



Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 09:58 PM JST

PDB ID : 7V9J
EMDB ID : EMD-31816
Title : Telomeric trinucleosome
Authors : Soman, A.
Deposited on : 2021-08-25
Resolution : 8.00 Å(reported)
Based on initial model : 6KE9

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.dev92
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

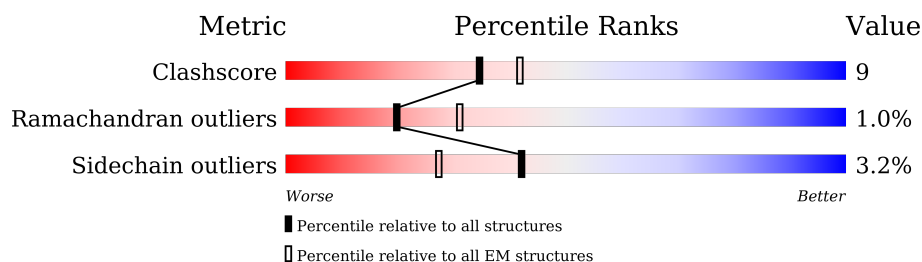
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	136	
1	E	136	
1	K	136	
1	O	136	
1	S	136	
1	W	136	
2	B	103	
2	F	103	

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Mol	Chain	Length	Quality of chain
2	L	103	
2	P	103	
2	T	103	
2	X	103	
3	C	130	
3	G	130	
3	M	130	
3	Q	130	
3	U	130	
3	Y	130	
4	D	99	
4	H	99	
4	N	99	
4	R	99	
4	V	99	
4	Z	99	
5	I	408	
6	J	408	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 35276 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	E	100	Total	C	N	O	S	0	0
			825	520	160	141	4		
1	K	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	O	100	Total	C	N	O	S	0	0
			825	520	160	141	4		
1	S	100	Total	C	N	O	S	0	0
			824	520	160	140	4		
1	W	100	Total	C	N	O	S	0	0
			825	520	160	141	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	S	0	0
			673	424	133	115	1		
2	F	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
2	L	87	Total	C	N	O	S	0	0
			703	442	142	118	1		
2	P	84	Total	C	N	O	S	0	0
			673	424	133	115	1		
2	T	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	X	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			840	529	166	145		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	120	Total	C	N	O	0	0
			927	582	185	160		
3	M	119	Total	C	N	O	0	0
			921	579	184	158		
3	Q	110	Total	C	N	O	0	0
			849	535	168	146		
3	U	109	Total	C	N	O	0	0
			840	529	166	145		
3	Y	110	Total	C	N	O	0	0
			849	535	168	146		

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	H	98	Total	C	N	O	S	0	0
			773	485	144	142	2		
4	N	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	R	98	Total	C	N	O	S	0	0
			773	485	144	142	2		
4	V	99	Total	C	N	O	S	0	0
			783	491	146	144	2		
4	Z	98	Total	C	N	O	S	0	0
			773	485	144	142	2		

- Molecule 5 is a DNA chain called DNA (408-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	399	Total	C	N	O	P	0	0
			8448	3990	1599	2460	399		

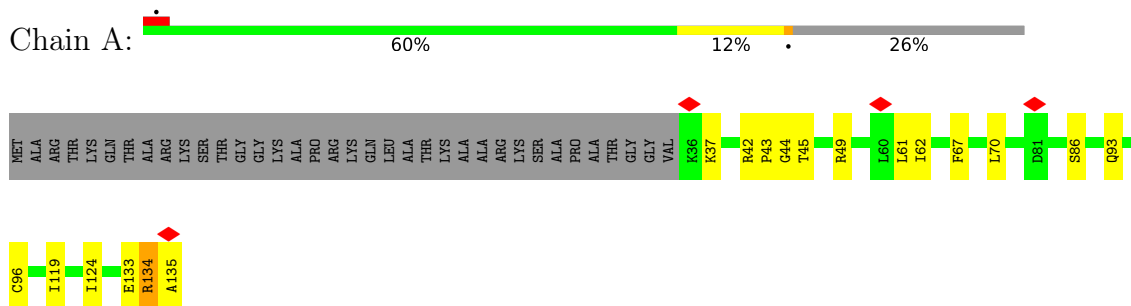
- Molecule 6 is a DNA chain called DNA (408-mer).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	399	Total	C	N	O	P	0	0
			7911	3789	1395	2328	399		

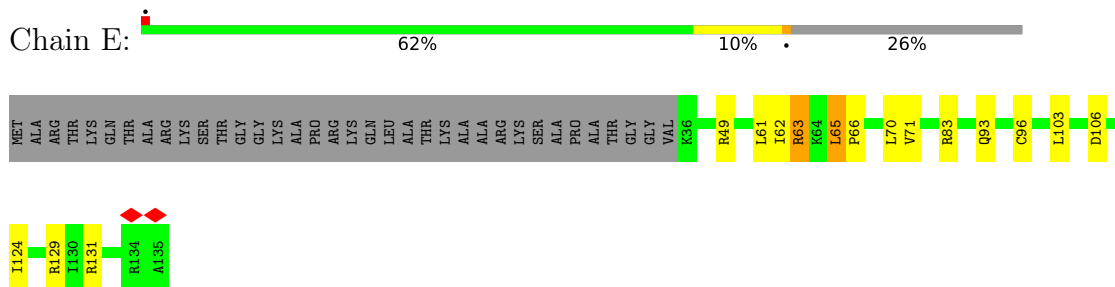
3 Residue-property plots [i](#)

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.

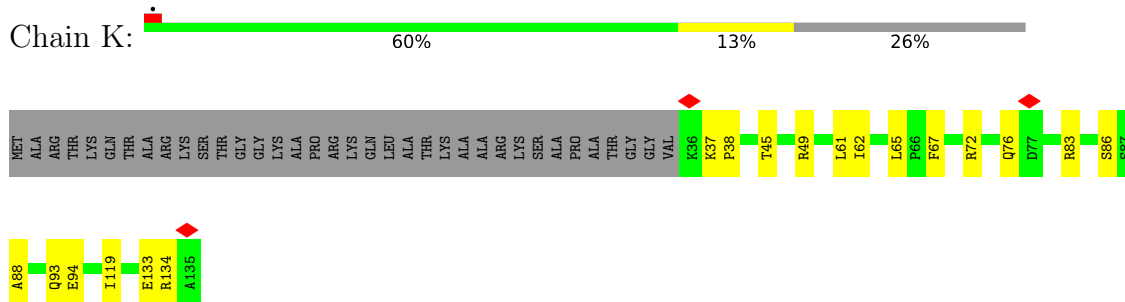
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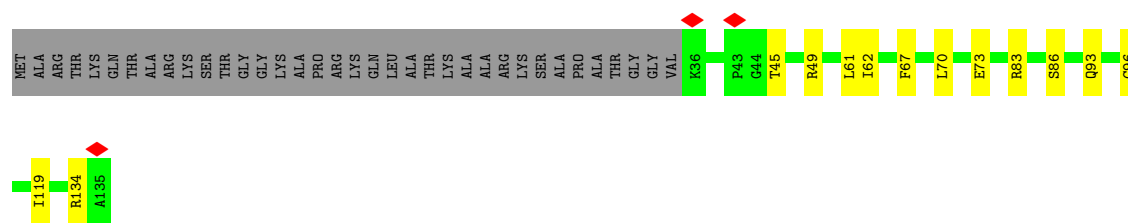


• Molecule 1: Histone H3.1

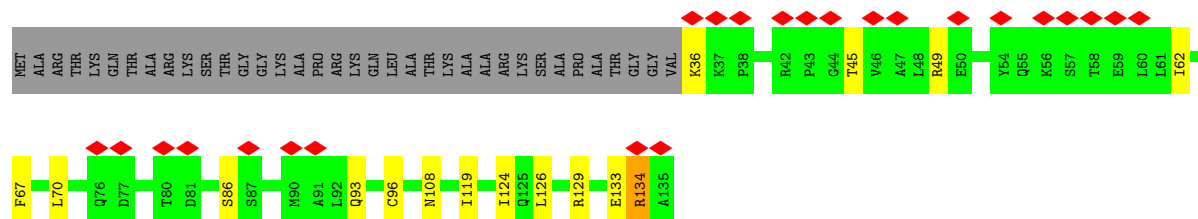


• Molecule 1: Histone H3.1

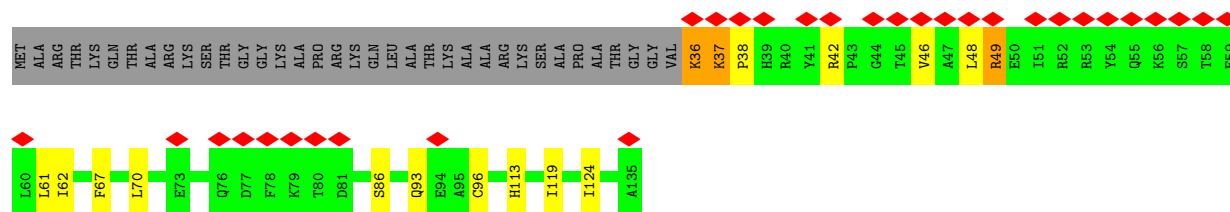




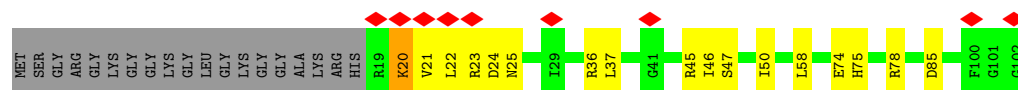
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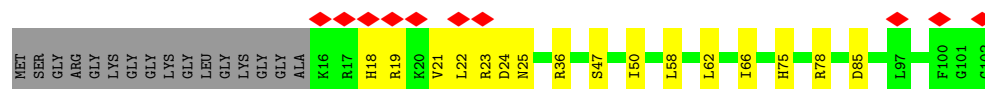
- Molecule 1: Histone H3.1



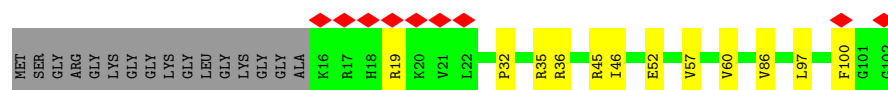
- Molecule 2: Histone H4



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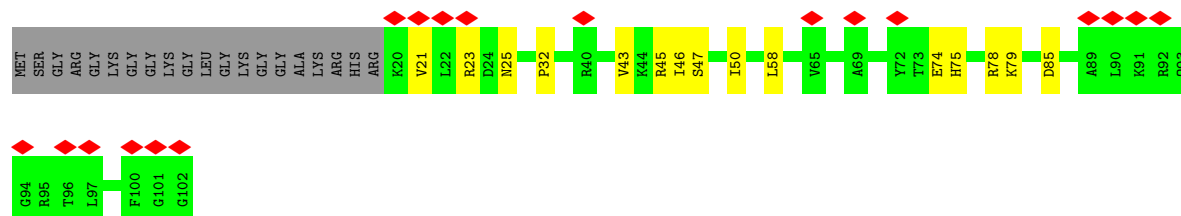
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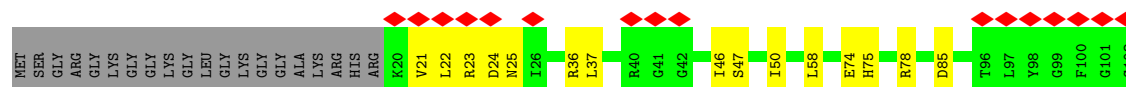
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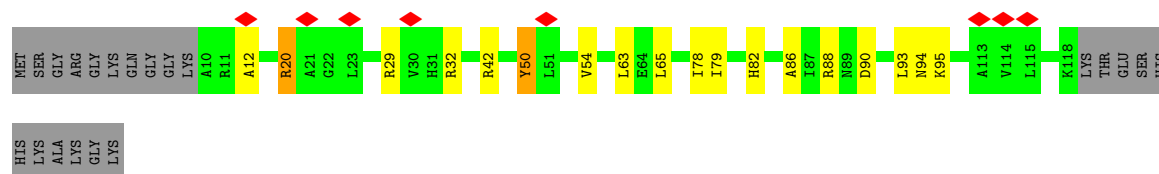
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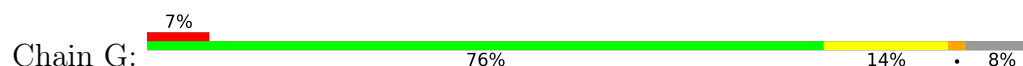
- Molecule 2: Histone H4



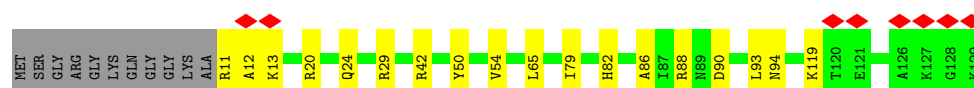
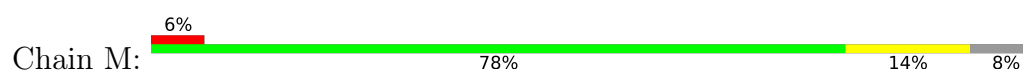
- Molecule 3: Histone H2A type 1-B/E



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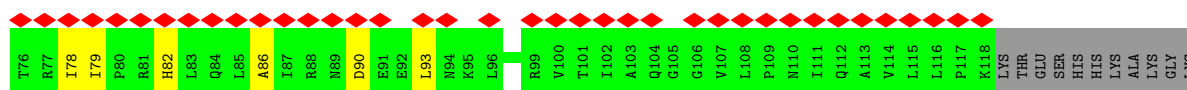
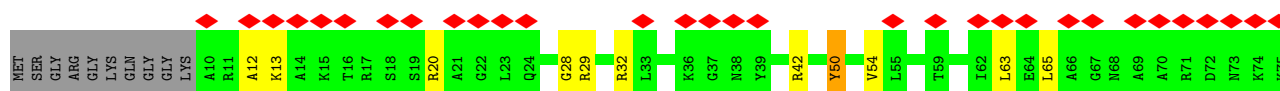
- Molecule 3: Histone H2A type 1-B/E

Chain Q: 



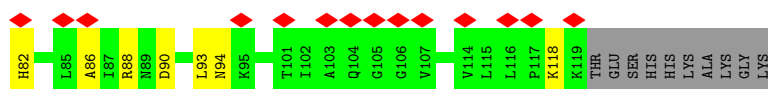
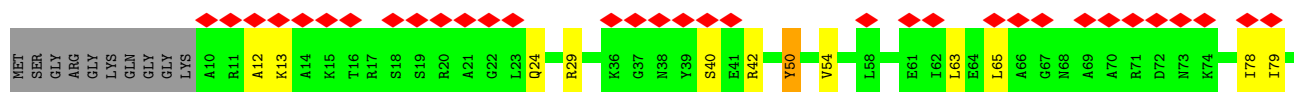
- Molecule 3: Histone H2A type 1-B/E

Chain U: 




- Molecule 3: Histone H2A type 1-B/E

Chain Y: 




- Molecule 4: Histone H2B type 1-K

Chain D: 




- Molecule 4: Histone H2B type 1-K

Chain H: 

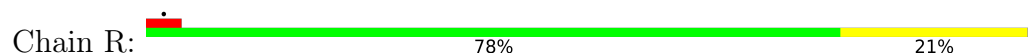


- Molecule 4: Histone H2B type 1-K

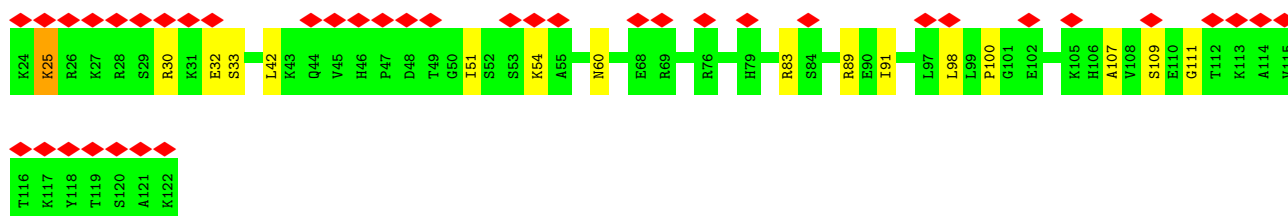
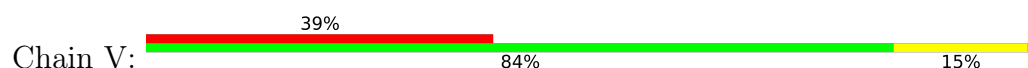
Chain N: 



