



wwPDB EM Validation Summary Report ⓘ

Mar 1, 2026 – 10:27 PM UTC

PDB ID : 7KHB / pdb_00007khhb
EMDB ID : EMD-21880
Title : Escherichia coli RNA polymerase and rrnBP1 promoter open complex
Authors : Shin, Y.; Qayyum, M.Z.; Murakami, K.S.
Deposited on : 2020-10-20
Resolution : 3.53 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

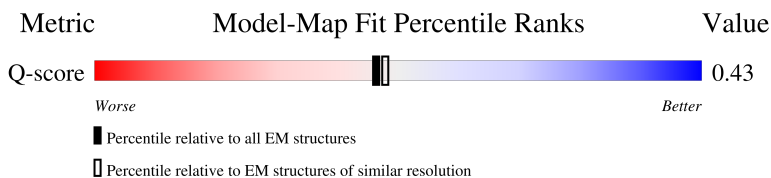
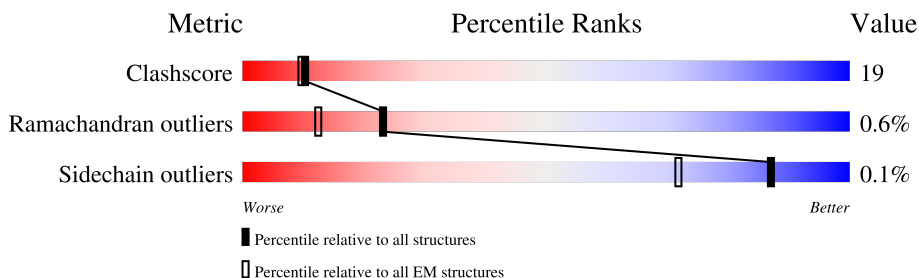
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	329	 47% 24% 30%
1	B	329	 42% 27% 30%
2	C	1342	 65% 34%
3	D	1407	 59% 36% 5%

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Mol	Chain	Length	Quality of chain
4	E	91	
5	F	613	
6	X	64	
7	Y	64	

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
10	ZN	D	2003	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 31608 atoms, of which 0 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	231	Total	C	N	O	S	0	0
			1794	1117	318	353	6		
1	B	230	Total	C	N	O	S	0	0
			1786	1112	317	351	6		

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0
			10570	6631	1841	2055	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1340	Total	C	N	O	S	0	0
			10382	6522	1849	1962	49		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	76	Total	C	N	O	S	0	0
			605	368	115	121	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	471	Total	C	N	O	S	0	0
			3836	2403	684	726	23		

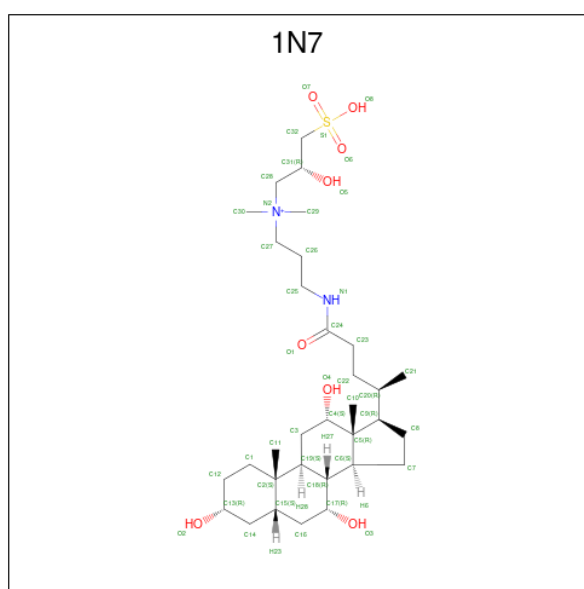
- Molecule 6 is a DNA chain called DNA (60-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	60	Total	C	N	O	P	0	0
			1221	582	219	360	60		

- Molecule 7 is a DNA chain called DNA (64-MER).

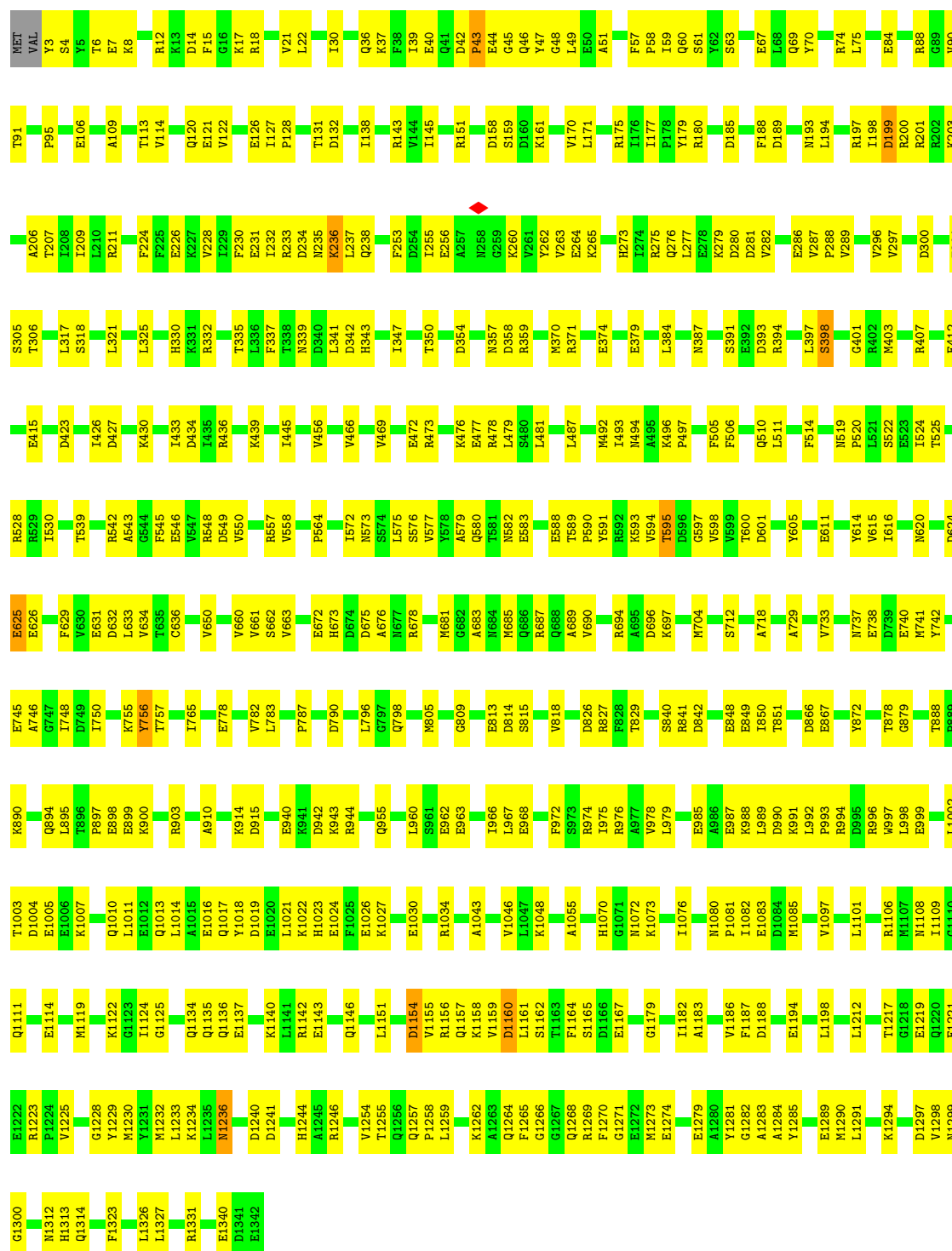
Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	64	Total	C	N	O	P	0	0
			1325	628	248	385	64		

