



Full wwPDB EM Validation Report ⓘ

Jan 8, 2024 – 07:44 pm GMT

PDB ID : 8REB
EMDB ID : EMD-19081
Title : Cryo-EM structure of bacterial RNA polymerase-sigma54 initial transcribing complex - 6nt complex
Authors : Gao, F.; Zhang, X.
Deposited on : 2023-12-10
Resolution : 3.40 Å(reported)

This is a Full wwPDB EM Validation 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:

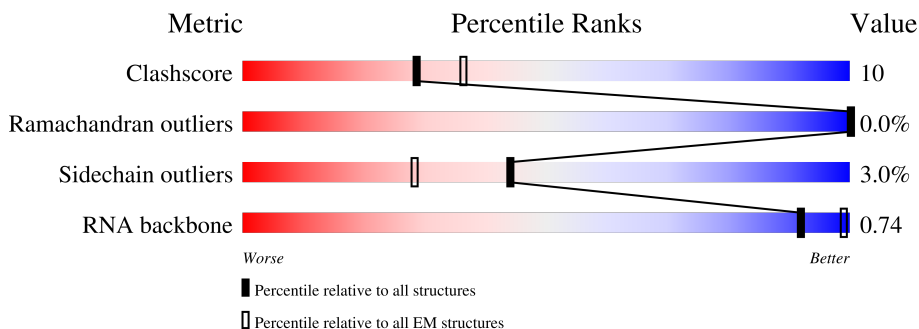
EMDB validation analysis : 0.0.1.dev70
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.40 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
RNA backbone	4643	859

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	43	
2	R	6	
3	T	52	
4	A	321	
4	B	321	
5	C	1341	
6	D	1373	

Continued on next page...

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Mol	Chain	Length	Quality of chain
7	E	74	
8	M	350	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 28681 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 DNA chain called DNA (43-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	N	43	875	419	148	265	43	0	0

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*CP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	R	6	129	57	24	42	6	0	0

- Molecule 3 is a DNA chain called DNA (52-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	T	52	1072	507	207	306	52	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	A	308	2365	1481	415	461	8	0	0
4	B	235	1735	1085	305	340	5	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	C	1341	10080	6328	1748	1964	40	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	D	1330	9682	6085	1738	1818	41	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	E	74	546	337	105	103	1	0	0

- Molecule 8 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	M	350	2194	1385	403	403	3	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

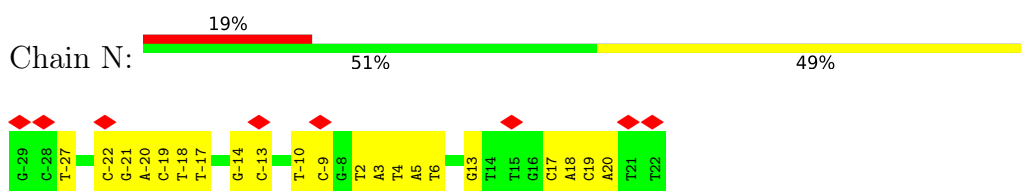
- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

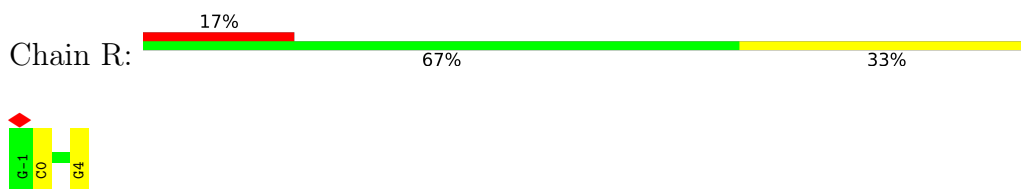
3 Residue-property plots

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.

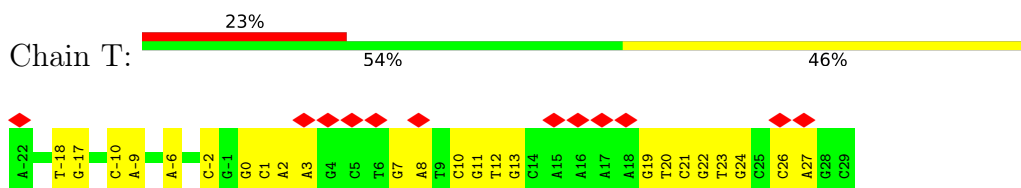
- Molecule 1: DNA (43-MER)



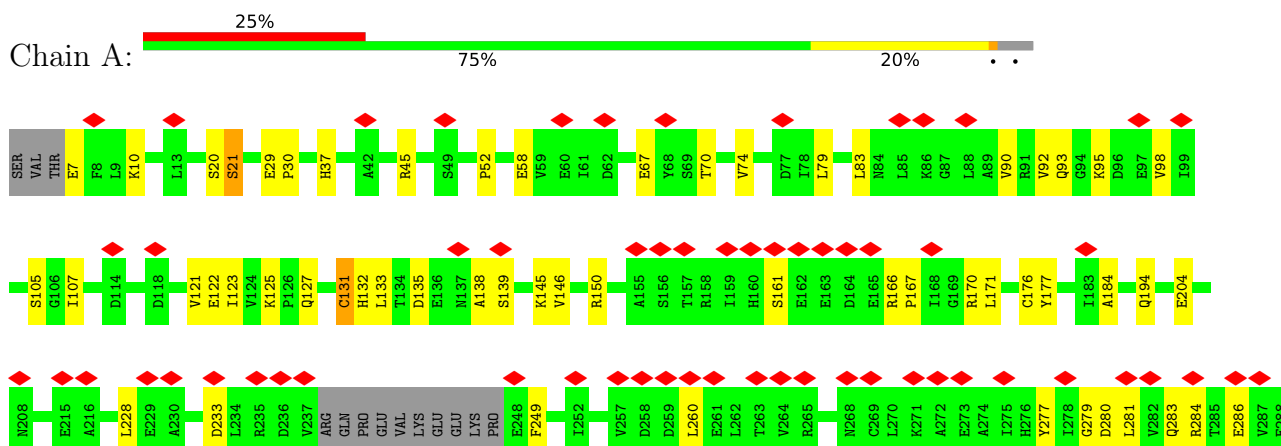
- Molecule 2: RNA (5'-R(P*GP*CP*CP*GP*CP*G)-3')

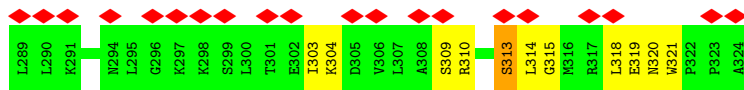


- Molecule 3: DNA (52-MER)

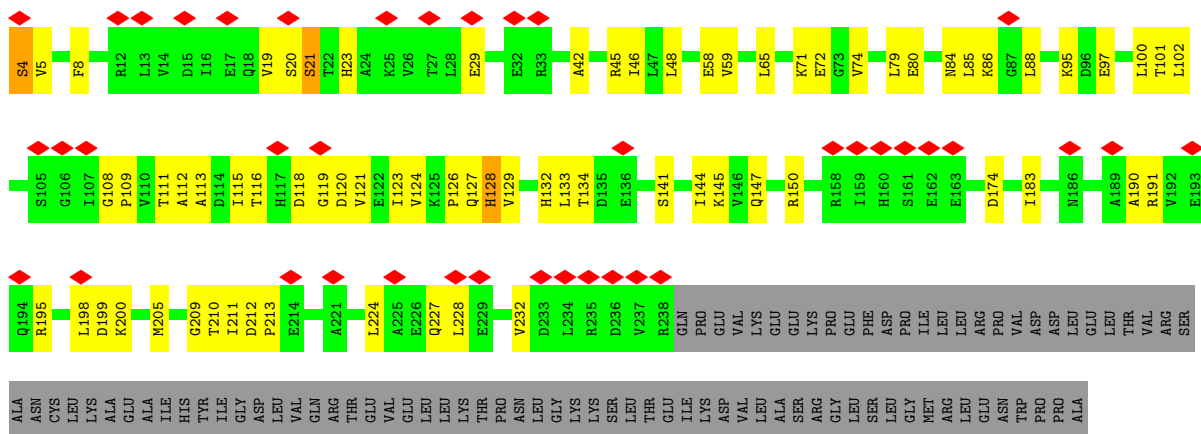


- Molecule 4: DNA-directed RNA polymerase subunit alpha

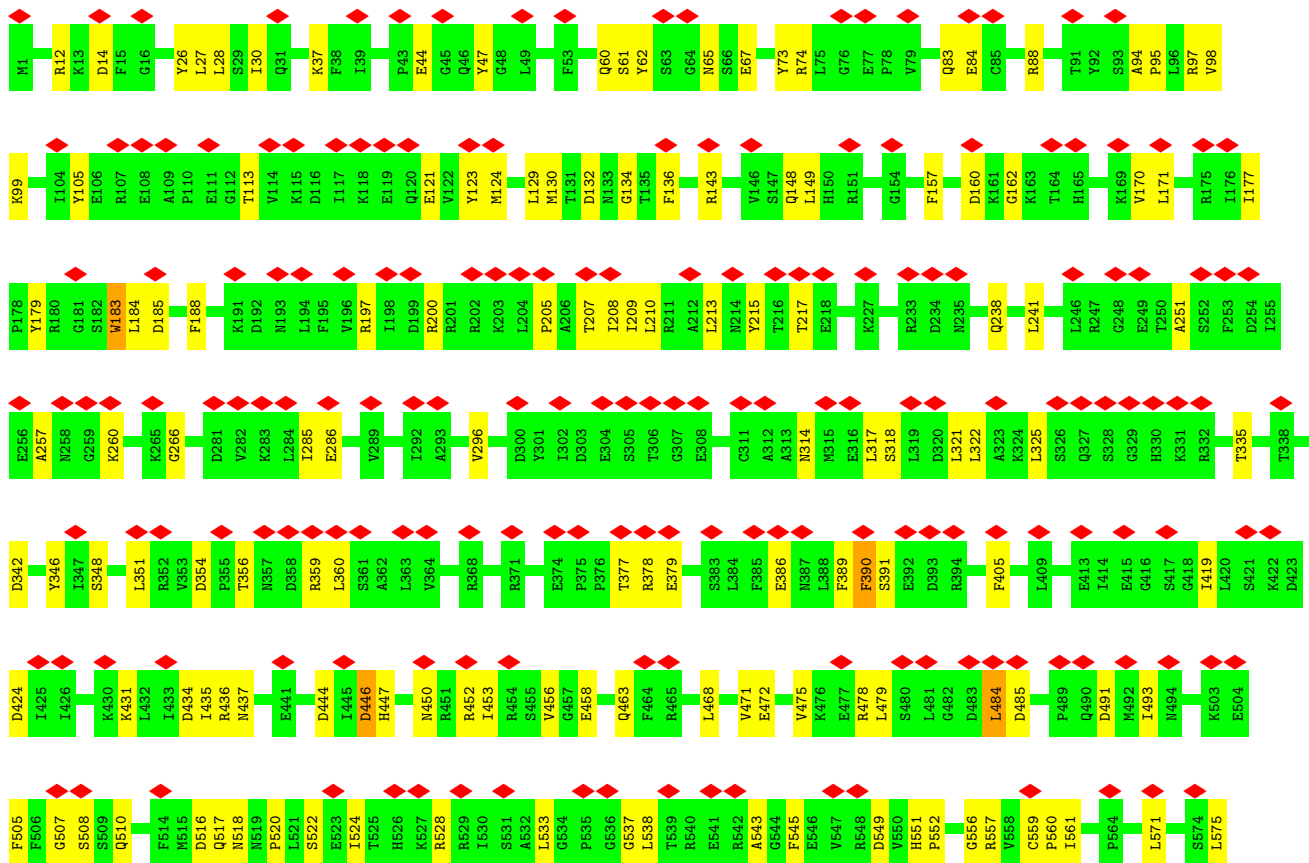
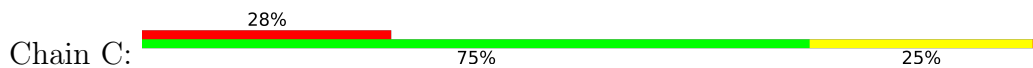