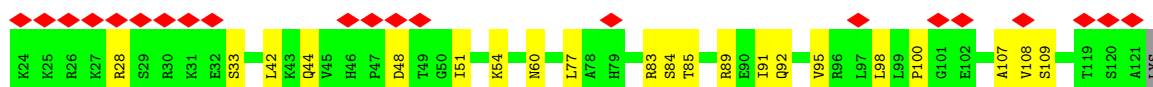
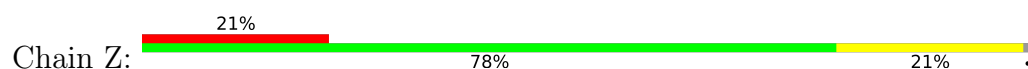
- Molecule 4: Histone H2B type 1-K



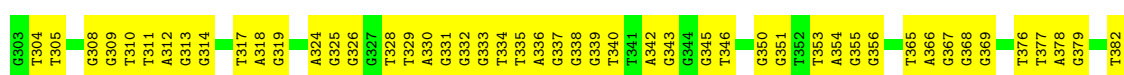
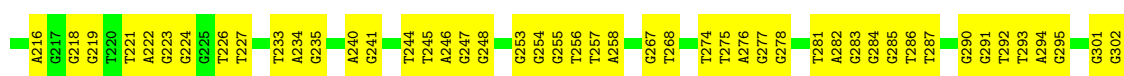
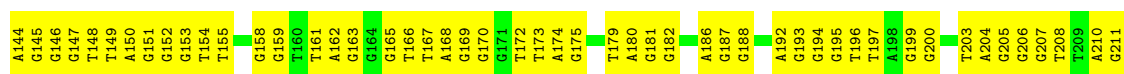
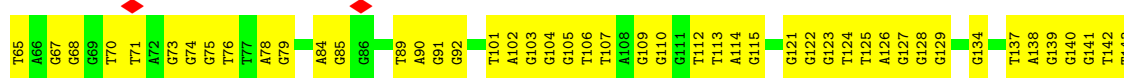
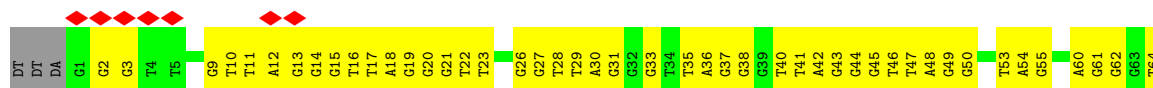
- Molecule 4: Histone H2B type 1-K



- Molecule 4: Histone H2B type 1-K



- Molecule 5: DNA (408-mer)



T383	T384	T385	T386	T387	T388	T389	T390	T391	T392	T393	T394	T395	T396	T397	T398	T399	T400	T401	T402	T403	T404	T405	T406	T407	T408	T409	T410	T411	T412	T413	T414	T415	T416	T417	T418	T419	T420	T421	T422	T423	T424	T425	T426	T427	T428	T429	T430	T431	T432	T433	T434	T435	T436	T437	T438	T439	T440	T441	T442	T443	T444	T445	T446	T447	T448	T449	T450	T451	T452	T453	T454	T455	T456	T457	T458	T459	T460	T461	T462	T463	T464	T465	T466	T467	T468	T469	T470	T471	T472	T473	T474	T475	T476	T477	T478	T479	T480	T481	T482	T483	T484	T485	T486	T487	T488	T489	T490	T491	T492	T493	T494	T495	T496	T497	T498	T499	T500	T501	T502	T503	T504	T505	T506	T507	T508	T509	T510	T511	T512	T513	T514	T515	T516	T517	T518	T519	T520	T521	T522	T523	T524	T525	T526	T527	T528	T529	T530	T531	T532	T533	T534	T535	T536	T537	T538	T539	T540	T541	T542	T543	T544	T545	T546	T547	T548	T549	T550	T551	T552	T553	T554	T555	T556	T557	T558	T559	T560	T561	T562	T563	T564	T565	T566	T567	T568	T569	T570	T571	T572	T573	T574	T575	T576	T577	T578	T579	T580	T581	T582	T583	T584	T585	T586	T587	T588	T589	T590	T591	T592	T593	T594	T595	T596	T597	T598	T599	T600	T601	T602	T603	T604	T605	T606	T607	T608	T609	T610	T611	T612	T613	T614	T615	T616	T617	T618	T619	T620	T621	T622	T623	T624	T625	T626	T627	T628	T629	T630	T631	T632	T633	T634	T635	T636	T637	T638	T639	T640	T641	T642	T643	T644	T645	T646	T647	T648	T649	T650	T651	T652	T653	T654	T655	T656	T657	T658	T659	T660	T661	T662	T663	T664	T665	T666	T667	T668	T669	T670	T671	T672	T673	T674	T675	T676	T677	T678	T679	T680	T681	T682	T683	T684	T685	T686	T687	T688	T689	T690	T691	T692	T693	T694	T695	T696	T697	T698	T699	T700	T701	T702	T703	T704	T705	T706	T707	T708	T709	T710	T711	T712	T713	T714	T715	T716	T717	T718	T719	T720	T721	T722	T723	T724	T725	T726	T727	T728	T729	T730	T731	T732	T733	T734	T735	T736	T737	T738	T739	T740	T741	T742	T743	T744	T745	T746	T747	T748	T749	T750	T751	T752	T753	T754	T755	T756	T757	T758	T759	T760	T761	T762	T763	T764	T765	T766	T767	T768	T769	T770	T771	T772	T773	T774	T775	T776	T777	T778	T779	T780	T781	T782	T783	T784	T785	T786	T787	T788	T789	T790	T791	T792	T793	T794	T795	T796	T797	T798	T799	T800	T801	T802	T803	T804	T805	T806	T807	T808	T809	T810	T811	T812	T813	T814	T815	T816	T817	T818	T819	T820	T821	T822	T823	T824	T825	T826	T827	T828	T829	T830	T831	T832	T833	T834	T835	T836	T837	T838	T839	T840	T841	T842	T843	T844	T845	T846	T847	T848	T849	T850	T851	T852	T853	T854	T855	T856	T857	T858	T859	T860	T861	T862	T863	T864	T865	T866	T867	T868	T869	T870	T871	T872	T873	T874	T875	T876	T877	T878	T879	T880	T881	T882	T883	T884	T885	T886	T887	T888	T889	T890	T891	T892	T893	T894	T895	T896	T897	T898	T899	T900	T901	T902	T903	T904	T905	T906	T907	T908	T909	T910	T911	T912	T913	T914	T915	T916	T917	T918	T919	T920	T921	T922	T923	T924	T925	T926	T927	T928	T929	T930	T931	T932	T933	T934	T935	T936	T937	T938	T939	T940	T941	T942	T943	T944	T945	T946	T947	T948	T949	T950	T951	T952	T953	T954	T955	T956	T957	T958	T959	T960	T961	T962	T963	T964	T965	T966	T967	T968	T969	T970	T971	T972	T973	T974	T975	T976	T977	T978	T979	T980	T981	T982	T983	T984	T985	T986	T987	T988	T989	T990	T991	T992	T993	T994	T995	T996	T997	T998	T999	T1000	T1001	T1002	T1003	T1004	T1005	T1006	T1007	T1008	T1009	T1010	T1011	T1012	T1013	T1014	T1015	T1016	T1017	T1018	T1019	T1020	T1021	T1022	T1023	T1024	T1025	T1026	T1027	T1028	T1029	T1030	T1031	T1032	T1033	T1034	T1035	T1036	T1037	T1038	T1039	T1040	T1041	T1042	T1043	T1044	T1045	T1046	T1047	T1048	T1049	T1050	T1051	T1052	T1053	T1054	T1055	T1056	T1057	T1058	T1059	T1060	T1061	T1062	T1063	T1064	T1065	T1066	T1067	T1068	T1069	T1070	T1071	T1072	T1073	T1074	T1075	T1076	T1077	T1078	T1079	T1080	T1081	T1082	T1083	T1084	T1085	T1086	T1087	T1088	T1089	T1090	T1091	T1092	T1093	T1094	T1095	T1096	T1097	T1098	T1099	T1100	T1101	T1102	T1103	T1104	T1105	T1106	T1107	T1108	T1109	T1110	T1111	T1112	T1113	T1114	T1115	T1116	T1117	T1118	T1119	T1120	T1121	T1122	T1123	T1124	T1125	T1126	T1127	T1128	T1129	T1130	T1131	T1132	T1133	T1134	T1135	T1136	T1137	T1138	T1139	T1140	T1141	T1142	T1143	T1144	T1145	T1146	T1147	T1148	T1149	T1150	T1151	T1152	T1153	T1154	T1155	T1156	T1157	T1158	T1159	T1160	T1161	T1162	T1163	T1164	T1165	T1166	T1167	T1168	T1169	T1170	T1171	T1172	T1173	T1174	T1175	T1176	T1177	T1178	T1179	T1180	T1181	T1182	T1183	T1184	T1185	T1186	T1187	T1188	T1189	T1190	T1191	T1192	T1193	T1194	T1195	T1196	T1197	T1198	T1199	T1200	T1201	T1202	T1203	T1204	T1205	T1206	T1207	T1208	T1209	T1210	T1211	T1212	T1213	T1214	T1215	T1216	T1217	T1218	T1219	T1220	T1221	T1222	T1223	T1224	T1225	T1226	T1227	T1228	T1229	T1230	T1231	T1232	T1233	T1234	T1235	T1236	T1237	T1238	T1239	T1240	T1241	T1242	T1243	T1244	T1245	T1246	T1247	T1248	T1249	T1250	T1251	T1252	T1253	T1254	T1255	T1256	T1257	T1258	T1259	T1260	T1261	T1262	T1263	T1264	T1265	T1266	T1267	T1268	T1269	T1270	T1271	T1272	T1273	T1274	T1275	T1276	T1277	T1278	T1279	T1280	T1281	T1282	T1283	T1284	T1285	T1286	T1287	T1288	T1289	T1290	T1291	T1292	T1293	T1294	T1295	T1296	T1297	T1298	T1299	T1300	T1301	T1302	T1303	T1304	T1305	T1306	T1307	T1308	T1309	T1310	T1311	T1312	T1313	T1314	T1315	T1316	T1317	T1318	T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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.042	Depositor
Minimum map value	-0.009	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0089	Depositor
Map size (\AA)	313.6, 313.6, 313.6	wwPDB
Map dimensions	224, 224, 224	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

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	0.27	0/836	0.52	0/1120
1	E	0.23	0/837	0.50	0/1120
1	K	0.25	0/836	0.51	0/1120
1	O	0.23	0/837	0.50	0/1120
1	S	0.26	0/836	0.51	0/1120
1	W	0.29	0/837	0.51	0/1120
2	B	0.23	0/680	0.52	0/908
2	F	0.22	0/711	0.52	0/948
2	L	0.23	0/711	0.53	0/948
2	P	0.23	0/680	0.52	0/908
2	T	0.23	0/669	0.52	0/894
2	X	0.23	0/669	0.51	0/894
3	C	0.24	0/850	0.49	0/1146
3	G	0.27	0/939	0.51	0/1262
3	M	0.23	0/933	0.48	0/1253
3	Q	0.24	0/859	0.50	0/1157
3	U	0.23	0/850	0.49	0/1146
3	Y	0.24	0/859	0.49	0/1157
4	D	0.29	0/794	0.47	0/1061
4	H	0.23	0/784	0.44	0/1050
4	N	0.27	0/794	0.44	0/1061
4	R	0.24	0/784	0.47	0/1050
4	V	0.23	0/794	0.44	0/1061
4	Z	0.24	0/784	0.47	0/1050
5	I	0.50	0/9512	0.92	0/14765
6	J	0.48	0/8840	0.86	0/13556
All	All	0.39	0/37515	0.73	0/53995

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	824	0	869	16	0
1	E	825	0	869	13	0
1	K	824	0	869	10	0
1	O	825	0	869	10	0
1	S	824	0	869	11	0
1	W	825	0	869	14	0
2	B	673	0	722	18	0
2	F	703	0	755	13	0
2	L	703	0	755	10	0
2	P	673	0	722	15	0
2	T	662	0	709	14	0
2	X	662	0	709	14	0
3	C	840	0	902	15	0
3	G	927	0	994	15	0
3	M	921	0	989	11	0
3	Q	849	0	915	16	0
3	U	840	0	902	12	0
3	Y	849	0	915	14	0
4	D	783	0	821	20	0
4	H	773	0	808	12	0
4	N	783	0	821	14	0
4	R	773	0	808	16	0
4	V	783	0	821	13	0
4	Z	773	0	808	15	0
5	I	8448	0	4522	197	0
6	J	7911	0	4456	178	0
All	All	35276	0	29068	563	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 9.