- Molecule 8 is CHAPSO (CCD ID: 1N7) (formula: $C_{32}H_{59}N_2O_8S$) (labeled as "Ligand of Interest" by depositor).



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

Chain C:  65% 34%

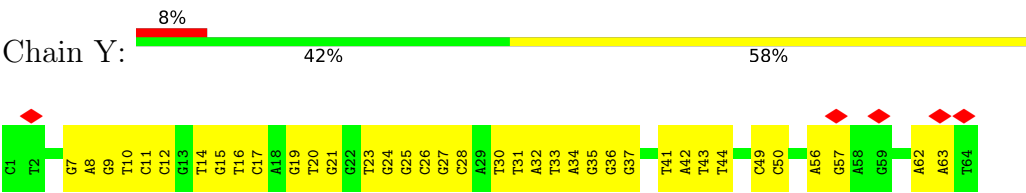


• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D:  59% 36% 5%

SER	Q1279	K1172	G1092	V1027	K953	H865	R764	E648	T528	K378	L291	M180	V92	MET
ALA	E1280	R1173	T1093	E1030	N954	E866	L767	K649	K531	Y382	I291	G181	V97	LYS
LEU	E1281	R1174	D1094	E1031	K955	K867	L768	K650	E532	E295	E295	E183	V99	ASP
ALA	Y1282	V1176	M1095	V1032	G956	K868	V769	I654	E533	R388	M298	I185	R99	LEU
GLU	S1283	T1177	L1101	S1032	K959	D870	L770	E658	E534	K395	L299	L188	R101	LEU
LEU	E1284	T1178	P1102	F1034	L960	L871	Q771	E659	V548	V407	Q300	L196	M102	PHE
LEU	V1285	V1179	G1103	V1035	S961	L872	F772	E661	K549	E301	E301	E195	E106	LEU
ASN	K1286	V1180	K1104	T1038	N962	E873	F773	E662	E552	D304	D304	Q196	G103	LYS
ALA	I1287	S1183	A1105	M1040	S963	K874	T774	E663	T553	I411	I411	I105	H104	GLN
LEU	V1288	D1184	L1106	T1045	K964	N875	S775	E664	E554	I416	I416	E197	E106	THR
GLY	F1289	P1185	V1107	T1046	S965	S876	T776	E665	Y555	R417	R417	C198	P110	LYS
GLY	F1290	Y1186	V1107	T1047	V966	S877	G782	E666	E556	H418	H418	Q200	T111	THR
GLY	A1300	E1187	N968	M1049	N968	A879	T786	E667	K557	H419	H419	E199	E106	LYS
ASP	T1301	E1188	K972	Q1044	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
ASN	S1313	M1189	K972	T1045	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
GLU	I1314	I1190	L973	T1046	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	A1315	I1190	V974	T1047	N968	A879	T786	E667	K557	H419	H419	Q200	E106	THR
	T1316	N1197	T975	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	E1317	V1198	T976	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	S1318	F1199	S977	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	A1323	E1201	T980	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	S1324	R1202	T981	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	F1325	R1203	L982	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	Q1326	E1204	K983	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	E1327	E1205	L984	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	V1331	R1206	T985	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	D1342	G1207	D986	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	E1343	E1208	R990	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	L1344	E1215	S994	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	R1345	A1216	Y995	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	G1346	E1220	K996	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	L1347	H1227	V997	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	K1348	E1230	A1001	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	E1349	K1251	L1002	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	M1350	E1252	L1003	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	V1351	I1253	A1004	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	I1352	E1254	K1005	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
	V1353	V1257	G1006	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
	L1356	I1266	E1007	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
	G1376	V1267	L1073	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
GLU	A1376	K1251	L1074	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
ALA	PRO	E1252	R1075	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
ALA	ALA	E1254	P1076	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
PRO	ALA	V1257	A1077	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
ALA	ALA	I1266	V1081	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
GLN	VAL	V1267	D1082	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
THR	THR	D1273	A1083	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
ALA	ALA	F1274	Q1084	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
ASP	ASP	L1275	G1085	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
ALA	ALA	E1276	N1086	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	E106	GLN
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
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			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
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			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	P110	LYS
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			T1024	Q1049	N968	A879	T786	E667	K557	H419	H419	Q200	T111	THR
			T1024	Q1049	N968	A879	T786	E667	K557	H419	H			

● Molecule 7: DNA (64-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	349752	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.104	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1N7, 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	0.24	0/1816	0.46	0/2461
1	B	0.22	0/1808	0.51	0/2450
2	C	0.27	0/10739	0.49	0/14489
3	D	0.26	0/10539	0.52	1/14234 (0.0%)
4	E	0.17	0/607	0.43	0/817
5	F	0.22	0/3887	0.56	0/5224
6	X	0.33	0/1366	0.56	0/2101
7	Y	0.32	0/1488	0.57	0/2298
All	All	0.26	0/32250	0.52	1/44074 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2
3	D	0	3
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1203	ARG	CG-CD-NE	-5.89	99.04	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	Peptide
3	D	860	ARG	Peptide
3	D	901	ARG	Peptide

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	1794	0	1819	62	0
1	B	1786	0	1813	73	0
2	C	10570	0	10582	389	0
3	D	10382	0	10571	447	0
4	E	605	0	612	24	0
5	F	3836	0	3907	198	0
6	X	1221	0	677	40	0
7	Y	1325	0	721	38	0
8	C	86	0	116	2	0
9	D	1	0	0	0	0
10	D	2	0	0	2	0
All	All	31608	0	30818	1195	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 19.

