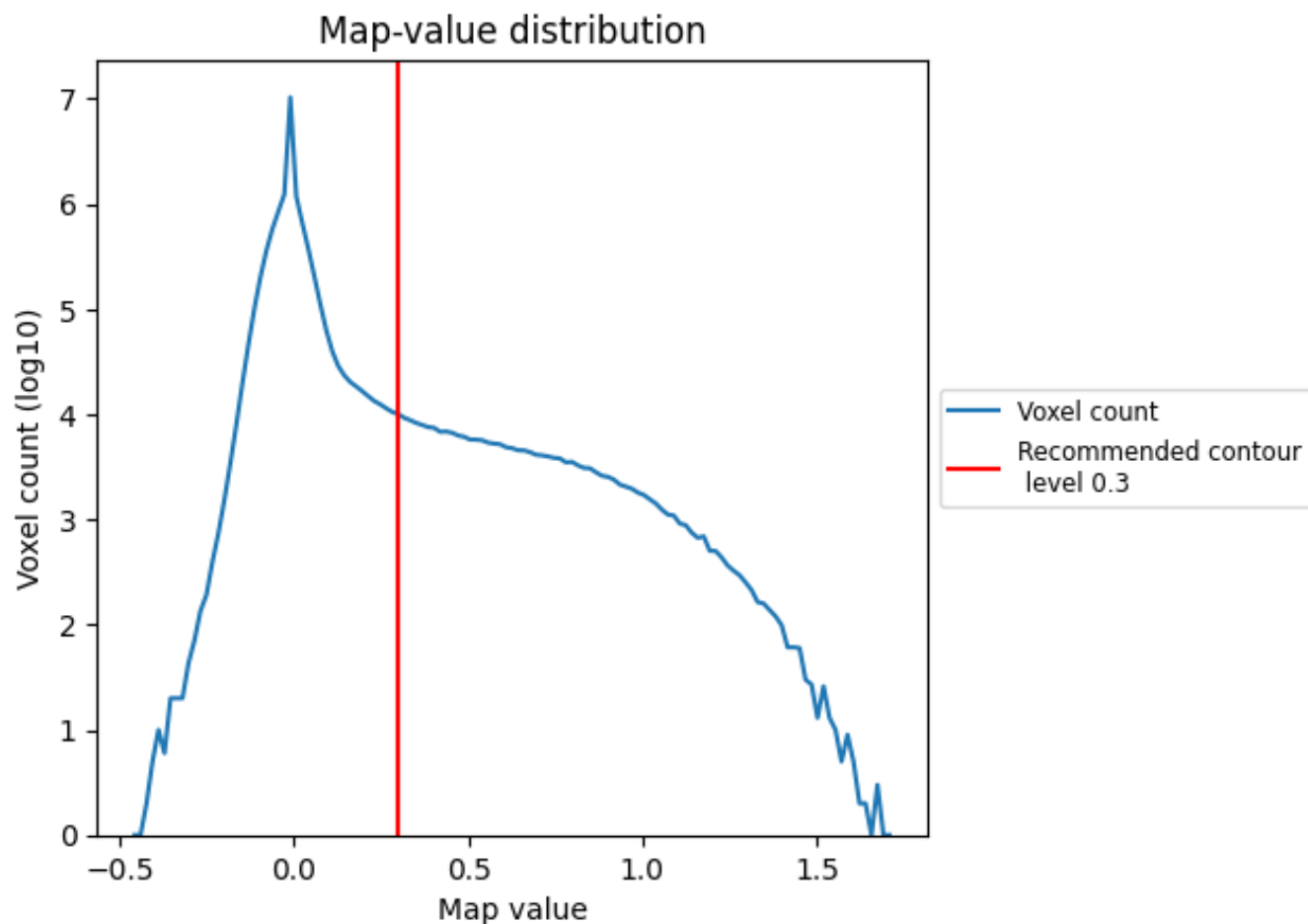
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