All (563) 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)
1:A:135:ALA:HB1	3:C:95:LYS:HE3	1.15	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ALA:CB	3:C:95:LYS:HE3	2.00	0.92
4:N:30:ARG:HB3	6:J:118:DT:H4'	1.69	0.75
2:B:21:VAL:HB	2:B:24:ASP:HB2	1.68	0.74
6:J:141:DC:H2''	6:J:142:DT:C5	2.25	0.72
2:L:32:PRO:HA	2:L:35:ARG:HB2	1.74	0.70
1:S:119:ILE:HD11	2:T:46:ILE:HG23	1.73	0.70
1:W:46:VAL:HA	1:W:49:ARG:HE	1.57	0.70
5:I:325:DG:H2''	5:I:326:DG:C8	2.28	0.69
5:I:332:DG:H1	6:J:68:DC:H42	1.40	0.68
5:I:61:DG:H2''	5:I:62:DG:C8	2.28	0.68
1:W:119:ILE:HD11	2:X:46:ILE:HG23	1.76	0.68
2:T:21:VAL:HG12	2:T:23:ARG:H	1.58	0.68
5:I:193:DG:H2''	5:I:194:DG:C8	2.31	0.66
2:P:30:THR:HG21	6:J:56:DC:H5''	1.78	0.66
1:A:119:ILE:HD11	2:B:46:ILE:HG23	1.78	0.66
6:J:177:DC:H2'	6:J:178:DT:H71	1.77	0.66
1:E:49:ARG:HD2	5:I:134:DG:H5'	1.78	0.65
5:I:18:DA:H2''	5:I:19:DG:C8	2.31	0.65
3:C:90:ASP:HB3	3:C:93:LEU:HB2	1.79	0.64
3:G:90:ASP:HB3	3:G:93:LEU:HB2	1.79	0.64
6:J:271:DC:H2'	6:J:272:DC:C6	2.33	0.64
3:Q:90:ASP:HB3	3:Q:93:LEU:HB2	1.79	0.64
5:I:244:DT:H2''	5:I:245:DT:C5	2.33	0.64
3:Y:90:ASP:HB3	3:Y:93:LEU:HB2	1.79	0.64
5:I:311:DT:H2'	5:I:312:DA:C8	2.33	0.64
3:U:90:ASP:HB3	3:U:93:LEU:HB2	1.79	0.64
5:I:47:DT:H2'	5:I:48:DA:C8	2.34	0.63
5:I:67:DG:H2''	5:I:68:DG:C8	2.34	0.63
3:M:90:ASP:HB3	3:M:93:LEU:HB2	1.79	0.63
5:I:226:DT:H2''	5:I:227:DT:H72	1.79	0.63
1:O:119:ILE:HD11	2:P:46:ILE:HG23	1.81	0.62
1:O:83:ARG:HE	6:J:46:DT:H5'	1.64	0.62
5:I:122:DG:H2''	5:I:123:DG:C8	2.35	0.62
5:I:353:DT:H2'	5:I:354:DA:C8	2.35	0.62
5:I:46:DT:H2'	5:I:47:DT:H71	1.81	0.61
1:E:62:ILE:O	1:E:93:GLN:NE2	2.33	0.61
5:I:35:DT:H2''	5:I:36:DA:C8	2.36	0.61
5:I:313:DG:H2''	5:I:314:DG:C8	2.35	0.61
6:J:238:DT:H2''	6:J:239:DA:C8	2.36	0.61
5:I:200:DG:H1	6:J:200:DC:H42	1.47	0.61
5:I:89:DT:H2'	5:I:90:DA:C8	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:ARG:HG2	3:M:119:LYS:HA	1.83	0.60
5:I:143:DT:H2''	5:I:144:DA:N7	2.16	0.60
5:I:68:DG:H1	6:J:332:DC:H42	1.49	0.60
5:I:376:DT:H2''	5:I:377:DT:C5	2.36	0.60
3:M:54:VAL:HG22	4:N:107:ALA:HB1	1.84	0.60
5:I:172:DT:H2''	5:I:173:DT:H72	1.84	0.60
3:M:42:ARG:HB3	6:J:107:DA:H4'	1.84	0.59
5:I:355:DG:H2''	5:I:356:DG:C8	2.36	0.59
6:J:370:DT:H2''	6:J:371:DA:C8	2.37	0.59
6:J:106:DT:H2''	6:J:107:DA:C8	2.37	0.59
5:I:342:DA:H2''	5:I:343:DG:C8	2.38	0.59
5:I:203:DT:H2''	5:I:204:DA:C8	2.38	0.59
5:I:210:DA:H2''	5:I:211:DG:C8	2.38	0.59
1:K:45:THR:HB	1:K:49:ARG:HH21	1.68	0.58
6:J:9:DC:H2''	6:J:10:DT:C5	2.37	0.58
4:H:95:VAL:HG13	4:H:99:LEU:HD12	1.85	0.58
3:Y:78:ILE:HB	4:Z:51:ILE:HG13	1.85	0.58
5:I:37:DG:H2'	5:I:38:DG:C8	2.38	0.58
3:G:54:VAL:HG22	4:H:107:ALA:HB1	1.86	0.58
5:I:167:DT:H2''	5:I:168:DA:C8	2.39	0.58
5:I:49:DG:H2''	5:I:50:DG:C8	2.38	0.58
1:A:45:THR:HB	1:A:49:ARG:HH21	1.68	0.58
5:I:78:DA:H2''	5:I:79:DG:C8	2.39	0.58
5:I:169:DG:H2'	5:I:170:DG:C8	2.39	0.58
5:I:70:DT:H2''	5:I:71:DT:C5	2.39	0.58
5:I:233:DT:H2''	5:I:234:DA:C8	2.38	0.57
1:A:134:ARG:O	1:A:135:ALA:HB2	2.04	0.57
2:X:22:LEU:O	2:X:25:ASN:ND2	2.36	0.57
4:N:95:VAL:HG13	4:N:99:LEU:HD12	1.85	0.57
1:S:45:THR:HB	1:S:49:ARG:HH21	1.68	0.57
1:O:45:THR:HB	1:O:49:ARG:HH21	1.68	0.57
6:J:202:DT:H2''	6:J:203:DA:C8	2.40	0.57
5:I:11:DT:H2''	5:I:12:DA:C5	2.40	0.57
5:I:162:DA:H2''	5:I:163:DG:C8	2.40	0.57
6:J:46:DT:H2''	6:J:47:DA:H8	1.70	0.57
5:I:313:DG:N2	6:J:88:DT:O2	2.36	0.57
5:I:365:DT:H2''	5:I:366:DA:N7	2.20	0.57
6:J:70:DT:H2''	6:J:71:DA:C8	2.40	0.57
5:I:91:DG:H2''	5:I:92:DG:C8	2.40	0.57
5:I:286:DT:H2''	5:I:287:DT:C5	2.40	0.57
6:J:225:DC:H2''	6:J:226:DT:C5	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:267:DG:H2'	5:I:268:DT:H71	1.87	0.56
6:J:255:DC:H2''	6:J:256:DT:C5	2.40	0.56
6:J:164:DC:H2''	6:J:165:DC:C5	2.41	0.56
2:T:75:HIS:O	4:V:89:ARG:NH1	2.37	0.56
2:X:75:HIS:O	4:Z:89:ARG:NH1	2.39	0.56
5:I:294:DA:H2''	5:I:295:DG:C8	2.41	0.56
3:Q:54:VAL:HG22	4:R:107:ALA:HB1	1.88	0.56
5:I:22:DT:H2''	5:I:23:DT:C5	2.41	0.56
5:I:30:DA:H2''	5:I:31:DG:C8	2.41	0.56
5:I:335:DT:H2''	5:I:336:DA:C8	2.41	0.56
6:J:239:DA:H2'	6:J:240:DA:C8	2.41	0.56
5:I:284:DG:H2''	5:I:285:DG:C8	2.41	0.56
6:J:334:DT:H2''	6:J:335:DA:C8	2.41	0.56
3:Y:24:GLN:HG3	4:Z:44:GLN:HE22	1.71	0.56
6:J:247:DC:H2''	6:J:248:DC:C5	2.41	0.56
4:D:83:ARG:NH2	4:D:85:THR:OG1	2.38	0.55
5:I:49:DG:N2	6:J:352:DT:O2	2.38	0.55
5:I:103:DG:H2''	5:I:104:DG:N7	2.22	0.55
5:I:367:DG:H2''	5:I:368:DG:N7	2.21	0.55
5:I:154:DT:H2''	5:I:155:DT:C5	2.41	0.55
5:I:331:DG:H2'	5:I:332:DG:C8	2.42	0.55
6:J:21:DC:H2''	6:J:22:DT:C5	2.42	0.55
6:J:92:DC:H2''	6:J:93:DC:C5	2.42	0.55
6:J:287:DA:H2''	6:J:288:DA:C8	2.42	0.55
4:D:83:ARG:NH1	4:D:90:GLU:OE2	2.41	0.54
5:I:304:DT:H2''	5:I:305:DT:H72	1.88	0.54
2:P:75:HIS:HD2	4:R:77:LEU:HD22	1.71	0.54
6:J:178:DT:C2	6:J:179:DA:N7	2.76	0.54
6:J:379:DC:H2''	6:J:380:DC:C5	2.42	0.54
3:G:32:ARG:NH1	4:H:32:GLU:OE2	2.37	0.54
6:J:327:DC:H2''	6:J:328:DT:C6	2.43	0.54
6:J:152:DC:H2''	6:J:153:DC:C5	2.43	0.54
5:I:385:DG:H2''	5:I:386:DG:C8	2.41	0.54
6:J:219:DC:H2''	6:J:220:DT:C5	2.43	0.54
6:J:353:DA:H2''	6:J:354:DA:H5''	1.88	0.54
5:I:17:DT:H2''	5:I:18:DA:C8	2.43	0.54
6:J:371:DA:H2'	6:J:372:DA:C8	2.43	0.54
1:E:83:ARG:HD2	6:J:178:DT:H5'	1.90	0.54
5:I:223:DG:H2''	5:I:224:DG:C8	2.43	0.54
1:K:119:ILE:HD11	2:L:46:ILE:HG23	1.90	0.54
6:J:89:DA:H2''	6:J:90:DA:H5''	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:32:DC:H2''	6:J:33:DC:C5	2.44	0.53
2:B:47:SER:HB3	2:B:50:ILE:HG12	1.91	0.53
1:E:63:ARG:HH21	6:J:187:DC:H5''	1.73	0.53
5:I:9:DG:N2	6:J:392:DC:O2	2.41	0.53
5:I:328:DT:H2''	5:I:329:DT:C5	2.43	0.53
5:I:390:DA:H2''	5:I:391:DG:C8	2.42	0.53
6:J:296:DC:H2''	6:J:297:DC:C5	2.43	0.53
3:U:65:LEU:HB3	3:U:86:ALA:HB1	1.91	0.53
5:I:75:DG:H2'	5:I:76:DT:H71	1.91	0.53
3:Q:65:LEU:HB3	3:Q:86:ALA:HB1	1.91	0.53
5:I:36:DA:H2''	5:I:37:DG:C8	2.44	0.53
6:J:268:DT:H2''	6:J:269:DA:C8	2.44	0.53
3:U:63:LEU:HD13	4:V:42:LEU:HB2	1.91	0.53
5:I:309:DG:H2'	5:I:310:DT:C6	2.44	0.53
6:J:262:DT:H2''	6:J:263:DA:C8	2.43	0.53
3:C:65:LEU:HB3	3:C:86:ALA:HB1	1.91	0.53
2:F:47:SER:HB3	2:F:50:ILE:HG12	1.91	0.53
1:K:61:LEU:O	2:L:36:ARG:NH2	2.42	0.53
3:G:65:LEU:HB3	3:G:86:ALA:HB1	1.91	0.52
3:U:42:ARG:HB3	6:J:371:DA:H4'	1.92	0.52
5:I:150:DA:H2''	5:I:151:DG:C8	2.43	0.52
1:W:119:ILE:HG13	2:X:50:ILE:HG13	1.90	0.52
6:J:115:DC:H2''	6:J:116:DC:C5	2.43	0.52
2:B:75:HIS:O	4:D:89:ARG:NH1	2.43	0.52
5:I:168:DA:H2''	5:I:169:DG:C8	2.44	0.52
1:A:96:CYS:HB3	2:B:58:LEU:HD11	1.91	0.52
2:B:47:SER:HA	6:J:208:DT:H5''	1.90	0.52
3:U:29:ARG:NH1	4:V:33:SER:O	2.43	0.52
5:I:147:DG:H2'	5:I:148:DT:H71	1.92	0.52
6:J:12:DA:H2''	6:J:13:DC:C5	2.43	0.52
3:C:29:ARG:NH1	4:D:33:SER:O	2.42	0.52
1:E:65:LEU:HB2	5:I:216:DA:H3'	1.92	0.52
3:M:65:LEU:HB3	3:M:86:ALA:HB1	1.91	0.52
3:Q:78:ILE:HB	4:R:51:ILE:HG13	1.91	0.52
5:I:181:DG:H2''	5:I:182:DG:C8	2.44	0.52
6:J:175:DC:H2''	6:J:176:DC:C6	2.45	0.52
6:J:274:DT:H2''	6:J:275:DA:N7	2.24	0.52
2:X:47:SER:HB3	2:X:50:ILE:HG12	1.91	0.52
5:I:355:DG:N2	6:J:46:DT:O2	2.43	0.52
5:I:378:DA:H2''	5:I:379:DG:C8	2.45	0.52
5:I:106:DT:H2'	5:I:107:DT:H71	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:187:DG:H2''	5:I:188:DG:C8	2.45	0.52
6:J:368:DC:H2''	6:J:369:DC:C5	2.45	0.52
3:C:54:VAL:HG22	4:D:107:ALA:HB1	1.92	0.52
1:K:94:GLU:HG3	2:L:100:PHE:HE2	1.75	0.52
2:T:47:SER:HB3	2:T:50:ILE:HG12	1.91	0.52
6:J:214:DT:H2''	6:J:215:DA:C8	2.45	0.52
3:U:78:ILE:HB	4:V:51:ILE:HG13	1.92	0.52
3:Y:65:LEU:HB3	3:Y:86:ALA:HB1	1.91	0.52
6:J:387:DC:H2''	6:J:388:DT:C5	2.45	0.52
5:I:282:DA:H2''	5:I:283:DG:C8	2.45	0.51
3:Y:54:VAL:HG22	4:Z:107:ALA:HB1	1.91	0.51
5:I:221:DT:H2'	5:I:222:DA:C8	2.46	0.51
6:J:346:DT:H2''	6:J:347:DA:C8	2.44	0.51
6:J:142:DT:H2''	6:J:143:DA:C8	2.46	0.51
2:F:75:HIS:HD2	4:H:77:LEU:HD22	1.75	0.51
3:G:24:GLN:HG3	4:H:44:GLN:HE22	1.74	0.51
5:I:246:DA:H2''	5:I:247:DG:C8	2.45	0.51
6:J:220:DT:H2'	6:J:221:DA:C8	2.45	0.51
5:I:207:DG:H2'	5:I:208:DT:H71	1.91	0.51
4:H:99:LEU:HD22	4:H:103:LEU:HB3	1.93	0.51
3:Y:63:LEU:HD13	4:Z:42:LEU:HB2	1.92	0.51
5:I:73:DG:H2''	5:I:74:DG:C8	2.45	0.51
5:I:218:DG:H2''	5:I:219:DG:H8	1.76	0.51
6:J:276:DA:H4'	6:J:277:DC:H5'	1.93	0.51
5:I:365:DT:H2''	5:I:366:DA:C8	2.45	0.51
6:J:284:DC:H2''	6:J:285:DC:C5	2.45	0.51
1:A:49:ARG:HD3	6:J:135:DC:H4'	1.93	0.51
5:I:26:DG:H2''	5:I:27:DG:C8	2.46	0.51
5:I:199:DG:H2'	5:I:200:DG:C8	2.46	0.51
6:J:93:DC:H1'	6:J:94:DT:C2	2.46	0.51
6:J:357:DC:H2''	6:J:358:DT:C5	2.46	0.51
3:U:32:ARG:NH1	4:V:32:GLU:OE2	2.42	0.51
5:I:386:DG:H2''	5:I:387:DG:C8	2.46	0.51
2:P:47:SER:HB3	2:P:50:ILE:HG12	1.91	0.50
5:I:90:DA:H2''	5:I:91:DG:C8	2.46	0.50
5:I:290:DG:H2''	5:I:291:DG:C8	2.46	0.50
6:J:96:DA:H2''	6:J:97:DC:C5	2.46	0.50
6:J:322:DT:H2''	6:J:323:DA:C8	2.45	0.50
1:O:96:CYS:HB3	2:P:58:LEU:HD11	1.94	0.50
5:I:121:DG:H2''	5:I:122:DG:C8	2.47	0.50
6:J:211:DC:H2''	6:J:212:DC:H2'	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:155:DA:H2''	6:J:156:DA:C8	2.47	0.50
3:Q:50:TYR:HB3	4:R:91:ILE:HG21	1.94	0.50
2:B:74:GLU:O	4:D:89:ARG:NH2	2.44	0.50
5:I:123:DG:H2''	5:I:124:DT:C5	2.47	0.50
6:J:93:DC:H2''	6:J:94:DT:C5	2.47	0.50
6:J:166:DT:H2''	6:J:167:DA:C8	2.45	0.50
4:N:73:GLU:OE1	4:N:76:ARG:NH2	2.45	0.50
4:N:99:LEU:HD22	4:N:103:LEU:HB3	1.93	0.50
4:H:73:GLU:OE1	4:H:76:ARG:NH2	2.45	0.50
6:J:73:DC:H2''	6:J:74:DC:C5	2.46	0.50
6:J:123:DC:H2''	6:J:124:DT:C5	2.47	0.50
6:J:310:DT:H2''	6:J:311:DA:H8	1.77	0.49
1:S:96:CYS:HB3	2:T:58:LEU:HD11	1.93	0.49
5:I:31:DG:N2	6:J:370:DT:O2	2.45	0.49
5:I:158:DG:H2''	5:I:159:DG:C8	2.47	0.49
6:J:382:DT:H2''	6:J:383:DA:C8	2.47	0.49
6:J:107:DA:H2'	6:J:108:DA:C8	2.47	0.49
3:C:32:ARG:NH1	4:D:32:GLU:OE2	2.41	0.49
2:B:45:ARG:HH21	6:J:208:DT:H4'	1.78	0.49
5:I:113:DT:H2''	5:I:114:DA:N7	2.27	0.49
6:J:63:DC:H2''	6:J:64:DT:C6	2.47	0.49
6:J:285:DC:H2''	6:J:286:DT:C5	2.47	0.49
5:I:267:DG:H22	6:J:133:DC:H42	1.61	0.49
3:C:20:ARG:HD3	4:D:122:LYS:HA	1.93	0.49
5:I:254:DG:H2''	5:I:255:DG:C8	2.47	0.49
6:J:23:DA:H2''	6:J:24:DA:C8	2.48	0.49
1:E:106:ASP:OD2	1:E:131:ARG:NE	2.45	0.49
5:I:101:DT:H2''	5:I:102:DA:C8	2.48	0.49
5:I:152:DG:H2''	5:I:153:DG:C8	2.47	0.49
5:I:253:DG:H2''	5:I:254:DG:C8	2.47	0.49
3:C:42:ARG:HB3	6:J:239:DA:H4'	1.95	0.49
4:H:30:ARG:HB3	5:I:248:DG:H4'	1.94	0.48
6:J:190:DT:H2''	6:J:191:DA:C8	2.47	0.48
5:I:145:DG:H2''	5:I:146:DG:C8	2.48	0.48
5:I:301:DG:H2''	5:I:302:DG:O4'	2.12	0.48
6:J:95:DA:C6	6:J:96:DA:C6	3.01	0.48
1:O:73:GLU:OE2	2:P:25:ASN:ND2	2.46	0.48
2:T:74:GLU:O	4:V:89:ARG:NH2	2.46	0.48
6:J:80:DC:H2''	6:J:81:DC:C5	2.48	0.48
6:J:257:DA:H2''	6:J:258:DA:C8	2.48	0.48
2:B:75:HIS:HD2	4:D:77:LEU:HD22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:127:DG:H2''	5:I:128:DG:C8	2.49	0.48
6:J:163:DC:H2''	6:J:164:DC:C6	2.48	0.48
5:I:247:DG:H1'	5:I:248:DG:C8	2.48	0.48
6:J:87:DC:H2''	6:J:88:DT:C5	2.48	0.48
4:Z:83:ARG:NH2	6:J:300:DA:OP2	2.47	0.48
5:I:384:DA:H2''	5:I:385:DG:N7	2.29	0.48
6:J:122:DC:H2''	6:J:123:DC:C5	2.49	0.48
6:J:155:DA:H2''	6:J:156:DA:N7	2.29	0.48
5:I:140:DG:H2''	5:I:141:DG:C8	2.49	0.48
3:C:78:ILE:HB	4:D:51:ILE:HG13	1.95	0.48
3:M:24:GLN:HG3	4:N:44:GLN:HE22	1.77	0.48
5:I:11:DT:H2''	5:I:12:DA:N7	2.28	0.48
5:I:64:DT:H2''	5:I:65:DT:C5	2.49	0.48
5:I:350:DG:H2''	5:I:351:DG:H8	1.79	0.48
6:J:58:DT:H2''	6:J:59:DA:C8	2.48	0.48
4:H:45:VAL:HG12	4:H:46:HIS:HD2	1.79	0.47
6:J:124:DT:H2''	6:J:125:DA:C8	2.49	0.47
5:I:330:DA:H2'	5:I:331:DG:H8	1.79	0.47
3:G:13:LYS:HA	3:G:13:LYS:HD3	1.65	0.47
4:V:54:LYS:HA	4:V:54:LYS:HD3	1.71	0.47
5:I:47:DT:H2'	5:I:48:DA:H8	1.78	0.47
5:I:142:DT:H2''	5:I:143:DT:C5	2.49	0.47
1:K:62:ILE:O	1:K:93:GLN:NE2	2.48	0.47
1:A:62:ILE:O	1:A:93:GLN:NE2	2.48	0.47
2:L:45:ARG:HG2	6:J:77:DA:H5'	1.97	0.47
1:O:62:ILE:O	1:O:93:GLN:NE2	2.48	0.47
1:S:62:ILE:O	1:S:93:GLN:NE2	2.48	0.47
5:I:49:DG:H2''	5:I:50:DG:N7	2.30	0.47
1:W:62:ILE:O	1:W:93:GLN:NE2	2.48	0.47
5:I:2:DG:H2''	5:I:3:DG:C8	2.50	0.47
5:I:186:DA:H2''	5:I:187:DG:C8	2.50	0.47
6:J:250:DT:H2''	6:J:251:DA:C8	2.49	0.47
5:I:105:DG:H2'	5:I:106:DT:H71	1.96	0.47
5:I:274:DT:H3	6:J:126:DA:H61	1.62	0.47
6:J:221:DA:H2''	6:J:222:DA:H5''	1.96	0.47
5:I:29:DT:H2''	5:I:30:DA:C8	2.50	0.47
6:J:151:DC:H2''	6:J:152:DC:H5'	1.96	0.47
6:J:349:DC:H2''	6:J:350:DC:C5	2.50	0.47
5:I:102:DA:H2''	5:I:103:DG:C8	2.50	0.46
5:I:109:DG:H2''	5:I:110:DG:C8	2.49	0.46
3:G:121:GLU:O	3:G:123:HIS:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:54:VAL:HG21	4:R:95:VAL:HG21	1.96	0.46
3:Y:42:ARG:HB2	4:Z:85:THR:HG22	1.96	0.46
6:J:40:DT:H2''	6:J:41:DA:N7	2.31	0.46
5:I:13:DG:H2''	5:I:14:DG:C8	2.51	0.46
4:N:45:VAL:HG12	4:N:46:HIS:HD2	1.80	0.46
3:Y:50:TYR:HB3	4:Z:91:ILE:HG21	1.97	0.46
5:I:324:DA:H2''	5:I:325:DG:N7	2.31	0.46
