



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 12:17 AM UTC

PDB ID : 6PSW / pdb_00006psw
EMDB ID : EMD-20466
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPo)
with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

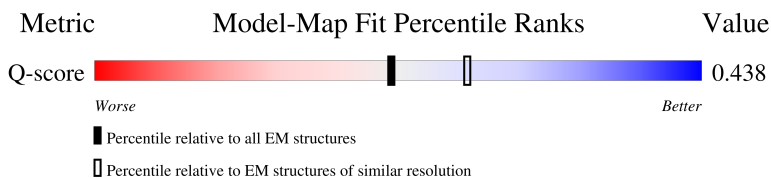
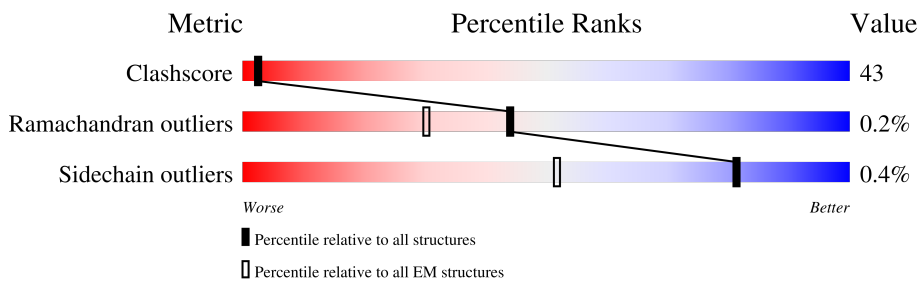
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	11569 (3.20 - 4.20)

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	G	329	36% 33% 30%
1	H	329	29% 37% 33%
1	M	329	8% 15% 78% 22%
2	I	1342	40% 60%

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Mol	Chain	Length	Quality of chain
3	J	1430	 5% 36% 58% 6%
4	K	91	 5% 27% 59% 13%
5	L	616	 13% 25% 51% 23%
6	N	72	 10% 56% 40% 4%
7	O	85	 12% 13% 60% 27%
8	P	85	 20% 9% 64% 27%

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 32773 atoms, of which 78 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	G	229	1762	1100	313	343	6	0	0
1	H	219	1678	1048	295	329	6	0	0
1	M	73	572	362	100	108	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	1341	10571	6633	1839	2056	43	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	J	1345	10460	6574	1864	1972	50	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	79	627	382	118	126	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	473	3854	2412	687	732	23	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 6 is a protein called Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	N	72	571	353	105	108	5	0	0

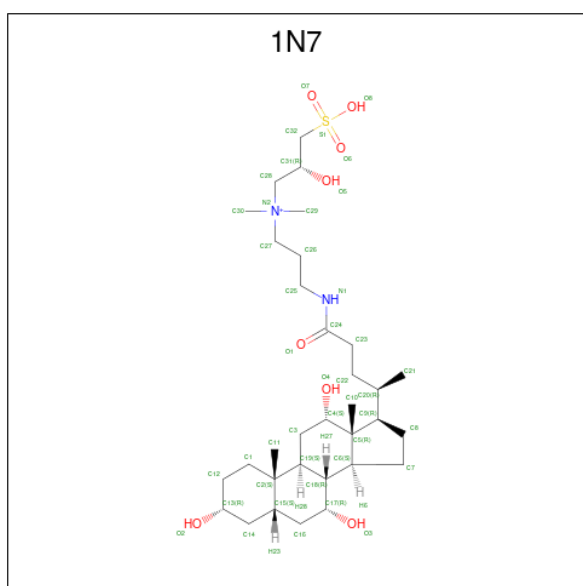
- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	O	62	1270	606	237	365	62	0	0

- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	P	62	1272	609	222	379	62	0	0

- Molecule 9 is CHAPSO (CCD ID: 1N7) (formula: C₃₂H₅₉N₂O₈S).



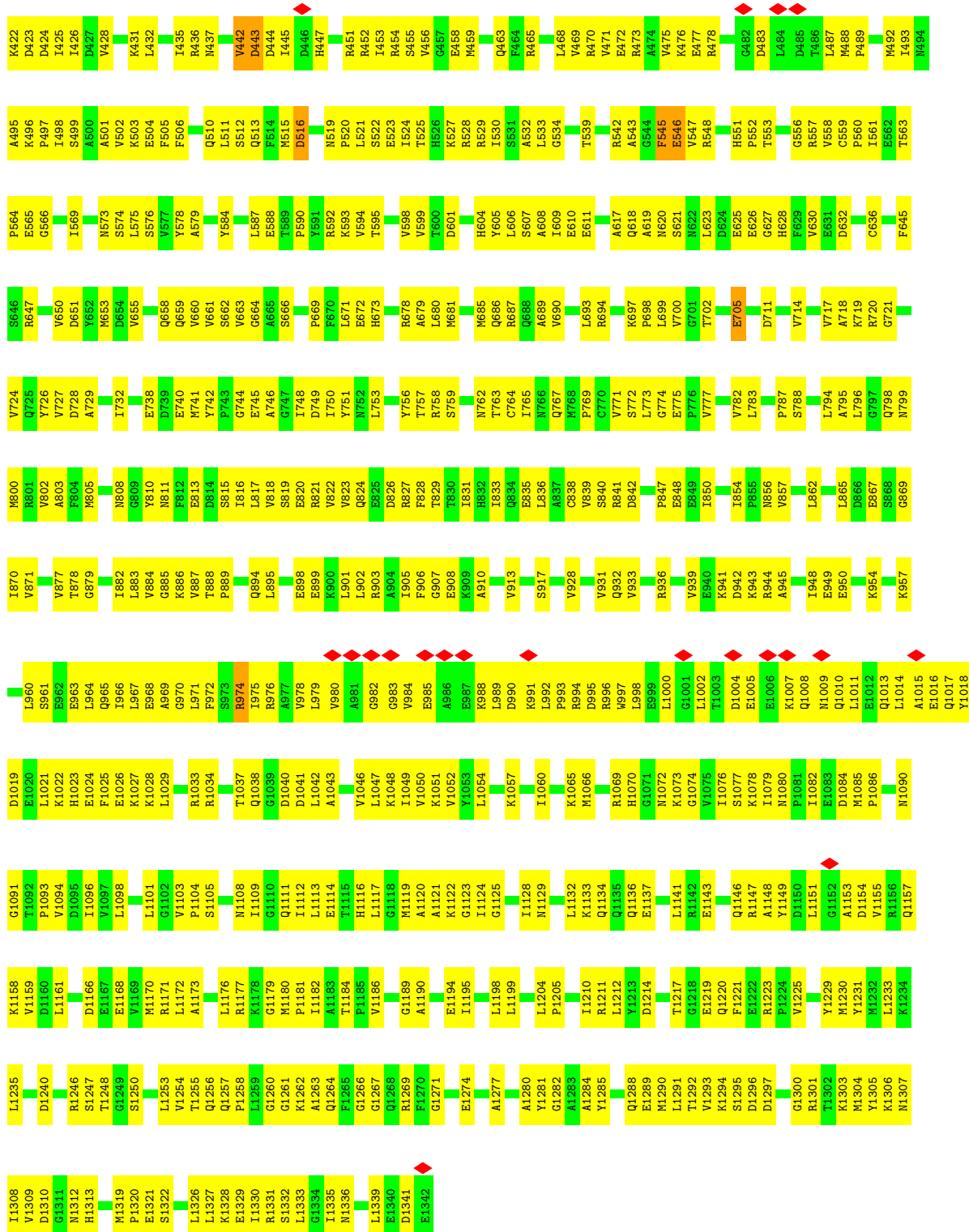
Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
9	I	1	66	24	39	3	0
9	J	1	66	24	39	3	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