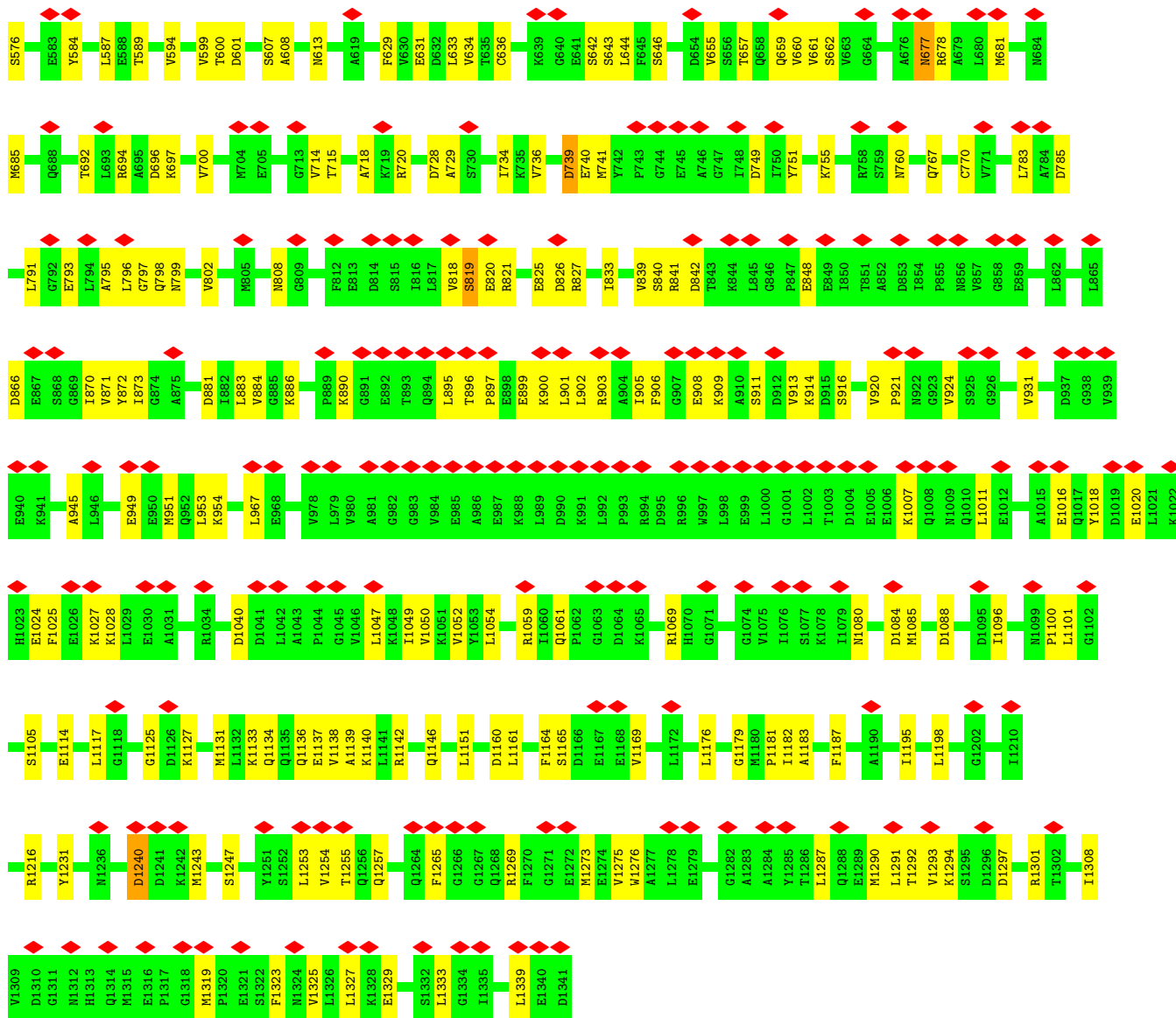


● Molecule 4: DNA-directed RNA polymerase subunit alpha

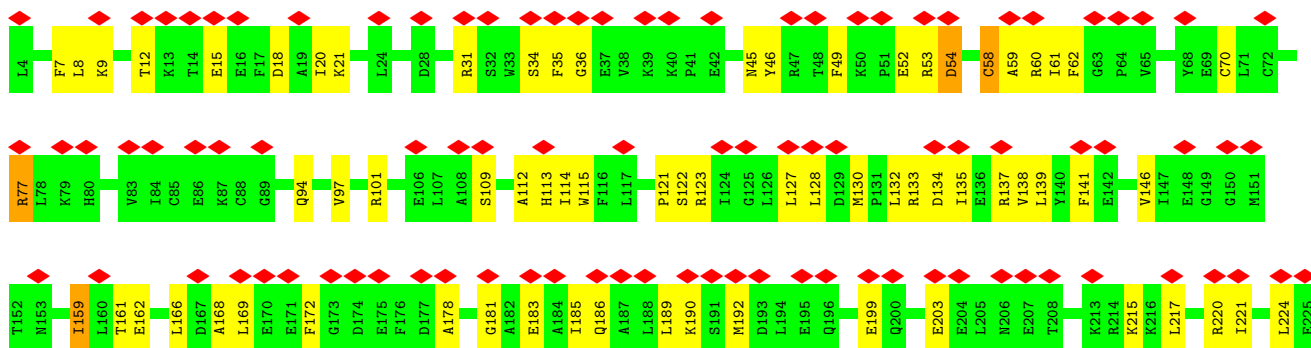
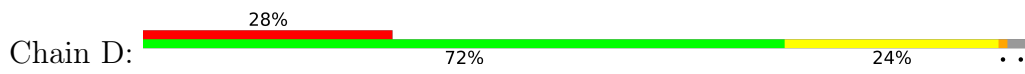


● Molecule 5: DNA-directed RNA polymerase subunit beta

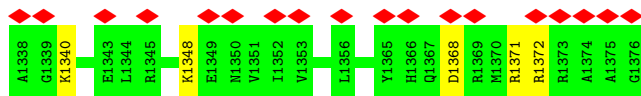




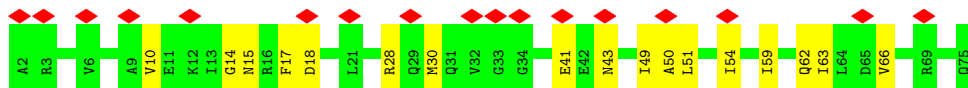
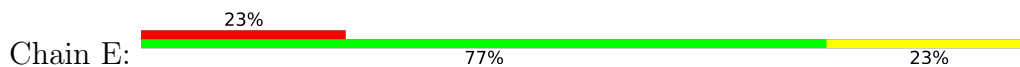
● Molecule 6: DNA-directed RNA polymerase subunit beta'



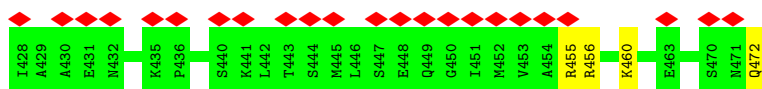
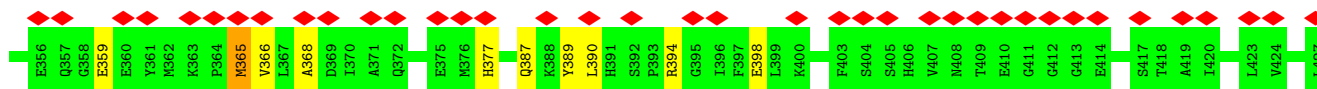
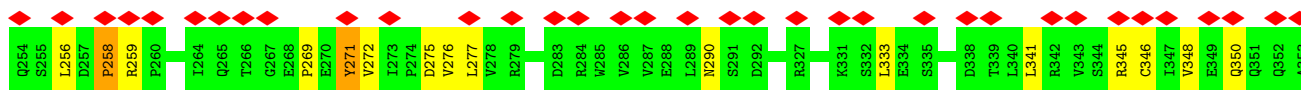
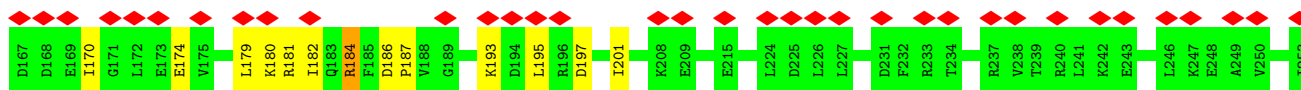
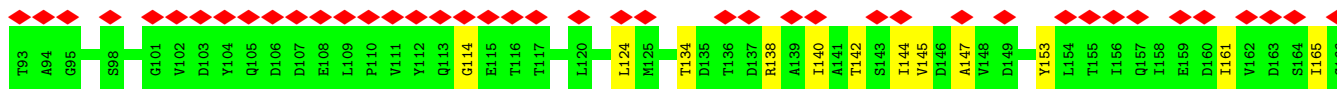
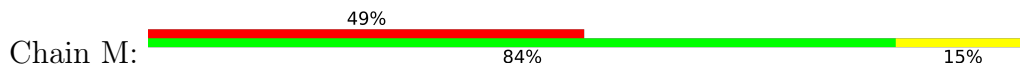
V228	V229	S230	G231	E235	I238	L239	L240	L245	D248	L249	R250	P251	L252	V253	P254	L255	D256	D264	T262	S263	D264	L265	N266	D267	L268	Y269	R270	R271	R275	R281	D284	L285	A286	A287	P288	D289	I290	L291	V292	E295	M298	L299	Q300	E301	A302	V303	D304	A305	L306	L307	R311	R312	G313	I316	T317	G318	S319	N320	K321	R322	P323	L324	K325	S326	L327	A328	D329	M330	I331	K332	G333	G336	R337	Q340	N341	L342	L343	G344	K345	R346	V347	Y349	S350	S353	G358	L363	H364	Q365	C366	G367	L368	K371	M372	A373	L374	E375	P379	F380	I381	Y382	G383	K384	L385	E386	L387	R388	G389	L390	A391	T392	T393	I394	K395	K398	K399	M400	R403	V407	V408	I411	L412	D413	V414	V415	I416	R417	E418	L422	L423	N424	R425	A426	P427	T428	R431	T434	Q435	R436	R437	E438	P439	G444	L449	H450	P451	L452	V453	A456	Q465	M466	A467	V470	P471	L472	L473	L474	E475	A476	E479	A480	R481	A482	L483	N488	N489	P493	G496	I500	D505	V506	V507	L508	G509	L510	C517	V518	N519	A520	P530	R535	S539	R547	V548	K549	H651	E652	I653	E656	V661	A662	E663	I664	Q665	E666	G671	L672	V673	T674	A675	Y679	N680	K681	V682	I685	M686	A687	D691	R692	V693	S694	M697	D699	E704	N708	E713	E714	K715	M725	A730	S733	I737	R738	L740	G742	N743	R744	G745	L746	M747	A748	D751	I754	P758	A761	N762	V769	L770	O771	V772	F773	I774	S775	T776	R780	A784	D785	L788	A791	N792	R798	R799	D802	V803	Q805	D806	L807	V808	V809	T810	T823	P824	V825	L826	E827	V831	K832	E833	D837	A845	E846	D847	K850	G852	T853	A854	D855	I856	V858	F859	R860	N861	T862	L863	C869	L872	V877	D878	K881	V885	D891	F892	G893	V894	C895	V899	D902	L903	A904	H907	G912	E913	A914	V915	G916	V917	A920	Q921	S922	I923	G924	E925	P926	G927	T928	L930	V931	M932	ARG	THR	PHE	HIS	ILE	GLY	GLY	ALA	ALA	SER	ARG	ALA	A945	A946	E947	S948	S949	N954	S957	L960	S961	N962	V963	K964	S965	V966	V967	N968	S969	S970	G971	V974	I975	I976	S977	R978	E981	L984	I985	F988	G989	R990	E993	L1003	A1004	D1007	Q1010	V1011	A1012	A1013	T1016	V1017	A1018	P1022	V1027	I1028	T1029	E1030	V1031	S1032	G1033	F1034	F1037	T1038	D1039	M1040	I1041	D1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	THR	ASP	GLU	LEU	THR	GLY	LEU	S1057	S1058	L1059	L1062	A1065	E1066	R1067	THR	ALA	GLY	LYS	ASP	ASP	R1147	R1148	R1149	P1150	K1151	E1152	P1153	A1154	I1155	L1156	I1159	I1162	V1163	S1164	K1167	E1168	T1169	K1170	R1173	I1177	P1179	V1180	D1181	G1182	S1183	D1184	P1185	Y1186	E1187	R1194	Q1195	L1196	M1197	V1198	G1207	E1215	A1216	F1217	H1218	R1222	G1225	V1226	T1230	E1236	V1237	R1242	L1243	Q1244	G1245	V1246	K1247	I1248	H1252	V1255	Q1259	R1262	K1263	A1264	V1267	N1268	A1269	G1270	S1271	S1272	D1273	F1274	L1275	E1278	Q1279	Y1282	K1286	N1289	R1290	E1293	A1294	N1295	G1296	K1297	V1298	T1301	D1305	I1309	T1310	K1311	L1314	A1315	T1316	E1317	S1318	F1319	S1321	A1322	A1323	S1324	F1325	T1329	R1330	V1331	L1332	T1333	A1336	V1337
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- Molecule 7: DNA-directed RNA polymerase subunit omega



- Molecule 8: RNA polymerase sigma-54 factor



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73619	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0067	Depositor
Map size (\AA)	211.99998, 211.99998, 211.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	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, 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	N	0.49	0/976	0.95	0/1501
2	R	0.40	0/143	0.85	0/221
3	T	0.54	0/1205	0.85	0/1858
4	A	0.28	0/2396	0.55	0/3252
4	B	0.29	0/1754	0.57	0/2388
5	C	0.30	0/10235	0.55	2/13877 (0.0%)
6	D	0.30	0/9818	0.56	5/13339 (0.0%)
7	E	0.30	0/548	0.57	0/743
8	M	0.31	1/2226 (0.0%)	0.60	2/3071 (0.1%)
All	All	0.32	1/29301 (0.0%)	0.60	9/40250 (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
6	D	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	M	258	PRO	CG-CD	-6.00	1.30	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	258	PRO	CA-N-CD	-12.20	94.43	111.50
8	M	258	PRO	N-CD-CG	-9.49	88.97	103.20
6	D	1139	PRO	CA-N-CD	-6.91	101.82	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	159	ILE	CG1-CB-CG2	-5.69	98.89	111.40
5	C	446	ASP	CB-CG-OD1	5.64	123.37	118.30
6	D	699	ASP	CB-CG-OD2	5.55	123.29	118.30
6	D	691	ASP	CB-CG-OD1	5.54	123.28	118.30
5	C	160	ASP	CB-CG-OD1	5.36	123.12	118.30
6	D	1138	LEU	C-N-CD	-5.14	109.28	120.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	D	1138	LEU	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	875	0	490	16	0
2	R	129	0	66	2	0
3	T	1072	0	582	25	0
4	A	2365	0	2387	46	0
4	B	1735	0	1724	47	0
5	C	10080	0	9757	221	0
6	D	9682	0	9408	216	0
7	E	546	0	537	12	0
8	M	2194	0	1711	45	0
9	D	1	0	0	0	0
10	D	2	0	0	0	0
All	All	28681	0	26662	574	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 10.

