



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 01:40 AM UTC

PDB ID : 6PST / pdb_00006pst
EMDB ID : EMD-20463
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi1.5b) with TraR and mutant rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

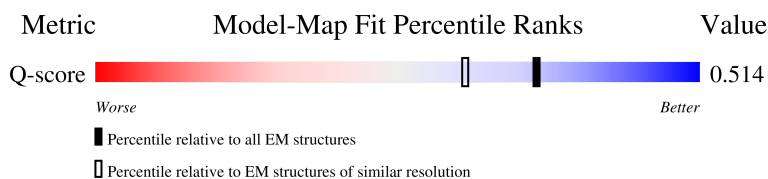
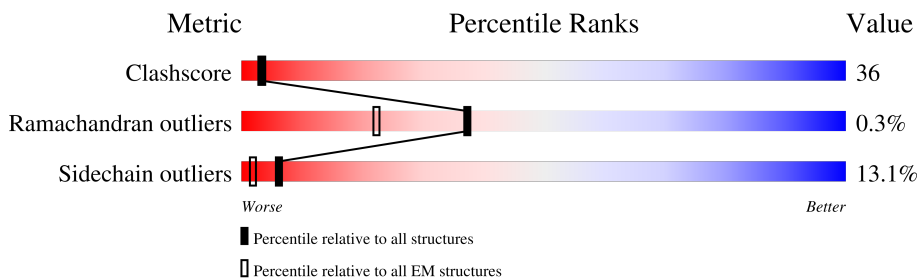
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	N	72	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">7%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">57%</div> <div style="text-align: right;">38%</div> <div style="text-align: right;">6%</div> </div>
2	O	85	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, grey);"></div> <div style="text-align: left;">9%</div> <div style="text-align: right;">49%</div> <div style="text-align: right;">41%</div> </div>
3	P	85	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">13%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, grey);"></div> <div style="text-align: left;">13%</div> <div style="text-align: right;">47%</div> <div style="text-align: right;">40%</div> </div>
4	G	329	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">5%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="text-align: left;">5%</div> <div style="text-align: right;">32%</div> <div style="text-align: right;">31%</div> <div style="text-align: right;">8%</div> <div style="text-align: right;">29%</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	329	<p>28% 32% 5% 34%</p>
4	M	329	<p>22% 5% 16% 78%</p>
5	I	1342	<p>8% 41% 50% 8%</p>
6	J	1430	<p>7% 35% 40% 6% 19%</p>
7	K	91	<p>11% 30% 44% 5% 21%</p>
8	L	616	<p>37% 31% 53% 6% 9%</p>

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 31608 atoms, of which 156 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 Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	72	566	350	103	108	5	0	0

- Molecule 2 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	O	50	1026	488	196	292	50	0	0

- Molecule 3 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	51	1045	499	182	313	51	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	73	572	362	100	108	2	0	0
4	G	232	1769	1106	315	342	6	0	0
4	H	218	1669	1044	293	326	6	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	1337	10512	6598	1831	2040	43	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	1164	9109	5730	1634	1698	47	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	72	577	352	110	114	1	0	0

- Molecule 8 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	558	4495	2804	788	876	27	0	0

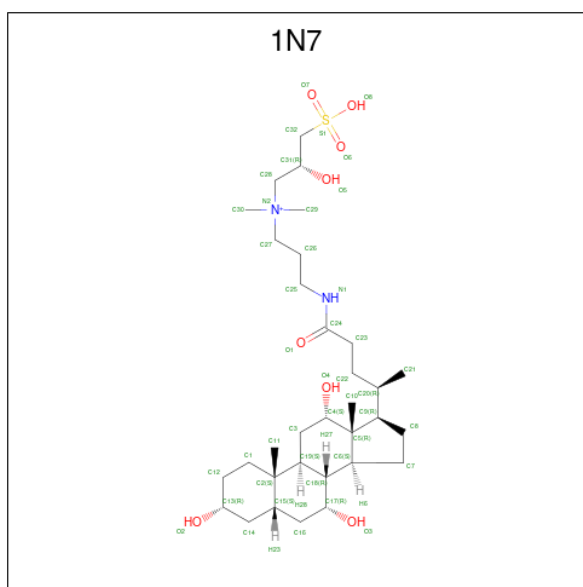
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
9	N	1	Total Zn 1 1	0
9	J	2	Total Zn 2 2	0

- Molecule 10 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms	AltConf
10	N	1	Total C H O 66 24 39 3	0
10	I	1	Total C H O 66 24 39 3	0
10	J	1	Total C H O 66 24 39 3	0
10	J	1	Total C H O 66 24 39 3	0

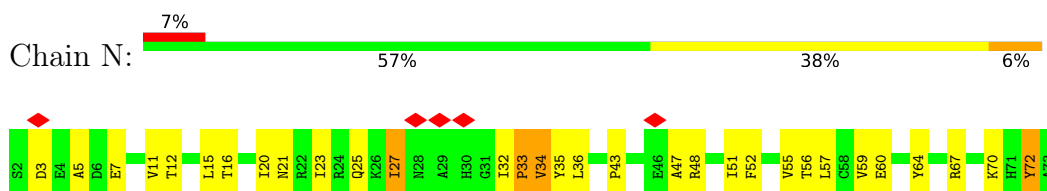
- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	J	1	Total	Mg	0
			1	1	

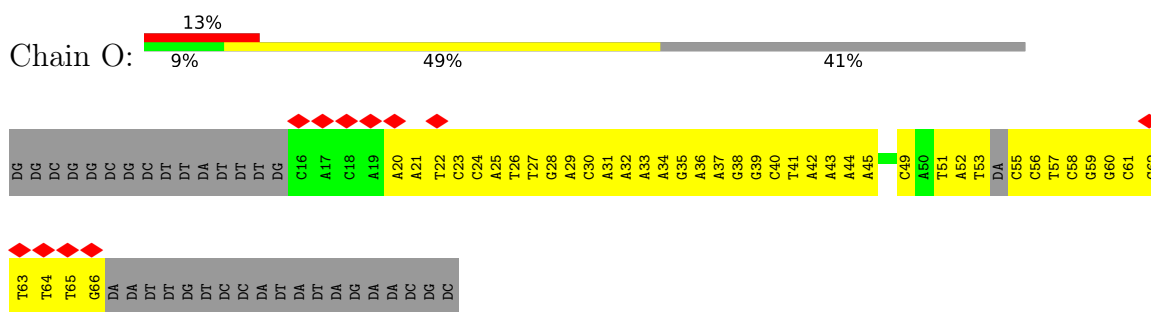
3 Residue-property plots

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.

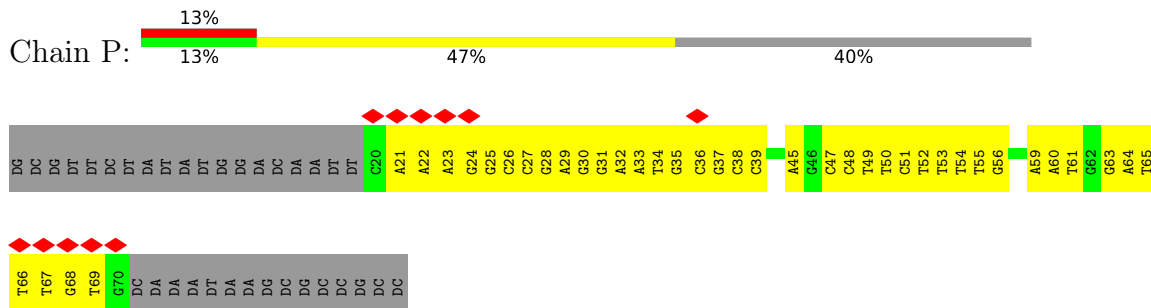
- Molecule 1: Protein TraR



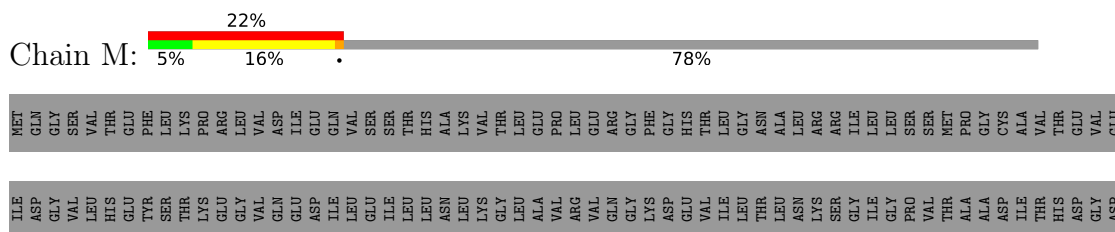
- Molecule 2: DNA (85-MER)



- Molecule 3: DNA (85-MER)