3:G:118:LYS:HB2	3:G:118:LYS:HE2	1.54	0.46
5:I:40:DT:H2''	5:I:41:DT:H72	1.97	0.46
5:I:42:DA:H2''	5:I:43:DG:N7	2.31	0.46
5:I:53:DT:H2''	5:I:54:DA:N7	2.30	0.46
5:I:125:DT:H2''	5:I:126:DA:H8	1.80	0.46
3:Q:42:ARG:HB3	5:I:369:DG:H4'	1.98	0.46
5:I:9:DG:H2''	5:I:10:DT:C5	2.51	0.46
6:J:20:DC:H2''	6:J:21:DC:C6	2.51	0.46
6:J:254:DC:H2''	6:J:255:DC:C5	2.51	0.46
4:D:54:LYS:HA	4:D:54:LYS:HD3	1.71	0.46
6:J:191:DA:H2''	6:J:192:DA:H8	1.81	0.46
2:L:97:LEU:HD11	3:Q:103:ALA:HB2	1.98	0.46
4:R:43:LYS:HD3	4:R:43:LYS:HA	1.79	0.46
3:U:54:VAL:HG22	4:V:107:ALA:HB1	1.97	0.46
1:W:61:LEU:O	2:X:36:ARG:NH2	2.49	0.45
5:I:281:DT:H2''	5:I:282:DA:C8	2.51	0.45
5:I:311:DT:H2'	5:I:312:DA:H8	1.78	0.45
6:J:366:DA:H1'	6:J:367:DC:H5'	1.98	0.45
1:S:119:ILE:HG13	2:T:50:ILE:HG13	1.98	0.45
5:I:48:DA:N6	6:J:353:DA:H61	2.15	0.45
6:J:209:DA:H2''	6:J:210:DA:H8	1.81	0.45
6:J:292:DT:H2''	6:J:293:DA:C8	2.51	0.45
6:J:269:DA:H2''	6:J:270:DA:H5'	1.99	0.45
1:E:96:CYS:HB3	2:F:58:LEU:HD11	1.98	0.45
6:J:33:DC:H2''	6:J:34:DT:H72	1.97	0.45
2:B:75:HIS:CE1	4:D:90:GLU:HG3	2.52	0.45
2:L:52:GLU:H	2:L:52:GLU:HG2	1.63	0.45
1:W:46:VAL:HA	1:W:49:ARG:NE	2.29	0.45
3:C:50:TYR:HB3	4:D:91:ILE:HG21	1.98	0.45
1:E:103:LEU:HD21	1:E:124:ILE:HG23	1.97	0.45
2:L:57:VAL:HA	2:L:60:VAL:HG22	1.98	0.45
5:I:125:DT:H3	6:J:275:DA:H2	1.64	0.45
1:W:96:CYS:HB3	2:X:58:LEU:HD11	1.98	0.45
5:I:293:DT:H2''	5:I:294:DA:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:344:DC:H2''	6:J:345:DC:C5	2.52	0.45
4:N:48:ASP:OD1	4:N:48:ASP:N	2.50	0.45
3:Q:42:ARG:HB2	4:R:85:THR:HG22	1.97	0.45
5:I:84:DA:H2''	5:I:85:DG:C8	2.52	0.45
4:D:26:ARG:HD2	4:D:26:ARG:HA	1.63	0.45
2:F:23:ARG:C	2:F:25:ASN:H	2.18	0.45
1:O:61:LEU:O	2:P:36:ARG:NH2	2.50	0.45
5:I:318:DA:H2''	5:I:319:DG:N7	2.32	0.45
6:J:323:DA:H2''	6:J:324:DA:H8	1.82	0.45
3:Q:29:ARG:NH1	4:R:33:SER:O	2.47	0.45
5:I:181:DG:H2''	5:I:182:DG:N7	2.32	0.45
1:S:108:ASN:HB2	2:T:43:VAL:HG22	2.00	0.44
3:U:50:TYR:CE1	4:V:111:GLY:HA3	2.52	0.44
5:I:54:DA:H2''	5:I:55:DG:C8	2.52	0.44
5:I:275:DT:H2''	5:I:276:DA:N7	2.31	0.44
5:I:277:DG:H2''	5:I:278:DG:C8	2.52	0.44
6:J:160:DT:H2''	6:J:161:DA:H8	1.81	0.44
6:J:92:DC:H2''	6:J:93:DC:C6	2.51	0.44
6:J:160:DT:H2''	6:J:161:DA:C8	2.52	0.44
3:C:63:LEU:HD13	4:D:42:LEU:HB2	1.98	0.44
5:I:168:DA:H2''	5:I:169:DG:N7	2.31	0.44
6:J:224:DC:H2''	6:J:225:DC:C5	2.52	0.44
6:J:236:DC:H2''	6:J:237:DC:C5	2.52	0.44
4:R:26:ARG:NH2	5:I:382:DT:OP1	2.50	0.44
5:I:141:DG:H2''	5:I:142:DT:H5'	1.99	0.44
2:P:75:HIS:O	4:R:89:ARG:NH1	2.50	0.44
5:I:174:DA:H2''	5:I:175:DG:N7	2.33	0.44
6:J:118:DT:H2''	6:J:119:DA:C8	2.53	0.44
6:J:286:DT:H2''	6:J:287:DA:C8	2.53	0.44
1:E:63:ARG:HB3	1:E:66:PRO:HD2	2.00	0.44
1:S:36:LYS:HE3	1:S:36:LYS:HB3	1.79	0.44
1:A:42:ARG:HG2	1:A:43:PRO:HD2	1.99	0.44
1:O:62:ILE:HD11	2:P:37:LEU:HD11	1.99	0.44
5:I:128:DG:H2''	5:I:129:DG:H8	1.83	0.44
5:I:277:DG:H2''	5:I:278:DG:C5	2.53	0.44
1:W:62:ILE:HD11	2:X:37:LEU:HD11	2.00	0.44
3:Y:29:ARG:NH1	4:Z:33:SER:O	2.50	0.44
6:J:227:DA:C6	6:J:228:DA:C6	3.06	0.44
1:A:70:LEU:HD13	2:B:25:ASN:HB3	1.99	0.43
6:J:194:DC:H2''	6:J:195:DC:C5	2.53	0.43
4:D:30:ARG:HG2	6:J:251:DA:H5'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:LEU:O	2:F:36:ARG:NH2	2.51	0.43
4:H:48:ASP:OD1	4:H:48:ASP:N	2.50	0.43
2:X:74:GLU:O	4:Z:89:ARG:NH2	2.51	0.43
5:I:181:DG:N2	6:J:220:DT:O2	2.51	0.43
6:J:23:DA:H2''	6:J:24:DA:N7	2.32	0.43
1:A:133:GLU:O	1:A:135:ALA:N	2.51	0.43
1:K:65:LEU:HD22	6:J:86:DC:OP2	2.18	0.43
5:I:161:DT:H2''	5:I:162:DA:C8	2.53	0.43
5:I:172:DT:H2''	5:I:173:DT:C7	2.48	0.43
5:I:255:DG:H2''	5:I:256:DT:C7	2.48	0.43
6:J:75:DC:H2''	6:J:76:DT:C5	2.54	0.43
6:J:224:DC:H2''	6:J:225:DC:C6	2.53	0.43
6:J:298:DT:H2''	6:J:299:DA:H8	1.83	0.43
1:A:119:ILE:HG13	2:B:50:ILE:HG13	2.01	0.43
1:K:88:ALA:HB1	2:L:86:VAL:HG21	1.99	0.43
2:L:46:ILE:N	6:J:77:DA:OP1	2.34	0.43
6:J:62:DC:H2''	6:J:63:DC:C5	2.53	0.43
6:J:380:DC:H2''	6:J:381:DC:C5	2.53	0.43
3:U:28:GLY:HA3	5:I:23:DT:H3'	2.01	0.43
5:I:368:DG:H2''	5:I:369:DG:C8	2.53	0.43
5:I:378:DA:H2''	5:I:379:DG:N7	2.34	0.43
6:J:80:DC:H2''	6:J:81:DC:C6	2.53	0.43
6:J:212:DC:H2''	6:J:213:DC:C5	2.53	0.43
1:K:83:ARG:HH11	6:J:96:DA:H5'	1.82	0.43
1:O:70:LEU:HD13	2:P:25:ASN:HB3	2.00	0.43
6:J:284:DC:H2''	6:J:285:DC:C6	2.54	0.43
6:J:386:DC:H2''	6:J:387:DC:C5	2.53	0.43
2:X:23:ARG:O	2:X:25:ASN:N	2.37	0.43
2:X:75:HIS:HD2	4:Z:77:LEU:HD22	1.84	0.43
3:Q:13:LYS:HG3	3:Q:14:ALA:N	2.33	0.43
1:S:129:ARG:HA	1:S:134:ARG:HA	2.01	0.43
4:V:30:ARG:HH22	5:I:20:DG:H21	1.67	0.43
3:Y:79:ILE:HG13	3:Y:82:HIS:H	1.84	0.43
5:I:114:DA:H2''	5:I:115:DG:N7	2.34	0.43
3:C:54:VAL:HG21	4:D:95:VAL:HG21	2.01	0.42
1:E:63:ARG:HA	1:E:63:ARG:HD3	1.57	0.42
3:G:121:GLU:C	3:G:123:HIS:H	2.22	0.42
3:M:79:ILE:HG13	3:M:82:HIS:H	1.84	0.42
4:N:81:ASN:O	4:N:83:ARG:N	2.52	0.42
1:S:70:LEU:HD13	2:T:25:ASN:HB3	2.00	0.42
5:I:234:DA:H2''	5:I:235:DG:N7	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:339:DG:H2'	5:I:340:DT:H71	2.00	0.42
5:I:366:DA:H2''	5:I:367:DG:C8	2.54	0.42
3:C:79:ILE:HG13	3:C:82:HIS:H	1.84	0.42
3:M:29:ARG:NH2	6:J:117:DC:H5''	2.34	0.42
1:S:124:ILE:HD11	2:T:50:ILE:HG23	2.01	0.42
3:U:50:TYR:HB3	4:V:91:ILE:HG21	2.01	0.42
1:W:36:LYS:HB2	1:W:37:LYS:H	1.61	0.42
1:W:70:LEU:HD13	2:X:25:ASN:HB3	2.00	0.42
5:I:137:DT:H2''	5:I:138:DA:C8	2.54	0.42
5:I:149:DT:H2''	5:I:150:DA:C8	2.54	0.42
6:J:12:DA:H2''	6:J:13:DC:C4	2.53	0.42
2:F:18:HIS:O	2:F:19:ARG:NE	2.52	0.42
1:O:119:ILE:HG13	2:P:50:ILE:HG13	2.01	0.42
3:Q:79:ILE:HG13	3:Q:82:HIS:H	1.84	0.42
5:I:101:DT:H2''	5:I:102:DA:N7	2.35	0.42
5:I:179:DT:H2'	5:I:180:DA:C8	2.55	0.42
6:J:323:DA:H2''	6:J:324:DA:C8	2.54	0.42
4:D:27:LYS:HE3	4:D:27:LYS:HB2	1.83	0.42
2:F:21:VAL:HG12	2:F:25:ASN:HD21	1.84	0.42
5:I:218:DG:H2''	5:I:219:DG:H5'	1.99	0.42
1:W:36:LYS:HB2	1:W:36:LYS:HE2	1.38	0.42
5:I:292:DT:H2'	5:I:293:DT:H71	2.01	0.42
5:I:294:DA:H2''	5:I:295:DG:N7	2.34	0.42
6:J:97:DC:H6	6:J:97:DC:H2'	1.67	0.42
4:D:30:ARG:HE	6:J:250:DT:H4'	1.84	0.42
3:G:54:VAL:HG21	4:H:95:VAL:HG21	2.02	0.42
4:N:65:ASP:OD2	4:N:69:ARG:NH2	2.50	0.42
4:V:25:LYS:H	4:V:25:LYS:HD2	1.85	0.42
5:I:313:DG:H2''	5:I:314:DG:N7	2.35	0.42
6:J:82:DT:H2''	6:J:83:DA:C8	2.55	0.42
6:J:202:DT:H2''	6:J:203:DA:N7	2.35	0.42
1:A:42:ARG:HH21	1:A:44:GLY:HA3	1.84	0.42
4:H:81:ASN:O	4:H:83:ARG:N	2.52	0.42
3:Y:40:SER:OG	4:Z:84:SER:O	2.38	0.42
5:I:36:DA:H2''	5:I:37:DG:N7	2.35	0.42
5:I:64:DT:H2''	5:I:65:DT:C6	2.54	0.42
5:I:257:DT:C2	5:I:258:DA:N7	2.88	0.42
6:J:212:DC:H1'	6:J:213:DC:C2	2.55	0.42
6:J:397:DC:H2''	6:J:398:DC:C6	2.55	0.42
2:F:23:ARG:C	2:F:25:ASN:N	2.73	0.42
1:S:126:LEU:HD22	1:W:113:HIS:ND1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:49:ARG:HE	1:W:49:ARG:HB3	1.65	0.42
5:I:151:DG:H2''	5:I:152:DG:C8	2.55	0.42
5:I:345:DG:H2''	5:I:346:DT:C7	2.49	0.42
5:I:389:DT:H2''	5:I:390:DA:H8	1.85	0.42
4:D:31:LYS:O	6:J:250:DT:H5''	2.19	0.42
5:I:20:DG:H2''	5:I:21:DG:C8	2.54	0.42
5:I:139:DG:H2''	5:I:140:DG:C8	2.55	0.42
5:I:312:DA:N6	6:J:89:DA:H61	2.18	0.42
6:J:225:DC:H1'	6:J:226:DT:C2	2.55	0.42
6:J:256:DT:H2''	6:J:257:DA:N7	2.34	0.42
4:R:54:LYS:HA	4:R:54:LYS:HD3	1.71	0.42
5:I:13:DG:H2''	5:I:14:DG:C5	2.55	0.42
5:I:44:DG:H2''	5:I:45:DG:H8	1.85	0.42
6:J:141:DC:H2''	6:J:142:DT:C4	2.55	0.42
6:J:178:DT:H2''	6:J:179:DA:H8	1.85	0.42
3:G:79:ILE:HG13	3:G:82:HIS:H	1.84	0.41
2:P:48:GLY:N	5:I:338:DG:O5'	2.53	0.41
5:I:318:DA:H2''	5:I:319:DG:C8	2.54	0.41
5:I:338:DG:H2''	5:I:339:DG:C8	2.54	0.41
6:J:73:DC:H2''	6:J:74:DC:C4	2.55	0.41
2:B:20:LYS:O	2:B:20:LYS:HG2	2.20	0.41
3:Q:32:ARG:NH1	4:R:32:GLU:OE2	2.49	0.41
5:I:102:DA:H2''	5:I:103:DG:H8	1.85	0.41
2:F:22:LEU:O	2:F:25:ASN:ND2	2.53	0.41
2:T:32:PRO:HG2	5:I:54:DA:H2'	2.01	0.41
4:V:83:ARG:HH21	5:I:33:DG:H3'	1.85	0.41
5:I:28:DT:H2'	5:I:29:DT:H71	2.02	0.41
5:I:240:DA:H2'	5:I:241:DG:C8	2.55	0.41
6:J:207:DC:H2''	6:J:208:DT:C6	2.54	0.41
6:J:220:DT:H2'	6:J:221:DA:H8	1.85	0.41
6:J:304:DT:H2''	6:J:305:DA:N7	2.34	0.41
3:Q:63:LEU:HD13	4:R:42:LEU:HB2	2.00	0.41
5:I:60:DA:H2''	5:I:61:DG:N7	2.35	0.41
6:J:235:DC:H6	6:J:235:DC:H2'	1.72	0.41
6:J:251:DA:H2''	6:J:252:DA:H8	1.85	0.41
6:J:297:DC:H2''	6:J:298:DT:H72	2.02	0.41
3:G:123:HIS:C	3:G:125:LYS:H	2.23	0.41
6:J:28:DT:H2''	6:J:29:DA:C8	2.55	0.41
6:J:104:DC:H2''	6:J:105:DC:C5	2.56	0.41
6:J:153:DC:H2''	6:J:154:DT:C5	2.55	0.41
1:E:70:LEU:HD22	2:F:62:LEU:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:47:SER:OG	5:I:338:DG:OP1	2.33	0.41
5:I:192:DA:H2''	5:I:193:DG:N7	2.35	0.41
5:I:196:DT:H2''	5:I:197:DT:C6	2.56	0.41
3:U:79:ILE:HG13	3:U:82:HIS:H	1.84	0.41
5:I:317:DT:H2''	5:I:318:DA:N7	2.36	0.41
5:I:333:DG:H2''	5:I:334:DT:H71	2.03	0.41
6:J:121:DC:H5'	6:J:121:DC:C6	2.56	0.41
6:J:361:DC:H1'	6:J:362:DC:O4'	2.21	0.41
2:B:78:ARG:NH2	2:B:85:ASP:OD2	2.54	0.41
2:F:78:ARG:NH2	2:F:85:ASP:OD2	2.54	0.41
4:N:43:LYS:HD3	4:N:43:LYS:HA	1.91	0.41
2:P:74:GLU:O	4:R:89:ARG:NH2	2.54	0.41
2:P:78:ARG:NH2	2:P:85:ASP:OD2	2.54	0.41
3:Y:54:VAL:HG21	4:Z:95:VAL:HG21	2.03	0.41
3:Y:88:ARG:NH1	3:Y:94:ASN:OD1	2.54	0.41
4:Z:54:LYS:HA	4:Z:54:LYS:HD3	1.71	0.41
5:I:112:DT:H2''	5:I:113:DT:C6	2.56	0.41
5:I:245:DT:H2''	5:I:246:DA:N7	2.36	0.41
5:I:291:DG:H1	6:J:109:DC:H42	1.69	0.41
6:J:167:DA:H2''	6:J:168:DA:C8	2.56	0.41
6:J:213:DC:H2''	6:J:214:DT:C5	2.55	0.41
6:J:329:DA:H2''	6:J:330:DA:C8	2.56	0.41
3:Q:40:SER:OG	4:R:84:SER:O	2.39	0.41
2:T:45:ARG:HH21	6:J:340:DT:H4'	1.86	0.41
5:I:337:DG:H2''	5:I:338:DG:C8	2.56	0.41
6:J:13:DC:H2''	6:J:14:DC:C5	2.56	0.41
1:A:62:ILE:HD11	2:B:37:LEU:HD11	2.02	0.40
3:C:88:ARG:NH1	3:C:94:ASN:OD1	2.54	0.40
3:G:88:ARG:HD3	3:G:88:ARG:HA	1.85	0.40
1:K:134:ARG:HA	1:K:134:ARG:HD3	1.78	0.40
3:M:88:ARG:NH1	3:M:94:ASN:OD1	2.54	0.40
5:I:15:DG:H2'	5:I:16:DT:H71	2.03	0.40
5:I:194:DG:H2''	5:I:195:DG:N7	2.36	0.40
5:I:205:DG:H2''	5:I:206:DG:C8	2.55	0.40
6:J:16:DT:H2''	6:J:17:DA:C8	2.56	0.40
6:J:152:DC:H2''	6:J:153:DC:C6	2.56	0.40
6:J:339:DC:H2''	6:J:340:DT:C6	2.56	0.40
6:J:356:DC:H2''	6:J:357:DC:C6	2.56	0.40
2:F:23:ARG:O	2:F:25:ASN:N	2.42	0.40
3:M:54:VAL:HG21	4:N:95:VAL:HG21	2.04	0.40
3:Q:88:ARG:NH1	3:Q:94:ASN:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:92:GLN:HE21	4:R:108:VAL:HG13	1.86	0.40
2:X:78:ARG:NH2	2:X:85:ASP:OD2	2.54	0.40
5:I:48:DA:H61	6:J:353:DA:N6	2.20	0.40
3:G:10:ALA:C	3:G:12:ALA:H	2.25	0.40
1:K:72:ARG:HH12	5:I:308:DG:H3'	1.85	0.40
3:Y:13:LYS:HD2	3:Y:13:LYS:HA	1.89	0.40
4:Z:92:GLN:HE21	4:Z:108:VAL:HG13	1.86	0.40
5:I:274:DT:H2''	5:I:275:DT:C5	2.56	0.40
5:I:377:DT:H2''	5:I:378:DA:N7	2.36	0.40
5:I:392:DG:H2''	5:I:393:DG:C8	2.56	0.40
6:J:81:DC:H2''	6:J:82:DT:C7	2.52	0.40
6:J:344:DC:H2''	6:J:345:DC:C6	2.55	0.40
1:A:61:LEU:O	2:B:36:ARG:NH2	2.54	0.40
1:A:124:ILE:HD11	2:B:50:ILE:HG23	2.04	0.40
2:B:22:LEU:HD12	2:B:23:ARG:HG2	2.04	0.40
1:E:71:VAL:HG13	2:F:66:ILE:HD11	2.03	0.40
4:N:26:ARG:HB2	4:N:27:LYS:H	1.60	0.40
2:T:78:ARG:NH2	2:T:85:ASP:OD2	2.54	0.40
2:T:79:LYS:HB3	2:T:79:LYS:HE3	1.88	0.40
1:W:124:ILE:HD11	2:X:50:ILE:HG23	2.02	0.40
5:I:165:DG:C2'	5:I:166:DT:H71	2.51	0.40
6:J:139:DC:C2	6:J:140:DC:C4	3.09	0.40
6:J:283:DC:H2''	6:J:284:DC:H5'	2.04	0.40
6:J:345:DC:H2''	6:J:346:DT:C5	2.56	0.40
3:M:29:ARG:NH2	4:N:37:TYR:OH	2.54	0.40
5:I:123:DG:H2''	5:I:124:DT:C7	2.52	0.40
5:I:206:DG:H2''	5:I:207:DG:C8	2.57	0.40
6:J:34:DT:H2''	6:J:35:DA:H8	1.87	0.40
6:J:326:DC:H2''	6:J:327:DC:C5	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	
1	A	98/136 (72%)	91 (93%)	6 (6%)	1 (1%)	15	55
1	E	98/136 (72%)	96 (98%)	2 (2%)	0	100	100
1	K	98/136 (72%)	89 (91%)	8 (8%)	1 (1%)	15	55
1	O	98/136 (72%)	91 (93%)	7 (7%)	0	100	100
1	S	98/136 (72%)	92 (94%)	6 (6%)	0	100	100
1	W	98/136 (72%)	91 (93%)	6 (6%)	1 (1%)	15	55
2	B	82/103 (80%)	77 (94%)	5 (6%)	0	100	100
2	F	85/103 (82%)	78 (92%)	6 (7%)	1 (1%)	13	50
2	L	85/103 (82%)	78 (92%)	7 (8%)	0	100	100
2	P	82/103 (80%)	75 (92%)	7 (8%)	0	100	100
2	T	81/103 (79%)	76 (94%)	5 (6%)	0	100	100
2	X	81/103 (79%)	75 (93%)	5 (6%)	1 (1%)	13	50
3	C	107/130 (82%)	101 (94%)	5 (5%)	1 (1%)	17	57
3	G	118/130 (91%)	103 (87%)	13 (11%)	2 (2%)	9	42
3	M	117/130 (90%)	102 (87%)	14 (12%)	1 (1%)	17	57
3	Q	108/130 (83%)	100 (93%)	7 (6%)	1 (1%)	17	57
3	U	107/130 (82%)	101 (94%)	5 (5%)	1 (1%)	17	57
3	Y	108/130 (83%)	100 (93%)	6 (6%)	2 (2%)	8	38
4	D	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	55
4	H	96/99 (97%)	88 (92%)	5 (5%)	3 (3%)	4	27
4	N	97/99 (98%)	88 (91%)	6 (6%)	3 (3%)	4	27
4	R	96/99 (97%)	92 (96%)	3 (3%)	1 (1%)	15	55
4	V	97/99 (98%)	91 (94%)	5 (5%)	1 (1%)	15	55
4	Z	96/99 (97%)	90 (94%)	5 (5%)	1 (1%)	15	55
All	All	2328/2808 (83%)	2157 (93%)	148 (6%)	23 (1%)	20	55

