



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 11:03 AM UTC

PDB ID : 8Q84 / pdb_00008q84
EMDB ID : EMD-18246
Title : Outer kinetochore Dam1 protomer dimer Ndc80-Nuf2 coiled-coil complex
Authors : Muir, K.W.; Barford, D.
Deposited on : 2023-08-17
Resolution : 3.15 Å(reported)
Based on initial model : .

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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

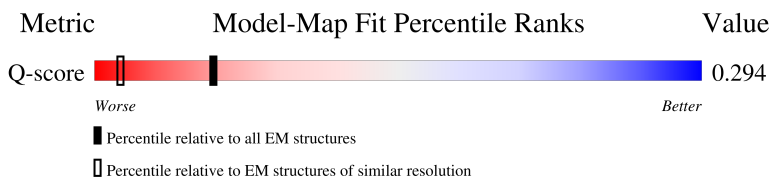
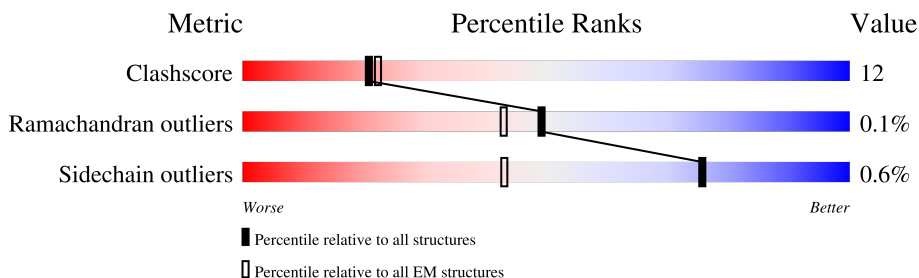
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.15 Å.

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



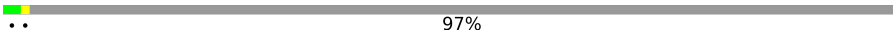
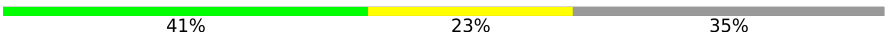
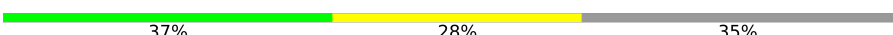
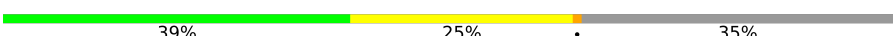
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14486 (2.65 - 3.65)

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	691	25% 42% 57%
1	F	691	26% 42% 57%
2	B	451	30% 52% 47%
2	G	451	31% 51% 48%

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Mol	Chain	Length	Quality of chain
3	I	343	
3	U	343	
3	e	343	
4	J	247	
4	V	247	
5	K	133	
5	W	133	
6	L	94	
6	X	94	
7	M	72	
7	Y	72	
8	N	94	
8	Z	94	
9	O	295	
9	a	295	
10	P	292	
10	b	292	
11	Q	69	
11	c	69	
12	R	165	
12	d	165	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 21802 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 Kinetochore protein NDC80.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	294	Total	C	N	O	0	0
			1463	875	294	294		
1	F	294	Total	C	N	O	0	0
			1463	875	294	294		

- Molecule 2 is a protein called Kinetochore protein NUF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	237	Total	C	N	O	0	0
			1180	706	237	237		
2	G	236	Total	C	N	O	0	0
			1175	703	236	236		

- Molecule 3 is a protein called DASH complex subunit DAM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	95	Total	C	N	O	S	0	0
			757	474	126	153	4		
3	U	95	Total	C	N	O	S	0	0
			757	474	126	153	4		
3	e	11	Total	C	N	O		0	0
			82	50	14	18			

- Molecule 4 is a protein called DASH complex subunit DUO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	117	Total	C	N	O	S	0	0
			935	580	167	185	3		
4	V	117	Total	C	N	O	S	0	0
			935	580	167	185	3		

- Molecule 5 is a protein called DASH complex subunit DAD2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	106	Total	C	N	O	S	0	0
			837	519	139	174	5		
5	W	106	Total	C	N	O	S	0	0
			837	519	139	174	5		

- Molecule 6 is a protein called DASH complex subunit DAD1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	61	Total	C	N	O	S	0	0
			485	304	79	101	1		
6	X	68	Total	C	N	O	S	0	0
			535	334	86	114	1		

- Molecule 7 is a protein called DASH complex subunit DAD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	72	Total	C	N	O	S	0	0
			571	351	106	111	3		
7	Y	72	Total	C	N	O	S	0	0
			571	351	106	111	3		

- Molecule 8 is a protein called DASH complex subunit DAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	92	Total	C	N	O	S	0	0
			744	461	130	152	1		
8	Z	94	Total	C	N	O	S	0	0
			761	471	132	156	2		

- Molecule 9 is a protein called DASH complex subunit SPC34.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	O	235	Total	C	N	O	S	0	0
			1929	1213	342	367	7		
9	a	234	Total	C	N	O	S	0	0
			1925	1211	341	366	7		

- Molecule 10 is a protein called DASH complex subunit ASK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	65	Total	C	N	O	S	0	0
			527	332	83	108	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	70	Total	C	N	O	S	0	0
			561	352	88	116	5		

- Molecule 11 is a protein called DASH complex subunit HSK3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	64	Total	C	N	O	S	0	0
			527	327	94	101	5		
11	c	64	Total	C	N	O	S	0	0
			527	327	94	101	5		

- Molecule 12 is a protein called DASH complex subunit SPC19.

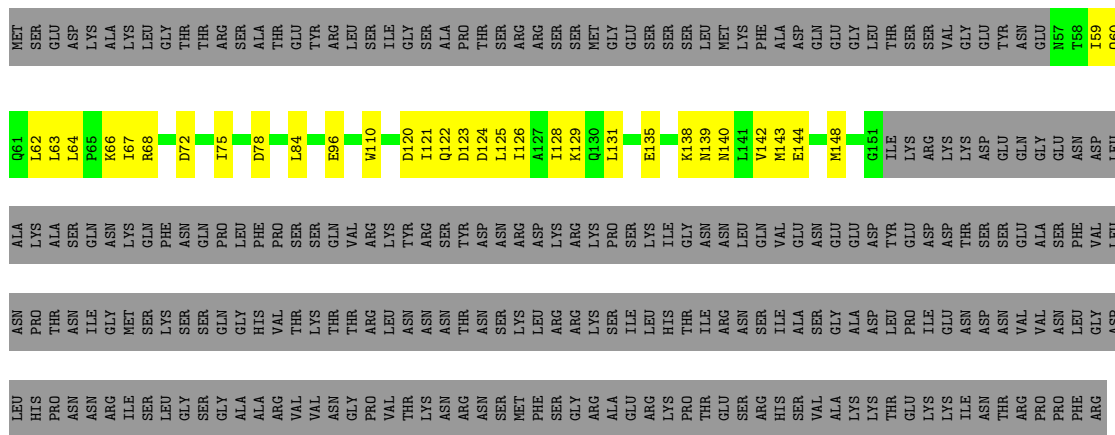
Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	108	Total	C	N	O	S	0	0
			859	532	149	172	6		
12	d	108	Total	C	N	O	S	0	0
			859	532	149	172	6		

V646	I647	H648	V649	I650	D651	I652	T653	K654	K655	F656	K657	I658	H659	I660	Q661	S662	S663	LEU	GLU	ASN	VAL	ILE	GLU	GLU	LEU	LEU	ARG	ASN	ASN	GLY	GLY	ASN	ASN	VAL	ILE	GLU	GLU	LEU	LEU	ARG	ASN	ASN	GLY	PHE	GLU	THR	GLU	HIS	ASN	ASN	VAL	THR	ASN																																																																																																																																																																																																																																																																																																																																																																																																																											
L496	L497	D498	R499	D500	F501	H502	E503	G504	I505	S506	E507	E508	Q509	L510	F511	F512	K513	G514	S515	G516	I517	N518	N519	E520	K521	L522	L523	S524	I525	L526	K527	R528	E529	T530	T531	L532	L533	L534	L535	L536	L537	L538	L539	L540	L541	L542	L543	L544	L545	L546	L547	L548	L549	L550	L551	L552	L553	L554	L555	L556	L557	L558	L559	L560	L561	L562	L563	L564	L565	L566	L567	L568	L569	L570	L571	L572	L573	L574	L575	L576	L577	L578	L579	L580	L581	L582	L583	L584	L585	L586	L587	L588	L589	L590	L591	L592	L593	L594	L595	L596	L597	L598	L599	L600	L601	L602	L603	L604	L605	L606	L607	L608	L609	L610	L611	L612	L613	L614	L615	L616	L617	L618	L619	L620	L621	L622	L623	L624	L625	L626	L627	L628	L629	L630	L631	L632	L633	L634	L635	L636	L637	L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650	L651	L652	L653	L654	L655	L656	L657	L658	L659	L660	L661	L662	L663	L664	L665	L666	L667	L668	L669	L670	L671	L672	L673	L674	L675	L676	L677	L678	L679	L680	L681	L682	L683	L684	L685	L686	L687	L688	L689	L690	L691	L692	L693	L694	L695	L696	L697	L698	L699	L700	L701	L702	L703	L704	L705	L706	L707	L708	L709	L710	L711	L712	L713	L714	L715	L716	L717	L718	L719	L720	L721	L722	L723	L724	L725	L726	L727	L728	L729	L730	L731	L732	L733	L734	L735	L736	L737	L738	L739	L740	L741	L742	L743	L744	L745	L746	L747	L748	L749	L750	L751	L752	L753	L754	L755	L756	L757	L758	L759	L760	L761	L762	L763	L764	L765	L766	L767	L768	L769	L770	L771	L772	L773	L774	L775	L776	L777	L778	L779	L780	L781	L782	L783	L784	L785	L786	L787	L788	L789	L790	L791	L792	L793	L794	L795	L796	L797	L798	L799	L800	L801	L802	L803	L804	L805	L806	L807	L808	L809	L810	L811	L812	L813	L814	L815	L816	L817	L818	L819	L820	L821	L822	L823	L824	L825	L826	L827	L828	L829	L830	L831	L832	L833	L834	L835	L836	L837	L838	L839	L840	L841	L842	L843	L844	L845	L846	L847	L848	L849	L850	L851	L852	L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960
Q421	E422	R423	E424	K425	L426	T427	R428	E429	L430	D431	K432	I433	N434	G435	Q436	S437	D438	K439	L440	T441	S442	S443	L444	K445	S446	R447	K448	L449	E450	A451	E452	G453	I454	F455	K456	S457	L458	L459	R463	D466	S467	S468	Q478	L479	G480	N484	D485	S486	S487	N491	I492	S493	E494	N495																																																																																																																																																																																																																																																																																																																																																																																																																										
GLU	ASN	TYR	VAL	ASN	ALA	MET	LYS	GLN	K370	S371	Q372	E373	W374	P375	G376	K377	L378	E379	K380	M381	K382	S383	E384	K385	E386	L387	K388	E389	E390	E391	I392	K393	A394	L395	Q396	S397	S398	I399	S400	E401	L402	H403	K404	I405	L406	R407	K408	K409	G410	I411	S412	T413	E414	Q415	F416	E417	L418	Q419	N420																																																																																																																																																																																																																																																																																																																																																																																																																					

Chain B: 30% 52% 47%

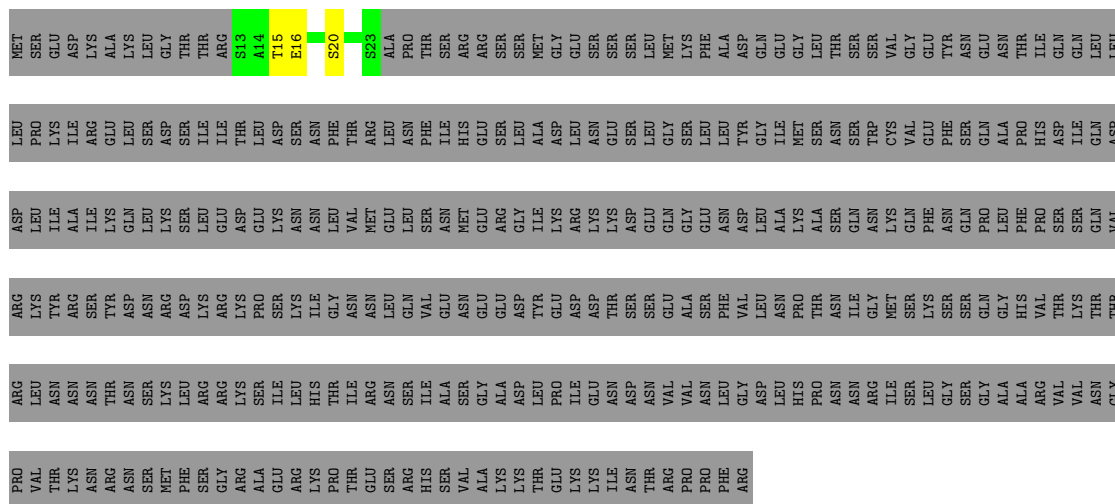
R241	R242	R243	R244	R245	R246	R247	R248	R249	R250	R251	R252	R253	R254	R255	R256	R257	R258	R259	R260	R261	R262	R263	R264	R265	R266	R267	R268	R269	R270	R271	R272	R273	R274	R275	R276	R277	R278	R279	R280	R281	R282	R283	R284	R285	R286	R287	R288	R289	R290	R291	R292	R293	R294	R295	R296	R297	R298	R299	R300	R301	R302	R303	R304	R305	R306	R307	R308	R309	R310	R311	R312	R313	R314	R315	R316	R317	R318	R319	R320	R321	R322	R323	R324	R325	R326	R327	R328	R329	R330	R331	R332	R333	R334	R335	R336	R337	R338	R339	R340	R341	R342	R343	R344	R345	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000	R1001	R1002	R1003	R1004	R1005	R1006	R1007	R1008	R1009	R1010	R1011	R1012	R1013	R1014	R1015	R1016	R1017	R1018	R1019	R1020	R1021	R1022	R1023	R1024	R1025	R1026	R1027	R1028	R1029	R1030	R1031	R1032	R1033	R1034	R1035	R1036	R1037	R1038	R1039	R1040	R1041	R1042	R1043	R1044	R1045	R1046	R1047	R1048	R1049	R1050	R1051	R1052	R1053	R1054	R1055	R1056	R1057	R1058	R1059	R1060	R1061	R1062	R1063	R1064	R1065	R1066	R1067	R1068	R1069	R1070	R1071	R1072	R1073	R1074	R1075	R1076	R1077	R1078	R1079	R1080	R1081	R1082	R1083	R1084	R1085	R1086	R1087	R1088	R1089	R1090	R1091	R1092	R1093	R1094	R1095	R1096	R1097	R1098	R1099	R1100	R1101	R1102	R1103	R1104	R1105	R1106	R1107	R1108	R1109	R1110	R1111	R1112	R1113	R1114	R1115	R1116	R1117	R1118	R1119	R1120	R1121	R1122	R1123	R1124	R1125	R1126	R1127	R1128	R1129	R1130	R1131	R1132	R1133	R1134	R1135	R1136	R1137	R1138	R1139	R1140	R1141	R1142	R1143	R1144	R1145	R1146	R1147	R1148	R1149	R1150	R1151	R1152	R1153	R1154	R1155	R1156	R1157	R1158	R1159	R1160	R1161	R1162	R1163	R1164	R1165	R1166	R1167	R1168	R1169	R1170	R1171	R1172	R1173	R1174	R1175	R1176	R1177	R1178	R1179	R1180	R1181	R1182	R1183	R1184	R1185	R1186	R1187	R1188	R1189	R1190	R1191	R1192	R1193	R1194	R1195	R1196	R1197	R1198	R1199	R1200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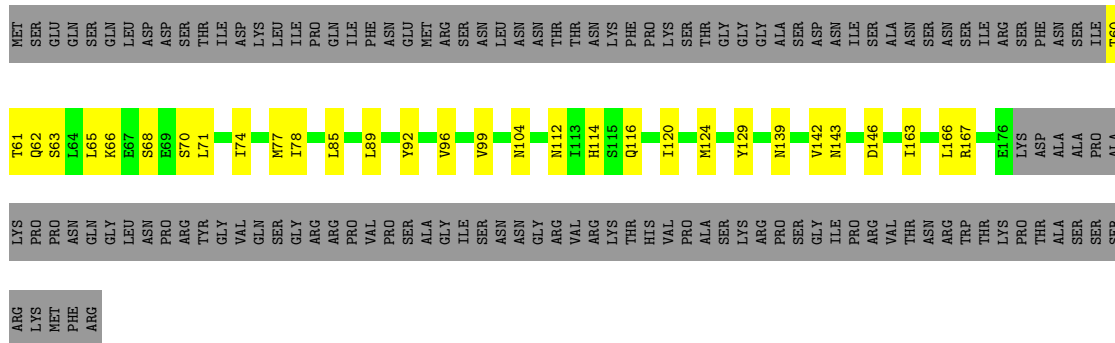
- Molecule 3: DASH complex subunit DAM1

