



wwPDB EM Validation Summary Report ⓘ

Nov 27, 2022 – 05:42 PM EST

PDB ID : 7KHC
EMDB ID : EMD-21879
Title : Escherichia coli RNA polymerase and rrnBP1 promoter closed complex
Authors : Shin, Y.; Qayyum, M.Z.; Murakami, K.S.
Deposited on : 2020-10-20
Resolution : 4.14 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

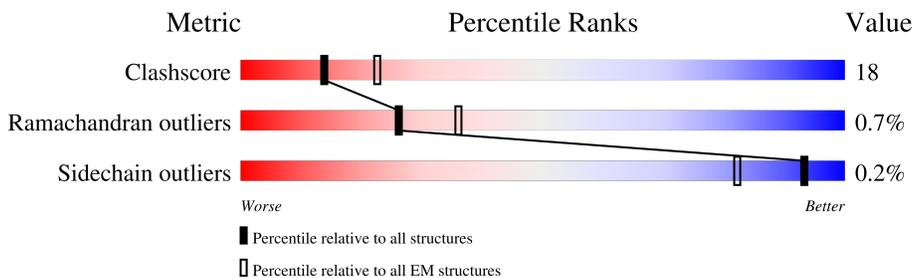
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.14 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



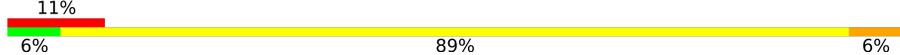
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	329	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">17%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 61% 32% • 6% </div> </div>
1	B	329	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">22%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 58% 38% • </div> </div>
2	C	1342	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">•</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 66% 33% • </div> </div>
3	D	1407	<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);"> 61% 34% • 5% </div> </div>
4	E	91	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">21%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 46% 36% • 16% </div> </div>
5	F	613	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">18%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 37% 35% • 27% </div> </div>
6	X	63	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">21%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 43% 51% 6% </div> </div>
7	Y	63	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">19%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red, orange, yellow, green, grey);"> 54% 43% • </div> </div>

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Mol	Chain	Length	Quality of chain
8	O	18	 39% 56% 6%
9	P	18	 11% 6% 89% 6%

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 33509 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
			Total	C	N	O	S		
1	A	309	Total	C	N	O	S	0	0
			2407	1504	424	472	7		
1	B	316	Total	C	N	O	S	0	0
			2472	1545	436	483	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	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
			Total	C	N	O	S		
3	D	1342	Total	C	N	O	S	0	0
			10396	6530	1852	1965	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
			Total	C	N	O	S		
5	F	447	Total	C	N	O	S	0	0
			3640	2283	648	689	20		

- Molecule 6 is DNA/RNA hybrid called DNA/RNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	X	63	1278	613	224	378	63	0	0

- Molecule 7 is a DNA chain called DNA (63-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	Y	63	1305	622	242	378	63	0	0

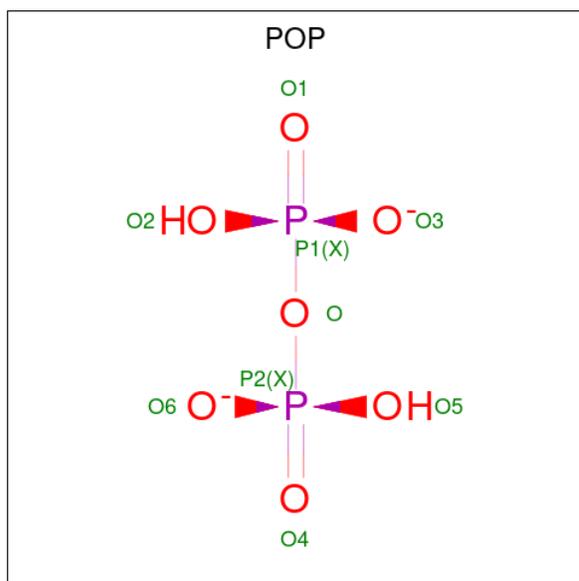
- Molecule 8 is a DNA chain called DNA (18 MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	O	18	370	175	71	106	18	0	0

- Molecule 9 is a DNA chain called DNA (18 MER).

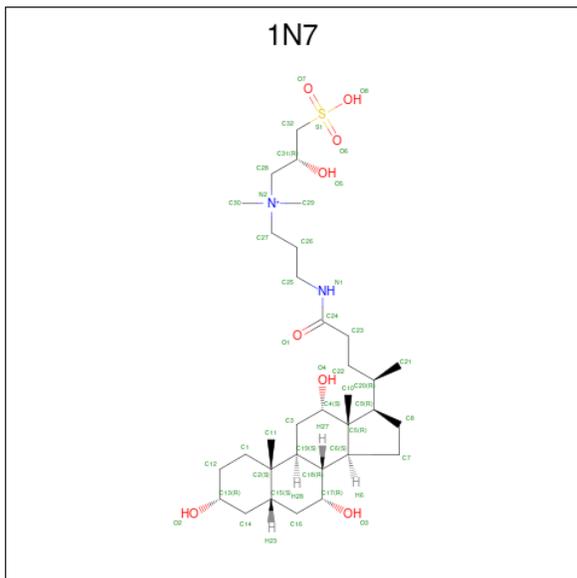
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	P	18	368	175	65	110	18	0	0

- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
10	C	1	9	7	2	0

- Molecule 11 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	C	1	Total	C	N	O	S	0
			86	64	4	16	2	
11	C	1	Total	C	N	O	S	0
			86	64	4	16	2	

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

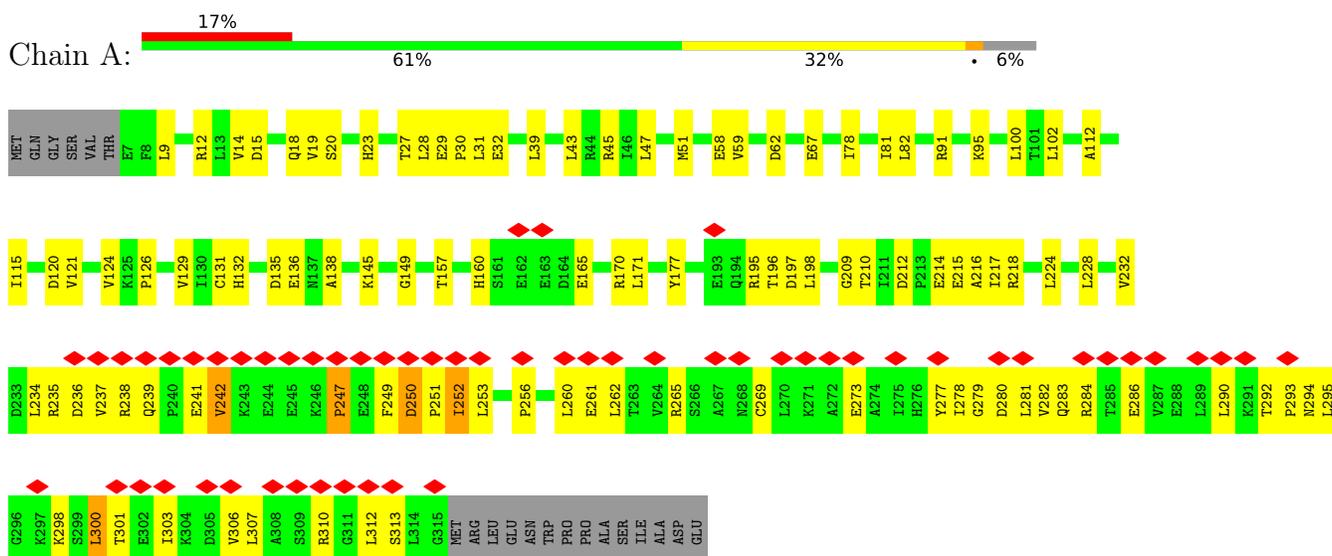
- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

