



wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 10:19 PM EST

PDB ID : 6EEC
EMDB ID : EMD-9041
Title : Mycobacterium tuberculosis RNAP promoter unwinding intermediate complex
with RbpA/CarD and AP3 promoter captured by Coralopyronin
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.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

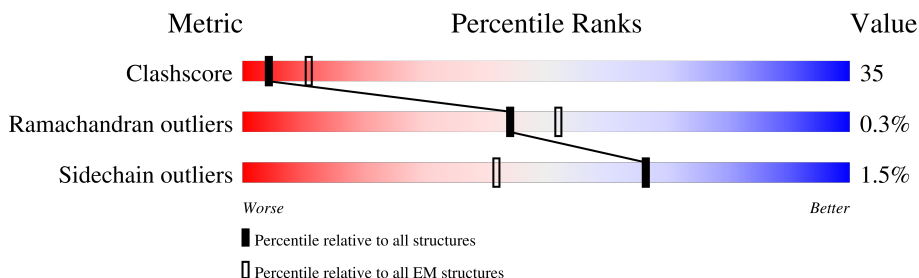
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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.




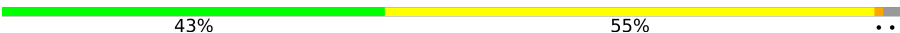
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
2	C	1179	
3	D	1326	
4	E	110	
5	F	531	
6	J	111	
7	O	90	

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Mol	Chain	Length	Quality of chain
8	P	90	 12% 58% 30%
9	M	162	 43% 55% ..

2 Entry composition

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
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
			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
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 (65-MER).

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

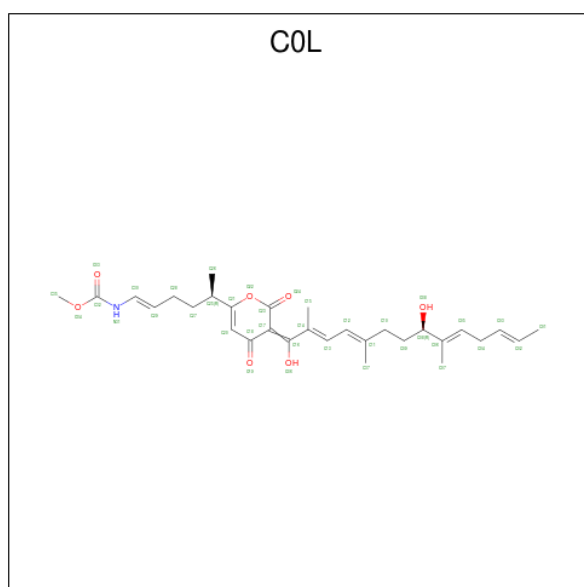
- Molecule 8 is a DNA chain called DNA (63-MER).

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

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

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

- 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 (three-letter code: C0L) (formula: C₃₀H₄₁NO₇) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

Chain C: 44% 49% 6%

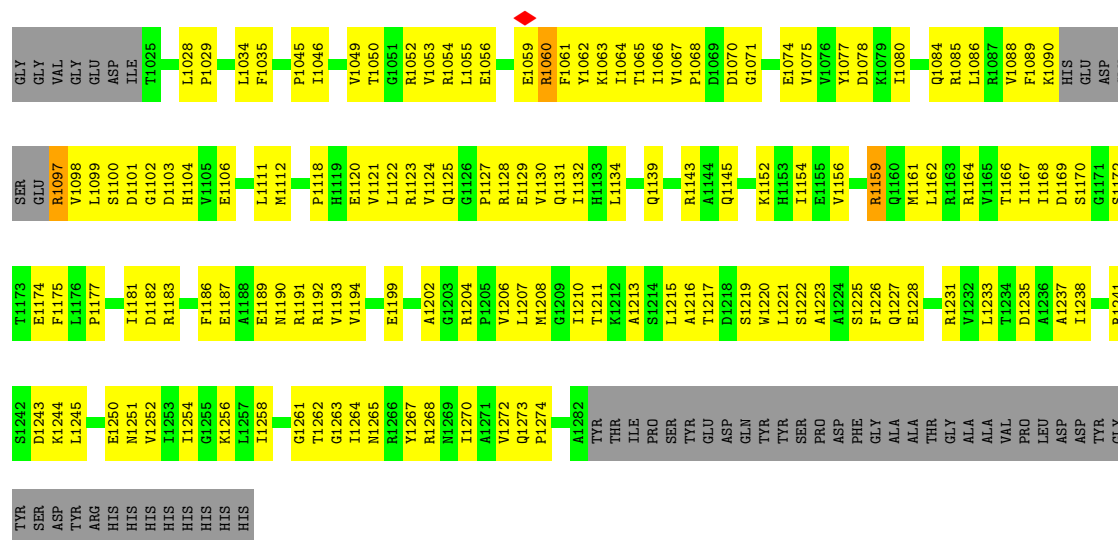


R1099	VAL
V1102	ASP
V1107	LEU
V1111	ALA
P1115	LEU
G1116	ALA
I1117	ARG
P1118	HIS
E1119	GLY
S1120	GLY
F1121	SER
L1128	
L1131	
G1132	
L1133	
N1134	
V1135	
E1136	
V1137	
L1138	
S1139	
S1140	
ASP	
GLY	
ALA	
ALA	
ILE	
GLU	
LEU	
L39	
Y106	
ARG	
GLU	
GLY	
GLU	
ASP	
C48	
ASP	
LEU	
GLU	
ARG	
ALA	
ALA	
ALA	
ASN	
LEU	
GLY	
ILE	
LEU	
ASN	
SER	
ARG	
ASN	
GLU	
SER	
ALA	

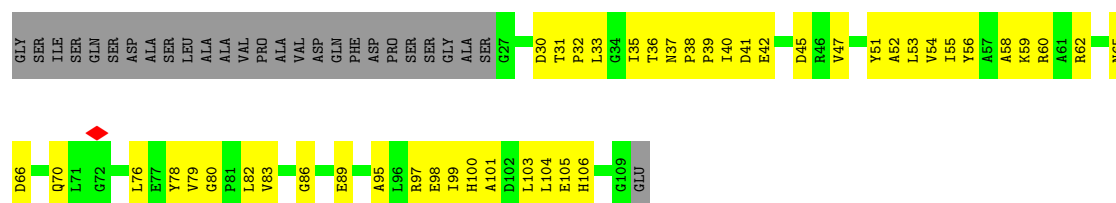
• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 45% 49% 5%

