



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 12:04 PM UTC

PDB ID : 6EEC / pdb_00006eec
EMDB ID : EMD-9041
Title : Mycobacterium tuberculosis RNAP promoter unwinding intermediate complex with RbpA/CarD and AP3 promoter captured by Corallopyronin
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.
Deposited on : 2018-08-13
Resolution : 3.55 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:

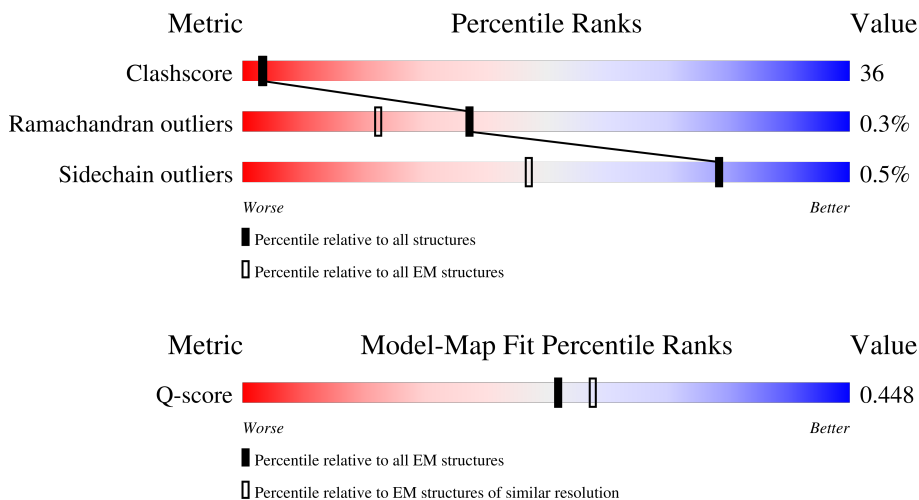
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.55 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.




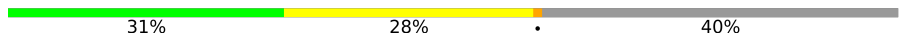



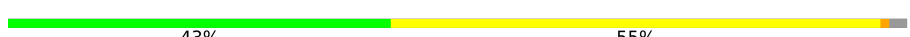
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12819 (3.05 - 4.05)

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	
1	B	347	
2	C	1179	
3	D	1326	

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Mol	Chain	Length	Quality of chain
4	E	110	
5	F	531	
6	J	111	
7	O	90	
8	P	90	
9	M	162	

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 29936 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
			Total	C	N	O	S		
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
			Total	C	N	O	S		
2	C	1111	Total	C	N	O	S	0	0
			8593	5381	1507	1666	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
			Total	C	N	O	S		
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
			Total	C	N	O		
4	E	83	649	414	108	127	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	319	2518	1571	456	482	9	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP 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
			Total	C	N	O	S		
6	J	108	881	543	168	167	3	0	0

- Molecule 7 is a DNA chain called DNA (65-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	65	1336	633	243	395	65	0	0

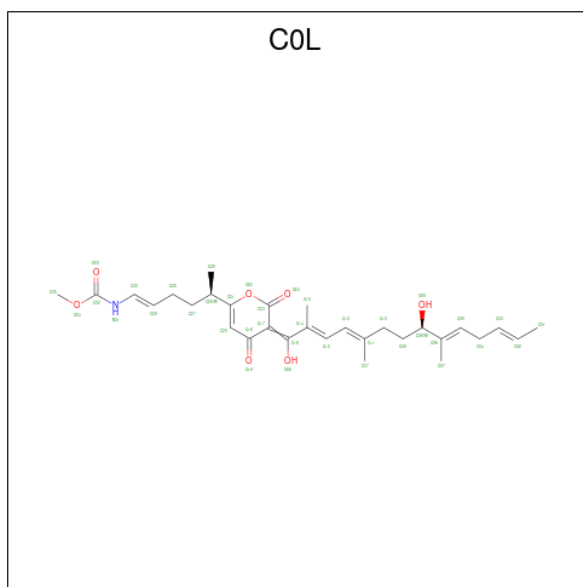
- Molecule 8 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	63	1289	610	242	374	63	0	0

- Molecule 9 is a protein called RNA polymerase-binding transcription factor CarD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	M	159	1241	777	224	239	1	0	0

- Molecule 10 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
			Total	C	H	N	O	
10	C	1	78	30	40	1	7	0

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

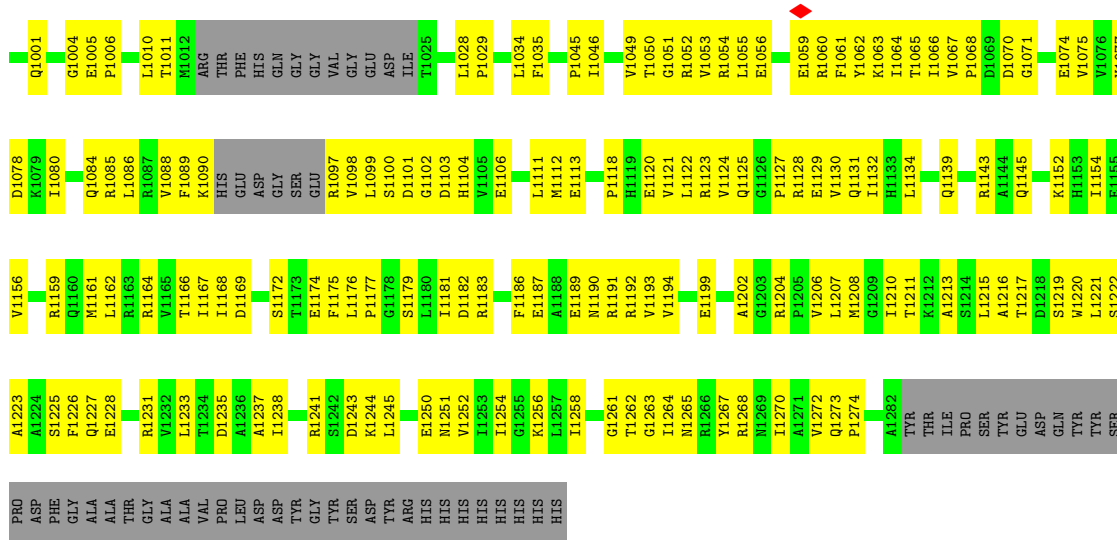
- Molecule 12 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