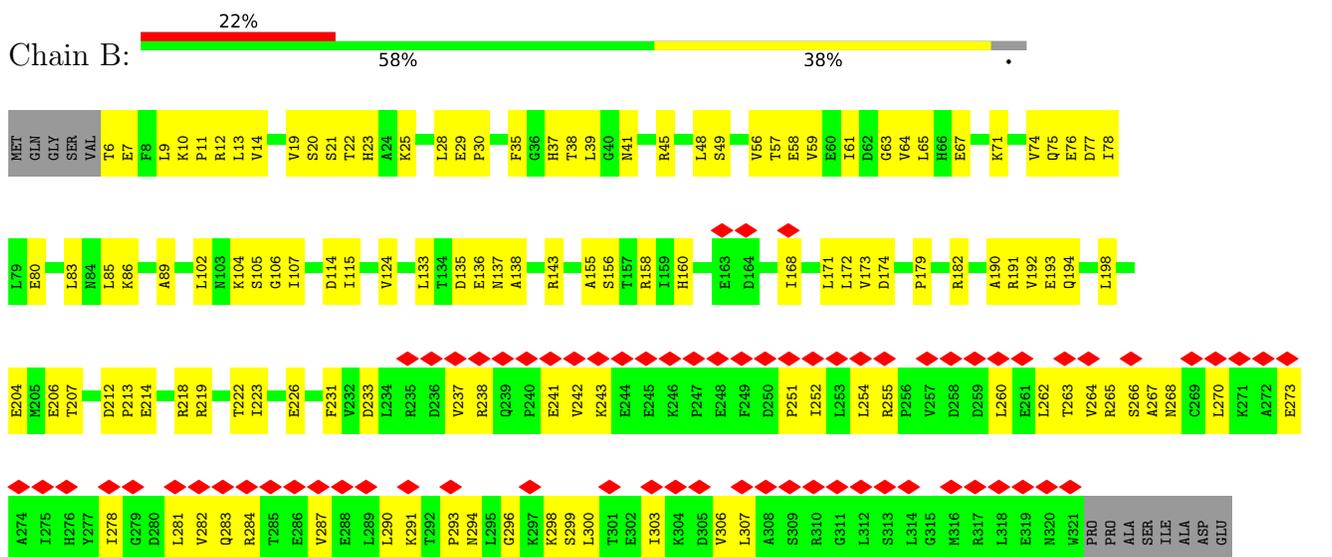
3 Residue-property plots

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.

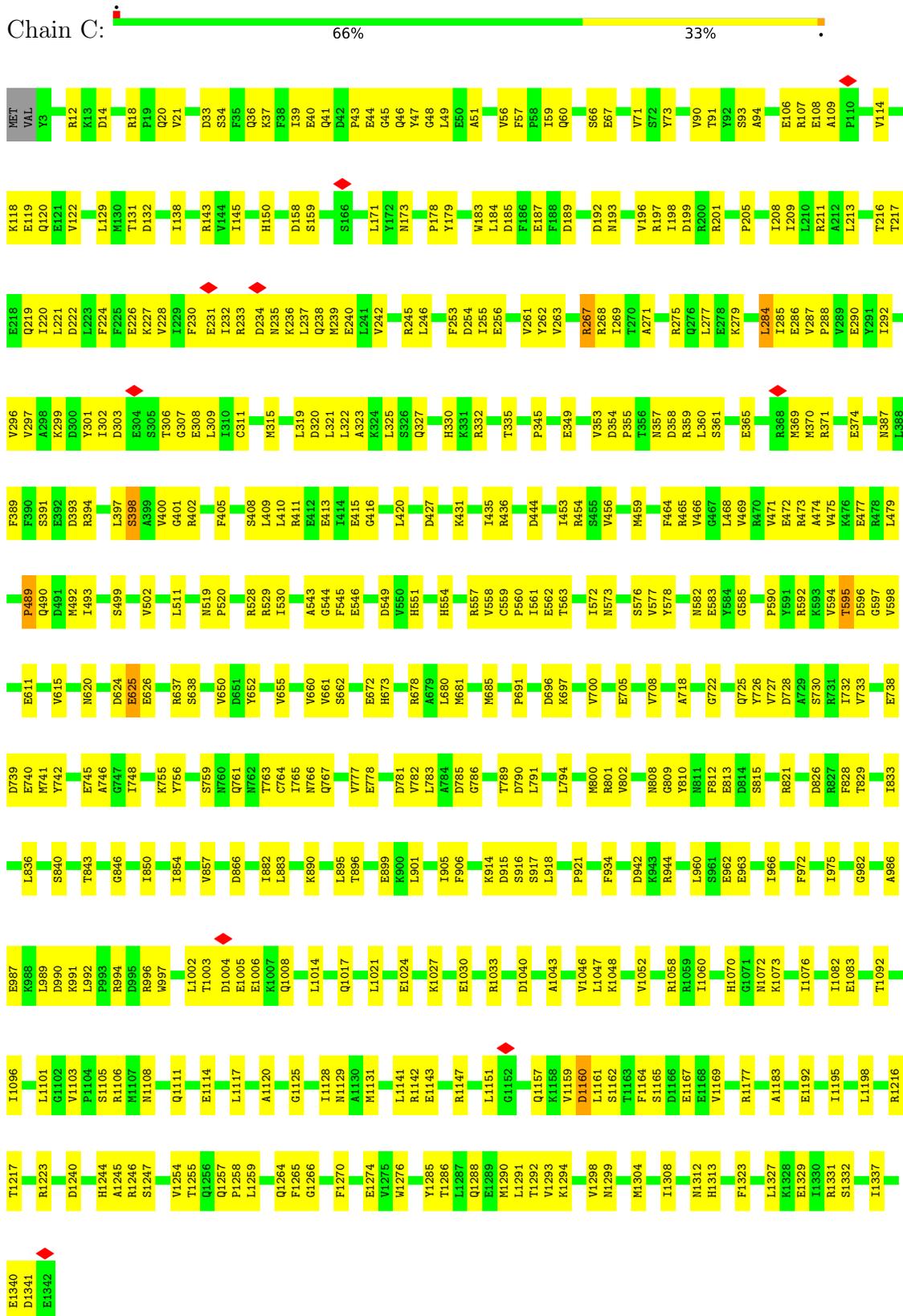
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha



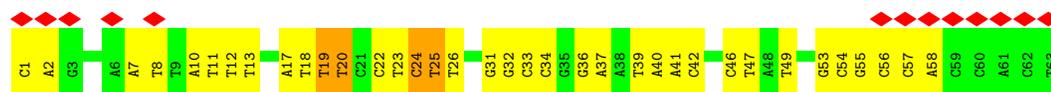
- Molecule 2: DNA-directed RNA polymerase subunit beta



