



Full wwPDB EM Validation Report ⓘ

Jun 25, 2025 – 06:33 PM JST

PDB ID : 8YQZ / pdb_00008yqz
EMDB ID : EMD-39511
Title : African swine fever virus RNA Polymerase–DNA complex
Authors : Feng, X.Y.
Deposited on : 2024-03-20
Resolution : 2.78 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.dev118
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

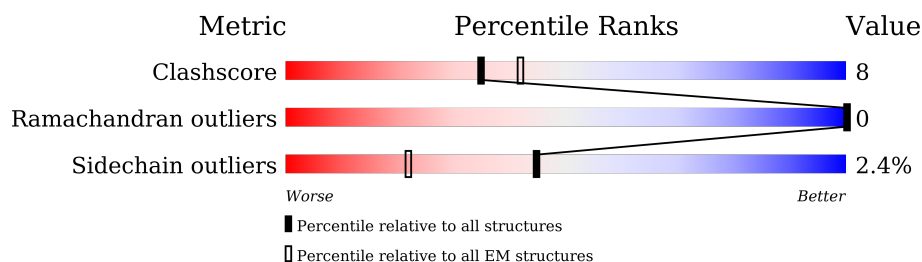
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1450	<div> <div>82%</div> <div>75% 19% 5%</div> </div>
2	B	1242	<div> <div>88%</div> <div>75% 21% .</div> </div>
3	C	359	<div> <div>82%</div> <div>86% 13% ..</div> </div>
4	D	205	<div> <div>81%</div> <div>83% 17%</div> </div>
5	E	147	<div> <div>56%</div> <div>60% 12% 28%</div> </div>
6	F	339	<div> <div>96%</div> <div>73% 27% .</div> </div>
7	G	105	<div> <div>41%</div> <div>44% 12% 44%</div> </div>
8	H	80	<div> <div>86%</div> <div>76% 22% .</div> </div>

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Mol	Chain	Length	Quality of chain
9	X	8	100%
			<div><div></div><div></div><div></div></div> 62%38%
10	Y	7	100%
			<div><div></div><div></div><div></div></div> 71%29%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29943 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1375	Total	C	N	O	S	0	0
			10954	6958	1906	2030	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1196	Total	C	N	O	S	0	0
			9459	5983	1653	1773	50		

- Molecule 3 is a protein called DNA-directed RNA polymerase RPB3-11 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	357	Total	C	N	O	S	0	0
			2897	1880	480	525	12		

- Molecule 4 is a protein called DNA-directed RNA polymerase RPB5 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	205	Total	C	N	O	S	0	0
			1668	1088	278	294	8		

- Molecule 5 is a protein called C147L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	106	Total	C	N	O	S	0	0
			829	528	143	153	5		

- Molecule 6 is a protein called D339L.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	339	Total	C	N	O	S	0	0
			2727	1753	451	509	14		

- Molecule 7 is a protein called C122R.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	59	Total	C	N	O	S	0	0
			468	295	80	85	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase RPB10 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	80	Total	C	N	O	S	0	0
			630	411	102	110	7		

- Molecule 9 is a DNA chain called DNA (5'-D(P*GP*CP*CP*GP*AP*GP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	X	8	Total	C	N	O	P	0	0
			165	77	34	46	8		

- Molecule 10 is a DNA chain called DNA (5'-D(P*TP*CP*GP*GP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	7	Total	C	N	O	P	0	0
			141	67	23	44	7		

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

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

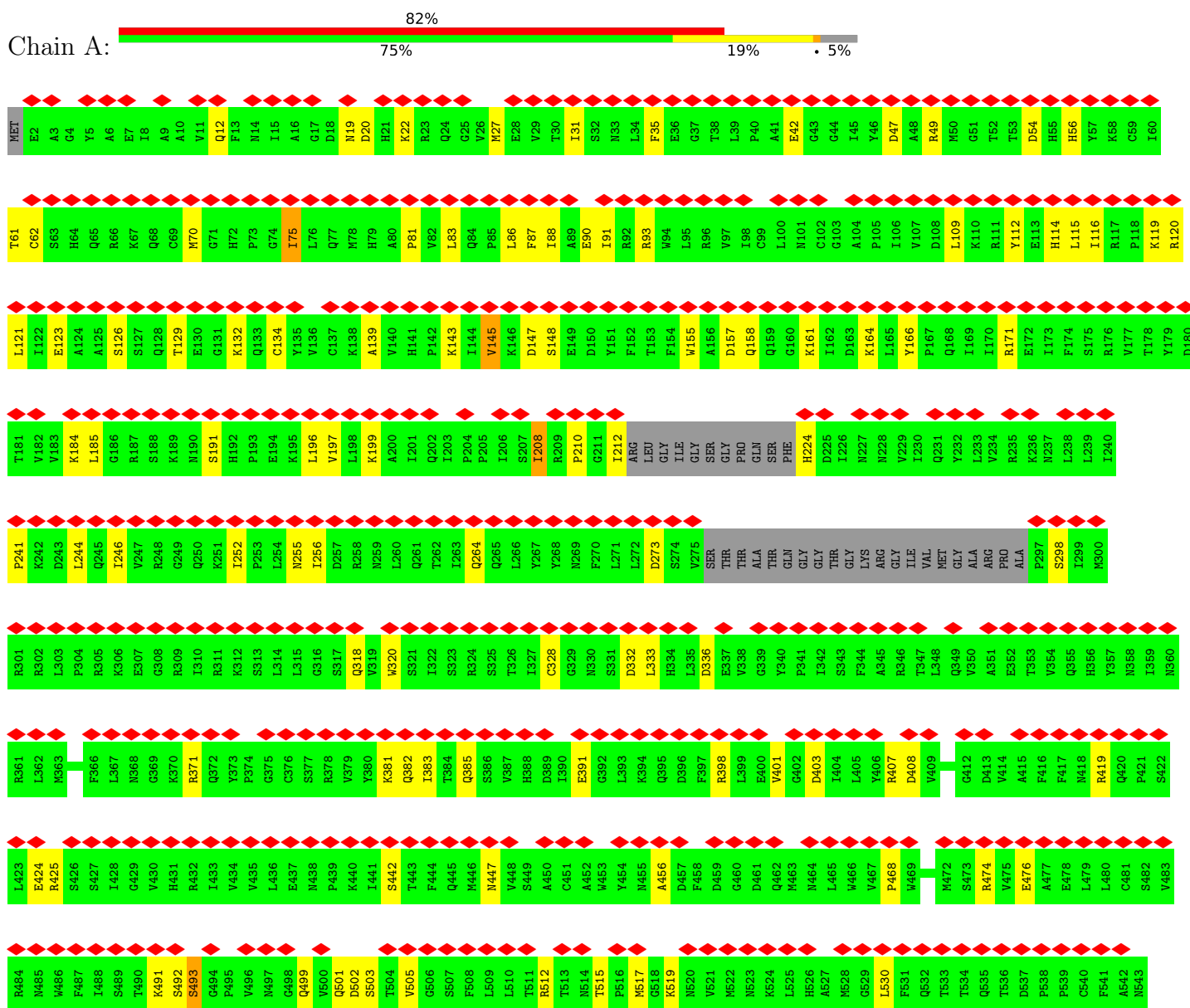
- Molecule 12 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	A	1	Total	Zn	0
			1	1	
12	B	1	Total	Zn	0
			1	1	
12	G	1	Total	Zn	0
			1	1	
12	H	1	Total	Zn	0
			1	1	

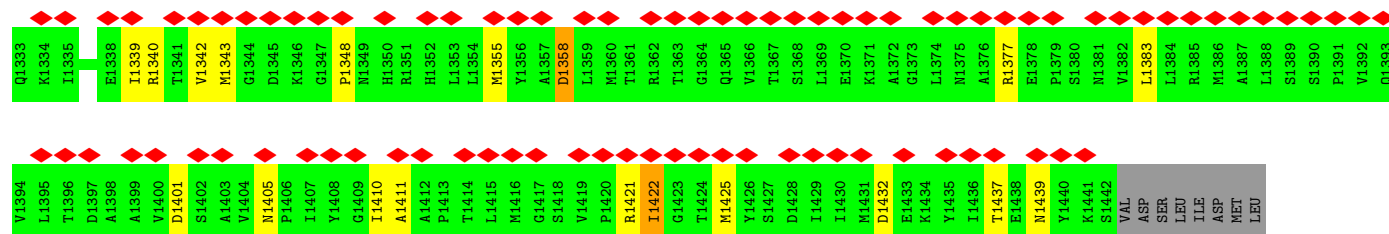
3 Residue-property plots

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

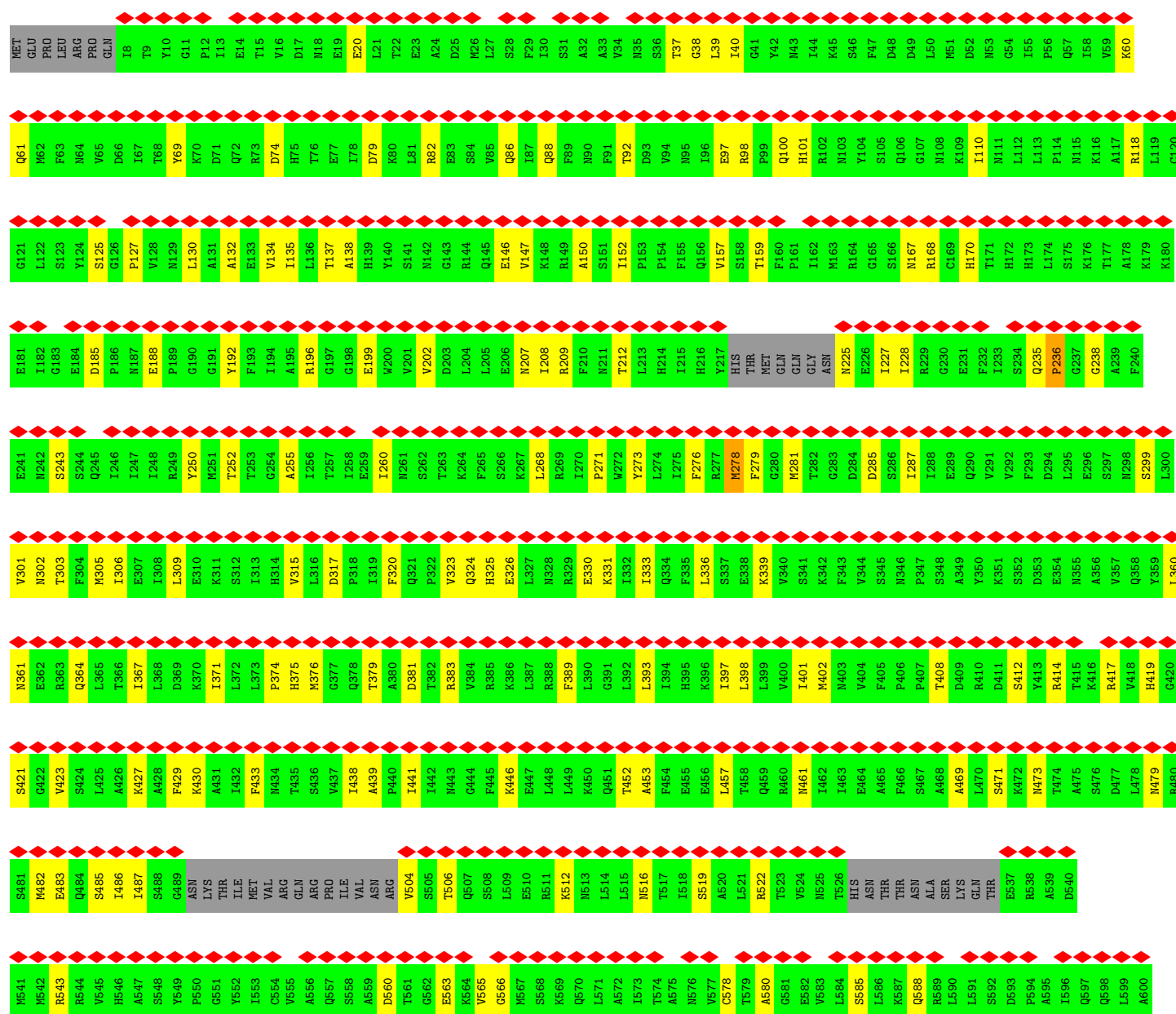
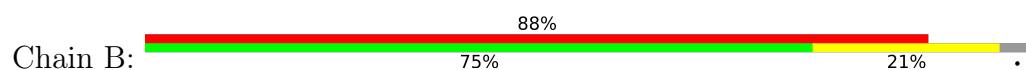
• Molecule 1: DNA-directed RNA polymerase subunit