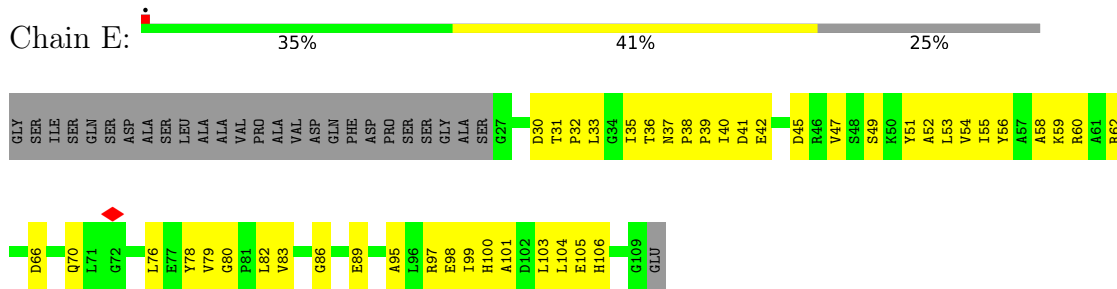
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C: 44% 49% 6%

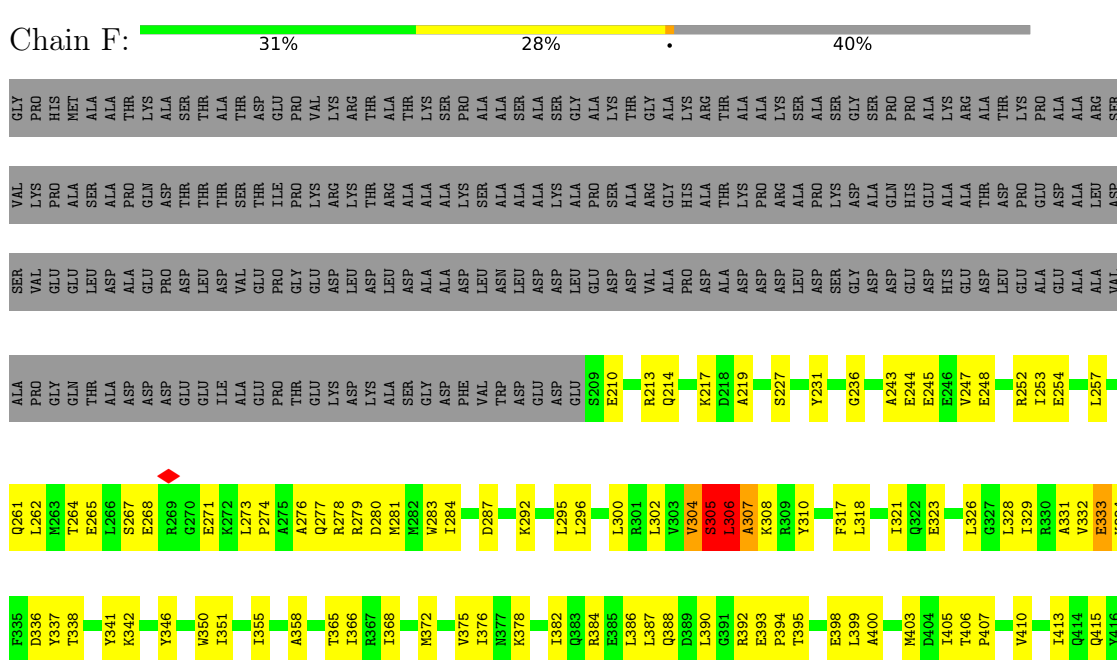
MET	ALA	ASP	SER	ARG	GLN	SER	PRO	THR	ALA	ALA	SER	PRO	SER	PRO	ARG	ARG	PRO	GLN	SER	SER	ASN	N30																																					
S84	P95	I96	E97	D98	G101	S102	M103	S104	L105	S106	F107	F112	V115	K116	A117	F118	V119	C122	D126	M127	T128	Y129	A130	A131	P132	L133	F134	V135	E138	F139	I140	M141	M142	N143	T144	G145	E146	I147	K148	Q150	R151	T152	V153	M154	K218	R219	D220	T221	V222	G223	F224	R225	K229	R230	R231	Q232	L233	L294	L296
T235	V236	L237	L238	K239	A240	W243	T244	E245	Q178	L179	S182	P183	F252	G253	F254	S255	E256	E189	D192	S194	T195	D196	K197	T198	D265	N266	T267	V268	G269	T270	D271	L272	E273	R274	K280	L281	R282	P283	G284	T285	P286	T288	K289	E290	S291	A292	Q293	L294	L296										
E297	M298	Y306	L308	A309	R310	V311	G312	R313	Y314	K315	L322	D408	V409	E410	A411	A412	T413	P414	Q415	T416	L417	I418	E343	Y344	L345	V346	R347	L348	H349	Q352	T353	T354	K355	T356	V357	P358	G359	D441	G360	V361	E362	V365	E366	T367	G374	N375	R376	R377	L378	R379	T380	V381	G459	P460	G461	G462			
L463	S464	R465	E466	R467	A468	G469	L470	V475	R401	E402	M404	D408	V409	E410	A411	A412	T413	P414	Q415	T416	L417	I418	L500	S501	V502	Y503	A504	R505	V506	N507	P508	F509	G510	F511	I512	E513	T514	P515	Y516	R517	K518	V519	G522	V523	V524	D525	R526	A527	R528	N603	R604	M607	N610						
D534	E535	E536	V540	V541	A542	S546	P547	I548	D549	R553	V559	L560	V561	R562	R563	K564	V568	V571	P572	E575	V576	D577	Y578	M579	D580	V581	S582	P583	R584	Q585	M586	V587	S588	T591	A592	M593	I594	F596	P599	E598	H599	D600	D601	A602	E527	R454	L455	I528	V529	Y530	L531	T532	A533						
M611	Q612	R613	P617	E622	A623	P624	P625	L626	V626	M630	E631	L632	R633	A634	A635	I636	D637	G638	G639	D640	V641	V642	V643	E646	S647	I650	S654	A655	D656	Y657	L658	T659	V660	M661	H662	R668	T669	Y670	R671	M672	R677	S678	M679	H680	G681	A602	P688	L455	R604	A698	V701	I702							
A703	D704	G705	P706	T707	T708	E712	M713	A714	L715	G716	K717	N718	L719	L720	R721	A722	I723	M724	P725	W726	E727	D728	Y731	E732	D733	A734	I735	I736	L737	S738	N739	R740	L741	L742	V746	H751	E756	I757	D758	A759	R760	D761	M762	G765	A766	E767	G681	P688	R771	D772	I773	P774	N775	I776					
S777	D778	E779	V780	L781	A782	D783	L784	D785	I789	V790	R791	I792	E795	L796	R797	D800	L801	L802	V803	G804	K805	V806	T807	P808	K809	T812	E813	L814	E817	R820	L821	R822	A823	I824	F825	G826	E827	K828	E831	V832	R833	D834	T835	S836	L837	K838	I848	M926	N927	I928	E860	L861	R862						
E833	T934	H935	L936	G943	Y946	H1034	H1035	L1036	V1037	L1038	D1039	D961	E962	L963	L964	Q967	P968	Y972	P1048	Y1049	S1050	M1051	I1052	A980	Q981	E982	A983	E984	L985	Q986	G987	L988	L989	E902	D903	M904	P905	F906	L907	A908	D909	G910	V913	D914	I915	L916	L917	N918	T919	V922	P923	D1012	G1013	R1014	S1015	F1019			
G1026	Y1027	M1028	Y1029	I1030	M1031	K1032	L1033	H1034	H1035	L1036	V1037	L1038	D1039	K1040	I1041	H1042	A1043	R1044	S1045	T1046	P1047	Y1048	Y1049	S1050	M1051	I1052	P1056	L1057	R1058	G1059	Q1062	F1063	Q1066	R1067	E1070	M1074	A1075	M1076	Q1077	A1078	Y1079	D999	G1080	A1081	A1082	Y1083	T1084	E1087	L1088	I1091	K1092	S1093	D1094						