All (574) 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)
4:B:190:ALA:O	4:B:198:LEU:HB2	1.71	0.89
5:C:883:LEU:HD11	5:C:920:VAL:HG23	1.58	0.86
6:D:825:VAL:HB	6:D:833:GLU:HB2	1.60	0.81
6:D:807:LEU:HD12	6:D:1259:GLN:HE21	1.45	0.80
4:B:183:ILE:HD13	4:B:205:MET:HE2	1.64	0.80
8:M:180:LYS:HG2	8:M:184:ARG:HH12	1.47	0.79
5:C:12:ARG:NH1	5:C:793:GLU:OE2	2.16	0.79
6:D:799:ARG:NH1	6:D:1146:GLU:OE1	2.15	0.79
5:C:1142:ARG:HG2	5:C:1169:VAL:HG11	1.68	0.75
6:D:1177:ILE:HG13	6:D:1179:PRO:HD3	1.70	0.73
5:C:105:TYR:HA	5:C:113:THR:HA	1.71	0.73
1:N:5:DA:H5'	5:C:200:ARG:HH12	1.53	0.72
4:A:281:LEU:HD11	4:A:303:ILE:HD11	1.71	0.72
6:D:342:LEU:HD22	6:D:1324:SER:HB2	1.72	0.71
6:D:46:TYR:O	8:M:387:GLN:NE2	2.24	0.70
4:B:210:THR:O	4:B:211:ILE:HD13	1.92	0.70
6:D:417:ARG:NH1	7:E:43:ASN:OD1	2.25	0.70
4:A:161:SER:OG	4:A:166:ARG:NH2	2.26	0.69
4:B:74:VAL:HA	4:B:134:THR:HA	1.72	0.69
5:C:88:ARG:NH2	5:C:1040:ASP:OD2	2.25	0.69
6:D:388:ARG:NH2	6:D:414:GLU:OE2	2.25	0.69
6:D:1144:LEU:HD11	6:D:1236:GLU:HB3	1.75	0.69
3:T:-2:DC:OP1	6:D:346:ARG:NH2	2.26	0.69
4:A:319:GLU:OE2	4:A:320:ASN:ND2	2.26	0.68
5:C:1276:TRP:HH2	6:D:798:ARG:HG2	1.58	0.68
6:D:275:ARG:NH2	6:D:298:MET:SD	2.65	0.68
5:C:241:LEU:HD11	5:C:285:ILE:HG12	1.75	0.68
6:D:741:ALA:O	6:D:762:ASN:ND2	2.24	0.67
6:D:20:ILE:HD11	6:D:1320:ILE:HG13	1.76	0.67
5:C:1117:LEU:HG	5:C:1182:ILE:HD11	1.75	0.67
3:T:3:DA:H4'	5:C:508:SER:HB2	1.76	0.66
6:D:770:LEU:O	6:D:774:ILE:HG13	1.95	0.66
6:D:342:LEU:HD11	6:D:1348:LYS:HD2	1.75	0.66
5:C:1117:LEU:HD13	5:C:1195:ILE:HG12	1.76	0.66
6:D:826:ILE:HD11	6:D:831:VAL:HG23	1.78	0.66
6:D:1140:ARG:HA	6:D:1143:ASP:HB2	1.78	0.66
6:D:1164:SER:HB3	6:D:1177:ILE:HD12	1.76	0.66
5:C:1061:GLN:NE2	5:C:1240:ASP:OD1	2.30	0.65
5:C:44:GLU:OE1	5:C:44:GLU:N	2.29	0.65
4:A:92:VAL:HG12	4:A:121:VAL:HG22	1.79	0.65
5:C:318:SER:H	5:C:321:LEU:HD12	1.62	0.65
5:C:714:VAL:O	5:C:767:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:5:DA:N6	5:C:537:GLY:O	2.30	0.64
4:B:4:SER:OG	4:B:5:VAL:N	2.30	0.64
6:D:190:LYS:HG2	6:D:235:GLU:HG2	1.79	0.64
4:A:98:VAL:HG23	4:A:146:VAL:HB	1.80	0.64
5:C:799:ASN:O	5:C:827:ARG:NH2	2.31	0.64
6:D:326:SER:OG	6:D:329:ASP:OD1	2.14	0.64
5:C:251:ALA:HB3	5:C:266:GLY:H	1.64	0.63
5:C:61:SER:HB3	5:C:479:LEU:HB2	1.81	0.63
5:C:545:PHE:HE1	6:D:788:LEU:HD12	1.64	0.63
4:A:194:GLN:OE1	4:A:194:GLN:N	2.25	0.63
6:D:385:LEU:HD12	6:D:411:ILE:HD13	1.81	0.63
4:B:113:ALA:HB2	4:B:126:PRO:HB2	1.81	0.63
6:D:1371:ARG:HG3	6:D:1372:ARG:HE	1.63	0.63
8:M:165:ILE:HG21	8:M:170:ILE:HG21	1.80	0.63
8:M:455:ARG:O	8:M:455:ARG:NH1	2.25	0.62
5:C:528:ARG:NH2	5:C:576:SER:O	2.31	0.62
6:D:127:LEU:O	6:D:220:ARG:NH2	2.32	0.62
5:C:207:THR:HA	5:C:210:LEU:HD23	1.79	0.62
6:D:932:MET:HA	6:D:1138:LEU:H	1.65	0.62
6:D:739:GLN:OE1	6:D:744:ARG:NH1	2.32	0.62
5:C:808:ASN:H	6:D:633:ALA:HB2	1.65	0.62
4:A:122:GLU:OE2	4:A:122:GLU:N	2.33	0.62
6:D:646:ILE:HD13	6:D:762:ASN:HD21	1.63	0.62
6:D:36:GLY:HA3	6:D:61:ILE:HG21	1.82	0.61
5:C:84:GLU:O	5:C:88:ARG:HG2	2.00	0.61
6:D:332:LYS:HD2	6:D:340:GLN:HG2	1.82	0.61
6:D:858:VAL:HG12	6:D:862:THR:HG21	1.82	0.61
5:C:739:ASP:OD2	5:C:740:GLU:N	2.33	0.61
5:C:185:ASP:HB2	5:C:197:ARG:HB2	1.83	0.61
6:D:417:ARG:HG3	6:D:418:GLU:HG2	1.83	0.61
5:C:561:ILE:HD11	6:D:772:TYR:HE2	1.64	0.60
6:D:49:PHE:HE1	8:M:387:GLN:HE22	1.47	0.60
8:M:144:ILE:HD12	8:M:179:LEU:HD13	1.83	0.60
4:B:97:GLU:HG3	4:B:147:GLN:HB3	1.83	0.60
5:C:677:ASN:O	5:C:681:MET:HG3	2.00	0.60
4:A:58:GLU:OE2	4:A:170:ARG:NH1	2.26	0.60
4:A:92:VAL:HG11	4:A:98:VAL:HG21	1.83	0.60
4:A:313:SER:HB3	8:M:181:ARG:HE	1.66	0.60
6:D:268:LEU:HD13	6:D:306:LEU:HA	1.83	0.60
6:D:833:GLU:OE1	6:D:1242:ARG:NH1	2.32	0.60
6:D:748:ALA:HB3	6:D:754:ILE:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:45:ASN:N	6:D:52:GLU:OE2	2.35	0.60
1:N:-20:DA:H2''	1:N:-19:DC:H5''	1.83	0.60
5:C:1069:ARG:NH1	5:C:1114:GLU:OE2	2.35	0.60
7:E:59:ILE:HA	7:E:63:ILE:HD11	1.84	0.60
5:C:517:GLN:HG3	5:C:760:ASN:H	1.66	0.59
6:D:846:GLU:HG2	6:D:881:LYS:HB3	1.84	0.59
4:A:10:LYS:NZ	4:B:227:GLN:OE1	2.35	0.59
3:T:7:DG:H1'	3:T:8:DA:C5	2.38	0.59
6:D:416:ILE:HG23	6:D:439:PRO:HG2	1.83	0.59
5:C:559:CYS:HB2	5:C:662:SER:HB3	1.84	0.59
5:C:897:PRO:HA	5:C:900:LYS:HG2	1.85	0.59
6:D:606:ASN:OD1	6:D:610:ARG:NH1	2.35	0.59
6:D:1011:VAL:HG22	6:D:1013:GLY:H	1.66	0.59
6:D:15:GLU:OE2	6:D:15:GLU:N	2.34	0.58
5:C:631:GLU:OE1	5:C:633:LEU:N	2.34	0.58
5:C:1269:ARG:NH1	6:D:344:GLY:O	2.36	0.58
5:C:1327:LEU:HD21	5:C:1339:LEU:HD21	1.85	0.58
6:D:493:PRO:HB3	6:D:904:ALA:HB2	1.85	0.58
4:A:127:GLN:OE1	4:A:127:GLN:N	2.36	0.58
6:D:374:LEU:HB2	6:D:412:LEU:HD22	1.86	0.58
4:A:131:CYS:SG	4:A:132:HIS:N	2.77	0.58
5:C:200:ARG:HG3	5:C:200:ARG:HH11	1.68	0.58
6:D:535:ARG:O	6:D:539:SER:OG	2.21	0.58
5:C:1308:ILE:HG21	6:D:379:PRO:HB2	1.85	0.57
6:D:805:GLN:HG3	6:D:806:ASP:N	2.17	0.57
5:C:478:ARG:HH12	5:C:491:ASP:HA	1.69	0.57
5:C:607:SER:OG	5:C:608:ALA:N	2.38	0.57
6:D:746:LEU:HA	6:D:758:PRO:HB3	1.87	0.57
4:A:37:HIS:HB2	4:B:45:ARG:HH21	1.70	0.57
4:B:113:ALA:N	4:B:126:PRO:O	2.36	0.57
8:M:180:LYS:O	8:M:184:ARG:NH1	2.38	0.57
6:D:52:GLU:N	6:D:52:GLU:OE1	2.38	0.57
6:D:596:LEU:HA	6:D:600:ALA:HB3	1.87	0.57
6:D:380:PHE:HB3	6:D:415:VAL:HG21	1.86	0.57
5:C:901:LEU:O	5:C:905:ILE:HG22	2.04	0.56
6:D:530:PRO:HB2	6:D:581:MET:HG3	1.87	0.56
5:C:60:GLN:HB3	5:C:67:GLU:HG2	1.88	0.56
5:C:1253:LEU:HB2	8:M:114:GLY:HA3	1.87	0.56
4:B:124:VAL:HG21	4:B:210:THR:HG22	1.87	0.56
3:T:2:DA:H2''	3:T:3:DA:C8	2.41	0.56
7:E:62:GLN:O	7:E:66:VAL:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:130:MET:SD	5:C:134:GLY:HA2	2.46	0.56
6:D:245:LEU:O	6:D:250:ARG:NH1	2.39	0.56
5:C:296:VAL:O	5:C:335:THR:OG1	2.17	0.56
5:C:390:PHE:HA	5:C:419:ILE:HG13	1.87	0.56
5:C:518:ASN:O	5:C:522:SER:HB3	2.05	0.56
5:C:890:LYS:HE3	5:C:890:LYS:HA	1.88	0.56
6:D:159:ILE:HG22	6:D:159:ILE:O	2.05	0.56
6:D:474:LEU:HD12	7:E:28:ARG:HE	1.70	0.56
5:C:12:ARG:HE	5:C:1183:ALA:HB2	1.70	0.56
6:D:808:VAL:HG12	6:D:914:ALA:HA	1.86	0.56
2:R:4:G:O2'	6:D:425:ARG:NH2	2.37	0.55
5:C:162:GLY:HA3	5:C:170:VAL:HG22	1.87	0.55
6:D:381:ILE:HD11	6:D:412:LEU:HD13	1.88	0.55
6:D:58:CYS:SG	6:D:59:ALA:N	2.78	0.55
5:C:660:VAL:HG13	5:C:661:VAL:HG13	1.88	0.55
5:C:883:LEU:HD23	5:C:1052:VAL:HG11	1.88	0.55
5:C:890:LYS:HD3	5:C:914:LYS:HD3	1.88	0.55
6:D:582:ILE:HD11	6:D:623:GLN:HB3	1.88	0.55
6:D:224:LEU:O	6:D:228:VAL:HG13	2.06	0.55
3:T:11:DG:H2'	3:T:12:DT:H71	1.89	0.55
4:A:105:SER:HB2	4:A:139:SER:HB3	1.88	0.55
5:C:797:GLY:N	5:C:1231:TYR:OH	2.38	0.55
6:D:968:ASN:HA	6:D:1118:GLY:HA3	1.89	0.55
6:D:708:ASN:HA	6:D:713:GLU:HA	1.89	0.55
4:B:80:GLU:O	4:B:84:ASN:ND2	2.40	0.54
5:C:207:THR:HG21	5:C:351:LEU:HB2	1.88	0.54
5:C:257:ALA:N	5:C:260:LYS:O	2.35	0.54
6:D:742:GLY:O	6:D:762:ASN:HB3	2.07	0.54
4:B:212:ASP:OD1	4:B:213:PRO:HD2	2.06	0.54
4:B:59:VAL:HG12	4:B:144:ILE:HG22	1.89	0.54
5:C:360:LEU:HD11	5:C:378:ARG:HD3	1.89	0.54
1:N:5:DA:H5'	5:C:200:ARG:NH1	2.20	0.54
5:C:906:PHE:CZ	8:M:258:PRO:HD3	2.43	0.54
5:C:1275:VAL:HG13	5:C:1287:LEU:HD11	1.89	0.54
5:C:903:ARG:HD2	5:C:908:GLU:O	2.08	0.54
5:C:209:ILE:HG13	5:C:210:LEU:HD22	1.90	0.54
5:C:629:PHE:CD2	5:C:634:VAL:HG11	2.42	0.54
5:C:533:LEU:HD21	5:C:571:LEU:HD13	1.91	0.53
6:D:926:PRO:HG2	6:D:1248:ILE:HD11	1.91	0.53
8:M:197:ASP:O	8:M:201:ILE:HG22	2.07	0.53
4:A:167:PRO:HD2	4:A:170:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:309:SER:O	8:M:184:ARG:NH2	2.41	0.53
6:D:53:ARG:HG3	6:D:54:ASP:OD2	2.09	0.53
8:M:144:ILE:HG22	8:M:161:ILE:HD13	1.90	0.53
4:A:90:VAL:HG12	4:A:123:ILE:HD13	1.89	0.53
4:A:95:LYS:HE2	4:A:98:VAL:HG12	1.89	0.53
5:C:472:GLU:HA	5:C:475:VAL:HG12	1.90	0.53
6:D:507:VAL:HG11	6:D:598:LYS:HB2	1.90	0.53
5:C:718:ALA:HB2	5:C:783:LEU:HD21	1.91	0.53
5:C:1146:GLN:HE22	5:C:1160:ASP:HA	1.74	0.53
5:C:424:ASP:OD1	5:C:424:ASP:N	2.41	0.53
8:M:275:ASP:O	8:M:290:ASN:ND2	2.41	0.53
4:B:20:SER:OG	4:B:21:SER:N	2.42	0.53
5:C:377:THR:OG1	5:C:379:GLU:OE1	2.19	0.53
5:C:1125:GLY:HA3	5:C:1179:GLY:HA2	1.90	0.52
4:A:90:VAL:HG21	4:A:146:VAL:HG11	1.91	0.52
5:C:95:PRO:HB3	5:C:123:TYR:HE2	1.73	0.52
5:C:561:ILE:HD11	6:D:772:TYR:CE2	2.43	0.52
5:C:444:ASP:O	5:C:450:ASN:ND2	2.42	0.52
5:C:560:PRO:HB2	6:D:776:THR:HG21	1.91	0.52
5:C:870:ILE:HG21	5:C:931:VAL:HG11	1.91	0.52
5:C:1290:MET:HG3	6:D:347:VAL:HG11	1.90	0.52
5:C:97:ARG:HB3	5:C:121:GLU:HG3	1.92	0.52
5:C:346:TYR:O	5:C:348:SER:N	2.38	0.52
5:C:692:THR:HG21	5:C:798:GLN:HE21	1.73	0.52
6:D:97:VAL:HG21	6:D:101:ARG:HH21	1.75	0.52