Chain e: 97%

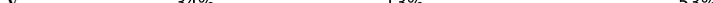


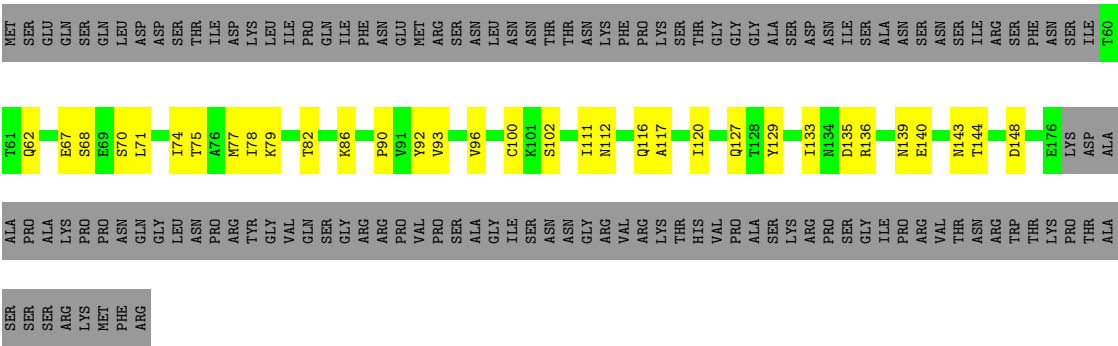
- Molecule 4: DASH complex subunit DUO1

Chain J: 35% 13% 53%

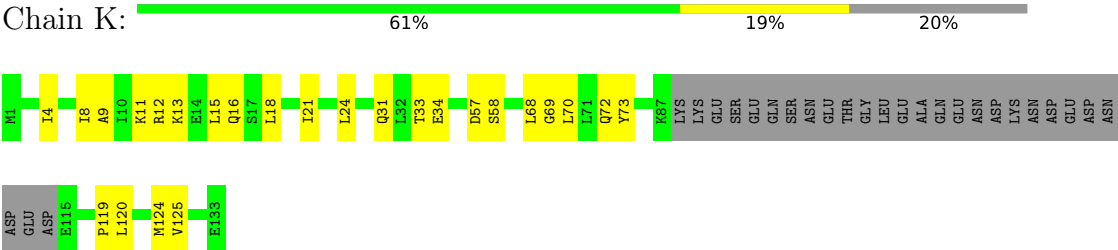


- Molecule 4: DASH complex subunit DUO1

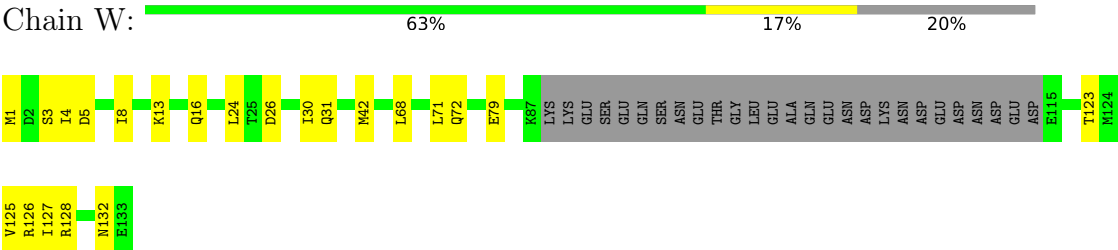
Chain V:  34% 13% 53%



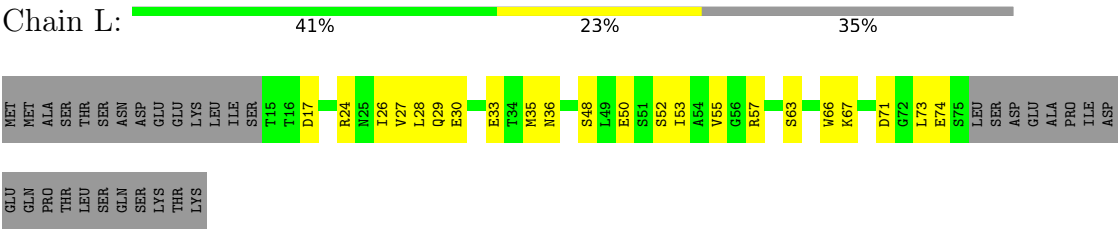
• Molecule 5: DASH complex subunit DAD2



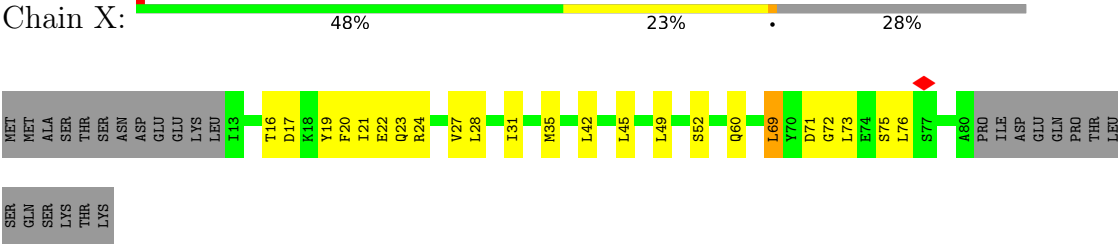
• Molecule 5: DASH complex subunit DAD2



• Molecule 6: DASH complex subunit DAD1



• Molecule 6: DASH complex subunit DAD1



- Molecule 7: DASH complex subunit DAD4

Chain M:  56% 44%



- Molecule 7: DASH complex subunit DAD4

Chain Y:  64% 36%



- Molecule 8: DASH complex subunit DAD3

Chain N:  64% 34%



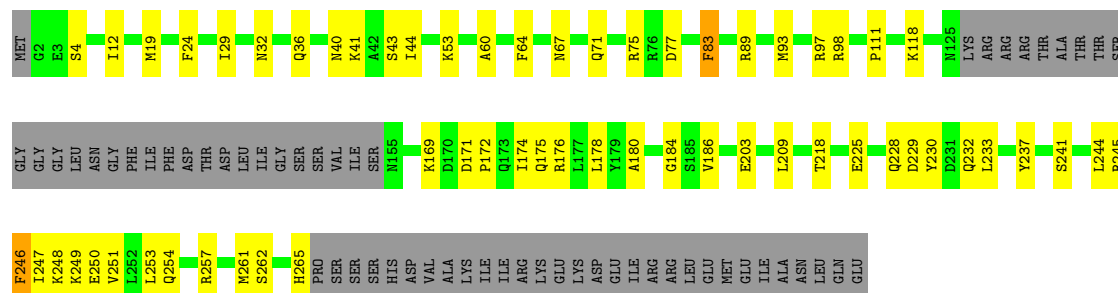
- Molecule 8: DASH complex subunit DAD3

Chain Z:  71% 29%



- Molecule 9: DASH complex subunit SPC34

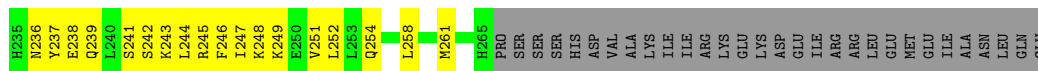
Chain O:  59% 20% 20%



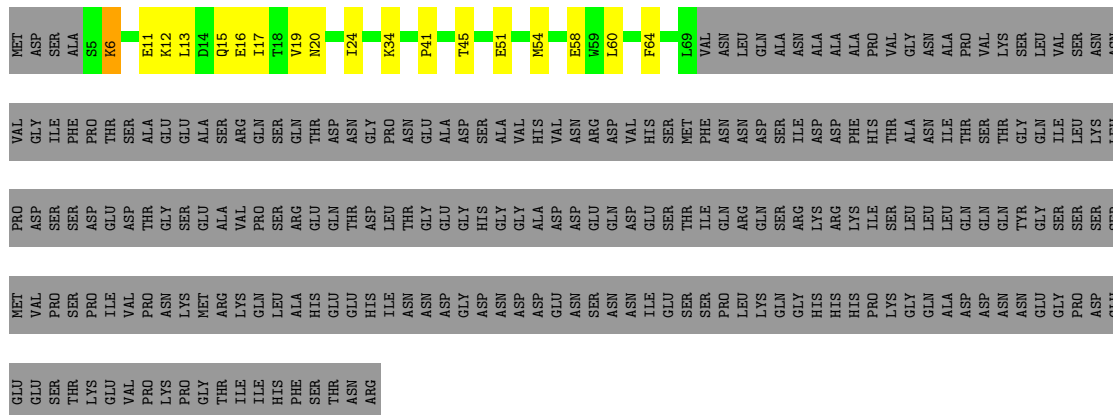
- Molecule 9: DASH complex subunit SPC34

Chain a:  57% 23% 21%

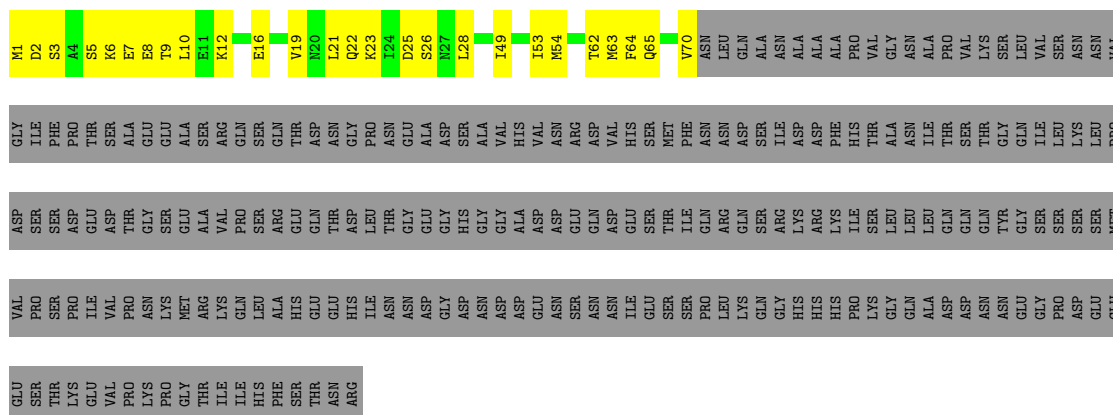




- Molecule 10: DASH complex subunit ASK1



- Molecule 10: DASH complex subunit ASK1



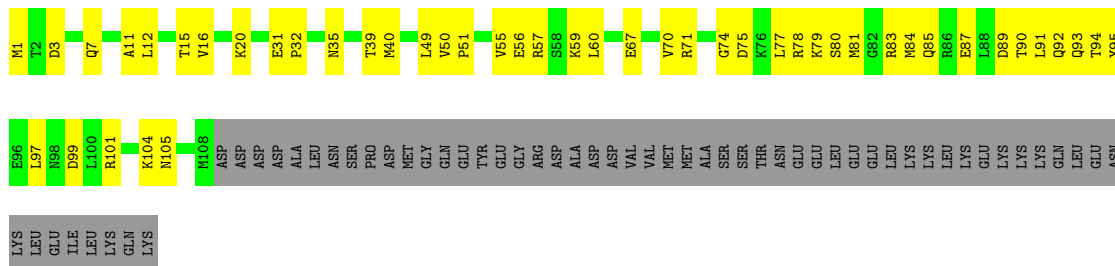
- Molecule 11: DASH complex subunit HSK3



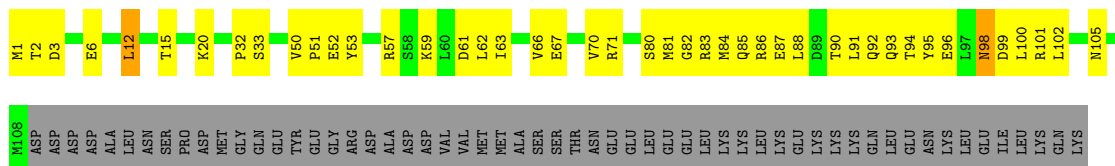
- Molecule 11: DASH complex subunit HSK3



- Molecule 12: DASH complex subunit SPC19



- Molecule 12: DASH complex subunit SPC19



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248732	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.815	Depositor
Minimum map value	-0.855	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/1462	0.29	0/2041
1	F	0.13	0/1462	0.30	0/2041
2	B	0.14	0/1179	0.35	0/1646
2	G	0.15	0/1174	0.35	0/1639
3	I	0.18	0/766	0.48	0/1034
3	U	0.21	0/766	0.56	0/1034
3	e	0.19	0/82	0.41	0/109
4	J	0.17	0/945	0.41	0/1275
4	V	0.16	0/945	0.39	0/1275
5	K	0.18	0/844	0.47	0/1135
5	W	0.17	0/844	0.38	0/1135
6	L	0.16	0/490	0.38	0/662
6	X	0.21	0/540	0.53	0/730
7	M	0.17	0/577	0.42	0/779
7	Y	0.17	0/577	0.44	0/779
8	N	0.32	0/751	0.57	0/1007
8	Z	0.19	0/768	0.56	0/1029
9	O	0.16	0/1962	0.41	0/2638
9	a	0.14	0/1958	0.37	0/2633
10	P	0.15	0/535	0.35	0/722
10	b	0.19	0/569	0.43	0/768
11	Q	0.18	0/534	0.45	0/716
11	c	0.14	0/534	0.35	0/716
12	R	0.17	0/864	0.50	0/1161
12	d	0.18	0/864	0.52	0/1161
All	All	0.17	0/21992	0.42	0/29865

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	1463	0	607	0	0
1	F	1463	0	607	1	0
2	B	1180	0	483	1	0
2	G	1175	0	481	2	0
3	I	757	0	753	21	0
3	U	757	0	753	27	0
3	e	82	0	79	4	0
4	J	935	0	952	33	0
4	V	935	0	952	31	0
5	K	837	0	837	30	0
5	W	837	0	837	21	0
6	L	485	0	475	18	0
6	X	535	0	522	23	0
7	M	571	0	578	28	0
7	Y	571	0	578	21	0
8	N	744	0	754	41	0
8	Z	761	0	772	30	0
9	O	1929	0	1929	63	0
9	a	1925	0	1926	61	0
10	P	527	0	513	21	0
10	b	561	0	548	25	0
11	Q	527	0	520	14	0
11	c	527	0	520	12	0
12	R	859	0	897	52	0
12	d	859	0	897	52	0
All	All	21802	0	18770	486	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 12.