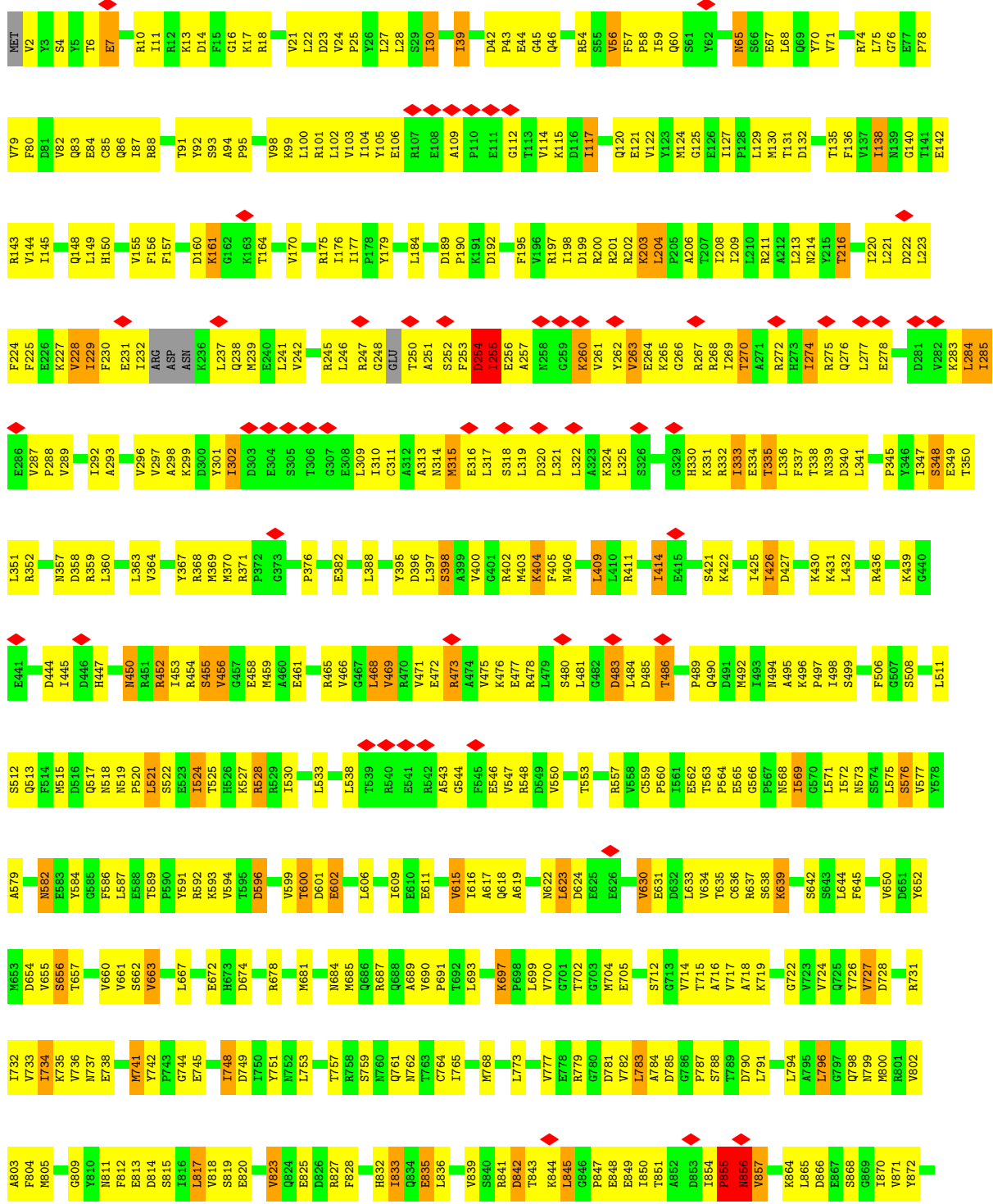


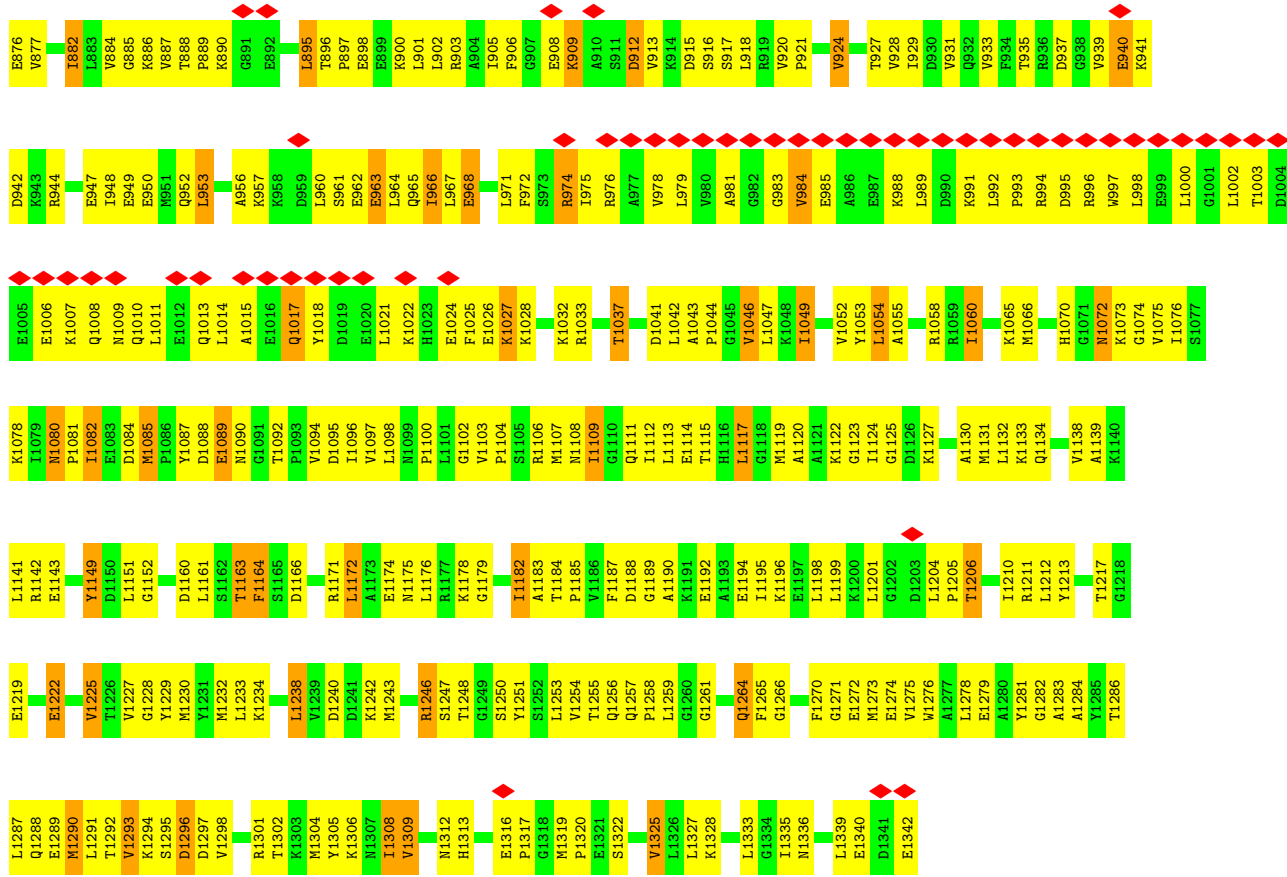
- Molecule 4: DNA-directed RNA polymerase subunit alpha



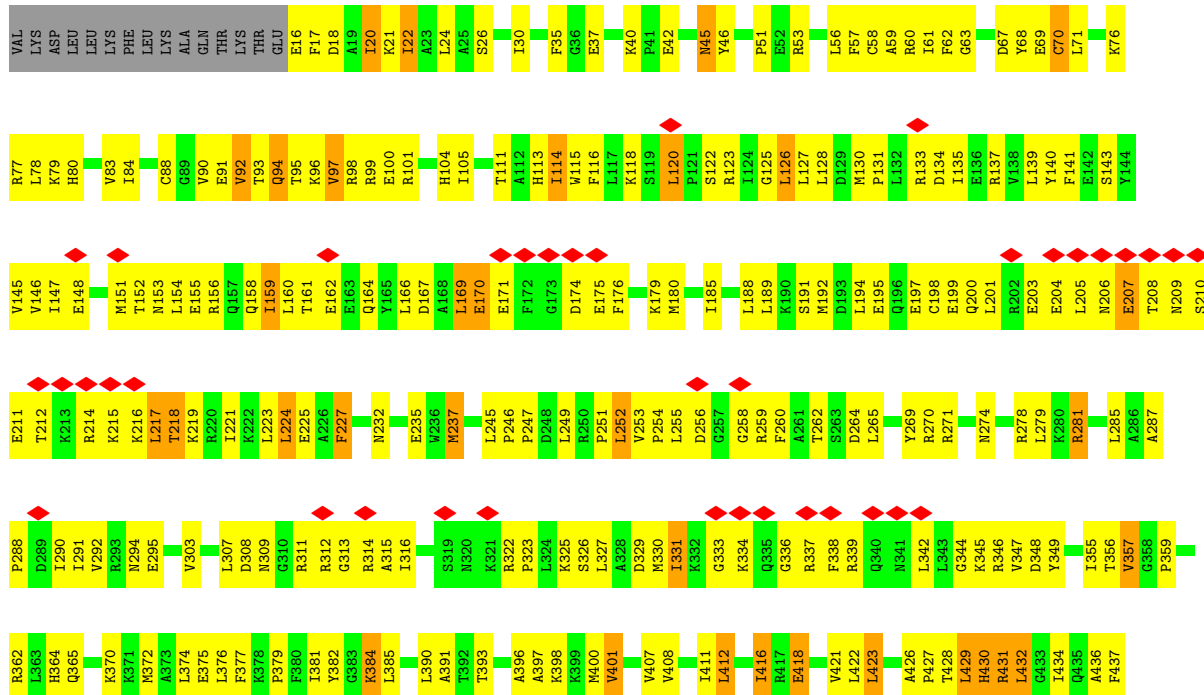
GLY	ASP	LEU	VAL	LEU	VAL	LEU	LEU	LEU	LYS	THR	PRO	ASN	LEU	GLY	LYS	ASP	VAL	LEU	ALA	ALA	SER	ARG	GLY	LEU	SER	SER	LEU	LEU	GLY	MET	ARG	LEU	GLY	ASN	TRP	PRO	PRO	ALA	ALA	ASP	GLU
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● Molecule 5: DNA-directed RNA polymerase subunit beta