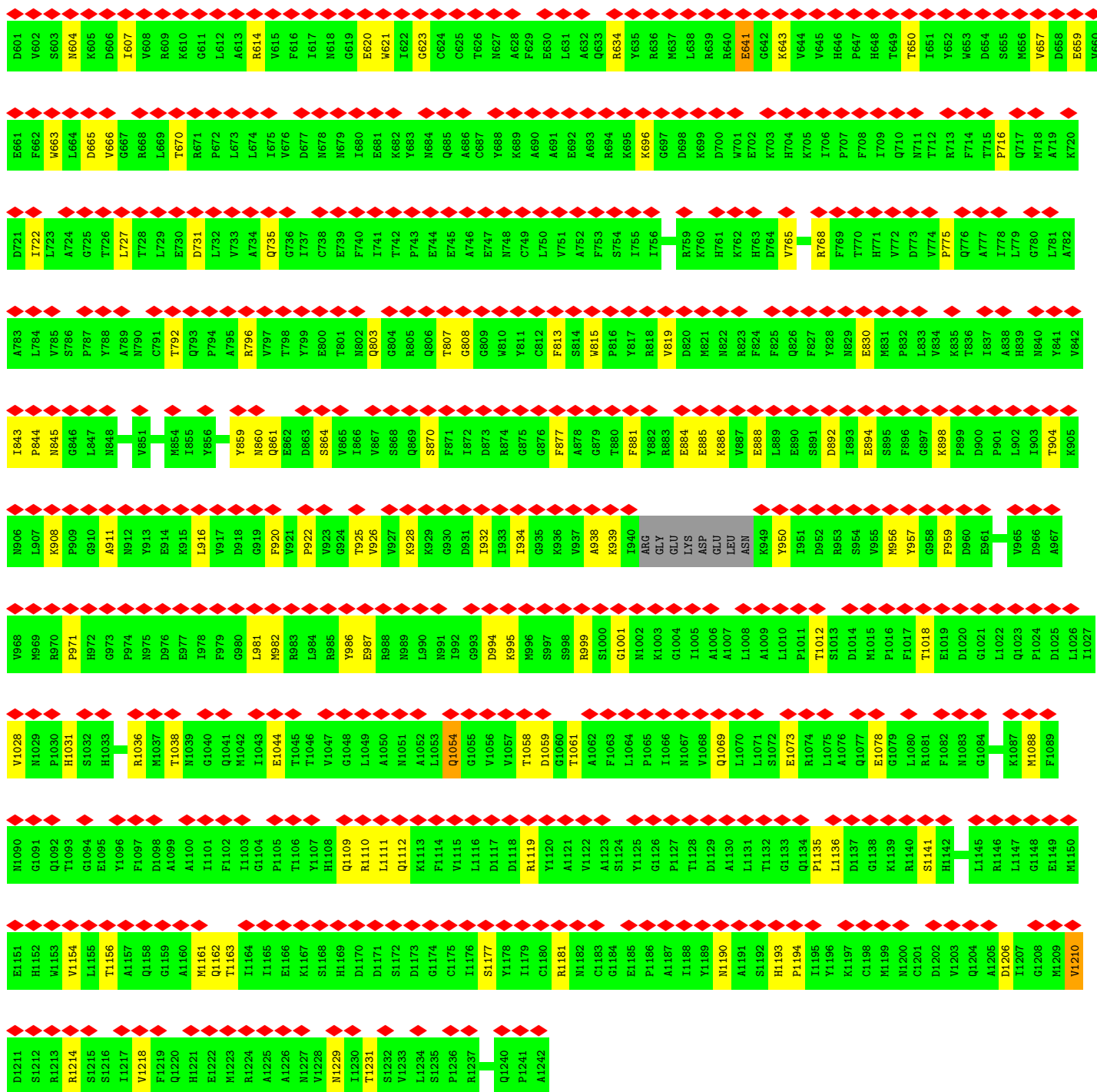


K1272	L1273	M1274	R1275	H1276	D1279	A1280	G1282	K1283	L1284	V1285	R1286	L1287	D1288	N1289	I1290	Y1291	A1292	I1293	K1294	T1295	N1296	G1297	T1298	N1299	I1300	F1301	G1302	A1303	M1304	L1305	D1306	D1307	N1308	I1309	D1310	P1311	Y1312	T1313	I1314	V1315	S1316	S1317	S1318	I1319	G1320	D1321	T1322	M1323	E1324	L1325	Y1326	G1327	I1328	E1329	A1330	A1331	R1332		
V1212	GLU	ASN	THR	ALA	SER	GLY	ILE	PRO	I1221	I1222	I1223	R1224	I1225	Y1226	L1227	R1228	E1229	S1230	A1231	F1232	R1233	R1234	S1235	T1236	N1237	T1238	R1239	M1240	A1241	T1242	D1243	E1244	K1245	I1246	A1247	V1248	N1249	V1250	V1251	D1252	K1253	L1254	L1255	N1256	S1257	T1258	I1259	R1260	G1261	I1262	P1263	K1264	I1265	K1266	N1267	A1268	N1269	V1270	V1271
S1091	S1092	E1093	M1094	L1095	L1096	R1097	L1098	K1099	N1100	P1101	E1102	V1103	E1104	T1105	N1106	K1107	T1108	Y1109	A1110	Q1111	E1112	I1113	A1114	N1115	S1116	I1117	E1118	L1119	I1120	T1121	F1122	E1123	R1124	L1125	I1126	L1127	Q1128	W1129	H1130	L1131	L1132	TVR	GLU	THR	TVR	SER	THR	LYS	ASN	V1143	M1144	Y1145	P1146	D1147	F1148	A1149	S1150		
D1151	V1152	E1153	W1154	M1155	T1156	D1157	F1158	L1159	E1160	M1161	H1162	P1163	L1164	L1165	Q1166	P1167	T1168	E1169	D1170	I1171	A1172	M1173	W1174	C1175	I1176	R1177	L1178	E1179	L1180	M1181	K1182	T1183	T1184	M1185	I1186	L1187	K1188	S1189	I1190	S1191	L1192	E1193	S1194	I1195	I1196	L1199	R1200	A1201	K1202	H1203	P1204	N1205	T1206	T1207	I1208	M1209	H1210	S1211	
T1031	Q1032	S1033	L1034	I1035	M1036	Y1037	G1038	E1039	A1040	V1041	G1042	I1043	L1044	A1045	A1046	Q1047	S1048	V1049	S1050	E1051	P1052	L1053	T1054	Q1055	Y1056	MET	LEU	ASP	SER	HIS	HIS	ARG	VAL	ALA	GLY	GLY	THR	ASN	LYS	SER	G1073	I1074	Y1075	R1076	P1077	Q1078	E1079	I1080	F1081	S1082	A1083	K1084	P1085	V1086	E1087	A1088	Q1089	Q1090	
N970	L971	P972	Y973	V974	F975	N976	N977	N978	I979	Q980	E981	R982	L983	Q984	T985	P986	I987	P988	V989	Y990	L991	K992	R993	A994	A995	S996	L997	M998	R999	M1000	L1001	R1002	I1003	I1004	E1005	Y886	G888	I889	Q890	S891	P892	L893	F894	E895	S896	I897	L988	Q899	S899	R900	L901	K902	K903	D904	Y905	D906	K907	Y908	R909
Q810	T911	F912	L913	N914	V915	E916	N917	F918	N919	P920	S921	Q922	L923	T924	T925	D926	R928	Q929	V930	P931	V932	N933	V934	A935	S936	I937	V938	K939	N940	I941	L942	L943	S944	S945	T946	S947	G948	V949	P951	F952	D953	E954	K955	S956	I957	L958	Q959	K960	Y961	A962	N963	V964	X965	T966	F967	C968	K969		
L850	V851	Q852	Q853	L854	Y855	G856	E857	D858	G859	L860	D861	A862	R863	Q864	L865	E866	T867	R869	F870	E871	T872	I873	M874	L875	S876	D877	Q878	E879	L880	E881	D882	K883	F884	K885	Y886	G888	I889	Q890	S891	P892	L893	F894	E895	S896	I897	L988	Q899	S899	R900	L901	K902	K903	D904	Y905	D906	K907	Y908	R909	
T727	N728	G729	L730	F731	Q732	M733	T736	G737	A738	K739	G740	I741	P743	N744	M745	I746	H747	I748	M749	A750	G751	I752	G753	Q754	I755	E756	I757	N758	T759	Q760	R761	I762	G763	F764	Q765	F766	S767	F768	G769	R770	T771	L772	P773	Y774	Y775	F776	R777	F778	A779	L780	R781	A782	Q783	A784	Y785	G786	F787		
Q667	E668	I669	N670	N671	E672	L673	L674	L675	E676	S677	E678	I680	N681	M682	R683	L684	L685	H686	G687	D688	I689	P691	P692	K631	M632	I633	F634	A635	Q638	L639	A640	L641	N642	Y643	V644	R645	N646	A647	G648	F649	T650	V651	S652	T653	A654	D655	M656	L657	L658	T659	P660	E661	A662	H663	Q664	E665	V666		
Y544	S545	P546	T547	D548	L549	L550	D551	G552	K553	S554	V555	V556	S557	M558	L559	L560	R561	Q562	T563	P564	I565	N566	Y567	Q568	R569	A570	P571	T572	W573	Y574	S575	E576	V577	Y578	A579	P580	Y581	M582	H583	Y584	N585	K586	Q587	D588	I589	S590	T591	Q592	I593	R594	N595	G596	E597	E600	G601	V602	L603	D604	

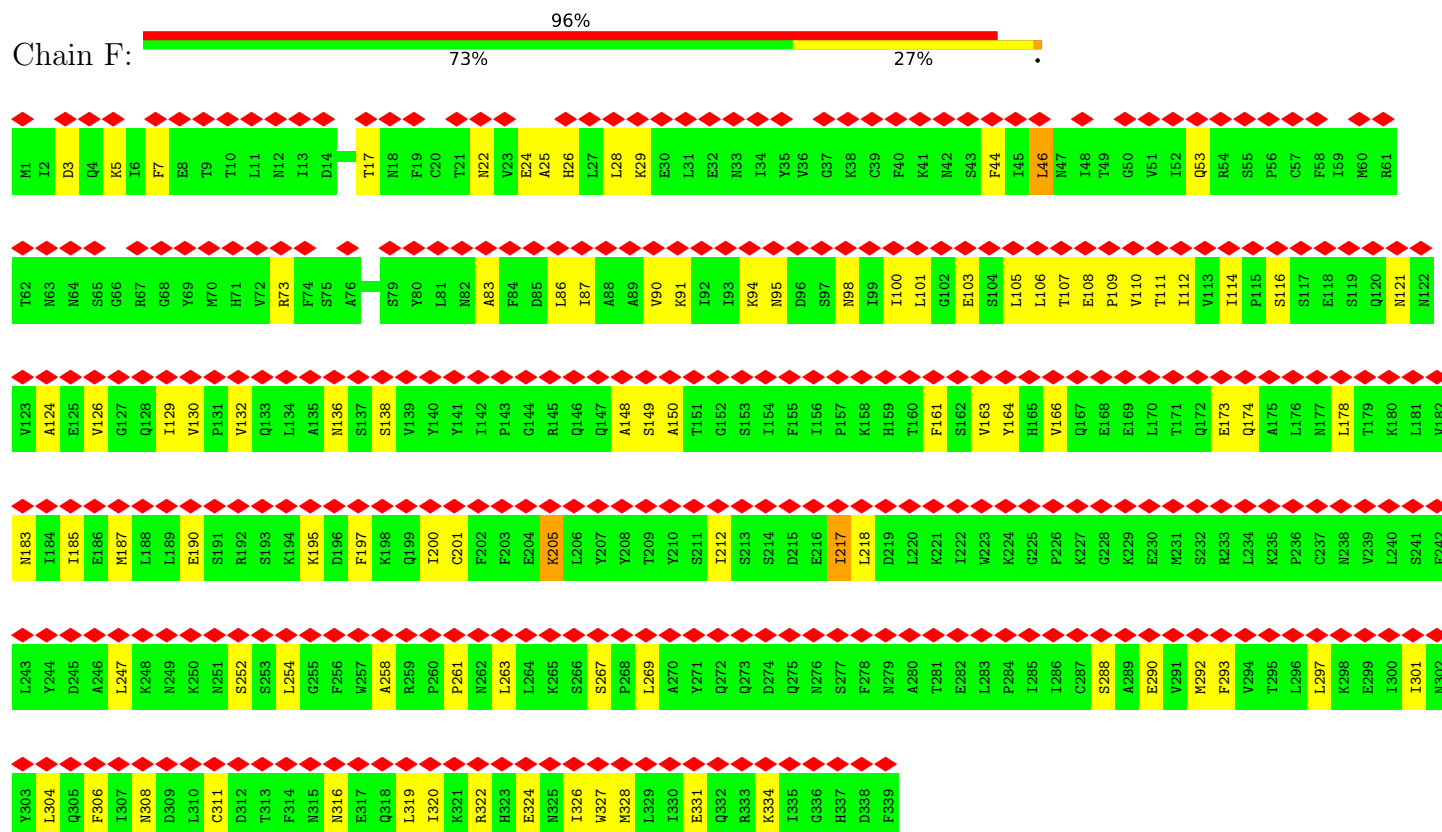


• Molecule 2: DNA-directed RNA polymerase subunit beta

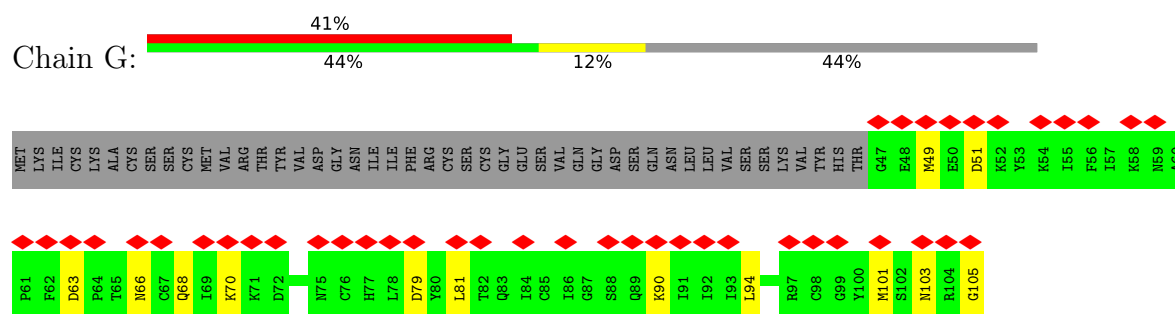




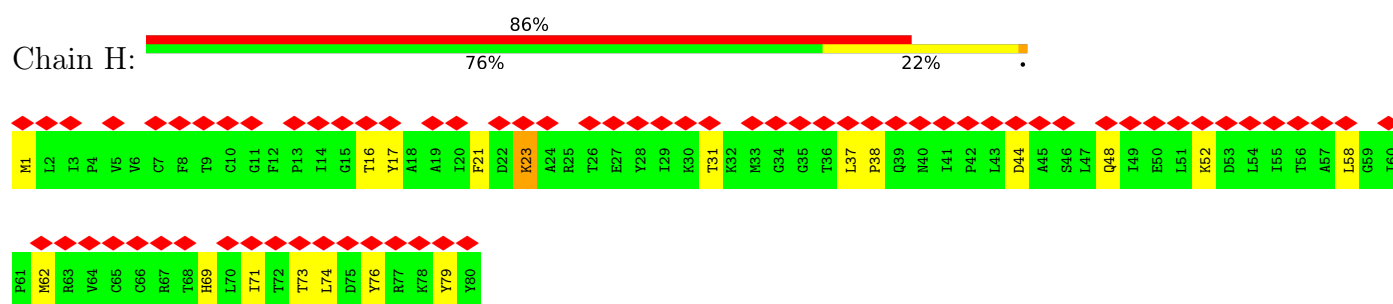
- Molecule 6: D339L



- Molecule 7: C122R

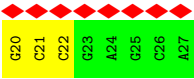


- Molecule 8: DNA-directed RNA polymerase RPB10 homolog

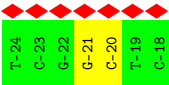


- Molecule 9: DNA (5'-D(P*GP*CP*CP*GP*AP*GP*CP*A)-3')





● Molecule 10: DNA (5'-D(P*TP*CP*GP*GP*CP*TP*C)-3')



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	266388	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 ($e^-/\text{\AA}^2$)	1.25	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.148	Depositor
Minimum map value	-0.090	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0129	Depositor
Map size (Å)	258.56, 258.56, 258.56	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.80799997, 0.80799997, 0.80799997	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	A	0.35	0/11163	0.45	2/15116 (0.0%)
2	B	0.30	0/9648	0.44	3/13055 (0.0%)
3	C	0.36	0/2959	0.41	0/4000
4	D	0.30	0/1707	0.44	0/2311
5	E	0.36	0/841	0.45	0/1139
6	F	0.20	0/2782	0.39	0/3767
7	G	0.26	0/476	0.41	0/638
8	H	0.37	0/643	0.46	0/872
9	X	0.19	0/185	0.40	0/283
10	Y	0.22	0/156	0.38	0/238
All	All	0.32	0/30560	0.44	5/41419 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1101	PRO	N-CD-CG	-8.09	91.07	103.20
2	B	323	VAL	N-CA-C	-6.03	107.25	113.10
1	A	1101	PRO	CA-N-CD	-5.49	104.31	112.00
2	B	971	PRO	N-CD-CG	-5.39	95.11	103.20
2	B	236	PRO	CA-N-CD	-5.29	104.59	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10954	0	11085	175	0
2	B	9459	0	9413	177	0
3	C	2897	0	2976	31	0
4	D	1668	0	1713	21	0
5	E	829	0	877	17	0
6	F	2727	0	2755	56	0
7	G	468	0	467	10	0
8	H	630	0	659	12	0
9	X	165	0	89	4	0
10	Y	141	0	80	3	0
11	A	1	0	0	0	0
12	A	1	0	0	0	0
12	B	1	0	0	0	0
12	G	1	0	0	0	0
12	H	1	0	0	0	0
All	All	29943	0	30114	466	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 8.