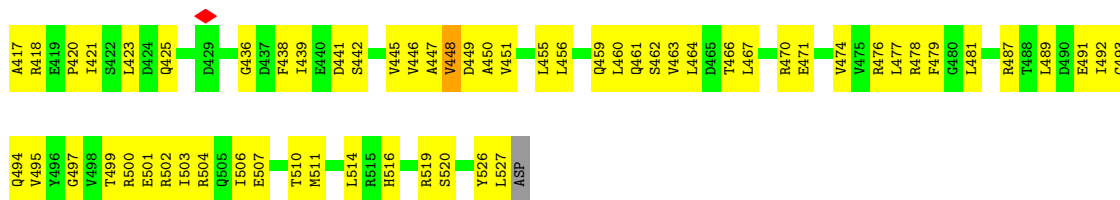


• Molecule 4: DNA-directed RNA polymerase subunit omega

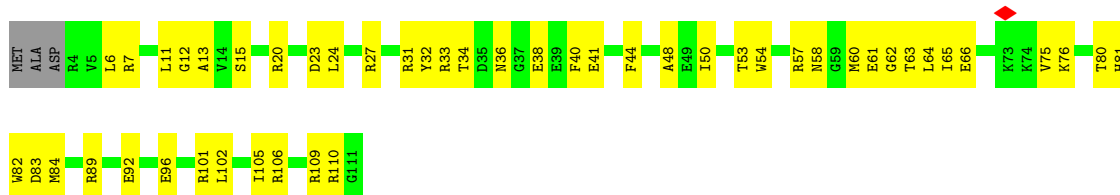


• Molecule 5: RNA polymerase sigma factor SigA

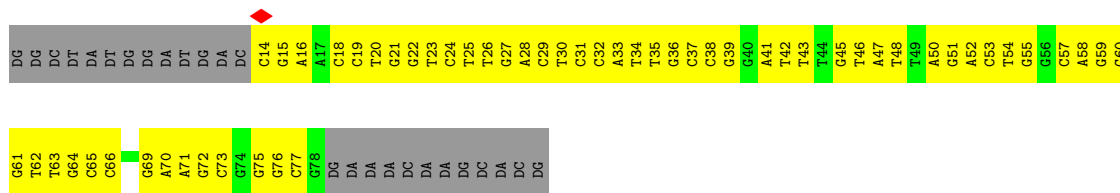
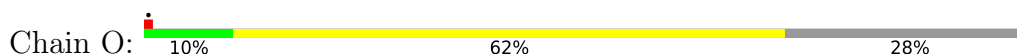




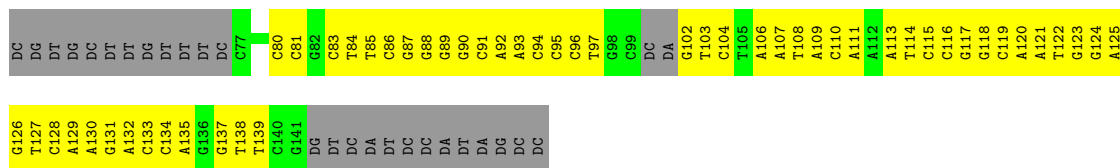
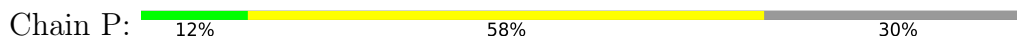
• Molecule 6: RNA polymerase-binding protein RbpA



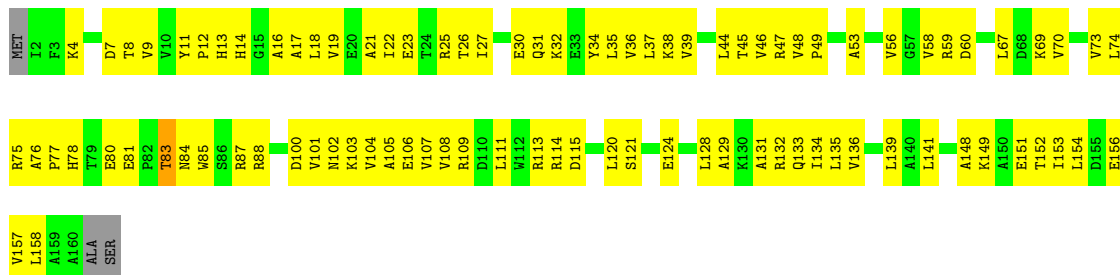
• Molecule 7: DNA (65-MER)



• Molecule 8: DNA (63-MER)



• Molecule 9: RNA polymerase-binding transcription factor CarD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246409	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	3.111	Depositor
Minimum map value	-1.642	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	325.0, 325.0, 325.0	wwPDB
Map dimensions	250, 250, 250	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, ZN, COL

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	0.43	0/1742	0.55	0/2370
1	B	0.39	0/1786	0.54	0/2435
2	C	0.57	7/8751 (0.1%)	0.67	13/11869 (0.1%)
3	D	0.63	24/10037 (0.2%)	0.65	16/13570 (0.1%)
4	E	0.37	0/662	0.51	0/901
5	F	0.55	6/2549 (0.2%)	0.63	3/3438 (0.1%)
6	J	0.32	0/897	0.62	2/1210 (0.2%)
7	O	0.35	0/1497	0.46	0/2310
8	P	0.32	0/1445	0.42	0/2224
9	M	0.29	0/1257	0.49	0/1700
All	All	0.54	37/30623 (0.1%)	0.61	34/42027 (0.1%)

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	656	TRP	CA-C	-8.86	1.41	1.52
3	D	389	ARG	CA-C	-8.74	1.43	1.52
3	D	661	ALA	CA-C	-8.66	1.41	1.52
5	F	305	SER	CA-C	-8.57	1.41	1.52
3	D	387	ARG	CA-C	-8.35	1.42	1.52

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	306	LEU	CA-C-N	-10.51	103.71	120.63
5	F	306	LEU	C-N-CA	-10.51	103.71	120.63
2	C	307	ASP	N-CA-C	8.87	122.75	110.06
2	C	288	THR	N-CA-C	-8.46	93.21	108.02
2	C	281	LEU	N-CA-C	-8.40	102.21	111.36

There are no chirality outliers.

