



wwPDB EM Validation Summary Report ⓘ

May 4, 2025 – 12:01 PM EDT

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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

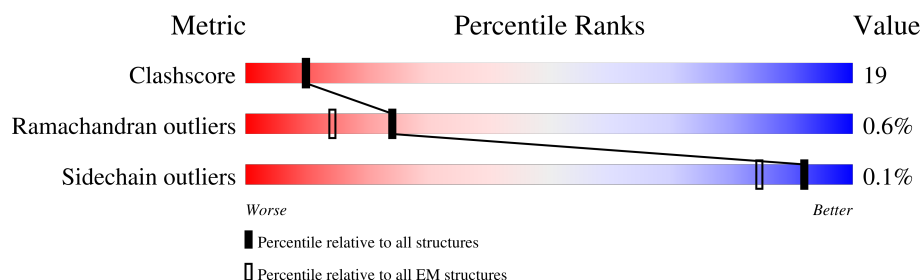
1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
1	B	329	
2	C	1342	
3	D	1407	
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 [i](#)

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		

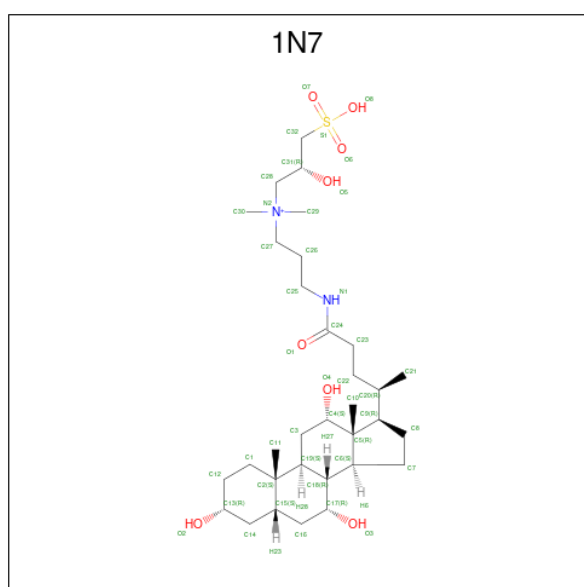
- Molecule 6 is a DNA chain called DNA (60-MER).

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: $\text{C}_{32}\text{H}_{59}\text{N}_2\text{O}_8\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
8	C	1	Total 43	C 32	N 2	O 8	S 1	0
8	C	1	Total 43	C 32	N 2	O 8	S 1	0

- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

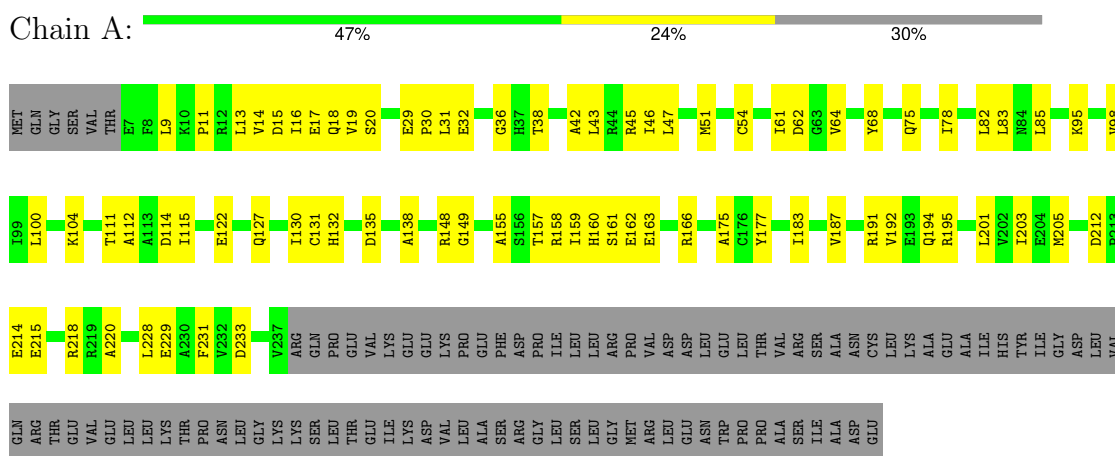
- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

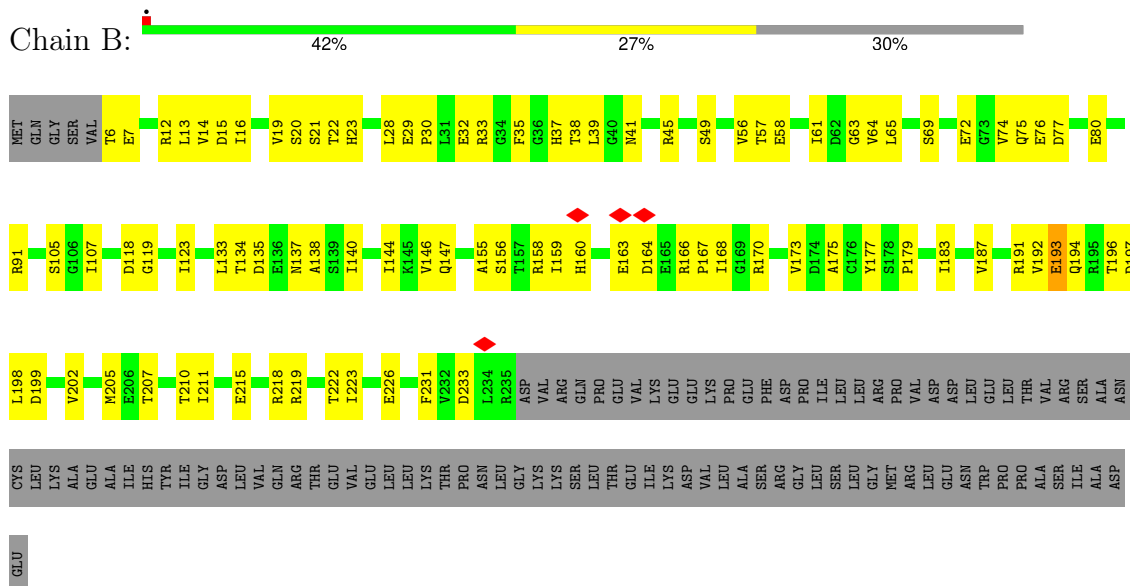
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