6:D:128:LEU:HB3	6:D:130:MET:HG2	1.92	0.52
5:C:734:ILE:HD12	5:C:751:TYR:HE1	1.74	0.52
5:C:1024:GLU:HA	5:C:1027:LYS:HG2	1.91	0.52
6:D:115:TRP:CH2	6:D:1329:THR:HG22	2.45	0.52
3:T:19:DG:H2'	3:T:20:DT:H71	1.91	0.52
4:B:111:THR:HA	4:B:129:VAL:HA	1.92	0.52
8:M:140:ILE:O	8:M:144:ILE:HG23	2.09	0.51
3:T:1:DC:H2''	3:T:2:DA:C8	2.45	0.51
6:D:94:GLN:O	6:D:94:GLN:HG3	2.11	0.51
5:C:551:HIS:CD2	5:C:552:PRO:HD2	2.44	0.51
1:N:6:DT:H73	3:T:-6:DA:C6	2.44	0.51
3:T:21:DC:H2''	3:T:22:DG:C8	2.44	0.51
5:C:1127:LYS:O	5:C:1131:MET:HG3	2.10	0.51
6:D:112:ALA:HA	6:D:238:ILE:HG22	1.91	0.51
6:D:390:LEU:HD21	6:D:407:VAL:HG21	1.91	0.51
8:M:186:ASP:HB3	8:M:187:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:35:PHE:CD2	6:D:101:ARG:HG2	2.45	0.51
6:D:925:GLU:HB3	6:D:926:PRO:HD3	1.93	0.51
6:D:1156:LEU:HD23	6:D:1207:GLY:HA2	1.93	0.51
5:C:434:ASP:OD2	5:C:435:ILE:N	2.44	0.51
6:D:135:ILE:HA	6:D:138:VAL:HG12	1.92	0.51
6:D:186:GLN:O	6:D:190:LYS:HG3	2.10	0.51
6:D:847:ASP:OD1	6:D:860:ARG:N	2.44	0.51
4:A:135:ASP:HB3	4:A:138:ALA:HB2	1.93	0.51
5:C:354:ASP:OD2	5:C:356:THR:OG1	2.28	0.50
6:D:652:GLU:O	6:D:656:GLU:HG3	2.10	0.50
1:N:-10:DT:H3	3:T:10:DC:H42	1.59	0.50
6:D:373:ALA:C	6:D:375:GLU:H	2.14	0.50
6:D:582:ILE:HG23	6:D:620:PHE:HE1	1.77	0.50
5:C:1291:LEU:HD13	6:D:345:LYS:HD2	1.92	0.50
5:C:452:ARG:NH2	5:C:458:GLU:OE2	2.44	0.50
8:M:142:THR:HA	8:M:145:VAL:HG12	1.93	0.50
6:D:1109:LEU:HD22	6:D:1113:VAL:HG21	1.92	0.50
1:N:13:DG:C3'	6:D:133:ARG:HH22	2.23	0.50
5:C:808:ASN:OD1	5:C:1216:ARG:NH2	2.45	0.50
5:C:871:VAL:HG13	5:C:883:LEU:HA	1.94	0.50
6:D:1004:ALA:N	6:D:1017:VAL:O	2.44	0.50
4:B:109:PRO:HA	4:B:132:HIS:HA	1.93	0.50
5:C:157:PHE:HE2	5:C:431:LYS:HZ3	1.60	0.50
8:M:276:VAL:HG23	8:M:277:LEU:HD23	1.93	0.50
5:C:342:ASP:O	5:C:437:ASN:HB3	2.12	0.50
5:C:538:LEU:HD13	5:C:543:ALA:HB2	1.93	0.50
6:D:271:ARG:O	6:D:275:ARG:HG2	2.12	0.50
6:D:475:GLU:O	6:D:479:GLU:HG3	2.12	0.50
6:D:733:SER:O	6:D:737:ILE:HG12	2.12	0.50
5:C:179:TYR:OH	5:C:458:GLU:OE2	2.22	0.49
5:C:1254:VAL:HG22	5:C:1255:THR:HG23	1.92	0.49
5:C:796:LEU:N	5:C:1231:TYR:OH	2.45	0.49
6:D:77:ARG:HH11	8:M:147:ALA:HA	1.75	0.49
6:D:451:PRO:HG2	6:D:625:MET:SD	2.52	0.49
4:B:101:THR:H	4:B:116:THR:HG22	1.76	0.49
6:D:957:SER:HA	6:D:1010:GLN:HA	1.94	0.49
6:D:1368:ASP:O	6:D:1372:ARG:HG2	2.12	0.49
7:E:41:GLU:HG2	7:E:49:ILE:HD11	1.93	0.49
5:C:728:ASP:OD1	5:C:729:ALA:N	2.44	0.49
6:D:1003:LEU:HA	6:D:1018:ALA:HA	1.95	0.49
8:M:366:VAL:HG13	8:M:368:ALA:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:890:LYS:HG2	5:C:913:VAL:HA	1.95	0.49
6:D:141:PHE:HE1	6:D:181:GLY:HA2	1.77	0.49
4:A:29:GLU:HB3	4:A:30:PRO:HD3	1.94	0.49
5:C:560:PRO:CB	6:D:776:THR:HG21	2.43	0.49
5:C:696:ASP:OD2	5:C:799:ASN:ND2	2.46	0.49
5:C:1136:GLN:HB3	5:C:1140:LYS:HD2	1.93	0.49
2:R:0:C:H5'	5:C:510:GLN:HE22	1.76	0.49
5:C:485:ASP:OD1	5:C:485:ASP:N	2.41	0.49
5:C:655:VAL:HG12	5:C:659:GLN:OE1	2.13	0.49
6:D:681:LYS:O	6:D:685:ILE:HG22	2.12	0.49
1:N:-18:DT:C6	1:N:-17:DT:H72	2.47	0.49
5:C:557:ARG:HG2	5:C:587:LEU:HB3	1.94	0.49
4:A:45:ARG:NH1	5:C:1084:ASP:OD1	2.33	0.48
6:D:948:SER:HB2	6:D:1022:PRO:HB3	1.95	0.48
6:D:1149:ARG:HB3	6:D:1149:ARG:NH1	2.27	0.48
4:B:29:GLU:HB2	4:B:200:LYS:HG3	1.96	0.48
5:C:1101:LEU:HD21	6:D:508:LEU:HD22	1.94	0.48
4:B:133:LEU:HG	4:B:134:THR:H	1.78	0.48
6:D:517:CYS:SG	6:D:520:ALA:HB2	2.54	0.48
6:D:872:LEU:HB2	6:D:877:VAL:HG21	1.95	0.48
6:D:1162:ILE:HD12	6:D:1162:ILE:H	1.78	0.48
6:D:1169:THR:O	6:D:1169:THR:OG1	2.28	0.48
3:T:23:DT:H2'	3:T:24:DG:C8	2.48	0.48
5:C:1319:MET:HE3	5:C:1323:PHE:HD2	1.78	0.48
5:C:1176:LEU:HD22	5:C:1181:PRO:HD2	1.95	0.48
6:D:1180:VAL:HA	6:D:1185:PRO:HB3	1.95	0.48
4:A:58:GLU:HG2	4:A:145:LYS:HB3	1.96	0.48
5:C:820:GLU:N	5:C:1080:ASN:O	2.47	0.48
5:C:1151:LEU:HD23	5:C:1198:LEU:HD13	1.96	0.48
6:D:640:GLY:N	6:D:643:ASP:OD2	2.44	0.48
5:C:643:SER:OG	5:C:644:LEU:N	2.47	0.48
5:C:715:THR:HG22	5:C:785:ASP:HA	1.96	0.48
8:M:144:ILE:HD11	8:M:182:ILE:HD12	1.94	0.48
6:D:554:GLU:OE2	6:D:570:LYS:NZ	2.36	0.48
6:D:847:ASP:HB3	6:D:856:ILE:HD12	1.95	0.48
4:B:118:ASP:OD2	4:B:119:GLY:N	2.46	0.48
4:B:133:LEU:HG	4:B:134:THR:N	2.28	0.48
6:D:332:LYS:HB3	6:D:337:ARG:HA	1.96	0.48
6:D:798:ARG:HH22	6:D:1325:PHE:HA	1.78	0.48
5:C:65:ASN:HB3	5:C:105:TYR:HB2	1.96	0.47
8:M:365:MET:HE3	8:M:365:MET:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:13:DG:H2''	8:M:377:HIS:CD2	2.49	0.47
5:C:317:LEU:HD13	5:C:322:LEU:HD21	1.94	0.47
5:C:468:LEU:O	5:C:471:VAL:HG12	2.14	0.47
6:D:7:PHE:HE1	6:D:9:LYS:HD3	1.78	0.47
6:D:141:PHE:CE1	6:D:181:GLY:HA2	2.48	0.47
5:C:205:PRO:O	5:C:208:ILE:HG12	2.14	0.47
5:C:524:ILE:O	5:C:528:ARG:HG2	2.14	0.47
5:C:636:CYS:O	5:C:642:SER:HA	2.15	0.47
5:C:1325:VAL:O	5:C:1329:GLU:HG3	2.15	0.47
6:D:322:ARG:HG3	6:D:323:PRO:HD2	1.97	0.47
6:D:307:LEU:HD23	6:D:307:LEU:HA	1.74	0.47
3:T:12:DT:H2''	3:T:13:DG:C8	2.50	0.47
6:D:1046:ILE:HD12	6:D:1059:LEU:HD13	1.96	0.47
4:B:85:LEU:HA	4:B:88:LEU:HD23	1.96	0.47
4:B:127:GLN:OE1	4:B:127:GLN:N	2.36	0.47
5:C:839:VAL:HG21	5:C:841:ARG:NH2	2.29	0.47
6:D:168:ALA:O	6:D:172:PHE:N	2.48	0.47
3:T:13:DG:H8	8:M:377:HIS:CG	2.33	0.47
4:B:71:LYS:O	4:B:72:GLU:HG2	2.14	0.47
5:C:484:LEU:HD12	5:C:484:LEU:H	1.80	0.47
5:C:1088:ASP:OD1	5:C:1088:ASP:N	2.36	0.47
6:D:337:ARG:O	6:D:342:LEU:HB3	2.14	0.47
6:D:438:GLU:OE2	6:D:481:ARG:NH2	2.48	0.47
6:D:598:LYS:HA	6:D:601:ILE:HG22	1.97	0.47
6:D:615:LYS:O	6:D:619:ILE:HG12	2.15	0.47
1:N:-22:DC:H2''	1:N:-21:DG:C8	2.50	0.47
4:A:228:LEU:HD11	4:B:224:LEU:HD23	1.96	0.47
5:C:833:ILE:HA	5:C:1054:LEU:O	2.15	0.47
5:C:902:LEU:HD13	8:M:259:ARG:NH2	2.30	0.47
5:C:1016:GLU:O	5:C:1020:GLU:HG3	2.14	0.47
3:T:26:DC:H2''	3:T:27:DA:C8	2.50	0.47
5:C:314:ASN:HD21	5:C:351:LEU:HD23	1.80	0.47
1:N:19:DC:H2''	1:N:20:DA:C8	2.51	0.46
8:M:174:GLU:OE1	8:M:174:GLU:N	2.38	0.46
6:D:183:GLU:HA	6:D:186:GLN:HG3	1.96	0.46
5:C:74:ARG:HH21	5:C:97:ARG:HG3	1.79	0.46
6:D:217:LEU:O	6:D:221:ILE:HG12	2.15	0.46
6:D:566:LYS:HB2	6:D:566:LYS:HE3	1.64	0.46
5:C:217:THR:HG23	5:C:351:LEU:HD21	1.96	0.46
5:C:557:ARG:HB3	5:C:587:LEU:HD13	1.97	0.46
5:C:802:VAL:HG22	5:C:1096:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:839:VAL:HG12	5:C:1049:ILE:HD13	1.96	0.46
5:C:866:ASP:HB3	5:C:872:TYR:CE1	2.51	0.46
6:D:199:GLU:O	6:D:203:GLU:HG2	2.16	0.46
5:C:895:LEU:HB3	5:C:900:LYS:HE3	1.96	0.46
3:T:8:DA:C8	8:M:333:LEU:HD21	2.50	0.46
4:A:184:ALA:HB3	4:A:204:GLU:HG2	1.98	0.46
5:C:149:LEU:HD12	5:C:453:ILE:HG13	1.97	0.46
6:D:1109:LEU:HB3	6:D:1113:VAL:HG11	1.98	0.46
1:N:2:DT:H2''	1:N:3:DA:C2	2.51	0.46
6:D:827:GLU:OE2	6:D:827:GLU:N	2.48	0.46
8:M:134:THR:O	8:M:138:ARG:N	2.40	0.46
8:M:341:LEU:O	8:M:345:ARG:HG2	2.15	0.46
6:D:1149:ARG:HH12	6:D:1153:PRO:HG2	1.81	0.46
3:T:2:DA:C8	3:T:2:DA:H5''	2.51	0.45
4:B:228:LEU:O	4:B:232:VAL:HG23	2.15	0.45
5:C:136:PHE:CZ	5:C:456:VAL:HG11	2.51	0.45
5:C:700:VAL:O	5:C:1069:ARG:NH2	2.48	0.45
5:C:1020:GLU:O	5:C:1024:GLU:HG2	2.15	0.45
5:C:1247:SER:HB3	6:D:375:GLU:O	2.16	0.45
6:D:134:ASP:OD2	6:D:137:ARG:NH2	2.47	0.45
7:E:10:VAL:O	7:E:14:GLY:HA2	2.16	0.45
4:A:107:ILE:HD12	4:A:107:ILE:HA	1.81	0.45
4:A:286:GLU:OE1	4:A:304:LYS:NZ	2.32	0.45
5:C:945:ALA:O	5:C:949:GLU:HG2	2.17	0.45
6:D:452:LEU:HB3	6:D:500:ILE:HG23	1.98	0.45
6:D:803:VAL:HG11	6:D:1309:ILE:HG22	1.98	0.45
5:C:951:MET:O	5:C:954:LYS:HG2	2.15	0.45
6:D:518:VAL:HA	6:D:547:ARG:NH2	2.31	0.45
3:T:7:DG:OP2	6:D:255:LEU:HD11	2.16	0.45
4:B:102:LEU:HB3	4:B:115:ILE:HG22	1.98	0.45
5:C:95:PRO:HB3	5:C:123:TYR:CE2	2.51	0.45
5:C:921:PRO:HG2	5:C:924:VAL:HG21	1.97	0.45
5:C:1297:ASP:O	5:C:1301:ARG:HG3	2.17	0.45
6:D:832:LYS:HA	6:D:832:LYS:HD2	1.63	0.45
6:D:1045:THR:HB	6:D:1062:LEU:HA	1.98	0.45
5:C:463:GLN:HG3	5:C:505:PHE:HB2	1.98	0.45
5:C:841:ARG:HD2	8:M:272:VAL:HG13	1.97	0.45
7:E:15:ASN:HB3	7:E:18:ASP:H	1.82	0.45
8:M:345:ARG:HA	8:M:348:VAL:HG12	1.99	0.45
6:D:804:ALA:O	6:D:916:GLY:HA3	2.17	0.45
6:D:850:LYS:HG3	6:D:851:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:24:DG:O6	8:M:460:LYS:NZ	2.40	0.44
5:C:452:ARG:HH22	5:C:458:GLU:CD	2.20	0.44
6:D:549:LYS:HG2	6:D:571:ASP:OD1	2.17	0.44
6:D:1267:VAL:HG23	6:D:1268:ASN:OD1	2.16	0.44
7:E:50:ALA:O	7:E:54:ILE:HG13	2.17	0.44
5:C:524:ILE:HD12	5:C:524:ILE:HA	1.84	0.44
6:D:114:ILE:HD11	6:D:311:ARG:HG3	1.99	0.44
8:M:346:CYS:O	8:M:350:GLN:HG3	2.16	0.44
5:C:1161:LEU:HD22	5:C:1164:PHE:HD2	1.82	0.44
6:D:902:ASP:OD1	6:D:902:ASP:N	2.50	0.44
4:A:70:THR:HG21	5:C:755:LYS:HG3	1.98	0.44