The worst 5 of 1195 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:277:MET:SD	5:F:362:ASN:ND2	2.28	1.07
3:D:816:THR:OG1	3:D:818:GLU:OE1	1.77	1.03
2:C:403:MET:SD	2:C:407:ARG:NH2	2.40	0.94
5:F:271:ASN:OD1	5:F:274:ARG:NH2	1.99	0.94
3:D:1344:LEU:O	3:D:1346:GLY:N	2.00	0.93

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	229/329 (70%)	211 (92%)	18 (8%)	0	100	100
1	B	228/329 (69%)	207 (91%)	19 (8%)	2 (1%)	14	47
2	C	1338/1342 (100%)	1228 (92%)	100 (8%)	10 (1%)	18	52
3	D	1334/1407 (95%)	1211 (91%)	117 (9%)	6 (0%)	30	61
4	E	74/91 (81%)	68 (92%)	6 (8%)	0	100	100
5	F	465/613 (76%)	430 (92%)	32 (7%)	3 (1%)	21	55
All	All	3668/4111 (89%)	3355 (92%)	292 (8%)	21 (1%)	23	55

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	SER
2	C	199	ASP
2	C	1160	ASP
3	D	338	PHE
3	D	1345	ARG

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	199/286 (70%)	199 (100%)	0	100	100
1	B	198/286 (69%)	198 (100%)	0	100	100
2	C	1155/1157 (100%)	1153 (100%)	2 (0%)	87	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	1113/1168 (95%)	1113 (100%)	0	100	100
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	419/540 (78%)	419 (100%)	0	100	100
All	All	3149/3512 (90%)	3147 (100%)	2 (0%)	87	87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	1154	ASP
2	C	1236	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	158	GLN
5	F	518	HIS
3	D	667	GLN
5	F	131	GLN
3	D	232	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
8	1N7	C	1402	-	44,46,46	4.20	20 (45%)	69,72,72	1.80	15 (21%)
8	1N7	C	1401	-	44,46,46	4.18	20 (45%)	69,72,72	2.14	21 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	1N7	C	1402	-	-	6/27/92/92	0/4/4/4
8	1N7	C	1401	-	-	4/27/92/92	0/4/4/4

The worst 5 of 40 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	1402	1N7	C3-C4	-12.87	1.32	1.53
8	C	1401	1N7	C3-C4	-12.78	1.32	1.53
8	C	1402	1N7	C5-C9	-11.25	1.36	1.55
8	C	1401	1N7	C5-C9	-10.72	1.37	1.55
8	C	1402	1N7	C3-C19	-9.49	1.38	1.53

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	1401	1N7	C5-C6-C18	-7.27	105.50	114.72
8	C	1402	1N7	C5-C6-C18	-5.39	107.89	114.72
8	C	1401	1N7	C6-C5-C4	-4.87	102.96	107.42
8	C	1401	1N7	C5-C9-C20	-4.77	113.70	119.48
8	C	1402	1N7	C6-C5-C4	-4.53	103.27	107.42

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1401	1N7	N2-C28-C31-C32

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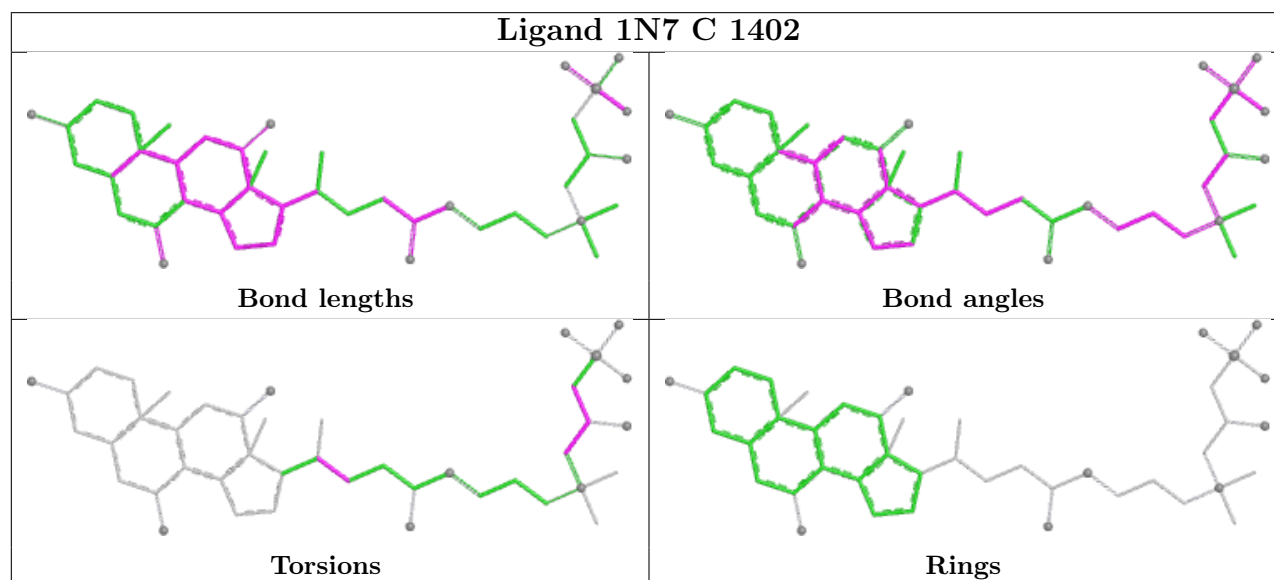
Mol	Chain	Res	Type	Atoms
8	C	1401	1N7	N2-C28-C31-O5
8	C	1402	1N7	N2-C28-C31-C32
8	C	1402	1N7	N2-C28-C31-O5
8	C	1402	1N7	C28-C31-C32-S1