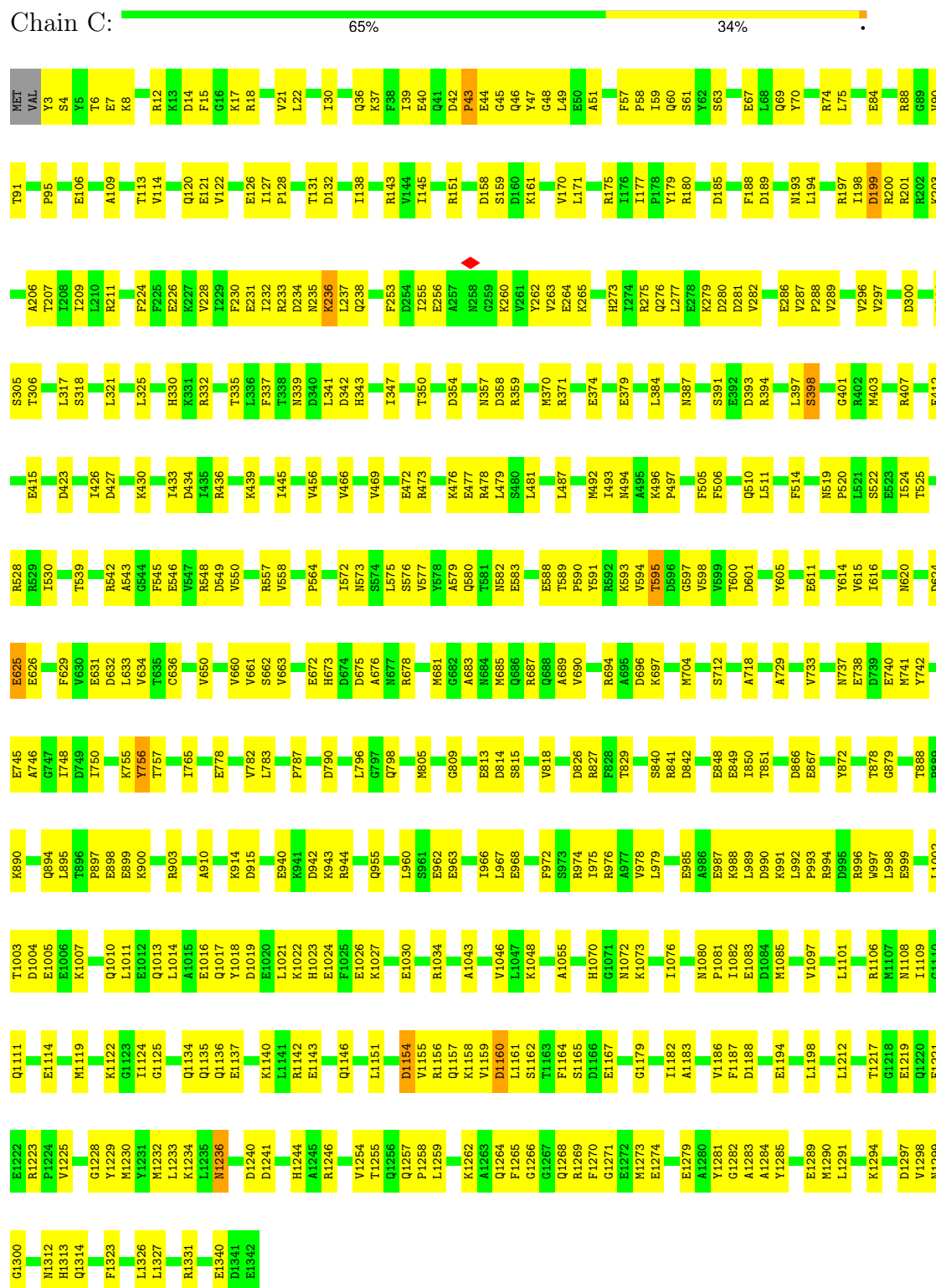
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta



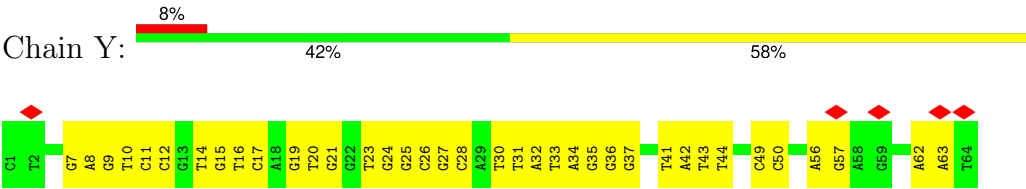
• Molecule 3: DNA-directed RNA polymerase subunit beta'