There are no planarity outliers.

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	1716	0	1756	120	0
1	B	1759	0	1783	146	0
2	C	8593	0	8517	721	0
3	D	9873	0	9938	772	0
4	E	649	0	645	55	0
5	F	2518	0	2540	186	0
6	J	881	0	861	63	0
7	O	1336	0	732	119	0
8	P	1289	0	706	88	0
9	M	1241	0	1259	111	0
10	C	38	40	0	1	0
11	D	2	0	0	0	0
12	D	1	0	0	0	0
All	All	29896	40	28737	2135	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 36.

The worst 5 of 2135 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)
2:C:281:LEU:CD2	2:C:295:LEU:HD21	1.62	1.30
2:C:271:ASP:O	2:C:275:LEU:HD12	1.25	1.27
2:C:1067:ARG:CZ	3:D:418:LEU:CD2	2.13	1.25
2:C:278:TYR:CE1	2:C:292:ALA:HB2	1.73	1.23
2:C:1067:ARG:NH1	3:D:418:LEU:CD2	2.04	1.21

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	223/347 (64%)	197 (88%)	26 (12%)	0	100	100
1	B	235/347 (68%)	194 (83%)	41 (17%)	0	100	100
2	C	1109/1179 (94%)	937 (84%)	168 (15%)	4 (0%)	30	61
3	D	1260/1326 (95%)	1141 (91%)	115 (9%)	4 (0%)	36	65
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	317/531 (60%)	296 (93%)	20 (6%)	1 (0%)	36	65
6	J	106/111 (96%)	87 (82%)	19 (18%)	0	100	100
9	M	157/162 (97%)	144 (92%)	12 (8%)	1 (1%)	21	54
All	All	3488/4113 (85%)	3072 (88%)	406 (12%)	10 (0%)	37	65

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	418	LEU
3	D	658	PRO
2	C	274	LEU
3	D	653	HIS
2	C	53	LEU

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	194/297 (65%)	194 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/297 (65%)	194 (100%)	0	100	100
2	C	935/997 (94%)	927 (99%)	8 (1%)	70	76
3	D	1042/1103 (94%)	1036 (99%)	6 (1%)	78	79
4	E	69/89 (78%)	69 (100%)	0	100	100
5	F	264/429 (62%)	262 (99%)	2 (1%)	73	77
6	J	93/97 (96%)	93 (100%)	0	100	100
9	M	129/131 (98%)	129 (100%)	0	100	100
All	All	2920/3440 (85%)	2904 (100%)	16 (0%)	78	80

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	305	SER
3	D	656	TRP
3	D	37	ARG
3	D	418	LEU
2	C	466	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	657	GLN
3	D	797	ASN
9	M	102	ASN
3	D	674	ASN
3	D	748	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
10	C0L	C	1201	-	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
10	C0L	C	1201	-	-	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)
10	C	1201	C0L	O24-C23	8.85	1.39	1.21
10	C	1201	C0L	O19-C18	5.65	1.39	1.24
10	C	1201	C0L	C17-C16	4.82	1.50	1.39
10	C	1201	C0L	O36-C16	-4.54	1.18	1.33
10	C	1201	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(°)
10	C	1201	C0L	O34-C32-N31	9.68	120.28	109.15
10	C	1201	C0L	C35-O34-C32	-6.27	108.38	115.63
10	C	1201	C0L	O22-C21-C25	5.53	116.21	111.35
10	C	1201	C0L	O36-C16-C17	4.94	128.90	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	C	1201	C0L	C23-C17-C18	4.42	121.98	119.41

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

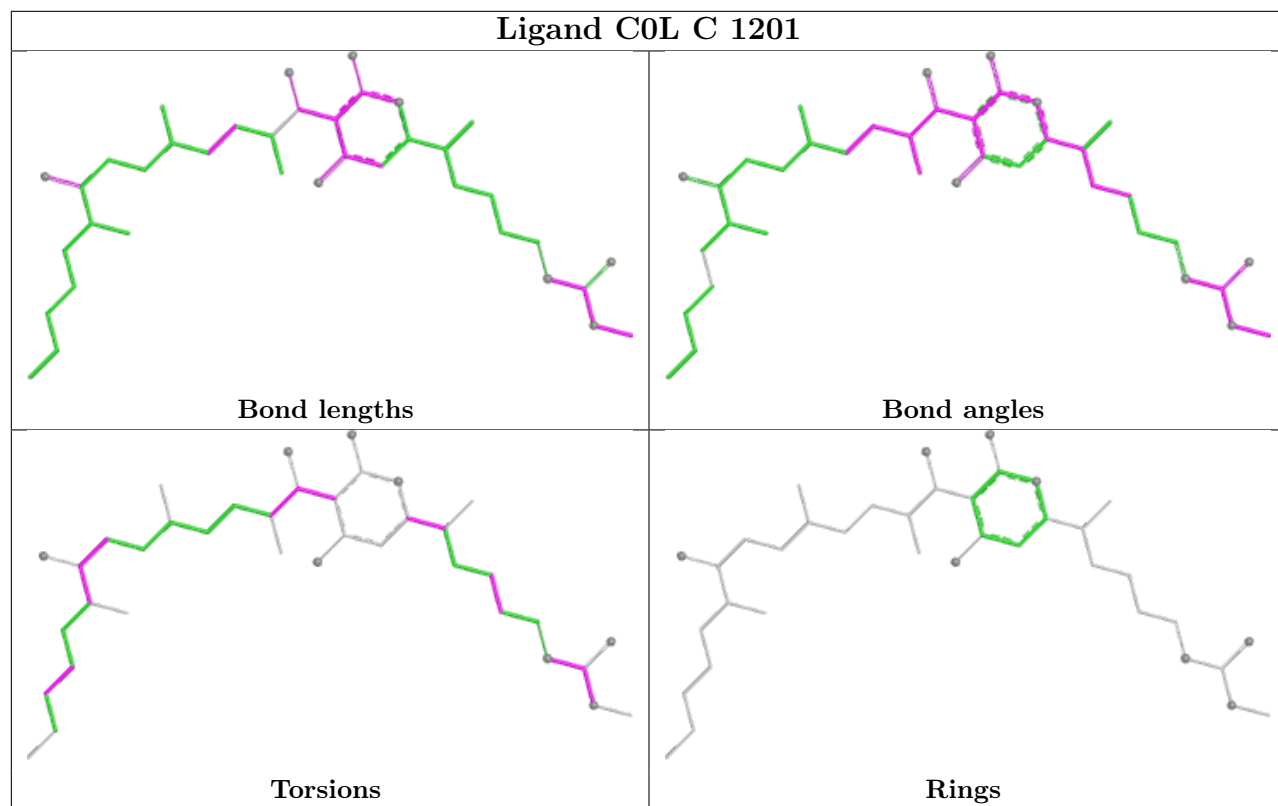
Mol	Chain	Res	Type	Atoms
10	C	1201	C0L	C13-C14-C16-O36
10	C	1201	C0L	C15-C14-C16-O36
10	C	1201	C0L	C14-C16-C17-C18
10	C	1201	C0L	C14-C16-C17-C23
10	C	1201	C0L	O36-C16-C17-C18

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1201	C0L	1	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.