All (486) 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)
5:W:24:LEU:HB3	12:d:12:LEU:HD22	1.61	0.82
9:a:182:GLU:OE2	9:a:183:ASN:ND2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:127:GLN:HE22	12:d:32:PRO:HB3	1.47	0.79
8:N:18:GLN:HA	8:N:21:LEU:HD12	1.65	0.77
9:O:176:ARG:HB3	9:O:186:VAL:HG21	1.67	0.76
7:M:17:ILE:HG13	11:Q:11:GLN:HE22	1.49	0.76
4:V:68:SER:O	8:Z:15:LYS:NZ	2.19	0.76
3:U:96:GLU:OE1	9:a:29:ILE:N	2.18	0.75
4:J:104:ASN:ND2	8:N:56:GLU:OE2	2.20	0.75
11:Q:8:GLN:HA	11:Q:11:GLN:HE21	1.51	0.75
9:O:247:ILE:O	12:R:95:TYR:OH	2.05	0.73
10:b:1:MET:SD	10:b:2:ASP:N	2.61	0.73
9:O:174:ILE:HD13	9:O:209:LEU:HD11	1.69	0.72
12:R:101:ARG:HA	12:R:104:LYS:HE2	1.71	0.72
3:I:121:ILE:HD12	3:I:121:ILE:H	1.54	0.71
12:d:70:VAL:HG13	12:d:71:ARG:HH11	1.55	0.71
4:V:79:LYS:NZ	8:Z:22:ASP:OD1	2.18	0.71
3:U:60:GLN:HA	3:U:63:LEU:HG	1.73	0.71
9:a:69:GLU:N	9:a:69:GLU:OE1	2.23	0.71
5:K:24:LEU:HD21	12:R:12:LEU:HB3	1.72	0.70
12:d:82:GLY:HA2	12:d:85:GLN:HE21	1.57	0.70
12:R:90:THR:O	12:R:94:THR:HG23	1.92	0.69
9:a:242:SER:OG	9:a:245:ARG:NH2	2.25	0.69
3:I:141:LEU:HD13	4:J:167:ARG:NH2	2.08	0.69
8:N:66:LEU:HA	8:N:70:LEU:HD22	1.73	0.68
12:R:3:ASP:O	12:R:7:GLN:HG3	1.94	0.68
8:Z:13:LEU:HD22	8:Z:16:TYR:HE2	1.59	0.68
9:a:83:PHE:HE1	12:d:51:PRO:HD2	1.59	0.68
4:J:166:LEU:HB3	4:J:167:ARG:HH22	1.58	0.67
5:W:3:SER:OG	5:W:5:ASP:OD1	2.12	0.67
7:Y:3:ASN:HB3	7:Y:6:GLU:HG2	1.76	0.67
12:d:83:ARG:HA	12:d:86:ARG:HH21	1.59	0.67
5:K:124:MET:HB3	12:R:49:LEU:HD12	1.75	0.67
9:O:67:ASN:O	9:O:71:GLN:N	2.28	0.67
9:O:261:MET:SD	12:R:101:ARG:NH1	2.67	0.67
9:O:203:GLU:OE1	12:R:83:ARG:NH1	2.28	0.66
5:K:13:LYS:O	5:K:16:GLN:NE2	2.28	0.66
8:N:21:LEU:HA	8:N:24:LYS:HZ3	1.61	0.65
9:O:218:THR:HG21	9:O:230:TYR:HB2	1.78	0.65
12:d:90:THR:O	12:d:94:THR:HG23	1.96	0.65
9:a:218:THR:HG21	9:a:230:TYR:HB2	1.78	0.65
9:a:96:ASN:OD1	9:a:101:ARG:NH1	2.30	0.64
9:a:254:GLN:NE2	12:d:99:ASP:OD1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:175:GLN:HB3	9:O:176:ARG:NH2	2.12	0.64
12:R:35:ASN:O	12:R:39:THR:HG23	1.98	0.64
12:R:93:GLN:O	12:R:97:LEU:HD22	1.99	0.63
4:V:102:SER:HB2	9:a:35:LEU:HD11	1.80	0.63
3:I:128:ILE:HD11	4:J:129:TYR:HB2	1.80	0.63
7:Y:12:ILE:HG21	10:b:21:LEU:HB3	1.81	0.63
11:c:1:MET:HE3	12:d:1:MET:HG3	1.79	0.63
4:J:163:ILE:O	4:J:167:ARG:HG2	1.98	0.63
5:W:127:ILE:HD12	12:d:50:VAL:HG21	1.79	0.63
9:a:251:VAL:HG11	12:d:91:LEU:HD12	1.80	0.63
7:Y:57:SER:HB3	8:Z:70:LEU:HD12	1.81	0.63
5:K:4:ILE:HG21	10:P:6:LYS:HE2	1.80	0.62
12:d:90:THR:O	12:d:93:GLN:HG2	1.98	0.62
9:O:254:GLN:NE2	12:R:99:ASP:OD1	2.32	0.62
7:M:45:GLU:OE2	7:M:45:GLU:N	2.27	0.62
9:O:93:MET:HE3	9:O:93:MET:HA	1.82	0.62
9:O:97:ARG:HH12	10:P:54:MET:HE3	1.63	0.62
8:N:58:ARG:O	8:N:62:VAL:HG13	2.00	0.62
3:U:110:TRP:CD1	9:a:52:ILE:HD12	2.35	0.62
8:N:58:ARG:HH12	7:Y:15:ARG:CZ	2.12	0.62
9:O:174:ILE:HG23	9:O:175:GLN:OE1	2.00	0.62
9:a:83:PHE:CE1	12:d:51:PRO:HD2	2.36	0.61
5:W:68:LEU:HD21	9:a:111:PRO:HG2	1.83	0.61
3:I:61:GLN:O	3:I:65:PRO:HD2	2.00	0.60
9:O:247:ILE:O	9:O:251:VAL:HG13	2.00	0.60
4:J:163:ILE:O	4:J:167:ARG:NH1	2.34	0.60
8:N:53:ILE:HG22	8:N:54:LEU:H	1.67	0.60
9:O:40:ASN:H	9:O:43:SER:HB2	1.66	0.60
5:W:125:VAL:HG23	12:d:52:GLU:HB3	1.84	0.60
9:O:118:LYS:NZ	12:R:57:ARG:HE	2.00	0.60
8:N:54:LEU:O	8:N:58:ARG:CB	2.50	0.60
9:O:83:PHE:HE1	12:R:51:PRO:HD2	1.65	0.60
4:J:166:LEU:HB3	4:J:167:ARG:NH2	2.17	0.59
12:d:80:SER:O	12:d:84:MET:HG2	2.02	0.59
6:L:28:LEU:HD21	8:N:16:TYR:HE2	1.68	0.59
11:c:50:GLY:O	11:c:54:ILE:HG12	2.02	0.58
9:a:105:LYS:NZ	10:b:62:THR:OG1	2.30	0.58
9:a:261:MET:SD	12:d:102:LEU:HA	2.43	0.58
12:R:75:ASP:OD1	12:R:78:ARG:NH2	2.36	0.58
5:W:5:ASP:OD1	5:W:5:ASP:N	2.37	0.58
12:d:83:ARG:O	12:d:87:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:23:LEU:HA	11:Q:26:THR:HG22	1.84	0.58
12:d:82:GLY:HA2	12:d:85:GLN:NE2	2.17	0.58
9:O:172:PRO:O	9:O:176:ARG:HG2	2.03	0.58
5:W:128:ARG:NH2	5:W:132:ASN:OD1	2.36	0.58
8:Z:12:VAL:HG12	8:Z:16:TYR:CZ	2.38	0.58
11:c:61:MET:HA	11:c:61:MET:HE2	1.86	0.58
4:V:117:ALA:O	11:c:51:SER:OG	2.22	0.58
6:X:24:ARG:HH21	6:X:28:LEU:HD23	1.69	0.58
11:c:42:VAL:HG11	12:d:33:SER:HB2	1.85	0.58
9:O:89:ARG:O	9:O:93:MET:HG2	2.04	0.57
9:O:248:LYS:O	9:O:251:VAL:HG22	2.03	0.57
12:R:80:SER:O	12:R:84:MET:HG3	2.03	0.57
10:b:3:SER:HA	10:b:6:LYS:HG2	1.86	0.57
7:Y:5:HIS:O	7:Y:9:GLN:HG2	2.04	0.57
7:Y:13:LEU:O	7:Y:17:ILE:HG12	2.04	0.57
7:Y:44:LEU:HD21	10:b:54:MET:HB3	1.87	0.57
2:G:304:ILE:O	2:G:309:GLN:N	2.29	0.57
8:N:53:ILE:O	8:N:56:GLU:N	2.30	0.57
10:P:20:ASN:O	10:P:24:ILE:HG12	2.04	0.57
4:V:136:ARG:NE	4:V:140:GLU:OE2	2.38	0.57
3:I:118:PRO:HB2	3:I:121:ILE:HG13	1.87	0.57
8:N:81:GLN:NE2	8:N:85:GLU:OE2	2.38	0.57
11:Q:17:ARG:NH2	12:R:7:GLN:OE1	2.38	0.56
9:a:244:LEU:HD13	12:d:88:LEU:HA	1.86	0.56
5:W:79:GLU:OE1	5:W:79:GLU:N	2.35	0.56
10:b:9:THR:HA	10:b:12:LYS:HG3	1.88	0.56
9:O:175:GLN:HB3	9:O:176:ARG:HH22	1.70	0.56
9:O:251:VAL:HG12	12:R:95:TYR:HE1	1.69	0.56
7:Y:33:GLU:O	7:Y:37:ILE:HG12	2.05	0.56
8:Z:79:ILE:HG22	8:Z:83:LYS:NZ	2.20	0.56
9:a:40:ASN:O	9:a:44:ILE:HG23	2.05	0.56
9:a:247:ILE:HG23	12:d:95:TYR:HE2	1.70	0.56
7:M:5:HIS:O	7:M:9:GLN:HG3	2.05	0.56
7:M:1:MET:HE2	7:M:1:MET:N	2.20	0.56
8:N:21:LEU:HA	8:N:24:LYS:NZ	2.20	0.56
9:O:250:GLU:HG3	12:R:95:TYR:OH	2.05	0.56
4:J:114:HIS:ND1	7:M:58:VAL:HG21	2.21	0.56
5:K:4:ILE:O	5:K:8:ILE:HG12	2.05	0.56
12:R:89:ASP:O	12:R:92:GLN:HG3	2.06	0.56
7:M:67:ASN:O	7:M:69:LYS:NZ	2.38	0.56
11:c:39:GLU:OE2	11:c:39:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:127:GLN:NE2	12:d:32:PRO:HB3	2.18	0.56
12:d:81:MET:SD	12:d:84:MET:HE3	2.46	0.55
3:U:124:ASP:O	3:U:128:ILE:HG12	2.07	0.55
5:K:125:VAL:HG12	9:O:53:LYS:HB2	1.88	0.55
7:Y:25:GLU:OE2	3:e:16:GLU:HB2	2.06	0.55
7:M:5:HIS:NE2	10:P:11:GLU:OE2	2.40	0.55
9:O:97:ARG:HG3	10:P:58:GLU:OE2	2.07	0.55
2:B:304:ILE:O	2:B:309:GLN:N	2.32	0.55
7:M:54:TYR:O	7:M:58:VAL:HG13	2.07	0.55
3:I:142:VAL:HA	3:I:145:LEU:HD12	1.89	0.55
7:M:46:ILE:O	7:M:50:ILE:HG23	2.06	0.55
8:N:58:ARG:HH22	7:Y:12:ILE:HG12	1.72	0.55
9:O:83:PHE:CE1	12:R:51:PRO:HD2	2.42	0.55
4:V:82:THR:O	4:V:86:LYS:HG2	2.07	0.55
5:W:1:MET:HE1	5:W:4:ILE:HG12	1.89	0.55
5:K:31:GLN:NE2	12:R:20:LYS:HD2	2.22	0.54
7:M:59:GLN:O	7:M:63:GLU:HG2	2.07	0.54
4:V:120:ILE:HD11	11:c:58:ILE:HD12	1.89	0.54
7:M:25:GLU:O	7:M:29:ILE:HG12	2.06	0.54
9:O:83:PHE:CE1	12:R:50:VAL:HG13	2.42	0.54
12:R:101:ARG:HA	12:R:104:LYS:CE	2.37	0.54
4:V:74:ILE:O	4:V:78:ILE:HG12	2.07	0.54
12:d:59:LYS:O	12:d:63:ILE:HG12	2.07	0.54
8:N:31:LYS:O	8:N:35:TYR:HD1	1.91	0.54
3:U:125:LEU:O	3:U:129:LYS:HG2	2.07	0.54
3:I:78:ASP:O	3:I:82:THR:HG23	2.08	0.54
9:a:62:LEU:HD22	9:a:223:LEU:HA	1.90	0.54
4:J:139:ASN:HA	4:J:142:VAL:HG22	1.90	0.54
5:W:42:MET:SD	11:c:33:MET:HE2	2.47	0.54
8:Z:13:LEU:HA	8:Z:16:TYR:CD2	2.42	0.54
6:X:52:SER:HB2	8:Z:53:ILE:HG23	1.90	0.54
5:K:11:LYS:O	5:K:15:LEU:HD23	2.08	0.53
9:O:241:SER:O	9:O:245:ARG:HG3	2.07	0.53
5:K:15:LEU:HD22	10:P:17:ILE:HD11	1.90	0.53
5:W:125:VAL:N	12:d:50:VAL:O	2.22	0.53
8:Z:79:ILE:HG22	8:Z:83:LYS:HZ3	1.74	0.53
9:a:254:GLN:NE2	12:d:98:ASN:HB2	2.23	0.53
6:L:17:ASP:OD1	6:L:17:ASP:N	2.41	0.53
4:V:71:LEU:HA	4:V:74:ILE:CG1	2.39	0.53
8:N:49:SER:OG	8:N:51:ASP:OD1	2.20	0.53
4:V:70:SER:O	4:V:74:ILE:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:24:LEU:HG	12:R:16:VAL:HG21	1.91	0.53
9:O:83:PHE:CZ	12:R:50:VAL:HG13	2.44	0.53
11:Q:7:ARG:O	11:Q:11:GLN:HG3	2.09	0.53
4:V:75:THR:O	4:V:79:LYS:HG2	2.09	0.53
9:a:237:TYR:HD1	9:a:241:SER:HG	1.57	0.53
4:J:71:LEU:HD21	8:N:16:TYR:CE1	2.44	0.52
3:U:140:ASN:HA	3:U:143:MET:SD	2.49	0.52
4:V:67:GLU:O	4:V:71:LEU:HD13	2.09	0.52
4:J:65:LEU:O	4:J:68:SER:OG	2.26	0.52
7:M:9:GLN:HA	7:M:12:ILE:HG22	1.90	0.52
7:M:53:ASN:ND2	8:N:77:SER:OG	2.43	0.52
9:O:246:PHE:O	9:O:250:GLU:HG2	2.09	0.52
9:O:261:MET:O	9:O:265:HIS:N	2.37	0.52
12:R:87:GLU:O	12:R:91:LEU:HD12	2.08	0.52
6:X:17:ASP:O	6:X:21:ILE:HG12	2.09	0.52
3:I:66:LYS:HB3	6:L:35:MET:HE3	1.90	0.52
3:U:62:LEU:O	3:U:66:LYS:HE2	2.10	0.52
6:L:24:ARG:O	6:L:28:LEU:HD23	2.09	0.52
7:M:44:LEU:HD11	10:P:54:MET:HG2	1.91	0.52
8:N:19:LEU:O	8:N:23:LEU:HD23	2.09	0.52
3:U:122:GLN:H	3:U:122:GLN:CD	2.17	0.52
6:X:42:LEU:HD13	6:X:45:LEU:HD23	1.92	0.52
8:Z:38:HIS:ND1	8:Z:47:THR:OG1	2.43	0.52
11:c:4:ASN:HA	11:c:7:ARG:HE	1.74	0.52
6:L:53:ILE:O	6:L:57:ARG:HG3	2.10	0.51
9:O:262:SER:OG	12:R:101:ARG:NH2	2.43	0.51
10:b:5:SER:HA	10:b:8:GLU:HB3	1.93	0.51
4:J:62:GLN:OE1	4:J:62:GLN:N	2.26	0.51
8:N:83:LYS:HG3	5:W:1:MET:HB3	1.91	0.51
9:a:97:ARG:NH2	9:a:98:ARG:HA	2.24	0.51
3:U:64:LEU:HD12	9:a:5:LEU:HB3	1.92	0.51
7:M:13:LEU:O	7:M:17:ILE:HG12	2.10	0.51
10:b:2:ASP:HB2	10:b:5:SER:HB3	1.91	0.51
4:J:85:LEU:HD13	4:J:89:LEU:HD22	1.93	0.51
5:K:18:LEU:HD23	5:K:21:ILE:HD12	1.92	0.51
9:O:174:ILE:O	9:O:178:LEU:HG	2.10	0.51
9:O:40:ASN:O	9:O:44:ILE:HG23	2.10	0.51
8:Z:22:ASP:OD2	8:Z:22:ASP:N	2.41	0.51
9:a:89:ARG:O	9:a:93:MET:HG3	2.09	0.51
9:a:248:LYS:O	9:a:252:LEU:HG	2.11	0.51
10:P:13:LEU:O	10:P:17:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:60:LEU:HD12	10:P:64:PHE:HE2	1.76	0.51
9:a:17:ASP:O	9:a:21:THR:HG23	2.10	0.51
3:e:16:GLU:N	3:e:16:GLU:OE1	2.44	0.51
1:F:587:ARG:HA	12:d:93:GLN:OE1	2.11	0.50
12:R:67:GLU:O	12:R:70:VAL:HG12	2.12	0.50
4:V:112:ASN:O	4:V:116:GLN:HG2	2.11	0.50
12:d:83:ARG:HA	12:d:86:ARG:NH2	2.26	0.50
6:L:74:GLU:N	6:L:74:GLU:OE1	2.44	0.50
4:V:116:GLN:HE22	7:Y:72:LEU:HD23	1.76	0.50
3:I:88:HIS:CE1	9:O:24:PHE:HB3	2.47	0.50
6:L:63:SER:O	6:L:67:LYS:HG2	2.12	0.50
12:R:67:GLU:O	12:R:71:ARG:HG2	2.10	0.50
4:V:77:MET:HA	4:V:77:MET:HE2	1.93	0.50
9:a:15:ALA:O	9:a:19:MET:HG2	2.11	0.50
4:J:146:ASP:OD2	4:J:146:ASP:N	2.39	0.50
7:M:24:ASN:ND2	11:Q:15:GLU:OE1	2.44	0.50
6:L:48:SER:HB2	8:N:53:ILE:HD13	1.93	0.50
4:V:92:TYR:O	4:V:96:VAL:HG12	2.12	0.50
9:a:97:ARG:NH1	10:b:54:MET:HE1	2.27	0.50
9:a:238:GLU:HA	9:a:242:SER:OG	2.11	0.50
4:J:71:LEU:HD23	8:N:15:LYS:HG2	1.93	0.50
8:N:54:LEU:O	8:N:58:ARG:HB3	2.11	0.50
12:R:71:ARG:HA	12:R:71:ARG:NH1	2.27	0.50
9:a:67:ASN:O	9:a:71:GLN:N	2.44	0.50
12:d:67:GLU:O	12:d:71:ARG:HG2	2.12	0.50
6:L:26:ILE:O	6:L:29:GLN:HG3	2.12	0.50
7:M:13:LEU:O	7:M:16:ILE:HG22	2.12	0.50
3:U:131:LEU:O	3:U:135:GLU:HG2	2.12	0.50
4:V:100:CYS:SG	8:Z:57:MET:HE1	2.52	0.49
7:Y:46:ILE:O	7:Y:50:ILE:HG23	2.11	0.49
9:a:113:GLU:OE1	9:a:113:GLU:N	2.34	0.49
4:V:129:TYR:CE2	4:V:133:ILE:HD11	2.47	0.49
6:X:16:THR:HA	8:Z:3:HIS:CE1	2.47	0.49
5:K:69:GLY:HA2	5:K:72:GLN:HG2	1.95	0.49
9:O:245:ARG:HB2	9:O:245:ARG:NH1	2.28	0.49
9:a:180:ALA:O	9:a:184:GLY:N	2.45	0.49
12:d:101:ARG:HH12	12:d:105:ASN:HB2	1.77	0.49
4:J:139:ASN:O	4:J:143:ASN:N	2.28	0.49
12:R:11:ALA:O	12:R:15:THR:HG23	2.13	0.49
12:R:94:THR:HA	12:R:97:LEU:HD23	1.94	0.49
3:U:122:GLN:O	3:U:126:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:16:THR:HA	8:Z:3:HIS:ND1	2.27	0.49
9:O:169:LYS:HZ3	9:O:171:ASP:HB3	1.77	0.49
3:U:62:LEU:HD21	6:X:28:LEU:HD13	1.94	0.49
12:R:56:GLU:HA	12:R:59:LYS:HZ3	1.78	0.49
9:a:118:LYS:HG2	12:d:53:TYR:OH	2.13	0.49
3:I:121:ILE:H	3:I:121:ILE:CD1	2.25	0.49
3:U:120:ASP:OD2	3:U:123:ASP:HB3	2.13	0.49
4:V:135:ASP:OD2	4:V:135:ASP:N	2.45	0.49
4:V:148:ASP:OD1	4:V:148:ASP:N	2.39	0.49