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



GLN	E1281	K1172	K1104	D1039	N861	E785	E688	E534	V407	V292	M180	MET
VAL	Y1282	R1173	A1105	M1040	L864	V769	Q665	R535	V408	R293	S191	LYS
THR	K1286	R1174	Q108	I1041	R883	Y966	Q666	L536	W409	R294	E197	ASP
ALA	L1175	L1176	L109	D1042	S884	Q771	T674	L536	D410	E295	E197	LEU
GLU	V1298	V1177	L1109	G1043	S884	Q772	E677	H545	I411	M298	L201	LEU
ASP	G1299	T1178	E1110	Q1044	V885	F773	R677	V548	I412	E301	E204	PHE
ALA	A1300	P1179	E1110	Q1045	F892	I774	Y679	K549	D413	A302	E204	LEU
SER	T1301	D1181	V1113	I1046	F892	T776	N680	V550	E414	V303	E204	LEU
LEU	T1310	D1181	Q1114	T1047	C895	H777	K681	R551	I416	D304	S210	LEU
ALA	S1313	D1184	I1115	Q1049	C898	R780	I683	K557	E418	R312	R214	ALA
LEU	L1314	M1189	S1116	I1050	D902	D785	D684	D568	M424	G343	K215	LEU
LEU	A1315	I1190	S1117	D1051	L903	K789	I685	E562	R425	R314	K216	LEU
ASN	E1316	P1191	D1119	E1052	L903	R978	D691	L563	A315	A315	L217	ASN
ALA	E1317	M1197	T1120	L1053	I909	T980	R692	T567	I316	T317	T218	ALA
GLY	E1318	V1198	L1421	L1054	N910	V693	V693	T573	A426	P427	K219	GLY
LEU	A1323	V1204	A1122	T1054	K911	S694	S694	I582	T428	R322	I221	LEU
GLY	S1324	R1204	R1123	G1055	G912	K695	K695	K570	P439	P323	K222	GLY
GLY	F1325	R1206	Q1126	L984	E925	R798	R798	D571	M466	K334	I221	GLY
SER	Q1326	G1207	GLU	L985	D926	E704	E704	T572	M466	K334	I221	SER
ASN	E1327	D1208	SER	D986	P926	T705	T705	T573	E443	K325	E225	ASN
GLY	V1331	P1215	GLY	E987	G927	D805	D805	I582	E443	S326	E225	GLY
GLY	S1334	A1215	GLY	F988	R807	T706	T706	I582	Q448	D329	V228	GLY
GLY	R1341	E1215	THR	G989	I918	T707	T707	I582	C454	M330	K233	GLY
GLY	D1342	A1216	LYS	Y999	E925	R709	R709	G556	M466	P234	K233	GLY
GLY	E1343	D1219	ASP	G1000	T810	D710	D710	G556	M466	E235	K233	GLY
GLY	L1344	I1220	ILE	V1002	C814	G711	G711	L587	M466	E235	K233	GLY
GLY	G1345	V1226	G1135	A1065	D805	T712	T712	P588	T473	R337	R133	GLY
GLY	G1346	H1227	G1136	A1065	D806	E713	E713	Y589	T474	F388	R133	GLY
GLY	V1331	V1228	G1137	L1003	I820	E475	E475	S590	A476	R339	R133	GLY
GLY	K1348	A1228	L1138	L1003	M821	I591	I591	V592	A476	Q340	E142	GLY
GLY	E1349	V1229	L1347	G1006	M822	K715	K715	V592	A476	Q340	E142	GLY
GLY	M1350	T1230	R1140	G1006	N720	N720	N720	V592	A476	Q340	E142	GLY
GLY	V1351	E1236	D1143	E1009	V825	M725	M725	V592	A476	Q340	E142	GLY
GLY	V1353	D1289	L1144	A1069	I826	I826	I826	V592	A476	Q340	E142	GLY
GLY	L1356	R1242	L1144	G1071	V831	R731	R731	V592	A476	Q340	E142	GLY
GLY	F1357	Q1244	L1144	A1072	K832	Q736	Q736	V592	A476	Q340	E142	GLY
GLY	P1358	Q1244	L1144	L1016	E833	G736	G736	V592	A476	Q340	E142	GLY
GLY	D1368	H1252	L1144	L1017	P834	R738	R738	V592	A476	Q340	E142	GLY
GLY	R1371	H1253	L1144	A1018	D837	Q739	Q739	V592	A476	Q340	E142	GLY
GLY	A1374	V1255	L1144	A1019	R838	L740	L740	V592	A476	Q340	E142	GLY
GLY	A1375	V1257	L1144	A1019	T844	G742	G742	V592	A476	Q340	E142	GLY
GLY	G1376	Q1289	L1144	A1019	T844	M743	M743	V592	A476	Q340	E142	GLY
GLY	GLU	H1252	L1144	P1022	V848	A741	A741	V592	A476	Q340	E142	GLY
ALA	PRD	I1253	L1144	H1023	L849	K749	K749	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
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ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1257	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	Q1244	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	H1252	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	I1253	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1254	L1144	H1023	K850	P750	P750	V592	A476	Q340	E142	ALA
ALA	PRD	V1255	L1144	H1023								



- Molecule 7: DNA (63-MER)



- Molecule 8: DNA (18 MER)



- Molecule 9: DNA (18 MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67187	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	0.075	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.013	Depositor
Map size (\AA)	388.80002, 388.80002, 388.80002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.08, 1.08, 1.08	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, POP, ZN, 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	A	0.29	0/2437	0.62	1/3301 (0.0%)
1	B	0.28	0/2504	0.63	0/3392
2	C	0.34	1/10739 (0.0%)	0.60	4/14489 (0.0%)
3	D	0.31	0/10553	0.60	1/14253 (0.0%)
4	E	0.37	1/607 (0.2%)	0.68	0/817
5	F	0.29	0/3689	0.63	0/4958
6	X	0.75	0/1430	1.17	7/2201 (0.3%)
7	Y	0.76	0/1466	1.14	3/2264 (0.1%)
8	O	0.81	0/415	1.14	1/638 (0.2%)
9	P	0.84	0/411	1.19	1/632 (0.2%)
All	All	0.39	2/34251 (0.0%)	0.70	18/46945 (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	3
3	D	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	489	PRO	CG-CD	-7.57	1.25	1.50
4	E	68	GLU	CG-CD	-5.59	1.43	1.51

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	489	PRO	N-CD-CG	-9.01	89.69	103.20
3	D	1189	MET	CB-CG-SD	7.67	135.41	112.40
6	X	24	DC	O4'-C1'-N1	7.64	113.35	108.00
7	Y	51	DT	O4'-C1'-N1	6.71	112.69	108.00
2	C	489	PRO	CA-N-CD	-6.48	102.43	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	198	ILE	Peptide
2	C	236	LYS	Peptide
2	C	595	THR	Peptide
3	D	1184	ASP	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	A	2407	0	2463	83	0
1	B	2472	0	2525	98	0
2	C	10570	0	10582	359	0
3	D	10396	0	10583	368	0
4	E	605	0	612	29	0
5	F	3640	0	3705	209	0
6	X	1278	0	713	30	0
7	Y	1305	0	713	31	0
8	O	370	0	202	10	0
9	P	368	0	204	21	0
10	C	9	0	0	1	0
11	C	86	0	116	8	0
12	D	1	0	0	0	0
13	D	2	0	0	0	0
All	All	33509	0	32418	1160	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 18.