5:C:840:SER:O	5:C:1047:LEU:HG	2.17	0.44
4:A:93:GLN:N	4:A:93:GLN:OE1	2.51	0.44
5:C:517:GLN:HG3	5:C:760:ASN:HB2	1.99	0.44
7:E:15:ASN:C	7:E:17:PHE:H	2.20	0.44
4:A:20:SER:OG	4:A:21:SER:N	2.51	0.44
5:C:434:ASP:HA	5:C:437:ASN:OD1	2.18	0.44
6:D:262:THR:HG21	6:D:270:ARG:HH21	1.81	0.44
6:D:398:LYS:HB3	6:D:398:LYS:HE3	1.81	0.44
6:D:1279:GLN:OE1	6:D:1279:GLN:N	2.44	0.44
4:A:260:LEU:HD22	4:A:310:ARG:HD2	2.00	0.44
5:C:694:ARG:HE	5:C:694:ARG:HB2	1.60	0.44
5:C:821:ARG:O	5:C:825:GLU:HG3	2.17	0.44
5:C:949:GLU:O	5:C:953:LEU:HD13	2.17	0.44
5:C:1134:GLN:H	5:C:1134:GLN:HG2	1.54	0.44
6:D:121:PRO:O	6:D:123:ARG:HD2	2.18	0.44
6:D:161:THR:OG1	6:D:162:GLU:N	2.50	0.44
6:D:805:GLN:OE1	6:D:1348:LYS:HG3	2.18	0.44
5:C:386:GLU:O	5:C:391:SER:HB2	2.18	0.44
5:C:1255:THR:O	5:C:1257:GLN:HG3	2.17	0.44
6:D:265:LEU:HD23	6:D:265:LEU:HA	1.83	0.44
6:D:1027:VAL:H	6:D:1120:THR:HG21	1.83	0.44
6:D:300:GLN:NE2	6:D:304:ASP:OD2	2.51	0.43
6:D:349:TYR:HE2	6:D:379:PRO:HG2	1.83	0.43
6:D:392:THR:OG1	6:D:393:THR:N	2.51	0.43
8:M:256:LEU:O	8:M:258:PRO:HD2	2.18	0.43
1:N:-10:DT:H2"	1:N:-9:DC:C6	2.53	0.43
4:A:7:GLU:OE1	4:B:150:ARG:NH2	2.37	0.43
4:B:19:VAL:HB	4:B:23:HIS:HB3	1.99	0.43
5:C:873:ILE:HD13	5:C:873:ILE:HA	1.86	0.43
6:D:253:VAL:HB	6:D:261:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:929:GLN:HE21	6:D:1246:VAL:HG22	1.83	0.43
8:M:124:LEU:HB3	8:M:145:VAL:HG21	1.99	0.43
4:B:48:LEU:HD13	4:B:183:ILE:HG22	2.00	0.43
5:C:94:ALA:HB2	5:C:129:LEU:HD11	2.00	0.43
5:C:452:ARG:NH1	5:C:584:TYR:O	2.47	0.43
5:C:755:LYS:HD2	5:C:755:LYS:HA	1.69	0.43
5:C:909:LYS:HG3	5:C:911:SER:H	1.83	0.43
6:D:290:ILE:HG13	6:D:291:ILE:N	2.34	0.43
6:D:663:GLU:O	6:D:666:GLU:HG3	2.18	0.43
6:D:1314:LEU:HA	6:D:1322:ALA:HB1	2.00	0.43
5:C:124:MET:HB3	5:C:493:ILE:HD11	2.01	0.43
5:C:148:GLN:O	5:C:453:ILE:HA	2.18	0.43
5:C:629:PHE:HD2	5:C:634:VAL:HG11	1.83	0.43
5:C:1276:TRP:CH2	6:D:798:ARG:HG2	2.46	0.43
6:D:373:ALA:O	6:D:374:LEU:HB3	2.18	0.43
8:M:195:LEU:HD12	8:M:195:LEU:HA	1.71	0.43
5:C:478:ARG:NH1	5:C:491:ASP:HA	2.31	0.43
5:C:916:SER:O	5:C:916:SER:OG	2.35	0.43
5:C:1319:MET:HE3	5:C:1323:PHE:CD2	2.53	0.43
8:M:359:GLU:N	8:M:394:ARG:HH22	2.16	0.43
3:T:-10:DC:H2''	3:T:-9:DA:C8	2.53	0.43
4:A:74:VAL:HG12	4:A:133:LEU:HD23	2.01	0.43
4:A:176:CYS:SG	4:A:177:TYR:N	2.90	0.43
5:C:770:CYS:SG	5:C:791:LEU:HD23	2.58	0.43
6:D:1340:LYS:H	6:D:1340:LYS:HG2	1.63	0.43
4:A:314:LEU:HD12	4:A:315:GLY:N	2.34	0.43
5:C:1292:THR:OG1	5:C:1293:VAL:N	2.51	0.43
6:D:878:ASP:OD1	6:D:878:ASP:N	2.52	0.43
8:M:389:TYR:HD1	8:M:398:GLU:HA	1.84	0.43
5:C:238:GLN:HA	5:C:286:GLU:HA	2.01	0.43
6:D:674:THR:OG1	6:D:675:ALA:N	2.52	0.43
6:D:1034:PHE:HA	6:D:1114:GLN:H	1.84	0.43
4:A:283:GLN:HE21	4:A:318:LEU:H	1.65	0.43
4:B:191:ARG:HB2	4:B:195:ARG:O	2.19	0.43
5:C:1133:LYS:HA	5:C:1133:LYS:HD3	1.81	0.43
6:D:262:THR:HG21	6:D:270:ARG:NH2	2.33	0.43
6:D:885:VAL:HG12	6:D:894:VAL:HG11	2.01	0.43
4:A:125:LYS:HG3	4:A:125:LYS:O	2.19	0.42
6:D:679:TYR:O	6:D:682:VAL:HG12	2.18	0.42
4:B:42:ALA:O	4:B:46:ILE:HG23	2.18	0.42
5:C:28:LEU:HD23	5:C:28:LEU:HA	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:453:ILE:HD12	5:C:587:LEU:HG	2.01	0.42
5:C:520:PRO:HG3	5:C:714:VAL:HG21	2.01	0.42
5:C:884:VAL:HG11	5:C:1050:VAL:HG11	1.99	0.42
8:M:193:LYS:HG2	8:M:197:ASP:OD2	2.19	0.42
4:A:277:TYR:HB2	4:A:280:ASP:OD2	2.18	0.42
6:D:9:LYS:HA	6:D:12:THR:HG22	2.01	0.42
6:D:113:HIS:CD2	6:D:307:LEU:HD13	2.55	0.42
6:D:653:ILE:HD12	6:D:692:ARG:HE	1.83	0.42
8:M:153:TYR:OH	8:M:258:PRO:O	2.33	0.42
4:A:284:ARG:N	4:A:284:ARG:HD2	2.35	0.42
5:C:184:LEU:HD21	5:C:389:PHE:CE1	2.54	0.42
5:C:1137:GLU:CD	5:C:1139:ALA:H	2.23	0.42
6:D:605:LEU:HD23	6:D:605:LEU:HA	1.80	0.42
1:N:-27:DT:H4'	8:M:472:GLN:HA	2.00	0.42
3:T:12:DT:H2''	3:T:13:DG:N7	2.34	0.42
6:D:61:ILE:HG13	6:D:62:PHE:CD2	2.55	0.42
6:D:112:ALA:CB	6:D:139:LEU:HD21	2.50	0.42
6:D:949:SER:HB2	6:D:1016:THR:HG21	2.01	0.42
3:T:-18:DT:H2''	3:T:-17:DG:C8	2.54	0.42
5:C:99:LYS:HB3	5:C:99:LYS:HE3	1.85	0.42
5:C:1138:VAL:HG12	5:C:1142:ARG:HD2	2.01	0.42
6:D:132:LEU:O	6:D:135:ILE:HG12	2.19	0.42
6:D:452:LEU:HD23	6:D:452:LEU:HA	1.90	0.42
5:C:26:TYR:O	5:C:27:LEU:HB2	2.18	0.42
5:C:478:ARG:HH21	5:C:479:LEU:HD23	1.84	0.42
6:D:426:ALA:HB3	6:D:427:PRO:HD3	2.02	0.42
6:D:603:LYS:HB3	6:D:603:LYS:HE3	1.80	0.42
5:C:30:ILE:HD11	5:C:528:ARG:HA	2.00	0.42
5:C:208:ILE:HG13	5:C:209:ILE:N	2.35	0.42
5:C:447:HIS:HA	5:C:551:HIS:CE1	2.55	0.42
5:C:657:THR:OG1	5:C:1187:PHE:HB2	2.20	0.42
6:D:422:LEU:HD13	6:D:434:ILE:HD11	2.00	0.42
5:C:967:LEU:HD23	5:C:967:LEU:HA	1.92	0.42
5:C:1333:LEU:HD23	6:D:307:LEU:HD22	2.01	0.42
6:D:58:CYS:SG	6:D:60:ARG:N	2.93	0.42
4:B:209:GLY:C	4:B:211:ILE:H	2.23	0.41
5:C:210:LEU:O	5:C:215:TYR:HB2	2.20	0.41
5:C:819:SER:HB2	5:C:1085:MET:HG3	2.00	0.41
6:D:215:LYS:H	6:D:215:LYS:HG3	1.72	0.41
6:D:263:SER:OG	6:D:266:ASN:ND2	2.53	0.41
6:D:450:HIS:CE1	6:D:452:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:697:MET:SD	6:D:741:ALA:HB3	2.60	0.41
6:D:985:ILE:HG23	6:D:988:PHE:O	2.20	0.41
1:N:4:DT:O2	1:N:4:DT:H5''	2.20	0.41
4:B:58:GLU:CB	4:B:145:LYS:HG2	2.50	0.41
5:C:1257:GLN:NE2	6:D:340:GLN:O	2.49	0.41
6:D:185:ILE:O	6:D:189:LEU:HB2	2.20	0.41
7:E:51:LEU:HD23	7:E:51:LEU:HA	1.91	0.41
5:C:188:PHE:HE1	5:C:436:ARG:HB2	1.84	0.41
6:D:166:LEU:HA	6:D:169:LEU:HG	2.02	0.41
6:D:239:LEU:HD23	6:D:239:LEU:H	1.84	0.41
6:D:324:LEU:HD23	6:D:324:LEU:HA	1.91	0.41
6:D:422:LEU:HA	6:D:436:ALA:HA	2.02	0.41
4:B:100:LEU:HD21	4:B:121:VAL:HG11	2.02	0.41
4:B:128:HIS:ND1	4:B:128:HIS:C	2.74	0.41
5:C:73:TYR:HB2	5:C:98:VAL:HG12	2.02	0.41
5:C:678:ARG:HA	5:C:678:ARG:HD2	1.79	0.41
5:C:896:THR:OG1	5:C:899:GLU:HG2	2.21	0.41
5:C:1294:LYS:HE3	6:D:472:LEU:HD22	2.01	0.41
6:D:34:SER:OG	6:D:36:GLY:O	2.37	0.41
4:A:52:PRO:HB3	4:B:5:VAL:HG21	2.02	0.41
4:B:79:LEU:HD12	4:B:79:LEU:HA	1.88	0.41
6:D:576:ARG:HD3	6:D:593:ASN:HA	2.01	0.41
6:D:1143:ASP:OD1	6:D:1148:ARG:HD2	2.21	0.41
4:A:279:GLY:HA3	4:A:321:TRP:CH2	2.55	0.41
5:C:177:ILE:HG23	5:C:183:TRP:CD1	2.56	0.41
8:M:365:MET:H	8:M:365:MET:CE	2.34	0.41
8:M:389:TYR:CD1	8:M:398:GLU:HA	2.55	0.41
1:N:-14:DG:H1'	1:N:-13:DC:H5'	2.02	0.41
3:T:2:DA:H5''	3:T:2:DA:H8	1.84	0.41
5:C:143:ARG:NH1	5:C:507:GLY:O	2.54	0.41
5:C:600:THR:OG1	5:C:601:ASP:N	2.52	0.41
5:C:848:GLU:OE1	5:C:886:LYS:HD2	2.21	0.41
5:C:900:LYS:N	5:C:900:LYS:HD3	2.36	0.41
5:C:1142:ARG:NH2	5:C:1161:LEU:O	2.47	0.41
6:D:615:LYS:N	6:D:616:PRO:HD2	2.36	0.41
7:E:30:MET:HB2	7:E:30:MET:HE2	1.77	0.41
8:M:455:ARG:NH1	8:M:456:ARG:HA	2.36	0.41
5:C:322:LEU:O	5:C:325:LEU:HG	2.21	0.41
5:C:791:LEU:HD23	5:C:791:LEU:HA	1.95	0.41
6:D:823:THR:OG1	6:D:824:PRO:HD2	2.21	0.41
4:A:67:GLU:HG2	4:A:171:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:233:ASP:OD1	4:A:233:ASP:O	2.39	0.41
4:B:95:LYS:HB3	4:B:95:LYS:NZ	2.36	0.41
4:B:112:ALA:HB1	4:B:123:ILE:HD11	2.03	0.41
4:B:190:ALA:O	4:B:198:LEU:CB	2.56	0.41
5:C:446:ASP:O	5:C:446:ASP:OD1	2.38	0.41
6:D:8:LEU:HD12	6:D:8:LEU:O	2.21	0.41
6:D:146:VAL:HA	6:D:178:ALA:HA	2.03	0.41
4:B:65:LEU:HD12	4:B:65:LEU:HA	1.88	0.41
4:B:86:LYS:HE3	4:B:174:ASP:HB2	2.02	0.41
5:C:696:ASP:O	5:C:795:ALA:HB1	2.21	0.41
5:C:1007:LYS:HA	5:C:1011:LEU:HD12	2.03	0.41
5:C:1100:PRO:HB2	6:D:725:MET:HE1	2.02	0.41
1:N:17:DC:H2''	1:N:18:DA:C8	2.56	0.40
3:T:0:DG:H2''	3:T:1:DC:H5'	2.03	0.40
5:C:37:LYS:HB2	5:C:37:LYS:HE3	1.74	0.40
6:D:954:ASN:OD1	6:D:954:ASN:N	2.54	0.40
6:D:1150:PRO:HD2	6:D:1216:ALA:HB2	2.03	0.40
5:C:594:VAL:HG22	5:C:599:VAL:HG22	2.03	0.40
3:T:7:DG:N2	6:D:319:SER:OG	2.54	0.40
4:A:79:LEU:O	4:A:83:LEU:HG	2.21	0.40
4:B:190:ALA:HB2	4:B:200:LYS:HB2	2.03	0.40
5:C:30:ILE:HD13	5:C:575:LEU:HD11	2.04	0.40
5:C:516:ASP:HB2	5:C:522:SER:OG	2.22	0.40
5:C:720:ARG:O	5:C:736:VAL:HG22	2.21	0.40
5:C:1117:LEU:HD12	5:C:1117:LEU:HA	1.69	0.40
5:C:1333:LEU:HD23	6:D:327:LEU:HD23	2.04	0.40
4:A:150:ARG:HD2	4:B:8:PHE:CZ	2.57	0.40
5:C:209:ILE:O	5:C:213:LEU:HD23	2.21	0.40
5:C:556:GLY:O	5:C:589:THR:OG1	2.38	0.40
5:C:1025:PHE:HA	5:C:1028:LYS:CE	2.51	0.40
5:C:1142:ARG:NH2	5:C:1164:PHE:O	2.54	0.40
6:D:255:LEU:HD11	6:D:261:ALA:HB2	2.02	0.40
6:D:661:VAL:HA	6:D:664:ILE:HG22	2.03	0.40
6:D:715:LYS:HB2	6:D:715:LYS:HE2	1.75	0.40
6:D:984:LEU:HD13	6:D:993:GLU:HB2	2.03	0.40
4:B:108:GLY:HA2	4:B:109:PRO:HD3	1.97	0.40
5:C:818:VAL:HG22	5:C:1096:ILE:HD13	2.03	0.40
6:D:58:CYS:SG	6:D:61:ILE:HG12	2.61	0.40
6:D:475:GLU:OE2	7:E:28:ARG:NH2	2.41	0.40
8:M:269:PRO:HA	8:M:271:TYR:CE1	2.57	0.40