6:X:71:ASP:OD1	6:X:71:ASP:N	2.46	0.49
9:a:40:ASN:H	9:a:43:SER:HB2	1.76	0.49
9:a:83:PHE:CZ	12:d:50:VAL:HG22	2.48	0.49
4:V:136:ARG:O	4:V:140:GLU:HG2	2.13	0.49
3:U:72:ASP:O	3:U:75:ILE:HG13	2.13	0.48
3:I:130:GLN:O	3:I:134:LEU:HG	2.13	0.48
5:K:34:GLU:HA	5:K:34:GLU:OE1	2.14	0.48
9:O:253:LEU:O	9:O:257:ARG:HG3	2.14	0.48
5:K:21:ILE:HG22	10:P:24:ILE:HD12	1.95	0.48
5:K:24:LEU:CD2	12:R:12:LEU:HB3	2.40	0.48
12:R:87:GLU:O	12:R:90:THR:OG1	2.22	0.48
8:Z:53:ILE:O	8:Z:56:GLU:N	2.24	0.48
10:P:15:GLN:O	10:P:19:VAL:HG12	2.14	0.48
8:Z:12:VAL:HG12	8:Z:16:TYR:CE1	2.49	0.48
9:a:236:ASN:HB3	12:d:81:MET:HE3	1.95	0.48
12:R:39:THR:OG1	12:R:40:MET:N	2.47	0.48
3:U:144:GLU:O	3:U:148:MET:HG2	2.13	0.48
7:Y:27:VAL:HG21	11:c:23:LEU:HD22	1.96	0.48
8:Z:53:ILE:HG22	8:Z:54:LEU:H	1.79	0.48
10:b:5:SER:O	10:b:9:THR:HG23	2.13	0.48
9:O:253:LEU:HB2	9:O:257:ARG:HH21	1.78	0.48
11:Q:32:ILE:O	11:Q:36:GLN:HG3	2.14	0.48
3:I:141:LEU:HD23	3:I:141:LEU:HA	1.73	0.47
4:J:71:LEU:HB3	8:N:15:LYS:HE3	1.96	0.47
7:M:21:LYS:NZ	11:Q:15:GLU:OE2	2.34	0.47
6:X:31:ILE:O	6:X:35:MET:HG2	2.14	0.47
4:J:60:THR:O	4:J:63:SER:OG	2.28	0.47
9:O:229:ASP:OD1	9:O:232:GLN:NE2	2.34	0.47
3:U:138:LYS:O	3:U:142:VAL:HG13	2.14	0.47
6:X:71:ASP:OD1	6:X:75:SER:HB3	2.13	0.47
3:U:78:ASP:HA	9:a:19:MET:HE1	1.96	0.47
2:G:335:VAL:O	2:G:340:ILE:N	2.38	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:60:GLN:HE21	3:I:61:GLN:HG3	1.80	0.47
7:M:39:ASN:O	7:M:42:LYS:NZ	2.48	0.47
7:M:60:PHE:CE1	10:b:12:LYS:HD3	2.49	0.47
8:N:31:LYS:HB3	8:N:35:TYR:HE1	1.80	0.47
9:O:251:VAL:HG12	12:R:95:TYR:CE1	2.49	0.47
6:X:23:GLN:O	6:X:27:VAL:HG22	2.14	0.47
8:Z:49:SER:O	8:Z:53:ILE:HG13	2.15	0.47
4:J:78:ILE:HD13	8:N:23:LEU:HD22	1.97	0.47
12:R:57:ARG:NH1	12:R:60:LEU:HD22	2.30	0.47
7:M:33:GLU:OE1	7:M:33:GLU:HA	2.15	0.47
12:R:79:LYS:O	12:R:79:LYS:NZ	2.48	0.47
12:d:92:GLN:O	12:d:96:GLU:HG2	2.15	0.47
4:J:116:GLN:HB3	11:Q:58:ILE:HD11	1.97	0.47
6:L:66:TRP:HE1	8:N:67:VAL:HG12	1.80	0.47
12:d:100:LEU:HD12	12:d:101:ARG:N	2.30	0.47
5:K:70:LEU:HD21	6:L:73:LEU:HD23	1.97	0.46
12:R:74:GLY:O	12:R:78:ARG:HG2	2.15	0.46
9:O:60:ALA:O	9:O:64:PHE:N	2.47	0.46
9:a:258:LEU:HD12	12:d:98:ASN:HB3	1.96	0.46
3:I:64:LEU:HD21	9:O:4:SER:HB3	1.96	0.46
7:Y:45:GLU:OE1	7:Y:45:GLU:N	2.33	0.46
9:a:19:MET:HA	9:a:19:MET:HE2	1.96	0.46
4:J:124:MET:HG2	12:R:40:MET:SD	2.55	0.46
12:d:70:VAL:HG13	12:d:71:ARG:HD2	1.97	0.46
4:J:120:ILE:HD11	11:Q:51:SER:O	2.15	0.46
3:U:122:GLN:OE1	3:U:122:GLN:N	2.28	0.46
5:W:26:ASP:O	5:W:30:ILE:HG12	2.16	0.46
9:a:246:PHE:HA	9:a:249:LYS:HG2	1.98	0.46
9:a:248:LYS:O	9:a:251:VAL:HG12	2.15	0.46
5:K:68:LEU:HD21	9:O:111:PRO:HG2	1.96	0.46
7:M:24:ASN:ND2	11:Q:18:GLU:OE1	2.48	0.46
6:X:35:MET:HE1	8:Z:23:LEU:HD12	1.98	0.46
6:X:35:MET:N	6:X:35:MET:HE2	2.31	0.46
10:b:8:GLU:O	10:b:12:LYS:HG3	2.16	0.46
4:J:60:THR:HG1	4:J:61:THR:N	2.14	0.46
5:K:125:VAL:N	12:R:50:VAL:O	2.37	0.46
9:a:247:ILE:HG23	12:d:95:TYR:CE2	2.51	0.46
7:M:2:GLU:OE2	7:M:2:GLU:N	2.31	0.46
7:M:18:GLY:O	7:M:22:ARG:HG2	2.16	0.46
8:N:31:LYS:O	8:N:34:ASN:N	2.49	0.46
8:N:54:LEU:HD23	10:b:26:SER:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:41:PRO:O	10:P:45:THR:HG23	2.17	0.45
6:X:19:TYR:HA	6:X:22:GLU:OE1	2.16	0.45
12:d:81:MET:O	12:d:85:GLN:HG3	2.15	0.45
9:O:172:PRO:O	9:O:176:ARG:NH1	2.49	0.45
12:d:2:THR:O	12:d:6:GLU:HG2	2.15	0.45
3:I:88:HIS:NE2	4:J:99:VAL:HG21	2.32	0.45
7:M:12:ILE:HG13	7:M:15:ARG:NH2	2.31	0.45
9:O:98:ARG:HH21	10:P:51:GLU:HB3	1.81	0.45
9:O:180:ALA:O	9:O:184:GLY:N	2.49	0.45
9:O:244:LEU:O	9:O:248:LYS:HG2	2.15	0.45
4:V:90:PRO:HA	4:V:93:VAL:HG22	1.98	0.45
10:b:65:GLN:HA	10:b:70:VAL:HG22	1.99	0.45
3:I:98:LEU:O	3:I:102:LEU:HD23	2.16	0.45
9:O:246:PHE:HA	9:O:249:LYS:HG2	1.96	0.45
11:Q:6:GLN:HA	12:R:1:MET:SD	2.57	0.45
10:b:19:VAL:O	10:b:23:LYS:HG3	2.16	0.45
11:c:20:GLN:HA	12:d:15:THR:HG22	1.99	0.45
5:K:8:ILE:HG22	5:K:12:ARG:NE	2.31	0.45
8:N:72:LYS:O	8:N:73:GLY:C	2.59	0.45
12:R:71:ARG:HA	12:R:71:ARG:CZ	2.47	0.45
4:V:71:LEU:HA	4:V:74:ILE:HG12	1.98	0.45
10:b:49:ILE:O	10:b:53:ILE:HG12	2.16	0.45
3:I:60:GLN:NE2	3:I:61:GLN:HG3	2.31	0.45
5:K:18:LEU:HD12	10:P:17:ILE:HD12	1.99	0.45
3:U:110:TRP:HE1	5:W:126:ARG:HG3	1.81	0.45
5:W:123:THR:O	12:d:52:GLU:HG3	2.17	0.45
11:Q:61:MET:O	11:Q:64:MET:HG3	2.17	0.45
4:J:63:SER:HA	4:J:66:LYS:HG2	1.99	0.44
6:X:60:GLN:HA	6:X:60:GLN:OE1	2.17	0.44
4:V:111:ILE:HG23	7:Y:62:LEU:HD21	1.98	0.44
5:W:13:LYS:HA	5:W:16:GLN:HG2	1.99	0.44
9:a:234:TYR:HD1	9:a:237:TYR:HD2	1.65	0.44
3:U:59:ILE:HA	3:U:62:LEU:HG	1.99	0.44
7:Y:23:LEU:HD12	7:Y:23:LEU:HA	1.87	0.44
5:W:68:LEU:HD13	9:a:115:TYR:CD1	2.52	0.44
8:N:54:LEU:O	8:N:58:ARG:HB2	2.17	0.44
6:X:69:LEU:HD23	10:b:63:MET:HE1	2.00	0.44
4:J:77:MET:HE3	9:O:12:ILE:HD13	1.99	0.44
9:O:41:LYS:O	9:O:44:ILE:HG12	2.18	0.44
6:X:73:LEU:HD23	6:X:73:LEU:H	1.82	0.44
8:Z:53:ILE:O	8:Z:55:GLN:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:122:GLN:CD	3:I:122:GLN:H	2.26	0.44
8:N:28:GLU:OE1	8:N:28:GLU:HA	2.18	0.44
8:Z:13:LEU:HD22	8:Z:16:TYR:CE2	2.47	0.44
8:Z:20:SER:O	8:Z:24:LYS:HG2	2.17	0.44
9:a:90:ASP:O	9:a:94:LYS:HG2	2.17	0.44
5:K:13:LYS:HA	5:K:16:GLN:HG3	2.00	0.43
3:I:103:TYR:O	3:I:106:MET:HG3	2.18	0.43
5:K:15:LEU:HD22	10:P:17:ILE:CD1	2.48	0.43
3:U:68:ARG:HG2	9:a:8:CYS:SG	2.58	0.43
7:M:31:ASN:OD1	11:Q:26:THR:HB	2.19	0.43
8:N:83:LYS:O	8:N:83:LYS:HD3	2.19	0.43
4:V:127:GLN:HA	4:V:127:GLN:OE1	2.18	0.43
12:d:67:GLU:O	12:d:70:VAL:HG12	2.19	0.43
8:N:26:LEU:HG	8:N:30:ILE:HD13	2.01	0.43
6:X:20:PHE:CD2	6:X:21:ILE:HD13	2.54	0.43
5:K:33:THR:HG22	10:P:34:LYS:HE3	2.01	0.43
9:O:67:ASN:O	9:O:71:GLN:CA	2.66	0.43
8:Z:31:LYS:O	8:Z:35:TYR:N	2.52	0.43
9:a:12:ILE:O	9:a:16:VAL:HG12	2.19	0.43
5:W:8:ILE:HD11	10:b:10:LEU:HB2	2.00	0.42
5:W:71:LEU:HD23	5:W:71:LEU:H	1.83	0.42
7:Y:1:MET:HE3	7:Y:1:MET:O	2.19	0.42
9:a:254:GLN:HE22	12:d:98:ASN:HB2	1.82	0.42
9:O:237:TYR:O	9:O:241:SER:OG	2.30	0.42
9:O:250:GLU:HA	9:O:253:LEU:HG	2.01	0.42
9:O:261:MET:SD	12:R:105:ASN:HB3	2.59	0.42
12:R:79:LYS:HZ2	12:R:83:ARG:NH1	2.17	0.42
12:R:85:GLN:NE2	12:R:89:ASP:OD2	2.52	0.42
4:V:71:LEU:HD22	8:Z:15:LYS:HD3	2.01	0.42
9:O:233:LEU:HD22	12:R:77:LEU:HD12	2.01	0.42
10:b:16:GLU:HA	10:b:19:VAL:HG12	2.01	0.42
7:M:57:SER:OG	8:N:70:LEU:HG	2.19	0.42
7:Y:15:ARG:HD2	10:b:25:ASP:OD1	2.19	0.42
9:a:238:GLU:O	9:a:242:SER:HB2	2.18	0.42
4:J:70:SER:O	4:J:74:ILE:HG12	2.20	0.42
4:J:89:LEU:HD11	9:O:19:MET:HE3	2.01	0.42
5:K:13:LYS:C	5:K:16:GLN:HE21	2.26	0.42
9:O:32:ASN:O	9:O:36:GLN:HG2	2.19	0.42
9:O:176:ARG:HG2	9:O:176:ARG:HH11	1.84	0.42
12:R:90:THR:O	12:R:93:GLN:HG3	2.20	0.42
3:I:96:GLU:OE2	3:I:96:GLU:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:120:ASP:OD2	3:U:120:ASP:O	2.37	0.42
12:d:57:ARG:HD3	12:d:61:ASP:OD2	2.19	0.42
4:J:62:GLN:HA	4:J:65:LEU:HD12	2.01	0.42
4:J:112:ASN:O	4:J:116:GLN:HG2	2.19	0.42
8:Z:18:GLN:NE2	8:Z:22:ASP:OD1	2.52	0.42
9:a:243:LYS:HA	9:a:246:PHE:CD1	2.55	0.42
10:b:6:LYS:HG3	10:b:7:GLU:N	2.35	0.42
5:K:57:ASP:OD1	5:K:58:SER:N	2.52	0.42
6:X:69:LEU:O	9:a:108:ILE:HB	2.19	0.42
7:Y:18:GLY:O	7:Y:22:ARG:HG2	2.19	0.42
9:a:41:LYS:O	9:a:44:ILE:HG12	2.20	0.42
5:K:11:LYS:HB2	10:P:13:LEU:HD13	2.01	0.42
8:N:33:LEU:HD23	8:N:33:LEU:HA	1.82	0.42
12:R:55:VAL:HG12	12:R:59:LYS:HZ2	1.84	0.42
3:U:63:LEU:HD12	3:U:64:LEU:N	2.35	0.42
4:V:62:GLN:H	4:V:62:GLN:CD	2.25	0.42
11:c:6:GLN:HE22	12:d:1:MET:HA	1.84	0.42
6:L:27:VAL:O	6:L:30:GLU:HG3	2.20	0.42
8:N:51:ASP:HA	8:N:55:GLN:OE1	2.20	0.42
12:R:78:ARG:HA	12:R:81:MET:HB2	2.02	0.42
9:a:4:SER:O	9:a:7:ARG:HG2	2.20	0.42
8:N:62:VAL:HA	10:b:22:GLN:NE2	2.34	0.41
4:V:139:ASN:O	4:V:143:ASN:N	2.32	0.41
6:X:49:LEU:HD13	6:X:49:LEU:HA	1.86	0.41
12:d:3:ASP:OD1	12:d:3:ASP:N	2.51	0.41
6:L:30:GLU:HA	6:L:33:GLU:HG3	2.02	0.41
6:L:36:ASN:OD1	3:e:20:SER:HB2	2.20	0.41
6:L:50:GLU:CD	3:e:15:THR:HG22	2.45	0.41
3:U:139:ASN:HA	3:U:142:VAL:HG22	2.02	0.41
6:X:72:GLY:O	6:X:76:LEU:HG	2.20	0.41
5:K:120:LEU:C	9:O:29:ILE:HD11	2.45	0.41
6:L:71:ASP:N	6:L:71:ASP:OD1	2.53	0.41
4:J:77:MET:SD	4:J:78:ILE:N	2.94	0.41
10:P:12:LYS:O	10:P:16:GLU:HG2	2.21	0.41
10:P:60:LEU:HD12	10:P:64:PHE:CE2	2.54	0.41
8:Z:51:ASP:OD2	8:Z:52:GLU:N	2.54	0.41
8:Z:71:LEU:HD21	10:b:64:PHE:CD1	2.55	0.41
5:K:73:TYR:CZ	5:K:119:PRO:HA	2.56	0.41
6:L:52:SER:OG	8:N:53:ILE:HG23	2.19	0.41
9:O:97:ARG:HH22	10:P:54:MET:HE2	1.85	0.41
9:a:83:PHE:HZ	12:d:50:VAL:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:Y:21:LYS:O	7:Y:25:GLU:HG3	2.21	0.41
9:a:173:GLN:NE2	9:a:205:PHE:HD2	2.19	0.41
6:L:55:VAL:HG11	8:N:54:LEU:HD12	2.03	0.41
9:O:225:GLU:O	9:O:228:GLN:HG2	2.20	0.41
3:U:121:ILE:H	3:U:121:ILE:HG13	1.55	0.41
12:d:101:ARG:HH22	12:d:105:ASN:ND2	2.19	0.41
4:J:92:TYR:O	4:J:96:VAL:HG23	2.21	0.41
3:U:63:LEU:O	3:U:67:ILE:HG12	2.21	0.41
4:V:140:GLU:HG2	4:V:140:GLU:H	1.77	0.41
5:W:31:GLN:NE2	12:d:20:LYS:HE2	2.35	0.41
5:W:125:VAL:CG1	9:a:55:CYS:HB2	2.51	0.41
9:a:239:GLN:O	9:a:243:LYS:HB3	2.21	0.41
12:R:31:GLU:HB3	12:R:32:PRO:HD3	2.03	0.41
5:K:9:ALA:HA	5:K:12:ARG:HE	1.85	0.40
7:M:13:LEU:HD23	7:M:13:LEU:HA	1.89	0.40
4:J:60:THR:OG1	4:J:61:THR:N	2.54	0.40
3:U:66:LYS:HD3	3:U:66:LYS:N	2.36	0.40
7:Y:19:ASN:HD21	10:b:28:LEU:HB2	1.85	0.40
3:I:132:LYS:HD2	3:I:132:LYS:O	2.21	0.40
8:N:62:VAL:HA	10:b:22:GLN:HE22	1.87	0.40
9:O:75:ARG:NH2	9:O:77:ASP:OD2	2.39	0.40
6:X:24:ARG:HE	6:X:28:LEU:CD2	2.34	0.40
9:a:189:GLU:HB3	9:a:195:GLN:NE2	2.35	0.40
9:a:247:ILE:O	9:a:251:VAL:HB	2.20	0.40
12:d:62:LEU:HA	12:d:66:VAL:HB	2.02	0.40
5:K:8:ILE:HG22	5:K:12:ARG:CZ	2.52	0.40
9:O:241:SER:HA	9:O:244:LEU:HB3	2.03	0.40
6:X:24:ARG:NH1	8:Z:16:TYR:CG	2.90	0.40
8:Z:51:ASP:OD2	8:Z:51:ASP:C	2.64	0.40
9:a:234:TYR:O	9:a:238:GLU:HG3	2.21	0.40
9:a:261:MET:HE3	12:d:101:ARG:NH2	2.37	0.40
8:N:71:LEU:HG	10:P:64:PHE:CE1	2.56	0.40
8:Z:15:LYS:O	8:Z:19:LEU:HD23	2.21	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	292/691 (42%)	291 (100%)	0	1 (0%)	36	64
1	F	292/691 (42%)	290 (99%)	1 (0%)	1 (0%)	36	64
2	B	235/451 (52%)	229 (97%)	6 (3%)	0	100	100
2	G	234/451 (52%)	228 (97%)	6 (3%)	0	100	100
3	I	93/343 (27%)	91 (98%)	2 (2%)	0	100	100
3	U	93/343 (27%)	92 (99%)	1 (1%)	0	100	100
3	e	9/343 (3%)	8 (89%)	1 (11%)	0	100	100
4	J	115/247 (47%)	113 (98%)	2 (2%)	0	100	100
4	V	115/247 (47%)	113 (98%)	2 (2%)	0	100	100
5	K	102/133 (77%)	100 (98%)	2 (2%)	0	100	100
5	W	102/133 (77%)	98 (96%)	4 (4%)	0	100	100
6	L	59/94 (63%)	59 (100%)	0	0	100	100
6	X	66/94 (70%)	63 (96%)	3 (4%)	0	100	100
7	M	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
7	Y	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
8	N	90/94 (96%)	79 (88%)	11 (12%)	0	100	100
8	Z	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
9	O	231/295 (78%)	228 (99%)	3 (1%)	0	100	100
9	a	230/295 (78%)	222 (96%)	8 (4%)	0	100	100
10	P	63/292 (22%)	62 (98%)	1 (2%)	0	100	100
10	b	68/292 (23%)	67 (98%)	1 (2%)	0	100	100
11	Q	62/69 (90%)	60 (97%)	2 (3%)	0	100	100
11	c	62/69 (90%)	62 (100%)	0	0	100	100
12	R	106/165 (64%)	105 (99%)	1 (1%)	0	100	100
12	d	106/165 (64%)	105 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3057/6235 (49%)	2984 (98%)	71 (2%)	2 (0%)	49 76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	411	ILE
1	F	411	ILE