The worst 5 of 1160 close contacts within the same asymmetric unit are listed below, sorted by

their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1142:ARG:NH2	2:C:1165:SER:O	1.87	1.08
3:D:1344:LEU:O	3:D:1346:GLY:N	1.97	0.97
3:D:210:SER:OG	9:P:7:DG:OP1	1.83	0.97
2:C:905:ILE:O	5:F:599:ARG:NH1	1.99	0.95
1:B:296:GLY:N	6:X:11:DT:OP1	2.00	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/329 (93%)	255 (83%)	47 (15%)	5 (2%)	9	44
1	B	314/329 (95%)	271 (86%)	41 (13%)	2 (1%)	25	64
2	C	1338/1342 (100%)	1227 (92%)	105 (8%)	6 (0%)	34	71
3	D	1336/1407 (95%)	1210 (91%)	115 (9%)	11 (1%)	19	59
4	E	74/91 (81%)	69 (93%)	5 (7%)	0	100	100
5	F	441/613 (72%)	397 (90%)	41 (9%)	3 (1%)	22	61
All	All	3810/4111 (93%)	3429 (90%)	354 (9%)	27 (1%)	26	61

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	GLU
3	D	338	PHE
3	D	1345	ARG
5	F	139	GLU
5	F	356	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/286 (94%)	268 (100%)	1 (0%)	91	94
1	B	276/286 (96%)	276 (100%)	0	100	100
2	C	1155/1157 (100%)	1153 (100%)	2 (0%)	93	96
3	D	1114/1168 (95%)	1112 (100%)	2 (0%)	93	96
4	E	65/75 (87%)	65 (100%)	0	100	100
5	F	397/540 (74%)	395 (100%)	2 (0%)	88	93
All	All	3276/3512 (93%)	3269 (100%)	7 (0%)	93	96

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	314	ARG
3	D	695	LYS
5	F	364	ARG
5	F	264	LYS
2	C	890	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	41	GLN
3	D	488	ASN
3	D	712	GLN
4	E	73	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	POP	C	1401	-	6,8,8	0.76	0	13,13,13	1.39	1 (7%)
11	1N7	C	1403	-	45,46,46	4.03	19 (42%)	69,72,72	2.00	20 (28%)
11	1N7	C	1402	-	45,46,46	4.10	20 (44%)	69,72,72	2.43	22 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	POP	C	1401	-	-	0/6/6/6	-
11	1N7	C	1403	-	-	6/27/92/92	0/4/4/4
11	1N7	C	1402	-	-	6/27/92/92	0/4/4/4

The worst 5 of 39 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1402	1N7	C3-C4	-12.69	1.31	1.53
11	C	1403	1N7	C3-C4	-12.45	1.32	1.53
11	C	1402	1N7	C5-C9	-11.28	1.36	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	1403	1N7	C5-C9	-10.92	1.36	1.55
11	C	1402	1N7	C3-C19	-9.14	1.38	1.53

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1402	1N7	C5-C6-C18	-8.07	104.43	114.74
11	C	1402	1N7	C5-C9-C20	-7.68	110.33	119.50
11	C	1403	1N7	C5-C6-C18	-6.29	106.70	114.74
11	C	1403	1N7	C6-C5-C4	-5.39	102.38	107.40
11	C	1402	1N7	C16-C17-C18	-5.33	105.79	111.48

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

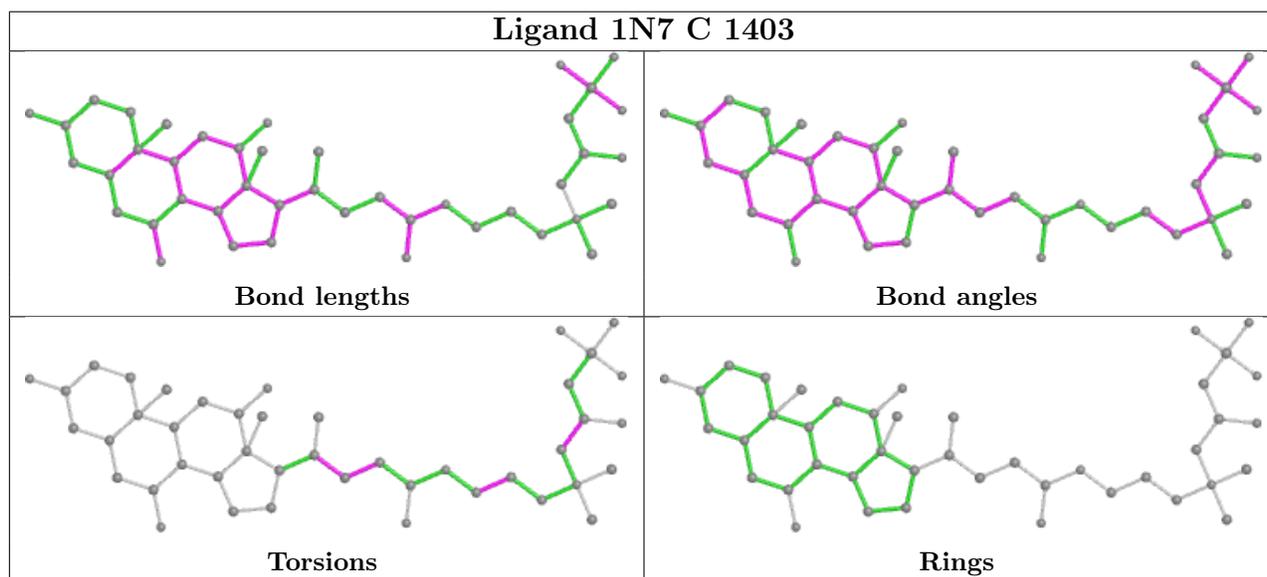
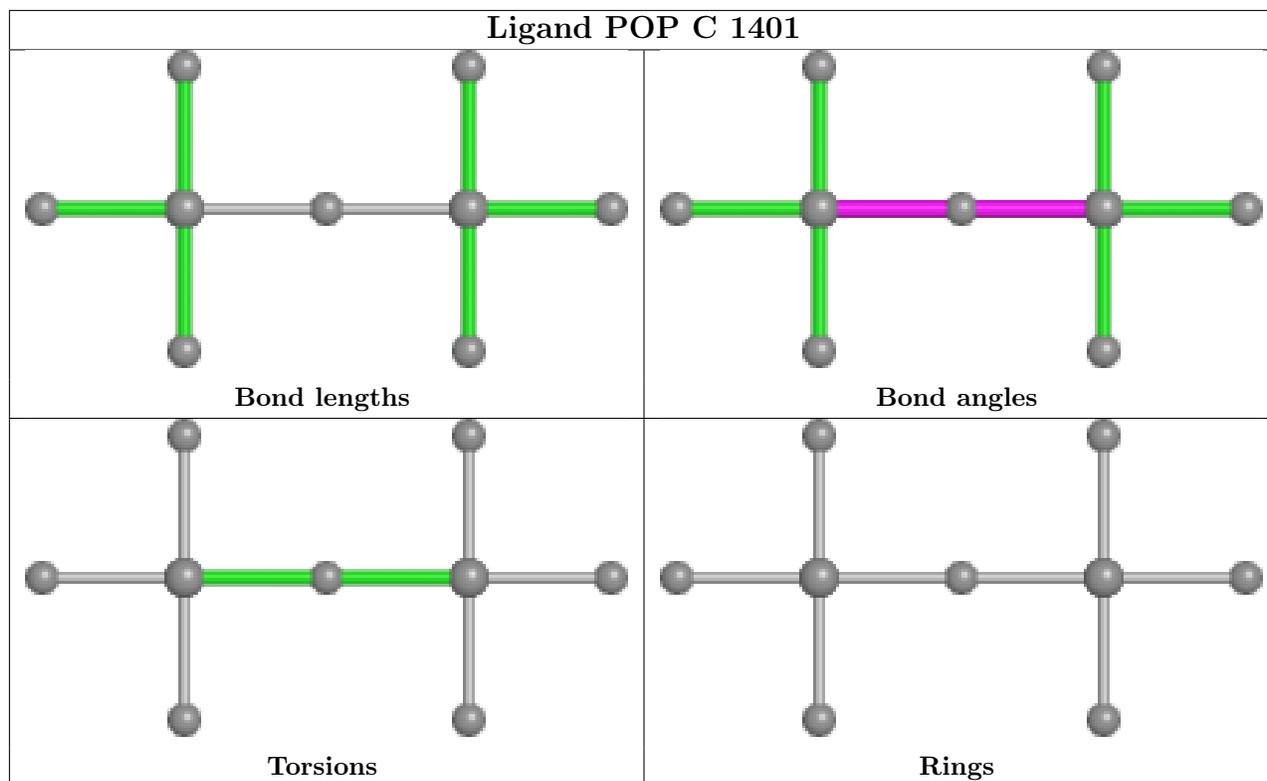
Mol	Chain	Res	Type	Atoms
11	C	1402	1N7	C21-C20-C9-C5
11	C	1402	1N7	C22-C20-C9-C5
11	C	1402	1N7	C22-C20-C9-C8
11	C	1402	1N7	N2-C28-C31-C32
11	C	1402	1N7	N2-C28-C31-O5