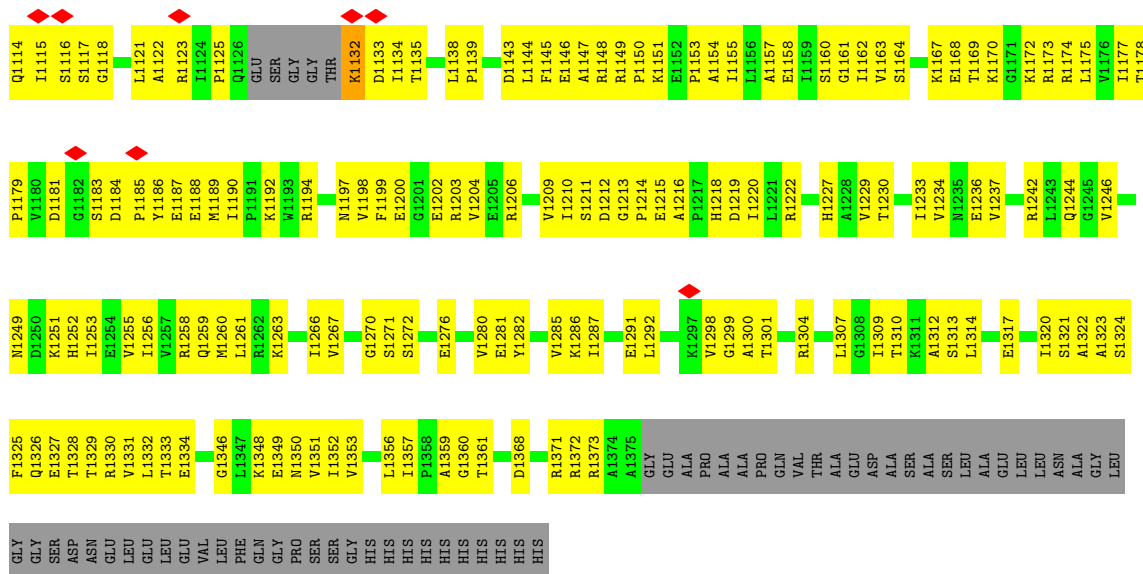


• Molecule 3: DNA-directed RNA polymerase subunit beta'