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
3	I	89/309 (29%)	89 (100%)	0	100 100
3	U	89/309 (29%)	88 (99%)	1 (1%)	65 75
3	e	9/309 (3%)	9 (100%)	0	100 100
4	J	109/222 (49%)	109 (100%)	0	100 100
4	V	109/222 (49%)	108 (99%)	1 (1%)	70 77
5	K	95/120 (79%)	95 (100%)	0	100 100
5	W	95/120 (79%)	94 (99%)	1 (1%)	65 75
6	L	56/87 (64%)	56 (100%)	0	100 100
6	X	62/87 (71%)	61 (98%)	1 (2%)	55 71
7	M	66/66 (100%)	66 (100%)	0	100 100
7	Y	66/66 (100%)	65 (98%)	1 (2%)	57 72
8	N	87/89 (98%)	87 (100%)	0	100 100
8	Z	89/89 (100%)	89 (100%)	0	100 100
9	O	217/269 (81%)	215 (99%)	2 (1%)	70 77
9	a	217/269 (81%)	217 (100%)	0	100 100
10	P	62/259 (24%)	61 (98%)	1 (2%)	55 71
10	b	66/259 (26%)	66 (100%)	0	100 100
11	Q	58/62 (94%)	57 (98%)	1 (2%)	53 70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	c	58/62 (94%)	58 (100%)	0	100	100
12	R	101/153 (66%)	101 (100%)	0	100	100
12	d	101/153 (66%)	99 (98%)	2 (2%)	48	68
All	All	1901/3581 (53%)	1890 (99%)	11 (1%)	76	81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	O	83	PHE
9	O	246	PHE
10	P	6	LYS
11	Q	27	THR
3	U	84	LEU
4	V	144	THR
5	W	72	GLN
6	X	69	LEU
7	Y	66	ASN
12	d	12	LEU
12	d	98	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
3	I	60	GLN
3	I	88	HIS
3	I	140	ASN
4	J	104	ASN
5	K	31	GLN
5	K	72	GLN
6	L	23	GLN
6	L	40	ASN
7	M	53	ASN
11	Q	8	GLN
11	Q	10	ASN
11	Q	11	GLN
11	Q	29	GLN
12	R	105	ASN
4	V	88	ASN
5	W	7	GLN
5	W	45	ASN