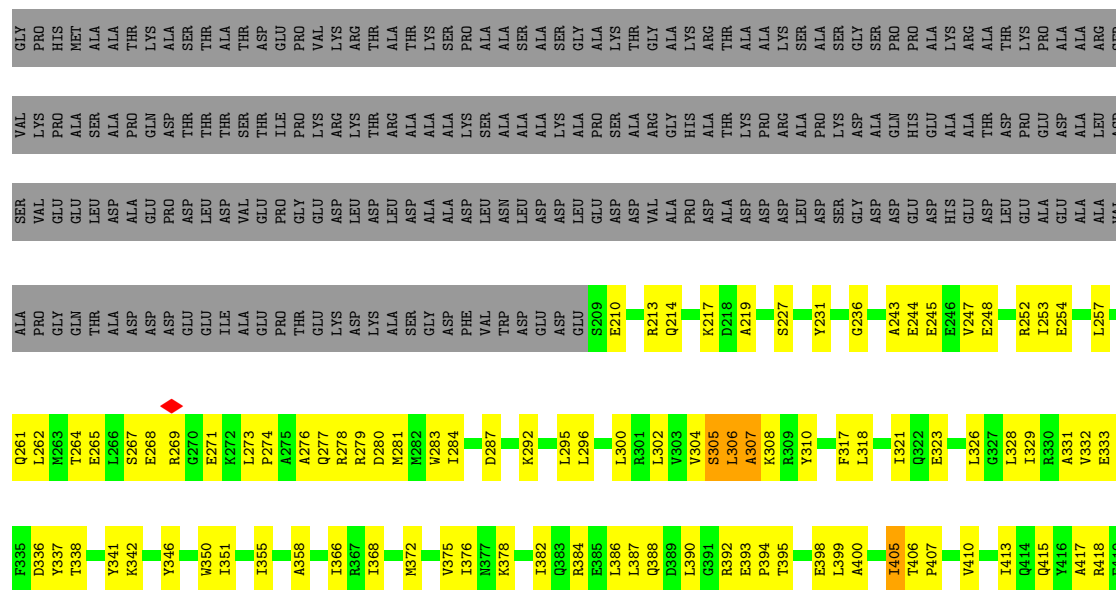
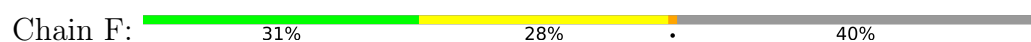
G-1	A0	N5	F6	F7	D8	E9	L10	R11	I12	G13	L14	A15	T16	A17	T20	R21	Q22	Q23	S24	Y25	G26	E27	F31	E32	T33	I34	N35	Y36	R37	T38	L39	K40	P41	E42	F47	C48	E49	K50	T51	F52	T55	R56	D57	W58	E59	C60	G63	K64	S138	V139	Y65	K66	R67	M143	R144
K71	G72	I73	L74	C75	E76	F77	C78	G79	W80	E81	W82	W83	R84	A85	K86	W87	R88	R89	E90	R91	N92	G93	H94	I95	E96	A98	V101	T102	H103	I104	W105	Y106	F107	R113	L114	L117	L118	E119	L120	D124	I129	Y130	Y134	V135	I136	T137	S138	R203	E204	K205	R206	Q207	L208	R209	
H145	M146	E147	L148	S149	T150	L151	E152	A153	V157	E158	R159	K160	A161	V162	K163	D164	R165	R166	D167	G168	E169	L170	R173	A174	L177	E178	A179	D180	L181	A182	E183	A186	E187	G188	A189	K190	A191	D192	A193	R194	K195	V197	R198	D199	G200	G201	E202	R203	E204	K205	R206	Q207	L208	R209	
A212	E215	L216	D217	R218	L219	E220	D221	W223	T227	K228	L229	A230	P231	G232	Q233	L234	T235	V236	D237	E238	N239	L240	Y241	R242	E243	L244	V245	D246	R247	Y248	Y251	F252	T253	M256	Q257	S260	L261	Q262	F268	D269	L270	D271	A272	E273	A274	E275	S276	L277	R278	L281					
R282	D285	R295	F302	Q303	P309	K310	G311	K312	V313	L314	V317	P318	V319	L320	P321	E322	E323	L324	K327	V328	K329	R334	P335	A336	L337	E338	L340	Y344	T348	N349	R353	L354	K355	R356	L357	L360	E364	L365	L366	V367	N368	K373	L374	E376											
D379	D383	G385	R386	R387	R389	P390	L399	S403	D404	L405	K409	Q410	R414	Q415	N416	L417	L418	G419	K420	R421	V422	S425	G426	R427	S428	V429	L430	V431	V432	Q435	L436	K437	L438	H439	Q440	C441	L443	P444	K445	L446	M447	L448	L449	K453	V456	M457									
K458	R459	L460	V461	D462	A466	Q467	N468	L469	K470	S471	A472	K473	V476	E477	R480	V483	V486	L487	V490	L491	L497	L498	N499	R500	L504	H505	R506	L507	G508	L509	G510	A511	F512	E513	P514	P515	L516	E518	G519	K520	Q523	L524	H525	P526	L527	V528	E530								
A534	E535	F536	D537	G538	D539	Q540	M541	L545	P546	L547	E550	E554	L557	L558	M559	L560	S561	S562	K563	L566	S567	P573	L574	A575	T576	P577	R578	L579	D580	N581	L585	G586	Y586	Y587	L588	T589	E591	G594	D595	T596	G597	E598	Y599	S603	H606	P607	G610								
V611	Y612	S613	G614	P615	A616	E617	A618	D623	R624	G625	V626	L627	S628	P629	R630	A631	G632	L633	K634	V635	R636	L637	T638	R641	P642	P643	W644	E645	P651	G652	H653	S654	G655	R656	Q657	D660	A661	W662	W663	A664	E665	L668	W671	P672	P673	N674	A753	D754	W755	L756	L777	Y681	P682		
F683	V684	N685	M688	Q693	N698	D699	L700	A701	W702	R703	Y704	P705	W706	L707	W708	V709	A710	Q711	T712	W713	D714	W715	F721	Y722	W723	A724	T725	W729	T730	W731	S732	W733	V736	L737	W738	D660	A661	W662	W663	A664	E665	L668	W671	P672	P673	N674	A753	D754	W755	L756	L777	Y681	P682		
R770	N771	L774	W775	A788	L789	W790	D791	W792	Y793	W797	P798	W799	I800	V803	D808	G809	L817	A818	G819	M820	K821	G822	L823	Y824	T825	N826	P827	L832	P833	R834	P835	V836	S839	T840	R841	L844	T845	W846	L847	E848	Y849	P850	L851	N852	T853	H854	R857	Q942							
A864	L865	R866	T867	T874	R875	R876	L877	W878	D879	W880	S881	V884	I885	W886	R887	E888	H889	D890	C891	Q892	T893	S894	A902	G908	T909	L910	L911	R912	D913	R914	Y915	I916	E917	A920	D921	A922	R923	T924	L925	G926	T927	T928	W846	L847	E848	Y849	P850	L851	N852	T853	H854	R857	Q942		
P943	L944	G945	D946	P947	E948	I949	L952	L953	A954	A955	G956	I957	V962	R963	L966	R967	C968	A969	T970	S971	T972	G973	V974	C975	A976	T977	L978	T979	T980	T981	Y982	G986	V989	D990	I991	G992	E993	G996	Q1001	G1004	E1005	P1006	L1010	T1011	M1012	ARG	THR	PHE	HIS	GLN					