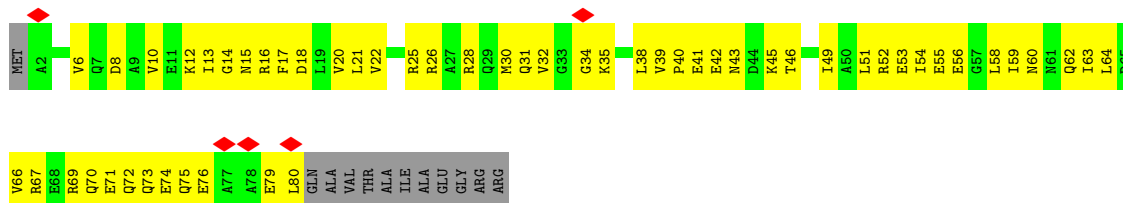


VAL	I1308	L1235	K1158	G1091	D1019	L960	I870	M800	V724	S646	P564	A495	K422
LYS	V1309	D1240	V1159	T1092	E1020	S961	V871	R801	Q725	R647	E565	K496	D423
ASP	D1310	G1178	L1161	P1093	K1021	E962	V877	V802	Y726	V650	G566	P497	D424
LEU	G1311	K1179	L1166	V1094	K1022	E963	V877	A803	Y727	D651	I569	I498	I425
LEU	N1312	M1180	D1166	D1095	H1023	E964	V887	F804	T878	D652	I569	A500	I426
LEU	H1313	M1181	E1167	I1096	E1024	L964	V887	M805	A729	Y653	I569	A501	V427
PHE	H1313	P1182	E1167	V1097	F1025	Q965	V888	M805	D728	D653	I569	A501	V428
LEU	M1319	L1176	E1168	L1098	E1026	L966	V888	M808	I732	D654	I569	A502	K431
LEU	P1320	R1177	V1169	L1098	K1027	L967	V889	G809	P743	D655	I569	K503	L432
LYS	E1321	R1177	V1169	L1101	L1027	L967	V889	G809	P743	D655	I569	K503	L432
ALA	S1322	M1170	V1169	G1102	L1029	E968	V889	G809	P743	D655	I569	F504	L432
THR	S1322	R1171	L1170	V1103	L1029	E968	V889	M811	E738	Q658	I569	F505	L432
LYS	L1326	A1172	L1172	V1103	L1029	E968	V889	M811	E738	Q658	I569	F505	L432
LYS	L1327	A1173	L1173	P1104	L1033	L971	V889	M811	E738	Q658	I569	F506	L432
THR	L1327	S1105	S1105	P1104	R1033	L971	V889	M811	E738	Q658	I569	F506	L432
GLU	L1328	L1176	L1176	S1105	R1034	F972	V889	M811	E738	Q658	I569	F506	L432
E16	K1328	R1177	R1177	M1108	T1037	S973	V889	M811	E738	Q658	I569	F506	L432
F17	E1329	R1177	R1177	I1109	T1037	S973	V889	M811	E738	Q658	I569	F506	L432
D18	I1330	G1178	K1178	I1109	T1037	S973	V889	M811	E738	Q658	I569	F506	L432
I22	R1331	L1259	G1260	G1110	G1038	R975	V889	M811	E738	Q658	I569	F506	L432
A23	R1331	G1260	G1261	Q1111	G1038	R975	V889	M811	E738	Q658	I569	F506	L432
L24	S1332	G1261	K1262	Q1111	D1040	A977	V889	M811	E738	Q658	I569	F506	L432
A25	L1333	K1262	P1181	I1112	D1041	V976	V889	M811	E738	Q658	I569	F506	L432
S26	G1334	L1185	V1186	L1114	L1042	L979	V889	M811	E738	Q658	I569	F506	L432
N29	N1336	F1265	P1185	T1115	A1043	V980	V889	M811	E738	Q658	I569	F506	L432
I30	L1339	G1266	V1186	H1116	V1046	A981	V889	M811	E738	Q658	I569	F506	L432
R31	E1340	G1267	L1117	L1117	L1047	Q982	V889	M811	E738	Q658	I569	F506	L432
S32	D1341	Q1268	G1118	G1118	K1048	Q983	V889	M811	E738	Q658	I569	F506	L432
W33	E1342	F1270	M1119	A1120	V1049	V984	V889	M811	E738	Q658	I569	F506	L432
S34	D1342	G1271	A1190	A1120	V1049	V984	V889	M811	E738	Q658	I569	F506	L432
F35	E1342	G1271	E1194	K1122	K1051	E986	V889	M811	E738	Q658	I569	F506	L432
G36	E1342	G1271	I1195	G1123	V1052	E987	V889	M811	E738	Q658	I569	F506	L432
E37	E1342	G1271	L1196	L1124	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
K40	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
P41	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
E42	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
T43	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
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Y46	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
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T48	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
F49	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
K50	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
P51	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
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R60	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
I61	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
F62	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
G63	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
R66	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
D67	E1342	G1271	L1199	G1125	L1054	K988	V889	M811	E738	Q658	I569	F506	L432
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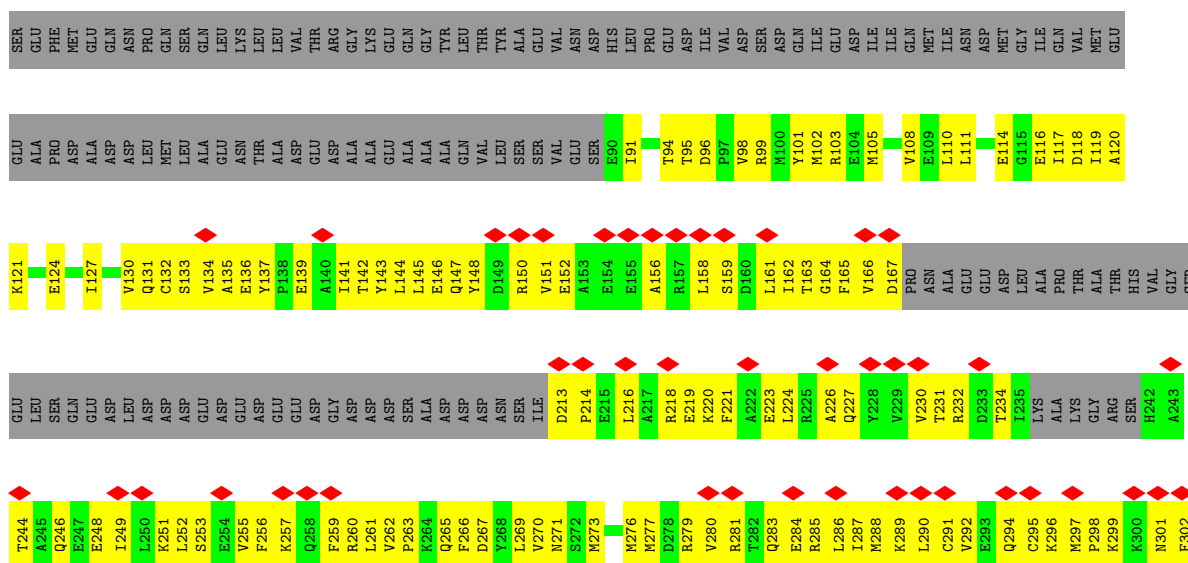
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L1059	Y995	R933	L857	T786	S718	K649	T573	S502	R431	H364	D289	K214	S143	K74
V1060	K985	R935	V858	K789	F719	K650	V574	Q504	G433	G433	I290	K215	Y144	Y75
V1061	P998	H936	P859	R860	M720	H651	G575	D506	A434	L368	I291	K216	V146	K76
D1062	Y999	GLY	L864	A791	S721	R652	R576	G509	A436	P369	V292	L217	V146	R77
D1063	A1001	GLY	H865	L796	I722	I653	A577	L510	P439	K370	N294	K218	V148	R78
S1064	L1003	ALA	E866	R798	Y723	I654	E578	M513	V440	K371	N294	K219	E148	K79
A1065	ALA	ALA	C869	R798	M724	S655	L579	L510	V440	A373	K296	R220	G149	H80
E1066	ALA	ALA	D870	M725	M725	A657	M581	M513	V440	L374	R297	K222	G150	V83
R1067	ALA	ALA	E858	R731	R731	E658	I582	T514	L441	E375	M298	K222	M151	R84
A1069	ALA	ALA	V661	G732	G732	V661	P584	R515	L441	L376	L299	K223	T152	C85
G1070	GLU	GLU	E803	S733	S733	V662	P584	D516	L441	L376	L299	L224	N153	C86
K1071	S948	S948	A804	A734	A734	E662	P584	C517	L441	L376	L299	L224	N153	C87
D1073	I950	I950	B805	A735	A735	E663	P584	V518	L441	L376	L299	L224	N153	C88
L1074	Q951	Q951	B806	Q736	Q736	E664	P584	M519	L441	L376	L299	L224	N153	C89
R1075	V952	V952	B807	Q737	Q737	E665	P584	A520	L441	L376	L299	L224	N153	V92
L1076	K953	K953	L807	Q737	Q737	E666	P584	K521	L441	L376	L299	L224	N153	V92
P1076	S957	S957	D812	G742	G742	S670	M593	M525	L441	L376	L299	L224	N153	V92
A1077	I958	I958	D813	M743	M743	E671	M593	V526	L441	L376	L299	L224	N153	V92
L1078	K959	K959	C814	R743	R743	E672	M593	L527	L441	L376	L299	L224	N153	V92
K1079	L960	L960	T816	L746	L746	E677	I601	P630	L441	L376	L299	L224	N153	V92
I1080	S961	S961	B820	L747	L747	E677	I601	K331	L441	L376	L299	L224	N153	V92
V1081	N962	N962	E821	L748	L748	R678	I601	A459	L441	L376	L299	L224	N153	V92
D1082	W963	W963	M822	A748	A748	E678	Y609	D460	L441	L376	L299	L224	N153	V92
A1083	K964	K964	M822	K749	K749	E678	Y609	D460	L441	L376	L299	L224	N153	V92
Q1084	S965	S965	M822	P750	P750	E678	Y609	D460	L441	L376	L299	L224	N153	V92
L1085	V966	V966	R824	S753	S753	E682	R610	Q465	L441	L376	L299	L224	N153	V92
N1086	V967	V967	R824	I754	I754	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1087	E967	E967	R824	I755	I755	E682	R610	Q465	L441	L376	L299	L224	N153	V92
V1088	N968	N968	E827	E756	E756	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1089	S969	S969	G828	T757	T757	E682	R610	Q465	L441	L376	L299	L224	N153	V92
I1090	R970	R970	D830	P758	P758	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1091	G971	G971	D830	I759	I759	E682	R610	Q465	L441	L376	L299	L224	N153	V92
P1091	K972	K972	E833	T760	T760	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1092	L973	L973	L835	A761	A761	E682	R610	Q465	L441	L376	L299	L224	N153	V92
T1093	V974	V974	L835	N762	N762	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1094	I975	I975	V839	F763	F763	E682	R610	Q465	L441	L376	L299	L224	N153	V92
M1095	T976	T976	L840	E765	E765	E682	R610	Q465	L441	L376	L299	L224	N153	V92
P1096	S977	S977	G841	G766	G766	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1097	R978	R978	R842	L767	L767	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Q1098	T980	T980	R843	N768	N768	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Y1099	L981	L981	R843	V769	V769	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1100	E981	E981	R843	E704	E704	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	K982	K982	R843	E704	E704	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	L983	L983	R843	Q771	Q771	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1098	L984	L984	R843	Y772	Y772	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Y1099	I985	I985	R843	F773	F773	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L986	L986	R843	I774	I774	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K987	K987	R843	T775	T775	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1099	L988	L988	R843	G776	G776	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Y1099	L989	L989	R843	I777	I777	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L990	L990	R843	T778	T778	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K989	K989	R843	G779	G779	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1100	L991	L991	R843	I780	I780	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Y1100	L992	L992	R843	T781	T781	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L993	L993	R843	G782	G782	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K990	K990	R843	I783	I783	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1103	L994	L994	R843	T784	T784	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L995	L995	R843	G785	G785	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K991	K991	R843	I786	I786	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1105	L996	L996	R843	T787	T787	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L997	L997	R843	G786	G786	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K992	K992	R843	I788	I788	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1106	L998	L998	R843	T789	T789	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1101	L999	L999	R843	G787	G787	E682	R610	Q465	L441	L376	L299	L224	N153	V92
F1102	K993	K993	R843	I790	I790	E682	R610	Q465	L441	L376	L299	L224	N153	V92
A1107	L1000	L1000	R843	T791	T791	E682	R610	Q465	L441	L376	L299	L224	N153	V92
Q1108	L1001	L1001	R843	G788	G788	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1109	L1002	L1002	R843	I792	I792	E682	R610	Q465	L441	L376	L299	L224	N153	V92
L1110	L1003	L1003	R843	T793	T793	E682	R610	Q465	L441	L376	L299	L224	N153	V92
G1112	L1004	L1004	R843	G789	G789	E682	R610	Q465	L441	L376	L299	L224	N153	V92
V1113	L1005	L1005	R843	I794	I794	E682	R610	Q465	L441	L376	L299	L224	N153	V92



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46650	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 ($e^-/\text{\AA}^2$)	80	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	0.154	Depositor
Minimum map value	-0.109	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	G	0.36	0/1784	0.55	0/2419
1	H	0.32	0/1697	0.53	0/2301
1	M	0.19	0/579	0.54	0/784
2	I	0.37	0/10740	0.57	0/14492
3	J	0.35	0/10619	0.55	0/14338
4	K	0.29	0/629	0.52	0/847
5	L	0.25	0/3906	0.53	2/5251 (0.0%)
6	N	0.24	0/581	0.64	1/785 (0.1%)
7	O	0.23	0/1426	0.40	0/2197
8	P	0.26	0/1424	0.45	0/2197
All	All	0.34	0/33385	0.54	3/45611 (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	I	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	N	27	ILE	N-CA-C	6.98	113.68	106.21
5	L	94	THR	CA-C-N	-6.16	113.32	122.56
5	L	94	THR	C-N-CA	-6.16	113.32	122.56

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	442	VAL	Peptide
2	I	545	PHE	Peptide
2	I	57	PHE	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	G	1762	0	1785	116	0
1	H	1678	0	1698	149	0
1	M	572	0	602	58	0
2	I	10571	0	10580	945	0
3	J	10460	0	10679	964	0
4	K	627	0	634	52	0
5	L	3854	0	3911	481	0
6	N	571	0	558	35	0
7	O	1270	0	698	88	0
8	P	1272	0	705	107	0
9	I	27	39	38	5	0
9	J	27	39	38	5	0
10	J	1	0	0	0	0
11	J	2	0	0	0	0
11	N	1	0	0	0	0
All	All	32695	78	31926	2753	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 43.