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Mol	Chain	Res	Type
5	W	62	ASN
5	W	72	GLN
6	X	36	ASN
7	Y	61	ASN
8	Z	86	GLN
9	a	40	ASN
9	a	235	HIS
10	b	20	ASN
10	b	22	GLN
11	c	8	GLN
11	c	38	ASN
11	c	63	GLN
12	d	98	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.

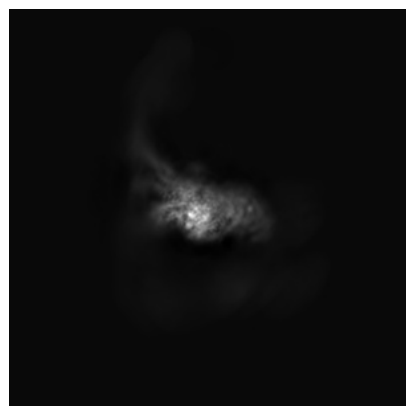
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18246. These allow visual inspection of the internal detail of the map and identification of artifacts.

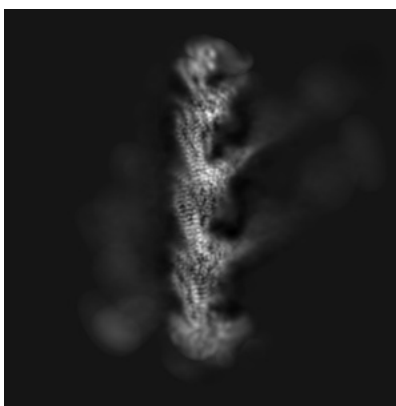
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

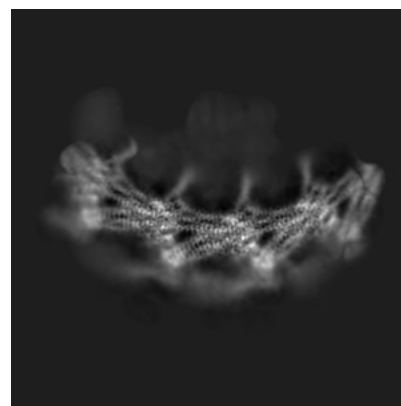
6.1.1 Primary map



X

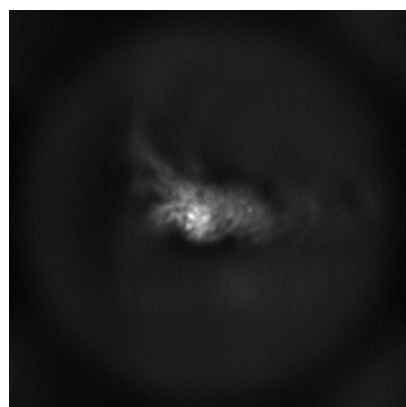


Y

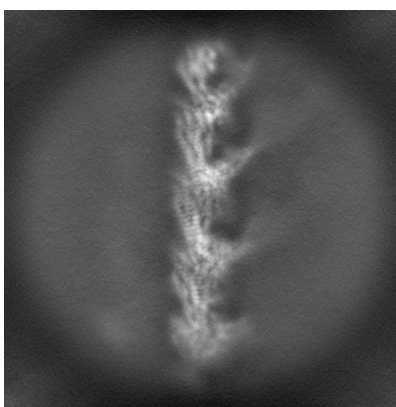


Z

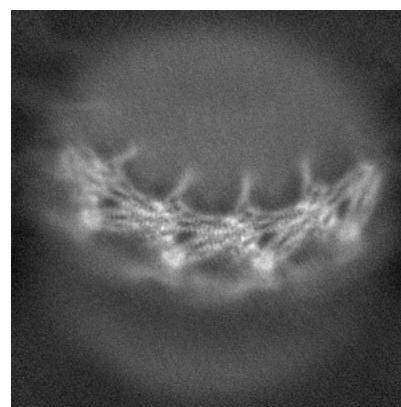
6.1.2 Raw map



X



Y

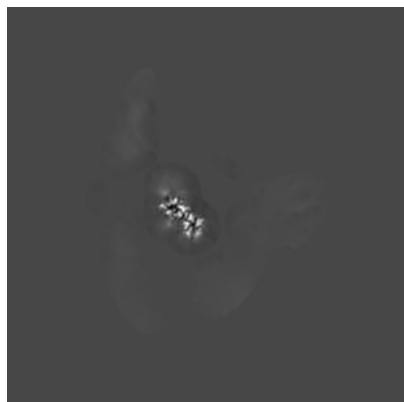


Z

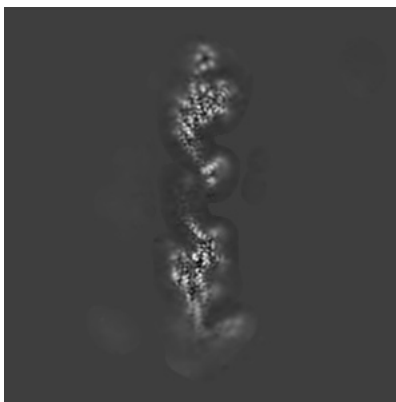
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 200



Y Index: 200

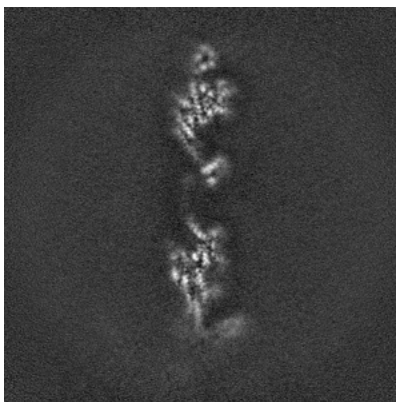


Z Index: 200

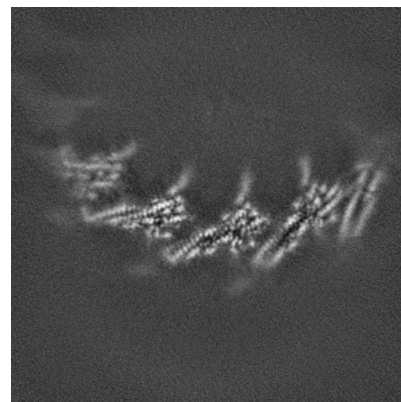
6.2.2 Raw map



X Index: 200



Y Index: 200

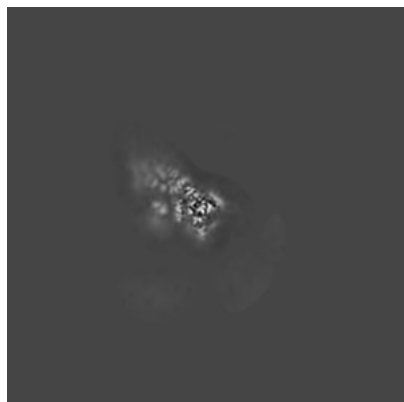


Z Index: 200

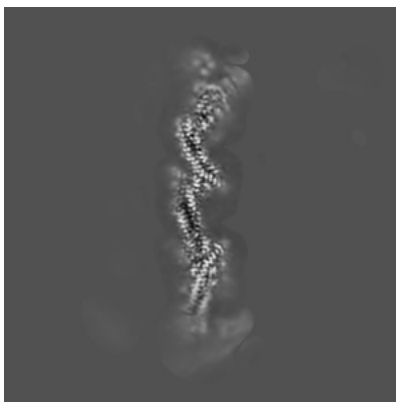
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

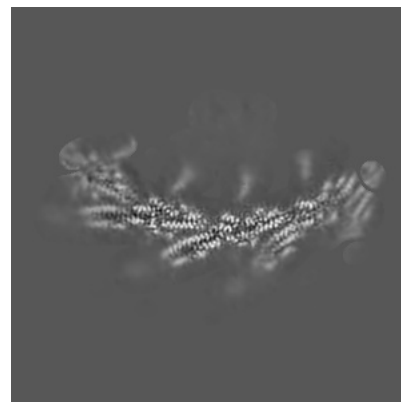
6.3.1 Primary map



X Index: 157

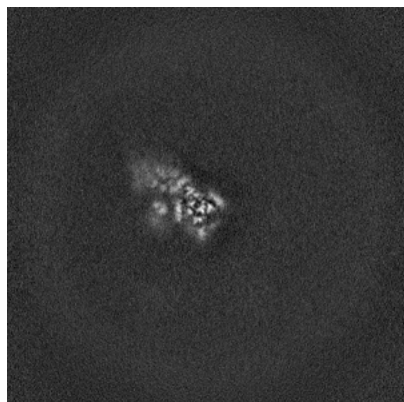


Y Index: 186

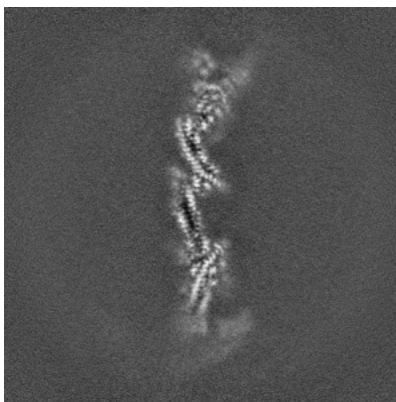


Z Index: 194

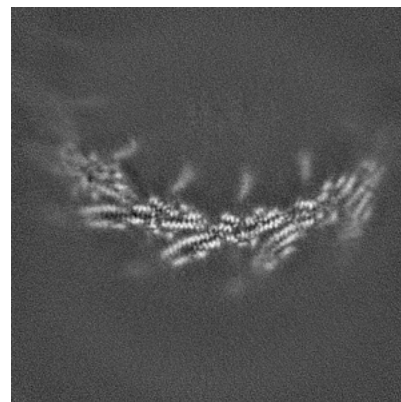
6.3.2 Raw map



X Index: 157



Y Index: 186

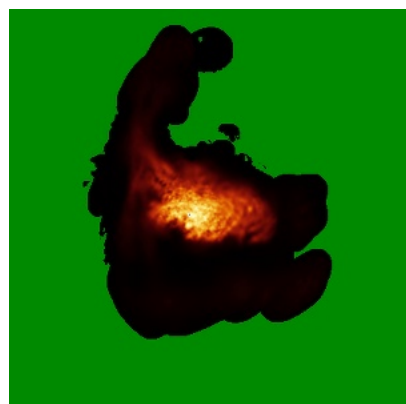


Z Index: 194

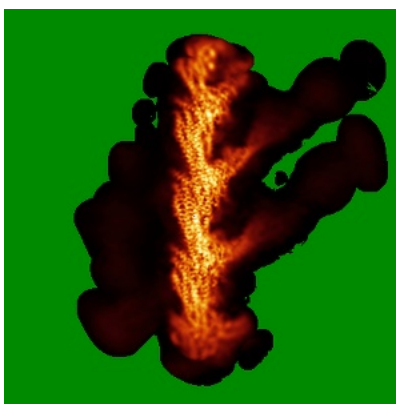
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