● Molecule 6: DNA-directed RNA polymerase subunit beta'



LEU	V1337	GLY	L1196	ALA	GLY	GLN	SER	GLY	E874	THR	T810	THR	L724	THR	E648	THR	I579	Y512	E438
LEU	R1341	THR	M1197	GLY	GLN	VAL	ILE	THR	N875	GLN	E811	THR	M725	GLN	K649	GLN	L579	M513	P439
LEU	D1342	LYS	V1198	LYS	VAL	ALA	VAL	LYS	D878	ALA	D812	VAL	A726	ALA	E652	VAL	I582	T514	V440
VAL	E1343	ASP	F1199	ASP	ASP	LEU	VAL	ASN	A879	GLY	D813	GLY	S728	GLY	I654	ASN	P584	C517	I442
LEU	G1346	ARG	G1201	ARG	GLU	THR	LYS	LYS	V880	GLY	T816	GLY	S733	LYS	E656	LYS	L587	V518	G444
PHE	L1273	PRO	L1138	PRO	THR	THR	THR	THR	V882	THR	H817	THR	I737	THR	A657	THR	P688	I519	K445
GLN	L1274	ALA	P1139	ALA	VAL	VAL	VAL	VAL	V883	VAL	I820	VAL	L740	VAL	E660	VAL	S590	A520	A446
PRO	L1275	LYS	R1140	LYS	ASN	ASN	ASN	ASN	S884	ASN	M822	ASN	A741	ASN	V661	ASN	I591	K521	I447
SER	G1277	ILE	L1144	ILE	TRP	TRP	TRP	TRP	V885	TRP	M822	TRP	G742	TRP	V662	TRP	V692	L452	
SER	Q1279	ASP	F1145	ASP	PRO	PRO	ASN	ASN	V886	PRO	P824	PRO	M743	ASN	E663	ASN	Q594	V453	
GLY	V1280	ASP	L1149	ASP	VAL	VAL	VAL	VAL	S887	VAL	R825	VAL	R744	VAL	I664	VAL	A595	C454	
HIS	E1281	ALA	H1149	ALA	HIS	HIS	VAL	VAL	T890	VAL	E827	VAL	M747	VAL	F668	VAL	L596	A455	
HIS	Y1282	GLN	P1150	GLN	THR	THR	THR	THR	F892	THR	G828	THR	G751	THR	L672	THR	A600	A456	
HIS	S1283	GLY	R1151	GLY	MET	MET	SER	SER	D891	SER	G829	SER	D751	SER	L673	SER	K603	V457	
HIS	R1284	ASN	K1151	ASN	PRO	PRO	VAL	VAL	F893	PRO	R831	VAL	I754	VAL	T674	PRO	M604	M458	
HIS	K1285	ASP	P1152	ASP	VAL	VAL	VAL	VAL	G894	VAL	G830	VAL	G752	VAL	R678	VAL	K603	M458	
HIS	K1286	VAL	P1153	VAL	THR	THR	THR	THR	V894	THR	D830	THR	G753	THR	R678	THR	M604	M458	
HIS	I1287	LEU	I1154	LEU	THR	THR	THR	THR	G900	THR	R831	THR	I754	THR	E677	THR	M604	M458	
HIS	A1288	PRO	L1156	PRO	VAL	VAL	VAL	VAL	R901	PRO	K832	VAL	I754	PRO	E677	PRO	M604	M458	
HIS	E1291	THR	A1157	THR	GLY	GLY	GLY	GLY	R905	THR	E833	THR	P758	THR	R678	THR	M604	M458	
HIS	L1292	THR	E1158	THR	THR	THR	THR	THR	G906	THR	P834	THR	I759	THR	R678	THR	M604	M458	
HIS	E1293	ASP	E1159	ASP	ASP	PHE	VAL	VAL	H907	ASP	R835	VAL	T760	ASP	R678	ASP	M604	M458	
HIS	A1294	MET	S1160	MET	VAL	VAL	VAL	VAL	I908	VAL	R836	VAL	T760	VAL	R678	VAL	M604	M458	
HIS	N1295	PRO	G1161	PRO	ARG	ARG	ARG	ARG	I909	PRO	R837	ARG	A761	ARG	R678	ARG	M604	M458	
HIS	G1296	ALA	I1162	ALA	PHE	PHE	SER	SER	N910	ALA	R838	SER	N762	SER	R678	SER	M604	M458	
HIS	K1297	GLN	V1163	GLN	THR	THR	THR	THR	K911	GLN	R839	THR	N762	GLN	R678	THR	M604	M458	
HIS	G1298	TVR	S1164	TVR	ASP	ASP	ASP	ASP	G912	TVR	L840	ASP	R764	ASP	R678	ASP	M604	M458	
HIS	V1298	PHE	F1165	PHE	MET	MET	THR	THR	E913	PHE	R840	THR	R764	THR	R678	THR	M604	M458	
HIS	L1299	PRO	G1166	PRO	ASP	ASP	THR	THR	A914	PRO	V843	THR	N768	PRO	R678	THR	M604	M458	
ALA	R1303	ALA	K1167	ALA	GLY	GLY	GLY	GLY	I915	ALA	D847	ALA	V769	ALA	R678	ALA	M604	M458	
ALA	D1304	LYS	E1168	LYS	LEU	LEU	LEU	LEU	G916	LYS	V848	LEU	L770	LYS	R678	LEU	M604	M458	
PRO	L1305	ALA	T1169	ALA	THR	THR	THR	THR	V917	THR	L849	THR	Q771	THR	R678	THR	M604	M458	
VAL	L1306	ILE	K1170	ILE	ILE	ILE	ILE	ILE	I918	ILE	K850	ILE	I774	ILE	R678	ILE	M604	M458	
THR	L1307	VAL	T1171	VAL	VAL	VAL	VAL	VAL	A919	VAL	R851	VAL	I774	VAL	R678	VAL	M604	M458	
ALA	G1308	GLN	G1171	GLN	ARG	ARG	PHE	PHE	A920	GLN	P851	ARG	T776	ARG	R678	ARG	M604	M458	
ALA	I1309	LEU	K1172	LEU	GLN	GLN	GLY	GLY	S922	LEU	G852	GLY	T776	GLY	R678	LEU	M604	M458	
ASP	T1310	GLU	R1173	GLU	THR	THR	THR	THR	S922	GLU	T853	THR	H777	THR	R678	GLU	M604	M458	
ALA	K1311	ASP	R1174	ASP	ASP	ASP	THR	THR	I923	ASP	A854	THR	H777	THR	R678	ASP	M604	M458	
ALA	L1314	VAL	L1175	VAL	GLY	GLY	LYS	LYS	T931	VAL	D855	LYS	L783	VAL	R678	VAL	M604	M458	
SER	E1317	VAL	V1176	VAL	LEU	LEU	GLY	GLY	M932	LEU	R855	GLY	T786	LEU	R678	LEU	M604	M458	
LEU	S1318	GLN	I1177	GLN	THR	THR	SER	SER	R933	THR	L857	THR	A787	THR	R678	THR	M604	M458	
ALA	F1319	SER	T1178	ILE	THR	THR	LYS	LYS	T934	SER	V858	LYS	L788	LYS	R678	SER	M604	M458	
LEU	I1320	THR	P1179	SER	LEU	LEU	VAL	VAL	I937	THR	R859	VAL	K789	VAL	R678	THR	M604	M458	
LEU	D1249	THR	V1180	SER	GLY	GLY	PRO	PRO	GLY	THR	R860	PRO	N792	THR	R678	THR	M604	M458	
LEU	D1250	THR	D1181	ASP	VAL	VAL	THR	THR	GLY	THR	T862	THR	L796	THR	R678	THR	M604	M458	
ASN	K1251	ALA	G1182	ALA	VAL	VAL	VAL	VAL	ALA	THR	L863	VAL	T797	THR	R678	VAL	M604	M458	
ALA	H1252	ALA	S1183	ALA	LEU	LEU	VAL	VAL	ALA	THR	R864	VAL	T797	THR	R678	VAL	M604	M458	
GLY	I1253	ALA	D1184	ALA	ARG	ARG	ASP	ASP	SER	THR	H865	ARG	V717	THR	R678	THR	M604	M458	
LEU	F1325	ILE	P1185	ILE	THR	THR	ALA	ALA	ALA	THR	Q867	THR	V801	THR	R678	THR	M604	M458	
GLY	I1254	PRO	Y1186	PRO	ALA	ALA	ALA	ALA	ALA	THR	R868	ALA	D802	THR	R678	THR	M604	M458	
GLY	E1327	GLN	E1187	GLN	ARG	ARG	GLY	GLY	ALA	THR	C869	ARG	V803	THR	R678	THR	M604	M458	
ASP	T1328	GLU	E1188	GLU	THR	THR	ASP	ASP	GLY	THR	R870	THR	A804	THR	R678	THR	M604	M458	
ASN	T1329	ASN	M1189	ASN	THR	THR	THR	THR	SER	THR	L871	THR	L872	THR	R678	THR	M604	M458	
ASN	T1333	ASN	I1190	ASN	THR	THR	THR	THR	GLY	THR	L872	THR	Q805	THR	R678	THR	M604	M458	
ASN		ASN	P1191	ASN	THR	THR	THR	THR	SER	THR	L873	THR	Q805	THR	R678	THR	M604	M458	
ASN		ASN	R1194	ASN	THR	THR	THR	THR	SER	THR	L873	THR	Q805	THR	R678	THR	M604	M458	
ASN		ASN	Q1195	ASN	THR	THR	THR	THR	SER	THR	L873	THR	Q805	THR	R678	THR	M604	M458	