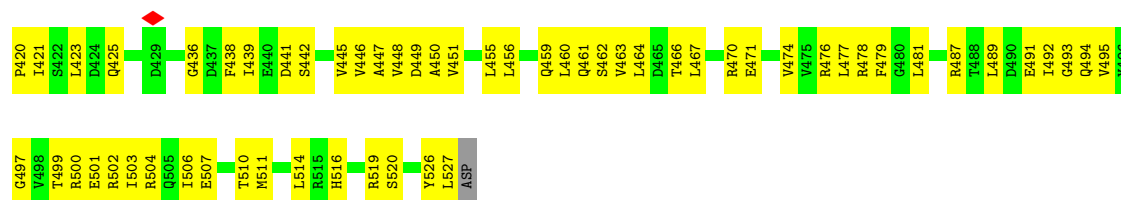


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor SigA

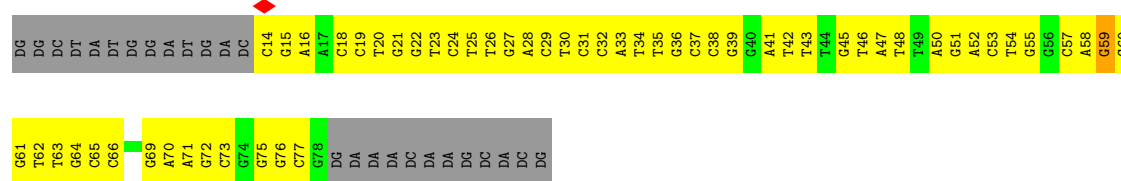
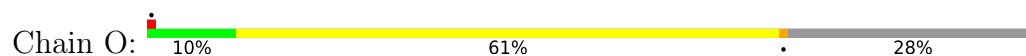




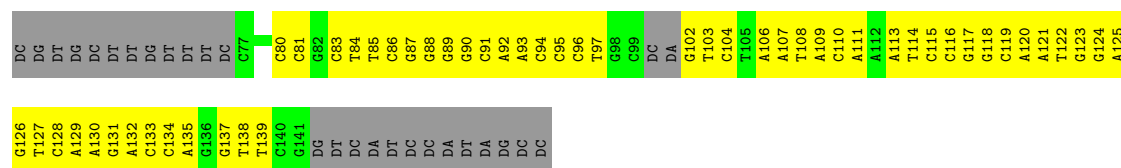
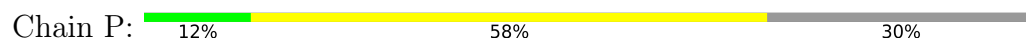
• Molecule 6: RNA polymerase-binding protein RbpA



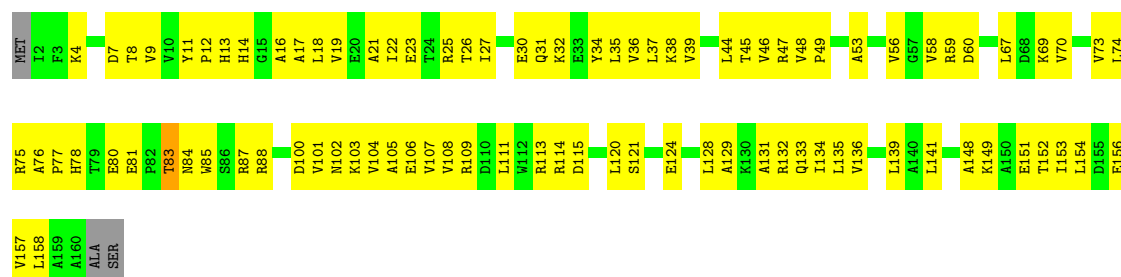
• Molecule 7: DNA (65-MER)



• 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, 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	0.47	0/1742	0.55	0/2370
1	B	0.43	0/1786	0.53	0/2435
2	C	0.55	0/8751	0.61	5/11869 (0.0%)
3	D	0.56	1/10037 (0.0%)	0.59	6/13570 (0.0%)
4	E	0.44	0/662	0.52	0/901
5	F	0.46	0/2549	0.55	3/3438 (0.1%)
6	J	0.38	0/897	0.55	1/1210 (0.1%)
7	O	0.80	0/1497	0.97	2/2310 (0.1%)
8	P	0.76	0/1445	0.91	0/2224
9	M	0.36	0/1257	0.49	0/1700
All	All	0.55	1/30623 (0.0%)	0.63	17/42027 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	656	TRP	CB-CG	-7.29	1.37	1.50

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	306	LEU	C-N-CA	-7.20	103.71	121.70
3	D	419	GLY	N-CA-C	7.08	130.80	113.10
3	D	655	GLY	N-CA-C	-6.73	96.27	113.10
2	C	275	LEU	CA-CB-CG	-6.63	100.04	115.30
2	C	288	THR	N-CA-C	-6.59	93.21	111.00

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	121	0
1	B	1759	0	1783	145	0
2	C	8593	0	8517	695	0
3	D	9873	0	9938	738	0
4	E	649	0	645	54	0
5	F	2518	0	2540	182	0
6	J	881	0	861	62	0
7	O	1336	0	732	116	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	2075	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 35.