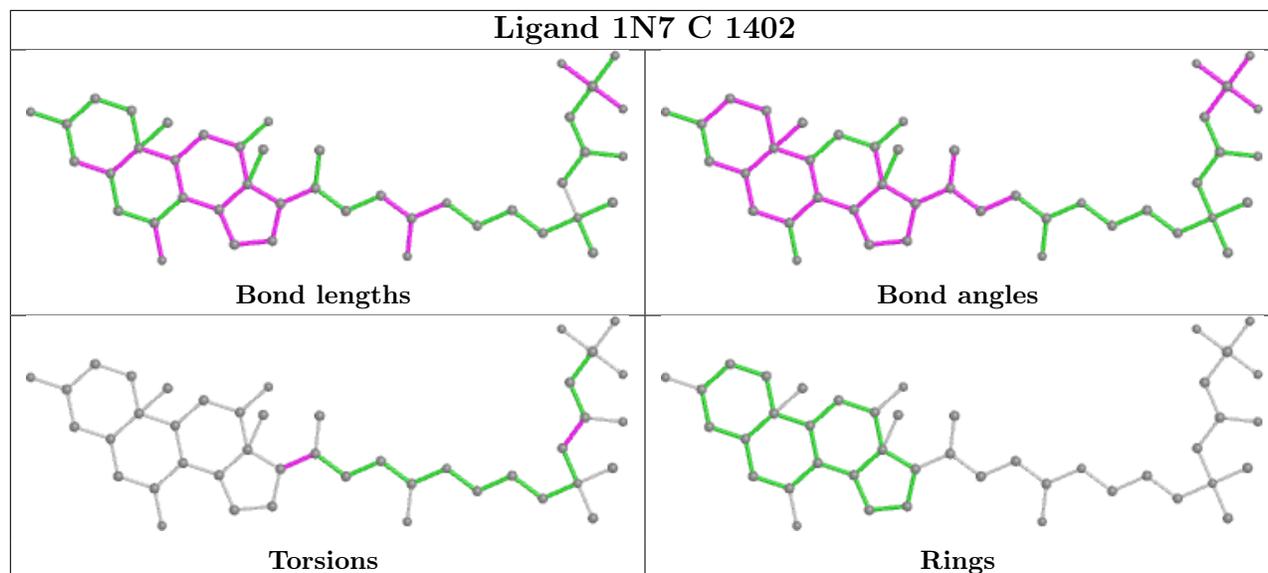
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	C	1401	POP	1	0
11	C	1403	1N7	5	0
11	C	1402	1N7	3	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.

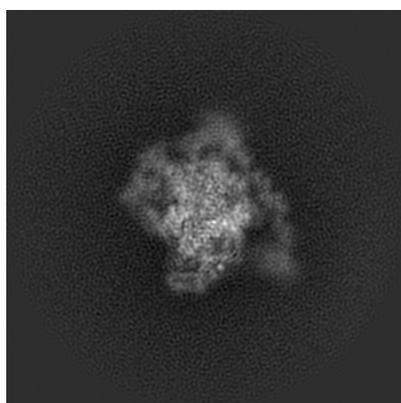
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21879. These allow visual inspection of the internal detail of the map and identification of artifacts.

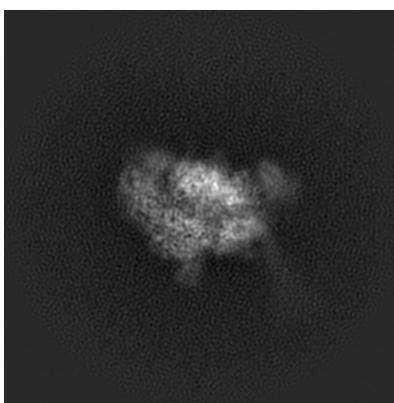
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

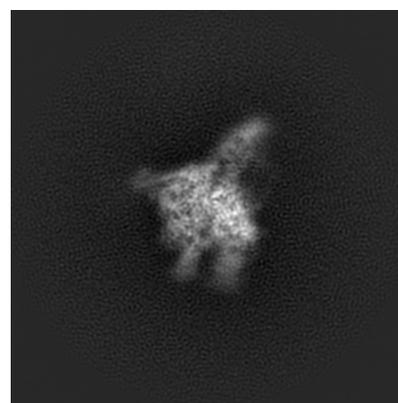
6.1.1 Primary map



X



Y

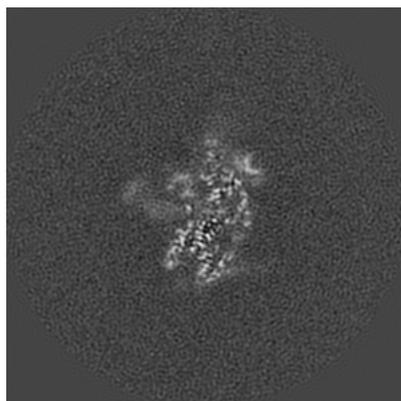


Z

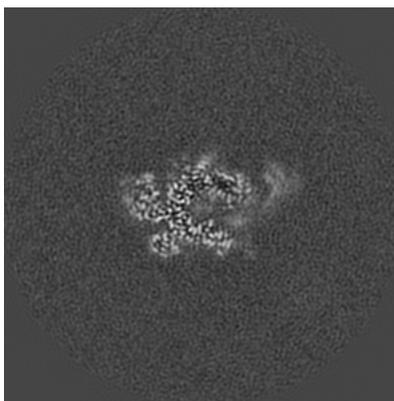
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

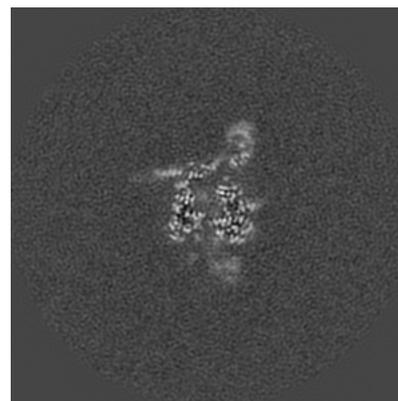
6.2.1 Primary map



X Index: 180



Y Index: 180

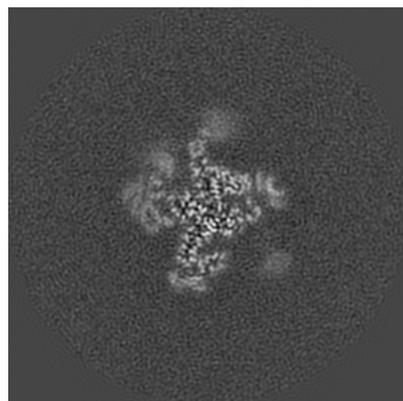


Z Index: 180

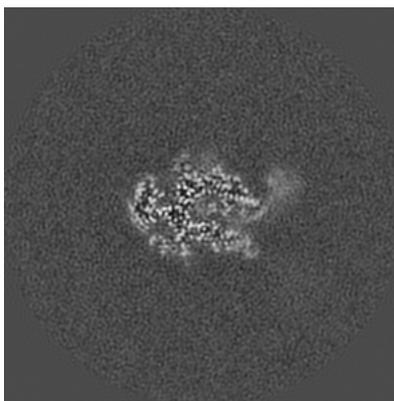
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