• Molecule 7: DNA-directed RNA polymerase subunit omega

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93666	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 ($e^-/\text{\AA}^2$)	50	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	0.172	Depositor
Minimum map value	-0.120	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 1N7

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	N	0.38	0/575	0.61	0/777
2	O	0.30	0/1152	0.44	0/1772
3	P	0.32	0/1169	0.47	0/1803
4	G	0.47	0/1791	0.57	0/2431
4	H	0.42	0/1688	0.60	2/2289 (0.1%)
4	M	0.14	0/579	0.37	0/784
5	I	0.48	0/10677	0.55	0/14406
6	J	0.48	1/9251 (0.0%)	0.57	2/12485 (0.0%)
7	K	0.34	0/579	0.50	0/779
8	L	0.28	0/4552	0.48	2/6130 (0.0%)
All	All	0.43	1/32013 (0.0%)	0.54	6/43656 (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
1	N	0	1
5	I	0	3
6	J	0	2
8	L	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	432	LEU	CA-C	-5.67	1.44	1.52

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	L	569	THR	CA-C-N	6.63	133.63	121.70
8	L	569	THR	C-N-CA	6.63	133.63	121.70
4	H	7	GLU	CA-C-N	-6.10	114.21	121.90
4	H	7	GLU	C-N-CA	-6.10	114.21	121.90
6	J	707	ILE	CA-C-N	5.53	131.66	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	254	ASP	Peptide
5	I	855	PRO	Peptide
5	I	857	VAL	Peptide
6	J	707	ILE	Peptide
1	N	33	PRO	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	566	0	552	30	0
2	O	1026	0	562	72	0
3	P	1045	0	579	57	0
4	G	1769	0	1789	137	0
4	H	1669	0	1698	132	0
4	M	572	0	602	88	0
5	I	10512	0	10521	787	0
6	J	9109	0	9308	653	0
7	K	577	0	588	39	0
8	L	4495	0	4517	443	0
9	J	2	0	0	0	0
9	N	1	0	0	0	0
10	I	27	39	37	6	0
10	J	54	78	75	12	0
10	N	27	39	37	5	0
11	J	1	0	0	0	0
All	All	31452	156	30865	2259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 36.

The worst 5 of 2259 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)
10:N:102:1N7:C19	10:N:102:1N7:C3	1.82	1.56
10:I:1401:1N7:C3	10:I:1401:1N7:C19	1.82	1.56
5:I:237:LEU:CD1	5:I:292:ILE:CD1	1.82	1.55
10:J:1505:1N7:C3	10:J:1505:1N7:C19	1.82	1.54
10:J:1504:1N7:C19	10:J:1504:1N7:C3	1.82	1.54

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	70/72 (97%)	60 (86%)	9 (13%)	1 (1%)	9	36
4	G	230/329 (70%)	210 (91%)	19 (8%)	1 (0%)	30	65
4	H	214/329 (65%)	184 (86%)	29 (14%)	1 (0%)	24	60
4	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
5	I	1331/1342 (99%)	1218 (92%)	107 (8%)	6 (0%)	24	60
6	J	1160/1430 (81%)	1065 (92%)	94 (8%)	1 (0%)	48	80
7	K	70/91 (77%)	65 (93%)	5 (7%)	0	100	100
8	L	552/616 (90%)	520 (94%)	31 (6%)	1 (0%)	43	76
All	All	3698/4538 (82%)	3390 (92%)	297 (8%)	11 (0%)	37	70

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	252	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	I	254	ASP
5	I	856	ASN
8	L	504	PRO
1	N	34	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	N	60/61 (98%)	57 (95%)	3 (5%)	22 56
4	G	192/286 (67%)	152 (79%)	40 (21%)	1 7
4	H	184/286 (64%)	155 (84%)	29 (16%)	2 13
4	M	65/286 (23%)	63 (97%)	2 (3%)	35 68
5	I	1145/1157 (99%)	980 (86%)	165 (14%)	3 15
6	J	976/1189 (82%)	853 (87%)	123 (13%)	4 20
7	K	63/75 (84%)	57 (90%)	6 (10%)	8 31
8	L	491/543 (90%)	442 (90%)	49 (10%)	7 29
All	All	3176/3883 (82%)	2759 (87%)	417 (13%)	6 19

5 of 417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	I	1296	ASP
6	J	468	VAL
8	L	498	LEU
5	I	1336	ASN
6	J	195	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
6	J	229	GLN

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Mol	Chain	Res	Type
6	J	665	GLN
8	L	338	HIS
6	J	274	ASN
6	J	450	HIS

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1N7	N	102	-	30,30,46	5.04	15 (50%)	47,48,72	2.27	19 (40%)
10	1N7	J	1505	-	30,30,46	4.97	14 (46%)	47,48,72	2.32	16 (34%)
10	1N7	J	1504	-	30,30,46	5.01	15 (50%)	47,48,72	2.52	14 (29%)
10	1N7	I	1401	-	30,30,46	4.96	15 (50%)	47,48,72	2.44	14 (29%)

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	1N7	N	102	-	-	1/7/72/92	0/4/4/4
10	1N7	J	1505	-	-	2/7/72/92	0/4/4/4
10	1N7	J	1504	-	-	4/7/72/92	0/4/4/4
10	1N7	I	1401	-	-	2/7/72/92	0/4/4/4

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1505	1N7	C3-C19	17.97	1.82	1.53
10	I	1401	1N7	C3-C19	17.79	1.82	1.53
10	N	102	1N7	C3-C19	17.76	1.82	1.53
10	J	1504	1N7	C3-C19	17.70	1.82	1.53
10	N	102	1N7	C3-C4	11.87	1.72	1.53

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	1504	1N7	C9-C5-C4	-9.29	109.31	117.67
10	I	1401	1N7	C9-C5-C4	-7.26	111.13	117.67
10	J	1505	1N7	C9-C5-C4	-5.48	112.74	117.67
10	J	1505	1N7	C7-C6-C18	-5.44	110.89	118.36
10	N	102	1N7	C9-C5-C6	5.27	105.40	100.11

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

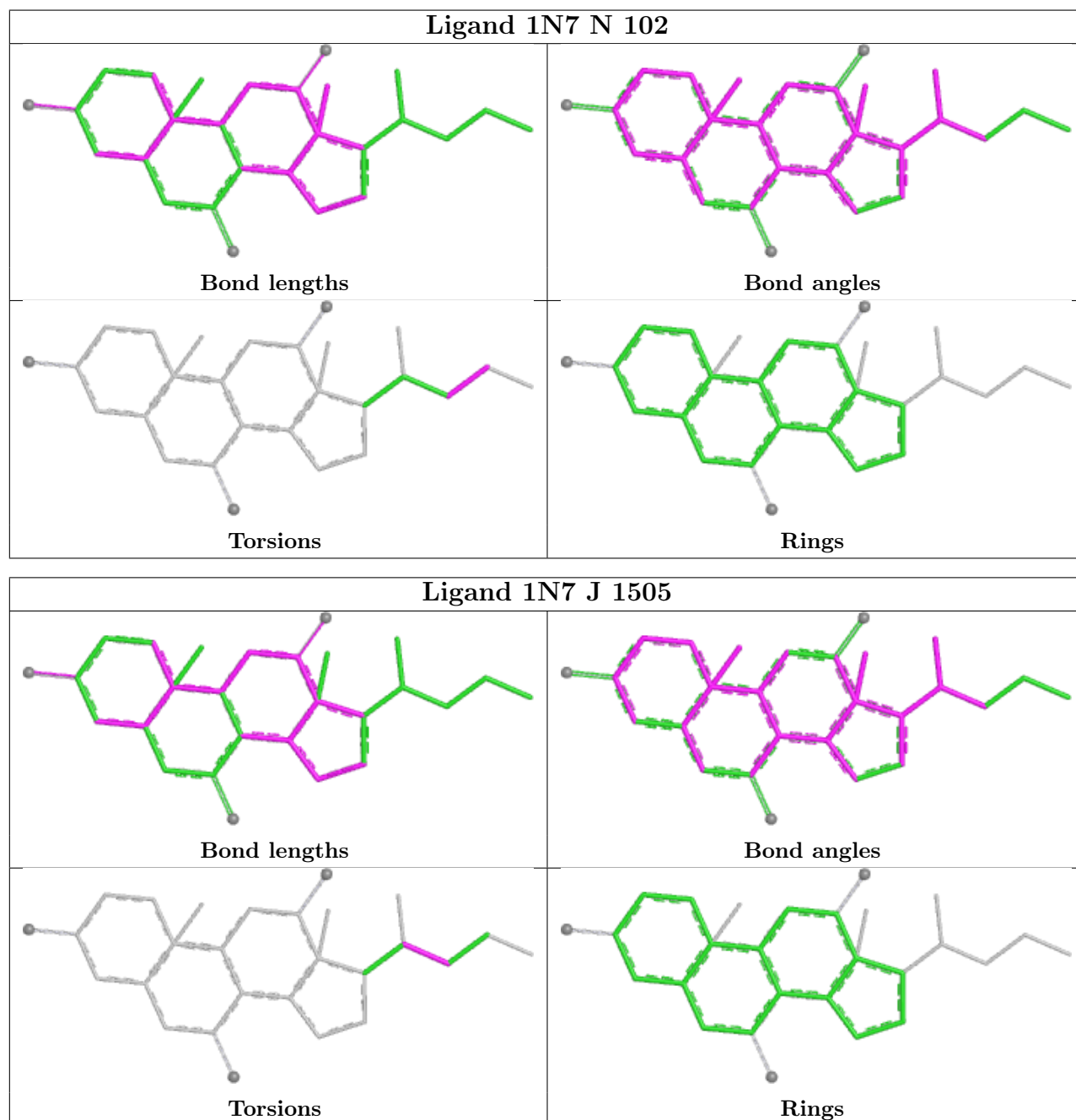
Mol	Chain	Res	Type	Atoms
10	J	1504	1N7	C21-C20-C9-C5
10	J	1504	1N7	C21-C20-C9-C8
10	J	1504	1N7	C22-C20-C9-C8
10	J	1504	1N7	C22-C20-C9-C5
10	J	1505	1N7	C9-C20-C22-C23