All (466) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:807:THR:OG1	2:B:845:ASN:ND2	1.99	0.95
6:F:91:LYS:HG3	6:F:105:LEU:HD11	1.56	0.87
5:E:42:SER:OG	5:E:43:PRO:HD3	1.74	0.86
1:A:121:LEU:HD23	1:A:185:LEU:HG	1.58	0.84
1:A:83:LEU:H	1:A:264:GLN:HE22	1.28	0.81
1:A:515:THR:HG22	1:A:517:MET:H	1.48	0.79
1:A:1078:GLN:OE1	1:A:1084:LYS:NZ	2.14	0.76
1:A:109:LEU:HD13	1:A:184:LYS:HD3	1.65	0.76
2:B:892:ASP:O	2:B:939:LYS:NZ	2.20	0.75
6:F:22:ASN:O	6:F:26:HIS:ND1	2.19	0.75
6:F:164:TYR:HB2	6:F:292:MET:HE1	1.68	0.75
2:B:138:ALA:HB3	2:B:146:GLU:HB3	1.70	0.73
1:A:1128:GLN:N	1:A:1179:GLU:OE1	2.22	0.73
2:B:886:LYS:NZ	2:B:888:GLU:OE2	2.22	0.72
9:X:21:DC:N3	10:Y:-21:DG:N1	2.31	0.72
5:E:96:LYS:HE3	5:E:96:LYS:HA	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:THR:HG22	1:A:905:ARG:HG3	1.73	0.70
6:F:95:ASN:ND2	6:F:124:ALA:O	2.24	0.70
1:A:1123:GLU:HG3	1:A:1255:LEU:HD12	1.72	0.70
1:A:1200:ARG:NE	1:A:1206:THR:O	2.23	0.70
2:B:543:ARG:NH1	2:B:563:GLU:O	2.24	0.70
6:F:173:GLU:OE2	6:F:174:GLN:NE2	2.25	0.70
8:H:17:TYR:HB3	8:H:58:LEU:HD22	1.74	0.69
2:B:911:ALA:HB2	2:B:956:MET:HE2	1.73	0.69
1:A:1126:ILE:HG21	1:A:1178:LEU:HD23	1.75	0.69
1:A:1432:ASP:OD2	5:E:139:ARG:NH2	2.23	0.69
1:A:381:LYS:NZ	1:A:403:ASP:OD2	2.25	0.69
2:B:130:LEU:HD22	2:B:157:VAL:HG21	1.76	0.68
1:A:1203:HIS:NE2	1:A:1257:SER:OG	2.25	0.68
1:A:1425:MET:HE2	2:B:1161:MET:HB3	1.74	0.67
1:A:91:ILE:HG12	1:A:196:LEU:HD23	1.77	0.67
1:A:501:GLN:O	2:B:1031:HIS:NE2	2.26	0.67
2:B:1229:ASN:HD22	5:E:45:ILE:HG13	1.60	0.67
1:A:145:VAL:HG13	1:A:155:TRP:HB2	1.76	0.67
6:F:46:LEU:HD21	6:F:108:GLU:HG2	1.76	0.66
5:E:67:THR:OG1	5:E:134:GLU:OE1	2.14	0.66
2:B:236:PRO:HD3	2:B:374:PRO:HB2	1.78	0.66
3:C:82:ASP:OD1	3:C:82:ASP:N	2.25	0.66
1:A:49:ARG:O	1:A:61:THR:OG1	2.14	0.66
6:F:293:PHE:O	6:F:297:LEU:HG	1.96	0.66
6:F:94:LYS:HB3	6:F:101:LEU:HB3	1.78	0.65
6:F:267:SER:HB2	6:F:269:LEU:HD22	1.79	0.65
2:B:792:THR:HG23	2:B:1038:THR:HA	1.76	0.65
2:B:1162:GLN:HE21	5:E:78:ARG:HH11	1.45	0.65
4:D:163:GLN:O	4:D:198:ARG:NH1	2.30	0.64
4:D:102:ILE:O	4:D:106:ILE:HG12	1.97	0.64
2:B:330:GLU:HA	2:B:333:ILE:HD12	1.80	0.64
2:B:486:ILE:HG13	2:B:487:ILE:HG13	1.80	0.64
2:B:330:GLU:OE2	2:B:361:ASN:ND2	2.31	0.64
2:B:486:ILE:O	2:B:506:THR:OG1	2.14	0.64
2:B:393:LEU:O	2:B:397:ILE:HD12	1.98	0.64
2:B:1059:ASP:OD2	2:B:1061:THR:OG1	2.15	0.64
1:A:886:TYR:HE2	1:A:889:ILE:HD12	1.64	0.63
3:C:110:VAL:HB	3:C:134:ALA:HB3	1.80	0.63
1:A:728:ASN:HD22	1:A:731:PHE:H	1.45	0.63
1:A:877:ASP:OD1	1:A:1282:GLY:HA3	1.99	0.62
1:A:1182:LYS:HA	1:A:1185:MET:HE1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:ARG:NH1	1:A:1226:TYR:OH	2.32	0.62
2:B:657:VAL:HG23	2:B:659:GLU:HG3	1.82	0.62
3:C:190:GLU:HB2	3:C:206:LYS:HD2	1.82	0.62
4:D:58:PHE:O	4:D:123:TYR:OH	2.17	0.61
2:B:621:TRP:NE1	2:B:623:GLY:O	2.33	0.61
2:B:908:LYS:HB3	2:B:956:MET:HE3	1.83	0.61
7:G:101:MET:HG2	7:G:105:GLY:HA3	1.82	0.61
1:A:1332:ARG:NH1	1:A:1358:ASP:OD1	2.34	0.60
2:B:278:MET:HE1	2:B:336:LEU:HD22	1.83	0.60
1:A:241:PRO:HG2	1:A:244:LEU:HB2	1.84	0.60
6:F:304:LEU:O	6:F:308:ASN:ND2	2.33	0.60
1:A:916:GLU:OE2	1:A:923:LEU:HD13	2.02	0.60
1:A:116:ILE:HG13	1:A:119:LYS:HG3	1.83	0.60
2:B:885:GLU:HB2	2:B:982:MET:HB3	1.83	0.60
1:A:676:GLU:HG2	1:A:708:ALA:HB1	1.83	0.59
1:A:681:ASN:OD1	1:A:701:TYR:OH	2.19	0.59
2:B:360:LEU:O	2:B:364:GLN:NE2	2.34	0.59
9:X:20:DG:H1	10:Y:-20:DC:H42	1.51	0.59
2:B:844:PRO:HG2	8:H:74:LEU:HD11	1.85	0.59
2:B:208:ILE:HD12	2:B:208:ILE:H	1.68	0.59
6:F:164:TYR:HB2	6:F:292:MET:CE	2.32	0.59
6:F:328:MET:HA	6:F:331:GLU:HB2	1.84	0.58
2:B:920:PHE:HE1	2:B:934:ILE:HG23	1.67	0.58
1:A:1274:MET:SD	1:A:1286:ARG:NH1	2.77	0.58
2:B:650:THR:HB	2:B:663:TRP:HB2	1.84	0.58
2:B:807:THR:HG1	2:B:845:ASN:HD21	1.46	0.58
6:F:163:VAL:HG22	6:F:258:ALA:HB2	1.86	0.58
6:F:166:VAL:HG23	6:F:292:MET:HE3	1.86	0.58
1:A:90:GLU:OE1	1:A:93:ARG:NH1	2.36	0.58
1:A:333:LEU:O	1:A:447:ASN:ND2	2.29	0.58
1:A:332:ASP:OD2	2:B:859:TYR:OH	2.21	0.58
1:A:696:THR:HG23	1:A:699:ASP:H	1.69	0.58
1:A:143:LYS:HB3	1:A:157:ASP:HB3	1.86	0.57
5:E:120:MET:HG3	5:E:135:ILE:HD13	1.85	0.57
1:A:491:LYS:HZ2	1:A:492:SER:HB3	1.70	0.57
1:A:1152:VAL:HG23	1:A:1155:MET:HE2	1.86	0.57
1:A:1184:THR:OG1	1:A:1185:MET:SD	2.62	0.57
2:B:485:SER:HG	2:B:504:VAL:N	2.02	0.57
1:A:1177:ARG:HH11	1:A:1222:ILE:HD11	1.70	0.57
7:G:81:LEU:HD23	7:G:94:LEU:HB3	1.86	0.57
6:F:319:LEU:HD23	6:F:322:ARG:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:324:GLU:HA	6:F:327:TRP:CD1	2.39	0.57
1:A:468:PRO:HB2	1:A:474:ARG:HG3	1.86	0.57
2:B:260:ILE:HG21	2:B:371:ILE:HD12	1.86	0.57
1:A:844:VAL:HG11	1:A:1355:MET:HE1	1.87	0.57
2:B:86:GLN:HB3	2:B:137:THR:HB	1.87	0.56
1:A:1410:ILE:HD12	2:B:1156:THR:HG21	1.88	0.56
2:B:202:VAL:HA	2:B:506:THR:HG22	1.86	0.56
1:A:273:ASP:N	1:A:298:SER:OG	2.35	0.56
5:E:42:SER:OG	5:E:43:PRO:CD	2.52	0.56
5:E:65:ARG:HG2	5:E:134:GLU:HG2	1.86	0.56
1:A:1150:SER:O	1:A:1154:TRP:N	2.33	0.56
2:B:999:ARG:NH2	2:B:1044:GLU:OE2	2.35	0.56
3:C:190:GLU:CD	3:C:190:GLU:H	2.13	0.56
3:C:328:SER:OG	3:C:331:ASP:OD1	2.24	0.56
1:A:1126:ILE:HD13	1:A:1129:TRP:HB3	1.86	0.56
2:B:1069:GLN:NE2	2:B:1073:GLU:OE2	2.35	0.56
6:F:116:SER:OG	6:F:121:ASN:ND2	2.39	0.56
2:B:302:ASN:O	2:B:306:ILE:HD12	2.05	0.56
1:A:1305:LEU:HB3	4:D:1:MET:HB3	1.86	0.56
1:A:872:THR:HG23	1:A:880:LEU:HD13	1.88	0.56
1:A:1096:LEU:HD22	1:A:1309:ILE:HG21	1.87	0.56
2:B:580:ALA:HB2	2:B:666:VAL:HG13	1.88	0.56
2:B:134:VAL:HB	2:B:150:ALA:HB3	1.88	0.56
2:B:118:ARG:NH2	2:B:192:TYR:OH	2.38	0.55
3:C:113:LEU:HD23	3:C:160:ILE:HD12	1.88	0.55
4:D:1:MET:HE3	4:D:5:LYS:HE2	1.88	0.55
2:B:235:GLN:NE2	2:B:238:GLY:O	2.35	0.55
1:A:54:ASP:OD2	1:A:56:HIS:ND1	2.38	0.55
1:A:134:CYS:HB3	1:A:139:ALA:H	1.71	0.55
6:F:53:GLN:OE1	6:F:73:ARG:NH1	2.39	0.55
3:C:6:GLN:HA	3:C:357:LEU:HD11	1.89	0.55
1:A:1209:MET:HE3	1:A:1209:MET:HA	1.89	0.54
1:A:1109:TYR:CZ	1:A:1113:ILE:HD11	2.43	0.54
1:A:1052:PRO:HG2	1:A:1348:PRO:HD3	1.90	0.54
6:F:183:ASN:O	6:F:187:MET:HG2	2.07	0.54
2:B:255:ALA:HB2	2:B:315:VAL:HG11	1.90	0.54
1:A:35:PHE:HE2	1:A:212:ILE:HG21	1.72	0.54
1:A:1340:ARG:NH2	4:D:189:GLU:OE2	2.41	0.54
2:B:429:PHE:O	2:B:433:PHE:HB2	2.08	0.54
1:A:255:ASN:OD1	1:A:256:ILE:N	2.41	0.53
1:A:147:ASP:OD1	1:A:148:SER:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:THR:O	1:A:1313:THR:HG22	2.08	0.53
1:A:158:GLN:HB3	1:A:161:LYS:HB3	1.90	0.53
1:A:1051:GLU:HB3	1:A:1052:PRO:HD3	1.91	0.53
1:A:336:ASP:OD1	1:A:336:ASP:N	2.42	0.53
2:B:20:GLU:HG2	2:B:716:PRO:HG2	1.90	0.53
4:D:30:LYS:O	4:D:34:MET:HG3	2.08	0.53
3:C:38:LEU:HD23	3:C:225:ALA:HB1	1.91	0.53
3:C:272:MET:HE2	3:C:276:LYS:HD2	1.91	0.53
1:A:442:SER:HB3	2:B:1119:ARG:HD3	1.91	0.52
1:A:850:LEU:HB3	4:D:162:MET:HE2	1.91	0.52
2:B:315:VAL:O	2:B:324:GLN:NE2	2.43	0.52
1:A:1208:ILE:HG13	1:A:1223:ILE:HD11	1.91	0.52
1:A:1195:ILE:O	1:A:1199:LEU:HD12	2.10	0.52
2:B:987:GLU:HG3	3:C:91:GLN:CD	2.34	0.52
1:A:1249:ASN:O	1:A:1253:LYS:N	2.36	0.52
2:B:417:ARG:NH1	2:B:665:ASP:OD2	2.43	0.52
2:B:60:LYS:HB2	2:B:61:GLN:OE1	2.10	0.52
2:B:74:ASP:N	2:B:74:ASP:OD1	2.41	0.52
3:C:61:VAL:HA	3:C:65:GLU:HB2	1.90	0.52
6:F:320:ILE:HG23	6:F:327:TRP:HE1	1.75	0.52
1:A:81:PRO:HD3	1:A:199:LYS:HE2	1.92	0.52
1:A:1174:TRP:HZ2	1:A:1243:ASP:HB3	1.75	0.52
2:B:320:PHE:CZ	2:B:339:LYS:HE3	2.45	0.52
2:B:722:ILE:HG13	2:B:727:LEU:HD23	1.92	0.51
1:A:22:LYS:HA	1:A:75:ILE:HD13	1.92	0.51
1:A:1185:MET:SD	1:A:1185:MET:N	2.83	0.51
2:B:881:PHE:HB3	2:B:986:TYR:HB2	1.91	0.51
7:G:49:MET:HE1	7:G:103:ASN:HB2	1.91	0.51
1:A:499:GLN:HB3	1:A:503:SER:HB2	1.93	0.51
2:B:101:HIS:N	2:B:110:ILE:O	2.35	0.51
6:F:24:GLU:CD	6:F:24:GLU:H	2.18	0.51
6:F:25:ALA:O	6:F:29:LYS:HG3	2.11	0.51
2:B:235:GLN:OE1	2:B:243:SER:OG	2.29	0.51
1:A:62:CYS:O	2:B:1190:ASN:ND2	2.41	0.51
2:B:299:SER:O	2:B:303:THR:HG23	2.11	0.51
2:B:482:MET:HG3	2:B:483:GLU:N	2.26	0.51
1:A:371:ARG:NH1	1:A:391:GLU:OE2	2.44	0.51
2:B:97:GLU:HG3	2:B:127:PRO:HD2	1.93	0.51
6:F:200:ILE:HG22	6:F:311:CYS:SG	2.51	0.51
2:B:375:HIS:HD2	2:B:620:GLU:HB3	1.75	0.51
2:B:132:ALA:HB3	2:B:152:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1439:ASN:HB3	5:E:94:MET:SD	2.51	0.50
2:B:877:PHE:O	2:B:1110:ARG:NH1	2.43	0.50
2:B:482:MET:O	2:B:486:ILE:HG23	2.11	0.50
4:D:1:MET:SD	4:D:4:GLN:HB3	2.50	0.50
2:B:79:ASP:HA	2:B:82:ARG:HH12	1.77	0.50
2:B:957:TYR:CZ	2:B:959:PHE:HB2	2.46	0.50
6:F:138:SER:O	6:F:150:ALA:HA	2.12	0.50
1:A:70:MET:HE1	2:B:1214:ARG:HG3	1.93	0.50
2:B:1177:SER:HB3	2:B:1210:VAL:HG22	1.93	0.50
1:A:493:SER:OG	1:A:862:ALA:O	2.17	0.50
1:A:407:ARG:NH1	1:A:408:ASP:O	2.45	0.49
2:B:486:ILE:HG13	2:B:487:ILE:N	2.27	0.49
8:H:21:PHE:HB2	8:H:58:LEU:HD11	1.94	0.49
9:X:21:DC:N4	10:Y:-21:DG:O6	2.20	0.49
2:B:209:ARG:NE	2:B:212:THR:HG21	2.26	0.49
2:B:604:ASN:HA	2:B:607:ILE:HG12	1.94	0.49
2:B:227:ILE:HG13	2:B:228:ILE:HG23	1.94	0.49
2:B:285:ASP:OD1	2:B:285:ASP:N	2.45	0.49
2:B:324:GLN:HG3	2:B:325:HIS:CD2	2.47	0.49
2:B:1190:ASN:O	2:B:1194:PRO:HA	2.13	0.49
4:D:103:LEU:O	4:D:107:VAL:HG12	2.12	0.49
1:A:1098:LEU:HD12	1:A:1104:GLU:HA	1.94	0.49
2:B:543:ARG:HD3	2:B:565:VAL:O	2.13	0.49
8:H:37:LEU:HD12	8:H:38:PRO:HD2	1.94	0.49
2:B:486:ILE:HG22	2:B:504:VAL:HB	1.95	0.49
2:B:389:PHE:O	2:B:393:LEU:HG	2.13	0.49
3:C:333:ILE:O	3:C:337:GLU:HG2	2.12	0.49
2:B:185:ASP:OD1	2:B:813:PHE:HB2	2.11	0.49
2:B:922:PRO:HG2	2:B:925:THR:HG21	1.95	0.49
6:F:263:LEU:HD11	6:F:269:LEU:HG	1.95	0.49
2:B:202:VAL:HG11	2:B:421:SER:HA	1.95	0.49
4:D:143:THR:OG1	4:D:146:GLU:HG3	2.13	0.49
1:A:1307:ASP:N	1:A:1307:ASP:OD1	2.45	0.48
1:A:586:LYS:HA	1:A:586:LYS:HD3	1.64	0.48
1:A:20:ASP:OD1	5:E:44:SER:OG	2.26	0.48
2:B:271:PRO:HB2	2:B:273:TYR:CE1	2.48	0.48
2:B:281:MET:HG2	2:B:287:ILE:HD13	1.96	0.48
3:C:3:LYS:NZ	3:C:357:LEU:HG	2.28	0.48
2:B:870:SER:HG	2:B:1012:THR:HG1	1.61	0.48
1:A:1174:TRP:HD1	1:A:1227:LEU:HD11	1.79	0.48
1:A:208:ILE:HD11	2:B:1218:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:TYR:CD2	2:B:199:GLU:HG2	2.49	0.47
2:B:1058:THR:HG22	8:H:48:GLN:HE22	1.79	0.47
6:F:3:ASP:N	6:F:3:ASP:OD1	2.46	0.47
2:B:1181:ARG:HB2	2:B:1206:ASP:HB3	1.96	0.47
1:A:1129:TRP:HB2	1:A:1178:LEU:HG	1.96	0.47
2:B:916:LEU:HD21	2:B:932:ILE:HG22	1.96	0.47
2:B:1162:GLN:NE2	5:E:78:ARG:HH11	2.10	0.47
2:B:457:LEU:HD22	2:B:461:ASN:HB3	1.96	0.47
2:B:894:GLU:HG2	2:B:938:ALA:HB2	1.96	0.47
5:E:127:PRO:HD2	5:E:128:GLU:OE2	2.14	0.47
2:B:995:LYS:HD2	2:B:1111:LEU:HD12	1.97	0.47
3:C:281:ILE:HD13	3:C:321:LEU:HD23	1.95	0.47
1:A:320:TRP:CE2	2:B:1135:PRO:HG3	2.50	0.47
1:A:501:GLN:O	2:B:1031:HIS:CE1	2.67	0.47
1:A:1185:MET:O	1:A:1189:SER:N	2.48	0.47
2:B:512:LYS:HD3	2:B:516:ASN:ND2	2.30	0.47
2:B:423:VAL:O	2:B:427:LYS:HG2	2.14	0.47
3:C:139:LYS:HA	3:C:139:LYS:HD3	1.66	0.47
2:B:727:LEU:HD12	2:B:731:ASP:OD1	2.15	0.46
5:E:120:MET:HG3	5:E:135:ILE:CD1	2.45	0.46
1:A:210:PRO:HD2	1:A:224:HIS:CE1	2.51	0.46
1:A:519:LYS:HE3	1:A:519:LYS:HB3	1.64	0.46
