



Full wwPDB EM Validation Report ⓘ

Dec 17, 2024 – 04:39 pm GMT

PDB ID : 9ESI
EMDB ID : EMD-19942
Title : Structure of a B-state intermediate committed to discard (Bd-II state)
Authors : Soni, K.; Wild, K.; Sinning, I.
Deposited on : 2024-03-26
Resolution : 3.10 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

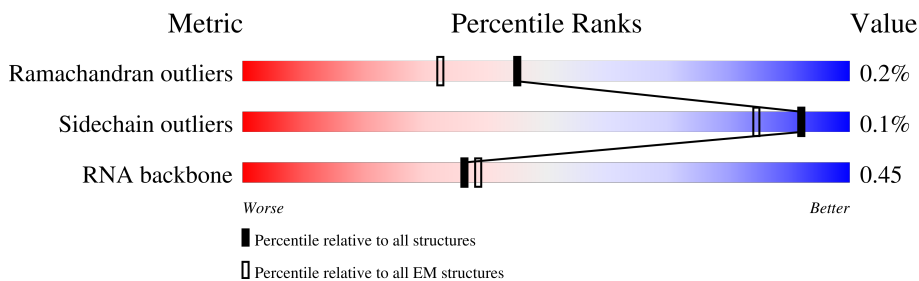
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	e	384	
2	p	299	
3	2	186	
4	5	120	
5	A	2363	
6	B	984	
7	C	340	
8	D	97	

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Mol	Chain	Length	Quality of chain
9	E	147	66% 34%
10	F	117	69% 31%
11	G	115	88% 11%
12	H	84	95% 5%
13	I	78	94% 6%
14	J	77	94% 5%
15	K	473	83% 17%
16	L	557	7% 44% 56%
17	M	354	31% 66% 34%
18	N	1284	100% 100%
19	O	146	99%
20	P	388	8% 70% 30%
21	Q	265	33% 66%
22	R	674	43% 89% 11%
23	S	488	27% 73%
23	T	488	22% 27% 73%
23	U	488	80% 88% 12%
23	V	488	26% 27% 73%
24	W	757	29% 65% 34%
25	X	790	68% 83% 17%
26	Y	229	36% 42% 57%
27	Z	187	48% 82% 17%
28	a	558	9% 27% 73%
29	b	293	24% 35% 65%
30	c	887	23% 77%

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Mol	Chain	Length	Quality of chain
31	d	155	<p>5% 99%</p>
32	m	797	<p>55% 58% 42%</p>
33	n	361	<p>8% 8% 92%</p>
34	y	534	<p>17% 37% 63%</p>
35	z	647	<p>65% 96%</p>
36	r	346	<p>14% 19% 81%</p>
37	q	56	<p>61% 100%</p>
38	6	99	<p>35% 45% 47% 7%</p>
39	1	29	<p>48% 34% 66%</p>
40	f	22	<p>68% 100%</p>

2 Entry composition [i](#)

There are 45 unique types of molecules in this entry. The entry contains 98220 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 Stress response protein bis1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	e	166	1329	838	221	268	2	0	0

- Molecule 2 is a protein called Protein saf4.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	p	60	487	304	89	94	0	0

- Molecule 3 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	2	24	500	224	79	173	24	0	0

- Molecule 4 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	5	102	2149	963	358	726	102	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1986	16424	10532	2887	2938	67	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	918	7298	4650	1251	1362	35	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	301	2328	1460	415	442	11	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	96	760	470	147	136	7	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	97	726	462	129	130	5	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	81	638	407	109	118	4	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	102	819	516	150	149	4	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	80	652	422	113	115	2	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	73	574	373	95	104	2	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	391	Total	C	N	O	S	0	0
			3053	1925	551	563	14		

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	246	Total	C	N	O	S	0	0
			1954	1221	364	363	6		

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	234	Total	C	N	O	S	0	0
			1818	1131	329	343	15		

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	1284	Total	C	N	O	S	0	0
			10461	6715	1732	1969	45		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	271	Total	C	N	O	S	0	0
			2178	1354	397	416	11		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	603	Total	C	N	O	S	0	0
			5108	3280	892	913	23		

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	132	Total	C	N	O	S	0	0
			1055	664	181	207	3		
23	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		
23	U	430	Total	C	N	O	S	0	0
			2870	1806	492	563	9		
23	V	131	Total	C	N	O	S	0	0
			1044	655	180	206	3		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	498	Total	C	N	O	S	0	0
			4126	2577	750	788	11		

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	654	Total	C	N	O	S	0	0
			5467	3534	918	996	19		

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	Y	98	Total	C	N	O	0	0
			845	522	157	166		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	155	1232	766	220	243	3	0	0

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	152	1035	644	185	205	1	0	0

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	104	822	503	148	169	2	0	0

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	204	1678	1071	280	315	12	0	0

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppl1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	154	1179	750	202	223	4	0	0

- Molecule 32 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	m	461	3813	2488	616	693	16	0	0

- Molecule 33 is a protein called Uncharacterized protein C17A2.08c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	n	30	248	153	44	50	1	0	0

- Molecule 34 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	y	200	Total	C	N	O	S	0	0
			1606	1000	279	323	4		

- Molecule 35 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	z	626	Total	C	N	O	S	0	0
			4980	3193	835	933	19		

- Molecule 36 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	r	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 37 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	q	56	Total	C	N	O	0	0
			295	182	57	56		

- Molecule 38 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	6	92	Total	C	N	O	P	0	0
			1970	882	365	631	92		

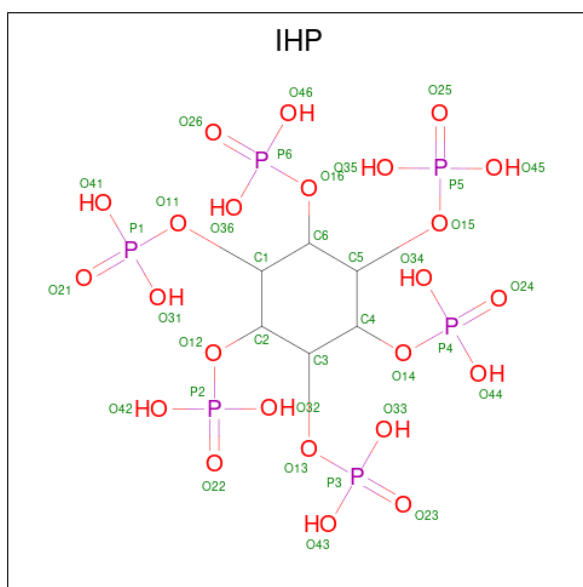
- Molecule 39 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	29	Total	C	N	O	P	0	0
			605	272	91	213	29		

- Molecule 40 is a protein called UNK3.

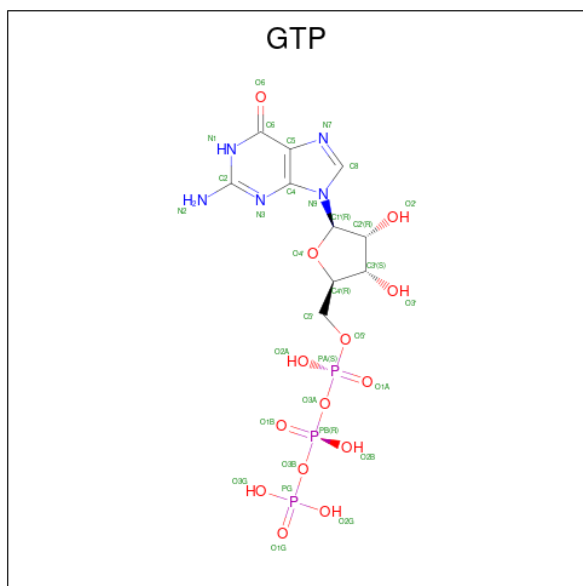
Mol	Chain	Residues	Atoms				AltConf	Trace
40	f	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C₆H₁₈O₂₄P₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
41	A	1	36	6	24	6	0

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
42	B	1	32	10	5	14	3	0

- Molecule 43 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

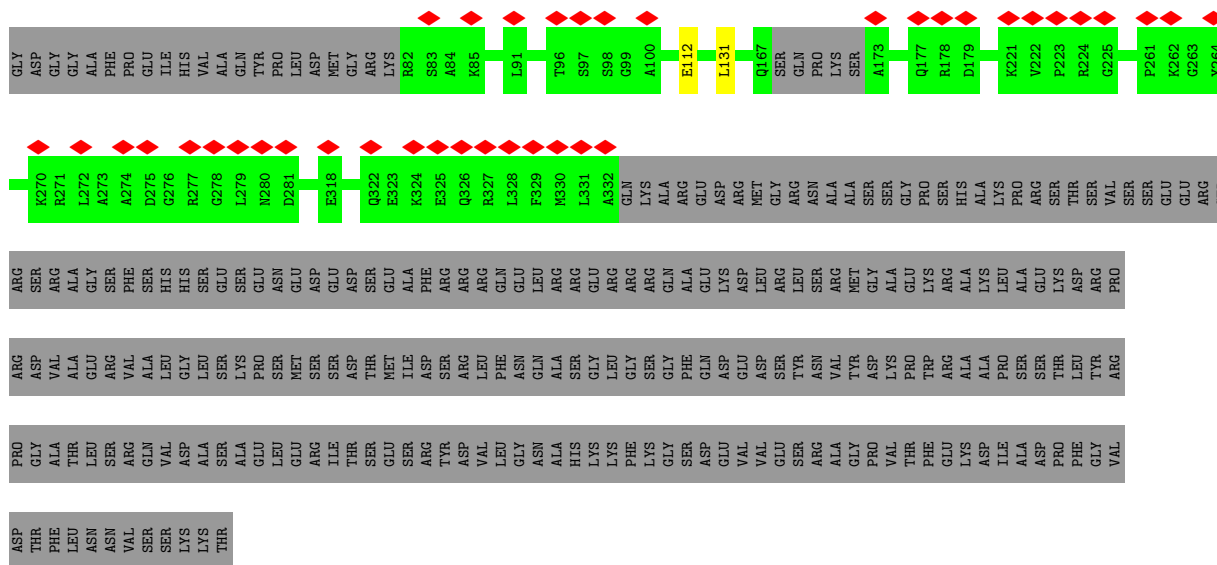
Mol	Chain	Residues	Atoms	AltConf
43	B	1	Total Mg 1 1	0
43	6	3	Total Mg 3 3	0