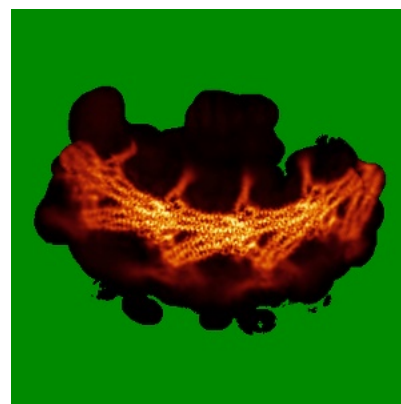
6.4.1 Primary map



X

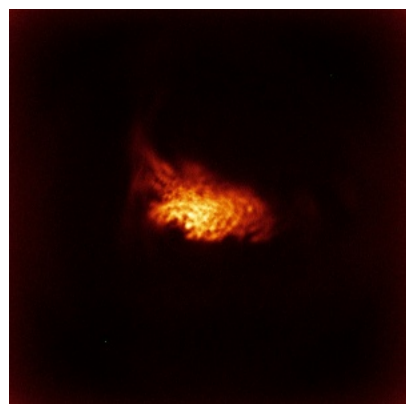


Y

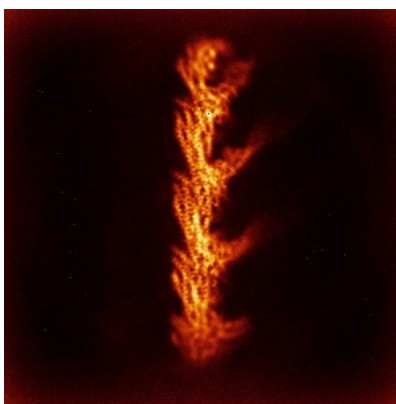


Z

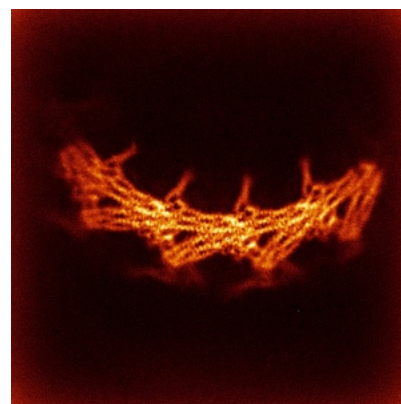
6.4.2 Raw map



X



Y

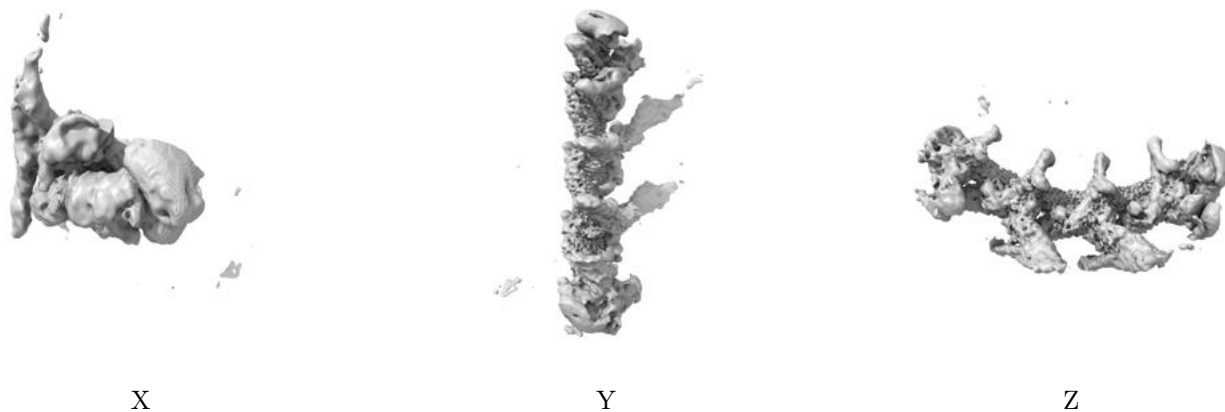


Z

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.

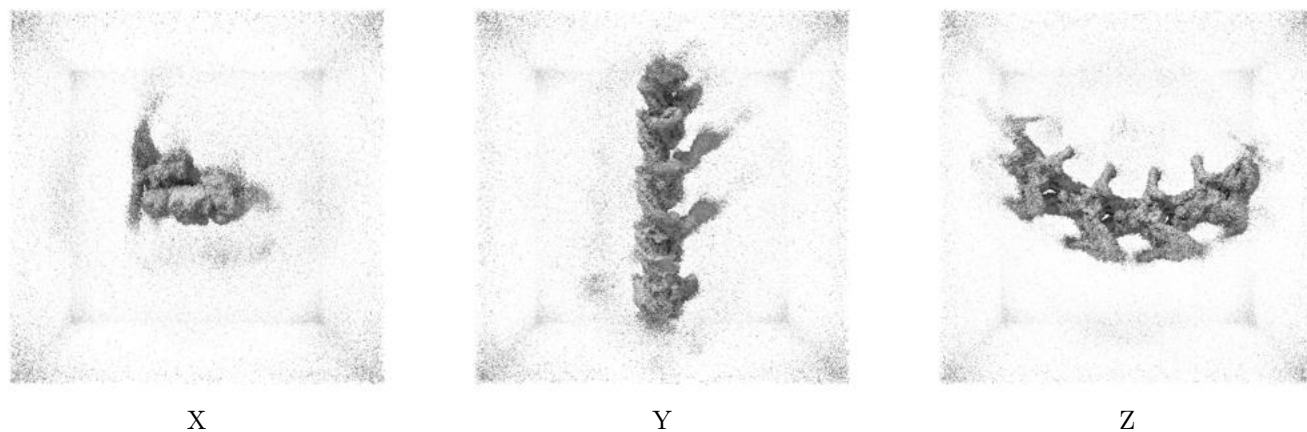
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

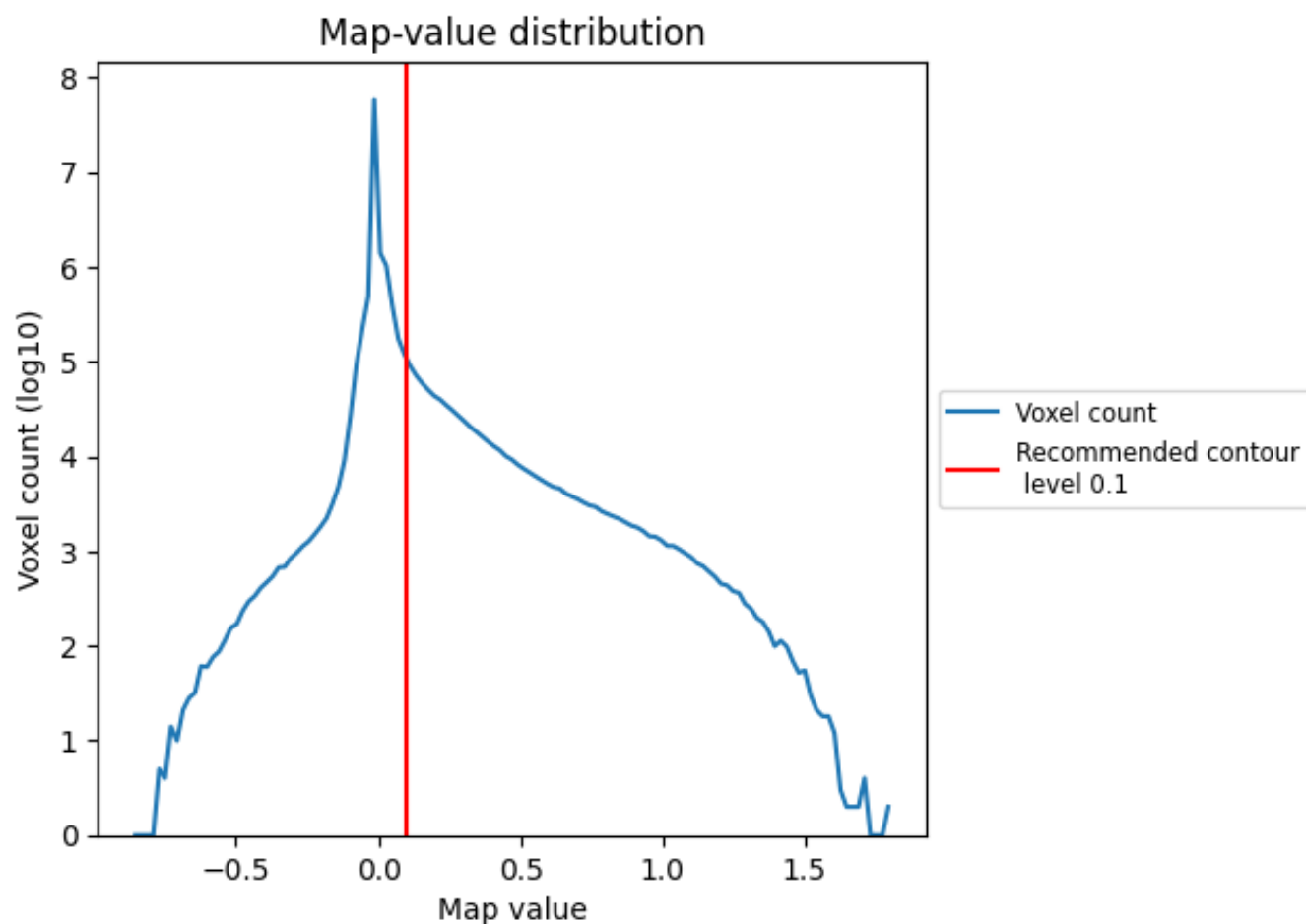
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

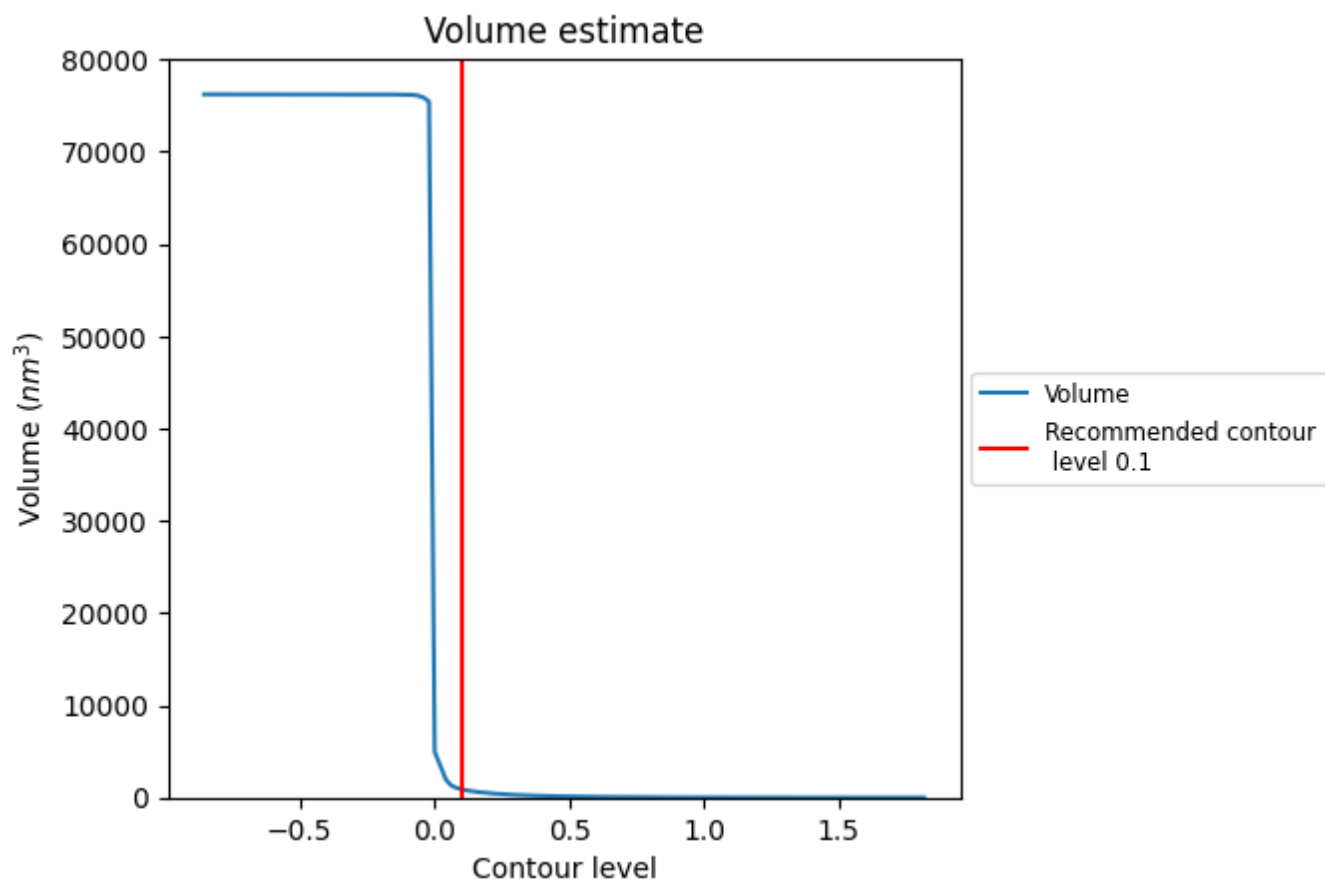
This section contains the results of statistical analysis of the map.

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.

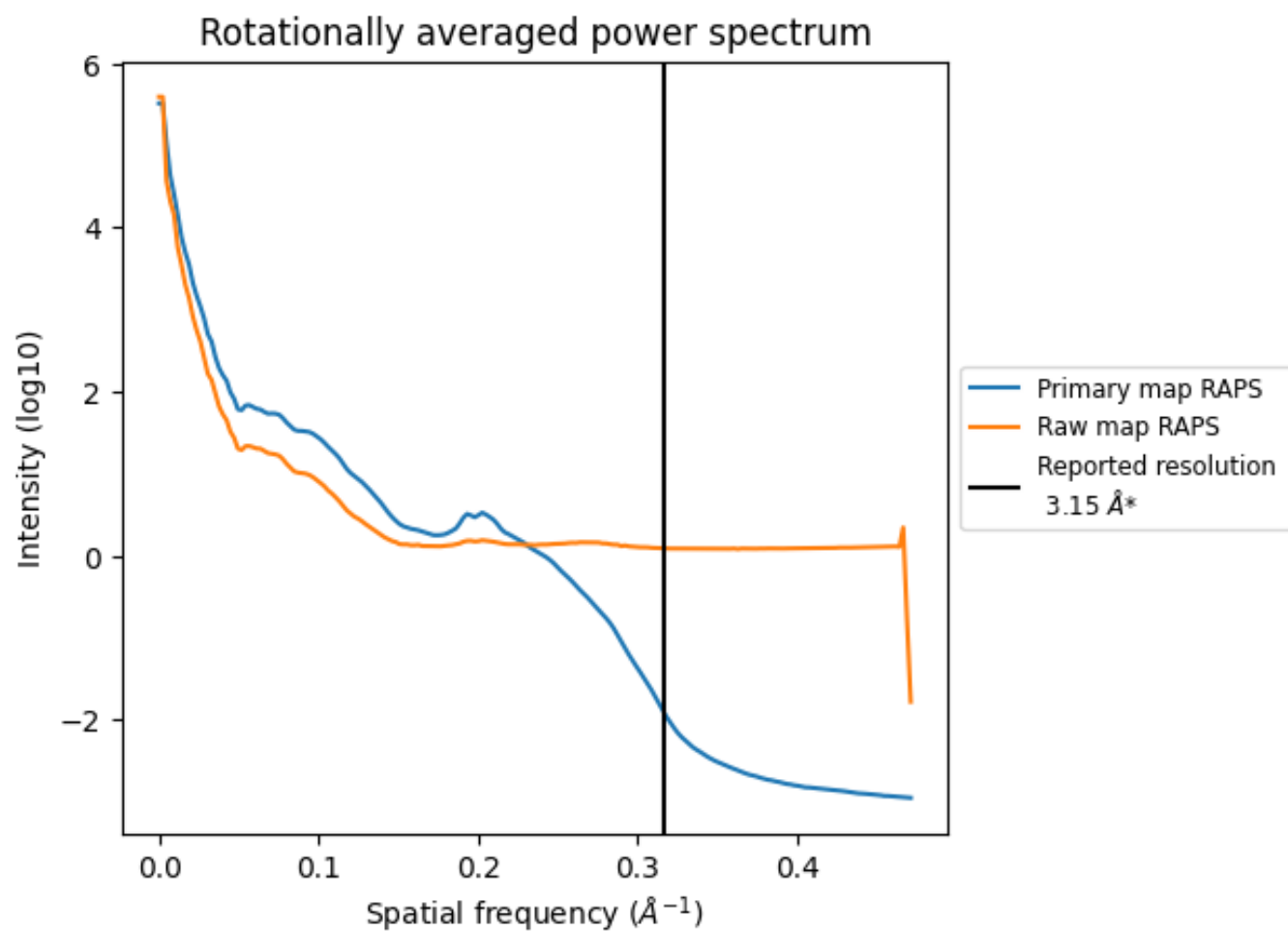
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 901 nm³; this corresponds to an approximate mass of 814 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 ⓘ