2:B:69:TYR:CZ	2:B:446:LYS:HG2	2.50	0.46
2:B:438:ILE:HG13	2:B:439:ALA:N	2.31	0.46
6:F:288:SER:OG	6:F:290:GLU:OE2	2.30	0.46
1:A:87:PHE:O	1:A:91:ILE:HG13	2.16	0.46
3:C:352:LYS:HE3	3:C:352:LYS:HB3	1.53	0.46
1:A:171:ARG:HB2	1:A:197:VAL:HG11	1.97	0.46
2:B:479:ASN:HA	2:B:482:MET:HG2	1.97	0.46
4:D:19:MET:HB3	4:D:45:ALA:HB1	1.96	0.46
2:B:39:LEU:O	2:B:522:ARG:NH1	2.42	0.46
6:F:98:ASN:O	6:F:116:SER:HB3	2.16	0.46
7:G:90:LYS:HB3	7:G:90:LYS:HE3	1.65	0.46
2:B:441:ILE:HA	2:B:469:ALA:HB1	1.98	0.46
2:B:796:ARG:HH22	2:B:1036:ARG:HH21	1.63	0.46
6:F:212:ILE:HG12	6:F:217:ILE:HG12	1.98	0.46
1:A:1233:ARG:HA	1:A:1233:ARG:HD2	1.74	0.46
2:B:379:THR:OG1	2:B:381:ASP:OD1	2.17	0.46
3:C:34:GLU:N	3:C:34:GLU:OE1	2.49	0.46
6:F:212:ILE:HG21	6:F:217:ILE:HD11	1.97	0.46
1:A:166:TYR:CD2	1:A:246:ILE:HG21	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:GLN:HA	2:B:367:ILE:HG22	1.98	0.46
2:B:870:SER:OG	2:B:1012:THR:OG1	2.33	0.46
3:C:70:MET:HG2	3:C:176:PHE:CE1	2.51	0.46
2:B:1054:GLN:NE2	2:B:1078:GLU:OE1	2.49	0.45
6:F:83:ALA:HB1	6:F:136:ASN:HA	1.98	0.45
1:A:1211:SER:OG	1:A:1212:VAL:N	2.48	0.45
2:B:803:GLN:OE1	2:B:1001:GLY:HA2	2.16	0.45
1:A:19:ASN:OD1	1:A:19:ASN:N	2.48	0.45
2:B:167:ASN:OD1	2:B:168:ARG:NH1	2.49	0.45
2:B:807:THR:HB	2:B:1109:GLN:HB3	1.99	0.45
1:A:559:LEU:HD22	1:A:639:LEU:HD22	1.99	0.45
1:A:1173:ASN:N	1:A:1173:ASN:OD1	2.50	0.45
2:B:904:THR:HA	2:B:950:TYR:HB2	1.99	0.45
5:E:60:ILE:HD12	5:E:134:GLU:HG3	1.98	0.45
1:A:112:TYR:HB3	1:A:120:ARG:HB2	1.98	0.45
1:A:252:ILE:HD12	1:A:256:ILE:HG22	1.99	0.45
1:A:952:PHE:C	1:A:952:PHE:CD2	2.95	0.45
2:B:196:ARG:NH2	2:B:487:ILE:HD13	2.32	0.45
2:B:830:GLU:HG2	8:H:73:THR:HA	1.99	0.45
6:F:87:ILE:HD12	6:F:112:ILE:HD11	1.99	0.45
6:F:108:GLU:O	6:F:110:VAL:HG23	2.17	0.45
1:A:798:SER:OG	2:B:775:PRO:HB3	2.17	0.45
1:A:1079:GLU:OE1	1:A:1089:GLU:HA	2.17	0.45
2:B:1018:THR:HG22	2:B:1088:MET:HG2	1.99	0.45
1:A:591:THR:HA	1:A:601:GLY:HA3	1.99	0.44
9:X:21:DC:H2"	9:X:22:DC:C6	2.52	0.44
1:A:1177:ARG:C	1:A:1178:LEU:HD12	2.42	0.44
2:B:430:LYS:HD2	2:B:430:LYS:HA	1.70	0.44
2:B:614:ARG:HD3	2:B:621:TRP:CZ2	2.52	0.44
6:F:110:VAL:HG13	6:F:148:ALA:HB3	1.98	0.44
1:A:31:ILE:HD11	1:A:42:GLU:O	2.17	0.44
1:A:114:HIS:CE1	1:A:115:LEU:HG	2.52	0.44
1:A:382:GLN:NE2	1:A:401:VAL:O	2.50	0.44
6:F:5:LYS:HD3	6:F:7:PHE:CZ	2.53	0.44
1:A:923:LEU:HD12	1:A:1276:HIS:HE1	1.83	0.44
3:C:180:VAL:HG22	3:C:222:CYS:HB3	1.99	0.44
6:F:106:LEU:HD12	6:F:107:THR:N	2.32	0.44
1:A:1251:VAL:HG13	1:A:1255:LEU:HD23	2.00	0.44
1:A:1401:ASP:OD2	1:A:1401:ASP:N	2.50	0.44
2:B:479:ASN:O	2:B:483:GLU:HG2	2.17	0.44
4:D:20:VAL:HG22	4:D:46:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ARG:HD2	1:A:456:ALA:HB2	2.00	0.44
1:A:923:LEU:HD12	1:A:1276:HIS:CE1	2.52	0.44
3:C:119:SER:OG	3:C:120:CYS:N	2.49	0.44
3:C:257:TYR:HB3	3:C:337:GLU:OE2	2.18	0.44
1:A:876:SER:HB3	1:A:1283:LYS:HG3	2.00	0.44
1:A:1015:THR:HG22	1:A:1016:CYS:H	1.83	0.44
2:B:60:LYS:HE2	2:B:92:THR:O	2.18	0.44
2:B:118:ARG:NE	2:B:199:GLU:OE1	2.40	0.44
1:A:960:LYS:NZ	1:A:1011:THR:O	2.45	0.44
2:B:543:ARG:HB3	2:B:566:GLY:HA3	2.00	0.44
6:F:44:PHE:CZ	6:F:109:PRO:HG2	2.53	0.44
2:B:305:MET:O	2:B:309:LEU:HD12	2.17	0.43
2:B:381:ASP:OD1	2:B:381:ASP:N	2.44	0.43
2:B:843:ILE:HD11	8:H:79:TYR:CD2	2.53	0.43
6:F:103:GLU:OE2	6:F:111:THR:OG1	2.34	0.43
1:A:208:ILE:HG13	2:B:1218:VAL:HG13	1.98	0.43
1:A:123:GLU:O	1:A:126:SER:OG	2.32	0.43
1:A:849:ARG:NH1	1:A:1377:ARG:O	2.49	0.43
1:A:1158:PHE:HA	1:A:1161:ASN:HD22	1.83	0.43
1:A:1208:ILE:HD12	1:A:1225:ILE:HG23	2.00	0.43
2:B:125:SER:HB3	2:B:159:THR:HB	2.00	0.43
2:B:994:ASP:OD2	2:B:1110:ARG:NH2	2.52	0.43
6:F:22:ASN:HB3	6:F:26:HIS:CE1	2.53	0.43
6:F:316:ASN:HD21	6:F:319:LEU:HG	1.82	0.43
1:A:318:GLN:NE2	2:B:1136:LEU:O	2.52	0.43
1:A:822:THR:HG21	1:A:1054:THR:HA	2.00	0.43
2:B:39:LEU:O	2:B:40:ILE:HD13	2.18	0.43
2:B:100:GLN:HG3	2:B:110:ILE:O	2.19	0.43
2:B:279:PHE:CG	2:B:383:ARG:HD2	2.53	0.43
1:A:834:GLN:HE22	1:A:1411:ALA:HB2	1.84	0.43
1:A:911:ILE:HD13	4:D:192:MET:O	2.19	0.43
2:B:185:ASP:HB3	2:B:188:GLU:HB3	2.01	0.43
2:B:225:ASN:O	2:B:252:THR:HG23	2.19	0.43
2:B:305:MET:HG3	2:B:398:LEU:HD23	2.00	0.43
2:B:471:SER:OG	2:B:473:ASN:OD1	2.32	0.43
2:B:860:ASN:OD1	2:B:860:ASN:N	2.51	0.43
1:A:920:PHE:CE2	1:A:1095:LEU:HB2	2.53	0.43
2:B:815:TRP:CD1	2:B:815:TRP:H	2.35	0.43
6:F:174:GLN:O	6:F:178:LEU:HG	2.19	0.43
6:F:205:LYS:HE2	6:F:205:LYS:N	2.34	0.43
1:A:164:LYS:HE3	1:A:164:LYS:HB2	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:ILE:O	1:A:1077:PRO:HD2	2.18	0.43
2:B:88:GLN:HB3	2:B:135:ILE:O	2.18	0.43
2:B:808:GLY:HA2	2:B:1112:GLN:OE1	2.19	0.43
6:F:324:GLU:HG3	6:F:327:TRP:HD1	1.84	0.43
8:H:1:MET:HB3	8:H:76:TYR:HB2	2.01	0.43
8:H:69:HIS:O	8:H:73:THR:OG1	2.29	0.43
1:A:425:ARG:HA	2:B:1154:VAL:HG13	2.00	0.43
1:A:1157:ASP:O	1:A:1160:GLU:HG3	2.19	0.43
1:A:1205:ASN:HA	1:A:1228:ARG:HD3	2.00	0.43
2:B:299:SER:OG	7:G:51:ASP:OD2	2.33	0.43
3:C:116:LEU:HD13	3:C:157:SER:HB3	2.00	0.43
1:A:35:PHE:CE2	1:A:212:ILE:HG21	2.51	0.43
1:A:698:HIS:HA	7:G:90:LYS:HD2	2.01	0.43
2:B:130:LEU:HB2	2:B:157:VAL:HG23	2.01	0.43
2:B:453:ALA:O	2:B:457:LEU:HG	2.19	0.43
2:B:885:GLU:O	2:B:981:LEU:HD12	2.18	0.43
3:C:187:LEU:HB2	3:C:216:HIS:CD2	2.54	0.43
1:A:1383:LEU:H	1:A:1405:ASN:ND2	2.17	0.42
7:G:49:MET:HE1	7:G:103:ASN:HD22	1.84	0.42
2:B:957:TYR:CE2	2:B:959:PHE:HB2	2.53	0.42
3:C:28:LYS:HD3	8:H:23:LYS:NZ	2.33	0.42
3:C:257:TYR:CZ	3:C:336:LEU:HD13	2.54	0.42
1:A:27:MET:HE3	1:A:47:ASP:OD2	2.19	0.42
1:A:512:ARG:HE	1:A:512:ARG:HB3	1.61	0.42
1:A:1120:ILE:HD12	1:A:1124:ARG:HD3	2.01	0.42
2:B:696:LYS:HE3	2:B:696:LYS:HB3	1.92	0.42
1:A:1174:TRP:CD1	1:A:1227:LEU:HD11	2.55	0.42
2:B:376:MET:HE1	2:B:389:PHE:HB2	2.01	0.42
2:B:665:ASP:OD1	2:B:665:ASP:N	2.52	0.42
3:C:11:LYS:HE2	3:C:11:LYS:HB2	1.56	0.42
3:C:276:LYS:NZ	3:C:326:LYS:HE2	2.35	0.42
5:E:126:THR:HG22	5:E:127:PRO:HD2	2.01	0.42
6:F:331:GLU:HA	6:F:334:LYS:HE3	2.01	0.42
1:A:767:SER:O	1:A:777:ARG:NH1	2.53	0.42
1:A:853:GLN:HE22	4:D:150:PHE:HZ	1.68	0.42
1:A:1017:GLU:H	1:A:1017:GLU:CD	2.27	0.42
1:A:1106:ASN:ND2	1:A:1109:TYR:HB2	2.34	0.42
2:B:235:GLN:HA	2:B:236:PRO:HD2	1.90	0.42
4:D:72:ARG:O	4:D:76:THR:HG23	2.19	0.42
7:G:70:LYS:HD2	7:G:70:LYS:HA	1.77	0.42
1:A:12:GLN:HB2	2:B:1231:THR:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG23	1:A:800:GLU:HG2	2.02	0.42
1:A:1177:ARG:HD2	1:A:1222:ILE:HD11	2.01	0.42
4:D:28:TYR:O	4:D:32:VAL:HG12	2.20	0.42
1:A:661:GLU:OE2	1:A:661:GLU:N	2.51	0.42
2:B:98:ARG:HB3	2:B:170:HIS:CE1	2.55	0.42
6:F:252:SER:OG	6:F:254:LEU:HG	2.19	0.42
8:H:44:ASP:O	8:H:48:GLN:HG2	2.20	0.42
1:A:1274:MET:HE3	1:A:1274:MET:HB2	1.89	0.42
1:A:476:GLU:OE2	2:B:1163:THR:OG1	2.30	0.42
1:A:874:MET:SD	1:A:1284:LEU:HD23	2.60	0.42
2:B:137:THR:HG23	2:B:147:VAL:HG22	2.01	0.42
3:C:13:PHE:HD2	3:C:40:PRO:HB2	1.84	0.42
6:F:185:ILE:HG13	6:F:301:ILE:HG12	2.01	0.42
1:A:1123:GLU:OE2	1:A:1255:LEU:HB3	2.19	0.42
1:A:1177:ARG:HG3	1:A:1224:ARG:HG2	2.02	0.42
2:B:207:ASN:HB3	2:B:419:HIS:CE1	2.55	0.42
1:A:1182:LYS:HA	1:A:1185:MET:CE	2.49	0.41
3:C:106:ASN:OD1	3:C:106:ASN:N	2.51	0.41
6:F:86:LEU:HD21	6:F:306:PHE:CD2	2.55	0.41
1:A:634:PHE:O	1:A:638:GLN:HG2	2.19	0.41
2:B:326:GLU:OE2	2:B:331:LYS:HB2	2.19	0.41
6:F:161:PHE:CD1	6:F:261:PRO:HD3	2.55	0.41
6:F:263:LEU:HD21	6:F:269:LEU:O	2.20	0.41
1:A:1262:ILE:HB	1:A:1265:ILE:HD12	2.00	0.41
1:A:1421:ARG:O	1:A:1422:ILE:HG13	2.20	0.41
3:C:256:ILE:HD13	3:C:256:ILE:HA	1.90	0.41
1:A:383:ILE:HD12	1:A:383:ILE:HA	1.97	0.41
1:A:385:GLN:N	1:A:385:GLN:OE1	2.53	0.41
1:A:661:GLU:CD	1:A:661:GLU:H	2.27	0.41
1:A:1002:ILE:O	1:A:1006:LEU:HB2	2.21	0.41
1:A:1177:ARG:HA	1:A:1224:ARG:HA	2.02	0.41
2:B:37:THR:HG22	2:B:38:GLY:O	2.20	0.41
2:B:641:GLU:OE1	2:B:643:LYS:N	2.52	0.41
2:B:641:GLU:CD	2:B:643:LYS:H	2.28	0.41
4:D:34:MET:HE2	4:D:34:MET:HB3	1.74	0.41
5:E:45:ILE:H	5:E:45:ILE:HG12	1.74	0.41
6:F:100:ILE:HB	6:F:114:ILE:HB	2.02	0.41
6:F:195:LYS:HE3	6:F:308:ASN:HA	2.01	0.41
1:A:70:MET:HE3	1:A:70:MET:HA	2.01	0.41
1:A:1178:LEU:HB2	1:A:1223:ILE:HG23	2.03	0.41
2:B:928:LYS:HE2	2:B:928:LYS:HB2	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:ASP:OD1	2:B:560:ASP:N	2.51	0.41
1:A:913:LEU:HD23	1:A:913:LEU:HA	1.88	0.41
2:B:207:ASN:ND2	2:B:208:ILE:HD12	2.36	0.41
6:F:187:MET:HA	6:F:190:GLU:HG2	2.02	0.41
6:F:200:ILE:HG13	6:F:201:CYS:N	2.34	0.41
1:A:381:LYS:NZ	1:A:398:ARG:O	2.50	0.41
1:A:965:LYS:HB3	1:A:965:LYS:HE3	1.71	0.41
2:B:412:SER:OG	2:B:414:ARG:HG2	2.21	0.41
1:A:881:GLU:O	1:A:885:LYS:HB3	2.21	0.41
1:A:1076:ARG:HB3	1:A:1077:PRO:HD3	2.03	0.41
1:A:1339:ILE:O	1:A:1343:MET:HG2	2.20	0.41
2:B:276:PHE:HD2	2:B:287:ILE:HG23	1.85	0.41
2:B:898:LYS:HG3	2:B:916:LEU:HB2	2.02	0.41
4:D:180:ASP:HB2	4:D:200:ILE:HD12	2.03	0.41
6:F:130:VAL:HG12	6:F:326:ILE:HG13	2.02	0.41
1:A:1170:ASP:OD1	1:A:1229:GLU:HB2	2.21	0.41
2:B:138:ALA:N	2:B:146:GLU:O	2.45	0.41
7:G:63:ASP:HB3	7:G:66:ASN:ND2	2.35	0.41
1:A:1150:SER:HA	1:A:1153:GLU:HB3	2.03	0.40
1:A:1210:HIS:HA	1:A:1223:ILE:HD13	2.03	0.40
1:A:1242:THR:OG1	1:A:1243:ASP:N	2.54	0.40
8:H:52:LYS:HE3	8:H:62:MET:HE3	2.03	0.40
1:A:779:ALA:O	1:A:785:TYR:OH	2.30	0.40
2:B:317:ASP:OD2	2:B:320:PHE:HD2	2.03	0.40
2:B:483:GLU:HA	2:B:486:ILE:HG12	2.03	0.40
2:B:585:SER:O	2:B:588:GLN:HG3	2.21	0.40
2:B:1193:HIS:O	2:B:1193:HIS:ND1	2.53	0.40
1:A:758:ASN:N	1:A:758:ASN:HD22	2.18	0.40
4:D:144:GLN:O	4:D:148:GLN:HB2	2.21	0.40
6:F:90:VAL:O	6:F:129:ILE:HA	2.20	0.40
6:F:197:PHE:CE1	6:F:218:LEU:HD22	2.56	0.40
1:A:129:THR:HG22	1:A:132:LYS:NZ	2.36	0.40
1:A:502:ASP:HB2	2:B:861:GLN:NE2	2.37	0.40
2:B:207:ASN:HD22	2:B:207:ASN:HA	1.72	0.40
2:B:768:ARG:NH2	7:G:68:GLN:OE1	2.54	0.40
3:C:304:ASP:OD2	3:C:304:ASP:N	2.54	0.40
2:B:228:ILE:HG12	2:B:250:TYR:HB3	2.02	0.40
2:B:543:ARG:HH12	2:B:563:GLU:HG2	1.86	0.40
2:B:819:VAL:HG12	2:B:884:GLU:HB2	2.03	0.40
4:D:61:ASN:HA	4:D:66:HIS:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1363/1450 (94%)	1314 (96%)	49 (4%)	0	100	100
2	B	1186/1242 (96%)	1143 (96%)	43 (4%)	0	100	100
3	C	355/359 (99%)	344 (97%)	11 (3%)	0	100	100
4	D	203/205 (99%)	196 (97%)	7 (3%)	0	100	100
5	E	104/147 (71%)	102 (98%)	2 (2%)	0	100	100
6	F	337/339 (99%)	321 (95%)	16 (5%)	0	100	100
7	G	57/105 (54%)	53 (93%)	4 (7%)	0	100	100
8	H	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
All	All	3683/3927 (94%)	3549 (96%)	134 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1219/1279 (95%)	1184 (97%)	35 (3%)	37	68
2	B	1038/1081 (96%)	1018 (98%)	20 (2%)	52	79
3	C	326/328 (99%)	318 (98%)	8 (2%)	42	73
4	D	185/185 (100%)	183 (99%)	2 (1%)	70	88
5	E	96/136 (71%)	95 (99%)	1 (1%)	73	89
6	F	312/312 (100%)	303 (97%)	9 (3%)	37	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	G	54/96 (56%)	53 (98%)	1 (2%)	52 79
8	H	70/70 (100%)	66 (94%)	4 (6%)	17 43
All	All	3300/3487 (95%)	3220 (98%)	80 (2%)	45 74