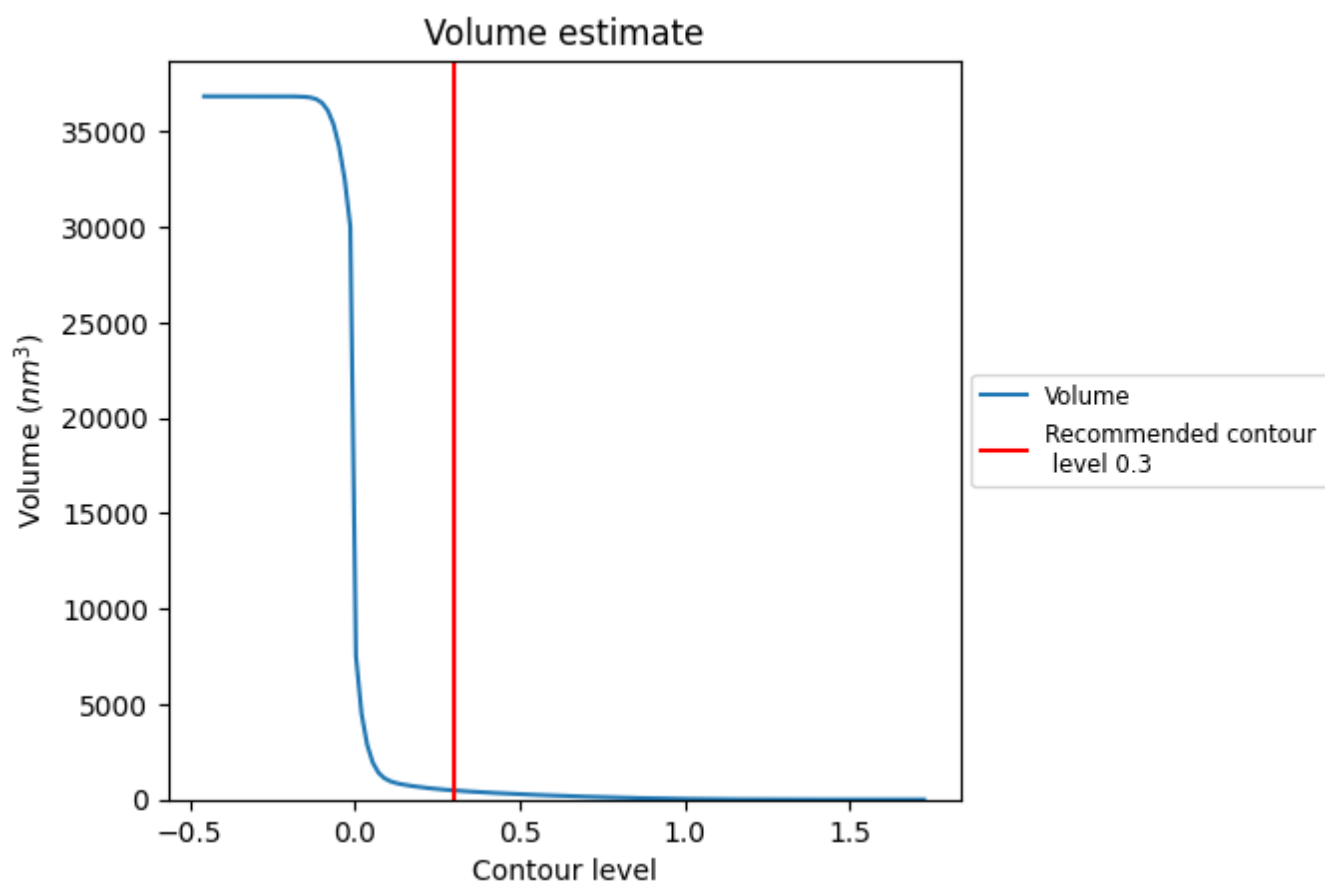
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