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	
4	A	304/321 (95%)	284 (93%)	20 (7%)	0	100	100
4	B	233/321 (73%)	215 (92%)	18 (8%)	0	100	100
5	C	1339/1341 (100%)	1261 (94%)	78 (6%)	0	100	100
6	D	1318/1373 (96%)	1220 (93%)	97 (7%)	1 (0%)	51	82
7	E	72/74 (97%)	66 (92%)	6 (8%)	0	100	100
8	M	346/350 (99%)	324 (94%)	22 (6%)	0	100	100
All	All	3612/3780 (96%)	3370 (93%)	241 (7%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	317	THR

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	
4	A	259/280 (92%)	255 (98%)	4 (2%)	65	82
4	B	183/280 (65%)	177 (97%)	6 (3%)	38	66
5	C	1038/1156 (90%)	1006 (97%)	32 (3%)	40	68
6	D	942/1145 (82%)	910 (97%)	32 (3%)	37	65
7	E	53/64 (83%)	53 (100%)	0	100	100
8	M	133/309 (43%)	129 (97%)	4 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2608/3234 (81%)	2530 (97%)	78 (3%)	44 68

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	21	SER
4	A	131	CYS
4	A	249	PHE
4	A	313	SER
4	B	4	SER
4	B	21	SER
4	B	120	ASP
4	B	128	HIS
4	B	141	SER
4	B	199	ASP
5	C	14	ASP
5	C	47	TYR
5	C	62	TYR
5	C	83	GLN
5	C	132	ASP
5	C	171	LEU
5	C	183	TRP
5	C	359	ARG
5	C	390	PHE
5	C	405	PHE
5	C	484	LEU
5	C	549	ASP
5	C	613	ASN
5	C	646	SER
5	C	677	ASN
5	C	685	MET
5	C	697	LYS
5	C	739	ASP
5	C	741	MET
5	C	749	ASP
5	C	819	SER
5	C	826	ASP
5	C	842	ASP
5	C	881	ASP
5	C	1018	TYR
5	C	1059	ARG
5	C	1105	SER

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Mol	Chain	Res	Type
5	C	1165	SER
5	C	1240	ASP
5	C	1243	MET
5	C	1265	PHE
5	C	1273	MET
6	D	18	ASP
6	D	21	LYS
6	D	31	ARG
6	D	54	ASP
6	D	58	CYS
6	D	70	CYS
6	D	77	ARG
6	D	109	SER
6	D	122	SER
6	D	192	MET
6	D	229	GLN
6	D	248	ASP
6	D	264	ASP
6	D	281	ARG
6	D	298	MET
6	D	329	ASP
6	D	350	SER
6	D	353	SER
6	D	366	CYS
6	D	400	MET
6	D	472	LEU
6	D	488	ASN
6	D	625	MET
6	D	651	HIS
6	D	694	SER
6	D	837	ASP
6	D	891	ASP
6	D	1149	ARG
6	D	1268	ASN
6	D	1271	SER
6	D	1301	THR
6	D	1321	SER
8	M	184	ARG
8	M	271	TYR
8	M	365	MET
8	M	390	LEU

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

sidechains are listed below:

Mol	Chain	Res	Type
5	C	551	HIS
6	D	1249	ASN
6	D	1259	GLN
8	M	387	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	N	1
8	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	-8:DG	O3'	2:DT	P	24.94
1	M	292:ASP	C	323:LEU	N	22.08

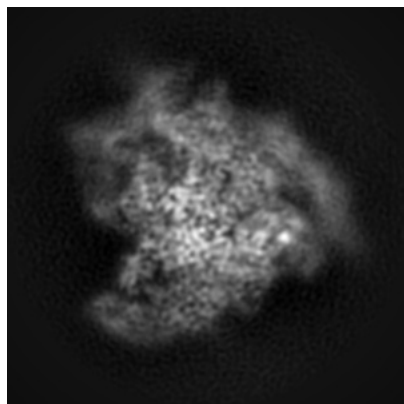
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19081. These allow visual inspection of the internal detail of the map and identification of artifacts.

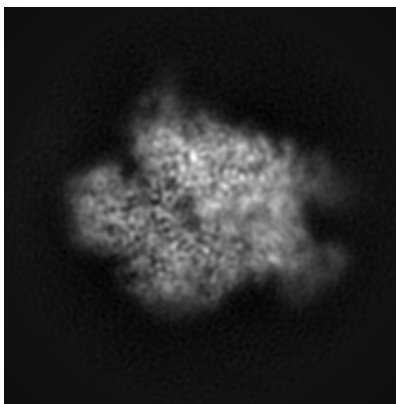
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

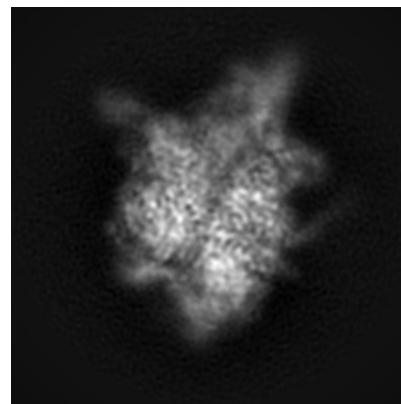
6.1.1 Primary map



X

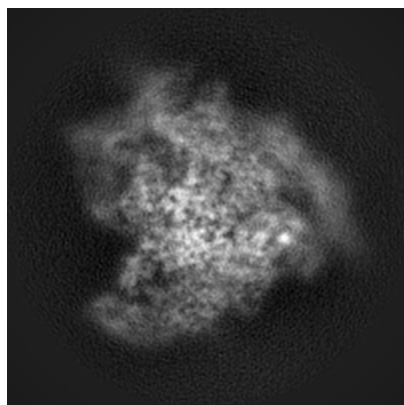


Y

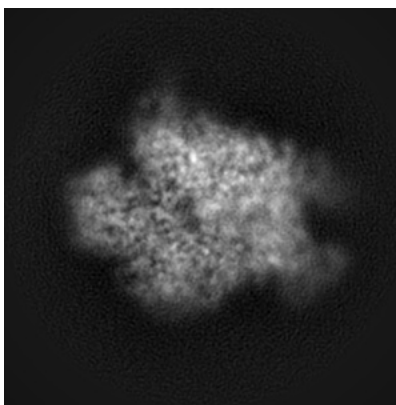


Z

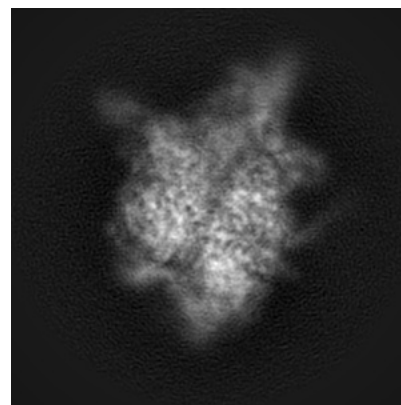
6.1.2 Raw map



X



Y

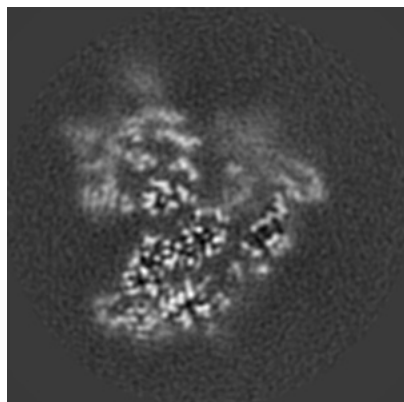


Z

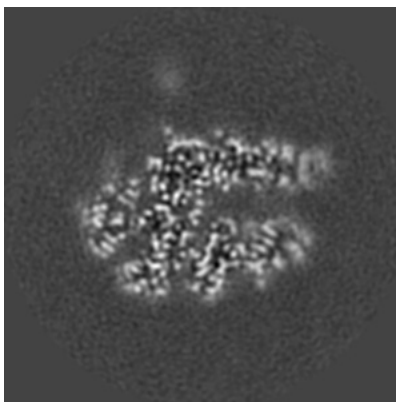
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

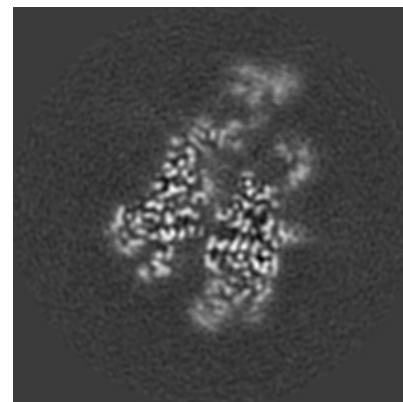
6.2.1 Primary map



X Index: 100

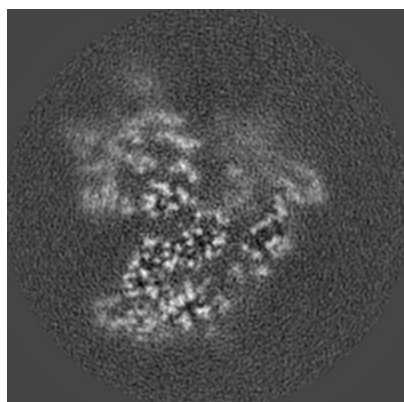


Y Index: 100

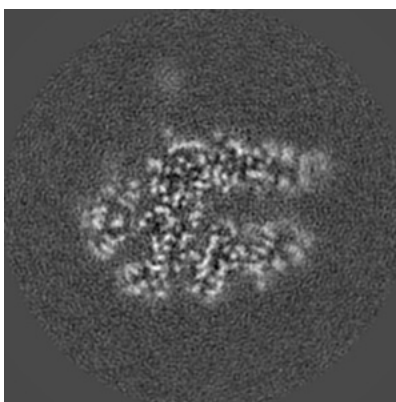


Z Index: 100

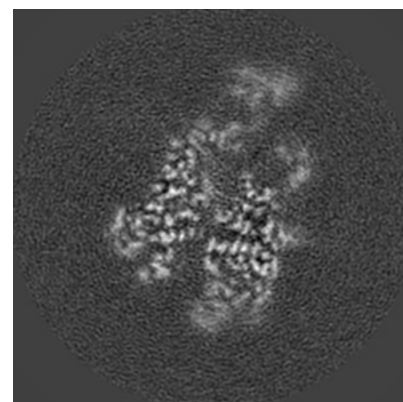
6.2.2 Raw map



X Index: 100



Y Index: 100

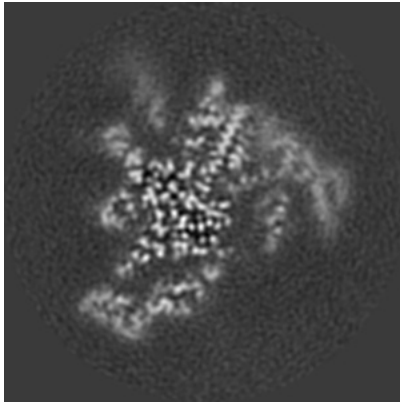


Z Index: 100

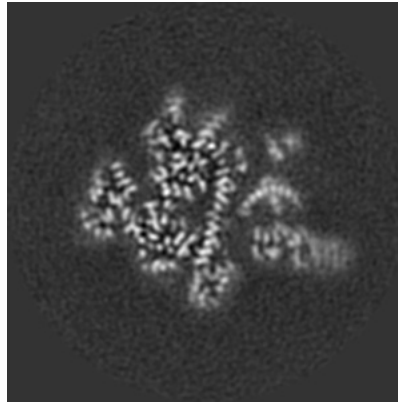
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

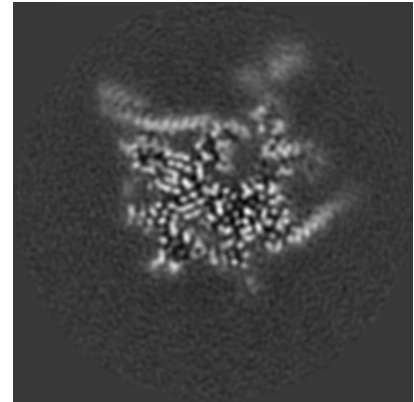
6.3.1 Primary map



X Index: 113

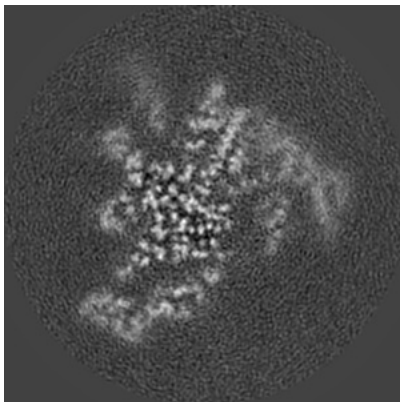


Y Index: 86

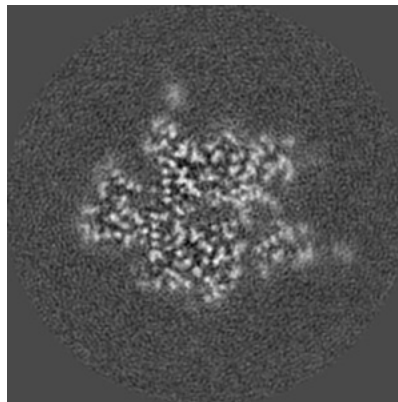


Z Index: 84

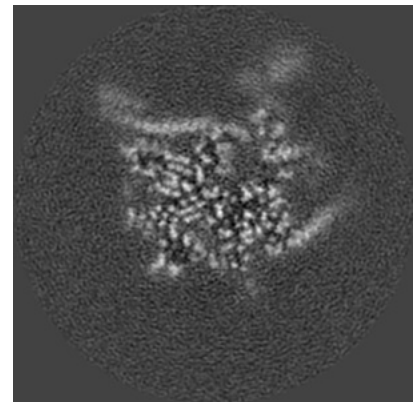
6.3.2 Raw map



X Index: 113



Y Index: 93

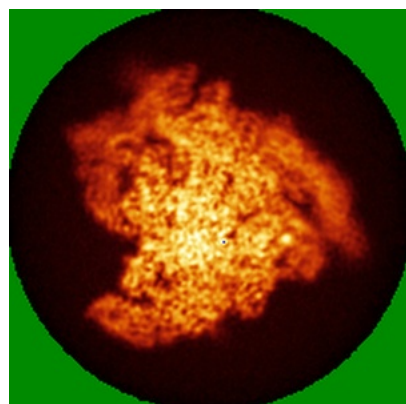


Z Index: 84

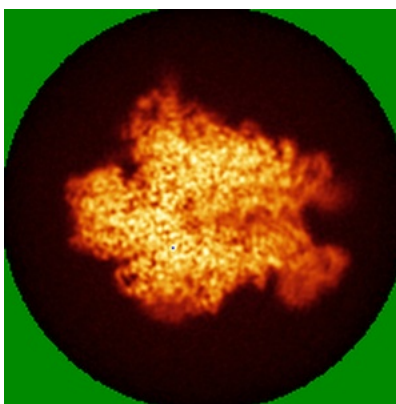
The images above show the largest variance slices of the map in three orthogonal directions.