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	ILE
1	A	86	LEU
1	A	88	ILE
1	A	145	VAL
1	A	191	SER
1	A	208	ILE
1	A	328	CYS
1	A	424	GLU
1	A	493	SER
1	A	505	VAL
1	A	530	LEU
1	A	562	GLN
1	A	659	THR
1	A	664	GLN
1	A	667	GLN
1	A	675	LEU
1	A	830	ILE
1	A	848	THR
1	A	922	GLN
1	A	941	ILE
1	A	943	LEU
1	A	959	GLN
1	A	974	VAL
1	A	1012	LEU
1	A	1015	THR
1	A	1086	VAL
1	A	1095	LEU
1	A	1105	THR
1	A	1171	ILE
1	A	1208	ILE
1	A	1227	LEU
1	A	1342	VAL
1	A	1358	ASP
1	A	1422	ILE

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Mol	Chain	Res	Type
1	A	1437	THR
2	B	268	LEU
2	B	278	MET
2	B	301	VAL
2	B	401	ILE
2	B	402	MET
2	B	408	THR
2	B	452	THR
2	B	519	SER
2	B	578	CYS
2	B	634	ARG
2	B	641	GLU
2	B	670	THR
2	B	735	GLN
2	B	765	VAL
2	B	864	SER
2	B	926	VAL
2	B	1028	VAL
2	B	1054	GLN
2	B	1141	SER
2	B	1210	VAL
3	C	5	PHE
3	C	29	LEU
3	C	82	ASP
3	C	116	LEU
3	C	120	CYS
3	C	194	THR
3	C	253	ILE
3	C	257	TYR
4	D	35	VAL
4	D	101	ASN
5	E	66	ILE
6	F	17	THR
6	F	28	LEU
6	F	46	LEU
6	F	126	VAL
6	F	132	VAL
6	F	149	SER
6	F	205	LYS
6	F	217	ILE
6	F	247	LEU
7	G	79	ASP

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Mol	Chain	Res	Type
8	H	16	THR
8	H	23	LYS
8	H	31	THR
8	H	71	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	21	HIS
1	A	64	HIS
1	A	68	GLN
1	A	114	HIS
1	A	224	HIS
1	A	228	ASN
1	A	264	GLN
1	A	265	GLN
1	A	269	ASN
1	A	418	ASN
1	A	420	GLN
1	A	455	ASN
1	A	464	ASN
1	A	501	GLN
1	A	566	ASN
1	A	592	GLN
1	A	646	ASN
1	A	663	HIS
1	A	698	HIS
1	A	728	ASN
1	A	758	ASN
1	A	763	GLN
1	A	834	GLN
1	A	853	GLN
1	A	878	GLN
1	A	1013	ASN
1	A	1106	ASN
1	A	1115	ASN
1	A	1161	ASN
1	A	1197	ASN
1	A	1276	HIS
1	A	1349	ASN
1	A	1439	ASN

Continued on next page...