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	V97	ASP
ALA	Y1282	V1176	M1095	V1031	G956	K868	V769	I654	E533	R388	M298	I185	R99	LEU
GLU	S1283	T1177	S1032	S1033	K959	D870	L770	E653	E534	K395	L299	L188	E100	LEU
LEU	E1284	T1178	L1101	F1034	L960	L871	Q771	E658	V548	V407	Q300	L196	R101	PHE
LEU	V1285	V1179	P1102	F1035	S961	L872	F772	E661	K549	E301	E301	E197	M102	LEU
ASN	K1286	V1180	G1103	T1038	N962	E873	F773	E662	E552	D304	D304	Q196	G103	LYS
ALA	I1287	S1183	K1104	M1040	S963	K874	T774	E663	T553	I411	I411	I105	H104	GLN
LEU	V1288	D1184	A1105	T1039	K964	N875	S775	E664	E554	I416	I416	E198	E106	THR
GLY	F1289	Y1185	L1106	M1041	S965	S876	T776	E665	Y555	R417	R417	C198	E106	LYS
GLY	A1300	Y1186	V967	M1042	V966	V877	G782	E666	E556	H418	H418	Q200	P110	THR
SER	T1301	E1187	N968	Q1044	N968	A879	T786	E669	K557	E419	E419	E199	T111	LYS
ASP	S1313	E1188	K881	T1045	N969	V880	T786	E670	E557	R312	R312	Q200	T111	LYS
ASN	L1314	M1189	K882	T1046	S970	K881	T786	E671	E558	G313	G313	R202	H113	LYS
GLU	A1315	I1190	S884	T1047	V974	S884	K789	E672	E559	R314	R314	L205	H113	LYS
GLY	T1316	N1197	Q1114	R1048	V975	D889	D802	E673	E560	A426	A426	L206	S119	LYS
ASP	E1317	F1199	T1115	Q1049	T976	D890	E811	E674	E561	R425	R425	T208	L120	LYS
ASN	S1318	E1200	S977	E1052	S977	D891	E811	E675	E562	P439	P439	N209	G125	LYS
GLY	A1323	E1201	T980	L1053	T980	V894	C814	E676	E563	E443	E443	T210	L126	LYS
GLY	S1324	G1202	E981	T1054	L981	C895	T816	E677	E564	R426	R426	E211	L127	LYS
GLY	F1325	R1203	L982	G1055	L982	C896	T816	E678	E565	A427	A427	E212	L128	LYS
GLY	Q1326	E1204	K983	S1057	K983	C897	H817	E679	E566	L449	L449	E213	L129	LYS
GLY	E1327	R1205	T985	S1058	T985	C898	E818	E680	E567	H450	H450	E214	L130	LYS
GLY	V1331	G1207	D986	L1059	D986	R901	M821	E681	E568	V453	V453	E215	L131	LYS
GLY	D1342	E1208	R990	V1060	R990	D902	T823	E682	E569	D460	D460	E216	L132	LYS
GLY	E1343	E1215	R991	L1062	R991	G906	T824	E683	E570	F461	F461	E217	L133	LYS
GLY	L1344	A1216	S994	D1063	S994	E925	H825	E684	E571	R337	R337	E218	L134	LYS
GLY	R1345	E1220	Y995	S1064	Y995	E926	T826	E685	E572	R338	R338	E219	L135	LYS
GLY	G1346	I1220	K996	A1065	K996	P926	E827	E686	E573	R339	R339	E220	L136	LYS
GLY	L1347	H1227	V997	E1066	V997	L930	V831	E687	E574	Q340	Q340	E221	L137	LYS
GLY	K1348	E1230	A1001	L1067	A1001	F931	K832	E688	E575	K345	K345	E222	L138	LYS
GLY	E1349	T1230	V1002	T1068	V1002	MET	E833	E689	E576	R346	R346	E223	L139	LYS
GLY	M1350	E1231	L1003	A1069	L1003	ARG	P834	E690	E577	V347	V347	E224	L140	LYS
GLY	V1351	D1239	A1004	G1070	A1004	THR	E835	E691	E578	D348	D348	E225	L141	LYS
GLY	V1353	R1242	K1005	G1071	K1005	PHE	D837	E692	E579	Y349	Y349	E226	L142	LYS
GLY	L1356	E1242	G1006	L1072	G1006	HIS	E846	E693	E580	R352	R352	E227	L143	LYS
GLY	G1376	D1250	E1009	D1073	E1009	ILE	E847	E694	E581	V352	V352	E228	L144	LYS
ALA	K1251	K1251	Q1010	L1074	Q1010	GLY	V848	E695	E582	T356	T356	E229	L145	LYS
PRO	I1253	E1253	V1011	R1075	V1011	ALA	L849	E696	E583	V357	V357	E230	L146	LYS
ALA	E1254	E1254	P1076	P1076	P1076	ALA	K850	E697	E584	Y357	Y357	E231	L147	LYS
ALA	V1257	V1257	A1077	A1077	A1077	SER	P851	E698	E585	R352	R352	E232	L148	LYS
ALA	V1257	V1257	G1014	L1078	G1014	ARG	C852	E699	E586	V357	V357	E233	L149	LYS
ALA	V1257	V1257	T1015	L1078	T1015	ALA	D855	E700	E587	T356	T356	E234	L150	LYS
ALA	V1257	V1257	T1016	K1079	T1016	ALA	L856	E701	E588	V357	V357	E235	L151	LYS
ALA	V1257	V1257	V1017	I1080	V1017	ALA	R857	E702	E589	Y357	Y357	E236	L152	LYS
ALA	V1257	V1257	A1018	V1081	A1018	ALA	V858	E703	E590	R352	R352	E237	L153	LYS
ALA	V1257	V1257	N1019	D1082	N1019	ALA	L859	E704	E591	V357	V357	E238	L154	LYS
ALA	V1257	V1257	W1020	A1083	W1020	ALA	V859	E705	E592	T356	T356	E239	L155	LYS
ALA	V1257	V1257	D1082	A1083	D1082	ALA	P859	E706	E593	R352	R352	E240	L156	LYS
ALA	V1257	V1257	Q1084	Q1084	Q1084	ALA	R860	E707	E594	V357	V357	E241	L157	LYS
ALA	V1257	V1257	G1085	G1085	G1085	ALA	N861	E708	E595	T356	T356	E242	L158	LYS
ALA	V1257	V1257	N1086	N1086	N1086	ALA	E862	E709	E596	R352	R352	E243	L159	LYS
ALA	V1257	V1257	D1087	D1087	D1087	ALA	V863	E710	E597	T356	T356	E244	L160	LYS
ALA	V1257	V1257	L1089	L1089	L1089	ALA	E864	E711	E598	V357	V357	E245	L161	LYS
ALA	V1257	V1257	I1090	I1090	I1090	ALA	E865	E712	E599	R352	R352	E246	L162	LYS
ALA	V1257	V1257	P1091	P1091	P1091	ALA	E866	E713	E600	T356	T356	E247	L163	LYS

- Molecule 4: DNA-directed RNA polymerase subunit omega

● 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: 1N7, MG, 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	49
2	C	1338/1342 (100%)	1228 (92%)	100 (8%)	10 (1%)	19	54
3	D	1334/1407 (95%)	1211 (91%)	117 (9%)	6 (0%)	30	63
4	E	74/91 (81%)	68 (92%)	6 (8%)	0	100	100
5	F	465/613 (76%)	430 (92%)	32 (7%)	3 (1%)	22	56
All	All	3668/4111 (89%)	3355 (92%)	292 (8%)	21 (1%)	24	56

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%)	92	97

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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%)	92	97

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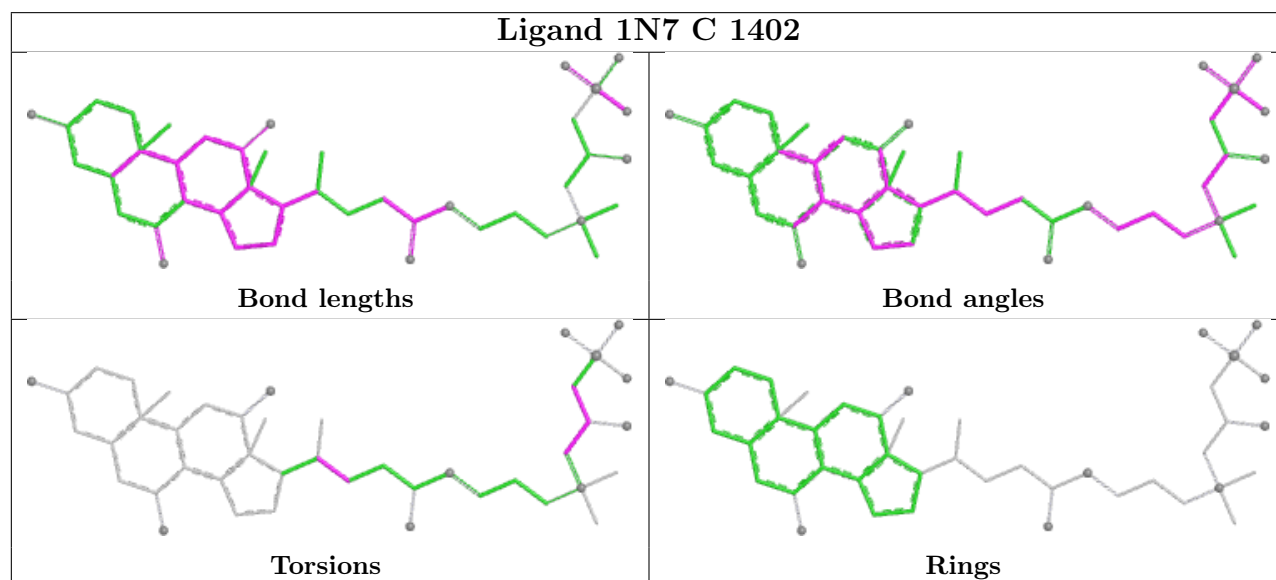
Mol	Chain	Res	Type	Atoms
8	C	1401	1N7	N2-C28-C31-O5
8	C	1402	1N7	N2-C28-C31-C32
8	C	1402	1N7	N2-C28-C31-O5
8	C	1402	1N7	C28-C31-C32-S1