- Molecule 44 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
44	M	2	Total Zn 2 2	0
44	O	3	Total Zn 3 3	0
44	P	1	Total Zn 1 1	0

- Molecule 45 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
45	6	1	Total K 1 1	0



• Molecule 17: Pre-mRNA-splicing factor *lfw5*



• Molecule 18: Pre-mRNA-splicing factor *lfw11*



T901	T902	N903	K904	D905	N906	F907	F908	D909	Y910	A911	T912	K913	L914	Y915	G916	E917	L918	E919	Y920	M921	F922	K923	Q924	L925	E926	E927	I928	R929	P930	F931	O932	L933	L934	R935	Y936	F937	E938	D939	Q940	E941	L942	M943	A944	L945	C946	Q947	Q948	S949	R950	F951	O952	G953	C954	T955	Y956	F957	S958	L959	S960	
Y121	Y122	M123	I124	Q125	F126	I127	T128	L129	C130	F131	Q132	F133	L134	N135	I136	E137	K138	L139	R140	K141	L142	V143	Y144	Q145	L146	T147	M148	I149	S150	I151	L152	M153	S154	L155	D156	M157	L158	D159	K160	V161	K162	Y163	L164	L165	L166	D167	S168	S169	L170	L171	T172	K173	A174	F175	D176	S177	Y178	K179	E180	
K181	R182	P183	S184	I185	V186	E187	K188	F189	P190	L191	H192	M193	L194	L195	S196	R197	V198	I199	H200	S201	L202	L203	I204	K205	S206	I207	S208	Y209	A210	Q211	T212	E213	K214	Q215	E216	A217	K218	V219	T220	P221	L222	L223	A224	I225	I226	N227	M228	S229	E230	V231	L232	L233	S234	A235	F236	P237	T238	R239	R240	
F241	A242	H243	P244	V245	I246	E247	D248	S249	C250	F251	Y252	T253	A254	L255	R256	M257	S258	L259	Y260	Y261	D262	S263	N264	E265	L266	F267	K268	K269	M270	T271	D272	D273	L274	N275	Y276	Z277	L278	K279	F280	P281	L282	D283	N284	L285	I286	G287	N288	E289	Y290	L291	K292	E293	Q294	K295	I296	R297	N298	D299	E300	
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Q421	M422	T423	A424	I425	Q426	Y427	L428	S429	L430	S431	F432	F433	M434	R435	Q436	S437	S438	K439	A440	Y441	K442	K443	L444	L445	L446	R447	S448	L449	Y450	A451	E452	L453	L454	M455	F456	S457	E458	Q459	Y460	R461	L462	G463	S464	I465	K466	M467	A468	T469	L470	M471	T472	T473	K474	D475	M476	F477	F478	S479	L480	
M481	M482	F483	K484	V485	L486	S487	V488	A489	P490	P491	Q492	L493	G494	Q495	V496	L497	P498	Q499	F500	V501	K502	C503	Q504	M505	G506	L507	S508	R509	P510	G511	P512	F513	H514	S515	A516	L517	R518	D519	L520	K521	N522	S523	I524	K525	S526	P527	F528	L529	C530	L531	I532	Y533	L534	S535	K536	D537	M538	E539	E540	
K541	L542	L543	H544	G545	N546	A547	L548	D549	P550	L551	E552	G553	V554	T555	D556	F557	T558	L559	A560	T561	I562	C563	N564	D565	V566	V567	G568	M569	F570	Q571	S572	D573	M574	Q575	S576	D577	S578	D579	N580	K581	S582	L583	N584	V585	S586	L587	S588	P589	F590	C591	Y592	H593	S594	L595	A596	G597	L598	G599	E600	
Y601	R602	P603	K604	Q605	L606	K607	F608	N609	F610	A611	L612	V613	L614	S615	P616	E617	A618	N619	K620	Y621	P622	L623	D624	L625	N626	L627	L628	V629	S630	L631	L632	N633	R634	A635	K636	E637	F638	P639	K640	M641	F642	E643	D644	L645	L646	L647	G648	F649	G650	T651	P652	D653	L654	C655	A656	F657	P658	N659	A660	
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S721	N722	R723	L724	T725	V726	Y727	N728	D729	K730	Q731	L732	E733	S734	I735	L736	R737	G738	S739	Q740	P741	L742	L743	T744	M745	V746	M747	G748	P749	L750	R751	C752	G753	K754	H755	L756	V757	L758	C759	K760	L761	E762	E763	V764	L765	L766	D767	T768	S769	P770	N771	D772	R773	T774	V775	V776	L777	S778	D779	S780	
M781	F782	S783	M784	N785	T786	L787	F788	T789	L790	L791	E792	K793	A794	R795	C796	F797	H798	Q799	G800	H801	L802	L803	H804	L805	S806	D807	E808	R809	K810	D811	E812	T813	L814	E815	R816	L817	G818	T819	L820	S821	M822	M823	I824	S825	K826	L827	P828	G829	L830	L831	R832	E833	T834	G835	K836	L837	L838	A839	S840	
I841	Q842	A843	P844	G845	S846	H847	D848	A849	S850	P851	D852	T853	A854	L855	Y856	F857	R858	D859	A860	Y861	I862	K863	R864	L865	W866	E867	K868	R869	L870	T871	T872	G873	D874	D875	K876	D877	S878	R879	D880	A881	Y882	M883	R884	F885	P886	F887	H888	S889	R890	F891	C892	D893	K894	S895	K896	R897	P898	L899	E900	
T901	Y902	N903	K904	D905	N906	F907	F908	D909	Y910	A911	T912	K913	L914	Y915	G916	E917	L918	E919	Y920	M921	F922	K923	Q924	L925	E926	E927	I928	R929	P930	F931	O932	L933	L934	R935	Y936	F937	E938	D939	Q940	E941	L942	M943	A944	L945	C946	Q947	Q948	S949	R950	F951	O952	G953	C954	T955	Y956	F957	S958	L959	S960	

TS961	R962	L963	G964	T965	L966	R967	E968	R969	G970	F971	C972	F973	N974	N975	L976	R977	N978	R979	N980	S981	Q982	N983	L984	S985	S986	S987	S988	R989	T990	S991	I992	L993	L994	S995	N996	C997	P998	T1000	G1001	F1002	D1003	L1004	L1005	V1006	L1007	L1008	G1009	N1010	Q1011	Y1012	L1013	T1014	S1015	G1016	N1017	Q1018	D1019	I1020	
N1021	N1022	T1023	S1024	N1025	G1026	S1027	F1028	L1029	K1030	R1031	L1032	R1033	Y1034	L1035	K1036	S1037	R1038	I1039	I1040	D1041	N1043	T1044	Q1045	Y1046	N1047	V1048	R1049	E1050	S1051	I1052	S1053	S1054	L1055	C1056	S1057	S1058	I1059	Y1060	P1061	L1062	D1063	L1064	K1065	T1066	V1067	D1068	S1069	N1070	P1071	N1072	K1073	R1074	L1075	D1076	Y1077	G1078	N1079	S1080	
G1081	F1082	A1083	H1084	E1085	V1086	Q1087	F1088	I1089	N1090	V1091	G1092	A1093	F1094	K1095	G1096	S1097	Q1098	E1099	T1100	E1101	V1103	S1104	G1105	V1106	K1107	Q1108	N1109	L1110	G1111	E1112	A1113	E1114	Y1115	A1116	V1117	A1118	L1119	F1120	Q1121	L1122	M1123	R1124	M1125	L1126	G1127	Y1128	P1129	T1130	M1131	E1132	L1133	V1134	I1135	C1136	L1137	L1138	Y1139	E1140	
S1141	Q1142	V1143	S1144	L1145	L1146	M1147	E1148	I1149	I1150	S1151	V1152	R1153	C1154	S1155	H1156	M1157	S1158	F1159	F1160	G1161	Q1162	P1163	A1164	F1165	V1166	G1167	T1168	V1169	E1170	K1171	L1172	P1173	S1174	D1175	K1176	V1177	V1178	M1179	F1180	V1181	I1182	F1183	T1184	M1185	T1186	E1187	S1188	K1189	E1190	A1191	S1192	D1193	H1194	W1195	M1196	F1197	K1198	T1199	F1200
Y1201	K1202	A1203	F1204	S1205	A1206	C1207	S1208	Y1209	G1210	L1211	Y1212	V1213	L1214	C1215	N1216	D1218	L1219	F1220	R1221	G1222	T1223	R1224	G1225	L1226	E1227	K1228	L1229	W1230	N1231	E1232	I1233	E1234	K1235	T1236	P1237	D1238	K1239	L1240	L1241	L1242	T1243	T1244	G1245	E1246	I1247	Y1248	P1249	S1250	S1251	H1252	K1253	I1254	G1255	S1256	S1257	V1258	E1259	T1260	
F1261	E1262	I1263	E1264	N1265	L1266	L1267	H1268	L1269	S1270	M1271	Y1272	V1273	V1274	E1275	M1276	T1277	K1278	L1279	R1280	L1281	N1282	T1283	M1284																																				