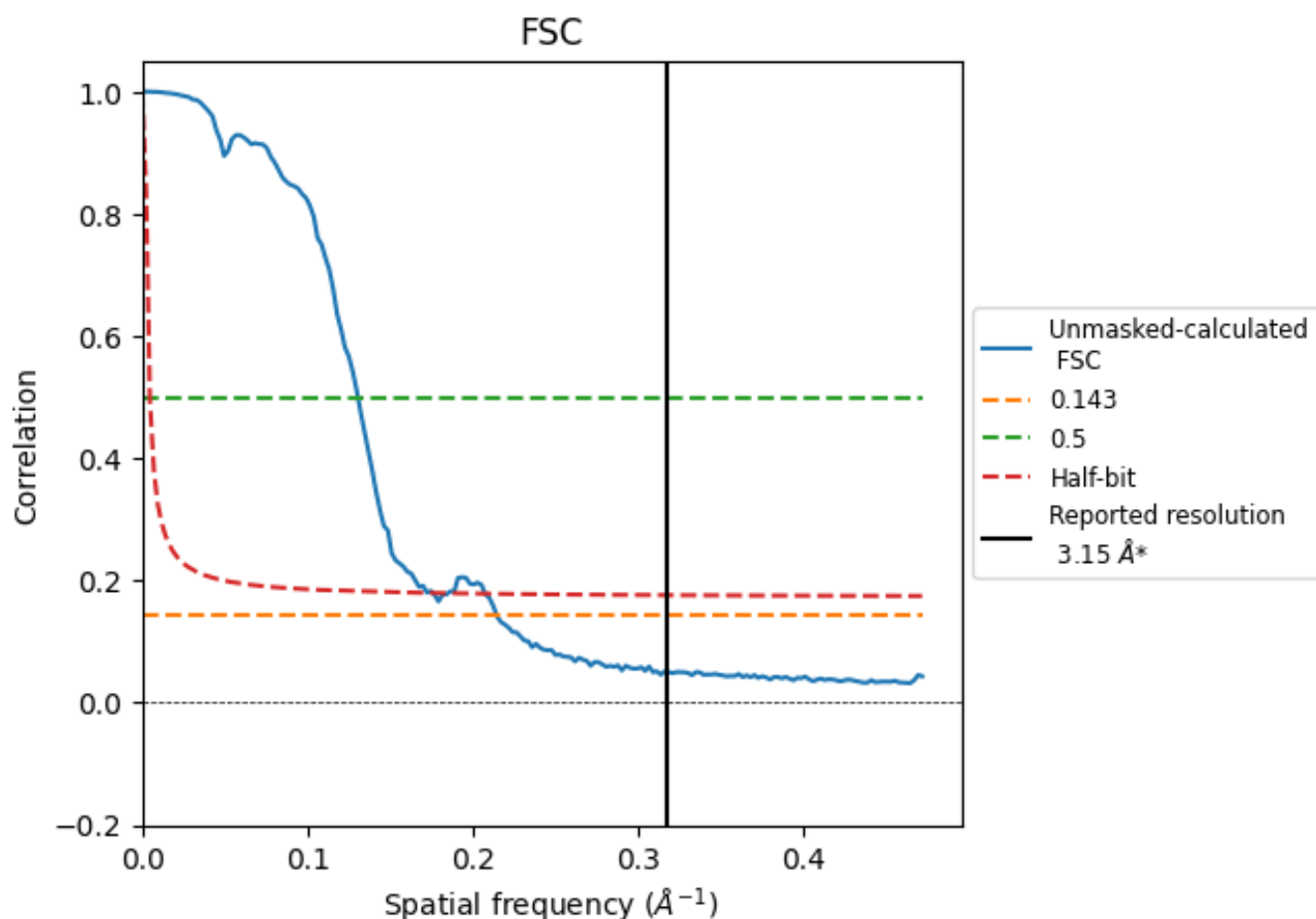


*Reported resolution corresponds to spatial frequency of $0.317 \text{ \AA}^{-1}$

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 $0.317 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

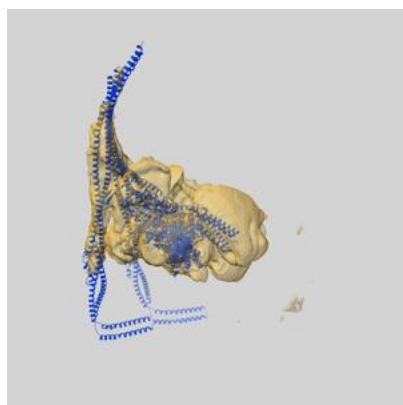
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.67	7.66	5.69

*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 4.67 differs from the reported value 3.15 by more than 10 %

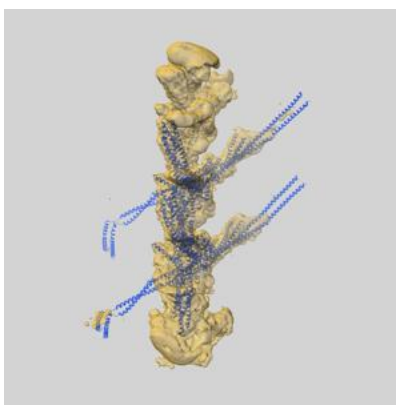
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18246 and PDB model 8Q84. Per-residue inclusion information can be found in section [3](#) on page [7](#).

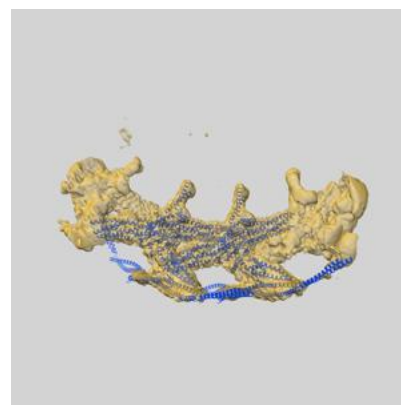
9.1 Map-model overlay [i](#)



X



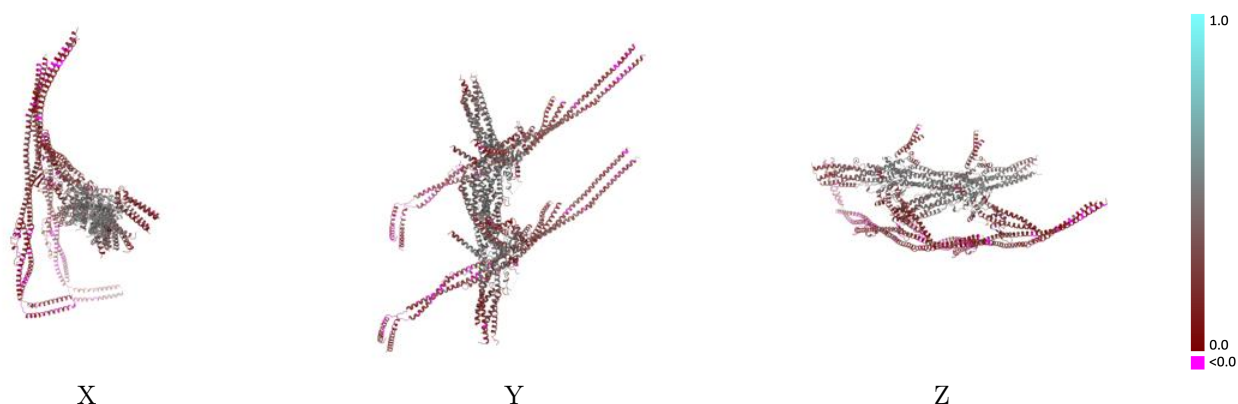
Y



Z

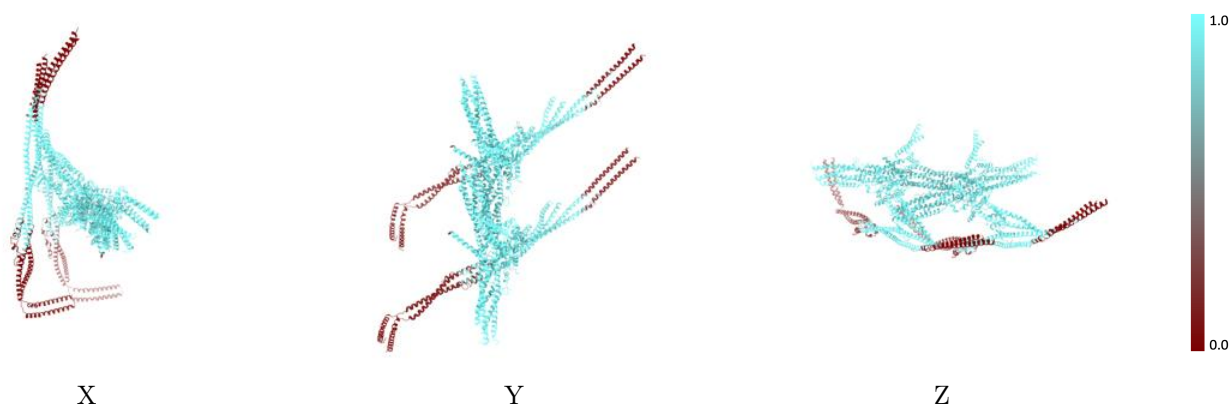
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



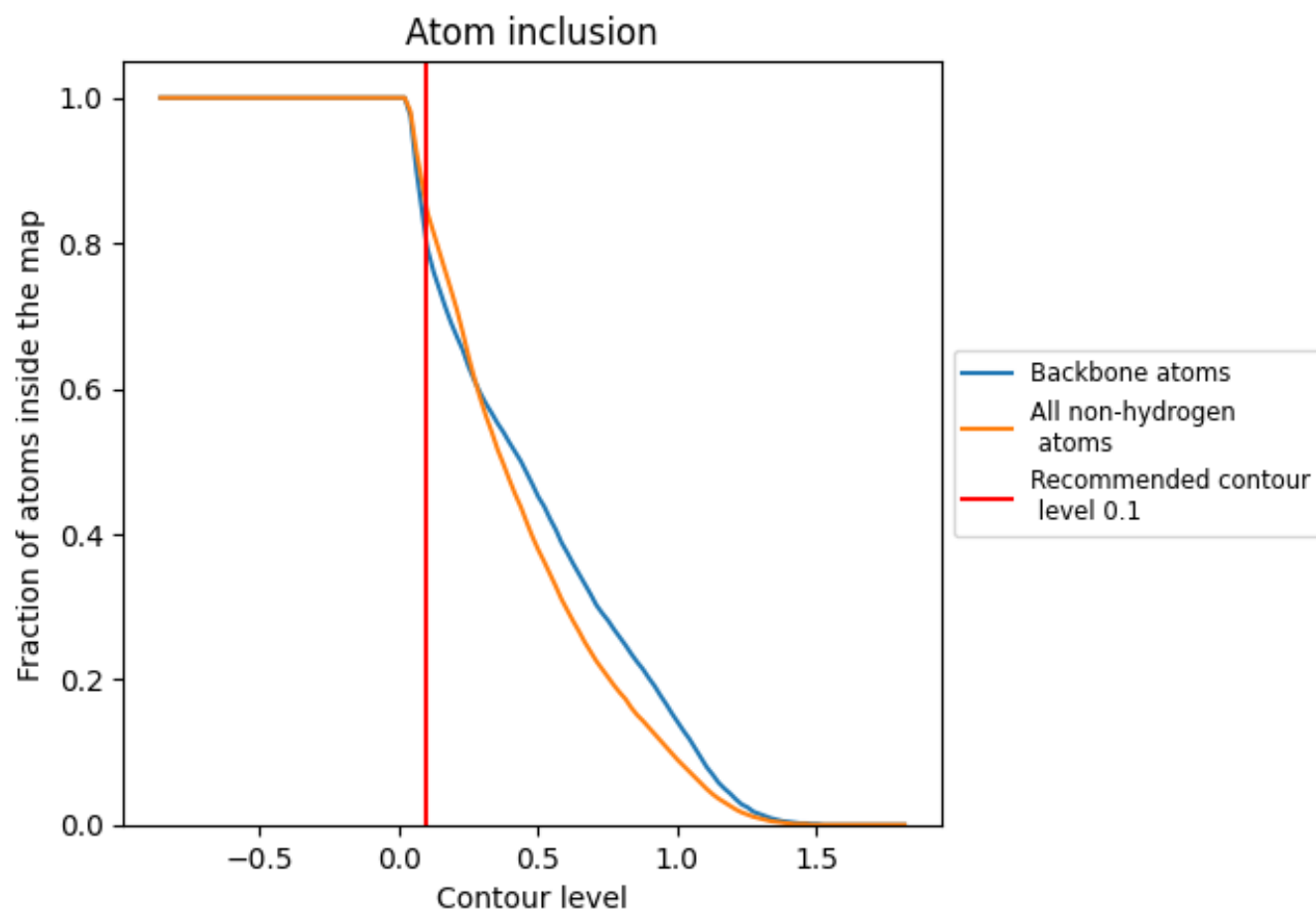
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 85% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8480	 0.2940
A	 0.4160	 0.1260
B	 0.4420	 0.1410
F	 0.3840	 0.1320
G	 0.4140	 0.1540
I	 0.9910	 0.3500
J	 0.9980	 0.3260
K	 0.9890	 0.4110
L	 0.9960	 0.4130
M	 0.9970	 0.4540
N	 0.9760	 0.3380
O	 0.9790	 0.2890
P	 1.0000	 0.4330
Q	 1.0000	 0.4430
R	 0.9940	 0.3240
U	 0.9960	 0.3210
V	 0.9950	 0.2900
W	 0.9950	 0.4120
X	 0.9740	 0.2880
Y	 1.0000	 0.4470
Z	 0.9800	 0.2990
a	 0.9880	 0.2590
b	 0.9890	 0.4140
c	 0.9960	 0.4640
d	 0.9940	 0.2970
e	 1.0000	 0.4850