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

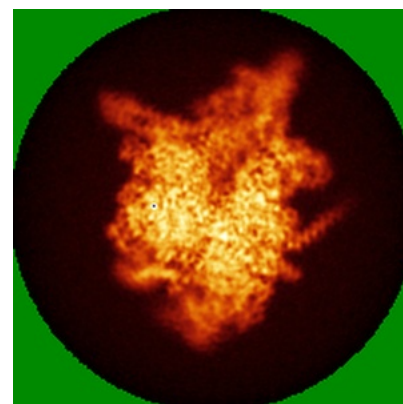
6.4.1 Primary map



X

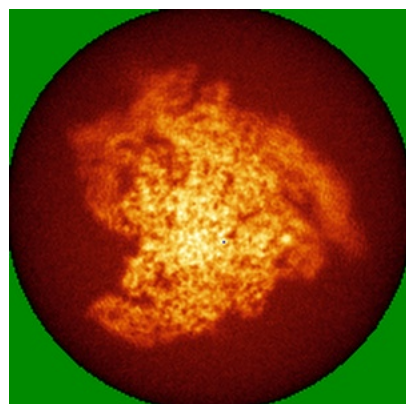


Y

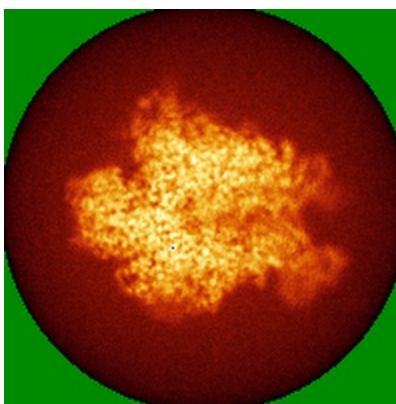


Z

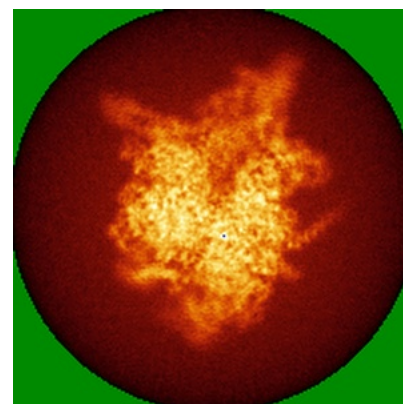
6.4.2 Raw map



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.

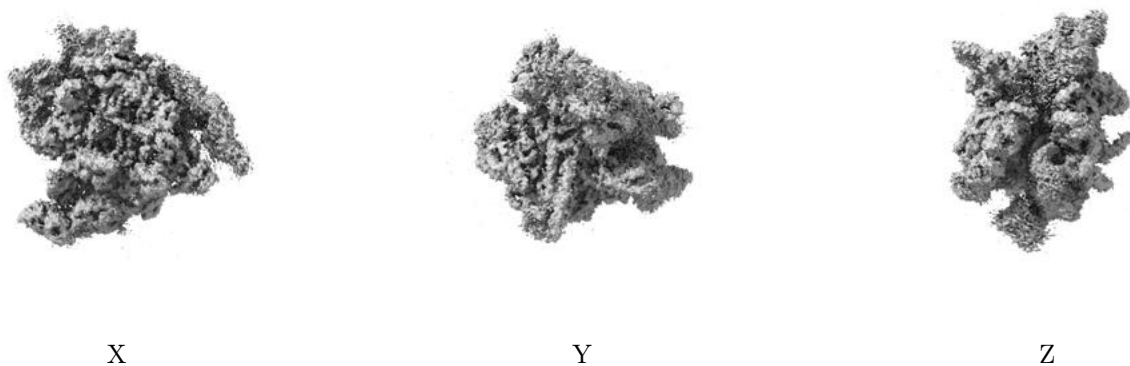
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0067. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

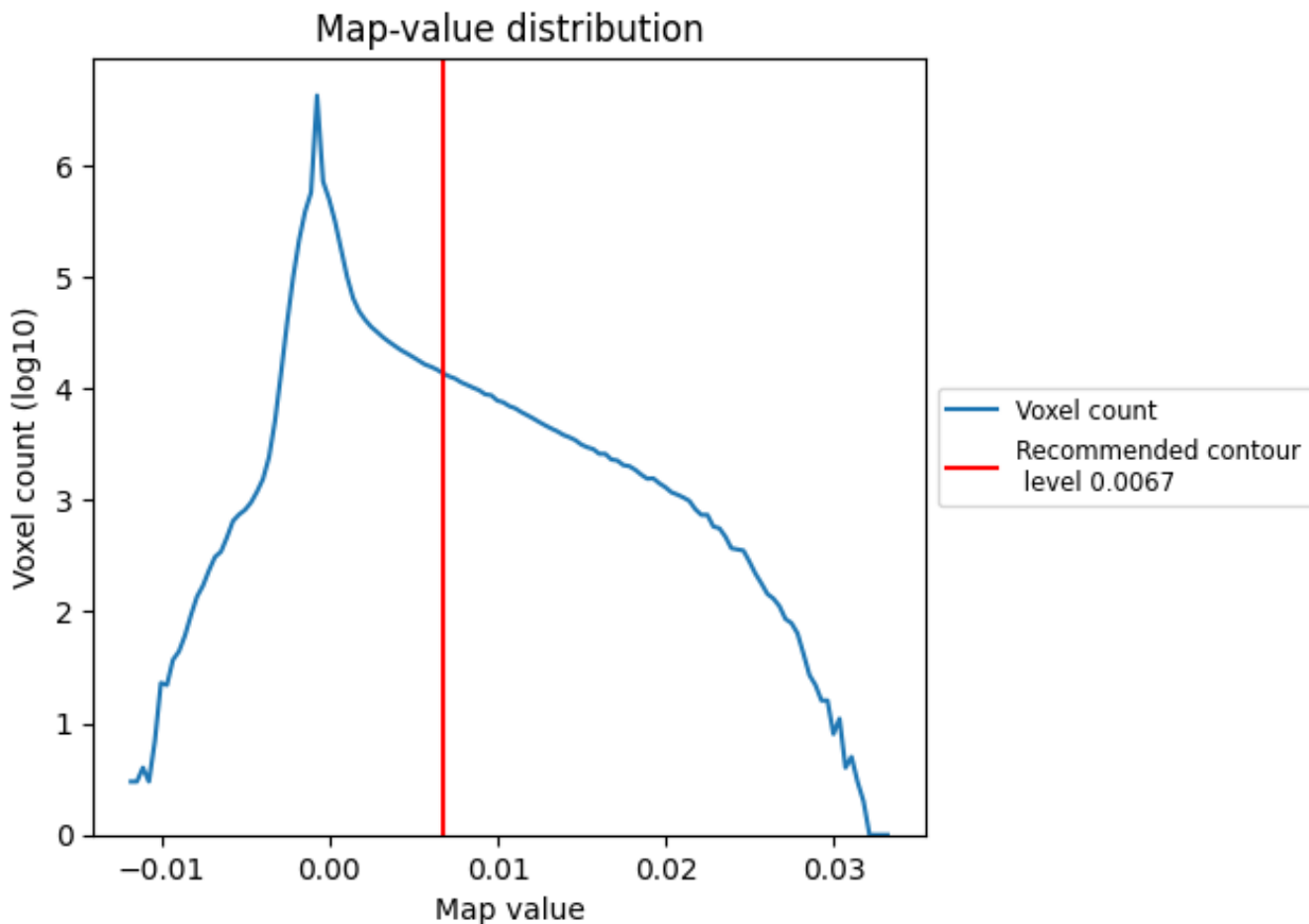
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

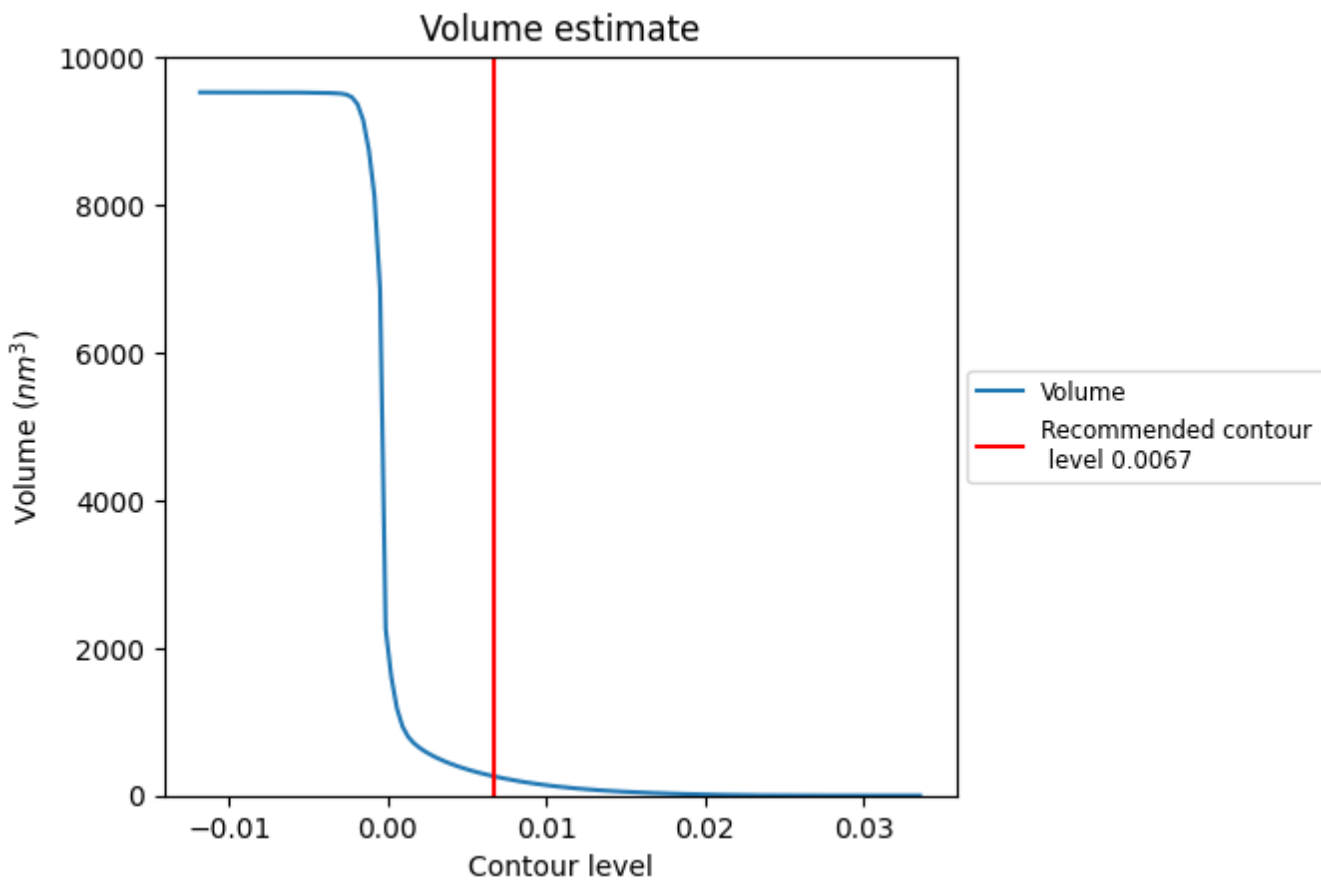
This section contains the results of statistical analysis of the map.

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.

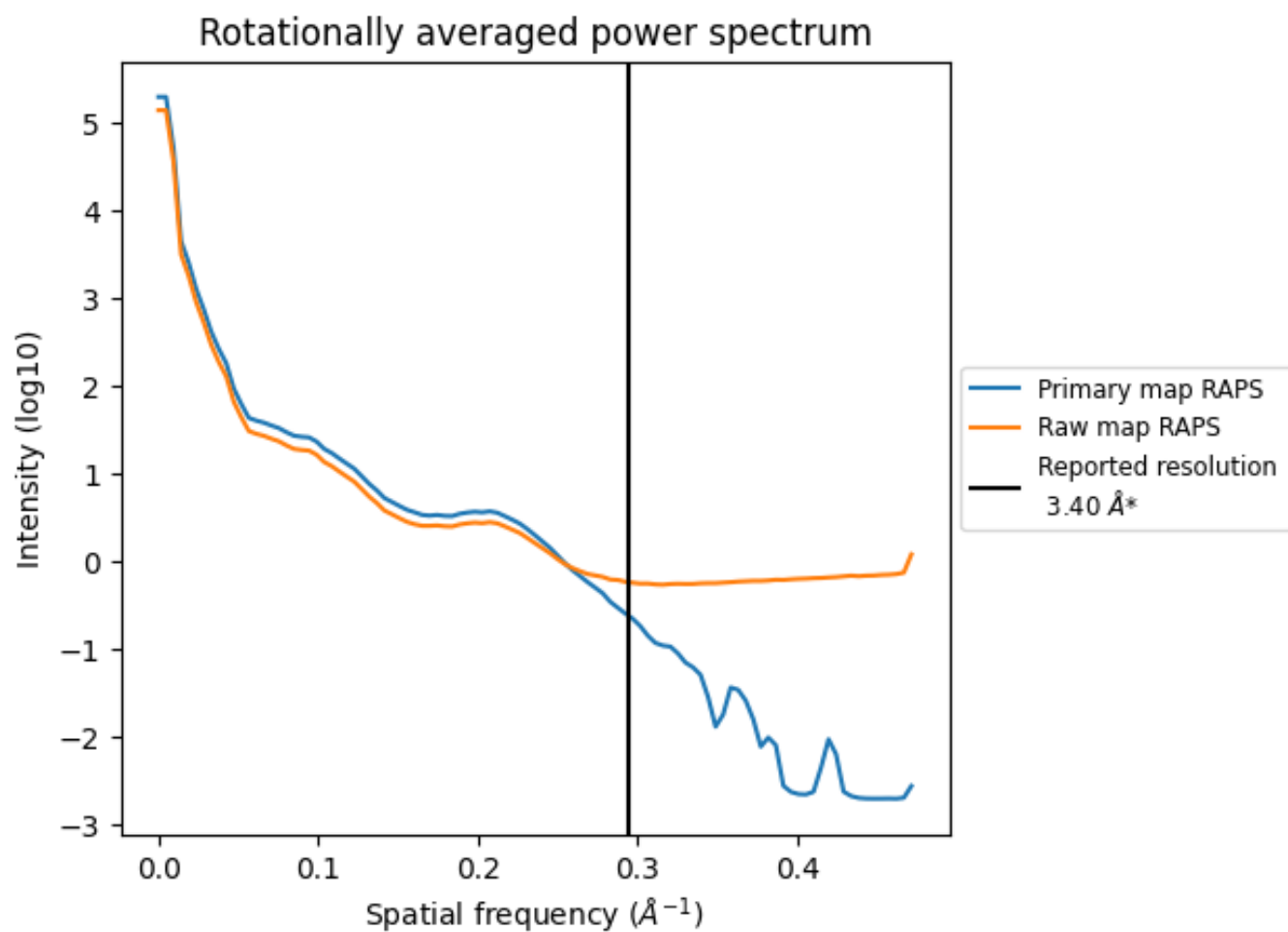
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261 nm³; this corresponds to an approximate mass of 235 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