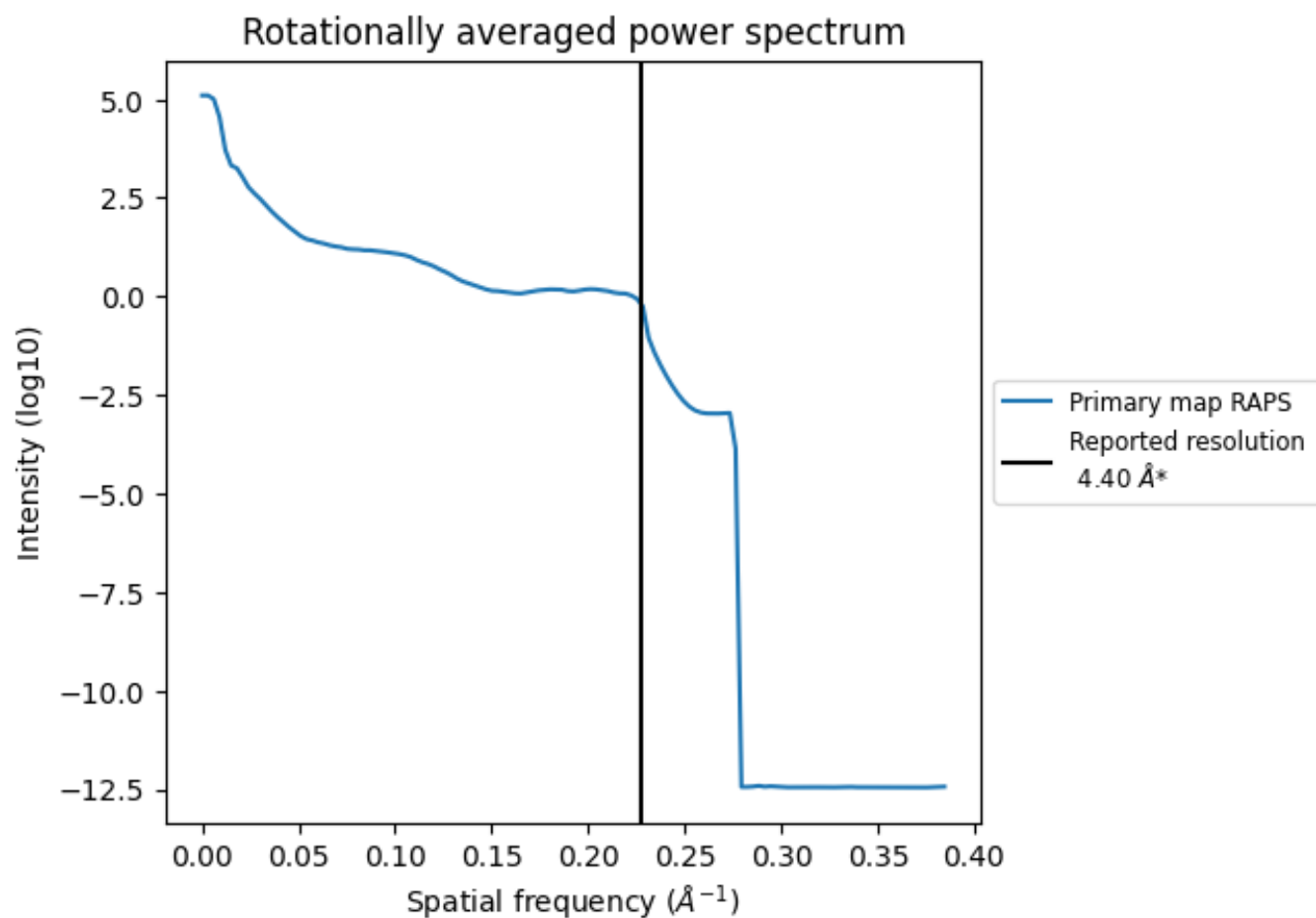
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 480 nm<sup>3</sup>; 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<sup>-1</sup>

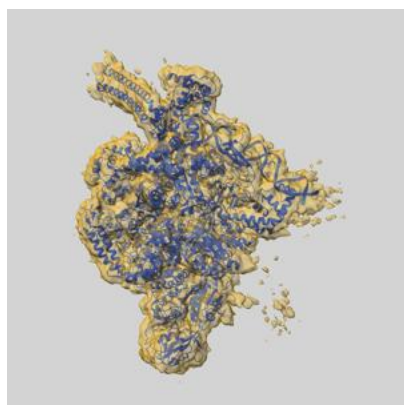
## 8 Fourier-Shell correlation

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

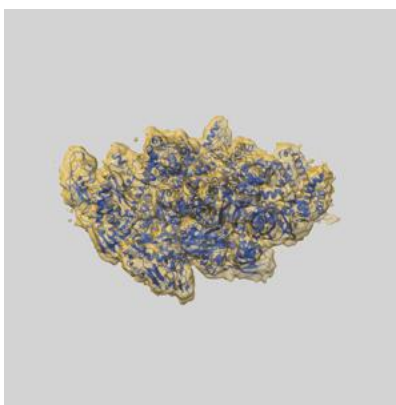
## 9 Map-model fit [i](#)

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](#).