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Mol	Chain	Res	Type
2	B	64	ASN
2	B	207	ASN
2	B	216	HIS
2	B	325	HIS
2	B	364	GLN
2	B	419	HIS
2	B	557	GLN
2	B	598	GLN
2	B	761	HIS
2	B	829	ASN
2	B	845	ASN
2	B	861	GLN
2	B	906	ASN
2	B	912	ASN
2	B	972	HIS
2	B	991	ASN
2	B	1039	ASN
2	B	1108	HIS
2	B	1112	GLN
2	B	1142	HIS
2	B	1162	GLN
2	B	1182	ASN
2	B	1227	ASN
2	B	1229	ASN
3	C	19	ASN
3	C	207	GLN
3	C	216	HIS
3	C	259	ASN
3	C	345	GLN
4	D	77	ASN
4	D	119	ASN
4	D	144	GLN
6	F	4	GLN
6	F	121	ASN
6	F	146	GLN
7	G	89	GLN
7	G	103	ASN
8	H	48	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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 [i](#)

There are no chain breaks in this entry.

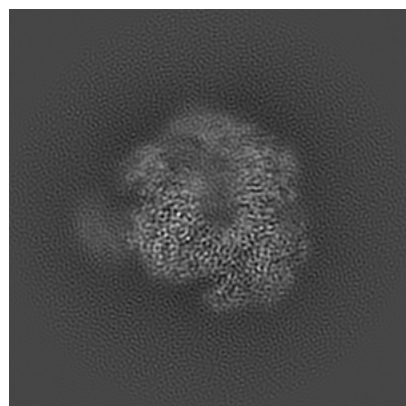
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39511. These allow visual inspection of the internal detail of the map and identification of artifacts.

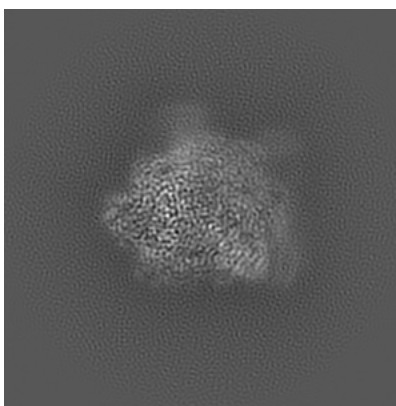
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

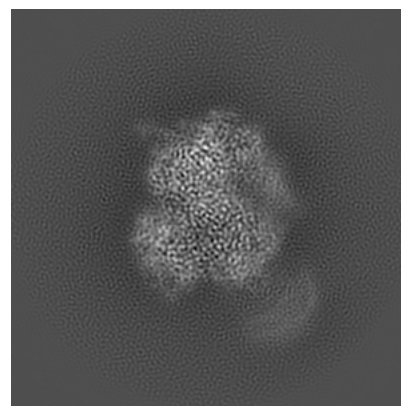
6.1.1 Primary map



X

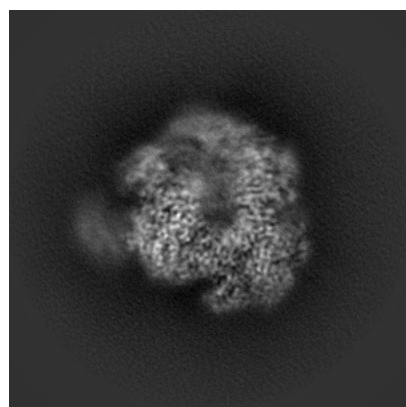


Y

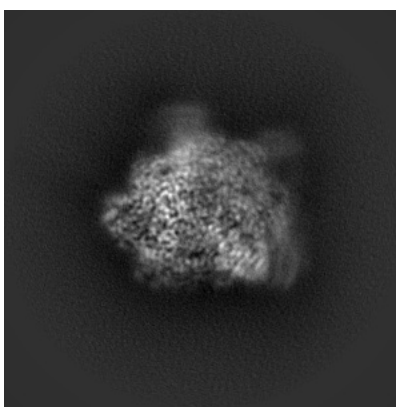


Z

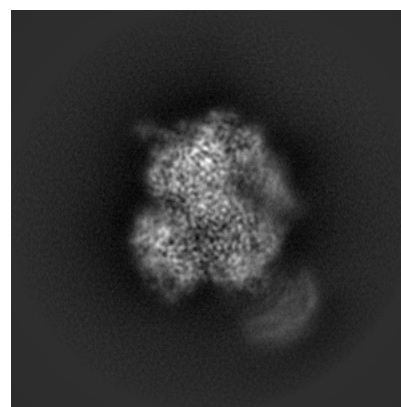
6.1.2 Raw map



X



Y

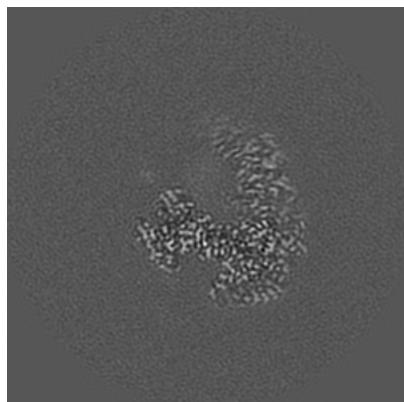


Z

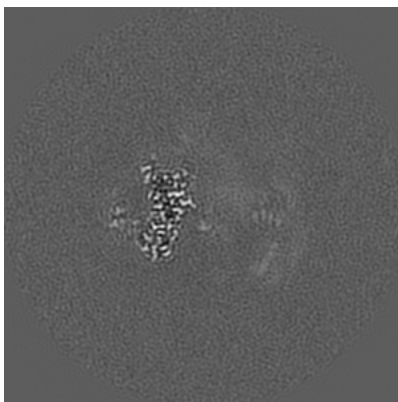
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

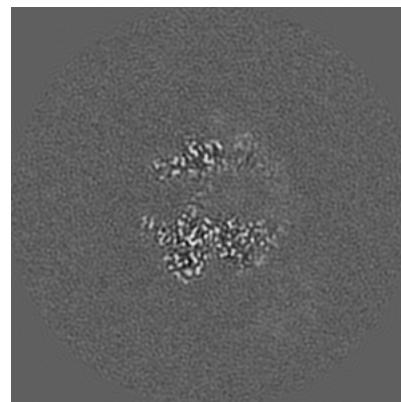
6.2.1 Primary map



X Index: 160

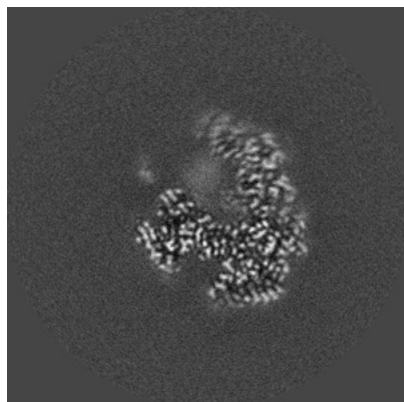


Y Index: 160

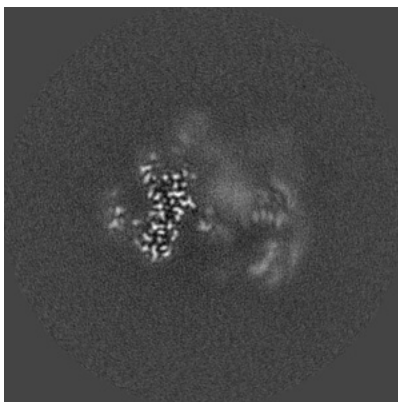


Z Index: 160

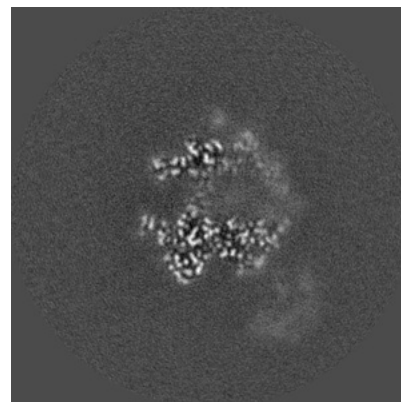
6.2.2 Raw map



X Index: 160



Y Index: 160

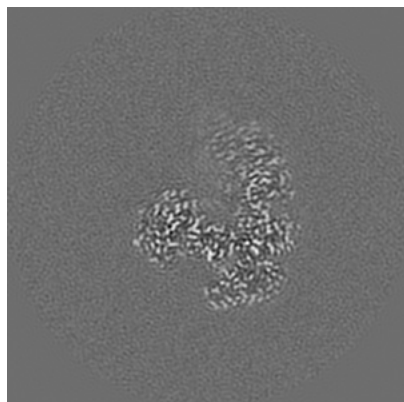


Z Index: 160

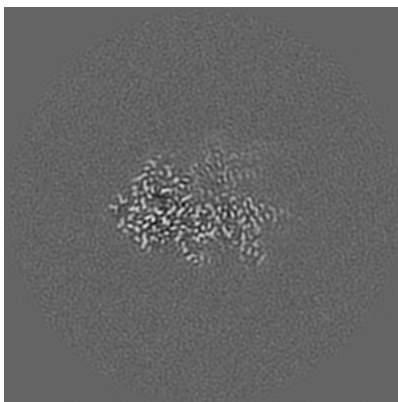
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

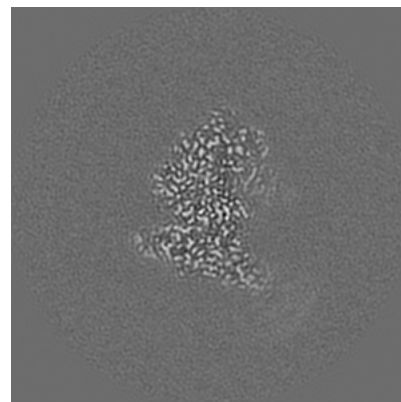
6.3.1 Primary map



X Index: 155

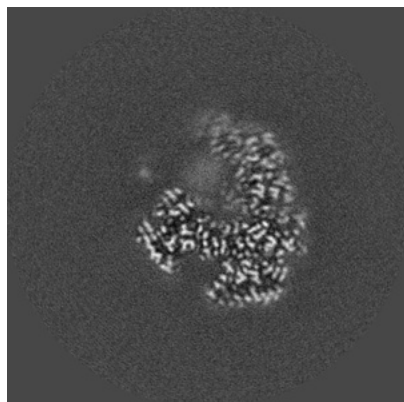


Y Index: 199

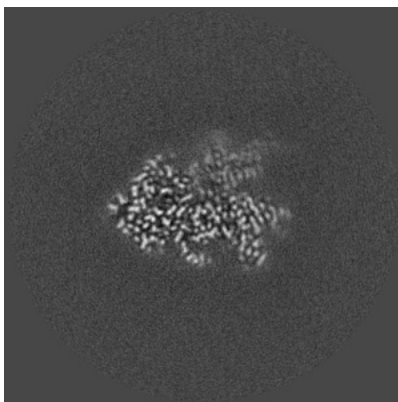


Z Index: 135

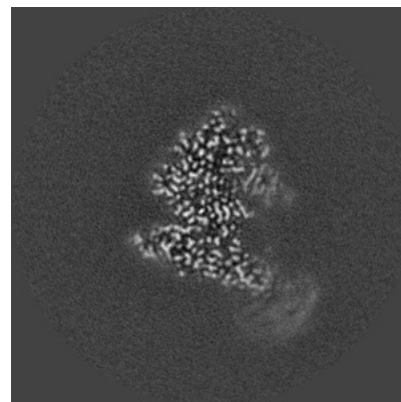
6.3.2 Raw map



X Index: 159



Y Index: 199

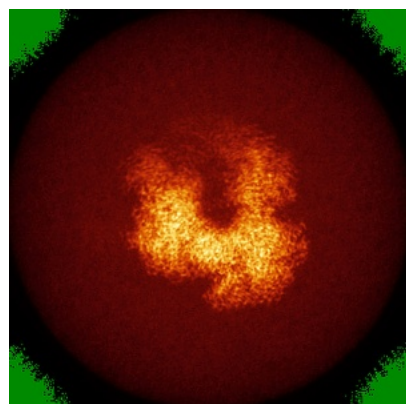


Z Index: 135

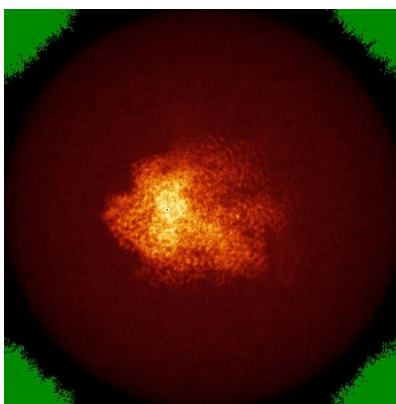
The images above show the largest variance slices of the map in three orthogonal directions.