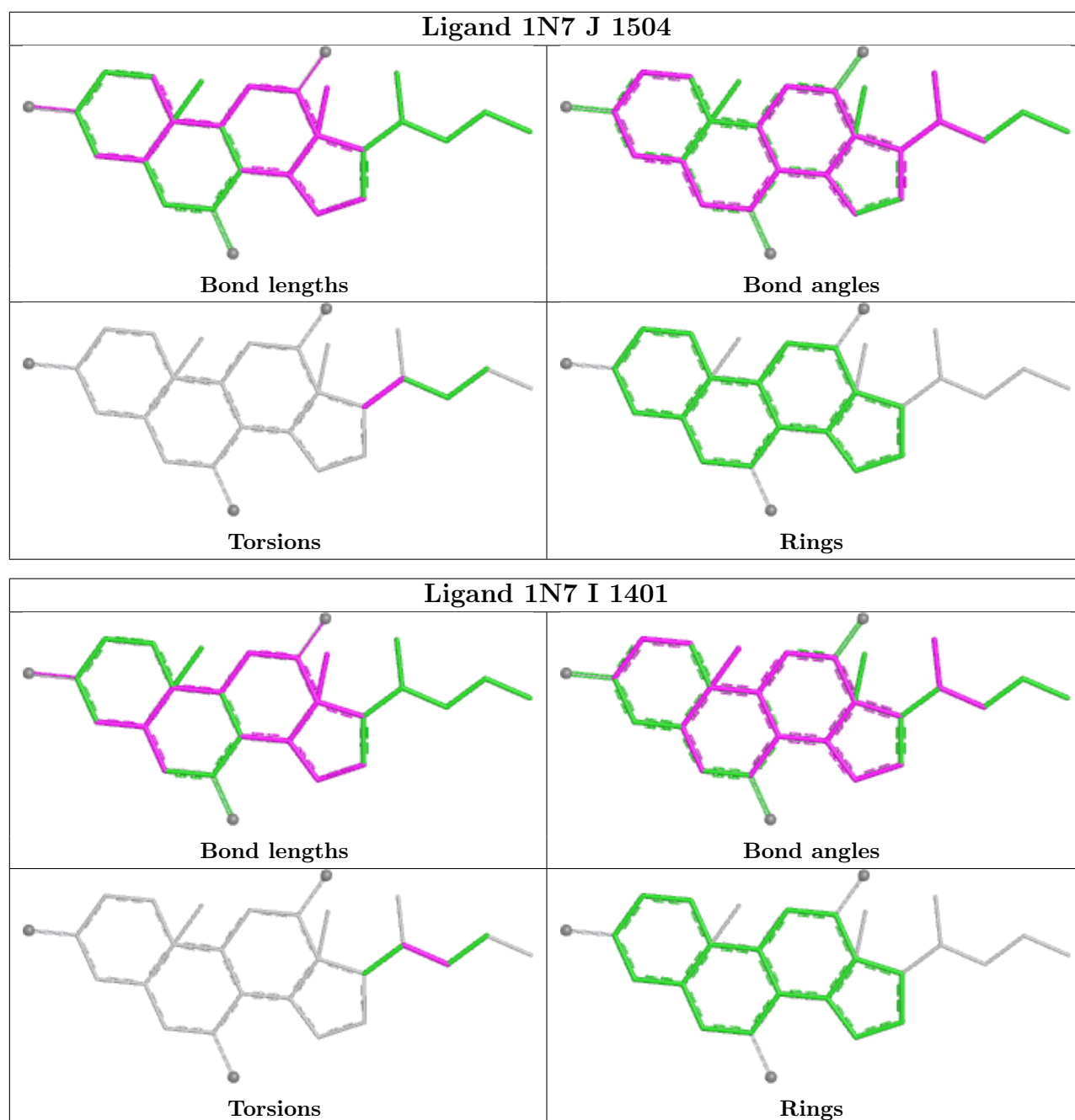
There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	102	1N7	5	0
10	J	1505	1N7	7	0
10	J	1504	1N7	6	0
10	I	1401	1N7	6	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.

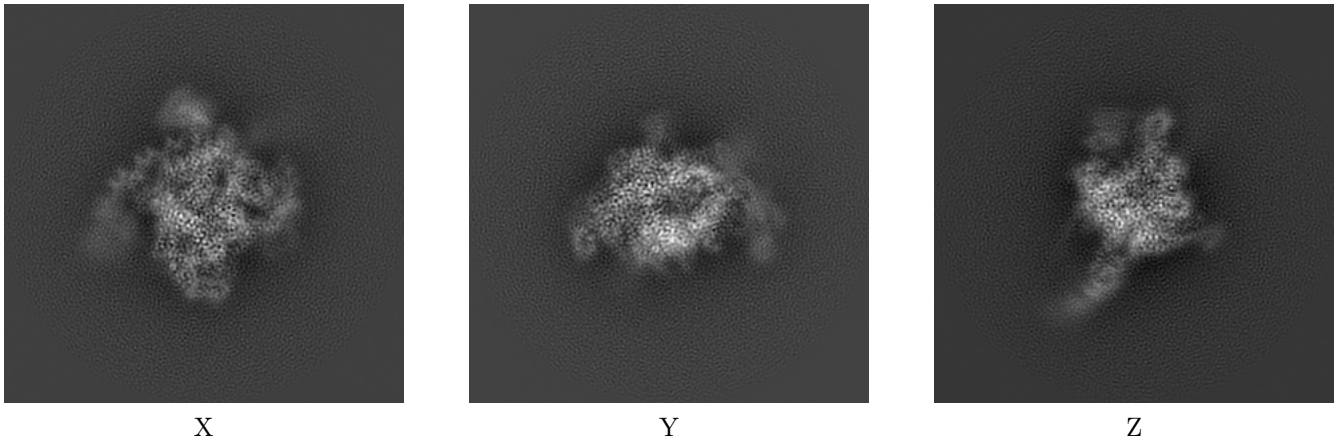
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20463. 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](#)

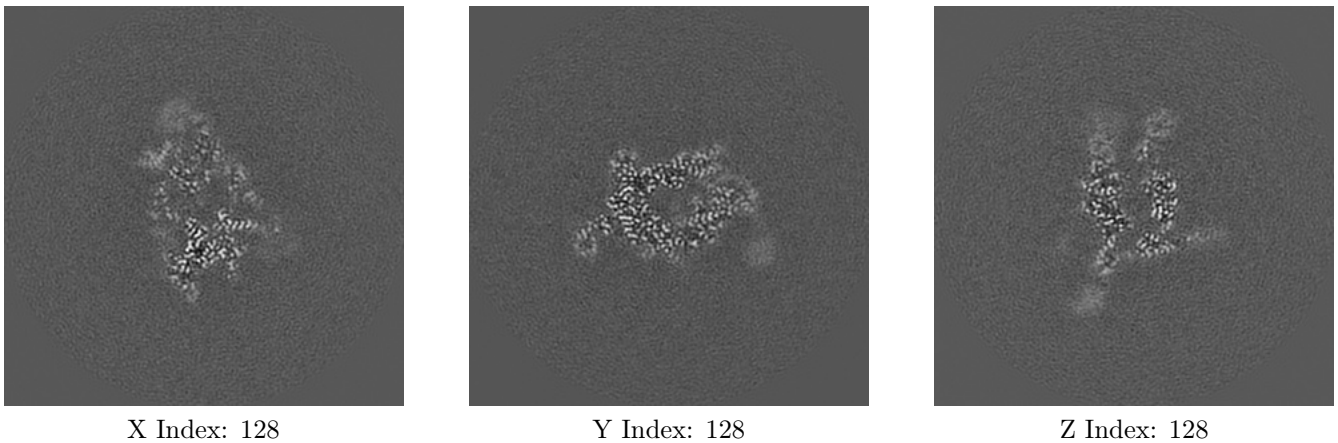
6.1.1 Primary map



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

6.2 Central slices [i](#)

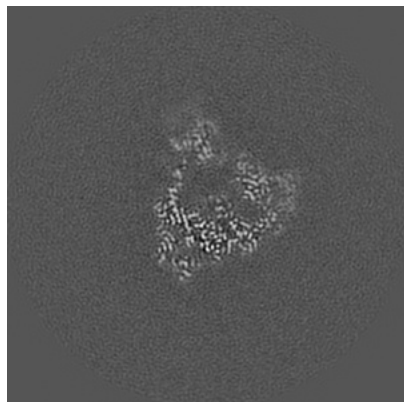
6.2.1 Primary map



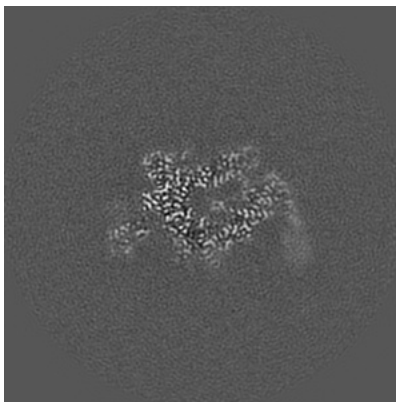
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