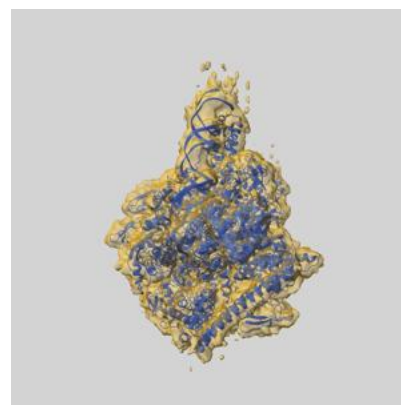
### 9.1 Map-model overlay [i](#)



X



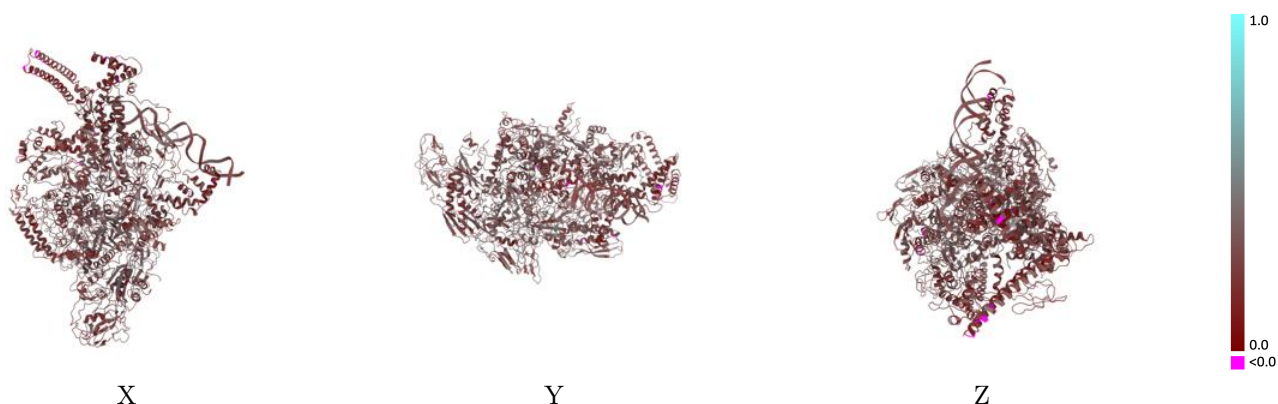
Y



Z

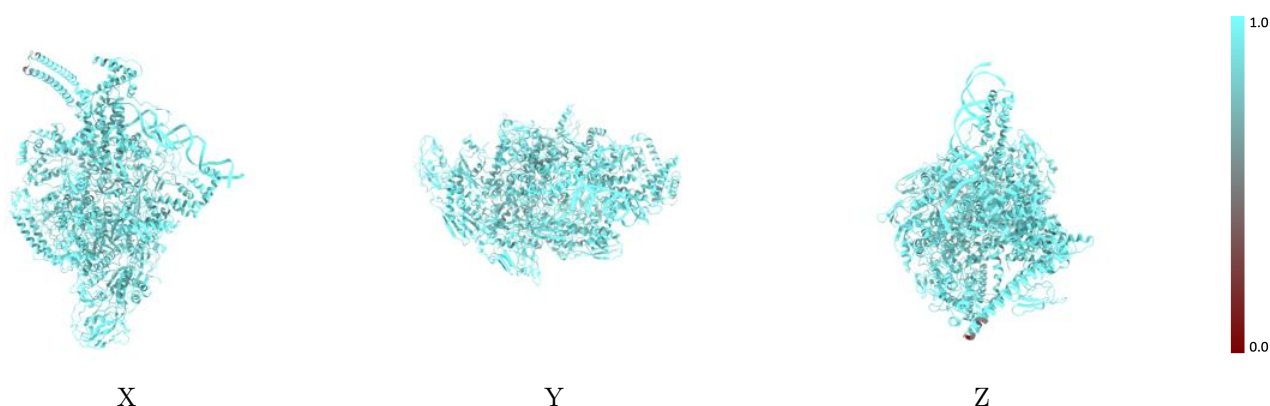
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