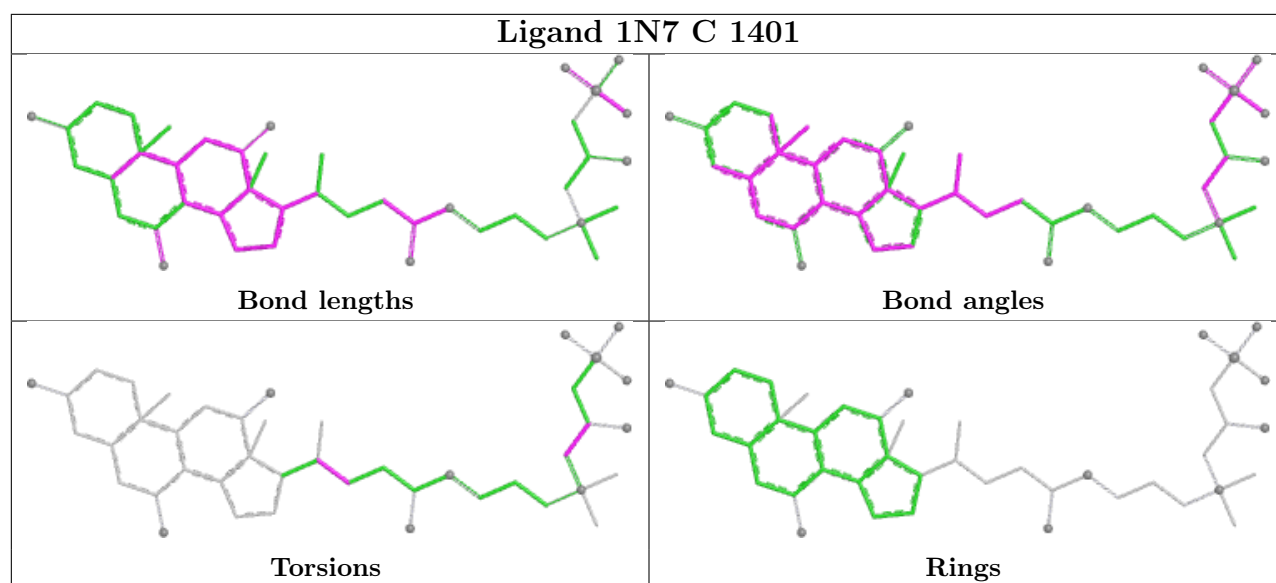
There are no ring outliers.

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.

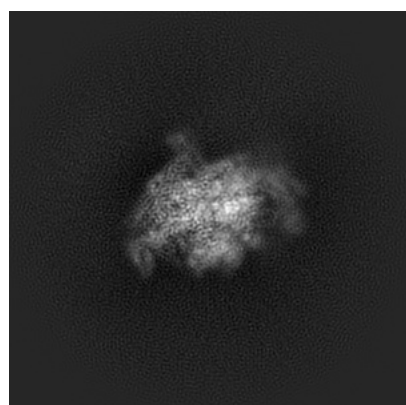
6 Map visualisation [i](#)

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.

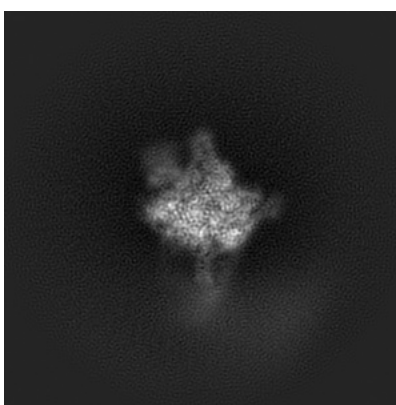
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

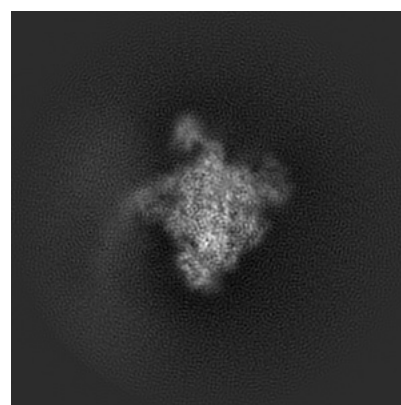
6.1.1 Primary map



X



Y

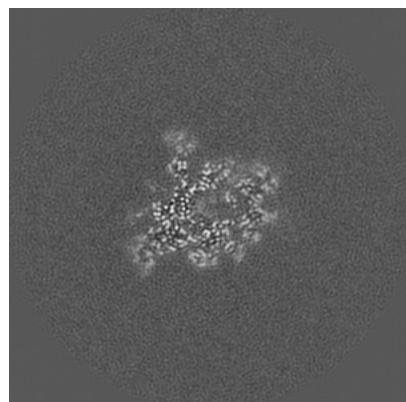


Z

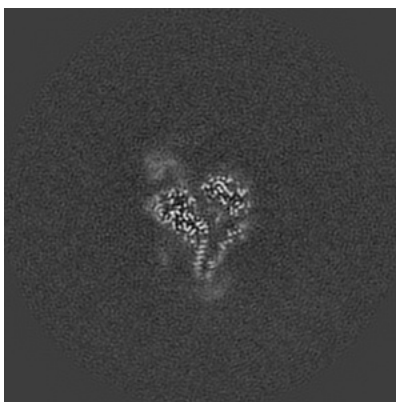
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