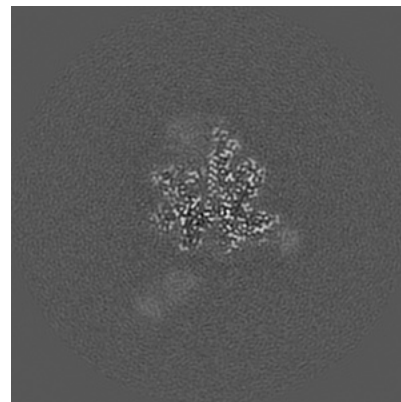
6.3.1 Primary map



X Index: 138



Y Index: 124

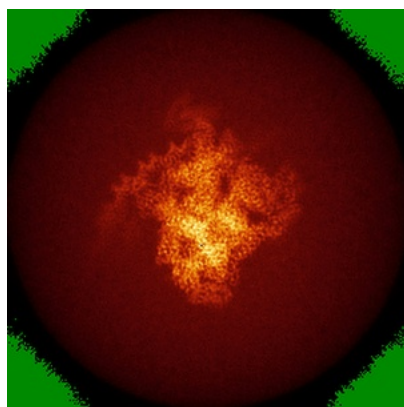


Z Index: 115

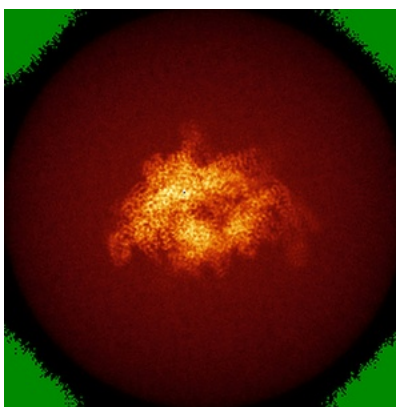
The images above show the largest variance slices of the map in three orthogonal directions.

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

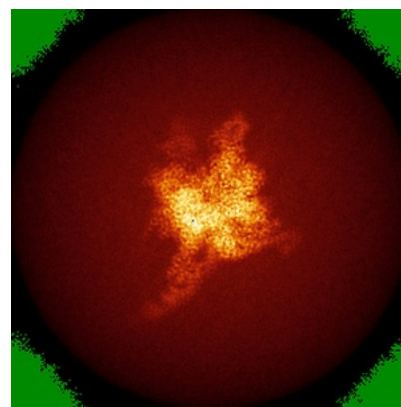
6.4.1 Primary map



X



Y

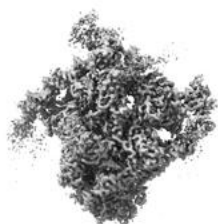


Z

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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

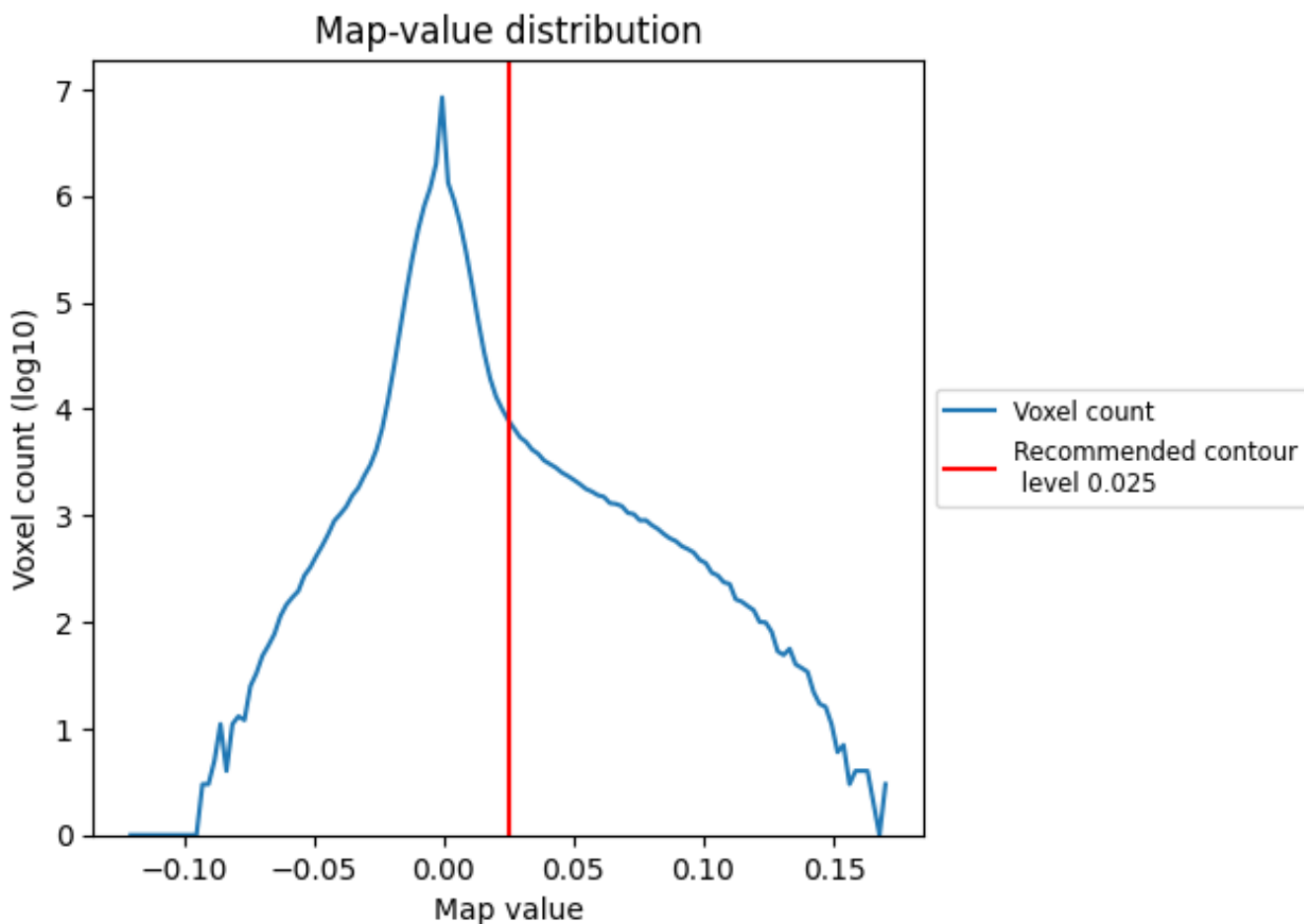
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

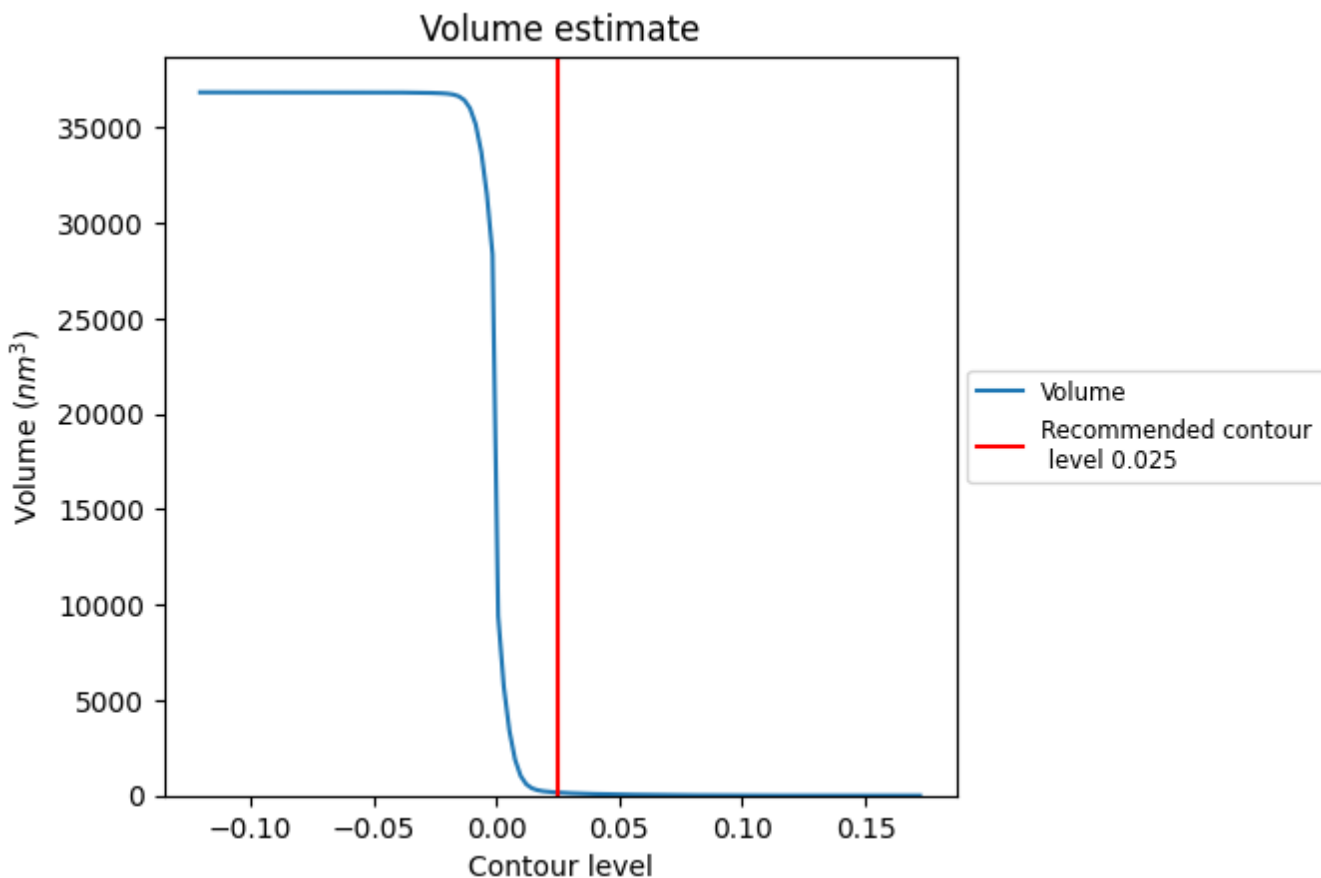
This section contains the results of statistical analysis of the map.