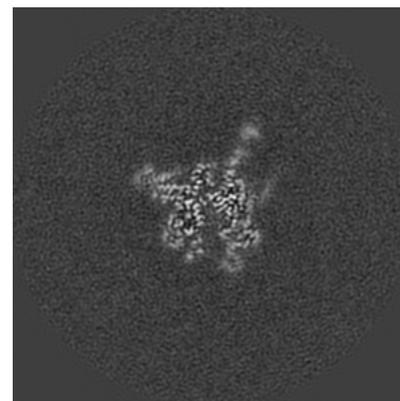
6.3.1 Primary map



X Index: 197



Y Index: 185



Z Index: 167

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

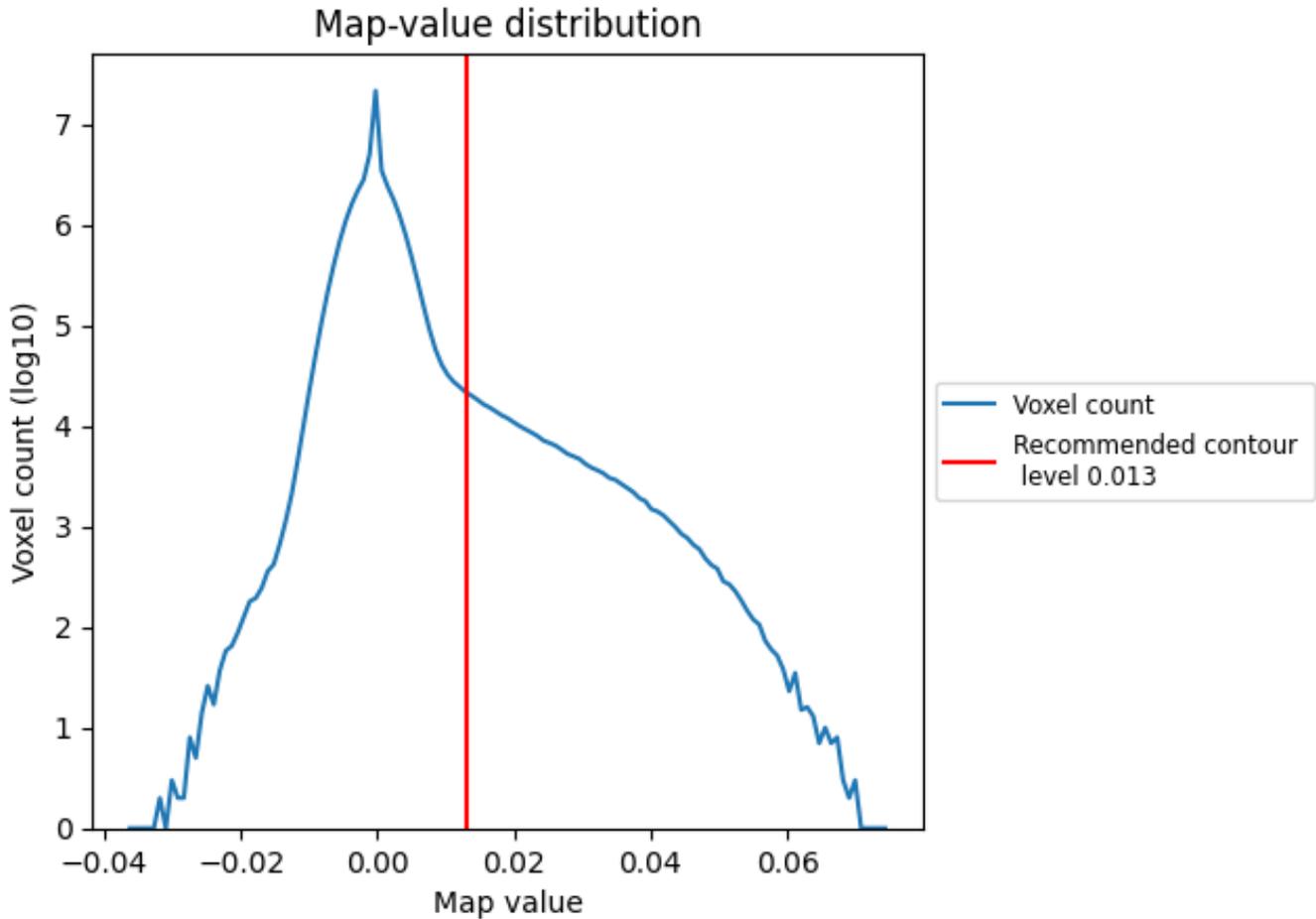
6.5 Mask visualisation

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

7 Map analysis [i](#)

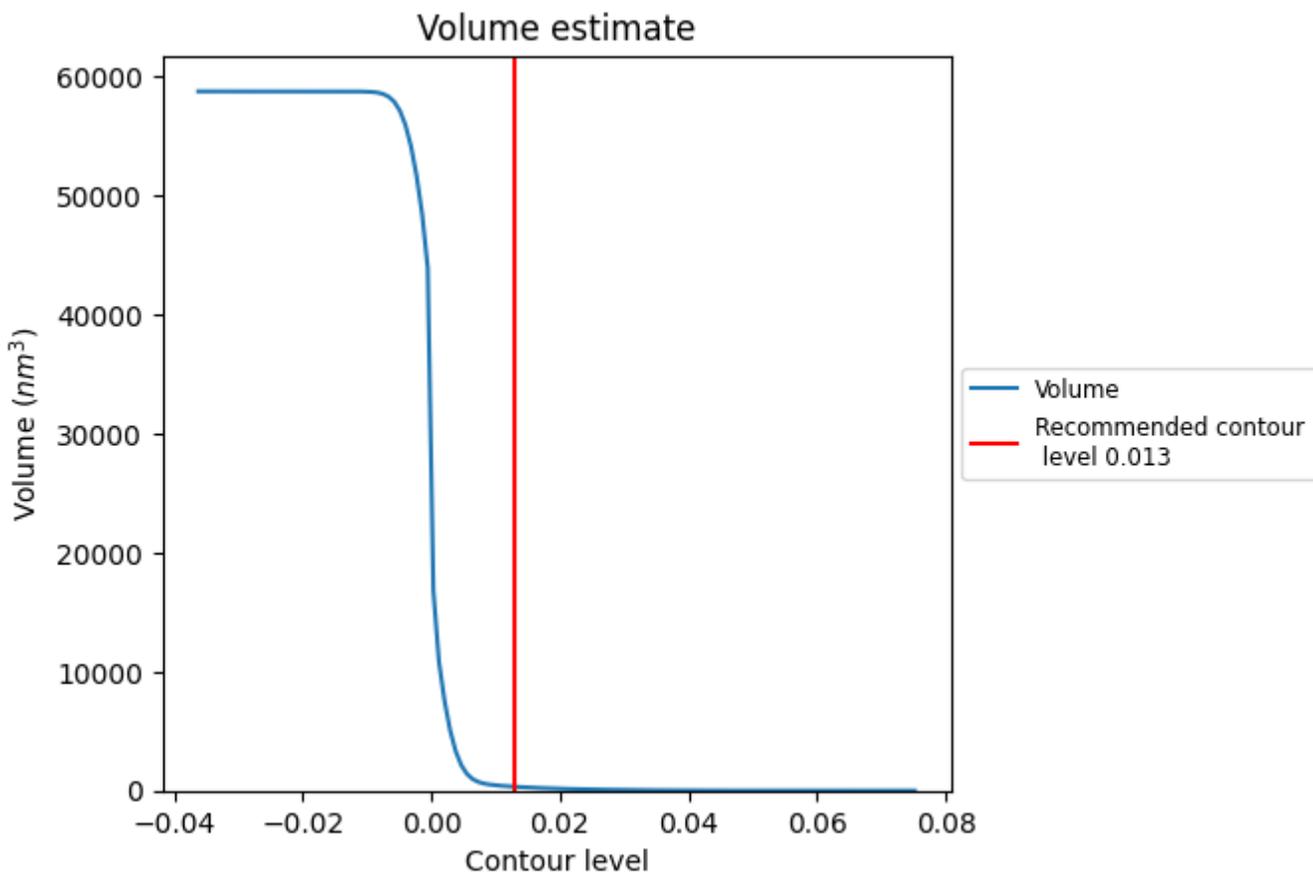
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