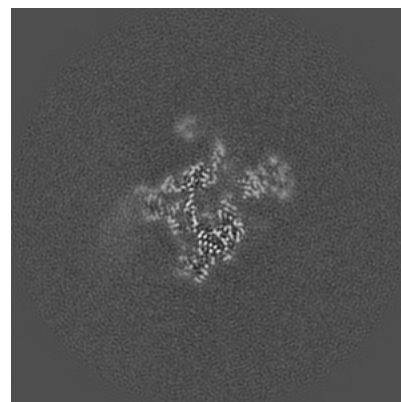
6.2.1 Primary map



X Index: 180



Y Index: 180

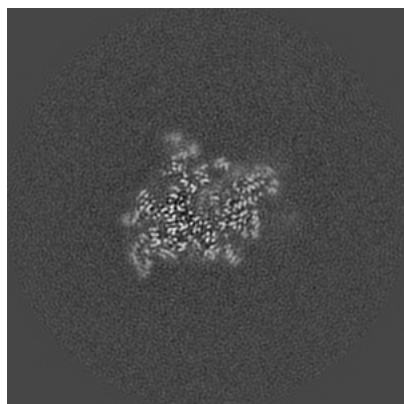


Z Index: 180

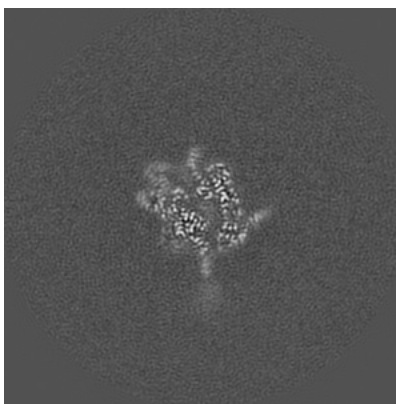
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

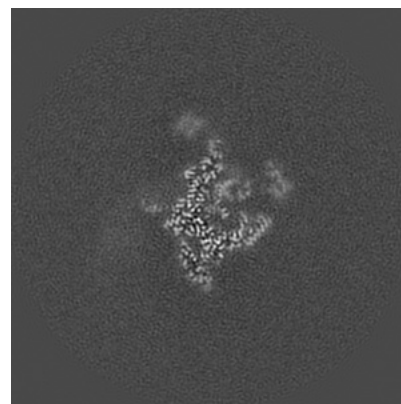
6.3.1 Primary map



X Index: 175



Y Index: 170

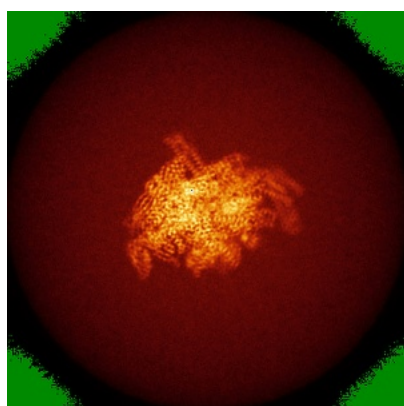


Z Index: 172

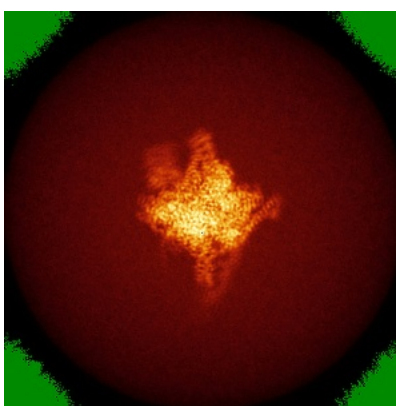
The images above show the largest variance slices of the map in three orthogonal directions.

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

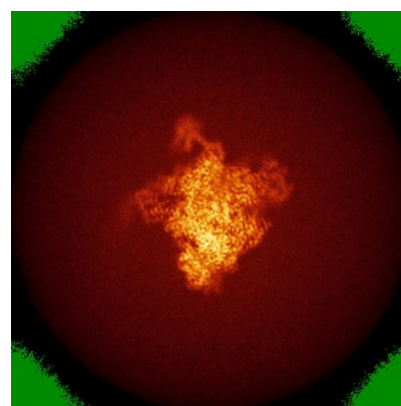
6.4.1 Primary map



X



Y

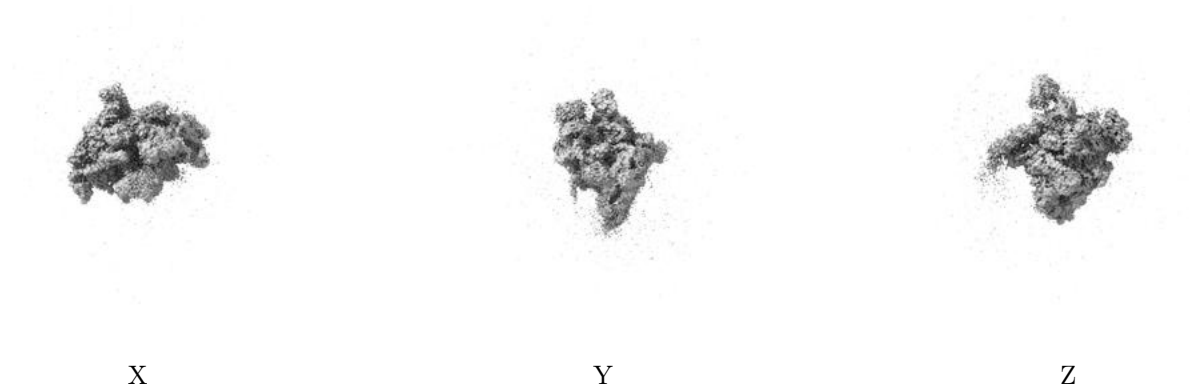


Z

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.