• Molecule 19: Pre-mRNA-splicing factor cwf14



MET	R3	K37	E110	D129	D146
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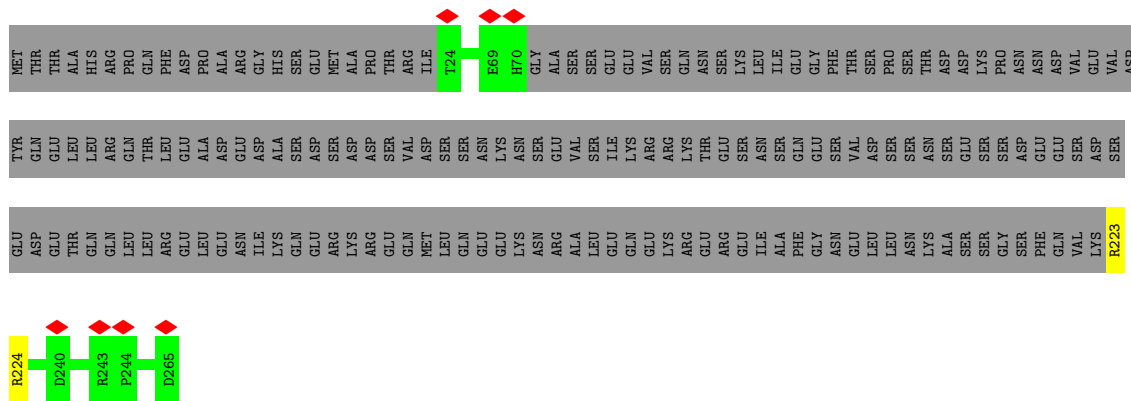
• Molecule 20: Pre-mRNA-splicing factor cwf2



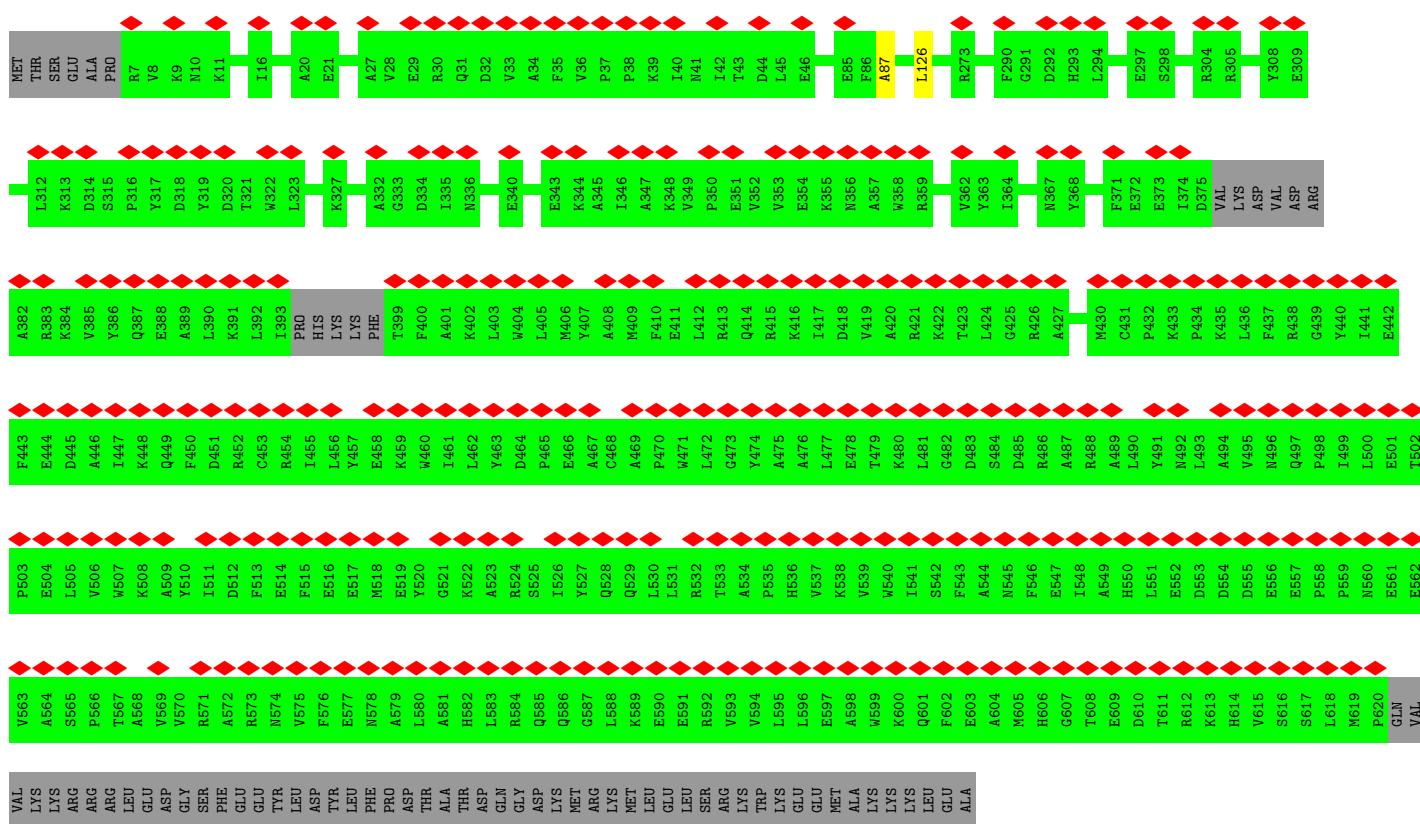
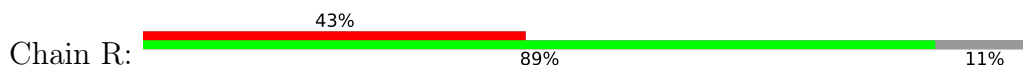
MET	SER	GLU	ASN	GLY	LEU	GLU	GLN	VAL	THR	VAL	GLU	GLU	LYS	ASN	ASP	VAL	THR	GLU	LYS	ILE	LEU	VAL	LEU	GLU	GLU	TYR	GLU	GLU	THR	PRO	ARG	VAL	LYS	ILE	VAL	VAL	ARG	ARG	LYS	K47	Q48	E55	E61	Q66	P67	M62	R83	Q84	D85				
P86	Q90	E94	D149	D161	G180	P183	T184	D185	E189	D200	N208	A213	E228	L235	ASP	HIS	ASP	LEU	GLU	C240	D249	R257	G288	K289	S290	G291	N292	R293	K294	R295	E300	PHE	GLY	LEU	LYS	GLY	TYR	R83	P308	N328	PHE	PRO											
ASN	LYS	SER	GLN	SER	GLU	GLU	GLY	SER	ASN	ASP	HIS	LYS	SER	VAL	THR	THR	GLU	SER	GLN	ASN	LYS	PHE	VAL	ASN	SER	GLN	ILE	LEU	SER	ASP	LEU	GLN	VAL	ALA	LYS	GLN	VAL	HIS	THR	ASN	GLN	SER	ALA	ALA	VAL	VAL	SER	TYR	ASP	SER	ASP	GLU	ASP