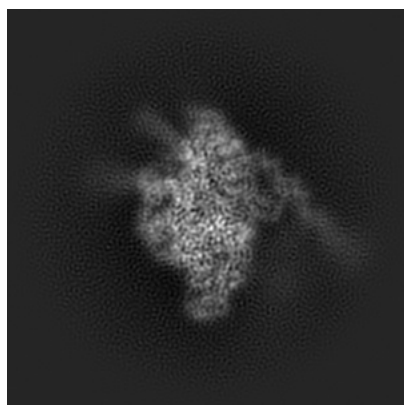
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9041. These allow visual inspection of the internal detail of the map and identification of artifacts.

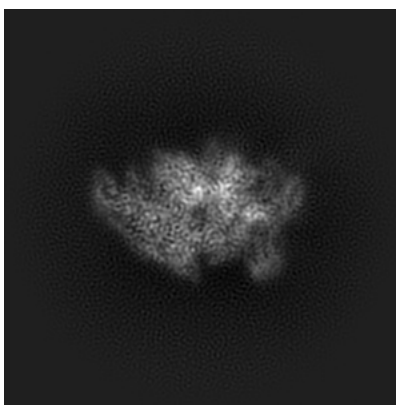
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

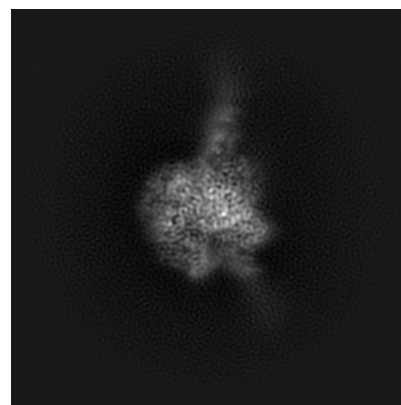
6.1.1 Primary map



X



Y

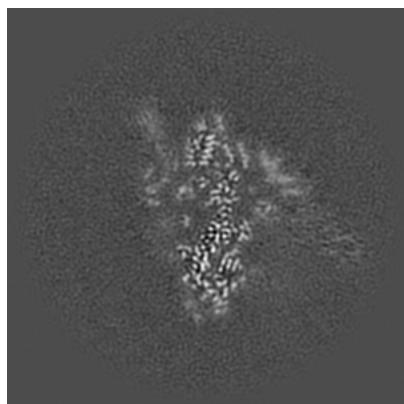


Z

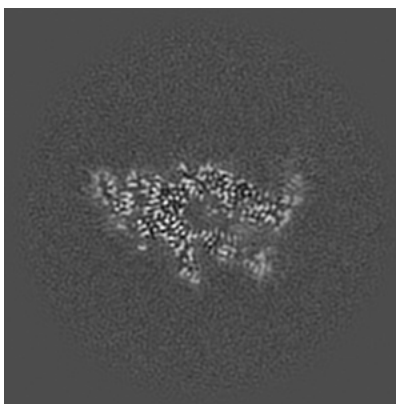
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

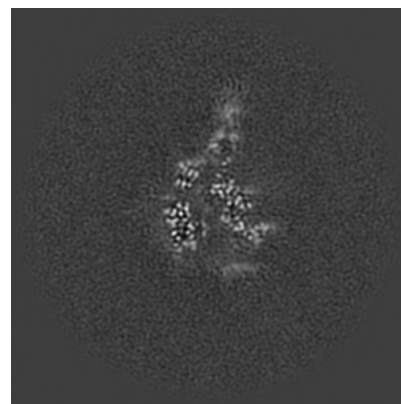
6.2.1 Primary map



X Index: 125



Y Index: 125

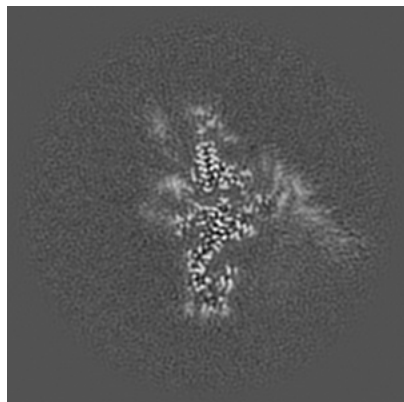


Z Index: 125

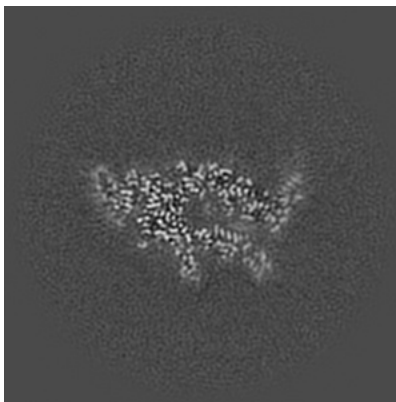
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

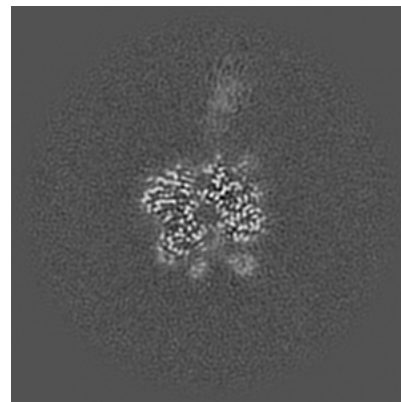
6.3.1 Primary map



X Index: 132



Y Index: 124

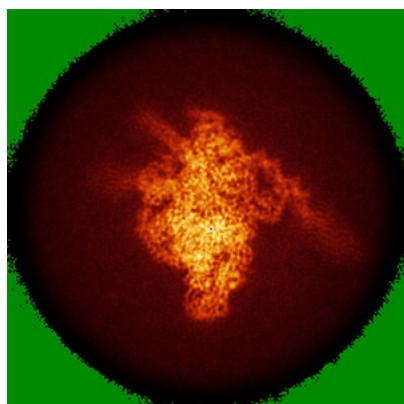


Z Index: 113

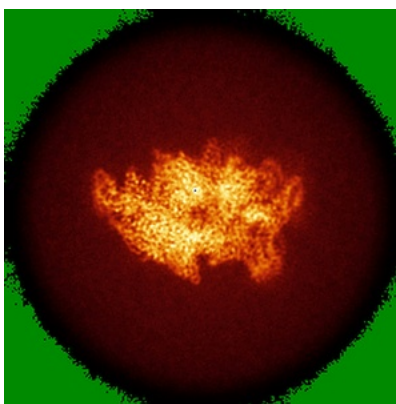
The images above show the largest variance slices of the map in three orthogonal directions.