The worst 5 of 2075 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

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%)	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%)	34	71
3	D	1260/1326 (95%)	1141 (91%)	115 (9%)	4 (0%)	41	74
4	E	81/110 (74%)	76 (94%)	5 (6%)	0	100	100
5	F	317/531 (60%)	296 (93%)	20 (6%)	1 (0%)	41	74
6	J	106/111 (96%)	87 (82%)	19 (18%)	0	100	100
9	M	157/162 (97%)	144 (92%)	12 (8%)	1 (1%)	25	64
All	All	3488/4113 (85%)	3072 (88%)	406 (12%)	10 (0%)	44	74

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 ⓘ

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%)	192 (99%)	2 (1%)	76	89
1	B	194/297 (65%)	193 (100%)	1 (0%)	88	95
2	C	935/997 (94%)	918 (98%)	17 (2%)	59	81
3	D	1042/1103 (94%)	1024 (98%)	18 (2%)	60	83
4	E	69/89 (78%)	68 (99%)	1 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	264/429 (62%)	262 (99%)	2 (1%)	81	92
6	J	93/97 (96%)	89 (96%)	4 (4%)	29	63
9	M	129/131 (98%)	129 (100%)	0	100	100
All	All	2920/3440 (85%)	2875 (98%)	45 (2%)	66	84

5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	416	ASN
3	D	1060	ARG
3	D	418	LEU
3	D	733	MET
3	D	1159	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	1001	GLN
5	F	494	GLN
3	D	1139	GLN
4	E	65	ASN
9	M	14	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	-	36,38,38	2.64	13 (36%)	38,49,49	2.96	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
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	8.59	1.39	1.21
10	C	1201	C0L	O19-C18	5.63	1.39	1.24
10	C	1201	C0L	C17-C16	4.61	1.50	1.39
10	C	1201	C0L	O36-C16	-4.53	1.18	1.33
10	C	1201	C0L	C17-C18	-4.06	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	10.50	120.28	109.16
10	C	1201	C0L	C23-O22-C21	-6.85	118.03	122.22
10	C	1201	C0L	C35-O34-C32	-6.17	108.38	115.66
10	C	1201	C0L	O36-C16-C17	4.90	128.90	119.87
10	C	1201	C0L	C13-C12-C11	-4.73	120.05	127.30

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

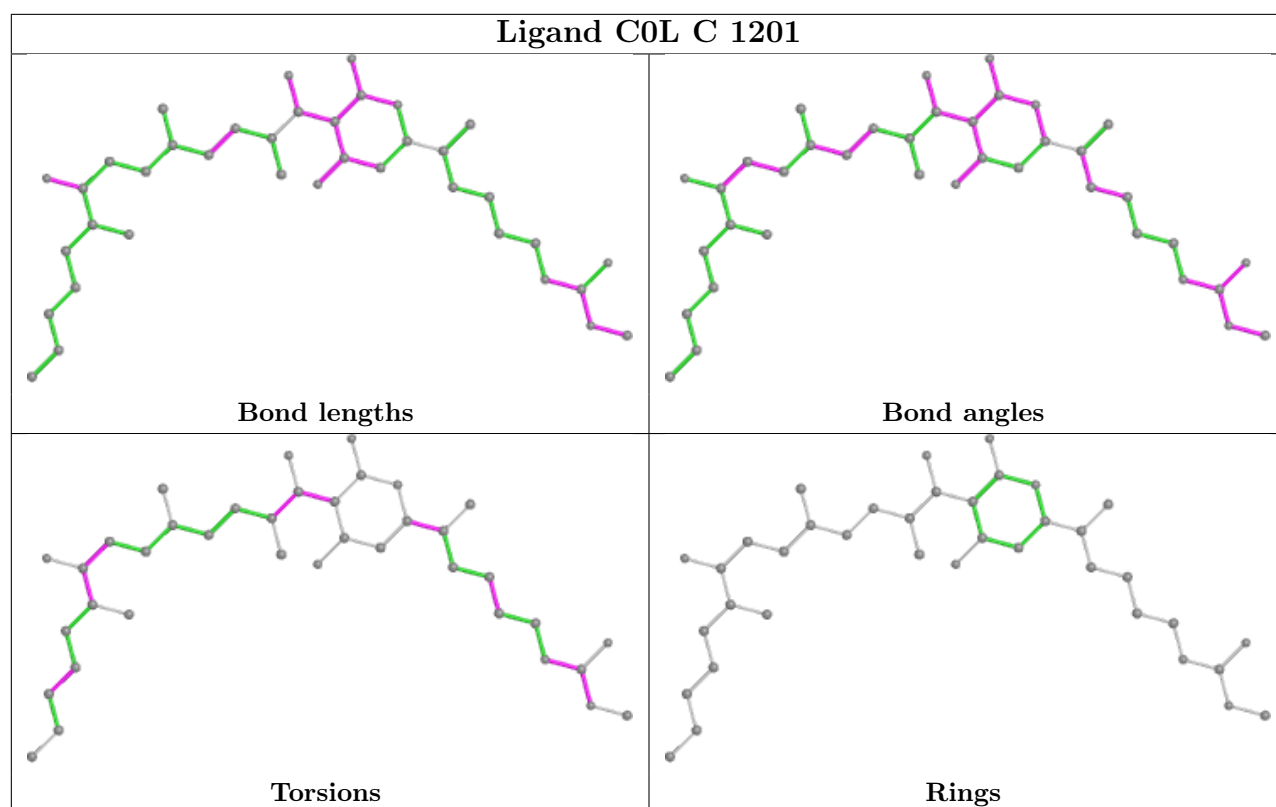
Mol	Chain	Res	Type	Atoms
10	C	1201	C0L	C05-C06-C08-C09
10	C	1201	C0L	C07-C06-C08-C09
10	C	1201	C0L	C13-C14-C16-O36
10	C	1201	C0L	C15-C14-C16-O36
10	C	1201	C0L	C14-C16-C17-C18

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.

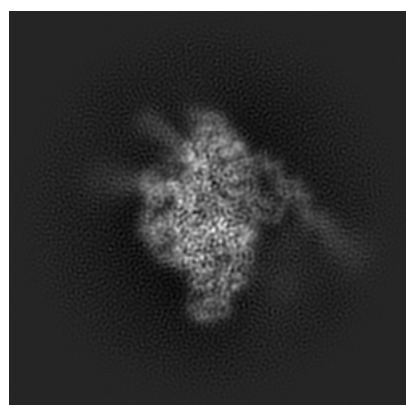
6 Map visualisation [i](#)

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.