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	24	ASP
4	H	26	ARG
3	M	12	ALA
2	X	24	ASP
1	A	134	ARG
4	D	100	PRO

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Mol	Chain	Res	Type
4	H	100	PRO
4	N	100	PRO
3	Q	12	ALA
4	R	100	PRO
4	V	100	PRO
4	Z	100	PRO
3	C	12	ALA
3	G	12	ALA
4	H	82	LYS
1	K	38	PRO
4	N	82	LYS
3	U	12	ALA
3	Y	118	LYS
3	G	125	LYS
4	N	26	ARG
3	Y	12	ALA
1	W	38	PRO

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	87/111 (78%)	84 (97%)	3 (3%)	37	60
1	E	87/111 (78%)	84 (97%)	3 (3%)	37	60
1	K	87/111 (78%)	82 (94%)	5 (6%)	20	45
1	O	87/111 (78%)	84 (97%)	3 (3%)	37	60
1	S	87/111 (78%)	83 (95%)	4 (5%)	27	52
1	W	87/111 (78%)	80 (92%)	7 (8%)	12	35
2	B	69/79 (87%)	68 (99%)	1 (1%)	67	80
2	F	72/79 (91%)	72 (100%)	0	100	100
2	L	72/79 (91%)	71 (99%)	1 (1%)	67	80
2	P	69/79 (87%)	69 (100%)	0	100	100
2	T	68/79 (86%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	68/79 (86%)	67 (98%)	1 (2%)	65	80
3	C	85/100 (85%)	83 (98%)	2 (2%)	49	69
3	G	94/100 (94%)	90 (96%)	4 (4%)	29	53
3	M	94/100 (94%)	90 (96%)	4 (4%)	29	53
3	Q	86/100 (86%)	85 (99%)	1 (1%)	71	83
3	U	85/100 (85%)	82 (96%)	3 (4%)	36	59
3	Y	86/100 (86%)	85 (99%)	1 (1%)	71	83
4	D	85/85 (100%)	82 (96%)	3 (4%)	36	59
4	H	84/85 (99%)	83 (99%)	1 (1%)	71	83
4	N	85/85 (100%)	81 (95%)	4 (5%)	26	51
4	R	84/85 (99%)	80 (95%)	4 (5%)	25	51
4	V	85/85 (100%)	81 (95%)	4 (5%)	26	51
4	Z	84/85 (99%)	79 (94%)	5 (6%)	19	44
All	All	1977/2250 (88%)	1913 (97%)	64 (3%)	42	61