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

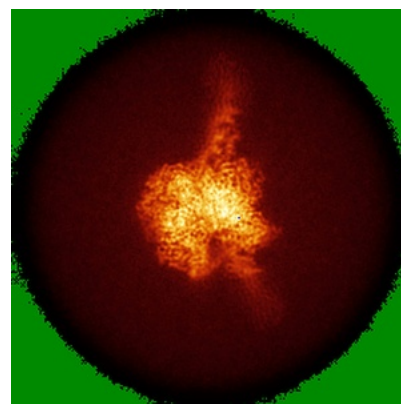
6.4.1 Primary map



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

This section was not generated.

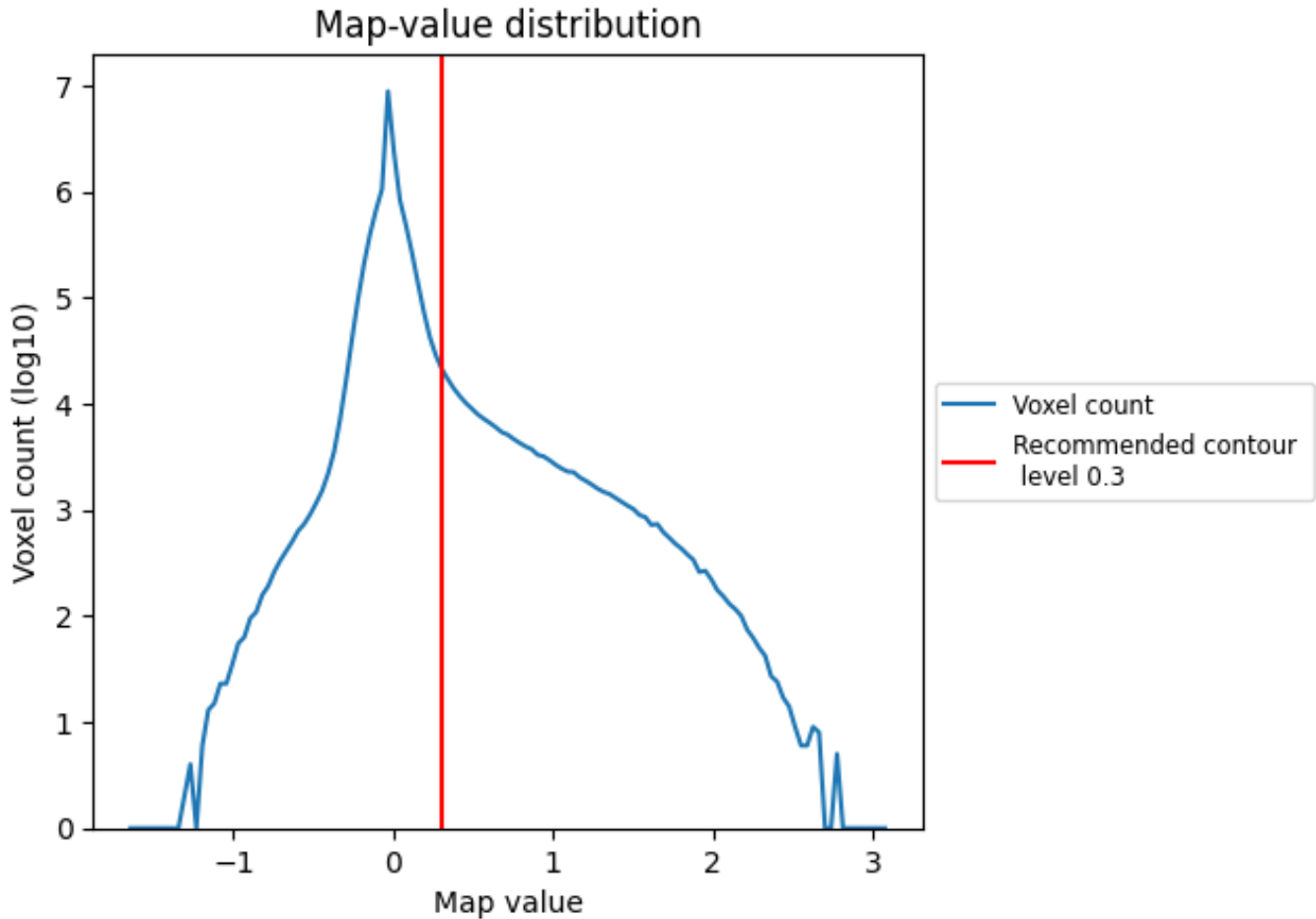
6.6 Mask visualisation

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

7 Map analysis [i](#)

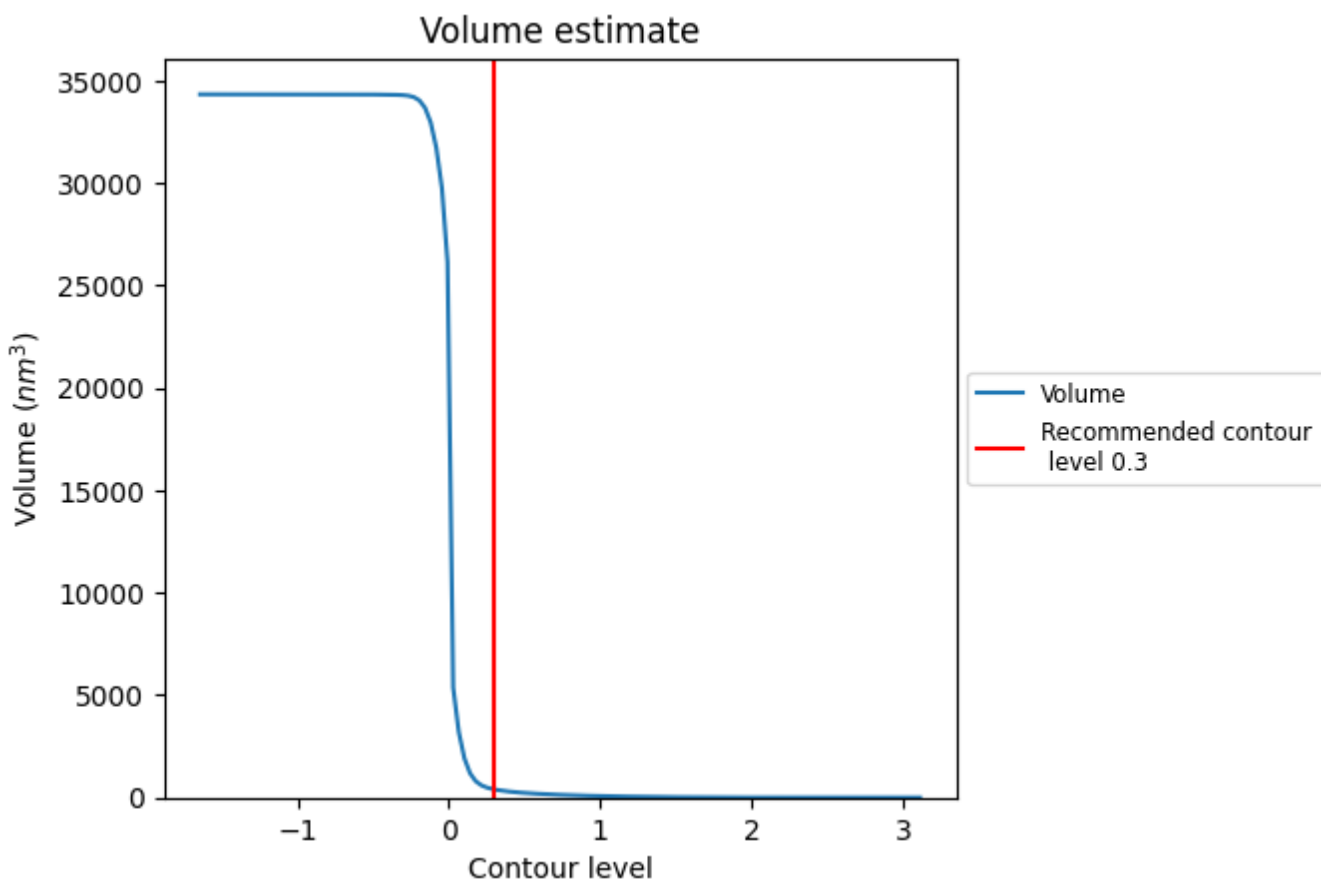
This section contains the results of statistical analysis of the map.