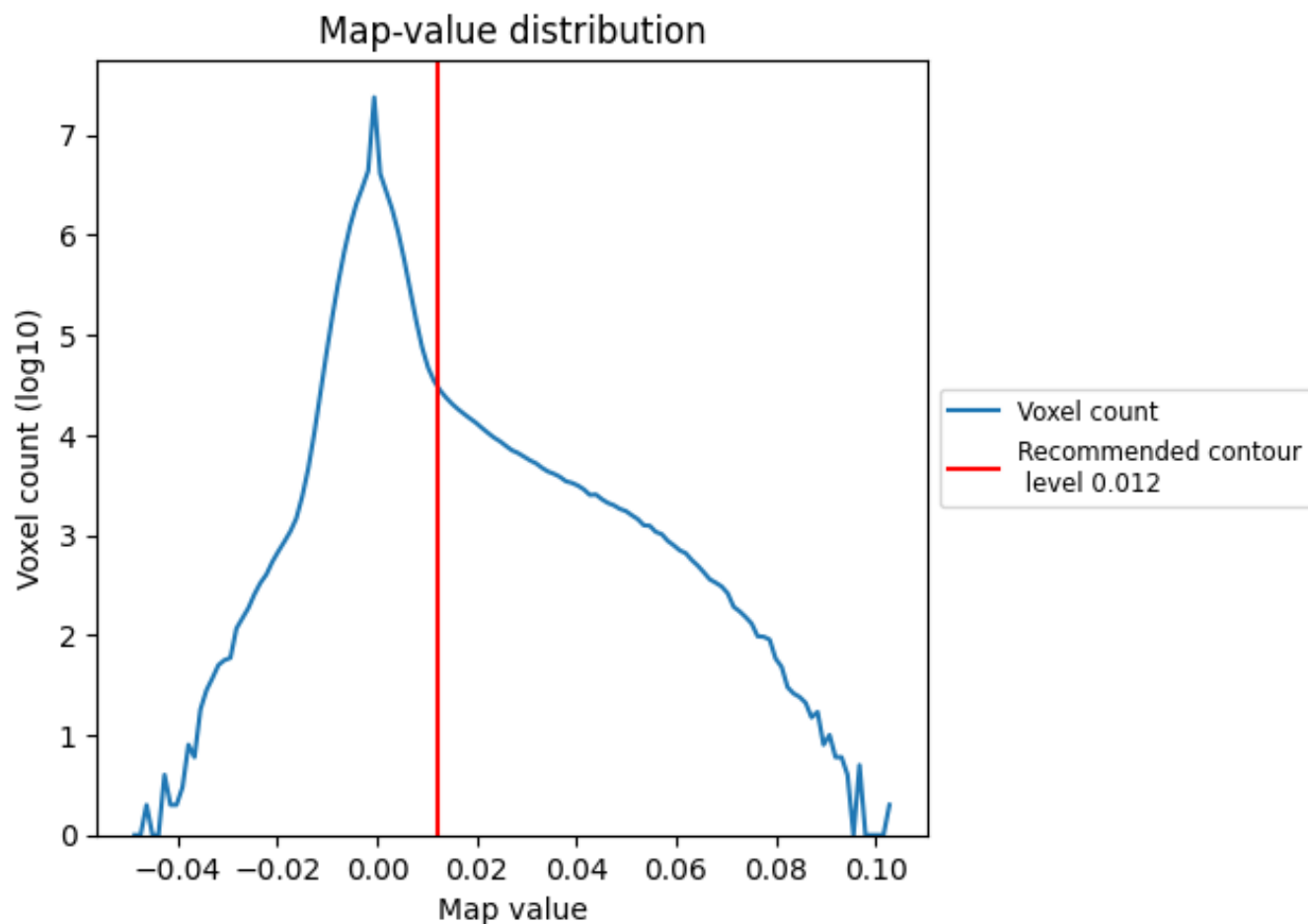
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

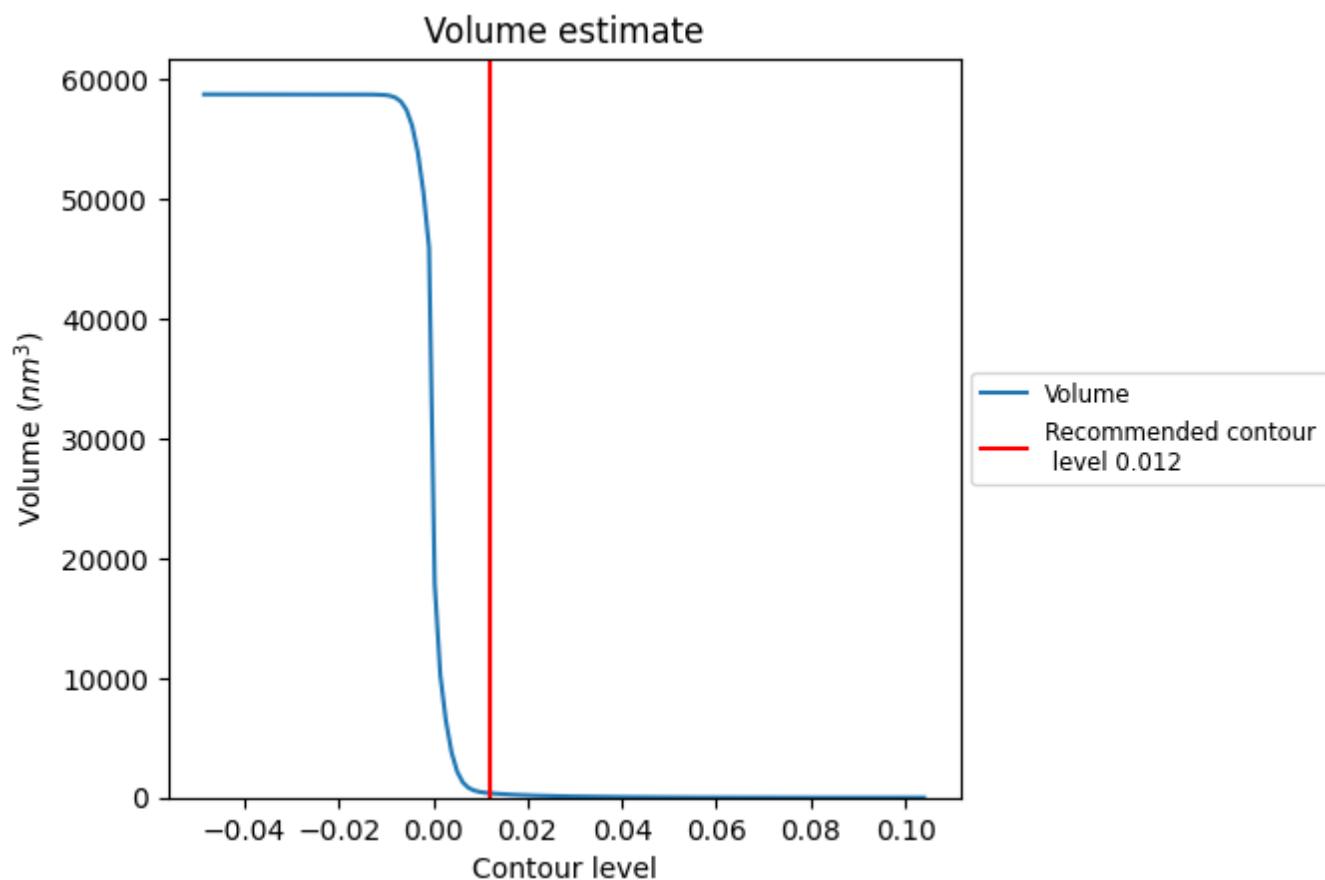
This section contains the results of statistical analysis of the map.

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.