The worst 5 of 2753 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)
9:J:1504:1N7:C19	9:J:1504:1N7:C3	1.84	1.54
9:I:1401:1N7:C3	9:I:1401:1N7:C19	1.82	1.52
5:L:146:GLU:O	5:L:150:ARG:HG3	1.48	1.10
3:J:145:VAL:HG23	3:J:159:ILE:HG22	1.36	1.05
3:J:965:SER:HB2	3:J:973:LEU:HD11	1.38	1.03

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	G	227/329 (69%)	195 (86%)	32 (14%)	0	100	100
1	H	215/329 (65%)	188 (87%)	26 (12%)	1 (0%)	24	56
1	M	71/329 (22%)	63 (89%)	8 (11%)	0	100	100
2	I	1339/1342 (100%)	1177 (88%)	158 (12%)	4 (0%)	36	65
3	J	1339/1430 (94%)	1187 (89%)	152 (11%)	0	100	100
4	K	77/91 (85%)	69 (90%)	8 (10%)	0	100	100
5	L	467/616 (76%)	422 (90%)	45 (10%)	0	100	100
6	N	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	3	26
All	All	3805/4538 (84%)	3363 (88%)	435 (11%)	7 (0%)	44	72

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	546	GLU
2	I	974	ARG
6	N	29	ALA
2	I	443	ASP
6	N	30	HIS

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	G	193/286 (68%)	191 (99%)	2 (1%)	68	74
1	H	184/286 (64%)	182 (99%)	2 (1%)	65	73
1	M	65/286 (23%)	65 (100%)	0	100	100
2	I	1155/1157 (100%)	1149 (100%)	6 (0%)	81	80
3	J	1127/1189 (95%)	1124 (100%)	3 (0%)	86	83
4	K	67/75 (89%)	67 (100%)	0	100	100
5	L	421/543 (78%)	421 (100%)	0	100	100
6	N	61/61 (100%)	61 (100%)	0	100	100
All	All	3273/3883 (84%)	3260 (100%)	13 (0%)	81	81

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	705	GLU
2	I	750	ILE
3	J	1132	LYS
3	J	316	ILE
3	J	1031	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	720	ASN
3	J	1023	HIS
3	J	777	HIS
3	J	910	ASN
3	J	1249	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 6 ligands modelled in this entry, 4 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
9	1N7	J	1504	-	30,30,46	5.20	15 (50%)	47,48,72	2.42	18 (38%)
9	1N7	I	1401	-	30,30,46	4.94	14 (46%)	47,48,72	2.22	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
9	1N7	J	1504	-	-	0/7/72/92	0/4/4/4
9	1N7	I	1401	-	-	2/7/72/92	0/4/4/4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	J	1504	1N7	C3-C19	19.11	1.84	1.53
9	I	1401	1N7	C3-C19	17.77	1.82	1.53
9	J	1504	1N7	C3-C4	12.46	1.73	1.53
9	I	1401	1N7	C3-C4	11.27	1.71	1.53
9	I	1401	1N7	C5-C4	-9.04	1.40	1.54

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C9-C5-C6	5.93	106.06	100.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1504	1N7	C9-C5-C4	-5.55	112.67	117.67
9	I	1401	1N7	C7-C6-C18	-5.00	111.49	118.36
9	I	1401	1N7	C19-C3-C4	-4.97	107.80	114.29
9	I	1401	1N7	C9-C5-C4	-4.62	113.51	117.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

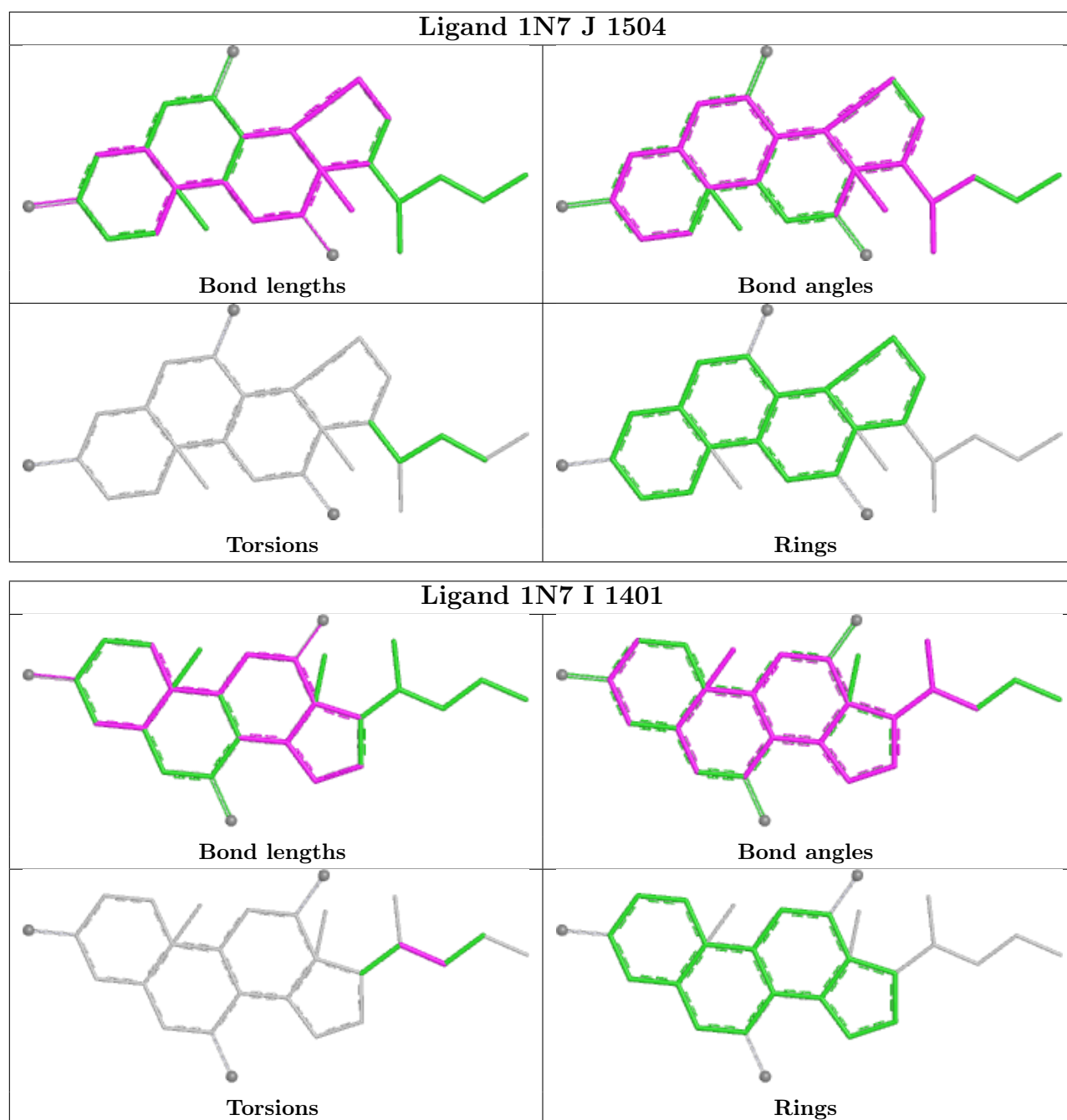
Mol	Chain	Res	Type	Atoms
9	I	1401	1N7	C9-C20-C22-C23
9	I	1401	1N7	C21-C20-C22-C23

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	J	1504	1N7	5	0
9	I	1401	1N7	5	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.

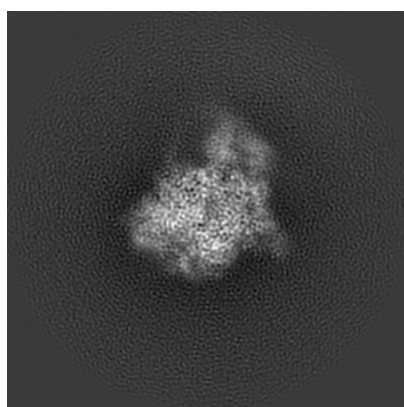
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20466. These allow visual inspection of the internal detail of the map and identification of artifacts.