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	67	PHE
1	A	86	SER
2	B	20	LYS
3	C	20	ARG
3	C	50	TYR
4	D	60	ASN
4	D	98	LEU
4	D	109	SER
1	E	63	ARG
1	E	65	LEU
1	E	129	ARG
3	G	50	TYR
3	G	118	LYS
3	G	119	LYS
3	G	120	THR
4	H	67	PHE
1	K	37	LYS
1	K	67	PHE

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Mol	Chain	Res	Type
1	K	76	GLN
1	K	86	SER
1	K	133	GLU
2	L	19	ARG
3	M	11	ARG
3	M	13	LYS
3	M	20	ARG
3	M	50	TYR
4	N	26	ARG
4	N	27	LYS
4	N	28	ARG
4	N	67	PHE
1	O	67	PHE
1	O	86	SER
1	O	134	ARG
3	Q	50	TYR
4	R	48	ASP
4	R	60	ASN
4	R	98	LEU
4	R	109	SER
1	S	67	PHE
1	S	86	SER
1	S	133	GLU
1	S	134	ARG
3	U	13	LYS
3	U	20	ARG
3	U	50	TYR
4	V	25	LYS
4	V	60	ASN
4	V	98	LEU
4	V	109	SER
1	W	36	LYS
1	W	37	LYS
1	W	42	ARG
1	W	48	LEU
1	W	49	ARG
1	W	67	PHE
1	W	86	SER
2	X	21	VAL
3	Y	50	TYR
4	Z	28	ARG
4	Z	48	ASP

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Mol	Chain	Res	Type
4	Z	60	ASN
4	Z	98	LEU
4	Z	109	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
2	B	75	HIS
3	C	110	ASN
4	D	60	ASN
4	D	92	GLN
2	F	25	ASN
2	F	27	GLN
2	F	75	HIS
3	G	24	GLN
3	G	110	ASN
3	G	124	HIS
4	H	44	GLN
4	H	46	HIS
1	K	68	GLN
3	M	24	GLN
3	M	110	ASN
4	N	44	GLN
4	N	46	HIS
1	O	68	GLN
2	P	75	HIS
3	Q	110	ASN
4	R	92	GLN
1	S	68	GLN
1	S	76	GLN
2	T	75	HIS
3	U	110	ASN
4	V	44	GLN
4	V	60	ASN
4	V	81	ASN
4	V	92	GLN
1	W	68	GLN
2	X	75	HIS
3	Y	24	GLN
3	Y	110	ASN
4	Z	44	GLN

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Mol	Chain	Res	Type
4	Z	81	ASN
4	Z	92	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

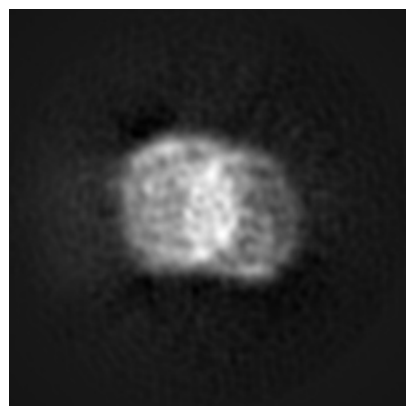
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31816. These allow visual inspection of the internal detail of the map and identification of artifacts.

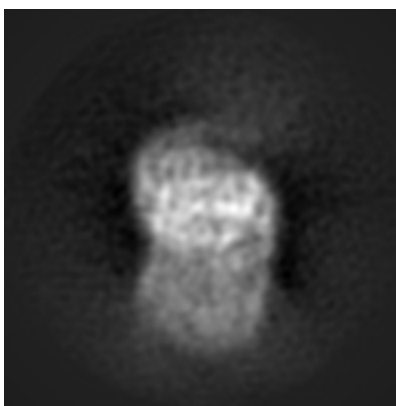
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

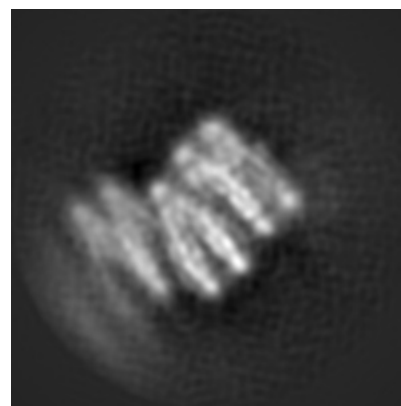
6.1.1 Primary map



X

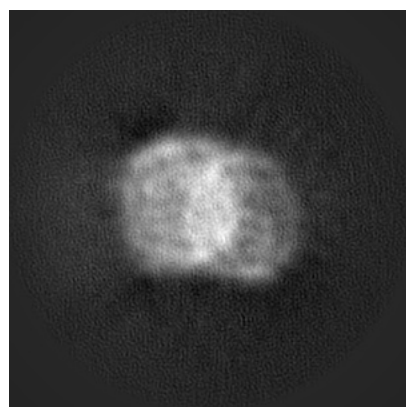


Y

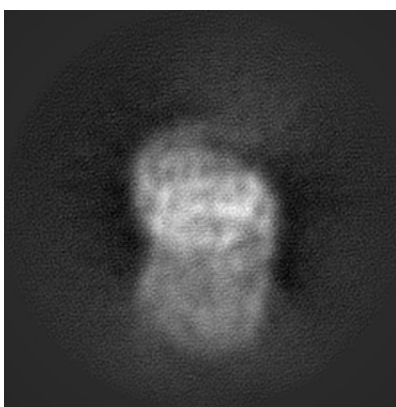


Z

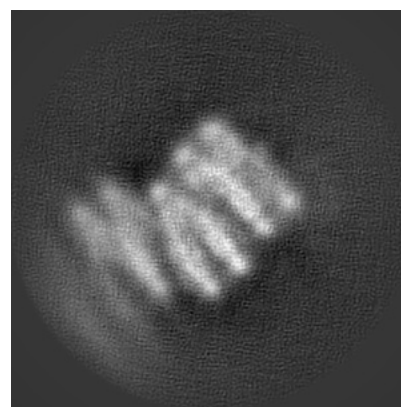
6.1.2 Raw map



X



Y

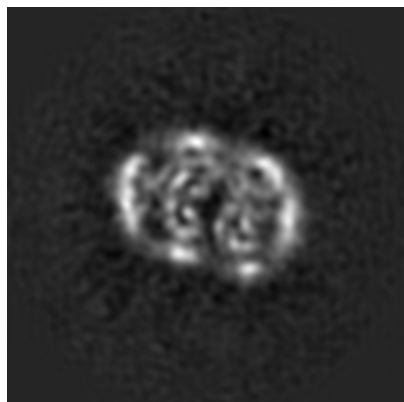


Z

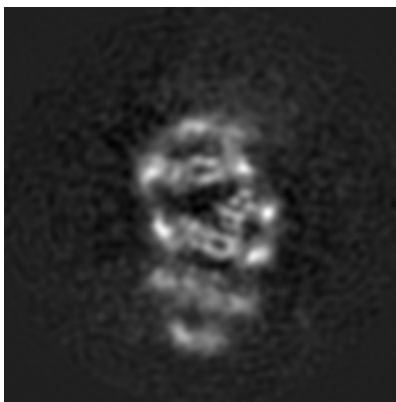
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

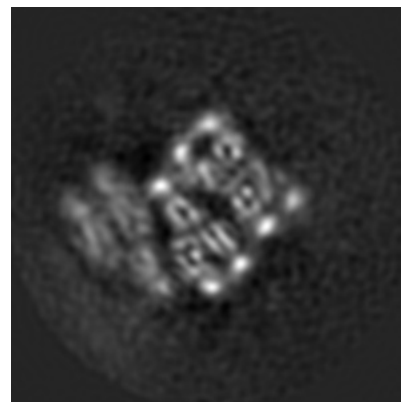
6.2.1 Primary map



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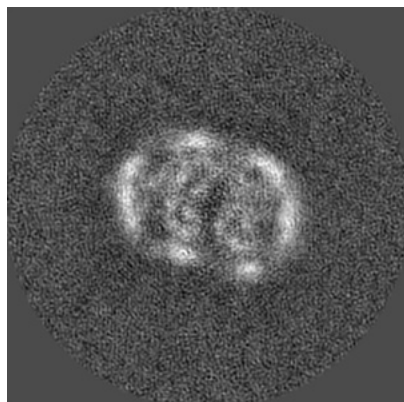


Y Index: 112

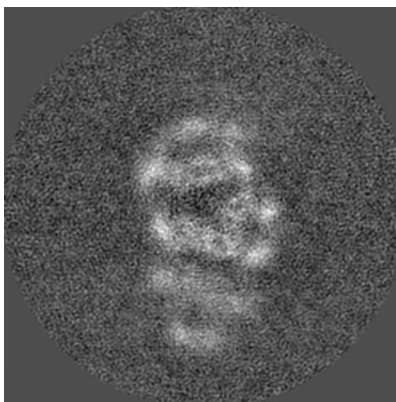


Z Index: 112

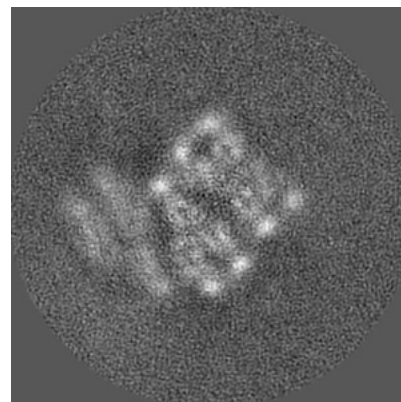
6.2.2 Raw map



X Index: 112



Y Index: 112

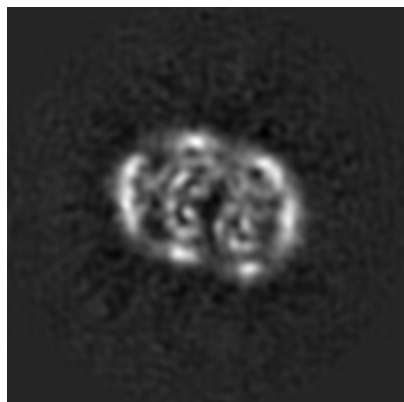


Z Index: 112

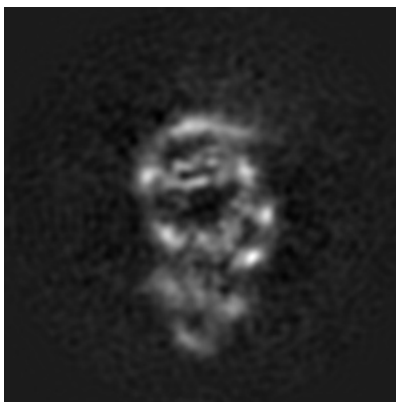
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

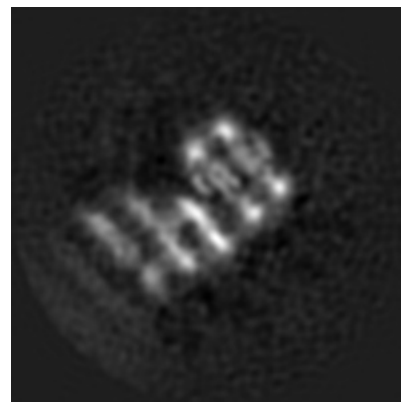
6.3.1 Primary map



X Index: 112

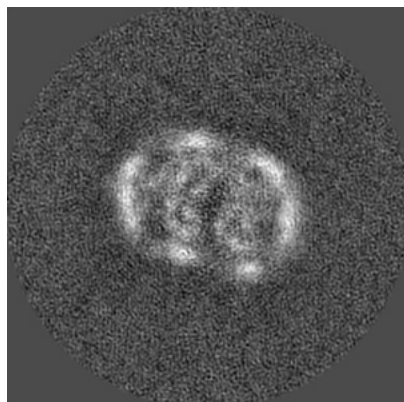


Y Index: 115

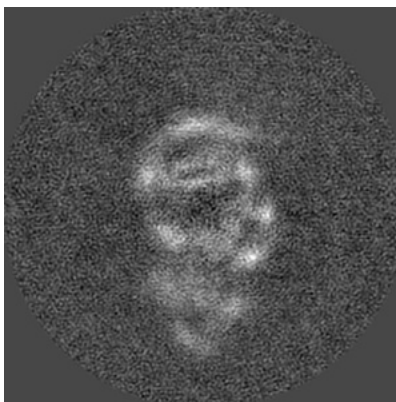


Z Index: 87

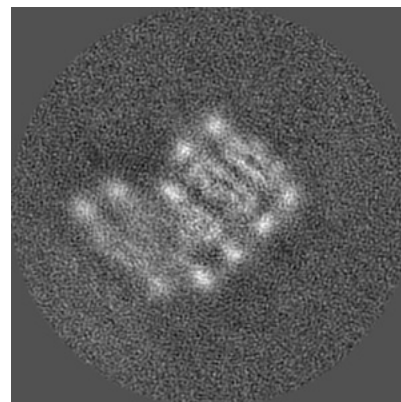
6.3.2 Raw map



X Index: 112



Y Index: 115

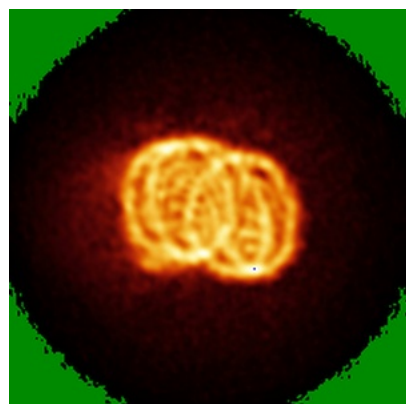


Z Index: 98

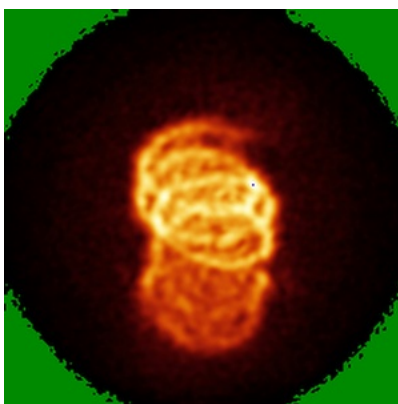
The images above show the largest variance slices of the map in three orthogonal directions.