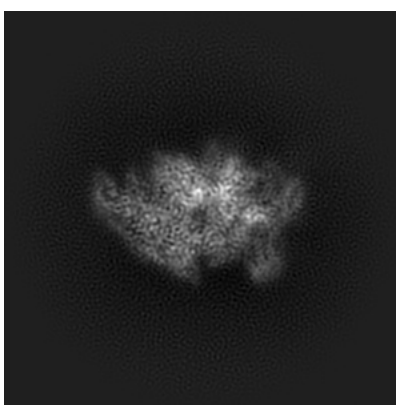
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

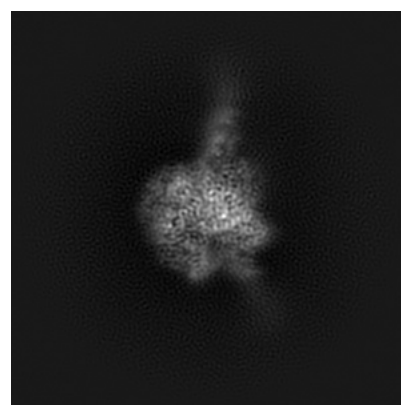
6.1.1 Primary map



X



Y

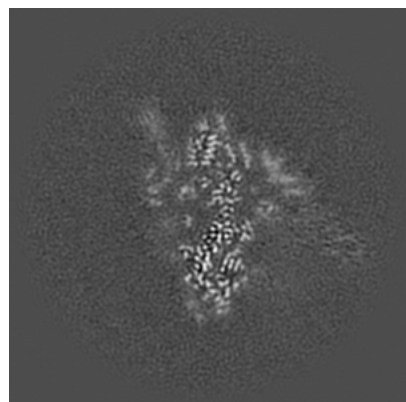


Z

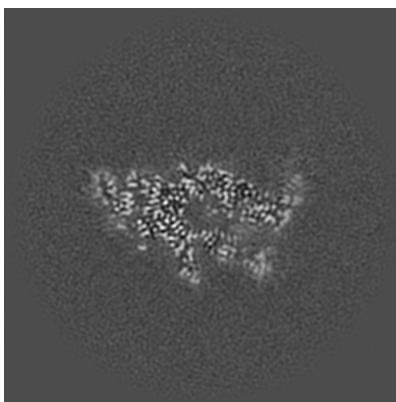
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

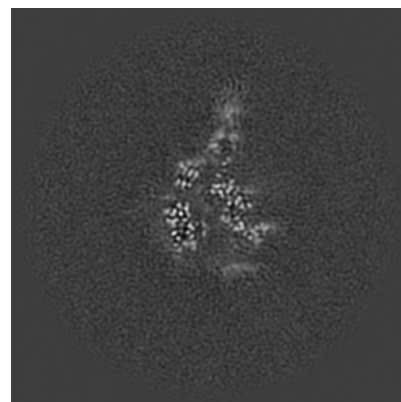
6.2.1 Primary map



X Index: 125



Y Index: 125

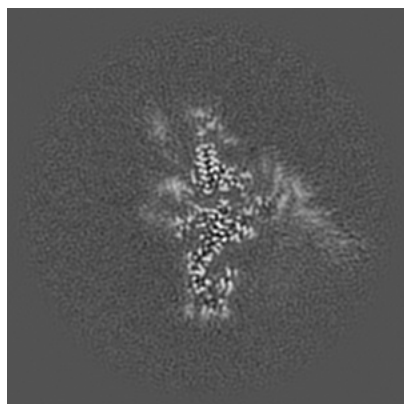


Z Index: 125

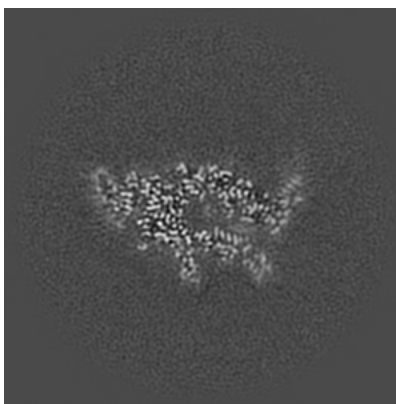
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

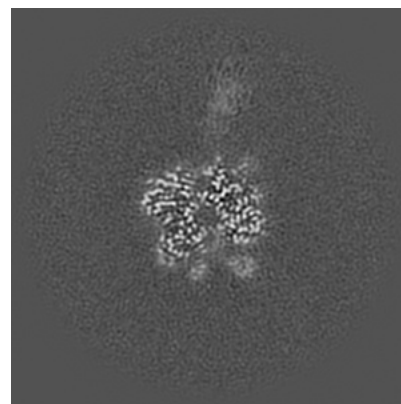
6.3.1 Primary map



X Index: 132



Y Index: 124

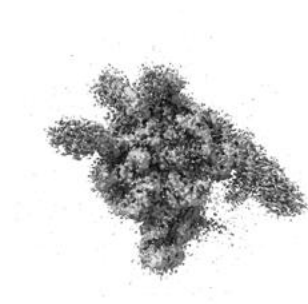


Z Index: 113

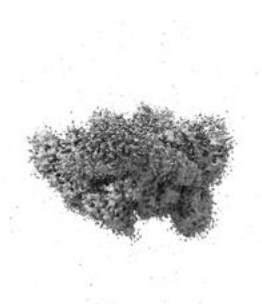
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

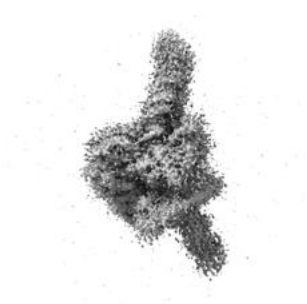
6.4.1 Primary map



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.