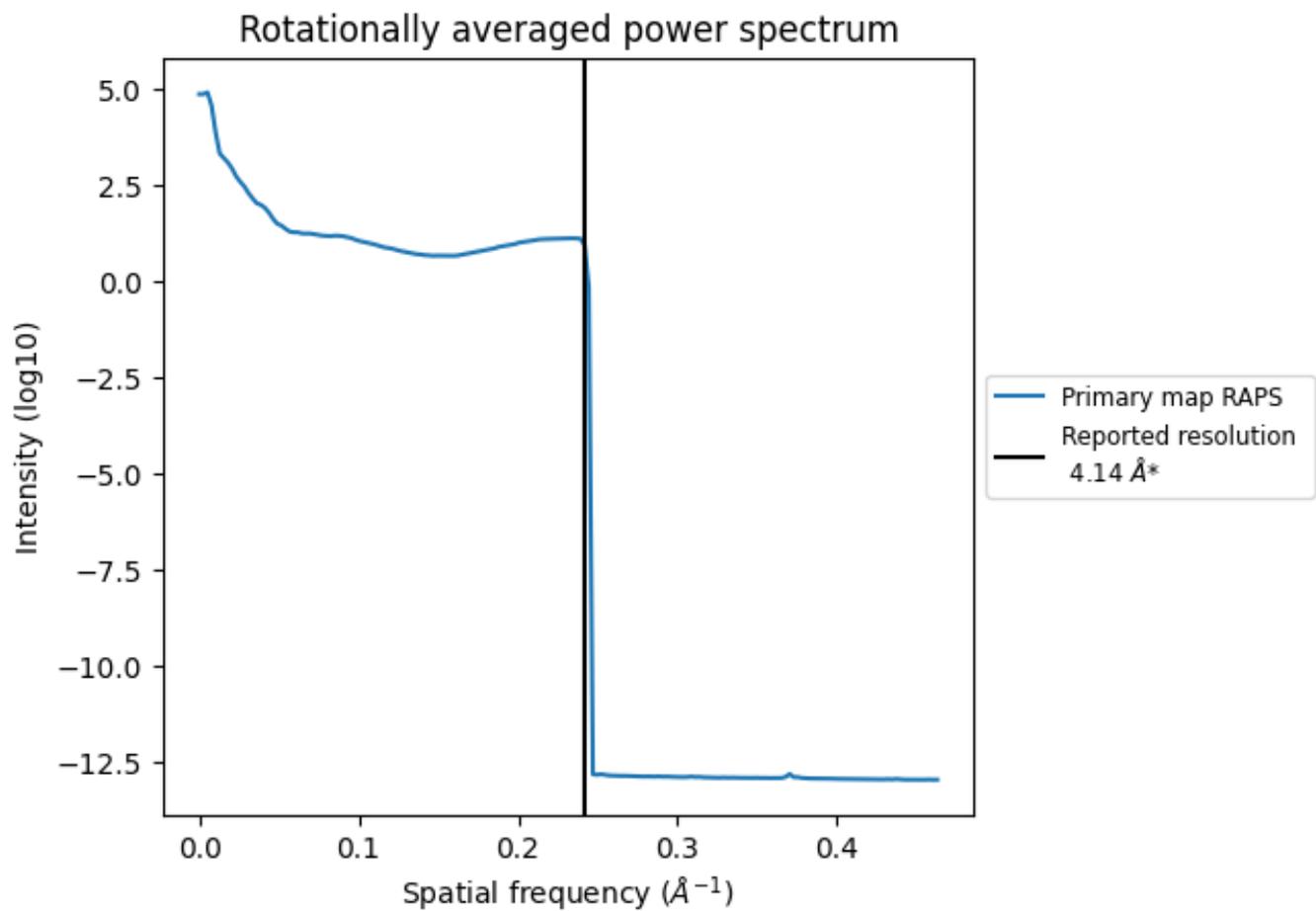
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 327 nm³; this corresponds to an approximate mass of 295 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 0.242 Å⁻¹

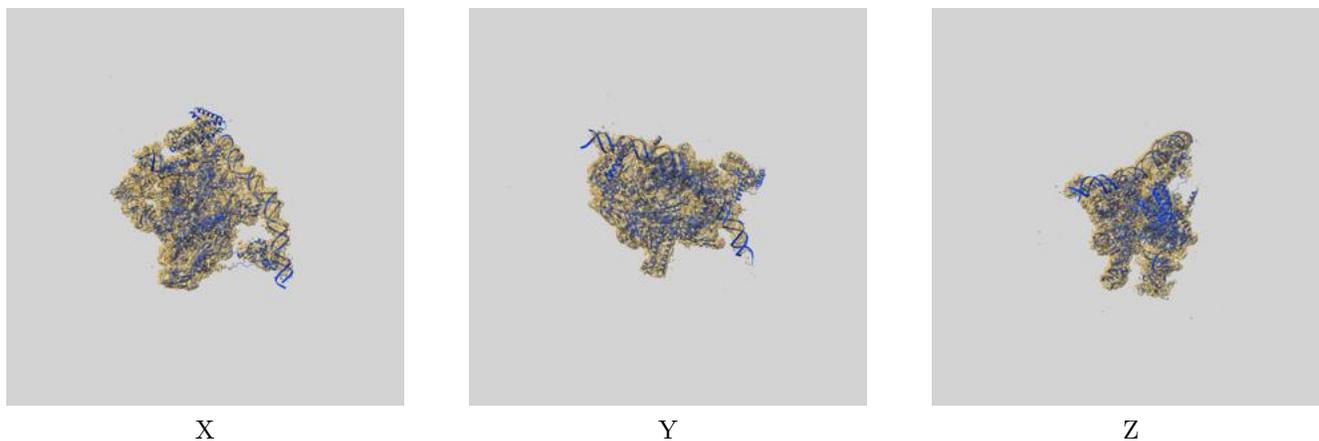
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