• Molecule 21: Pre-mRNA-splicing factor cwf15



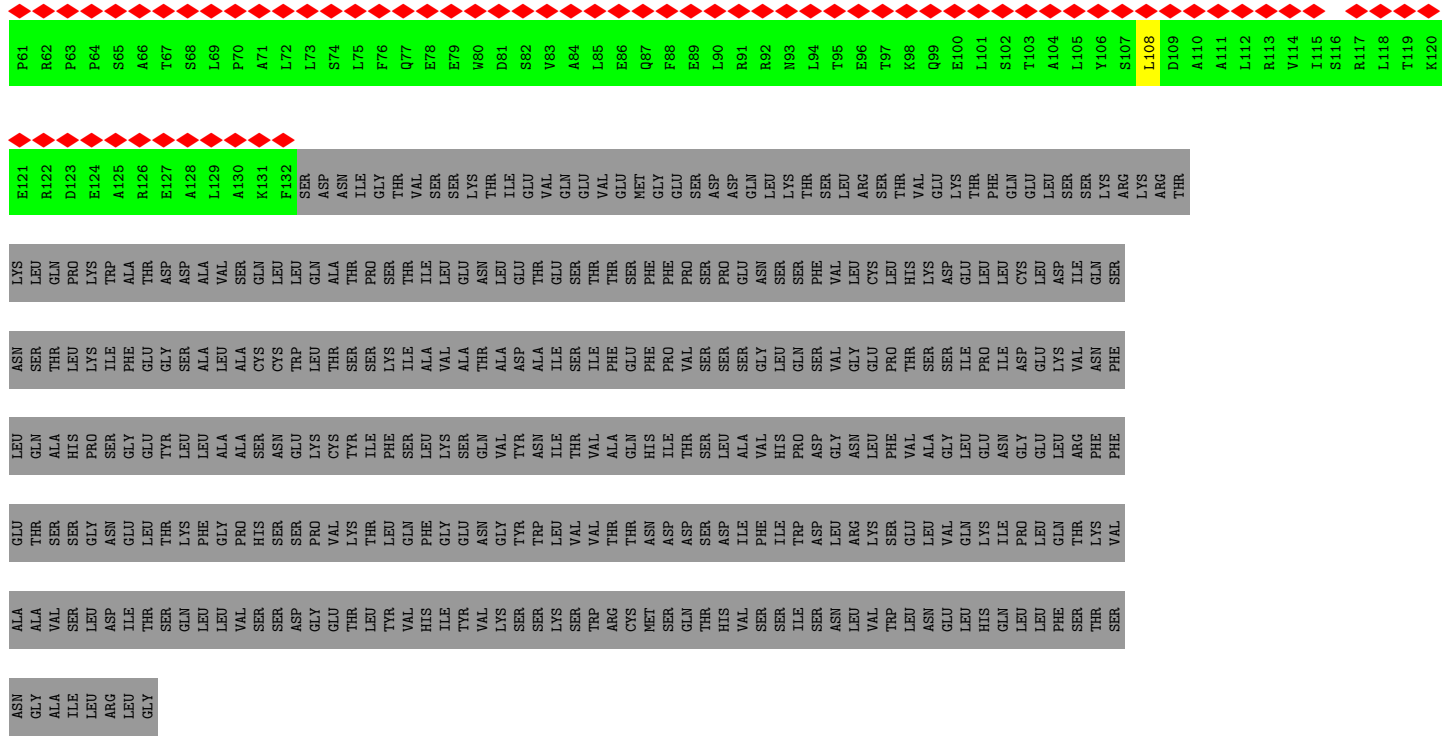


• Molecule 22: Pre-mRNA-splicing factor cwf4

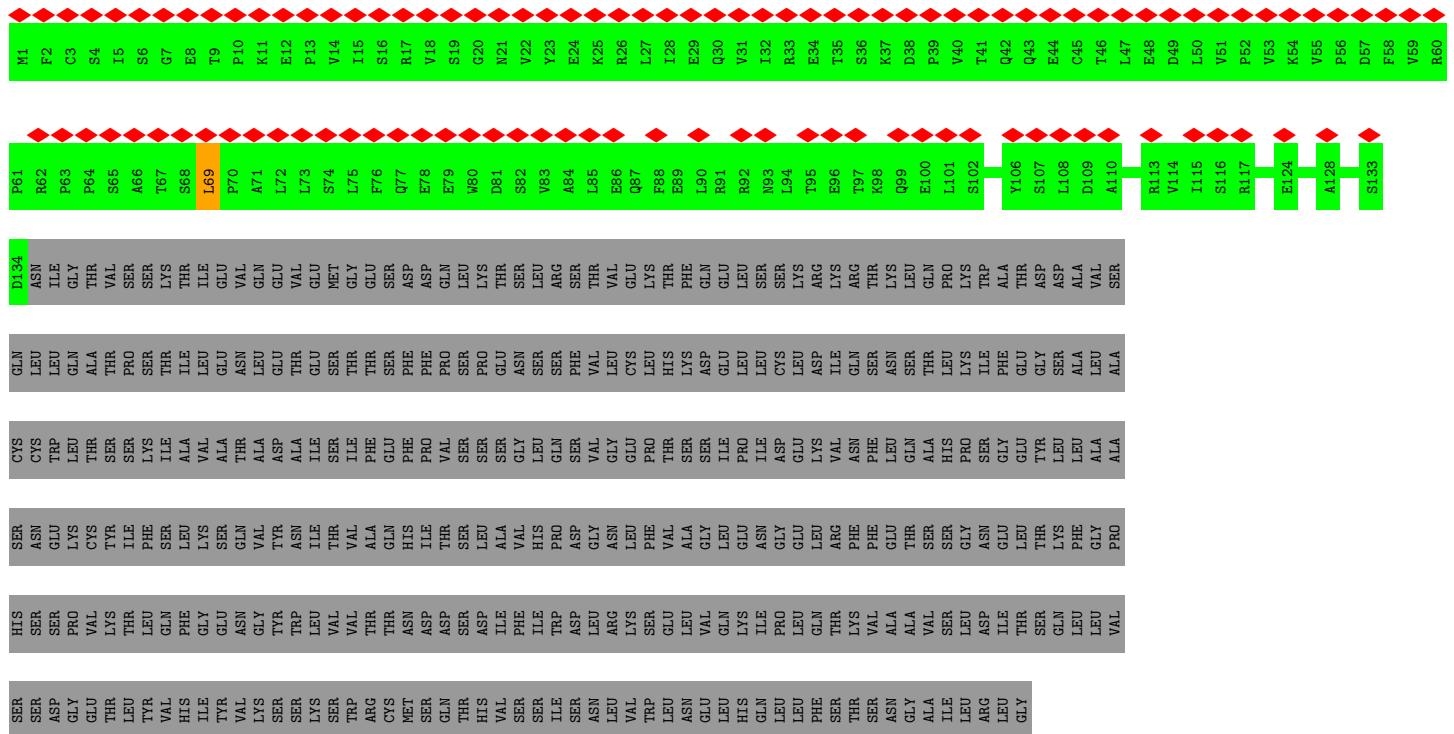


• Molecule 23: Pre-mRNA-processing factor 19



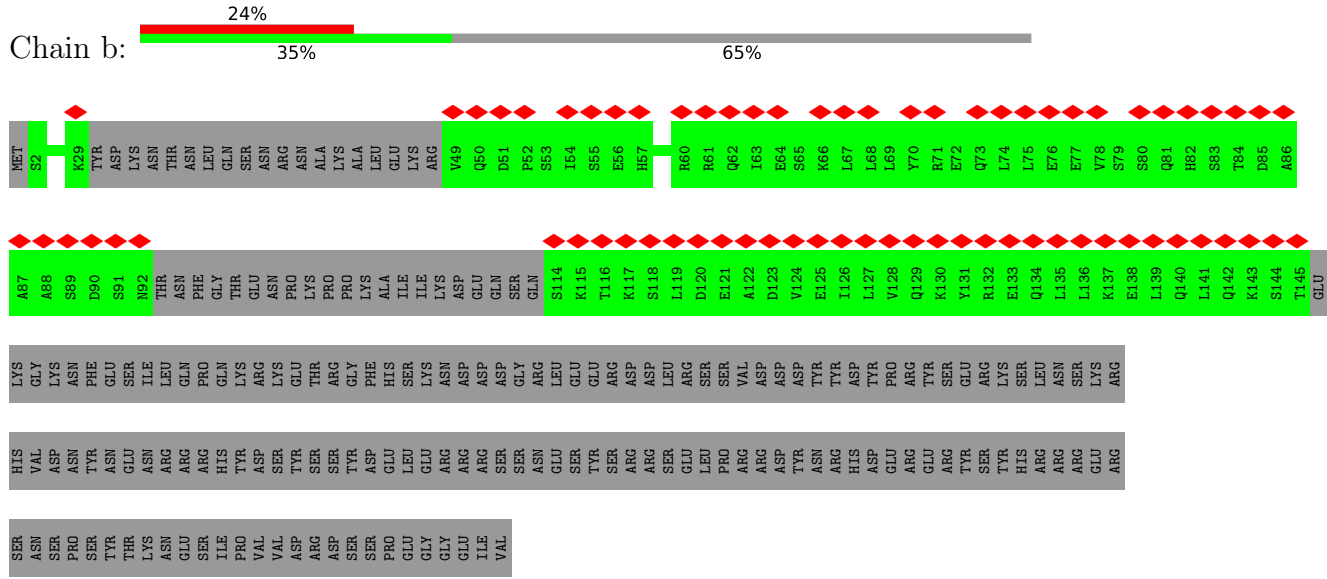


• Molecule 23: Pre-mRNA-processing factor 19

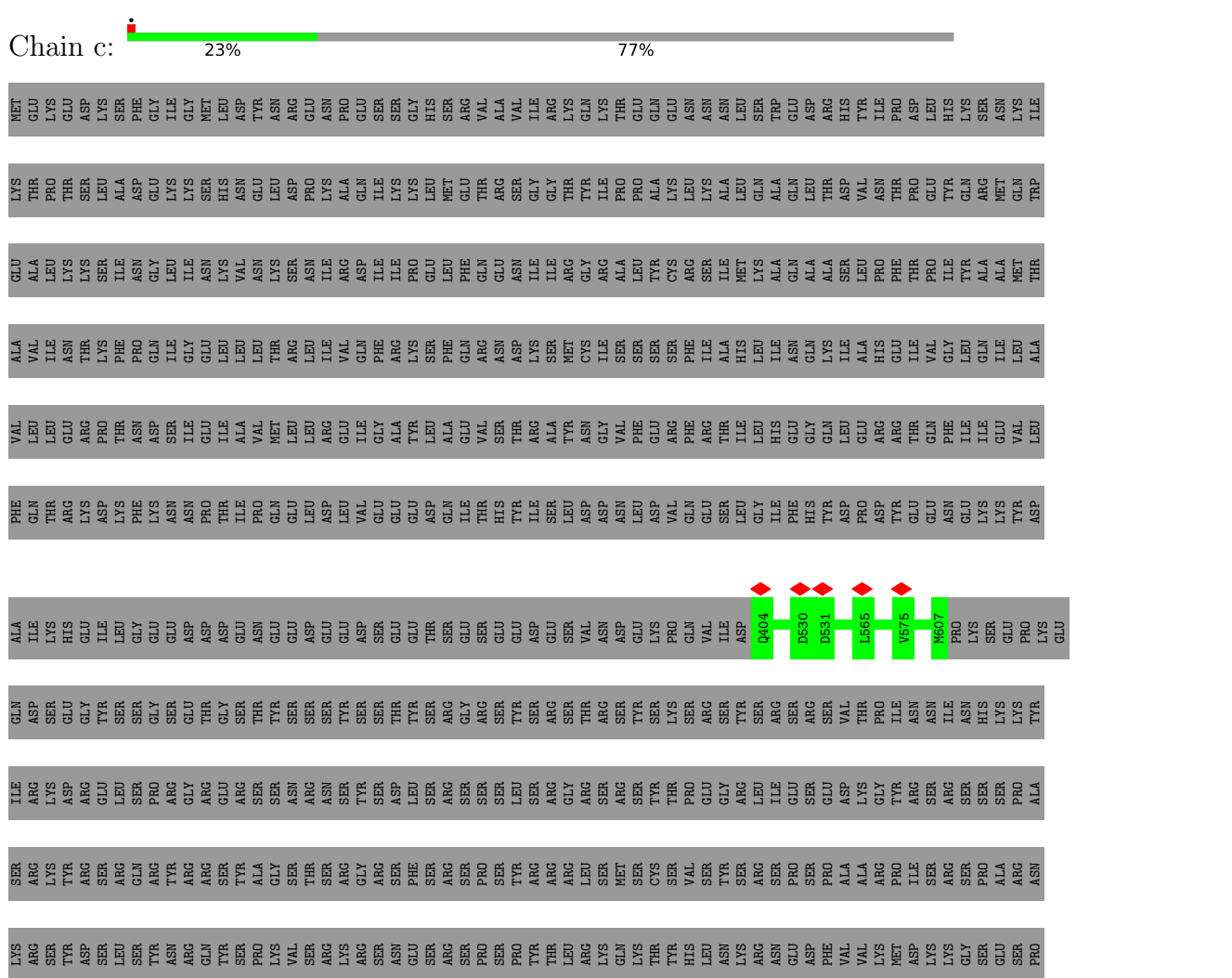


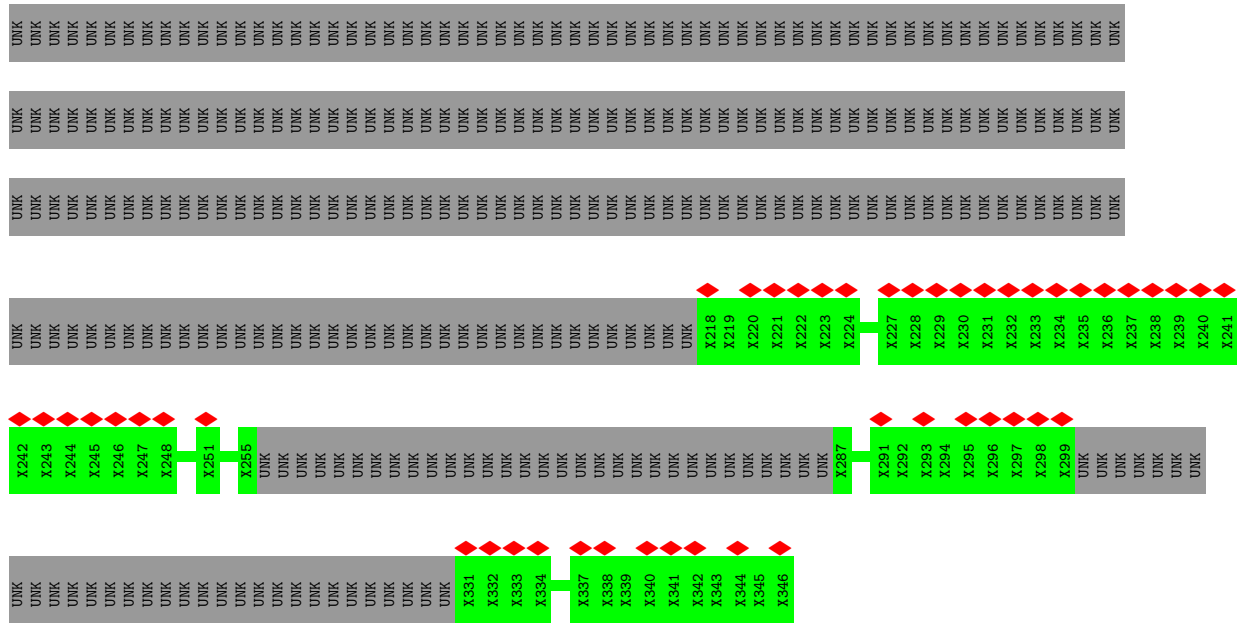
• Molecule 23: Pre-mRNA-processing factor 19

• Molecule 29: Pre-mRNA-splicing factor cwf21

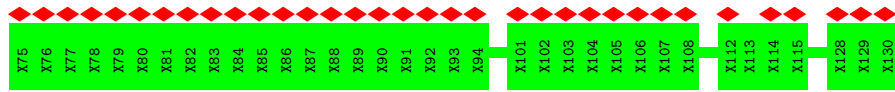


• Molecule 30: Pre-mRNA-splicing factor cwf22

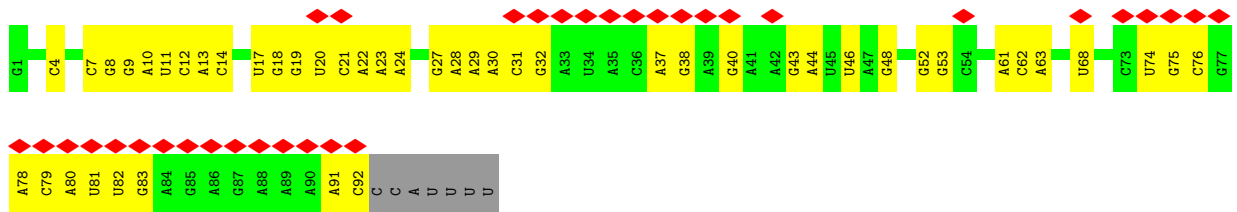
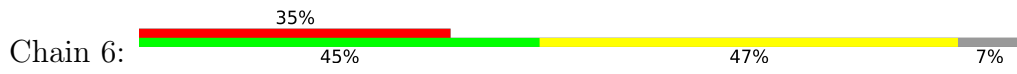




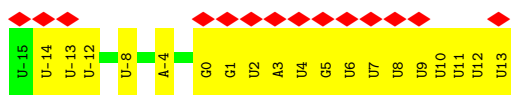
● Molecule 37: UNK2



● Molecule 38: U6snRNA

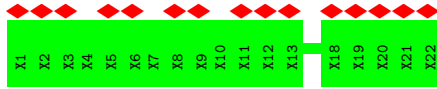


● Molecule 39: pre-mRNA



● Molecule 40: UNK3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	72631	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 ($e^-/\text{\AA}^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	37.664	Depositor
Minimum map value	-23.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.904	Depositor
Recommended contour level	3.2	Depositor
Map size (\AA)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, K, GTP, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	e	0.31	0/1354	0.50	0/1831
2	p	0.27	0/491	0.56	0/654