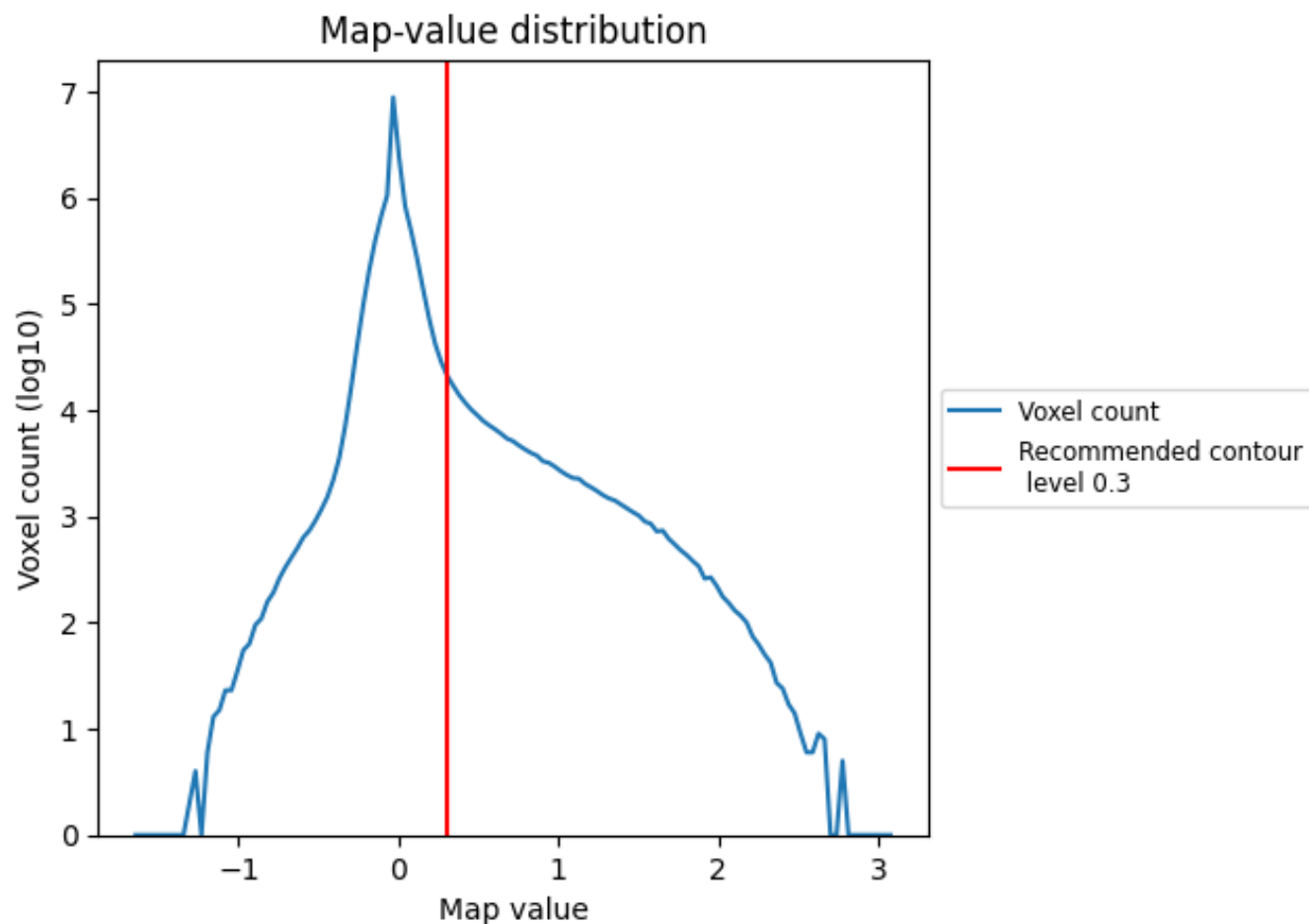
6.5 Mask visualisation

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

7 Map analysis [i](#)

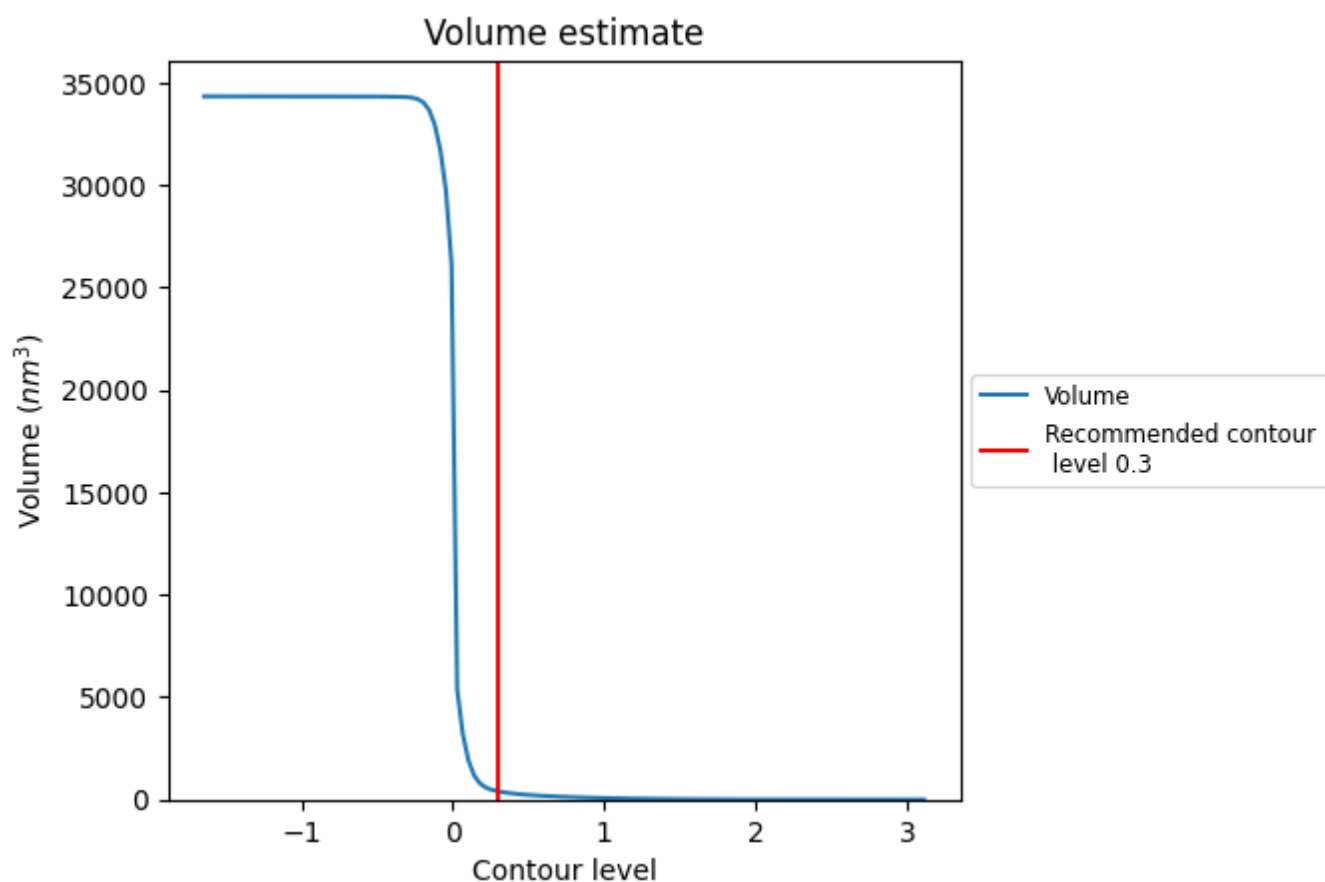
This section contains the results of statistical analysis of the map.