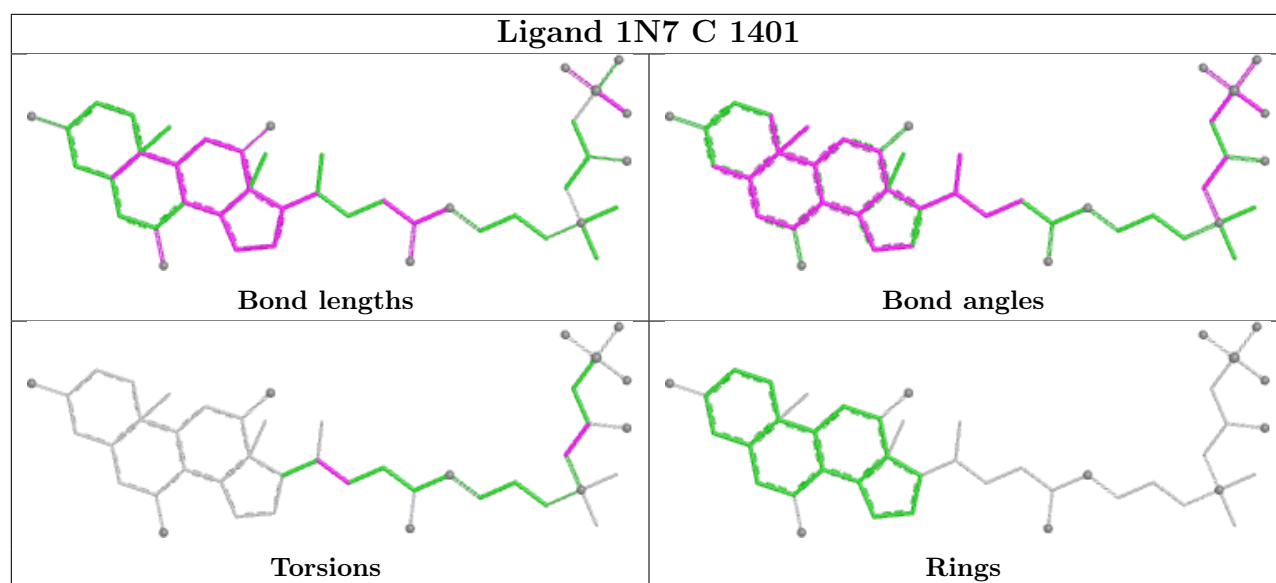
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	1402	1N7	1	0
8	C	1401	1N7	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.

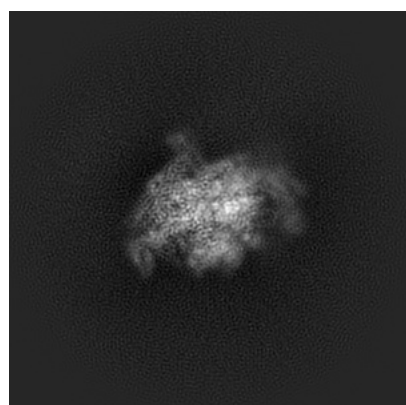
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21880. These allow visual inspection of the internal detail of the map and identification of artifacts.

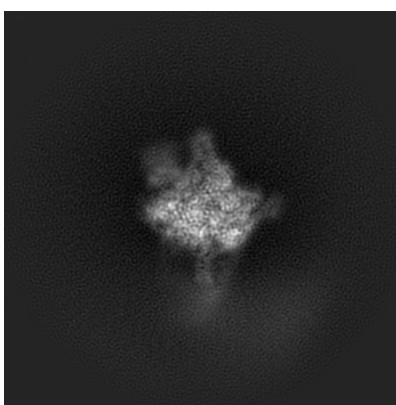
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

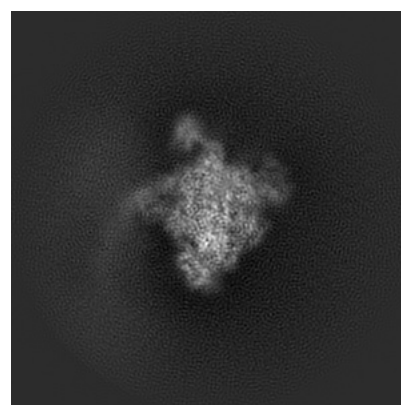
6.1.1 Primary map



X



Y

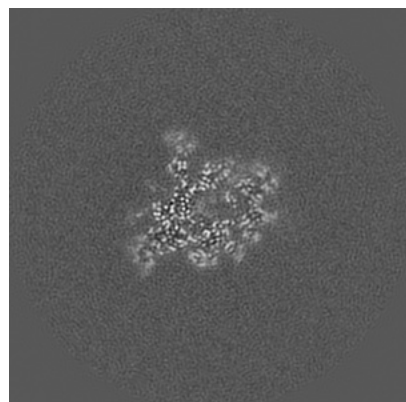


Z

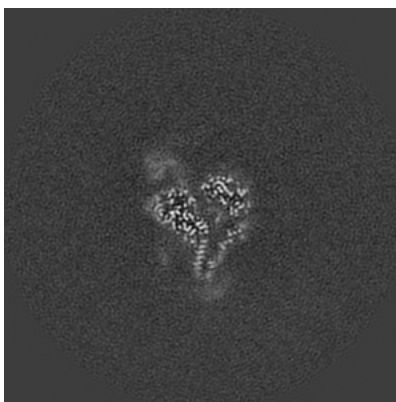
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

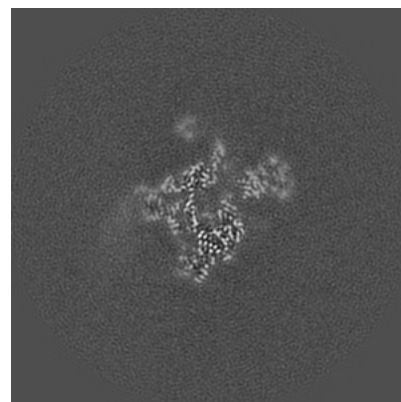
6.2.1 Primary map



X Index: 180



Y Index: 180

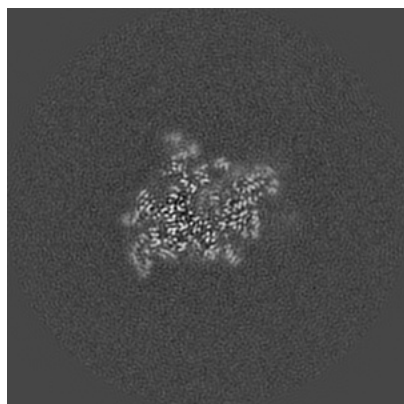


Z Index: 180

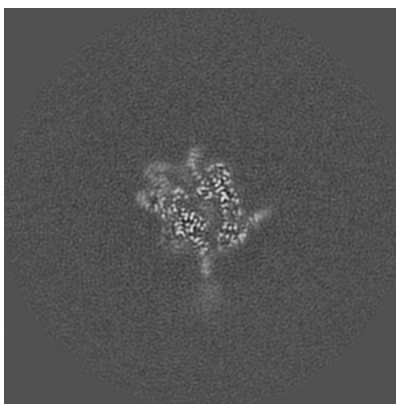
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