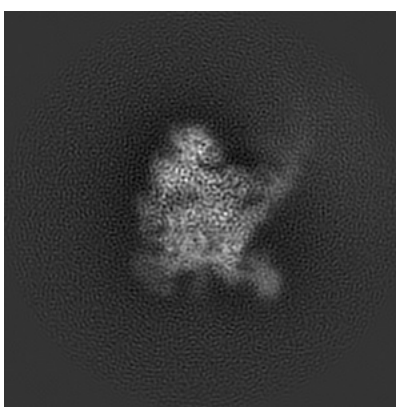
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

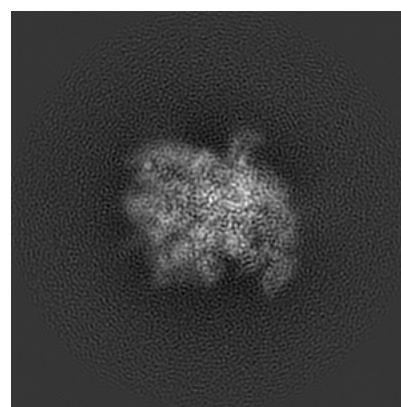
6.1.1 Primary map



X



Y

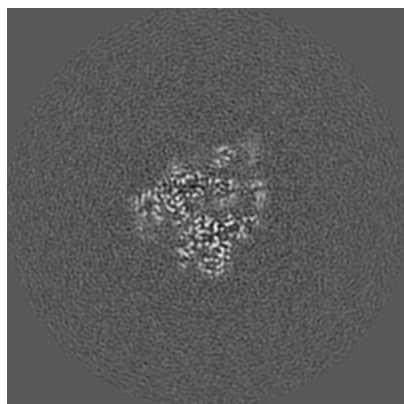


Z

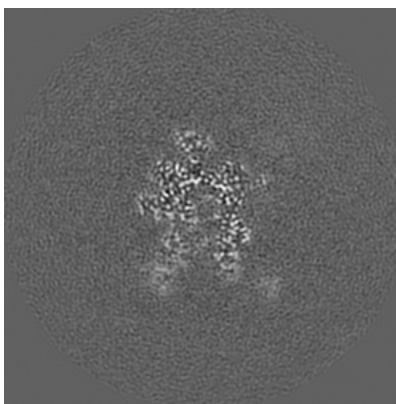
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

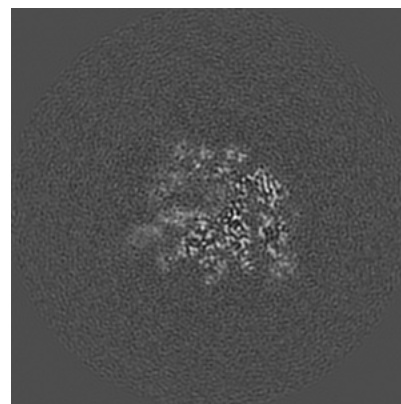
6.2.1 Primary map



X Index: 128



Y Index: 128

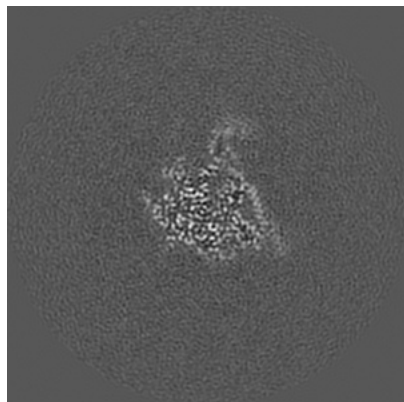


Z Index: 128

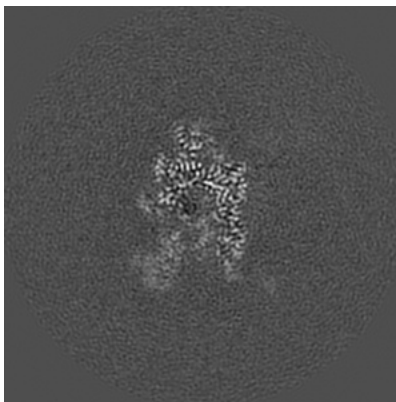
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

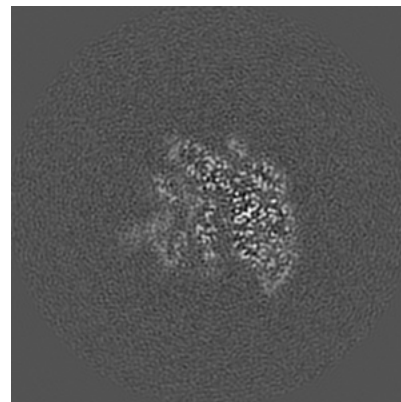
6.3.1 Primary map



X Index: 147



Y Index: 125

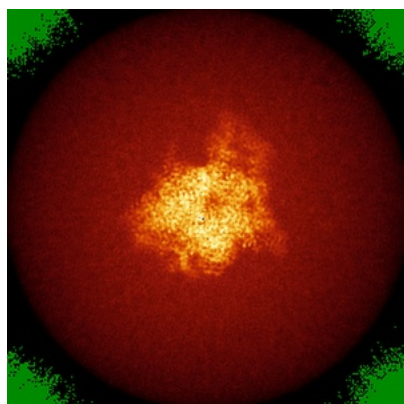


Z Index: 121

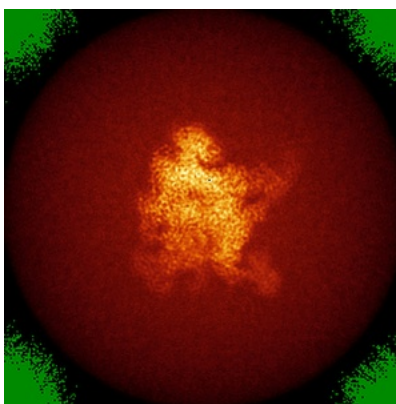
The images above show the largest variance slices of the map in three orthogonal directions.