3	2	0.47	0/554	0.77	0/856
4	5	0.93	0/2397	0.81	4/3727 (0.1%)
5	A	0.54	0/16857	0.59	2/22848 (0.0%)
6	B	0.51	0/7459	0.60	1/10117 (0.0%)
7	C	0.36	0/2376	0.56	0/3216
8	D	0.46	0/772	0.62	0/1038
9	E	0.38	0/737	0.64	0/993
10	F	0.38	0/646	0.70	0/875
11	G	0.34	0/829	0.63	0/1111
12	H	0.35	0/662	0.59	0/894
13	I	0.37	0/585	0.66	0/794
14	J	0.48	0/578	0.61	0/774
15	K	0.55	0/3130	0.61	0/4251
16	L	0.41	0/1991	0.61	0/2684
17	M	0.35	0/1841	0.58	0/2468
18	N	0.26	0/10690	0.48	0/14463
19	O	0.51	0/1199	0.59	0/1609
20	P	0.39	0/2222	0.63	0/2991
21	Q	0.41	0/767	0.60	0/1028
22	R	0.36	0/5235	0.57	1/7067 (0.0%)
23	S	0.29	0/1072	0.65	1/1453 (0.1%)
23	T	0.29	0/1086	0.61	1/1472 (0.1%)
23	U	0.26	0/2897	0.52	0/3914
23	V	0.27	0/1060	0.61	0/1437
24	W	0.33	0/4187	0.60	1/5613 (0.0%)
25	X	0.29	0/5599	0.55	1/7566 (0.0%)
26	Y	0.27	0/857	0.55	0/1138
27	Z	0.29	0/1244	0.59	0/1667
28	a	0.39	0/1055	0.56	0/1443
29	b	0.36	0/829	0.52	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	c	0.51	0/1711	0.59	0/2312
31	d	0.32	0/1206	0.58	0/1636
32	m	0.26	0/3916	0.48	0/5300
33	n	0.22	0/247	0.45	0/327
34	y	0.36	0/1641	0.65	0/2211
35	z	0.30	0/5079	0.54	2/6875 (0.0%)
37	q	0.30	0/32	0.21	0/43
38	6	0.44	0/2207	0.78	0/3438
39	1	0.63	0/673	0.85	0/1043
All	All	0.42	0/99970	0.59	14/136288 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	Q	0	1
24	W	0	3
35	z	0	1
All	All	0	5