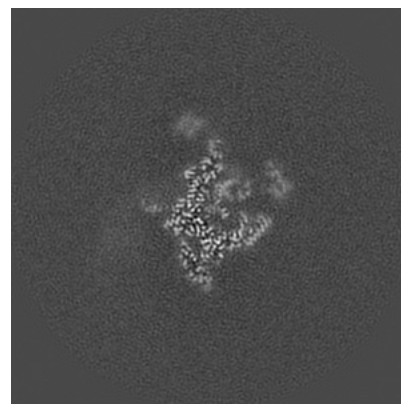
6.3.1 Primary map



X Index: 175



Y Index: 170

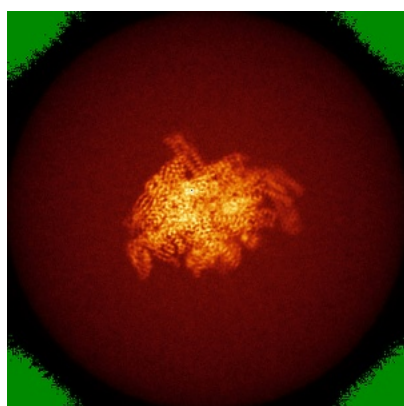


Z Index: 172

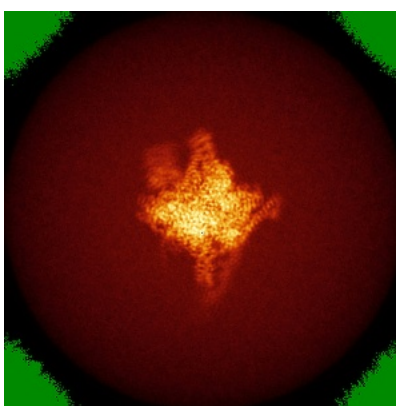
The images above show the largest variance slices of the map in three orthogonal directions.

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

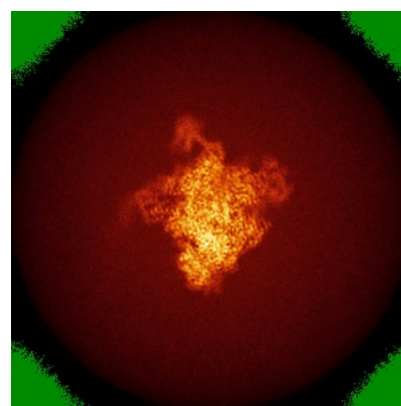
6.4.1 Primary map



X



Y

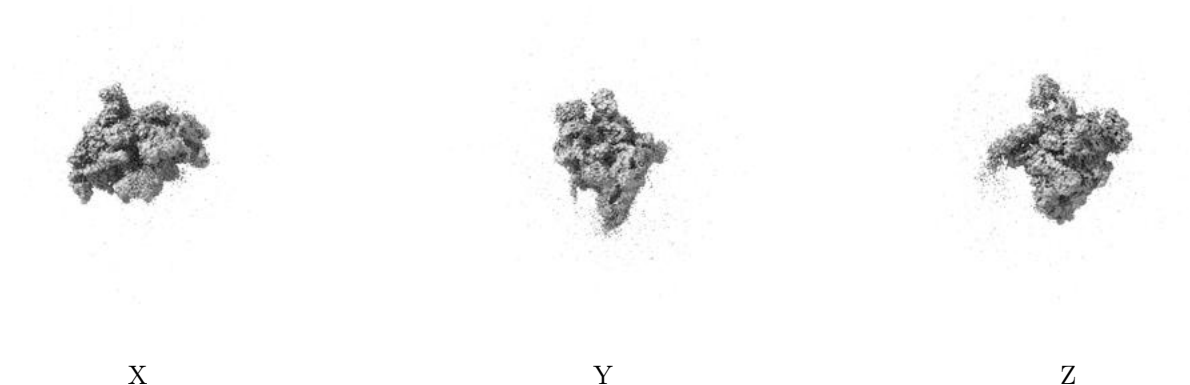


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

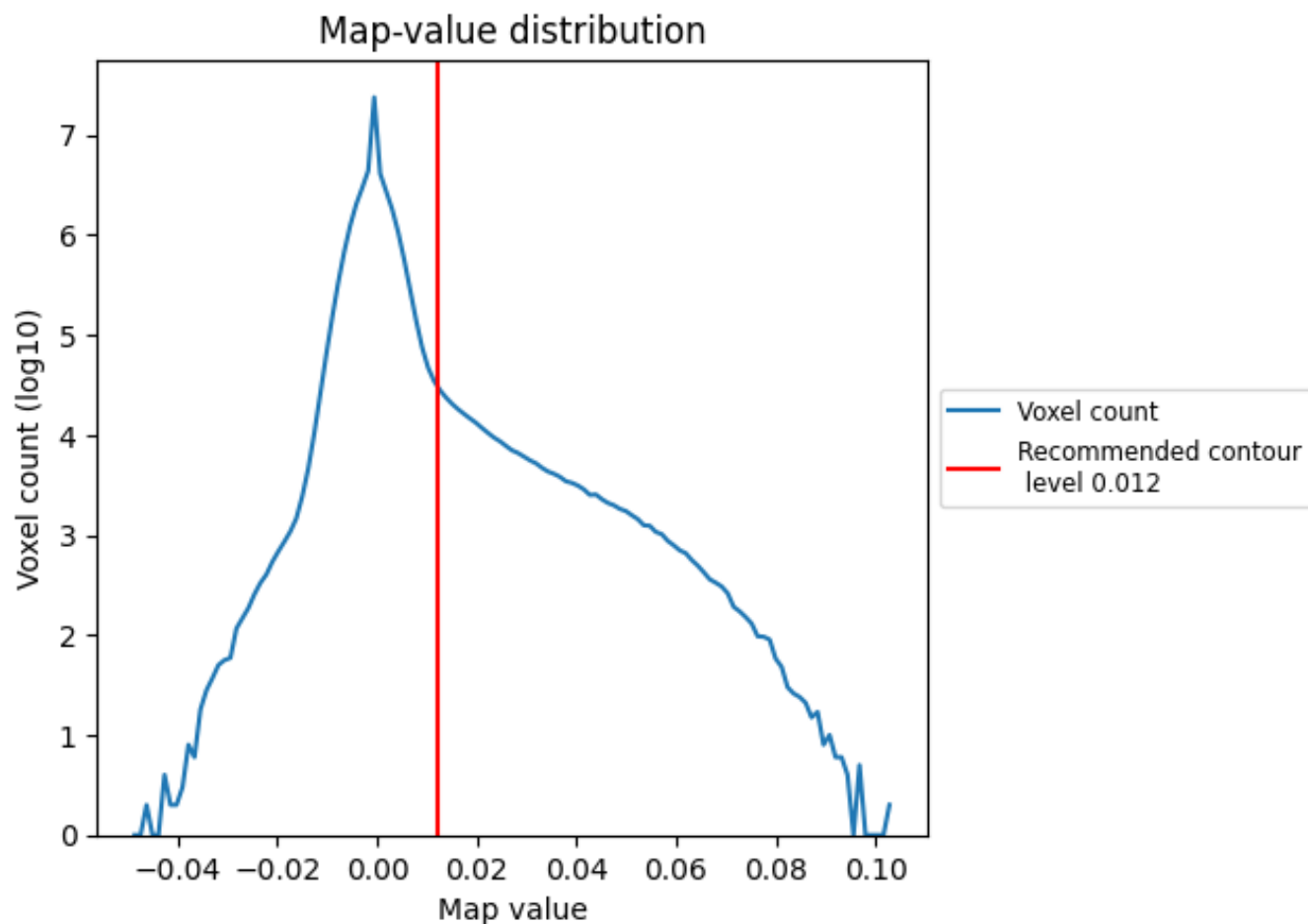
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