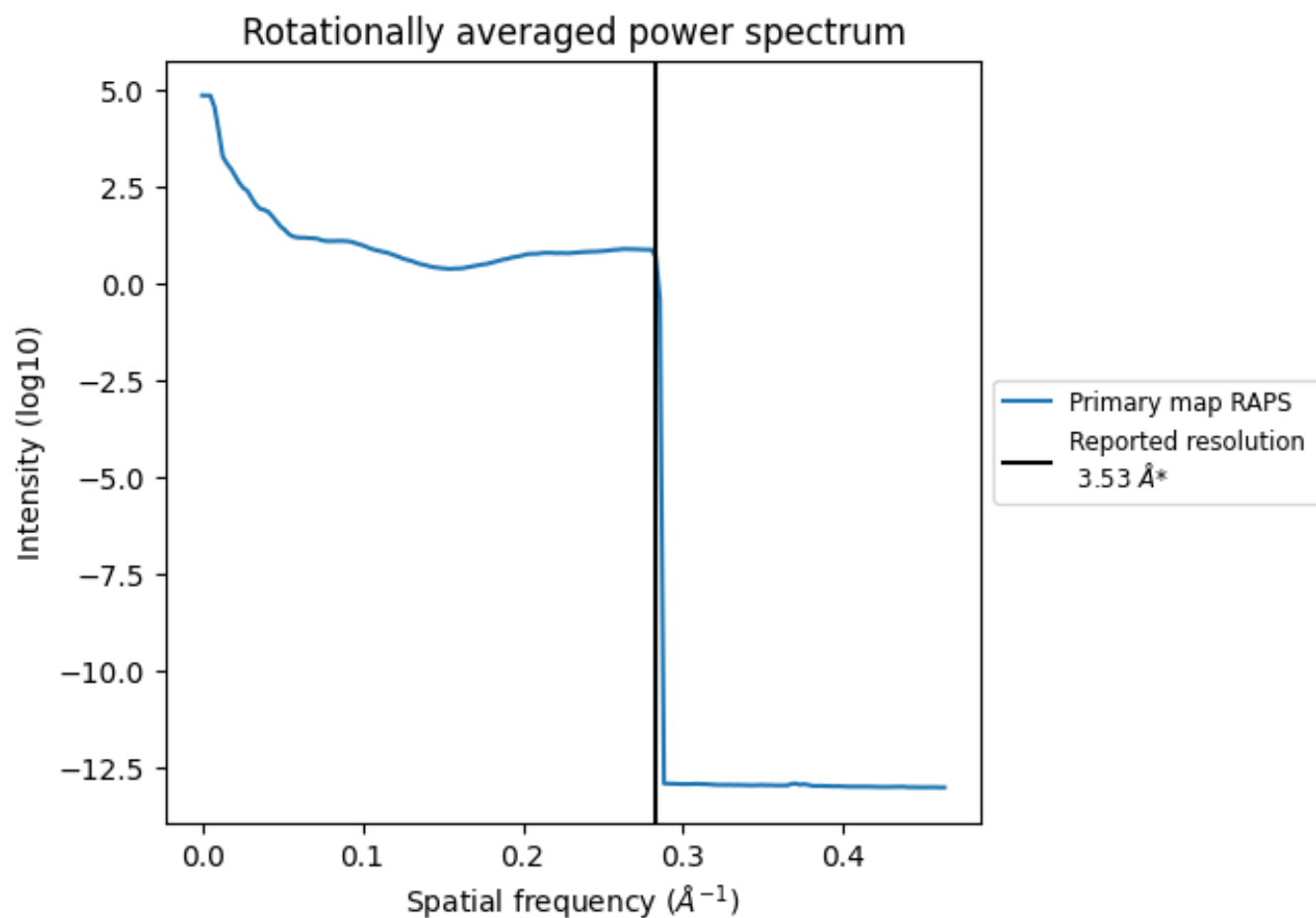
7.2 Volume estimate [i](#)



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

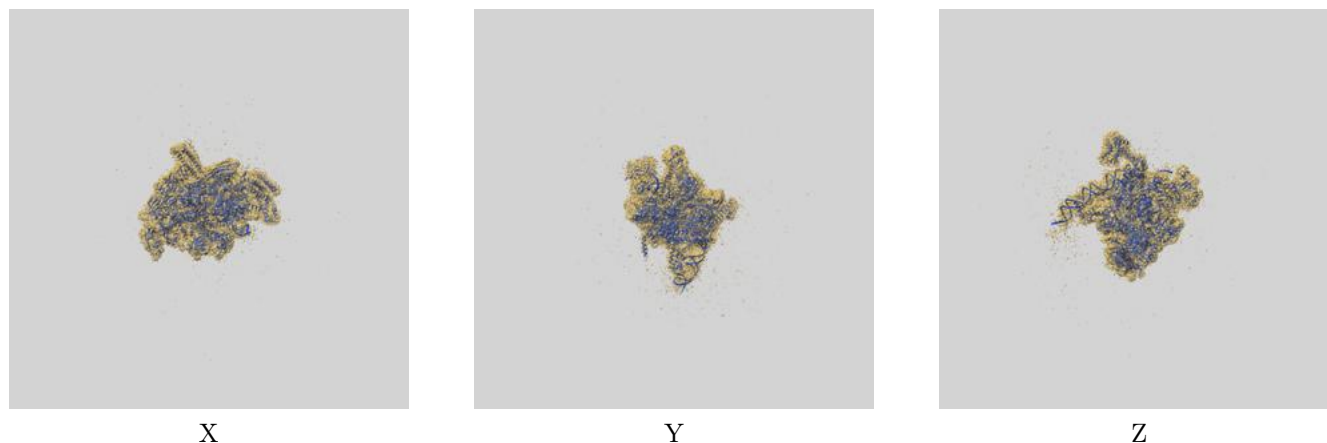
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

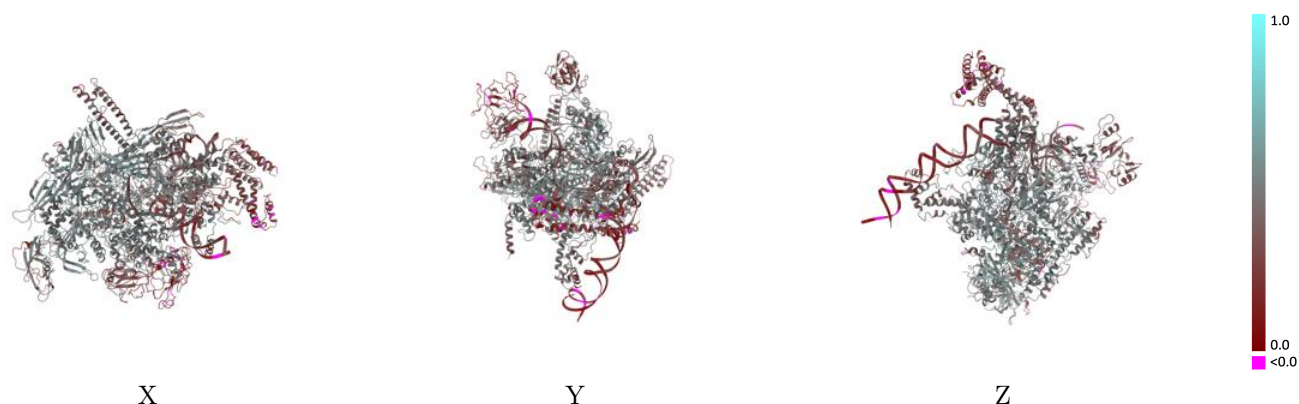
This section contains information regarding the fit between EMDB map EMD-21880 and PDB model 7KHB. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