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

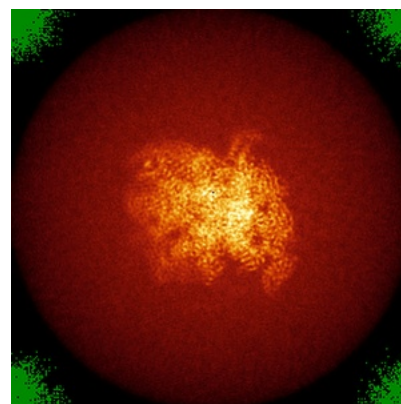
6.4.1 Primary map



X



Y

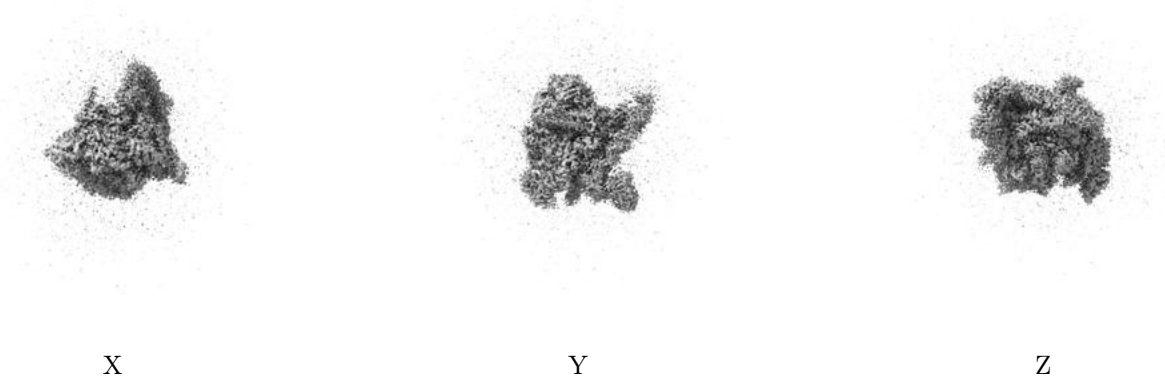


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

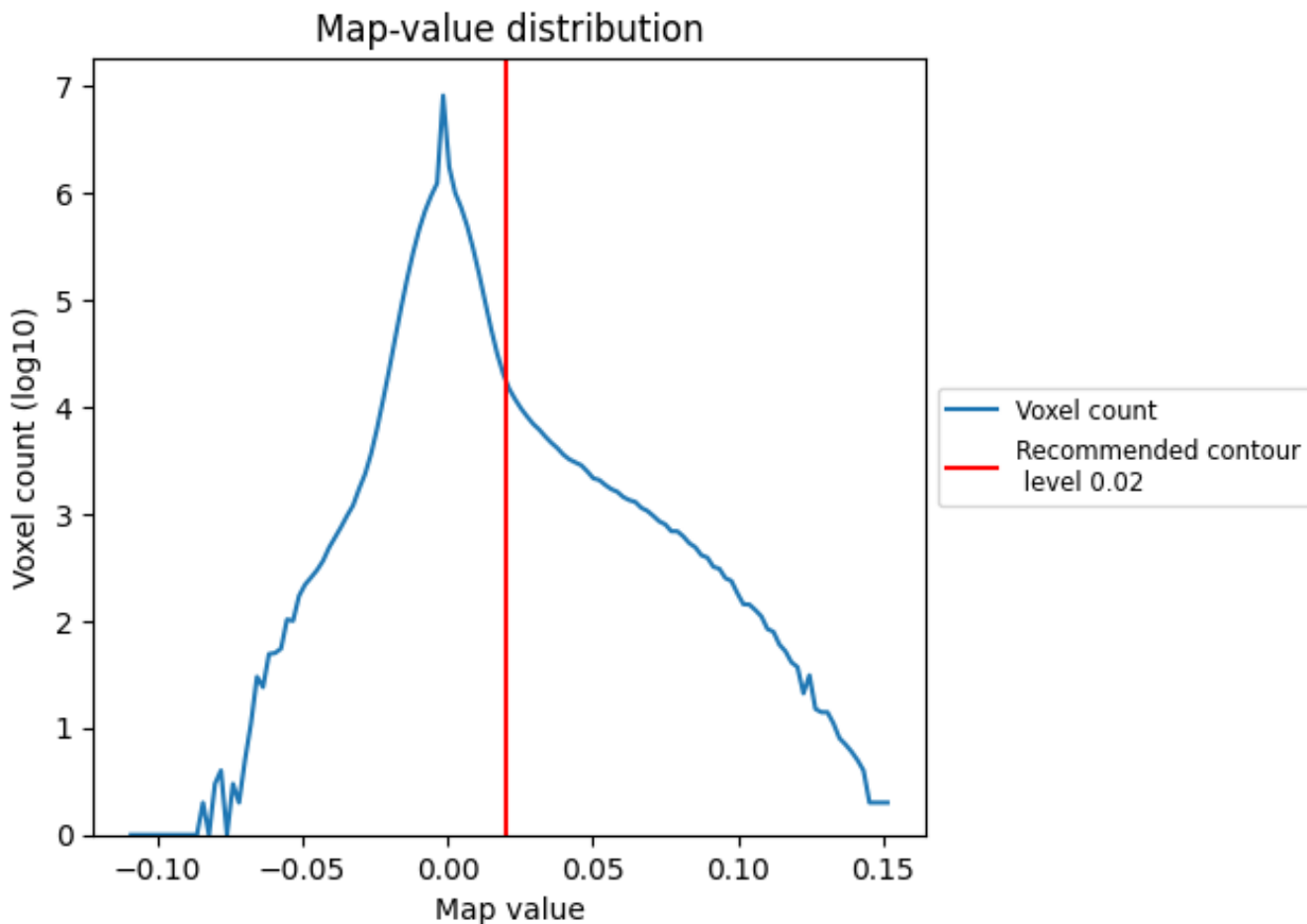
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

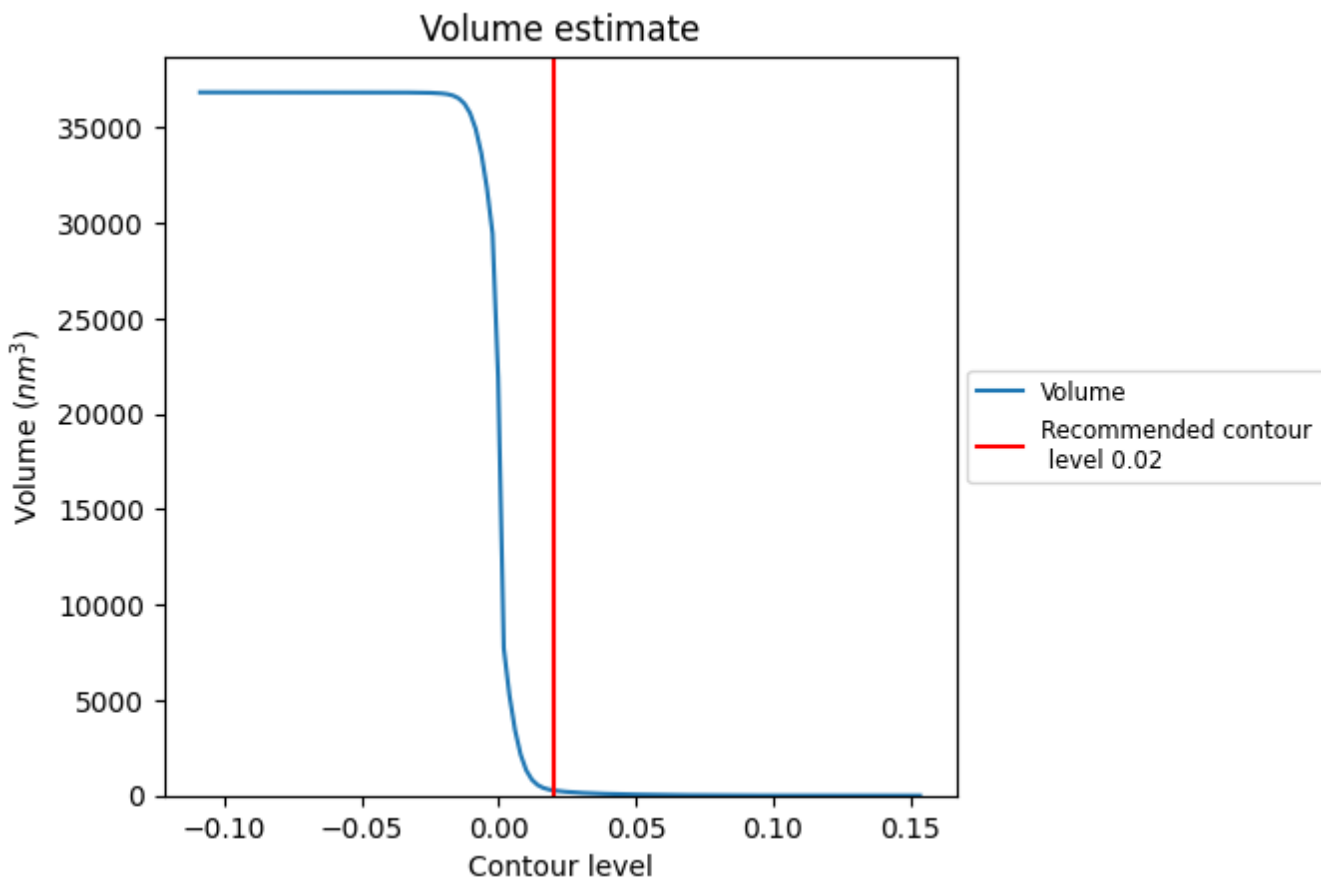
This section contains the results of statistical analysis of the map.

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.