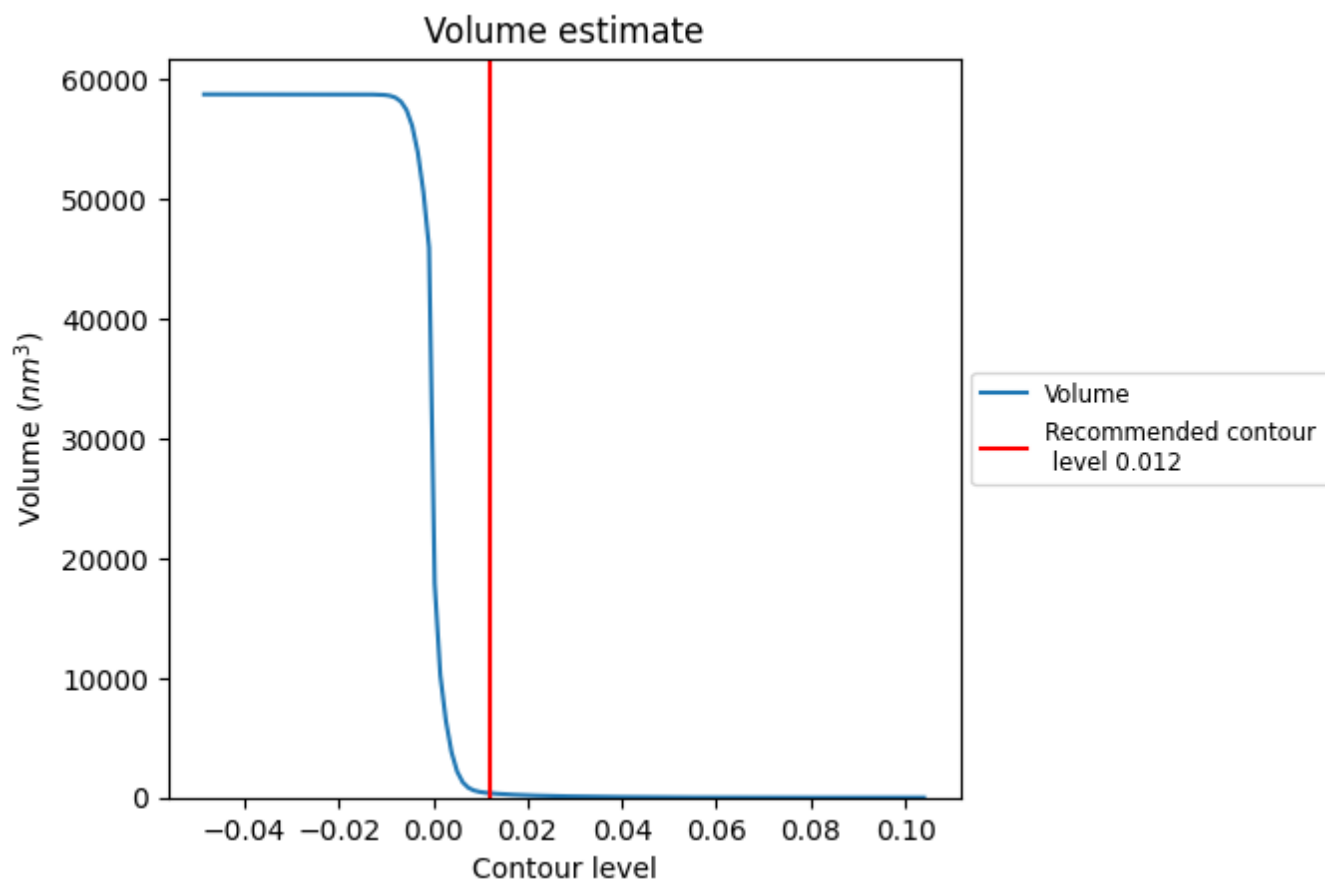
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