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.

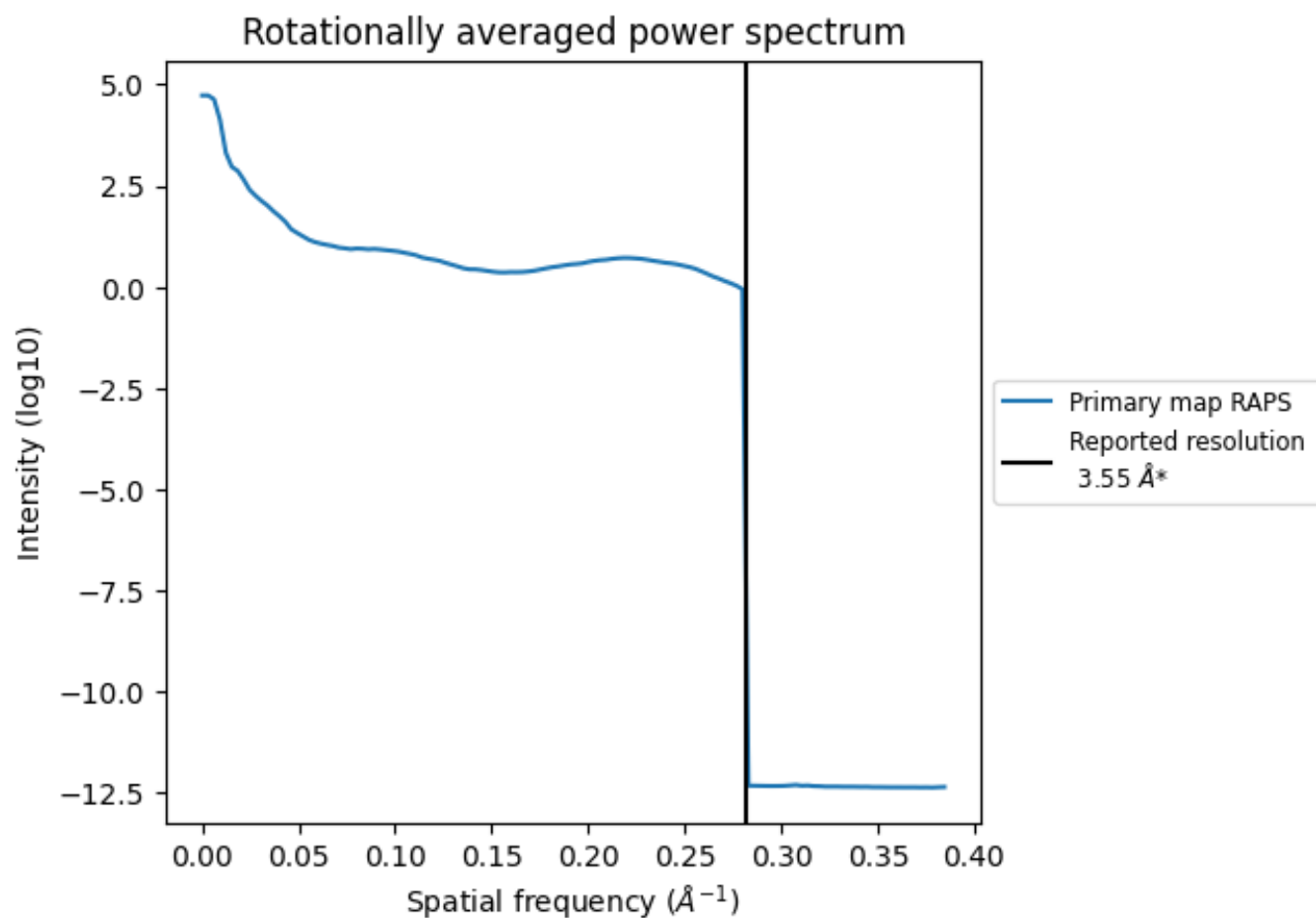
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm^3 ; this corresponds to an approximate mass of 362 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.282 Å⁻¹

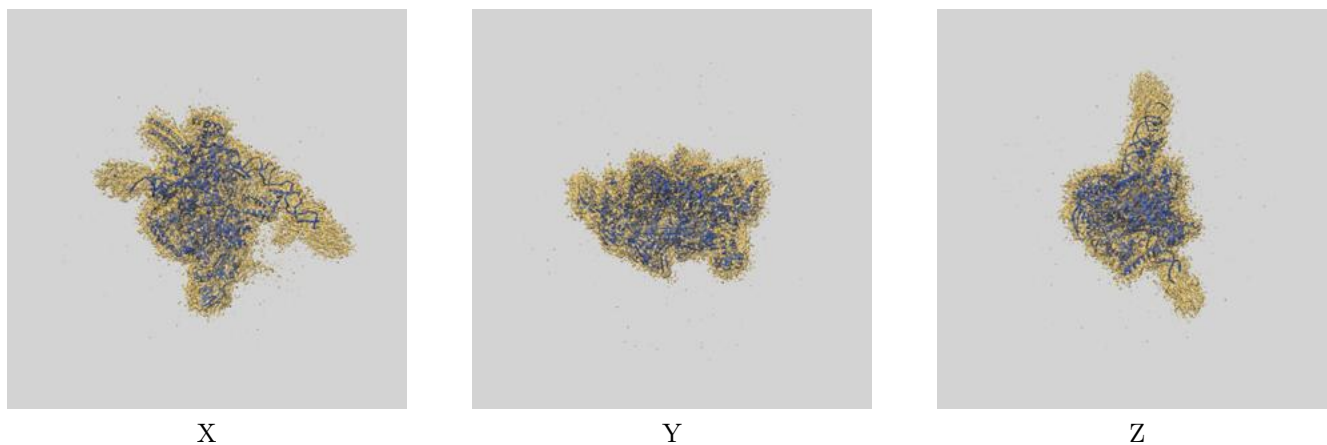
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