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

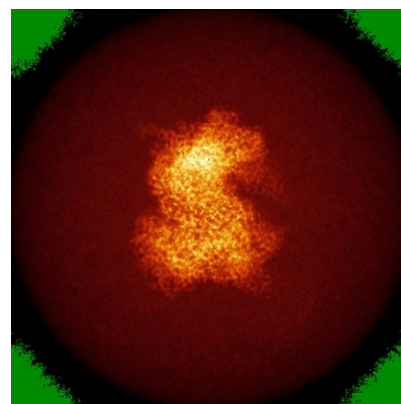
6.4.1 Primary map



X

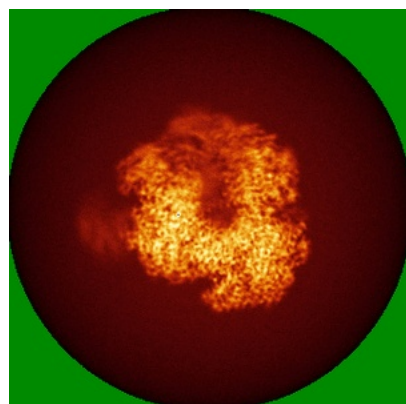


Y

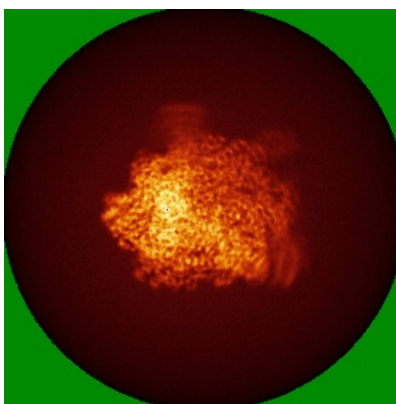


Z

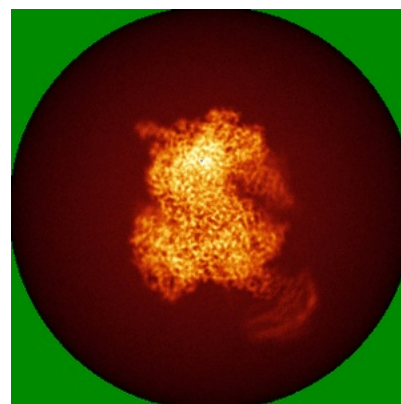
6.4.2 Raw map



X



Y

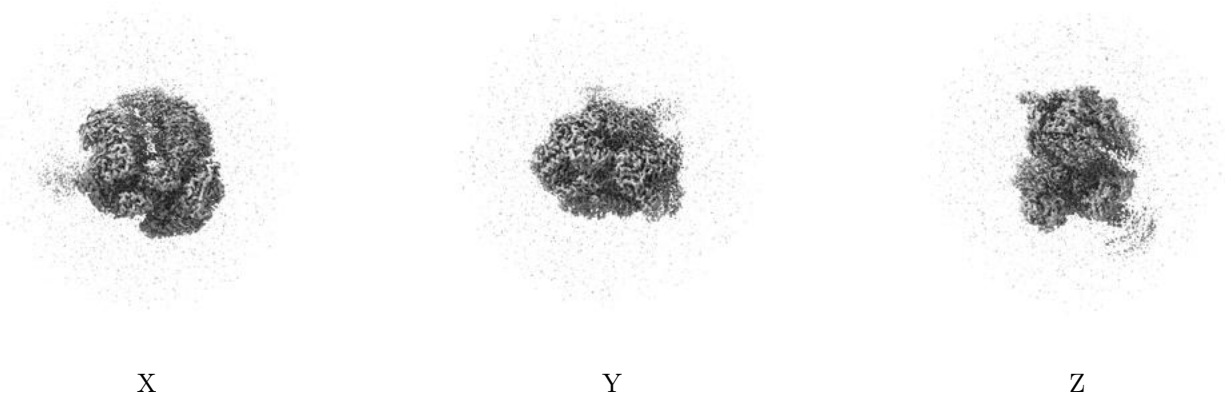


Z

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.

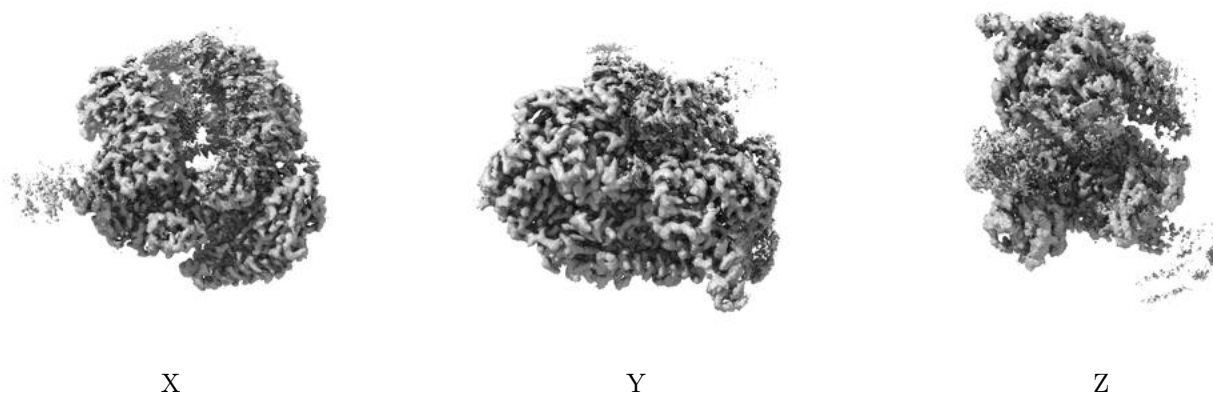
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0129. 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.

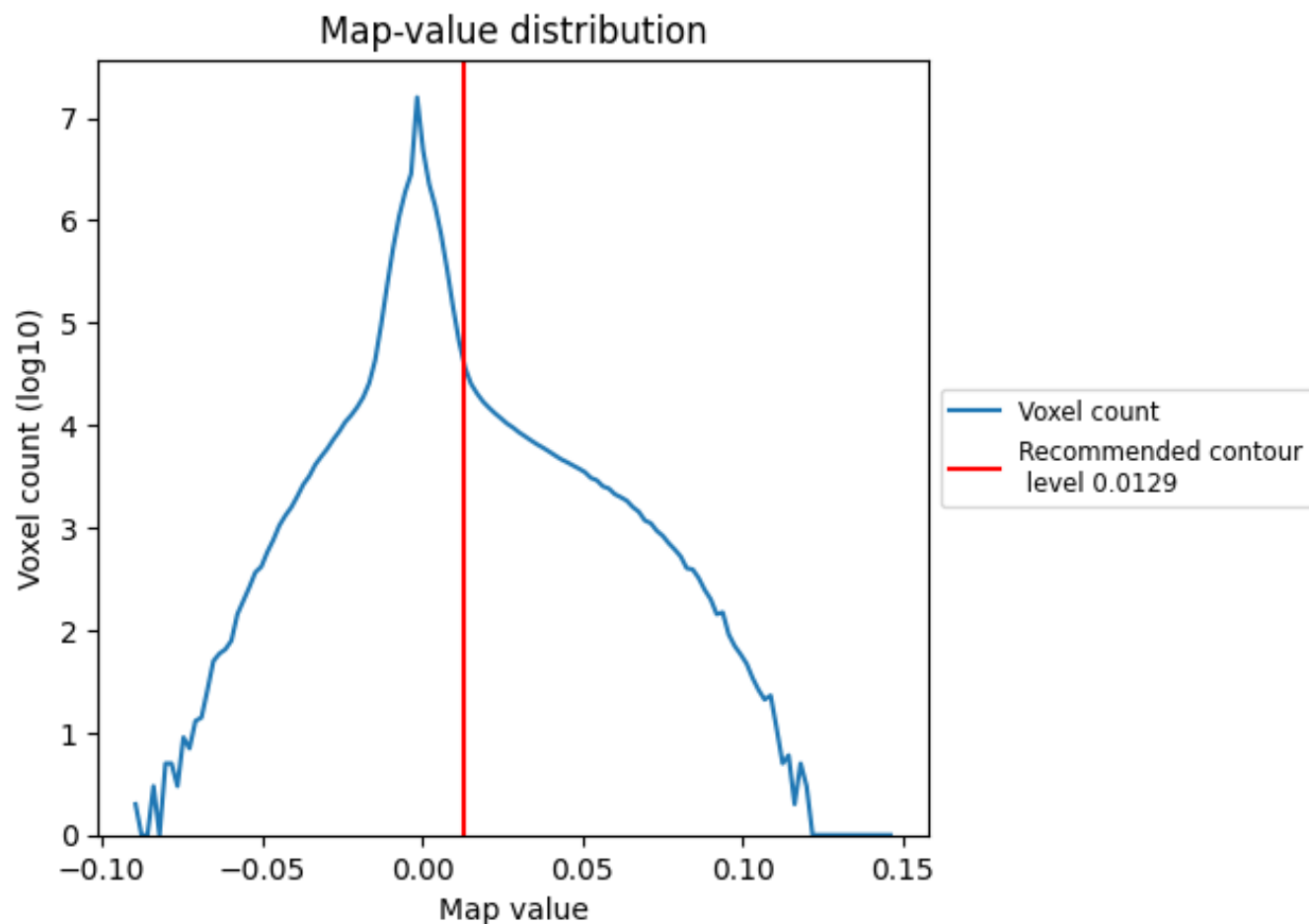
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

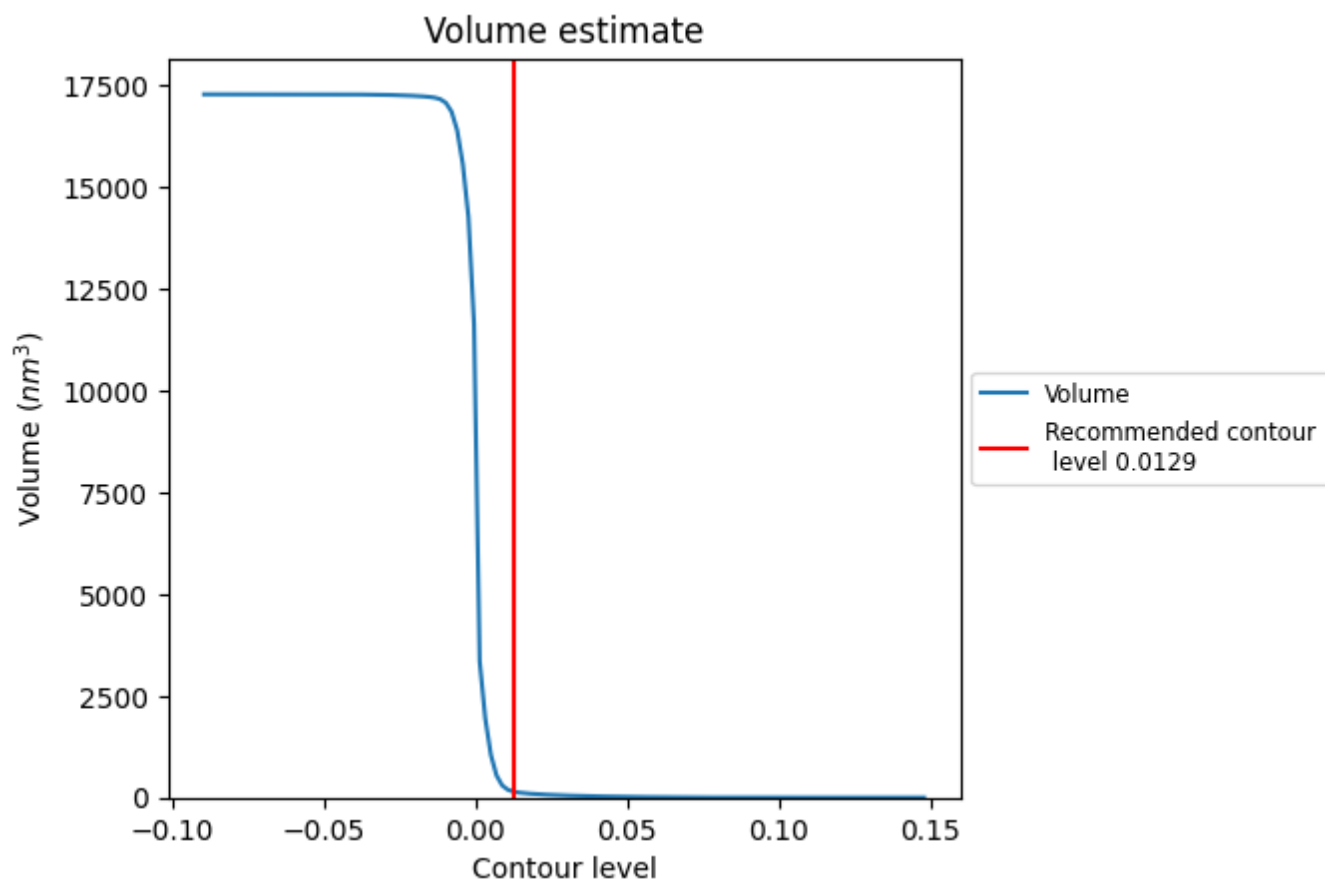
This section contains the results of statistical analysis of the map.

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.

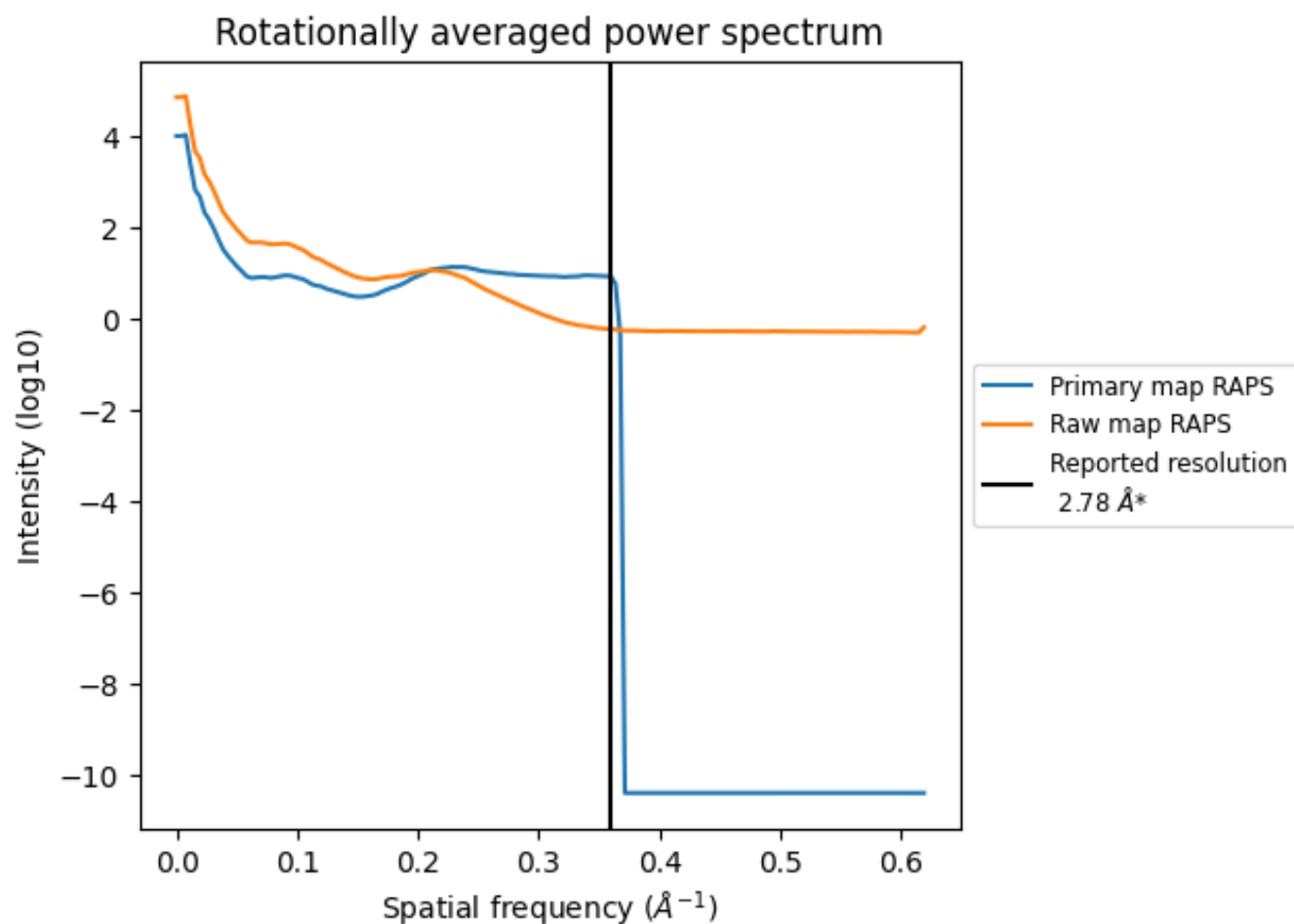
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 141 nm^3 ; this corresponds to an approximate mass of 127 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