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.

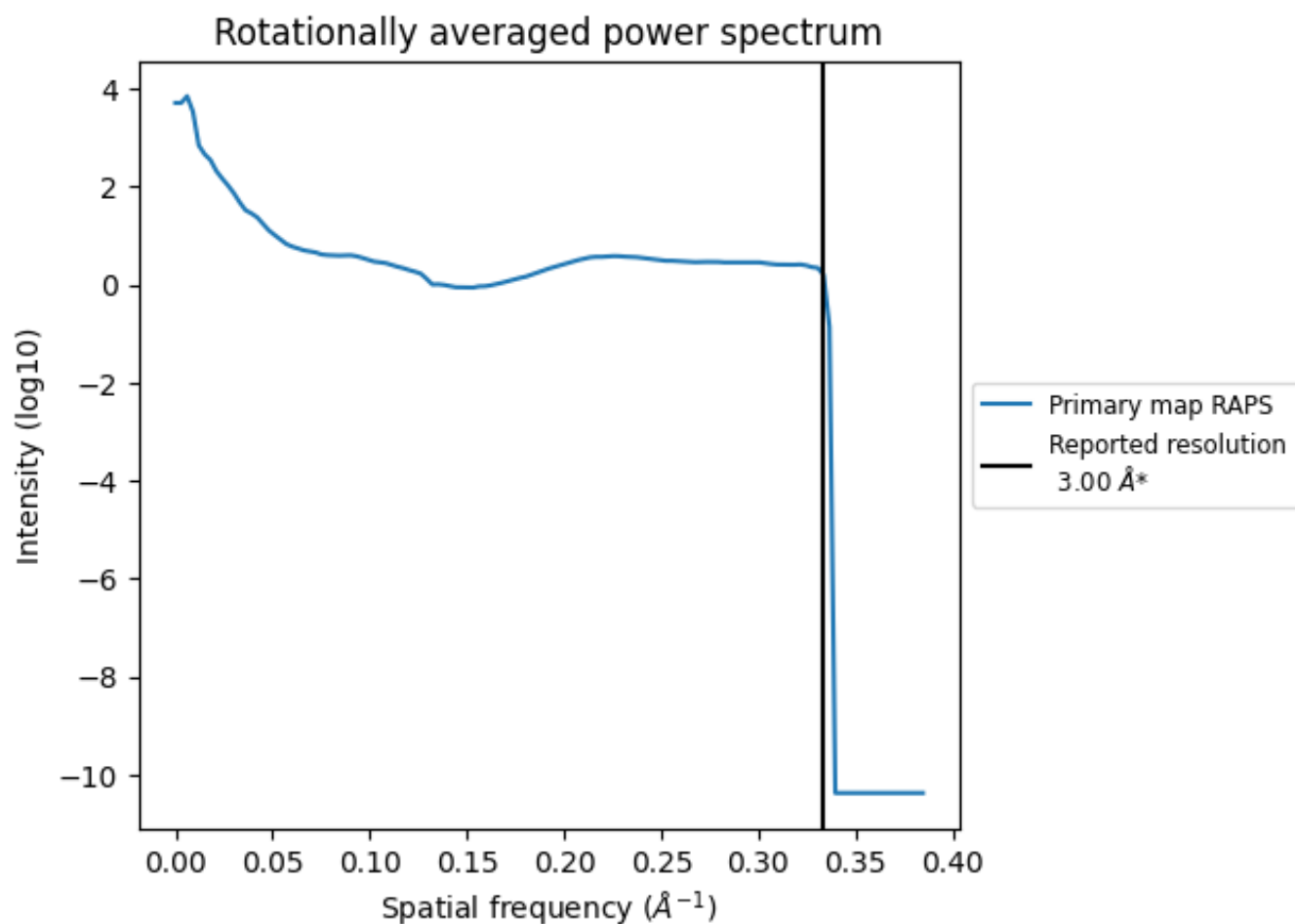
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 143 kDa.

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

7.3 Rotationally averaged power spectrum [\(i\)](#)

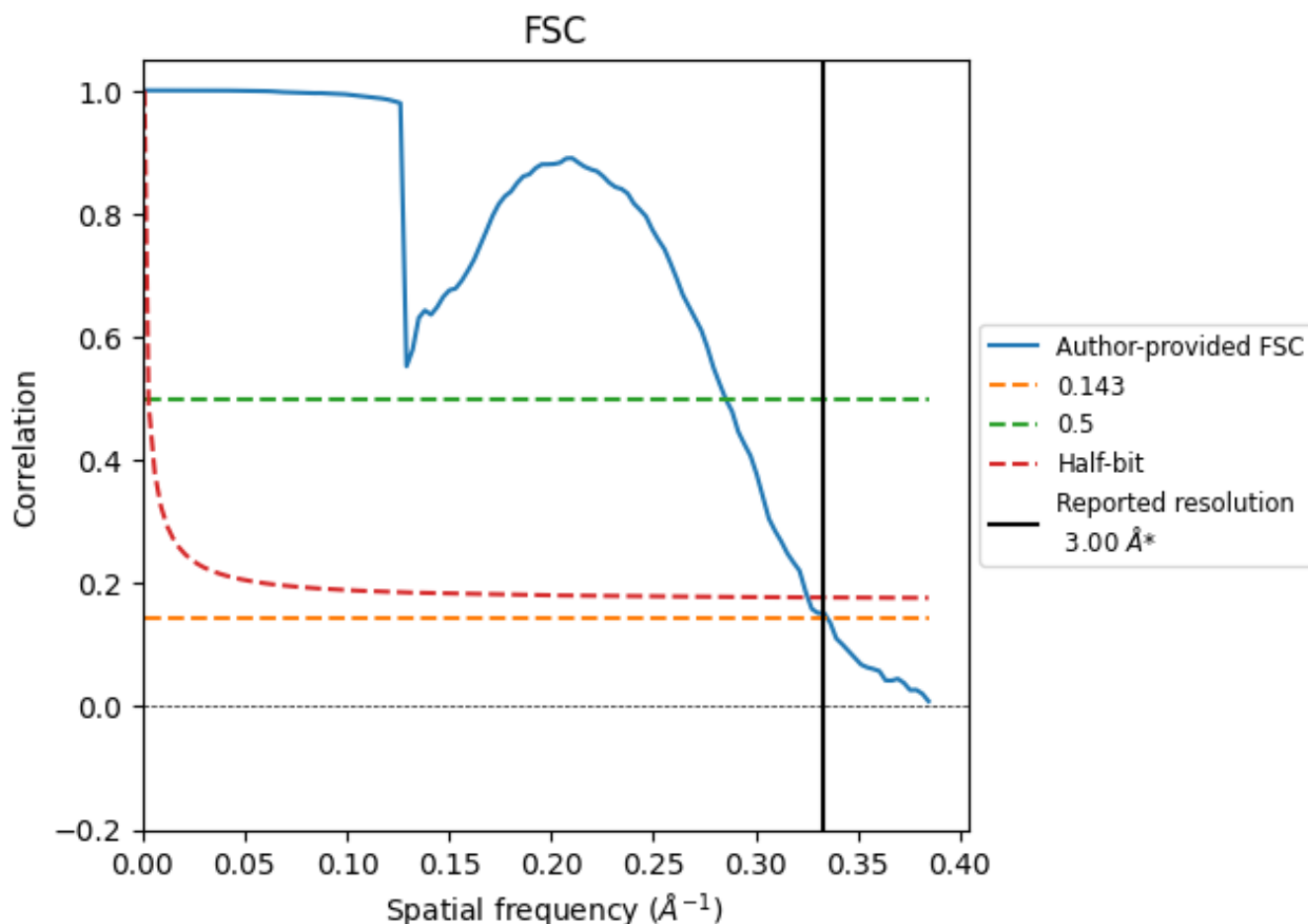


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8.2 Resolution estimates [i](#)