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.

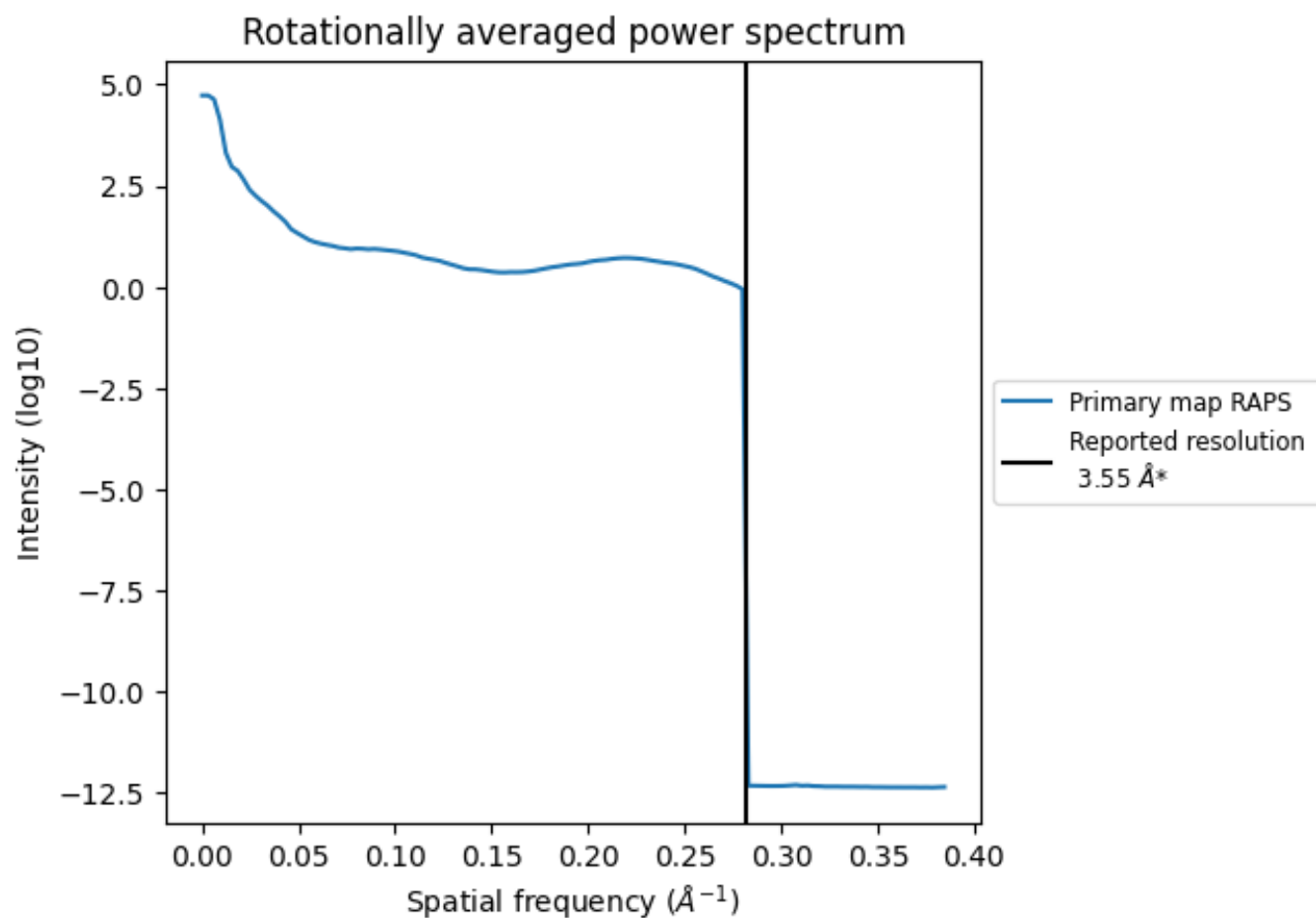
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 401 nm³; 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 ⓘ



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

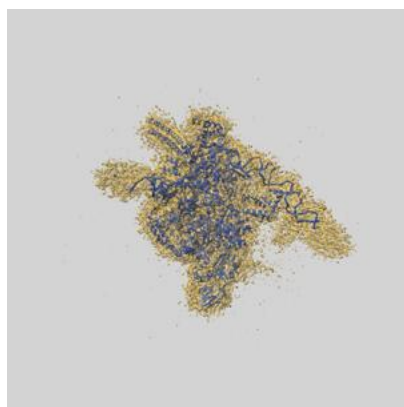
8 Fourier-Shell correlation

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

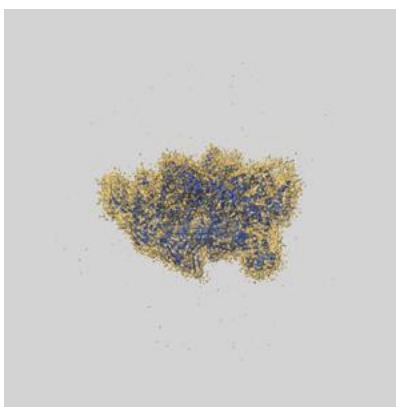
9 Map-model fit [i](#)

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](#).