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

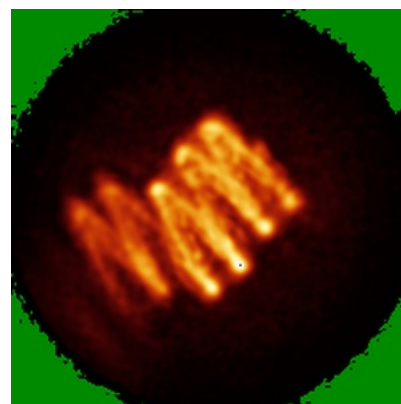
6.4.1 Primary map



X

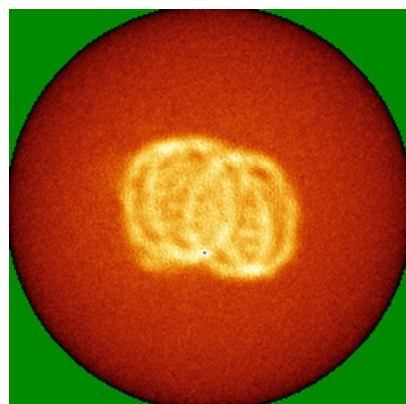


Y

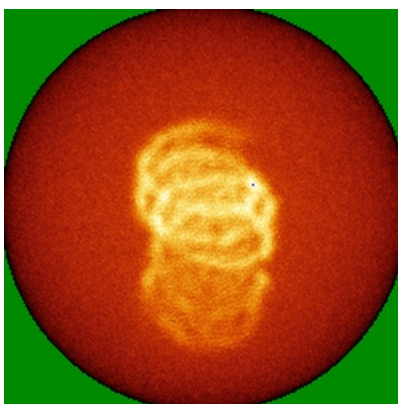


Z

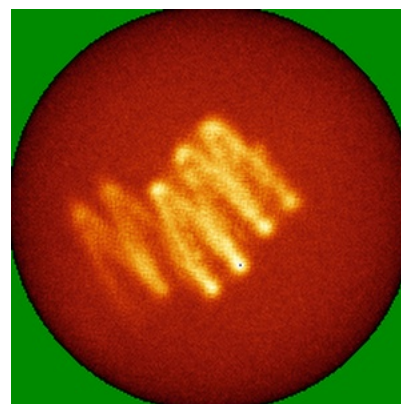
6.4.2 Raw map



X



Y

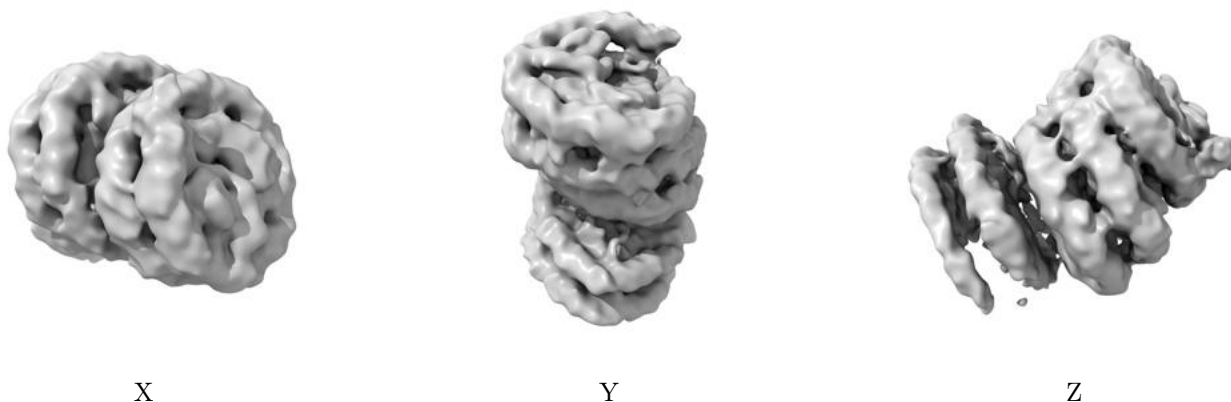


Z

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.

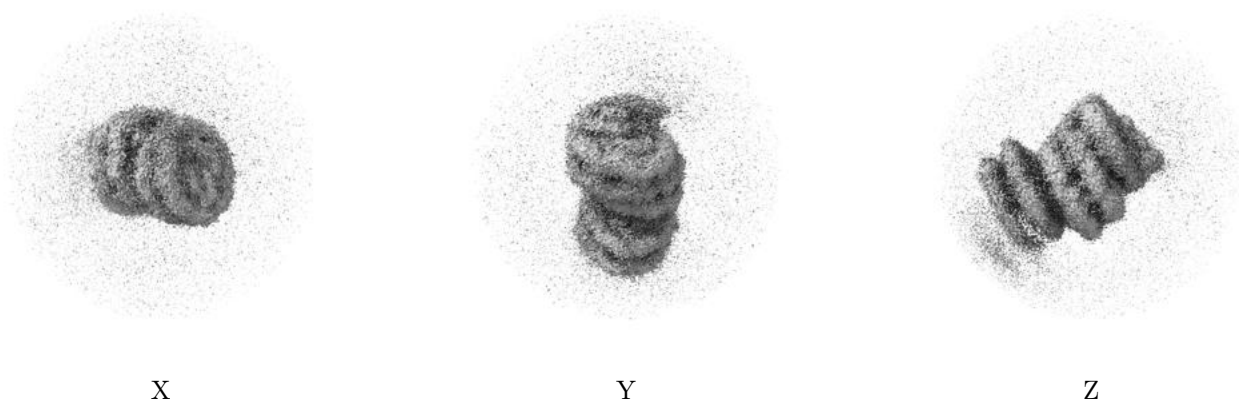
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0089. 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.

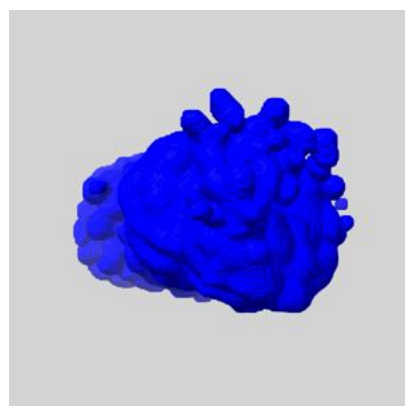
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

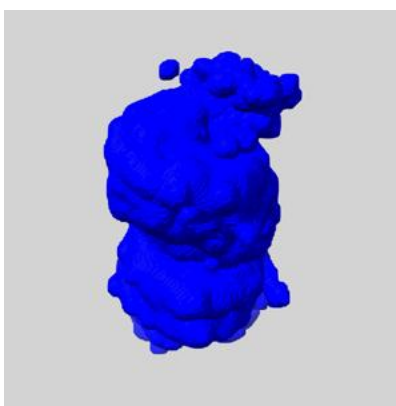
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

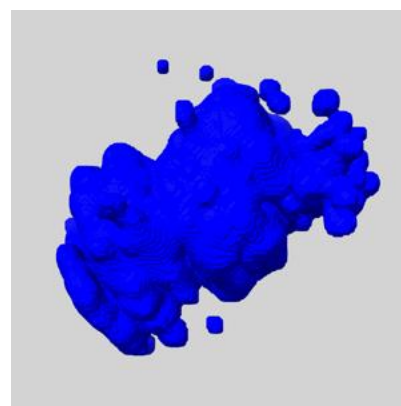
6.6.1 emd_31816_msk_1.map [i](#)



X



Y

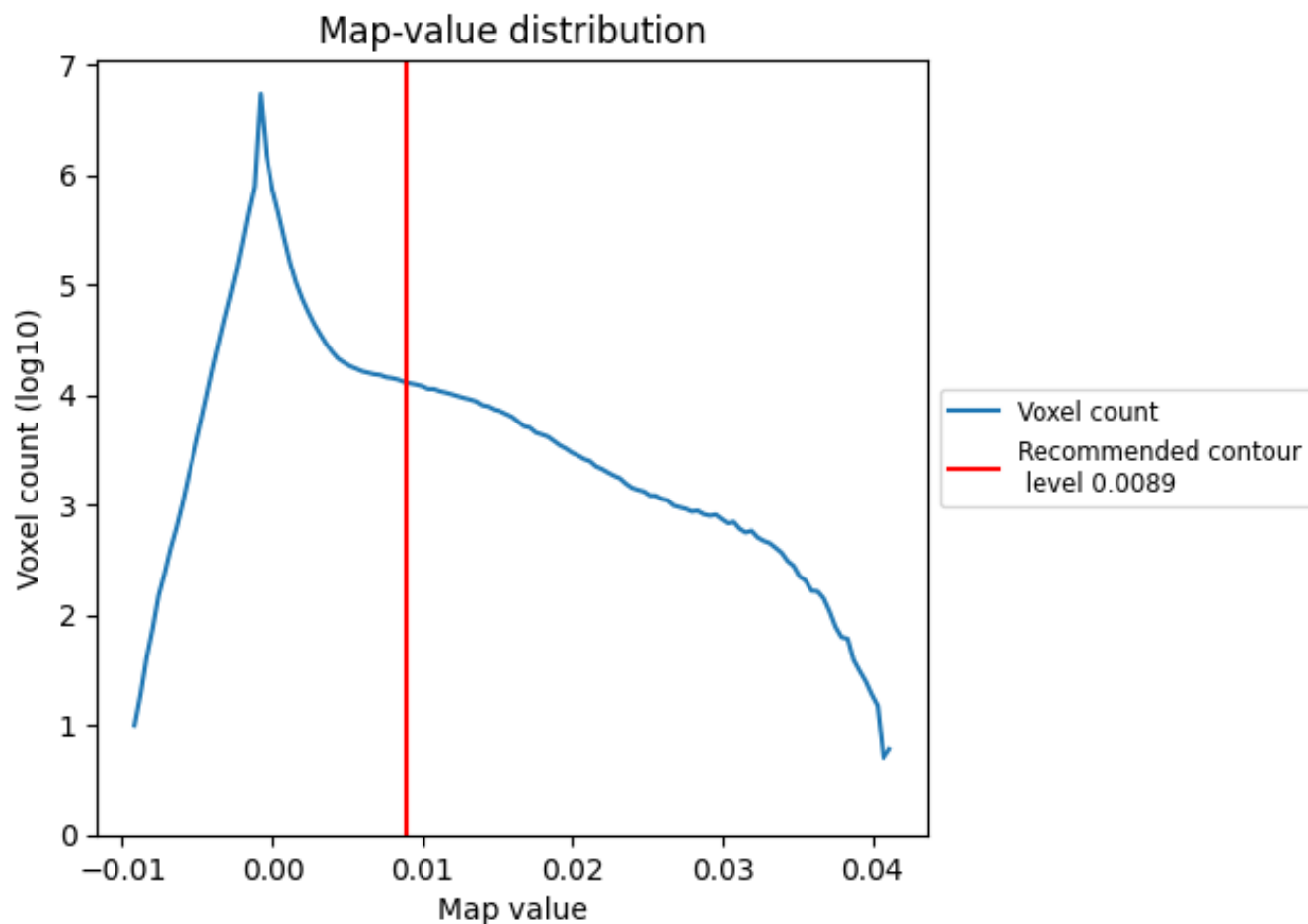


Z

7 Map analysis [i](#)

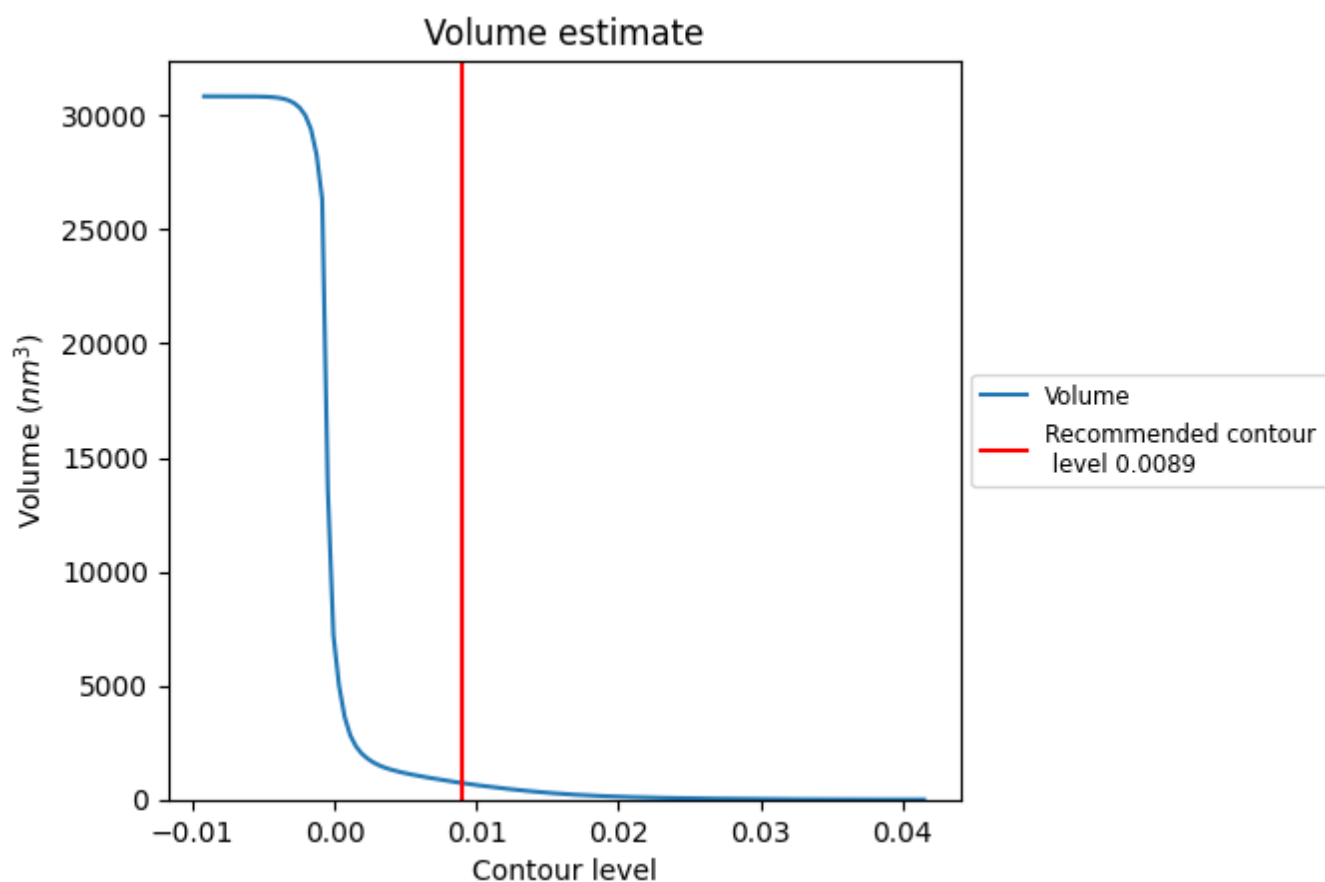
This section contains the results of statistical analysis of the map.

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.