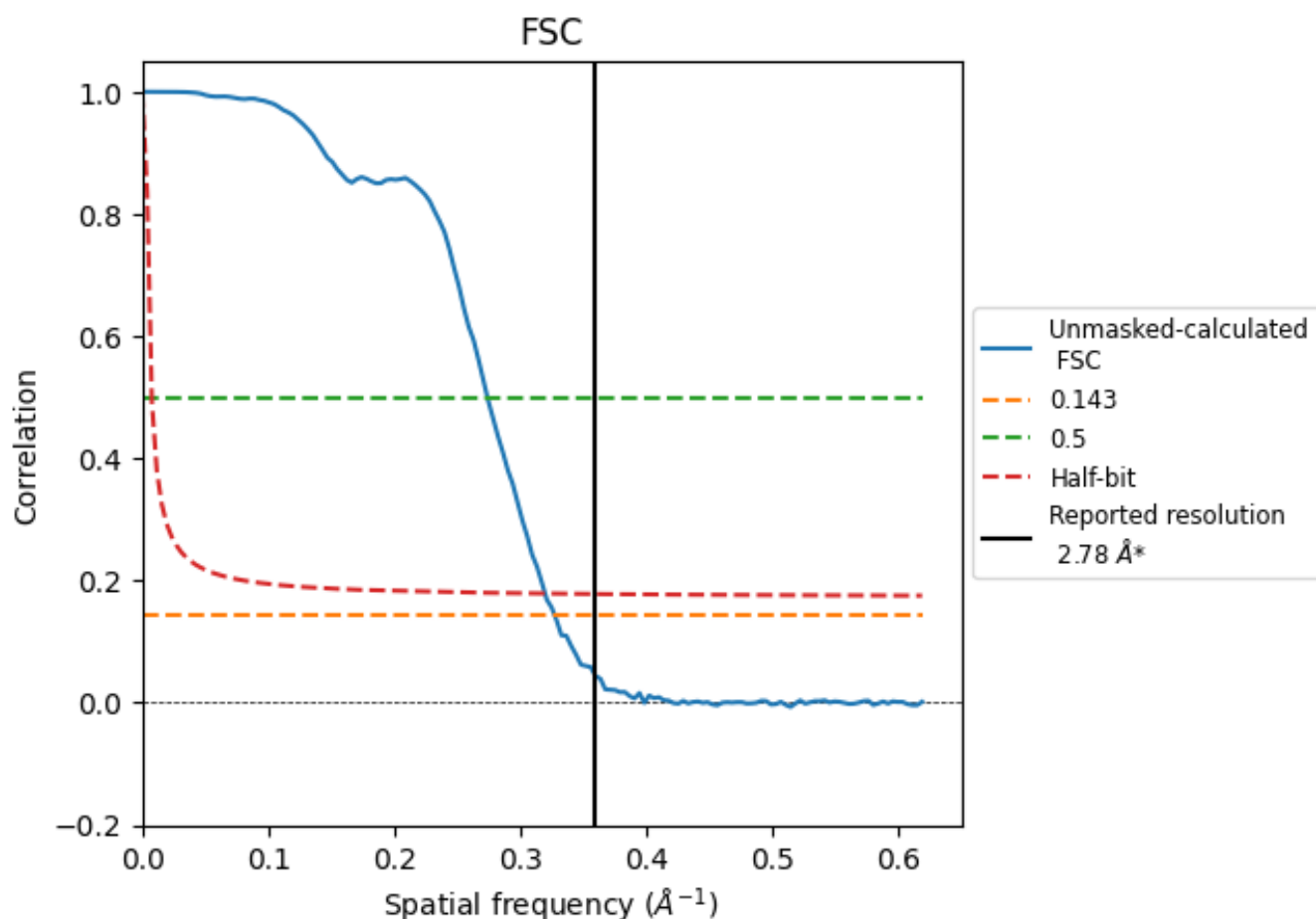


*Reported resolution corresponds to spatial frequency of 0.360 \AA^{-1}

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 0.360 \AA^{-1}

8.2 Resolution estimates [i](#)

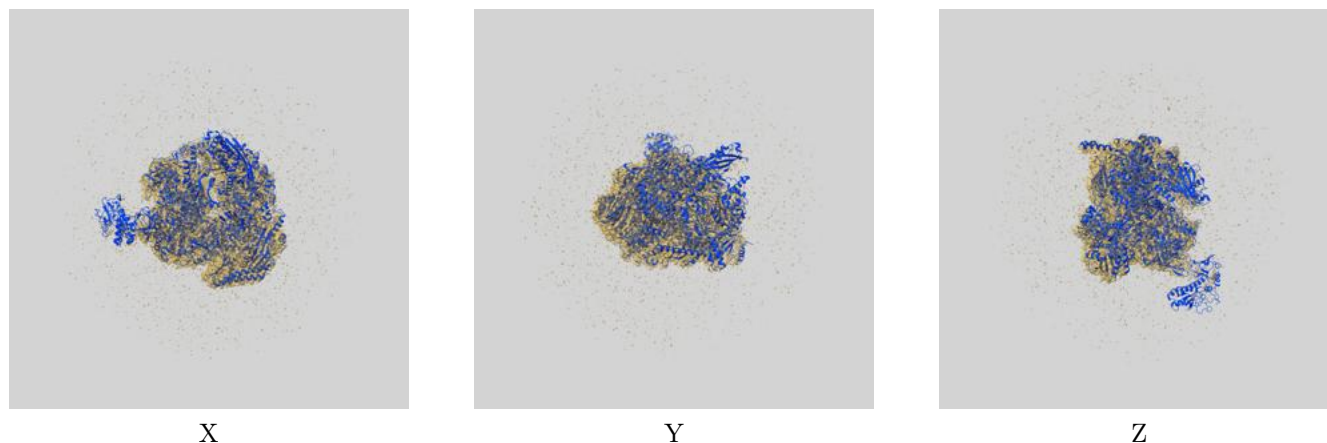
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.06	3.65	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.06 differs from the reported value 2.78 by more than 10 %

9 Map-model fit [i](#)

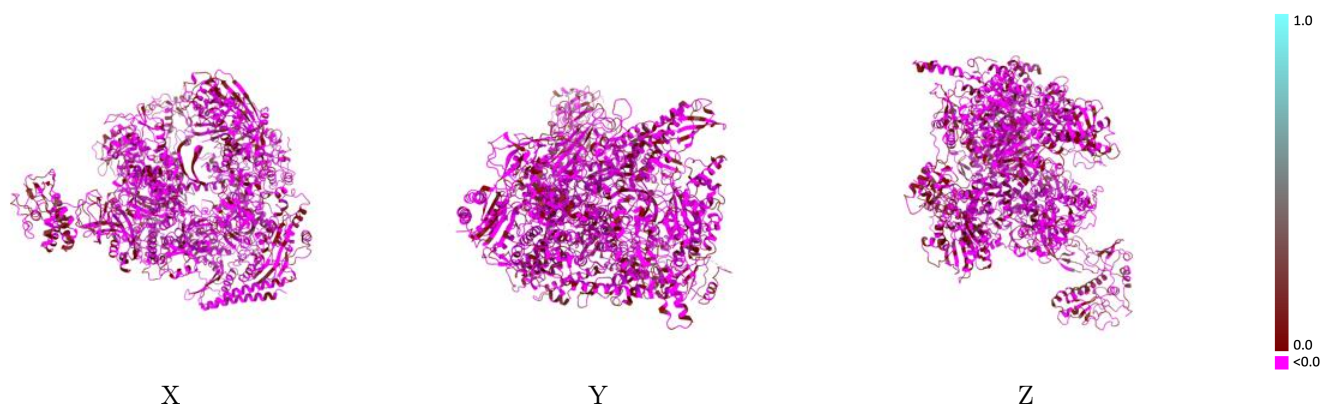
This section contains information regarding the fit between EMDB map EMD-39511 and PDB model 8YQZ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



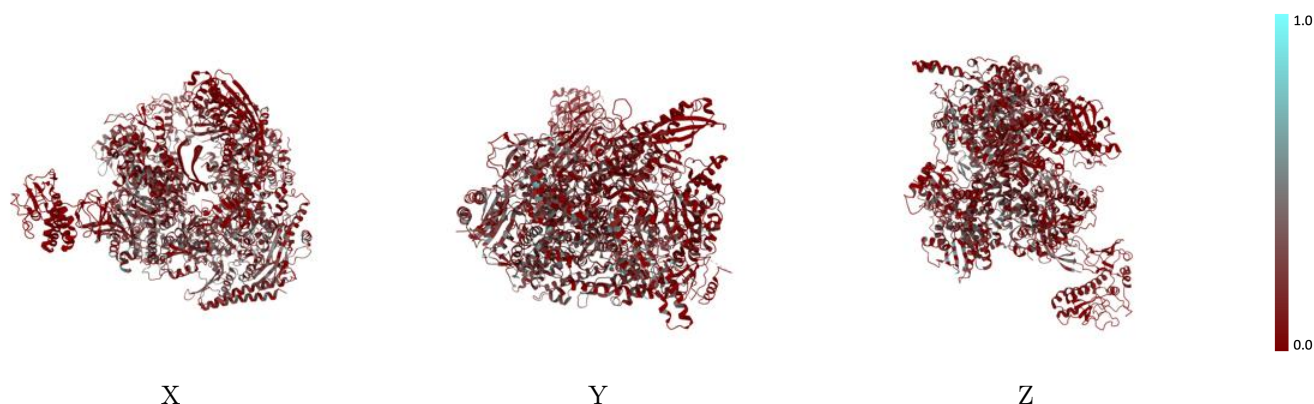
The images above show the 3D surface view of the map at the recommended contour level 0.0129 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



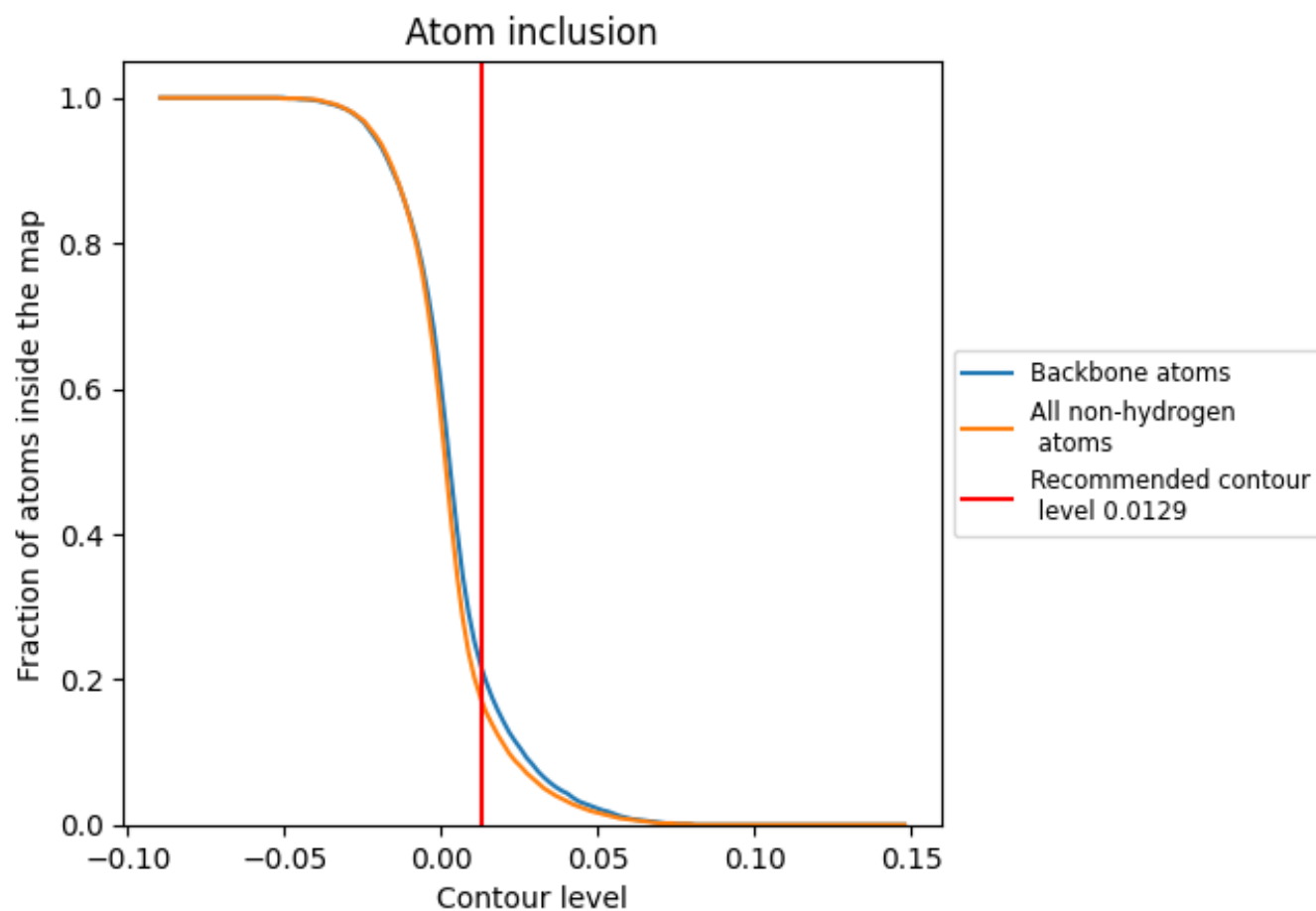
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0129).

9.4 Atom inclusion [i](#)



At the recommended contour level, 22% of all backbone atoms, 17% 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 (0.0129) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.1710	<div></div> -0.0810
A	<div></div> 0.2010	<div></div> -0.0910
B	<div></div> 0.1300	<div></div> -0.0990
C	<div></div> 0.2320	<div></div> -0.0920
D	<div></div> 0.2530	<div></div> -0.0250
E	<div></div> 0.2540	<div></div> -0.0690
F	<div></div> 0.0530	<div></div> -0.0120
G	<div></div> 0.2230	<div></div> -0.0700
H	<div></div> 0.1880	<div></div> -0.0890
X	<div></div> 0.0360	<div></div> 0.0190
Y	<div></div> 0.0140	<div></div> -0.0090