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	R	126	LEU	CB-CG-CD2	-8.60	96.39	111.00
4	5	32	C	C2-N1-C1'	8.29	127.92	118.80
4	5	32	C	N1-C2-O2	6.72	122.93	118.90
24	W	130	PRO	CA-N-CD	-6.48	102.43	111.50
4	5	32	C	C6-N1-C1'	-6.17	113.39	120.80
35	z	383	LEU	CA-CB-CG	5.97	129.04	115.30
25	X	637	LEU	CA-CB-CG	5.62	128.22	115.30
5	A	978	TRP	CB-CG-CD2	-5.60	119.32	126.60
4	5	32	C	N3-C2-O2	-5.57	118.00	121.90
23	T	69	LEU	CA-CB-CG	5.56	128.10	115.30
5	A	244	TYR	CB-CG-CD1	-5.51	117.70	121.00
35	z	62	LEU	CA-CB-CG	5.26	127.39	115.30
6	B	338	LEU	CA-CB-CG	5.03	126.87	115.30
23	S	108	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	Q	223	ARG	Sidechain
24	W	533	ARG	Sidechain
24	W	537	ARG	Sidechain
24	W	657	TYR	Peptide
35	z	326	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	e	156/384 (41%)	146 (94%)	10 (6%)	0	100	100
2	p	58/299 (19%)	55 (95%)	3 (5%)	0	100	100
5	A	1984/2363 (84%)	1893 (95%)	90 (4%)	1 (0%)	48	79
6	B	916/984 (93%)	867 (95%)	49 (5%)	0	100	100
7	C	297/340 (87%)	278 (94%)	19 (6%)	0	100	100
8	D	94/97 (97%)	93 (99%)	1 (1%)	0	100	100
9	E	91/147 (62%)	88 (97%)	3 (3%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	92 (94%)	6 (6%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	68 (96%)	3 (4%)	0	100	100
14	J	71/77 (92%)	68 (96%)	3 (4%)	0	100	100
15	K	389/473 (82%)	359 (92%)	30 (8%)	0	100	100
16	L	242/557 (43%)	226 (93%)	14 (6%)	2 (1%)	16	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	222/354 (63%)	215 (97%)	7 (3%)	0	100	100
18	N	1282/1284 (100%)	1261 (98%)	21 (2%)	0	100	100
19	O	142/146 (97%)	136 (96%)	6 (4%)	0	100	100
20	P	265/388 (68%)	247 (93%)	17 (6%)	1 (0%)	30	63
21	Q	86/265 (32%)	82 (95%)	3 (4%)	1 (1%)	11	38
22	R	597/674 (89%)	585 (98%)	11 (2%)	1 (0%)	44	74
23	S	130/488 (27%)	121 (93%)	9 (7%)	0	100	100
23	T	132/488 (27%)	127 (96%)	4 (3%)	1 (1%)	16	48
23	U	414/488 (85%)	399 (96%)	15 (4%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	488/757 (64%)	450 (92%)	33 (7%)	5 (1%)	13	42
25	X	642/790 (81%)	608 (95%)	33 (5%)	1 (0%)	44	74
26	Y	94/229 (41%)	89 (95%)	4 (4%)	1 (1%)	12	39
27	Z	151/187 (81%)	145 (96%)	5 (3%)	1 (1%)	19	51
28	a	150/558 (27%)	138 (92%)	12 (8%)	0	100	100
29	b	98/293 (33%)	92 (94%)	6 (6%)	0	100	100
30	c	202/887 (23%)	194 (96%)	8 (4%)	0	100	100
31	d	152/155 (98%)	138 (91%)	14 (9%)	0	100	100
32	m	455/797 (57%)	447 (98%)	7 (2%)	1 (0%)	44	74
33	n	28/361 (8%)	27 (96%)	1 (4%)	0	100	100
34	y	196/534 (37%)	168 (86%)	25 (13%)	3 (2%)	8	33
35	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	44	74
37	q	3/56 (5%)	3 (100%)	0	0	100	100
All	All	11306/17429 (65%)	10784 (95%)	502 (4%)	20 (0%)	45	74

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	Y	144	VAL
34	y	115	LYS
23	T	69	LEU
24	W	536	ILE
5	A	1115	ILE
16	L	131	LEU

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Mol	Chain	Res	Type
21	Q	224	ARG
20	P	90	GLN
22	R	87	ALA
24	W	538	PRO
27	Z	71	LYS
32	m	321	THR
35	z	437	ASP
24	W	221	TYR
16	L	112	GLU
25	X	83	ASN
24	W	537	ARG
24	W	530	VAL
34	y	127	ASP
34	y	28	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	e	149/346 (43%)	149 (100%)	0	100	100
2	p	56/274 (20%)	56 (100%)	0	100	100
5	A	1798/2138 (84%)	1796 (100%)	2 (0%)	92	97
6	B	821/881 (93%)	820 (100%)	1 (0%)	92	97
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	90 (99%)	1 (1%)	70	84
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100
14	J	63/67 (94%)	62 (98%)	1 (2%)	58	79
15	K	333/405 (82%)	333 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	L	211/477 (44%)	211 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1187 (100%)	1 (0%)	92	97
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	532 (100%)	0	100	100
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	222/443 (50%)	220 (99%)	2 (1%)	75	88
23	V	120/443 (27%)	120 (100%)	0	100	100
24	W	443/656 (68%)	443 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
26	Y	94/214 (44%)	93 (99%)	1 (1%)	70	84
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	78 (99%)	1 (1%)	65	82
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
32	m	425/719 (59%)	425 (100%)	0	100	100
33	n	28/335 (8%)	28 (100%)	0	100	100
34	y	173/478 (36%)	173 (100%)	0	100	100
35	z	564/585 (96%)	563 (100%)	1 (0%)	92	96
37	q	2/2 (100%)	2 (100%)	0	100	100
All	All	10038/15582 (64%)	10027 (100%)	11 (0%)	92	97

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

Mol	Chain	Res	Type
5	A	488	LYS
5	A	1244	ARG
6	B	583	ASN
11	G	74	MET
14	J	25	ARG

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Mol	Chain	Res	Type
18	N	505	MET
23	U	184	PRO
23	U	415	PRO
26	Y	142	ARG
28	a	106	ASN
35	z	358	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	e	204	HIS
1	e	219	GLN
5	A	256	ASN
5	A	1391	ASN
5	A	1490	GLN
5	A	1576	GLN
5	A	1607	GLN
5	A	1639	HIS
5	A	1752	GLN
6	B	371	GLN
6	B	821	GLN
7	C	213	HIS
9	E	81	GLN
10	F	64	ASN
12	H	82	GLN
16	L	191	GLN
16	L	301	GLN
16	L	322	GLN
17	M	88	GLN
17	M	120	GLN
17	M	134	GLN
20	P	224	GLN
20	P	268	ASN
22	R	225	GLN
23	S	21	ASN
23	U	342	HIS
23	V	99	GLN
27	Z	94	GLN
27	Z	108	ASN
27	Z	156	GLN
28	a	106	ASN
31	d	3	ASN

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Mol	Chain	Res	Type
31	d	101	GLN
31	d	116	HIS
34	y	117	ASN
34	y	208	ASN
35	z	108	GLN
35	z	384	ASN
35	z	415	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	22/186 (11%)	5 (22%)	0
38	6	91/99 (91%)	44 (48%)	7 (7%)
39	1	28/29 (96%)	19 (67%)	2 (7%)
4	5	101/120 (84%)	22 (21%)	2 (1%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

All (90) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	11	U
3	2	12	G
3	2	13	C
3	2	24	A
3	2	29	A
4	5	13	A
4	5	14	G
4	5	27	G
4	5	28	C
4	5	30	A
4	5	31	A
4	5	33	G
4	5	37	C
4	5	50	U
4	5	54	C
4	5	79	G
4	5	82	A
4	5	83	A
4	5	90	U
4	5	91	G
4	5	92	U

Continued on next page...

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Mol	Chain	Res	Type
4	5	98	U
4	5	99	U
4	5	102	G
4	5	103	U
4	5	105	A
4	5	108	U
38	6	4	C
38	6	7	C
38	6	8	G
38	6	9	G
38	6	10	A
38	6	11	U
38	6	12	C
38	6	14	C
38	6	18	G
38	6	19	G
38	6	20	U
38	6	21	C
38	6	22	A
38	6	23	A
38	6	24	A
38	6	27	G
38	6	28	A
38	6	29	A
38	6	30	A
38	6	31	C
38	6	32	G
38	6	38	G
38	6	40	G
38	6	43	G
38	6	44	A
38	6	46	U
38	6	48	G
38	6	52	G
38	6	53	G
38	6	61	A
38	6	62	C
38	6	63	A
38	6	68	U
38	6	74	U
38	6	75	G
38	6	76	C

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Mol	Chain	Res	Type
38	6	78	A
38	6	79	C
38	6	80	A
38	6	81	U
38	6	82	U
38	6	83	G
38	6	91	A
38	6	92	C
39	1	-14	U
39	1	-13	U
39	1	-12	U
39	1	-8	U
39	1	-4	A
39	1	0	G
39	1	1	G
39	1	2	U
39	1	3	A
39	1	4	U
39	1	5	G
39	1	6	U
39	1	7	U
39	1	8	U
39	1	9	U
39	1	10	U
39	1	11	U
39	1	12	U
39	1	13	U

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	5	27	G
4	5	49	U
38	6	13	A
38	6	17	U
38	6	29	A
38	6	30	A
38	6	37	A
38	6	52	G
38	6	74	U
39	1	0	G
39	1	1	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	GTP	B	1001	43	26,34,34	1.45	3 (11%)	32,54,54	1.75	8 (25%)
41	IHP	A	2401	-	36,36,36	1.54	13 (36%)	54,60,60	1.48	10 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
42	GTP	B	1001	43	-	0/18/38/38	0/3/3/3
41	IHP	A	2401	-	-	4/30/54/54	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	B	1001	GTP	C5-C6	-4.74	1.37	1.47
42	B	1001	GTP	C2'-C1'	-2.47	1.50	1.53
41	A	2401	IHP	P1-O31	-2.46	1.45	1.54
41	A	2401	IHP	P3-O33	-2.36	1.45	1.54
41	A	2401	IHP	P6-O46	-2.35	1.45	1.54
41	A	2401	IHP	P5-O45	-2.33	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	A	2401	IHP	P3-O43	-2.32	1.45	1.54
41	A	2401	IHP	P4-O34	-2.29	1.46	1.54
41	A	2401	IHP	P1-O11	2.29	1.63	1.59
42	B	1001	GTP	C5-C4	-2.26	1.37	1.43
41	A	2401	IHP	P6-O36	-2.24	1.46	1.54
41	A	2401	IHP	P1-O41	-2.22	1.46	1.54
41	A	2401	IHP	P5-O35	-2.21	1.46	1.54
41	A	2401	IHP	P4-O44	-2.21	1.46	1.54
41	A	2401	IHP	P2-O42	-2.20	1.46	1.54
41	A	2401	IHP	P2-O32	-2.13	1.46	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	B	1001	GTP	PB-O3B-PG	-5.21	114.95	132.83
42	B	1001	GTP	C5-C6-N1	3.71	120.51	113.95
42	B	1001	GTP	C2-N1-C6	-3.26	119.09	125.10
41	A	2401	IHP	C5-C6-C1	3.18	117.38	110.41
42	B	1001	GTP	PA-O3A-PB	-3.16	121.99	132.83
42	B	1001	GTP	C8-N7-C5	3.10	108.90	102.99
41	A	2401	IHP	O11-P1-O21	-2.87	98.32	109.39
41	A	2401	IHP	C6-C1-C2	2.82	116.58	110.41
41	A	2401	IHP	C6-C5-C4	2.62	116.14	110.41
41	A	2401	IHP	O41-P1-O31	2.61	117.60	107.64
42	B	1001	GTP	O6-C6-C5	-2.37	119.74	124.37
42	B	1001	GTP	O4'-C1'-C2'	-2.23	103.67	106.93
41	A	2401	IHP	C3-C2-C1	2.22	115.27	110.41
41	A	2401	IHP	O12-P2-O22	-2.14	101.13	109.39
42	B	1001	GTP	O3G-PG-O3B	2.06	111.55	104.64
41	A	2401	IHP	O44-P4-O34	2.03	115.40	107.64
41	A	2401	IHP	O42-P2-O32	2.02	115.37	107.64
41	A	2401	IHP	O41-P1-O21	2.02	118.59	110.68

There are no chirality outliers.