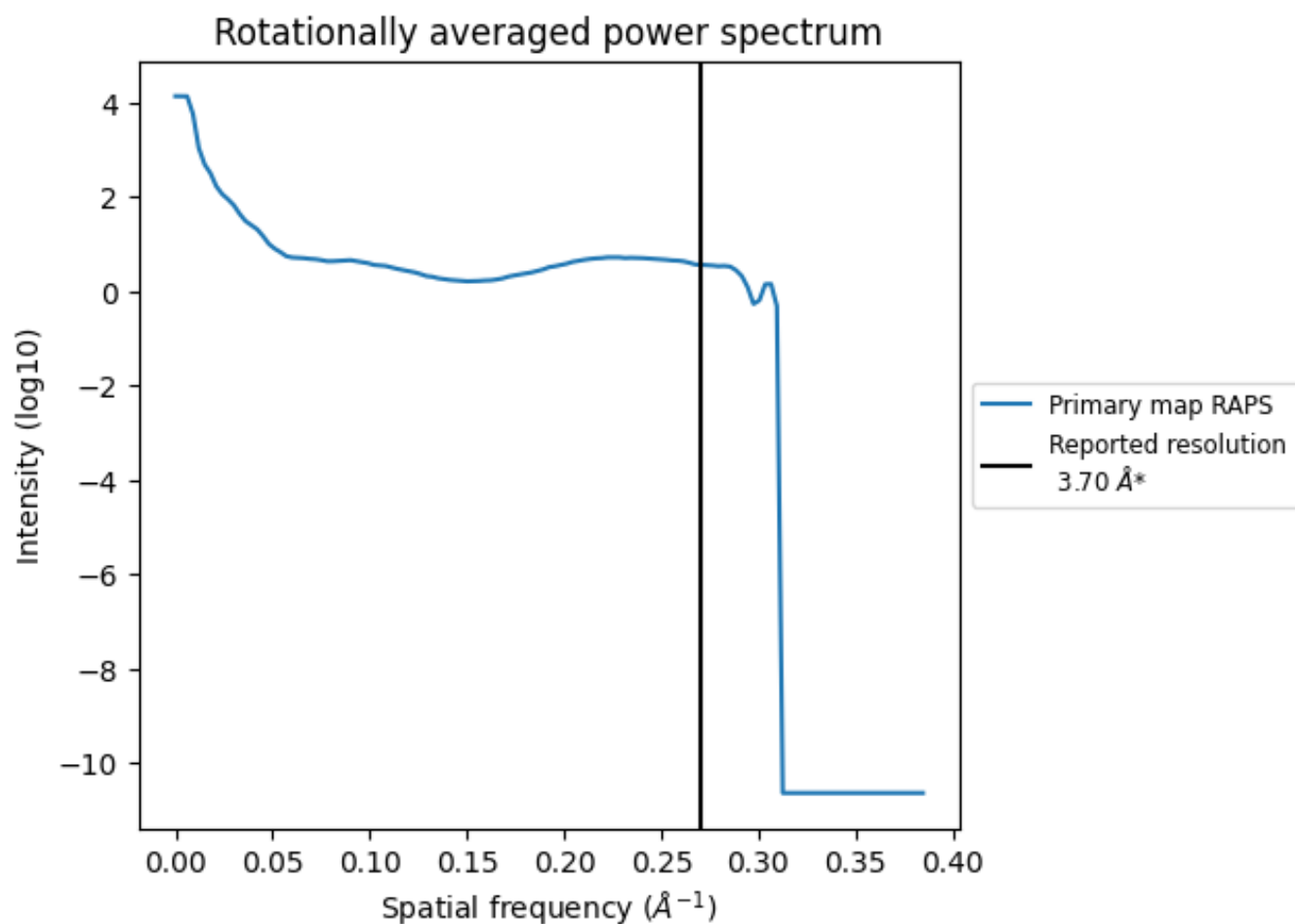
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 270 nm³; this corresponds to an approximate mass of 244 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 [\(i\)](#)

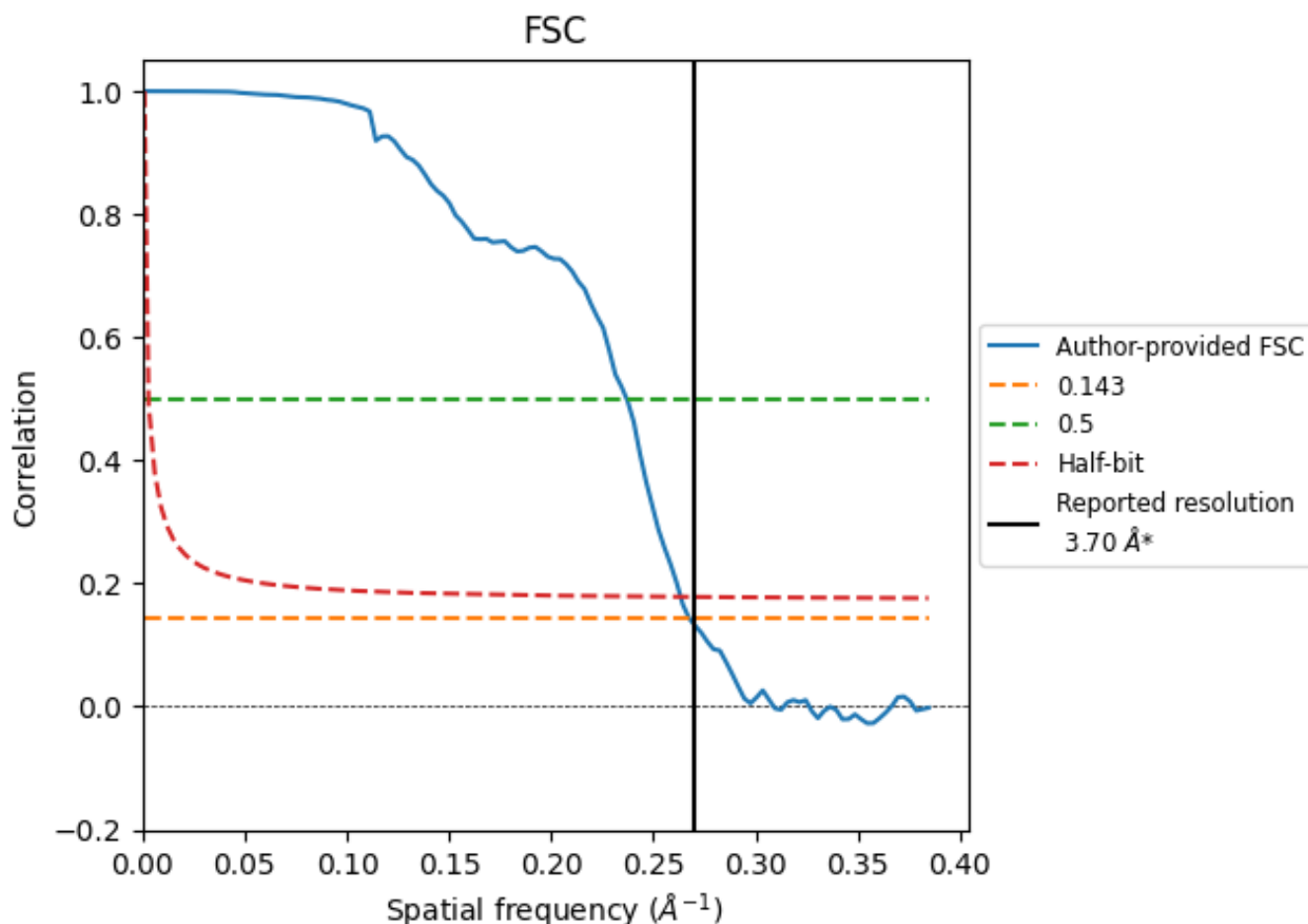


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

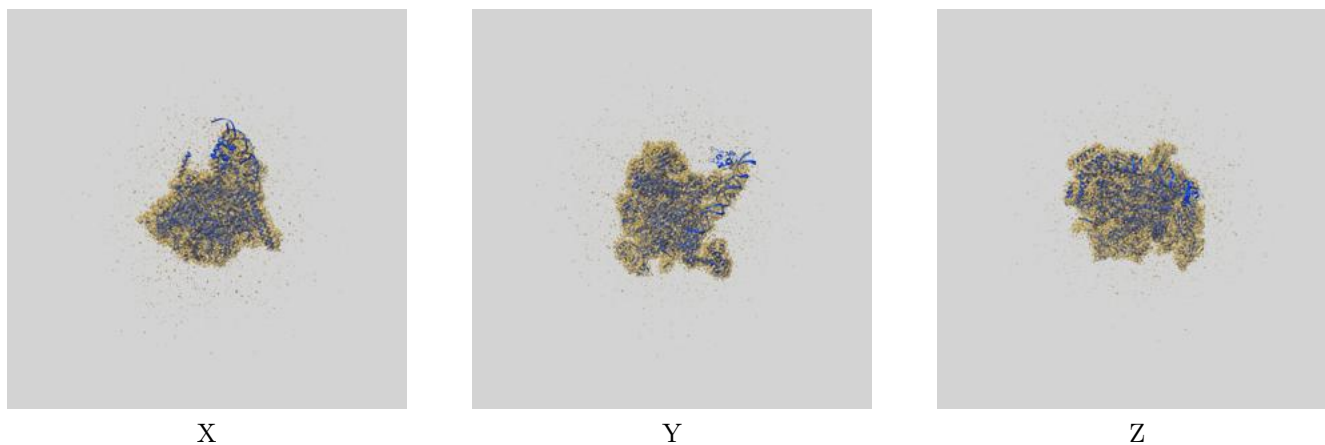
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.74	4.22	3.80
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