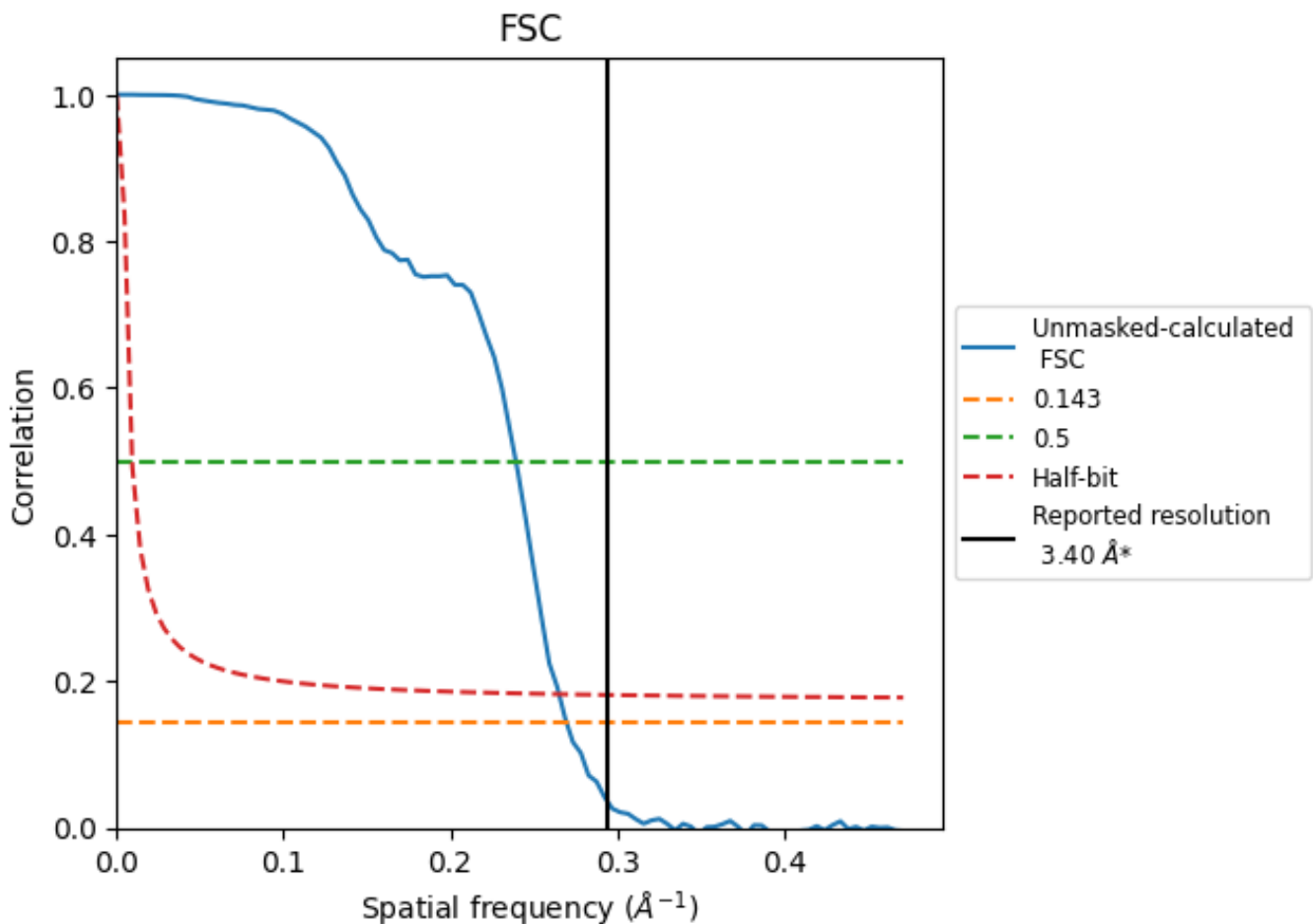


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

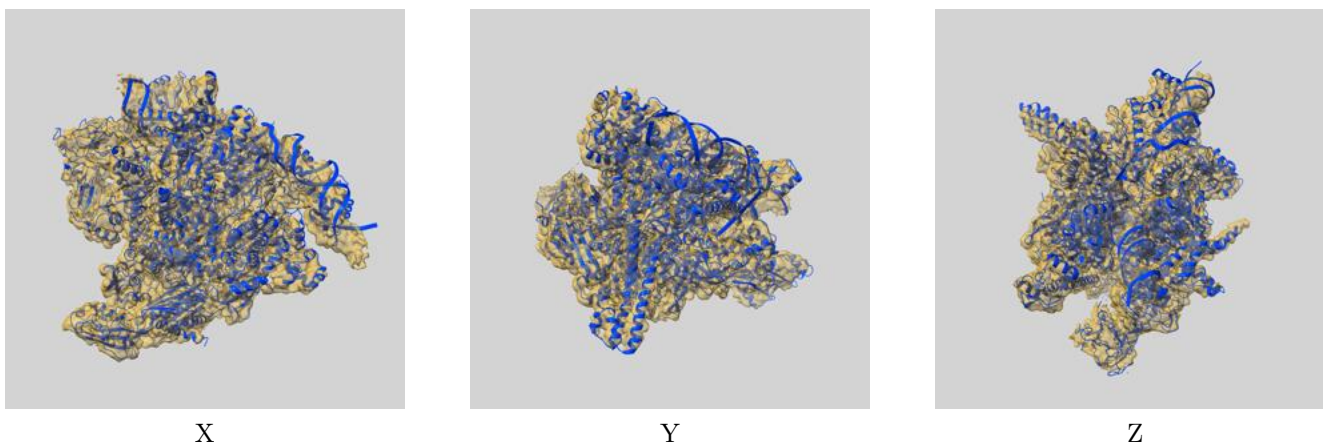
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.71	4.18	3.77

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

9 Map-model fit [i](#)

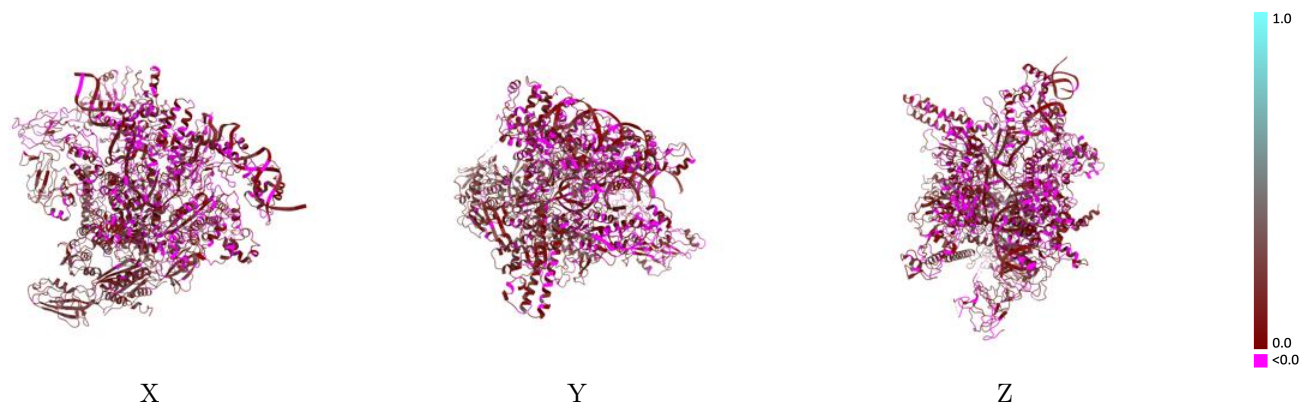
This section contains information regarding the fit between EMDB map EMD-19081 and PDB model 8REB. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



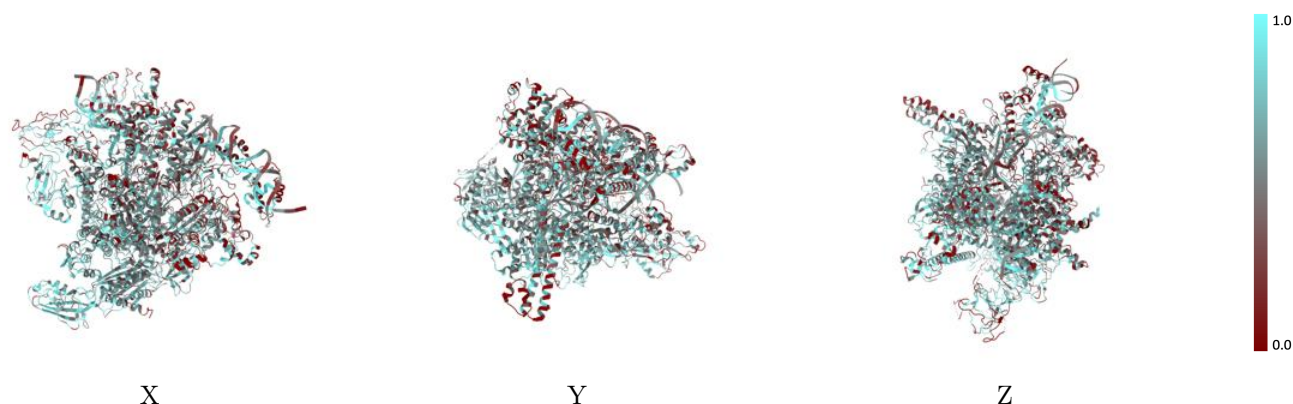
The images above show the 3D surface view of the map at the recommended contour level 0.0067 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



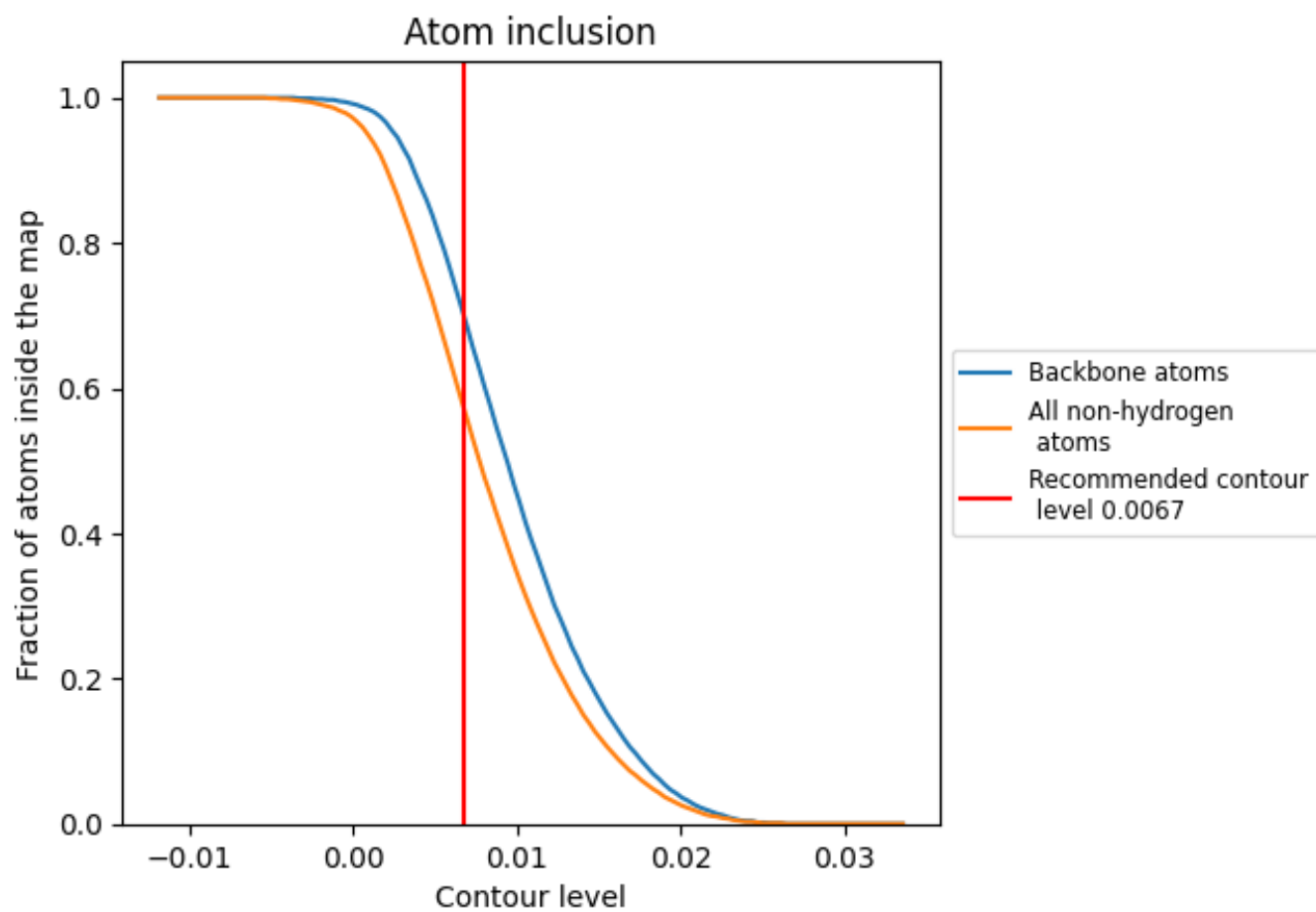
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0067).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 58% 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 (0.0067) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5760	 0.1080
A	 0.5830	 0.1490
B	 0.6630	 0.2110
C	 0.5720	 0.0980
D	 0.5760	 0.1030
E	 0.6300	 0.1060
M	 0.4770	 0.0570
N	 0.6390	 0.1020
R	 0.6430	 0.1140
T	 0.5860	 0.0950