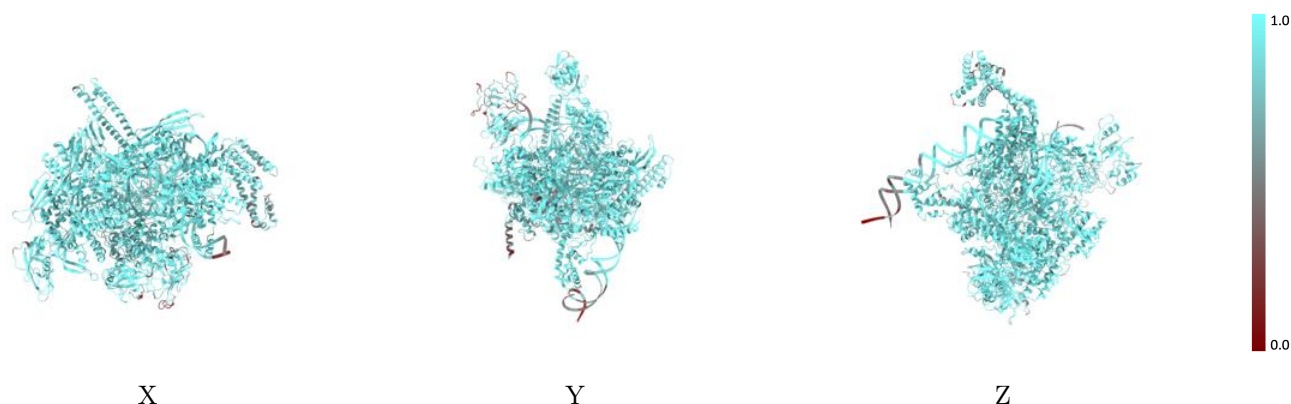
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



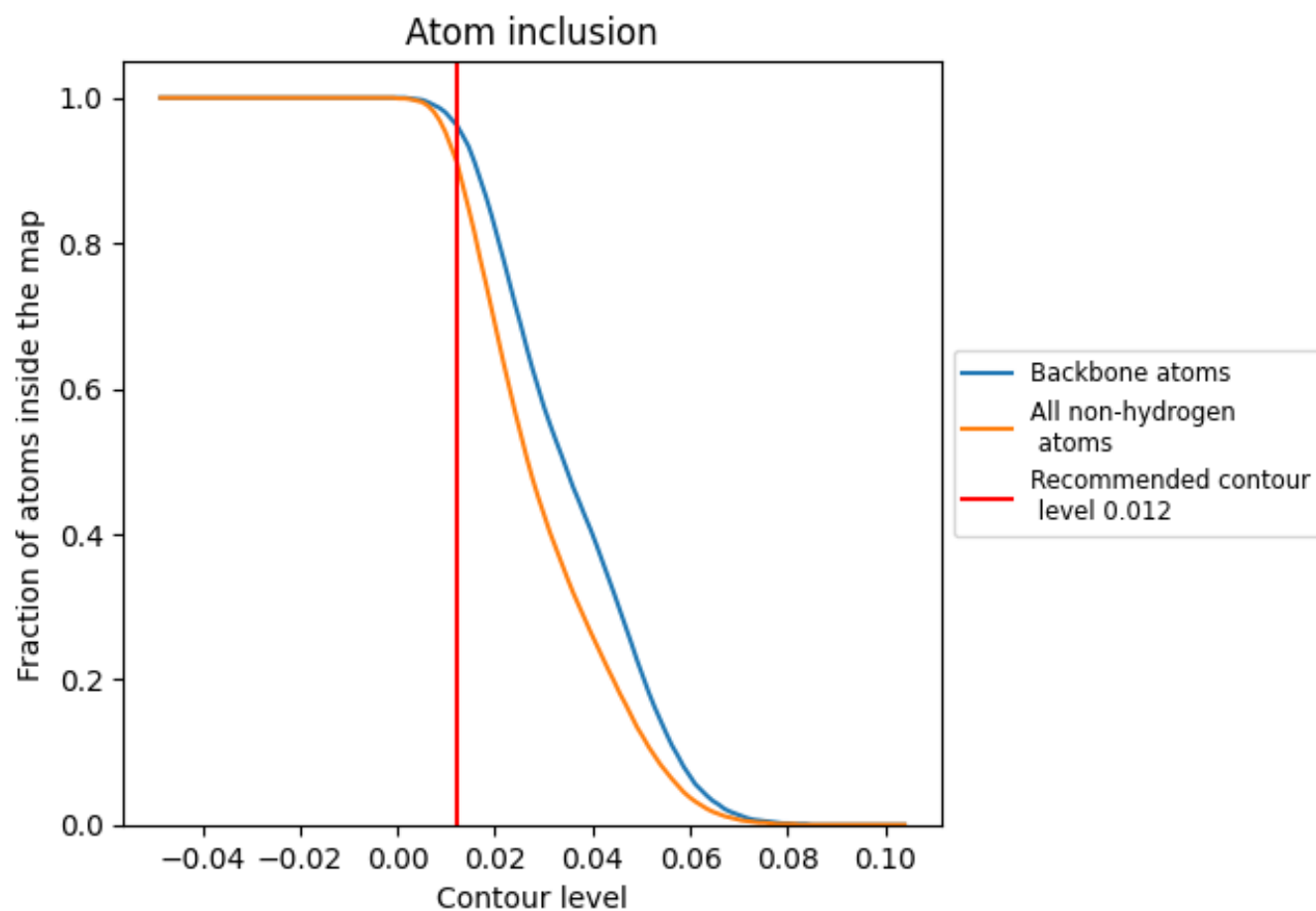
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div><div></div>0.9140</div>	<div><div></div>0.4300</div>
A	<div><div></div>0.9480</div>	<div><div></div>0.4870</div>
B	<div><div></div>0.9260</div>	<div><div></div>0.4500</div>
C	<div><div></div>0.9510</div>	<div><div></div>0.4760</div>
D	<div><div></div>0.9290</div>	<div><div></div>0.4500</div>
E	<div><div></div>0.6620</div>	<div><div></div>0.4320</div>
F	<div><div></div>0.8710</div>	<div><div></div>0.3410</div>
X	<div><div></div>0.7990</div>	<div><div></div>0.2310</div>
Y	<div><div></div>0.7970</div>	<div><div></div>0.2400</div>

1.0

0.0

<0.0