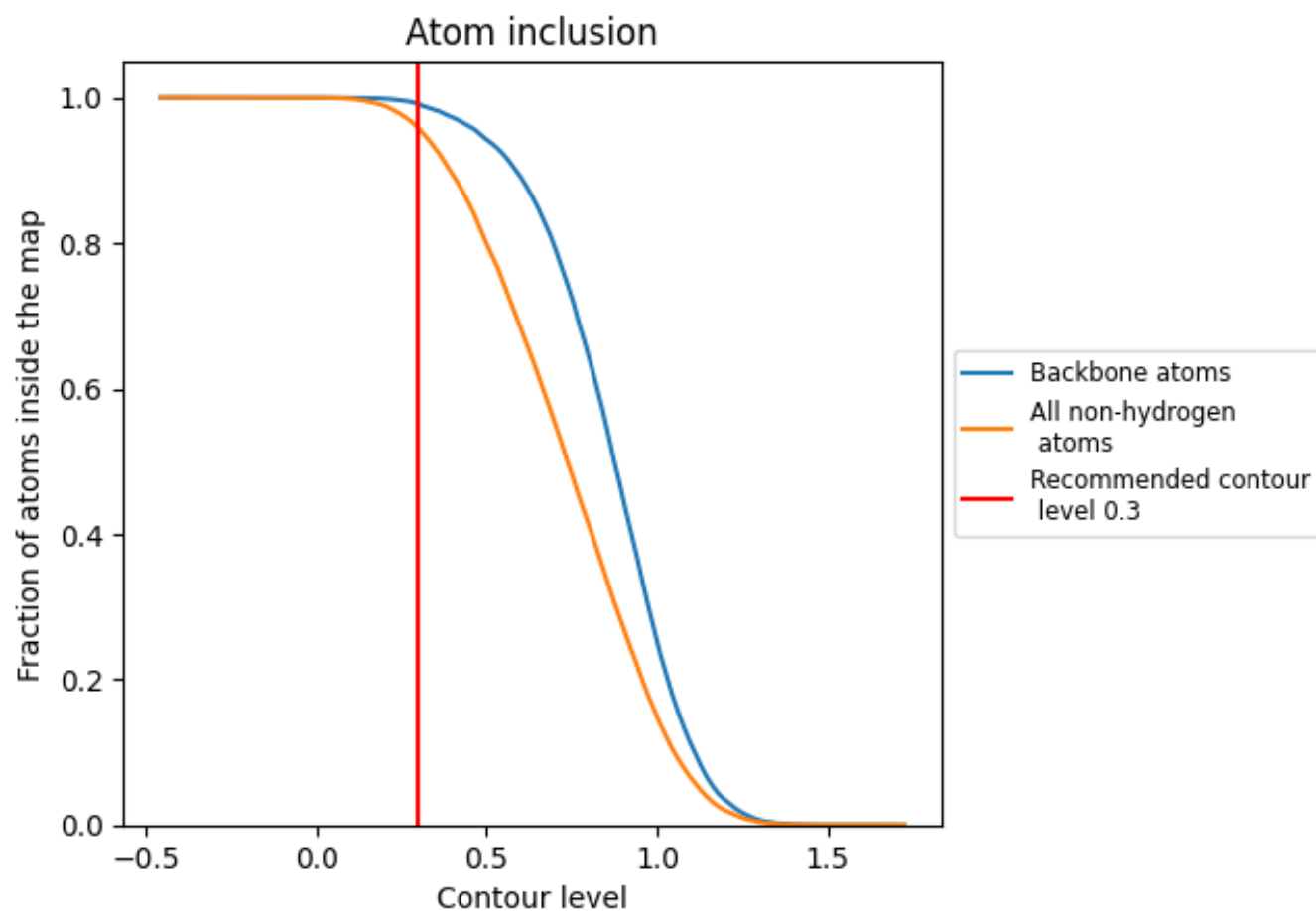
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div>0.9580</div>	<div><div></div>0.2970</div>
A	<div><div></div>0.9667</div>	<div><div></div>0.3200</div>
B	<div><div></div>0.9706</div>	<div><div></div>0.3000</div>
C	<div><div></div>0.9584</div>	<div><div></div>0.3070</div>
D	<div><div></div>0.9538</div>	<div><div></div>0.2960</div>
E	<div><div></div>0.9638</div>	<div><div></div>0.3080</div>
F	<div><div></div>0.9456</div>	<div><div></div>0.2500</div>
J	<div><div></div>0.9538</div>	<div><div></div>0.2830</div>
O	<div><div></div>0.9953</div>	<div><div></div>0.3060</div>
P	<div><div></div>0.9981</div>	<div><div></div>0.2990</div>

1.0

0.0

<0.0