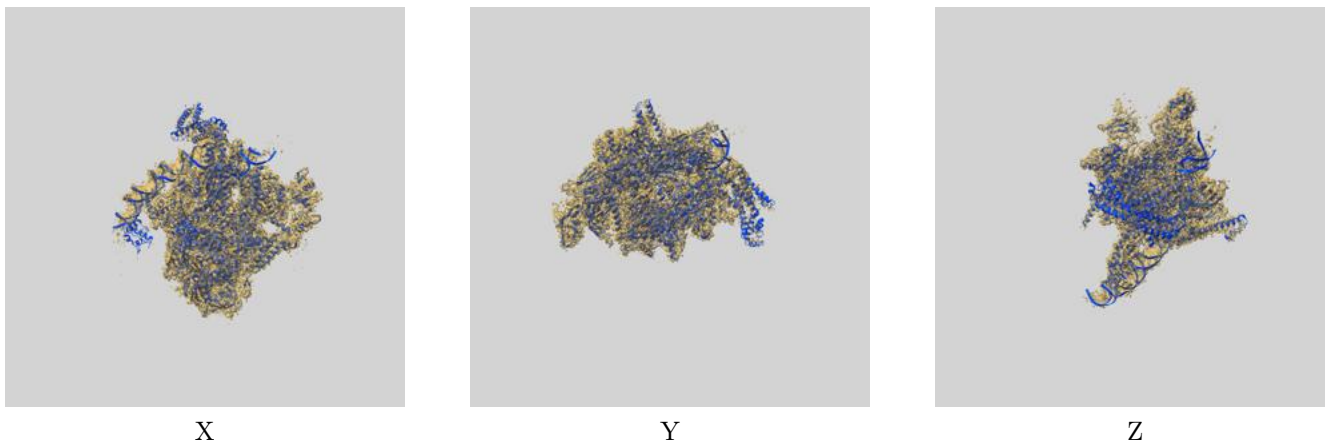
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.98	3.51	3.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

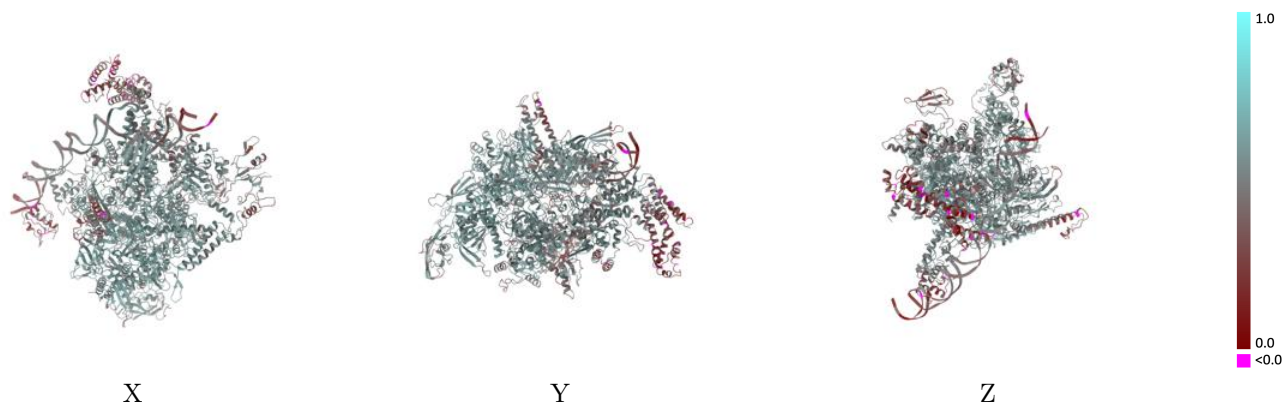
This section contains information regarding the fit between EMDB map EMD-20463 and PDB model 6PST. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



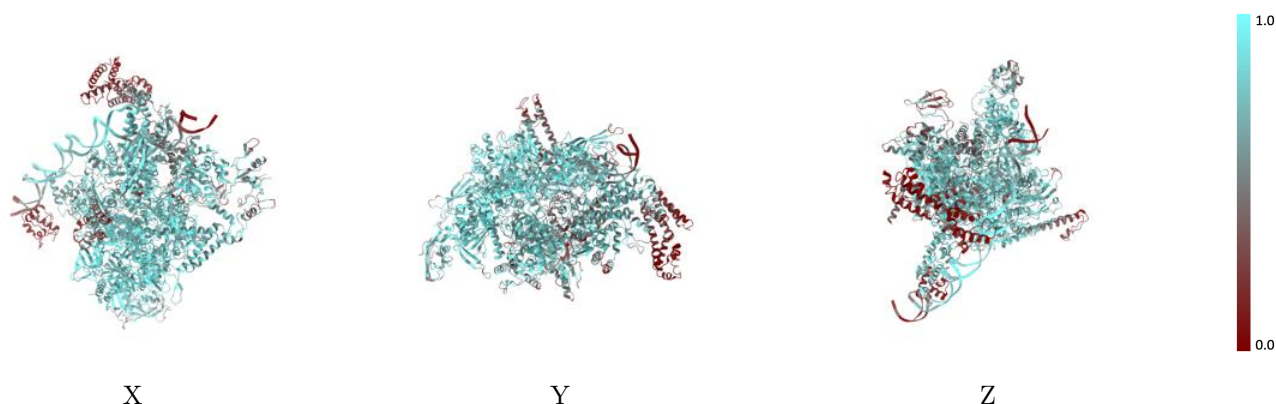
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



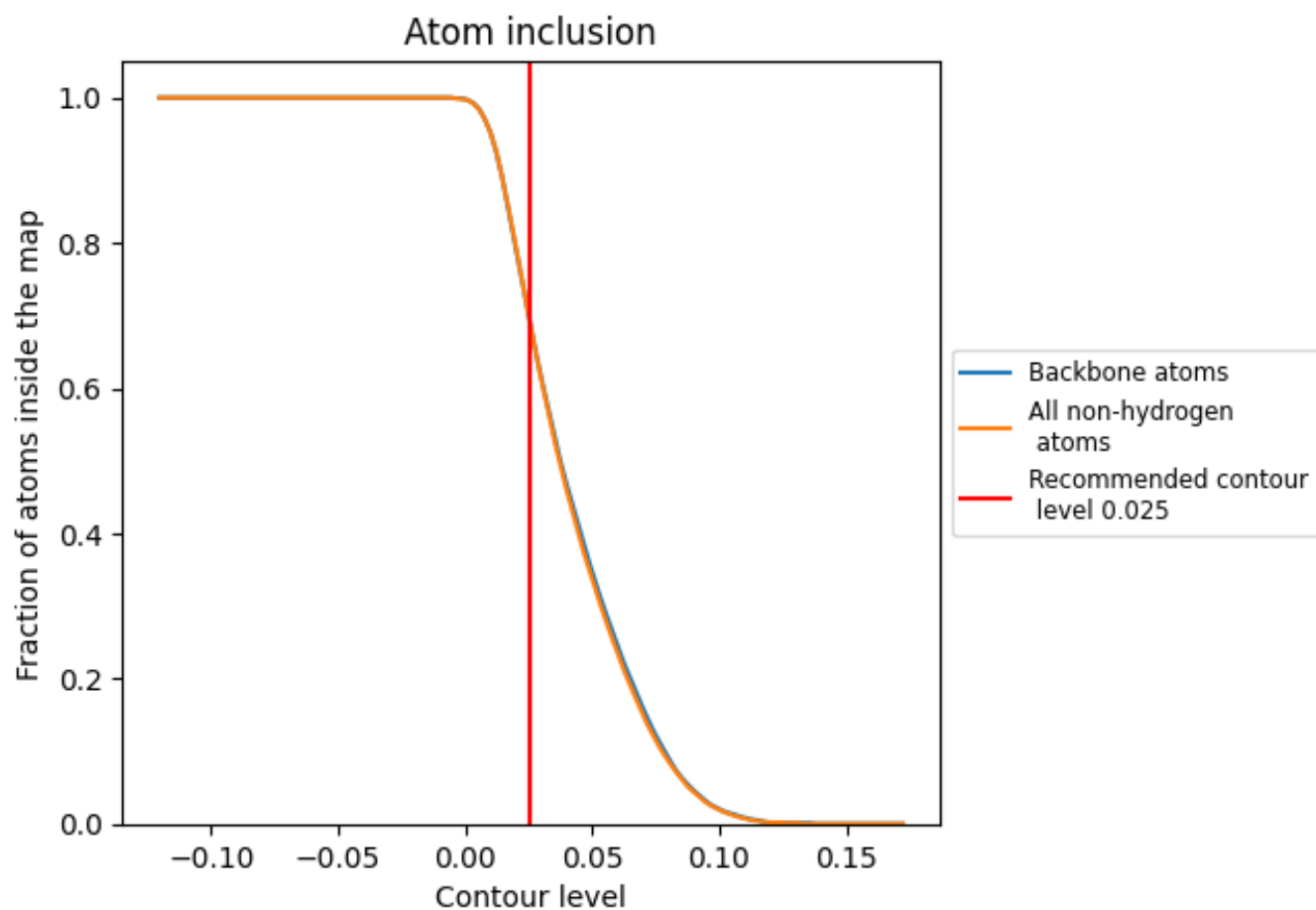
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).























9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6980	 0.5140
G	 0.8030	 0.5640
H	 0.7580	 0.5390
I	 0.7720	 0.5510
J	 0.7720	 0.5470
K	 0.6540	 0.5560
L	 0.4760	 0.4160
M	 0.0390	 0.2480
N	 0.7560	 0.5270
O	 0.6370	 0.4080
P	 0.6060	 0.3850