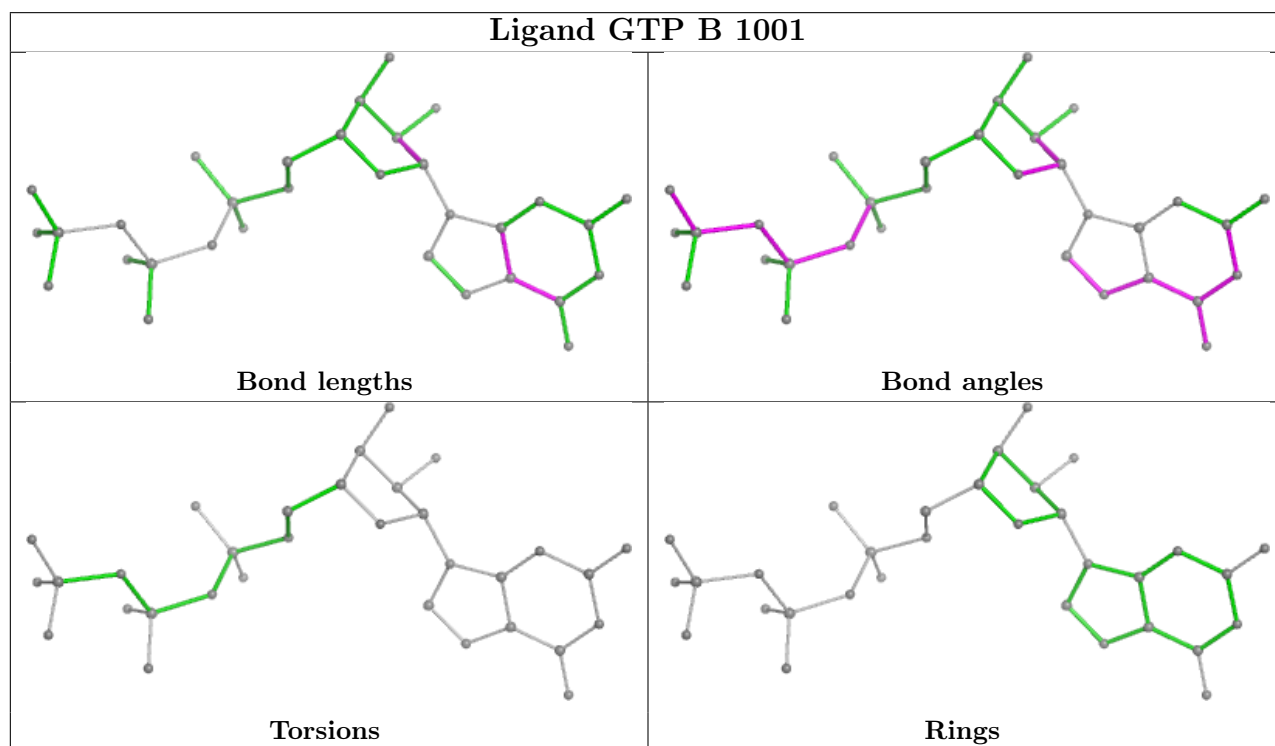
All (4) torsion outliers are listed below:

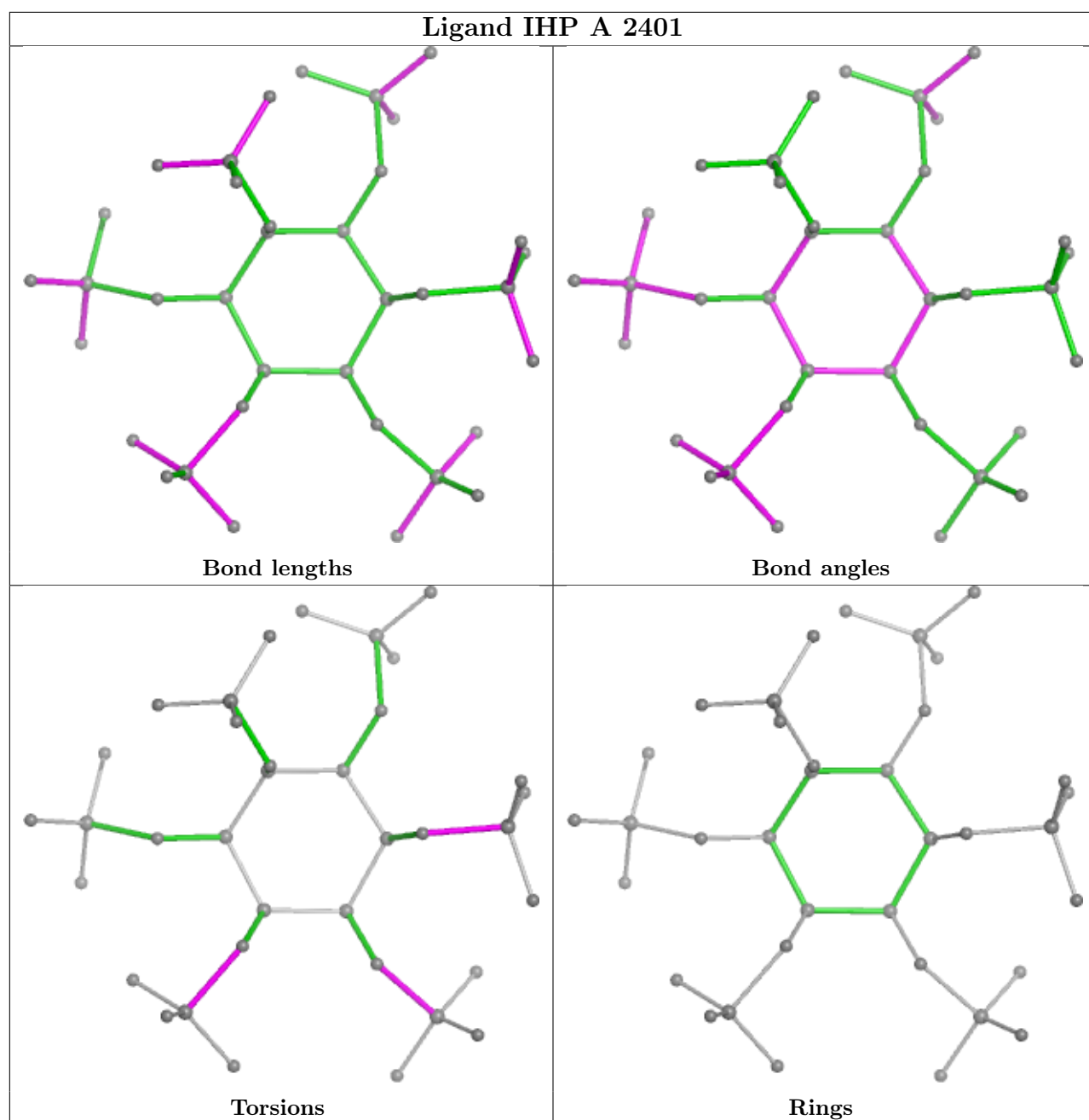
Mol	Chain	Res	Type	Atoms
41	A	2401	IHP	C6-O16-P6-O26
41	A	2401	IHP	C1-O11-P1-O41
41	A	2401	IHP	C6-O16-P6-O36
41	A	2401	IHP	C5-O15-P5-O35

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

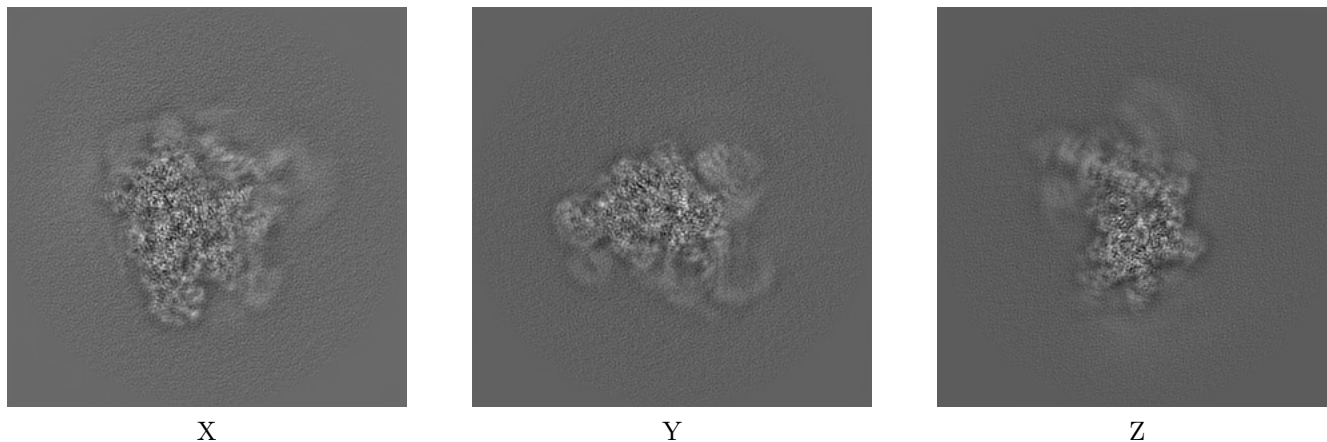
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19942. These allow visual inspection of the internal detail of the map and identification of artifacts.