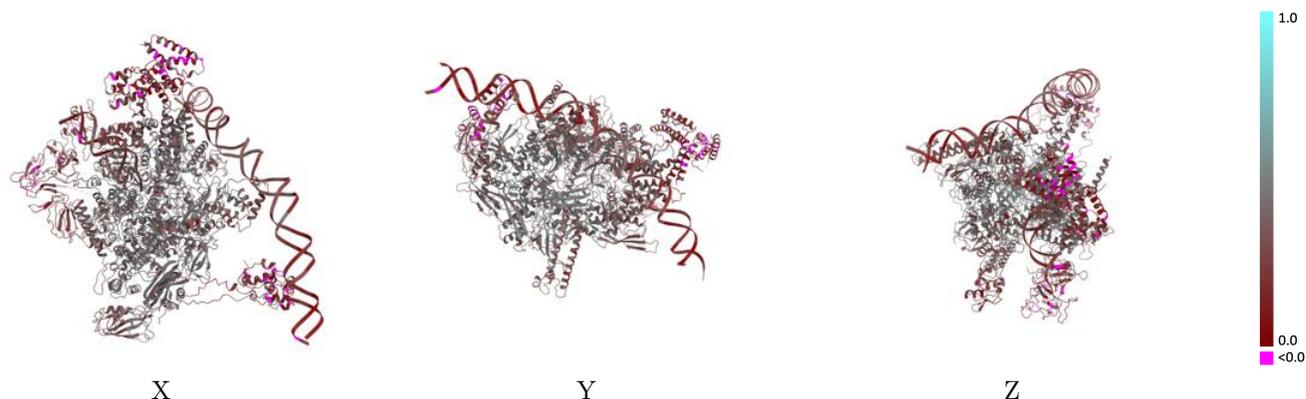
This section contains information regarding the fit between EMDB map EMD-21879 and PDB model 7KHC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



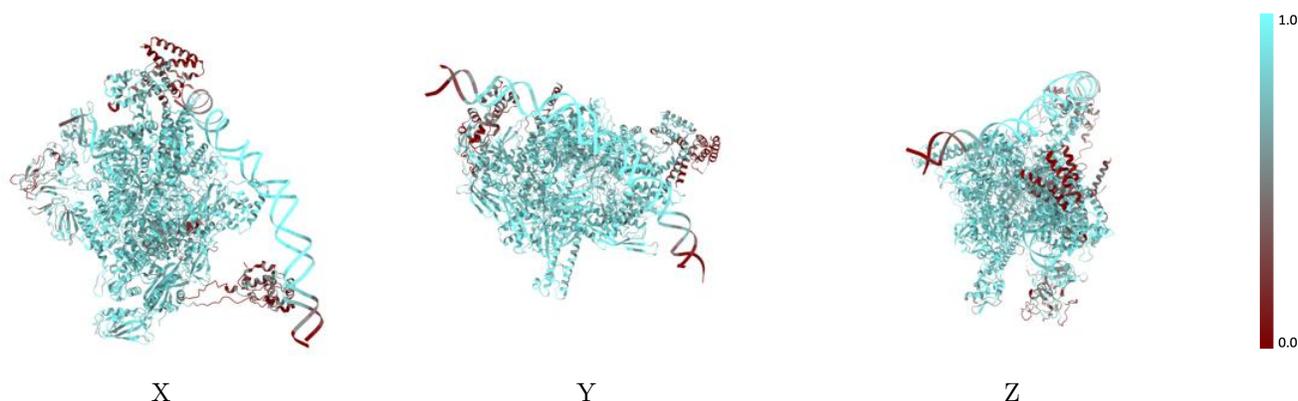
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



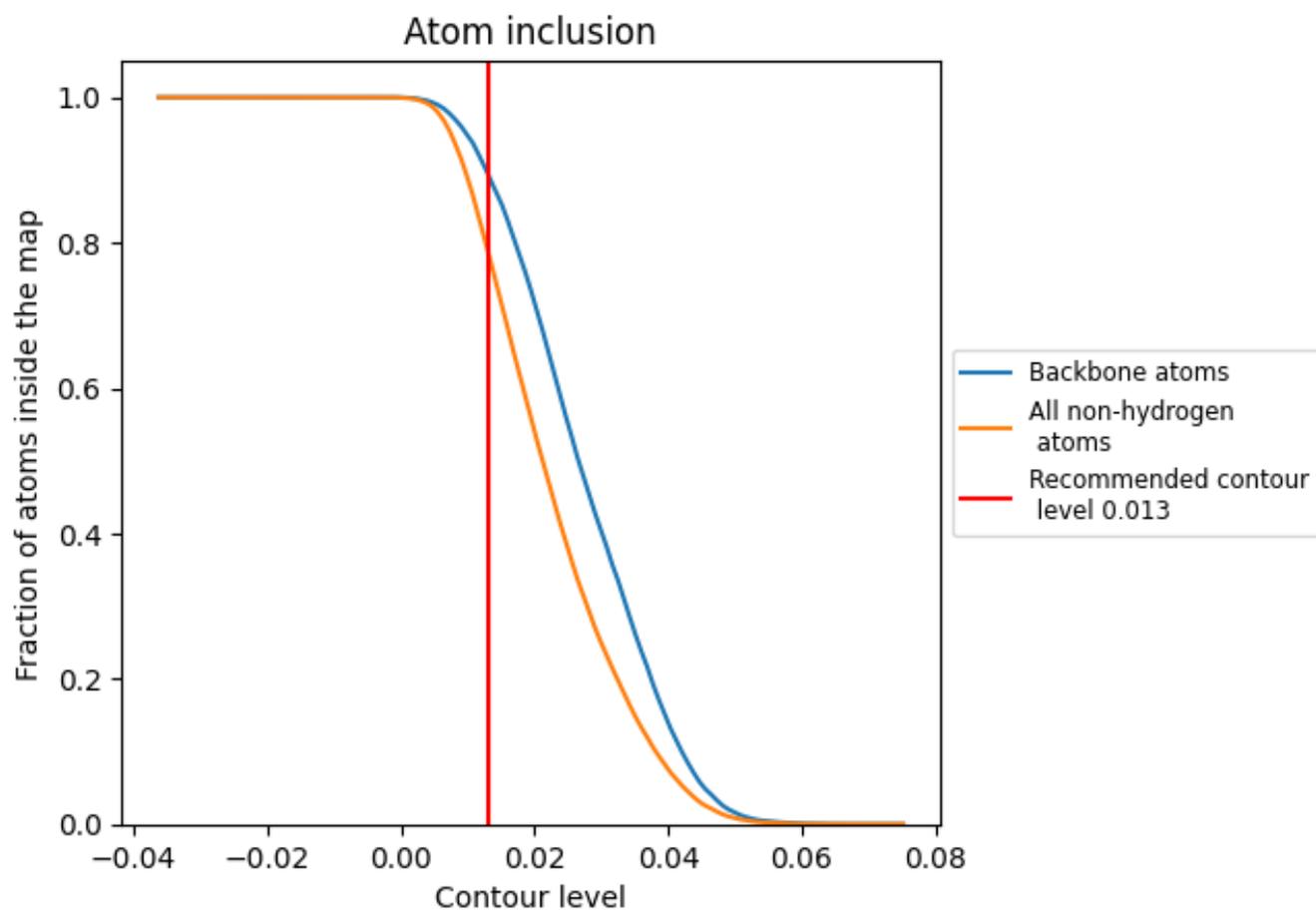
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 79% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.3570
A	 0.7057	 0.3580
B	 0.6599	 0.3310
C	 0.8696	 0.4070
D	 0.8314	 0.3870
E	 0.5671	 0.3720
F	 0.6537	 0.2600
O	 0.8351	 0.2130
P	 0.8505	 0.2720
X	 0.7214	 0.2050
Y	 0.7341	 0.2250