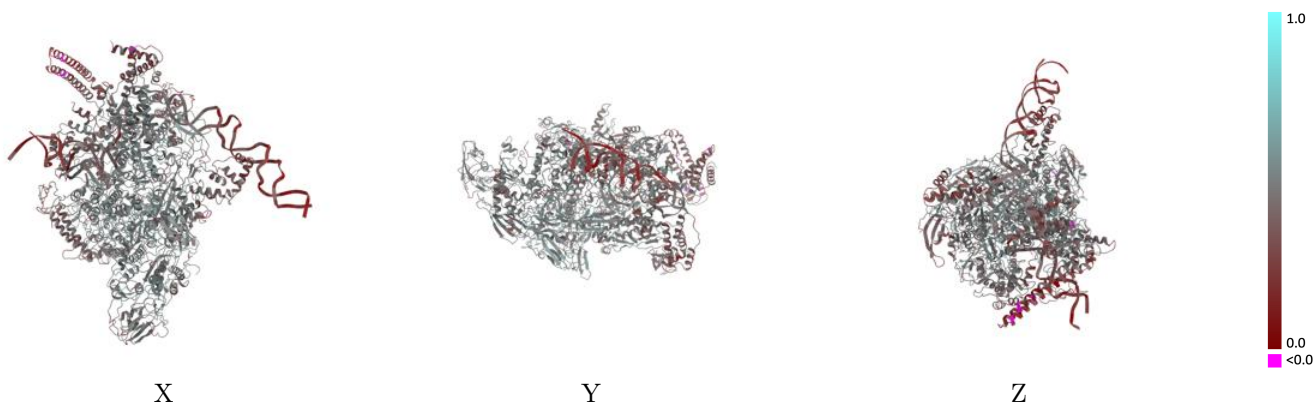
This section contains information regarding the fit between EMDB map EMD-9041 and PDB model 6EEC. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



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](#)

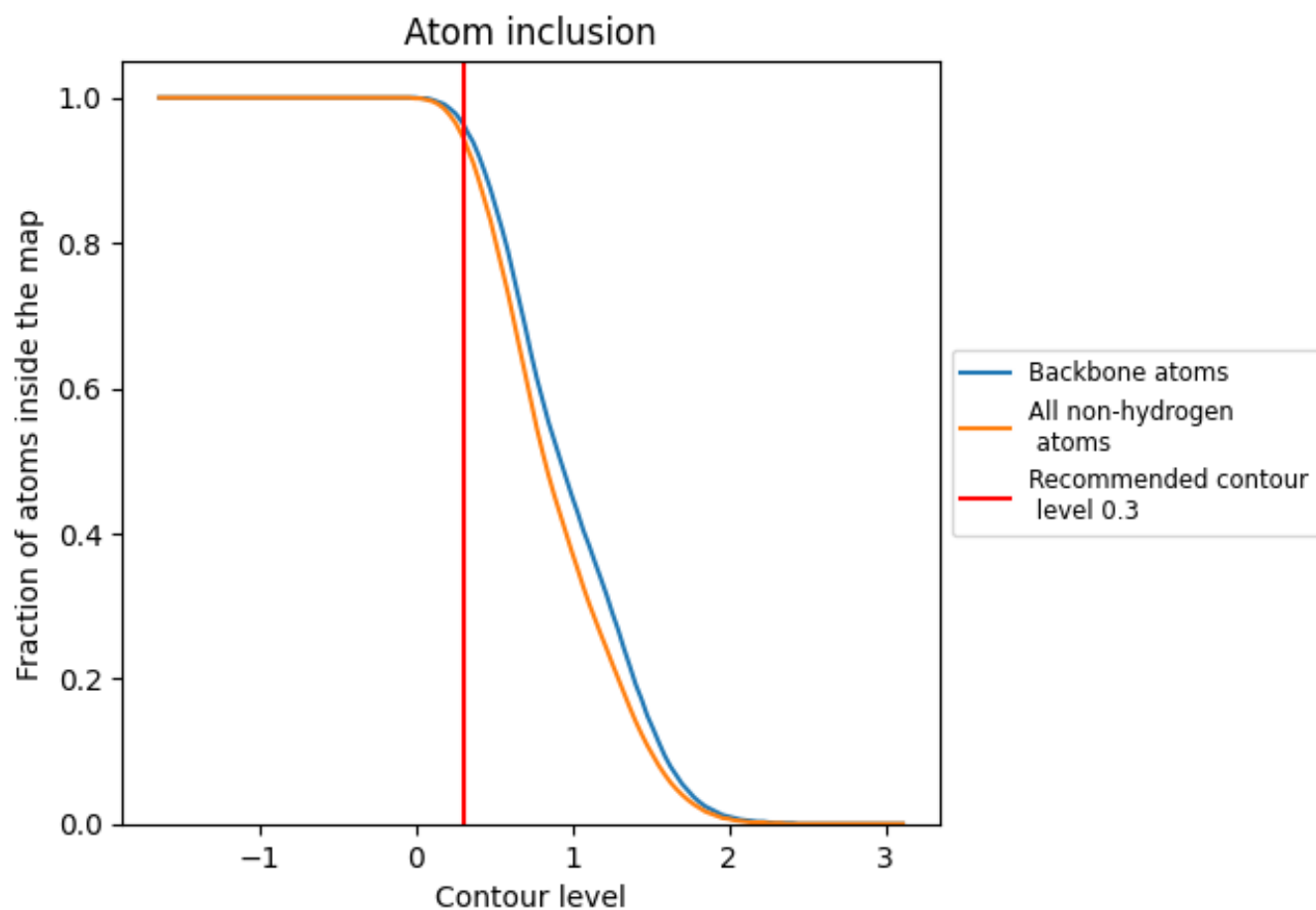


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.























9.4 Atom inclusion [i](#)



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

Chain	Atom inclusion	Q-score
All	 0.9450	 0.4480
A	 0.9670	 0.4860
B	 0.9500	 0.4650
C	 0.9520	 0.4860
D	 0.9440	 0.4640
E	 0.9020	 0.4470
F	 0.9310	 0.4170
J	 0.9390	 0.4170
M	 0.9160	 0.3740
O	 0.9510	 0.3070
P	 0.9660	 0.3020