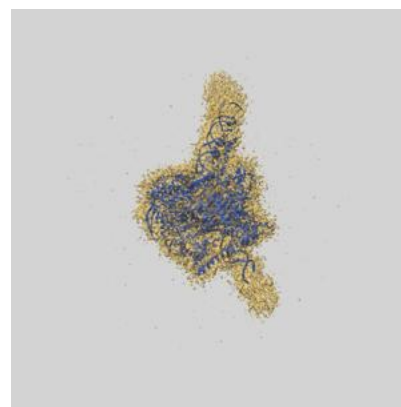
9.1 Map-model overlay [i](#)



X



Y



Z

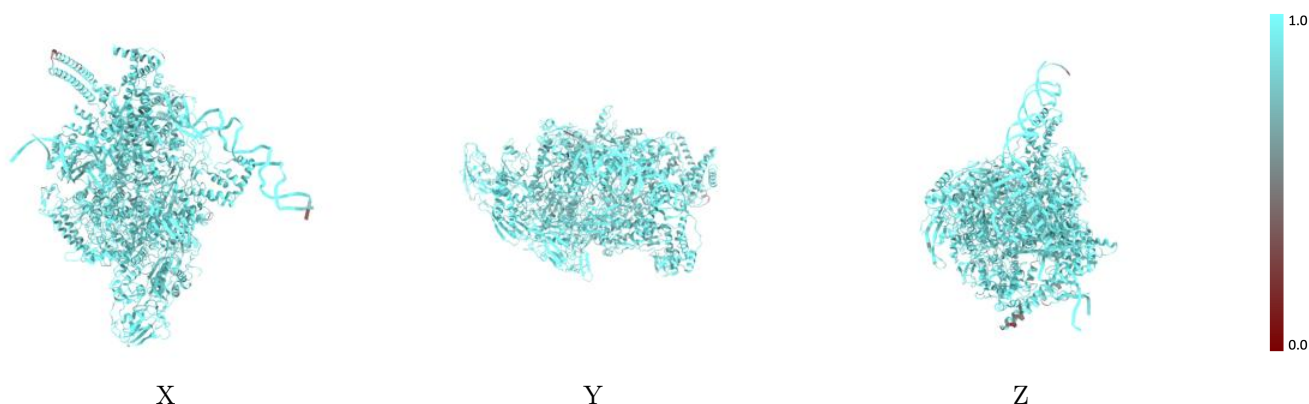
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



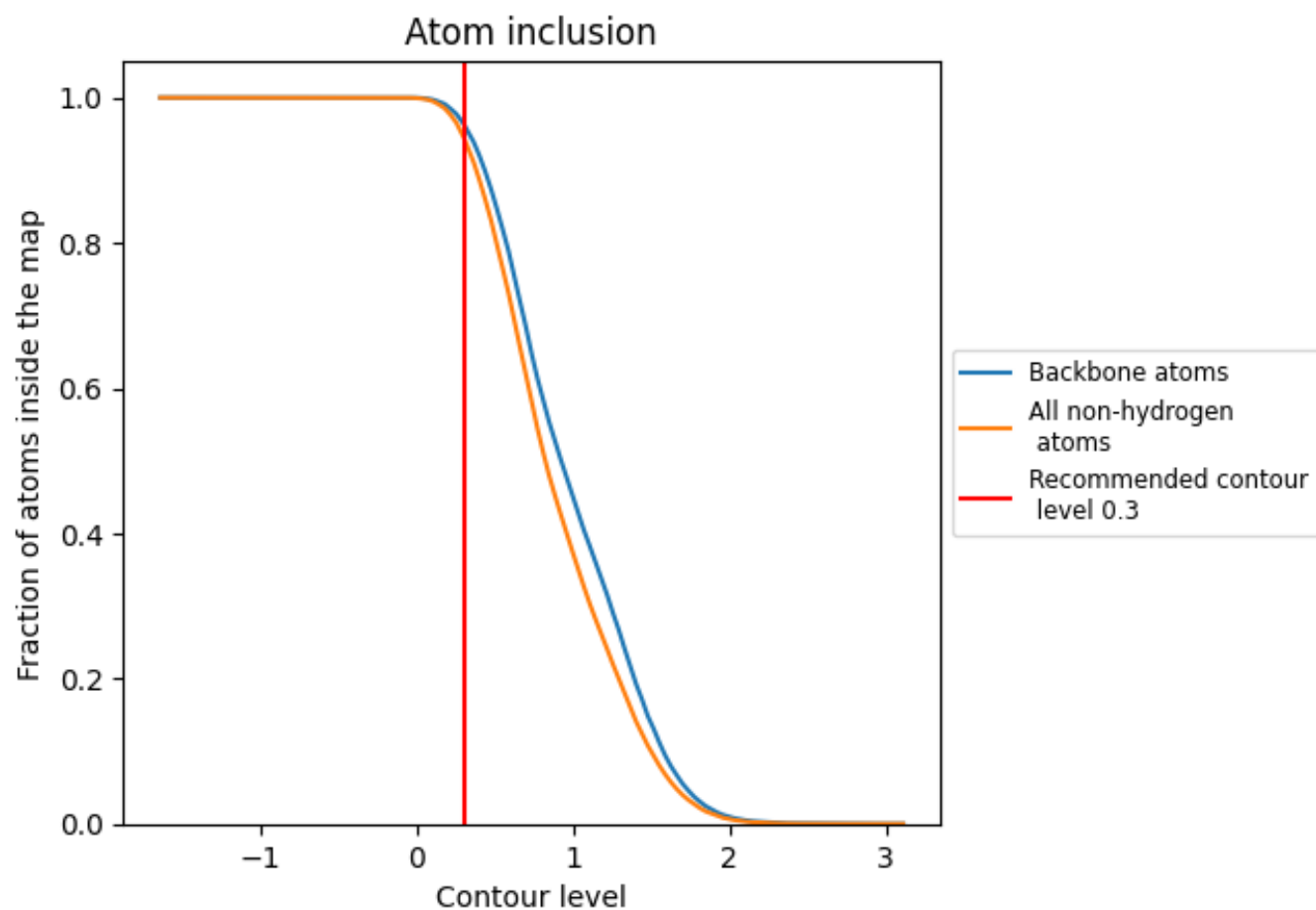
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 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	<div></div> 0.9447	<div></div> 0.4480
A	<div></div> 0.9667	<div></div> 0.4860
B	<div></div> 0.9498	<div></div> 0.4650
C	<div></div> 0.9519	<div></div> 0.4860
D	<div></div> 0.9444	<div></div> 0.4640
E	<div></div> 0.9024	<div></div> 0.4470
F	<div></div> 0.9309	<div></div> 0.4170
J	<div></div> 0.9385	<div></div> 0.4170
M	<div></div> 0.9158	<div></div> 0.3740
O	<div></div> 0.9506	<div></div> 0.3070
P	<div></div> 0.9659	<div></div> 0.3020

1.0

0.0

<0.0