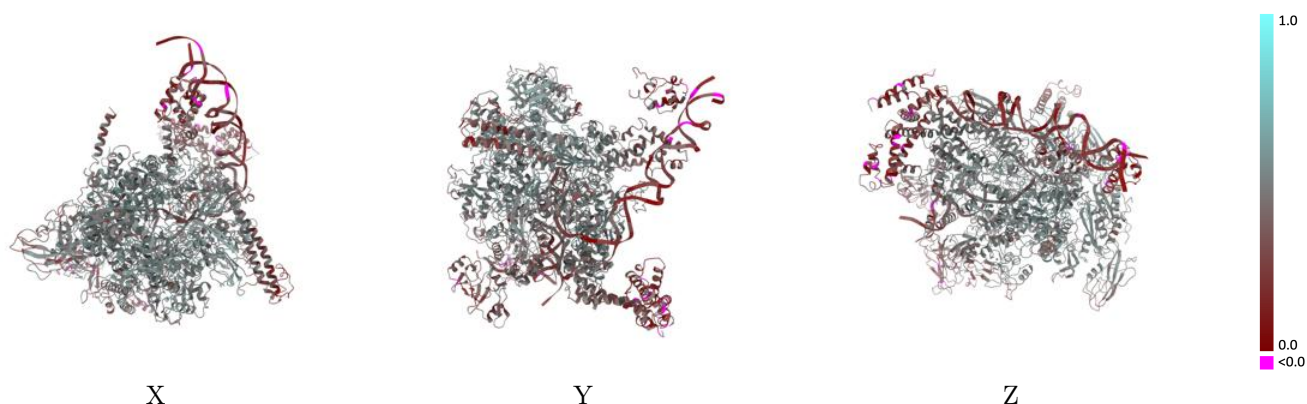
This section contains information regarding the fit between EMDB map EMD-20466 and PDB model 6PSW. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



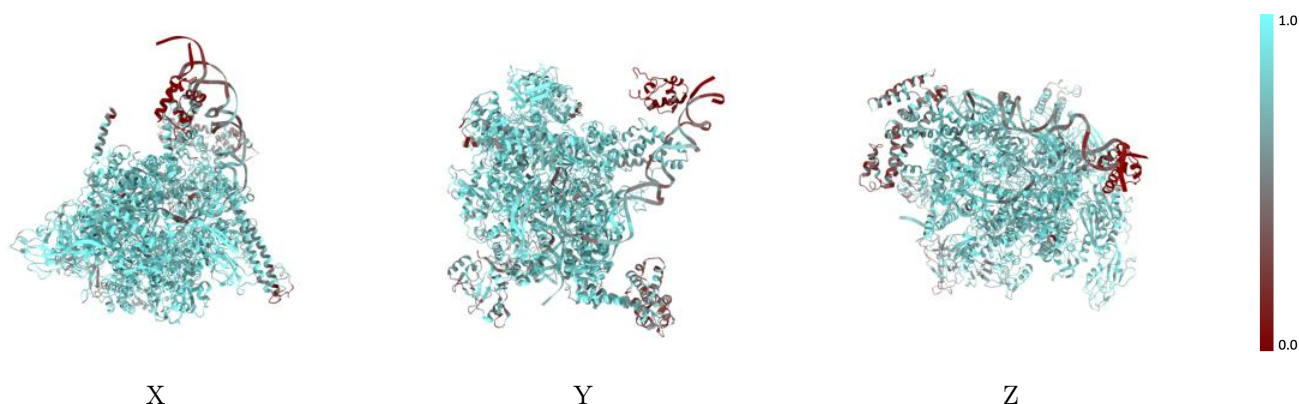
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



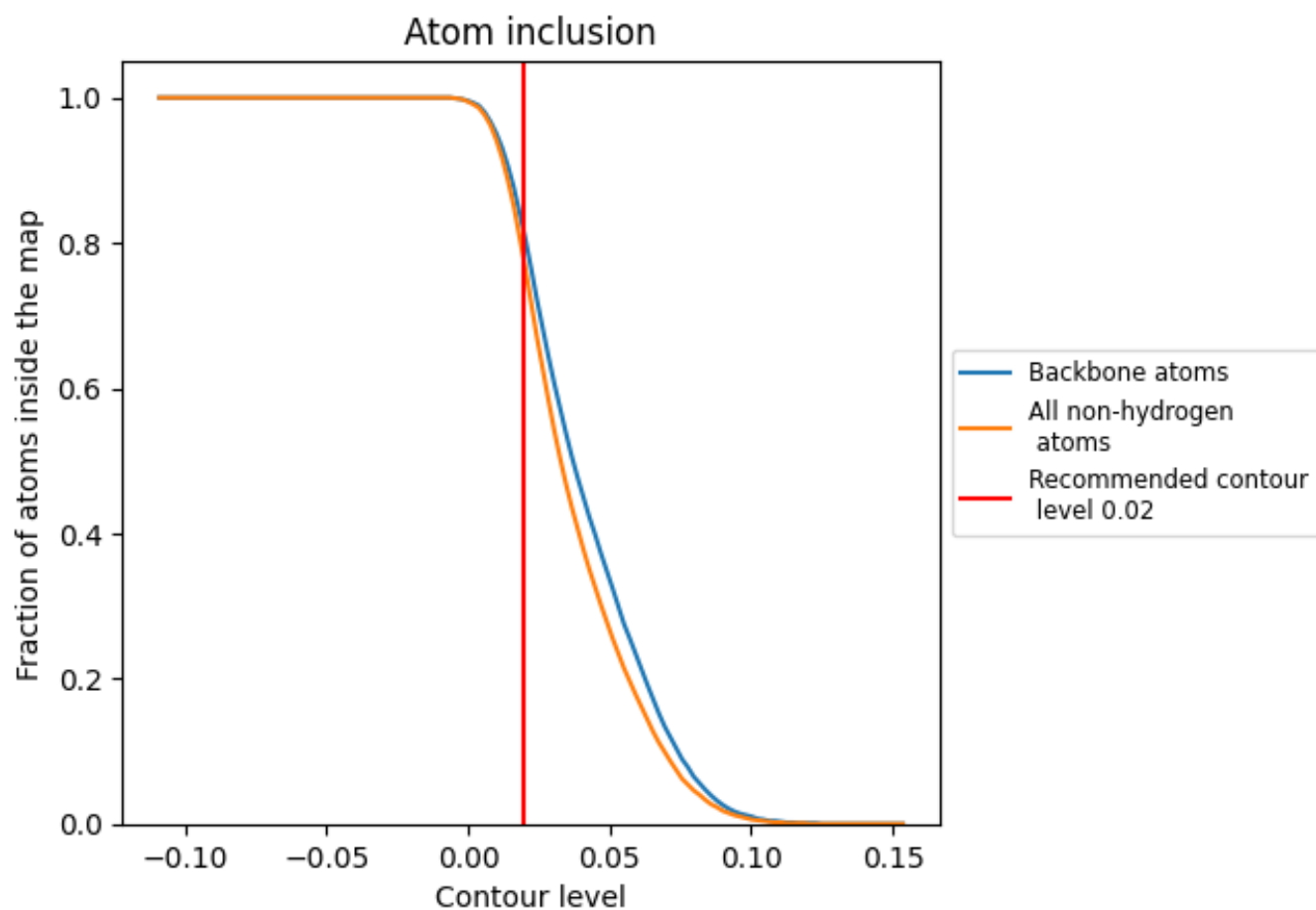
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).























9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7700	 0.4380
G	 0.8590	 0.5010
H	 0.8260	 0.4660
I	 0.8270	 0.4750
J	 0.8220	 0.4710
K	 0.7380	 0.4650
L	 0.6770	 0.3560
M	 0.0460	 0.2530
N	 0.6890	 0.3990
O	 0.6260	 0.2570
P	 0.5650	 0.2460