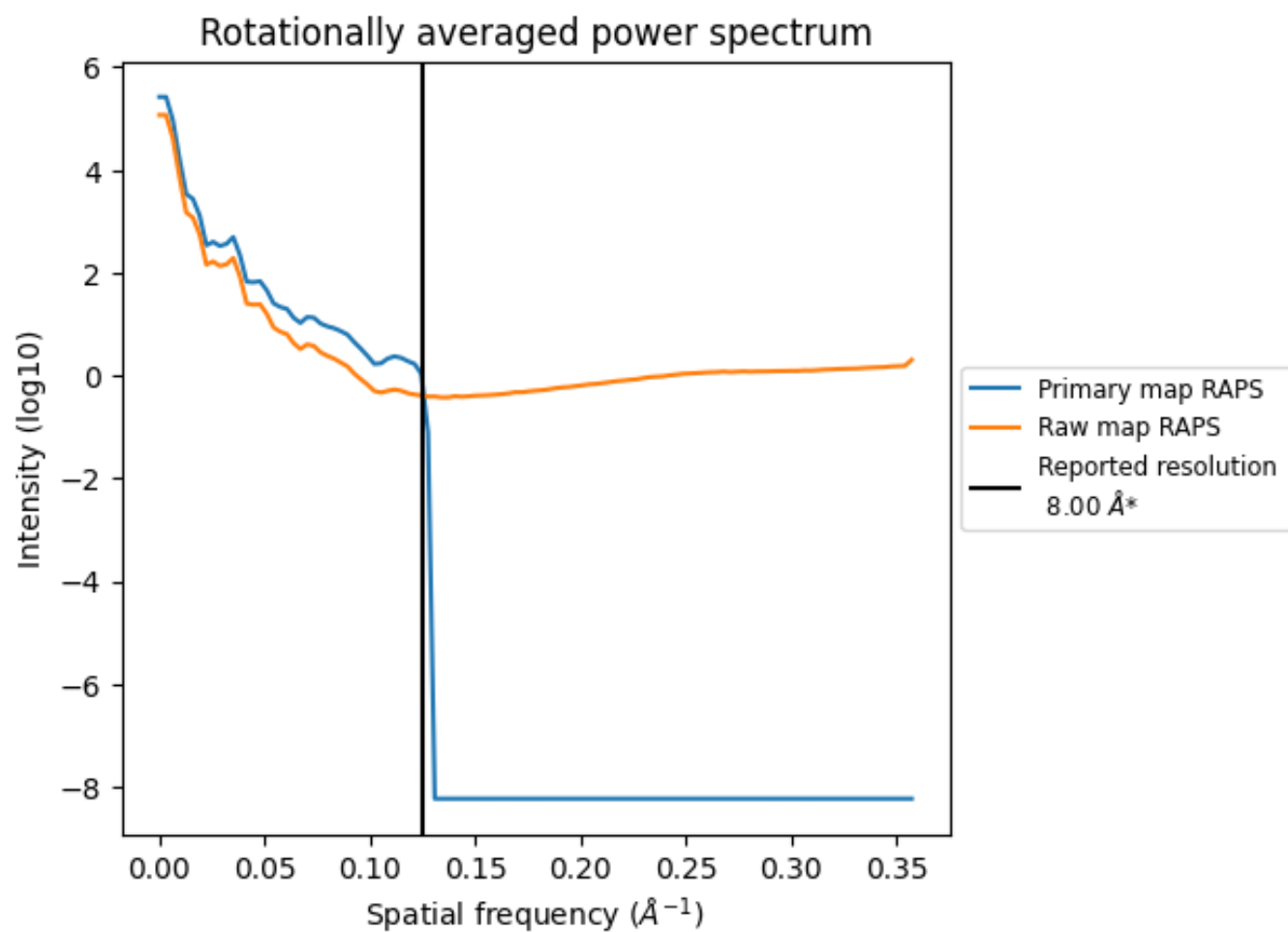
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 732 nm³; this corresponds to an approximate mass of 661 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 ⓘ

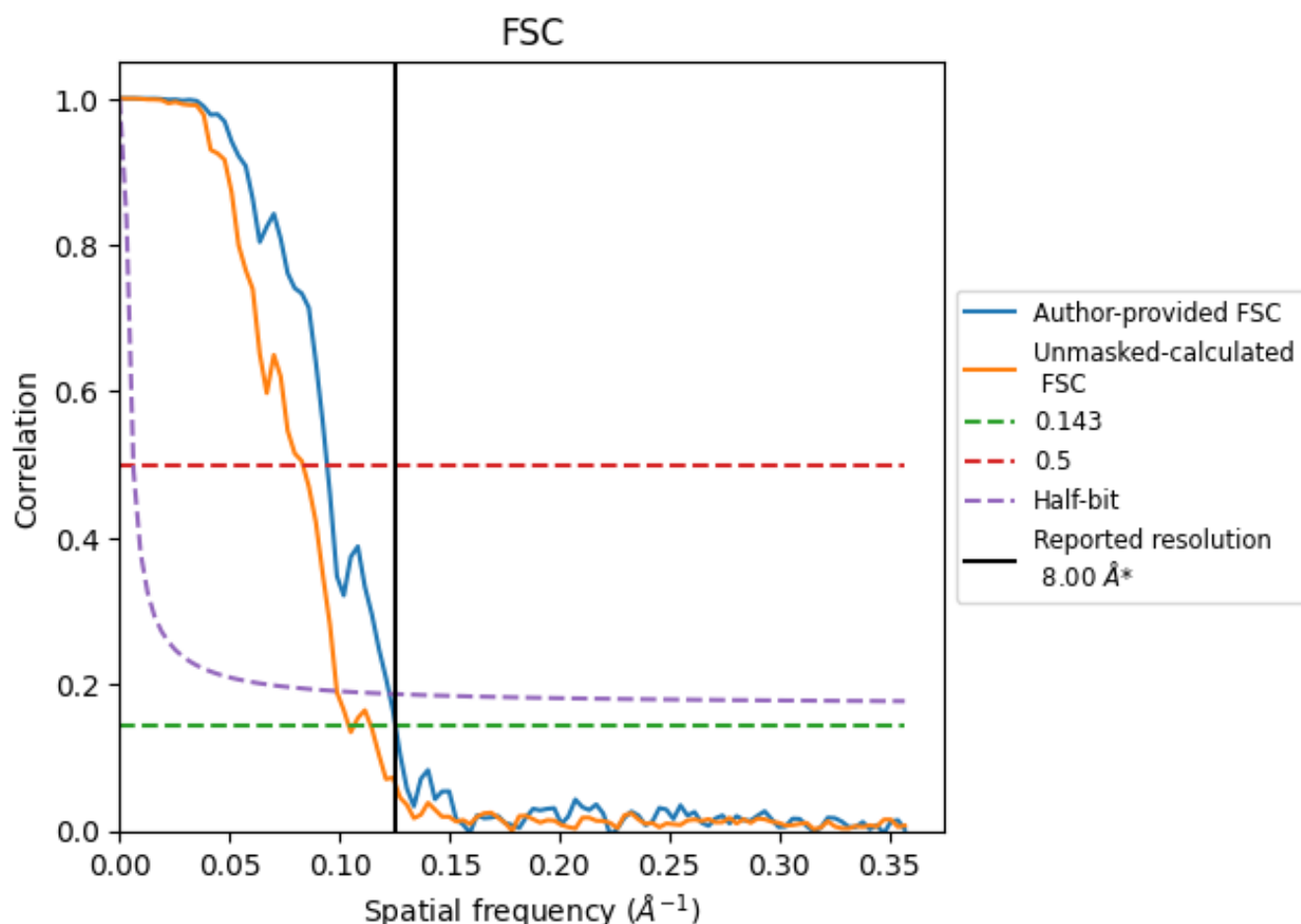


*Reported resolution corresponds to spatial frequency of 0.125 Å⁻¹

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 0.125 Å⁻¹

8.2 Resolution estimates [i](#)

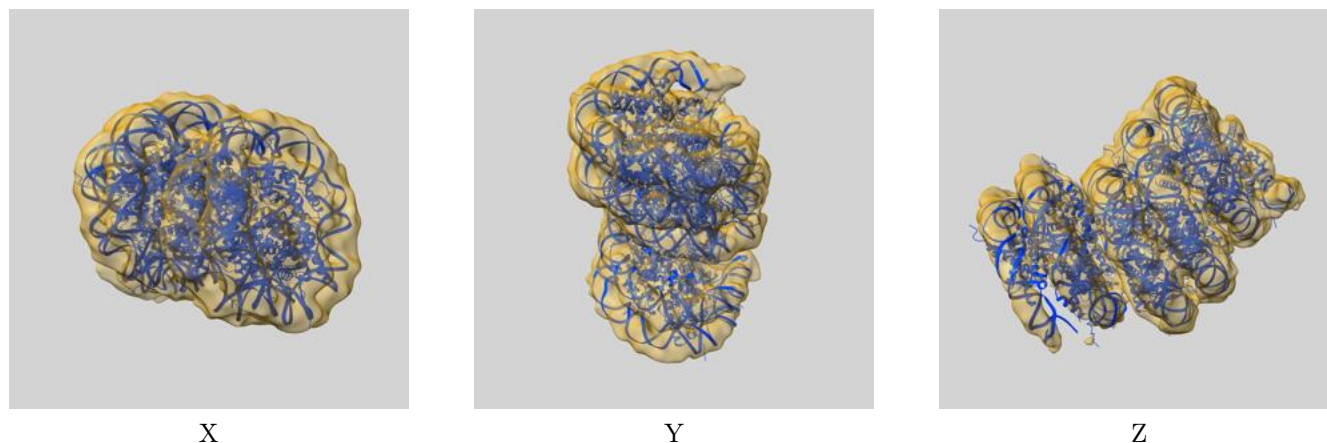
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	8.00	-	-
Author-provided FSC curve	7.97	10.60	8.15
Unmasked-calculated*	9.59	12.00	10.12

*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 9.59 differs from the reported value 8.0 by more than 10 %

9 Map-model fit [i](#)

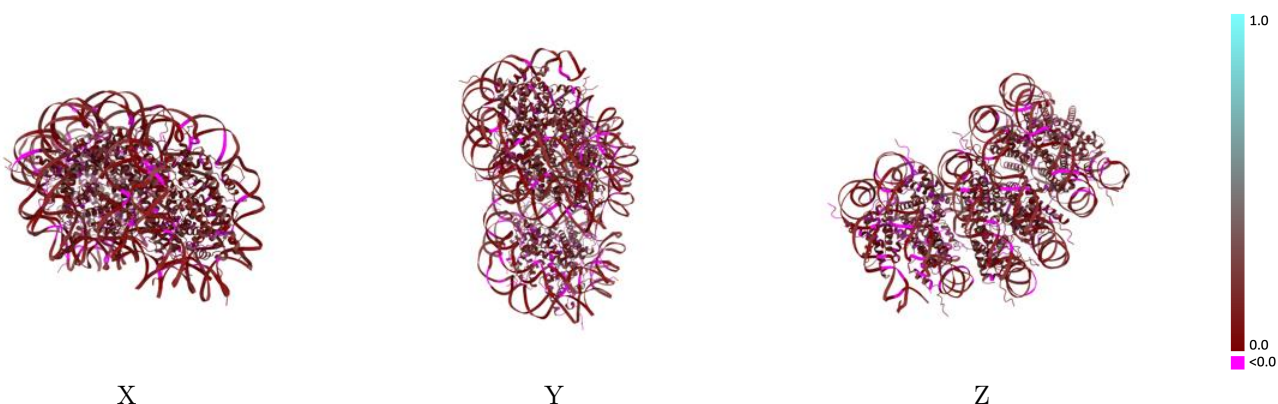
This section contains information regarding the fit between EMDB map EMD-31816 and PDB model 7V9J. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



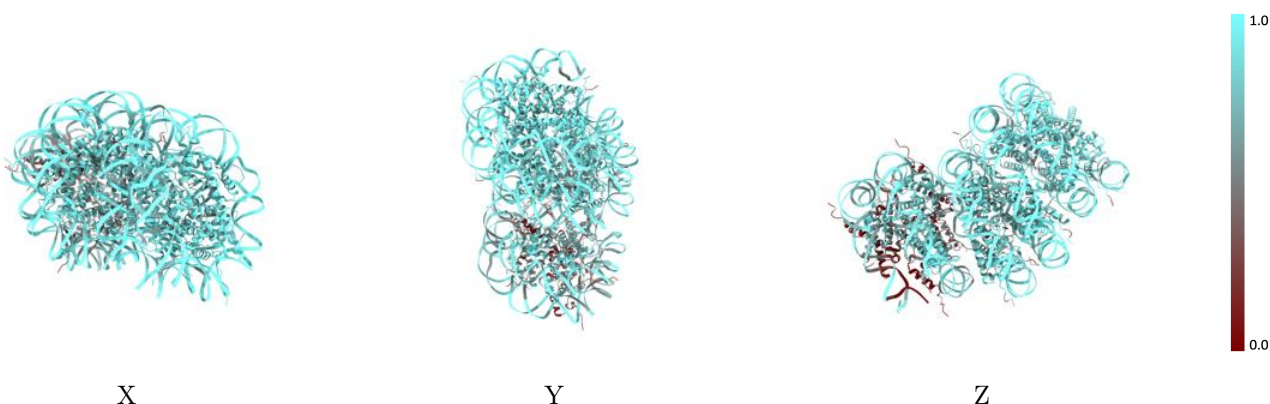
The images above show the 3D surface view of the map at the recommended contour level 0.0089 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



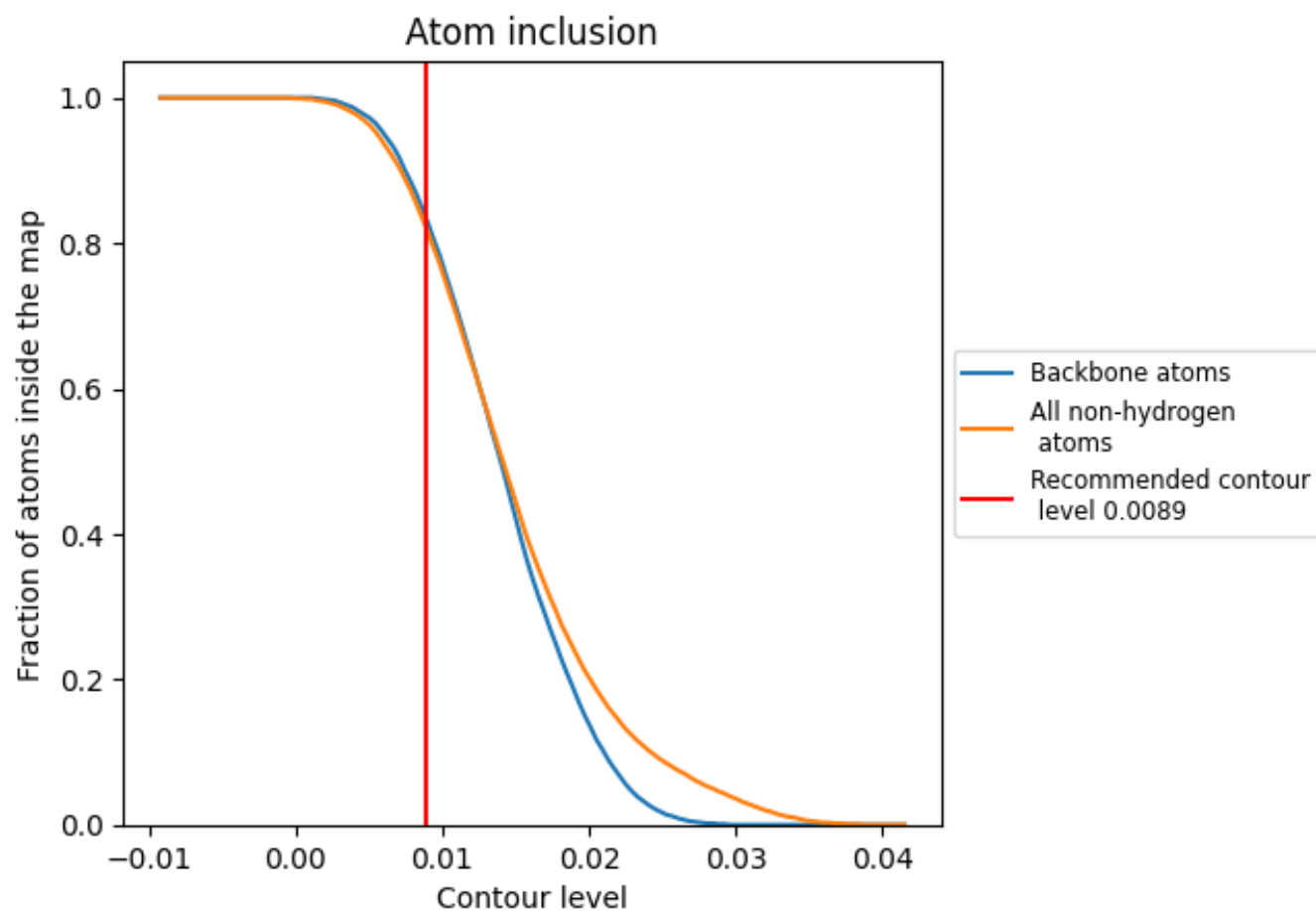
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0089).























































9.4 Atom inclusion ⓘ



At the recommended contour level, 84% of all backbone atoms, 82% 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 (0.0089) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.1070
A	 0.8530	 0.1330
B	 0.7880	 0.1160
C	 0.7980	 0.1320
D	 0.8180	 0.1380
E	 0.8770	 0.1290
F	 0.7650	 0.1060
G	 0.8140	 0.1250
H	 0.8780	 0.1360
I	 0.8840	 0.1020
J	 0.8830	 0.0960
K	 0.8830	 0.1310
L	 0.8310	 0.1130
M	 0.8420	 0.1200
N	 0.8740	 0.1310
O	 0.9020	 0.1240
P	 0.9130	 0.1220
Q	 0.8690	 0.1440
R	 0.8840	 0.1450
S	 0.6950	 0.1030
T	 0.7190	 0.0720
U	 0.3210	 0.0820
V	 0.5130	 0.0940
W	 0.6030	 0.0960
X	 0.7260	 0.0750
Y	 0.5350	 0.0610
Z	 0.6930	 0.1080