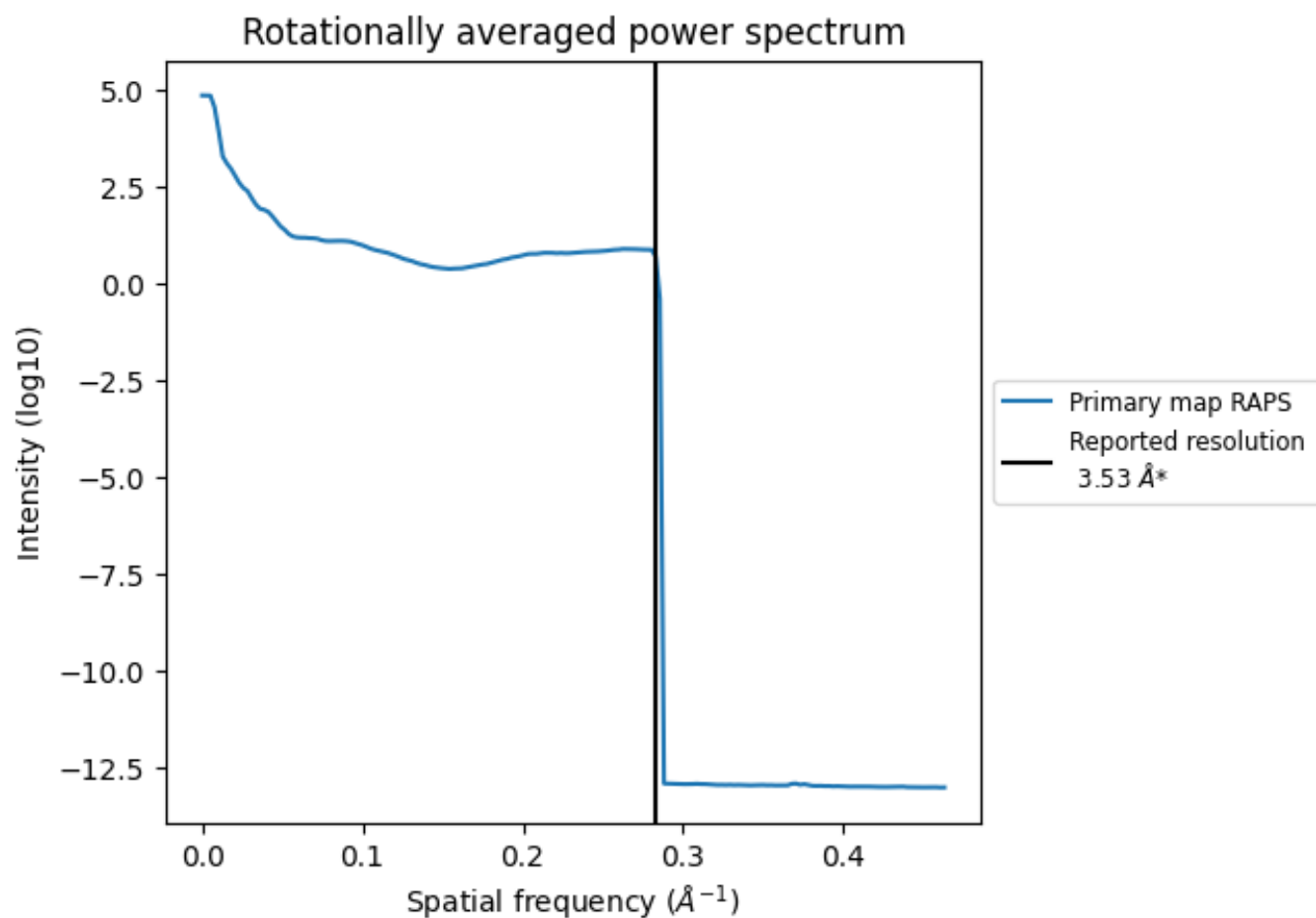
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm³; this corresponds to an approximate mass of 331 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 0.283 Å⁻¹

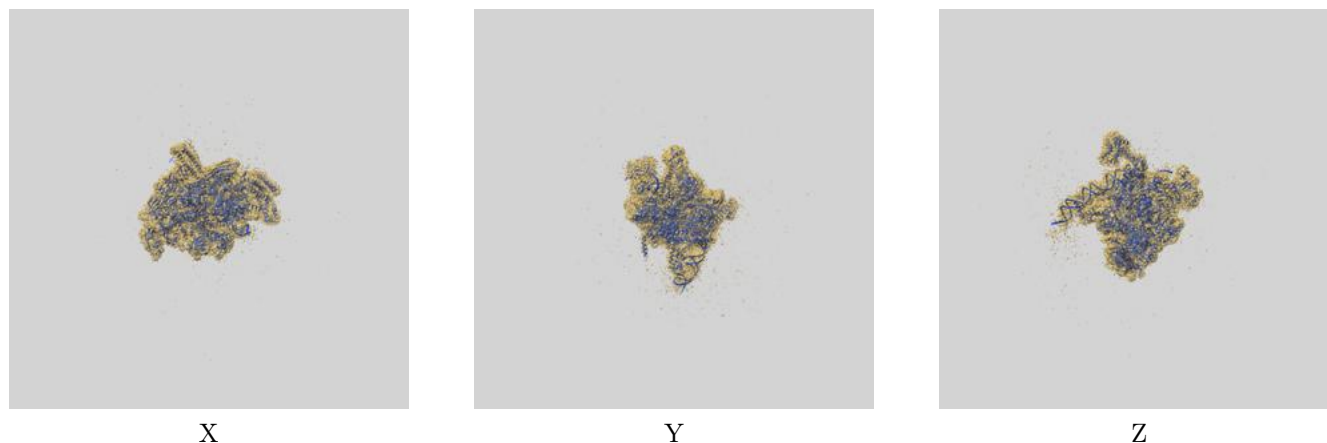
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

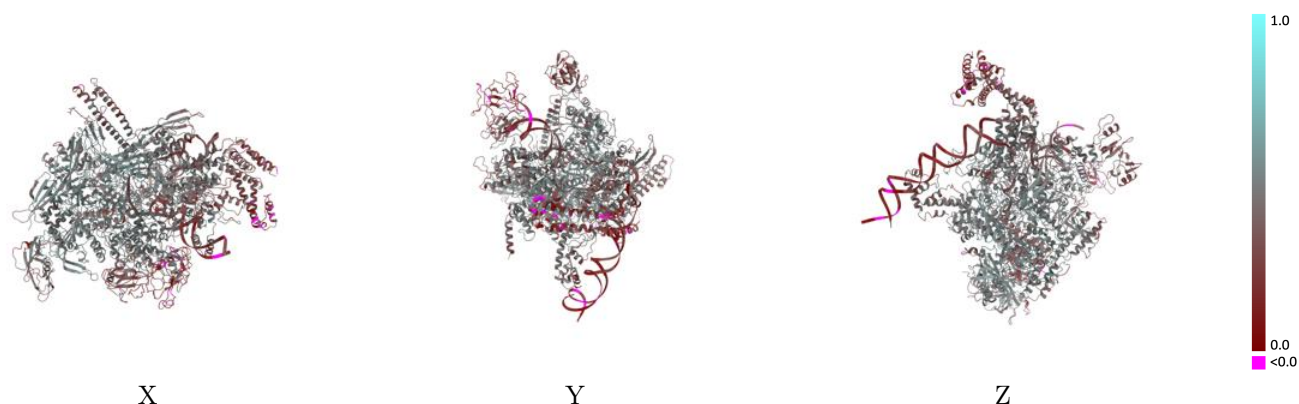
This section contains information regarding the fit between EMDB map EMD-21880 and PDB model 7KHB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



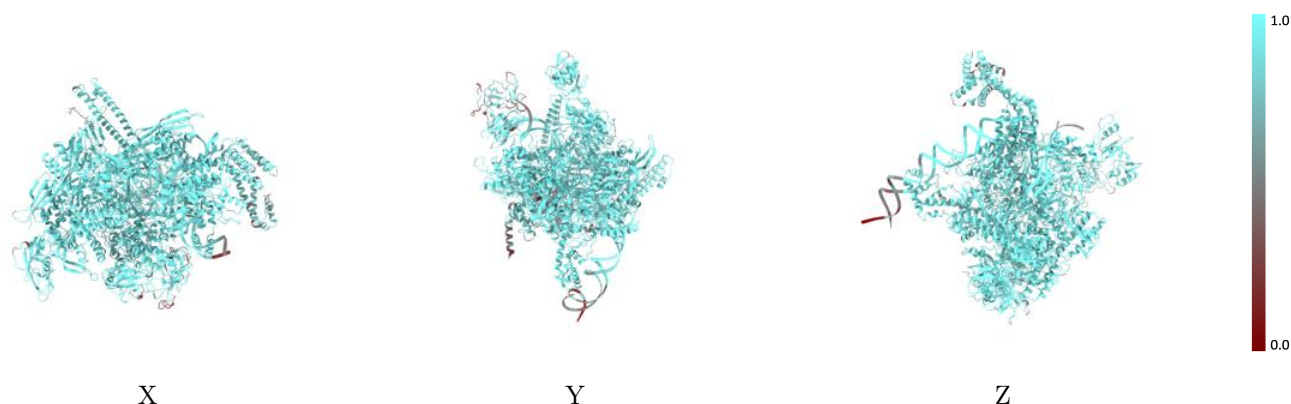
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



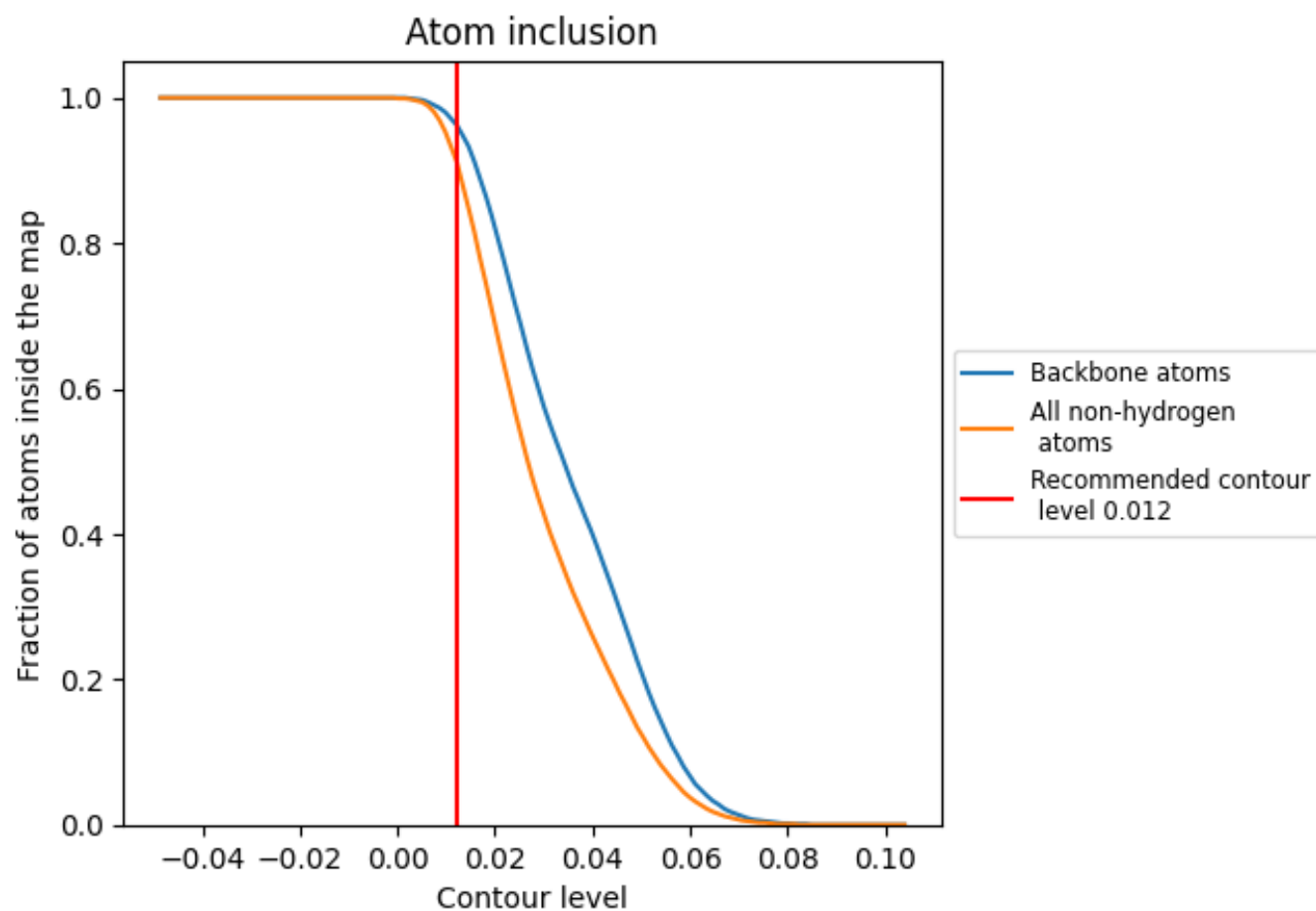
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 91% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9140	0.4300
A	0.9480	0.4870
B	0.9260	0.4500
C	0.9510	0.4760
D	0.9290	0.4500
E	0.6620	0.4320
F	0.8710	0.3410
X	0.7990	0.2310
Y	0.7970	0.2400

1.0

0.0

<0.0