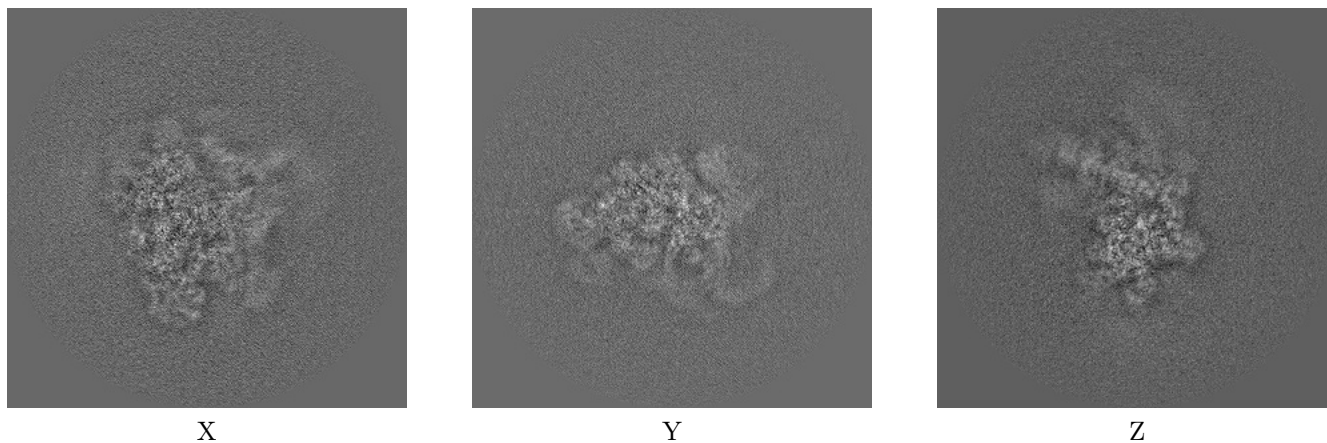
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



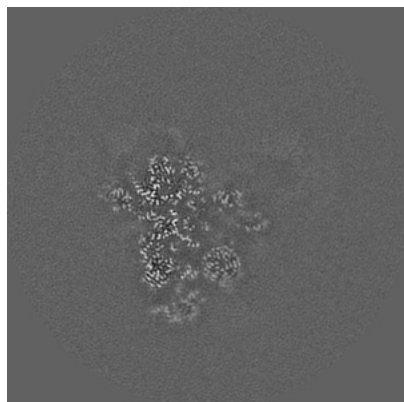
6.1.2 Raw map



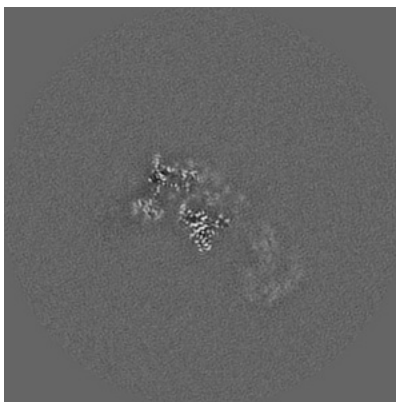
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

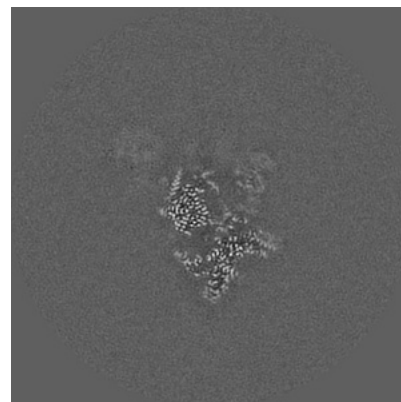
6.2.1 Primary map



X Index: 280

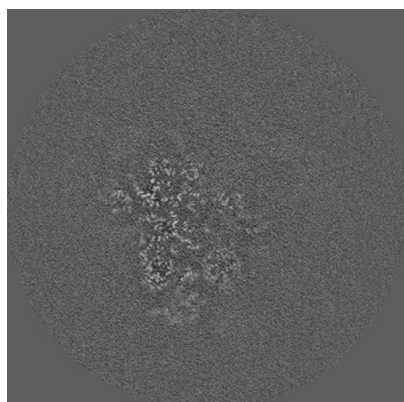


Y Index: 280

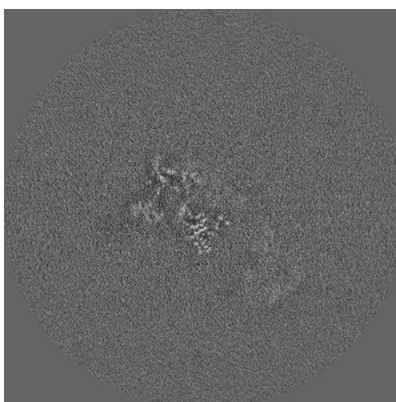


Z Index: 280

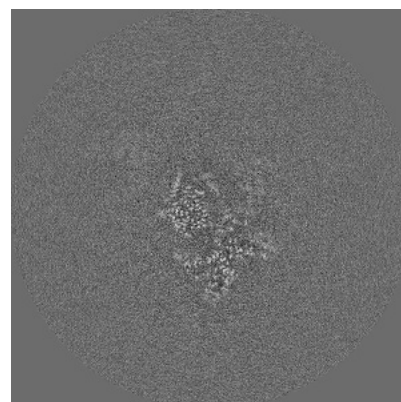
6.2.2 Raw map



X Index: 280



Y Index: 280

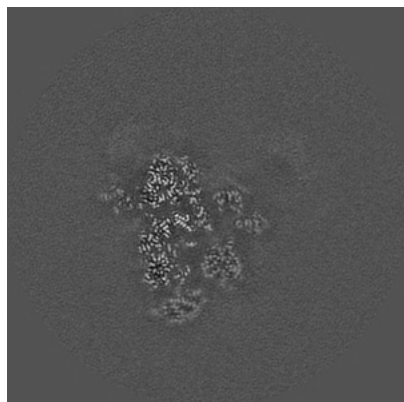


Z Index: 280

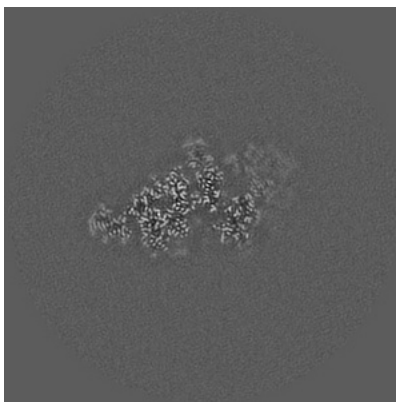
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

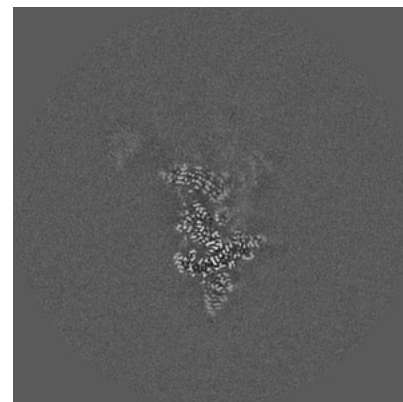
6.3.1 Primary map



X Index: 276

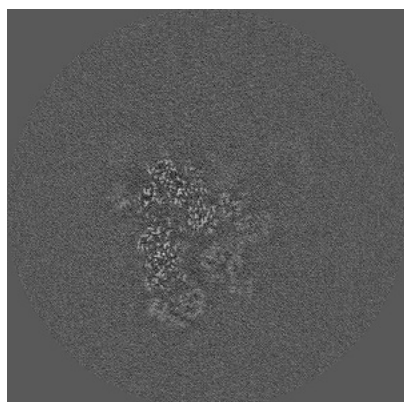


Y Index: 219

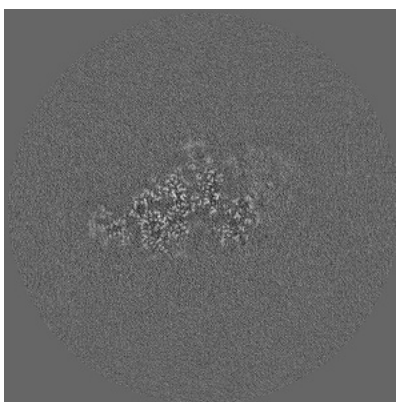


Z Index: 295

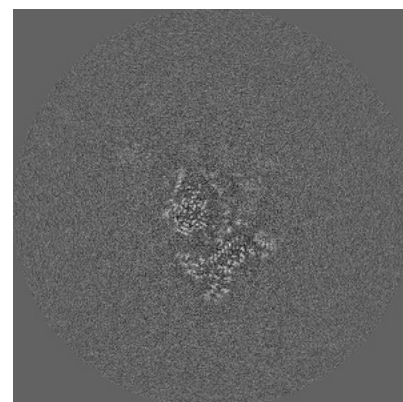
6.3.2 Raw map



X Index: 269



Y Index: 219

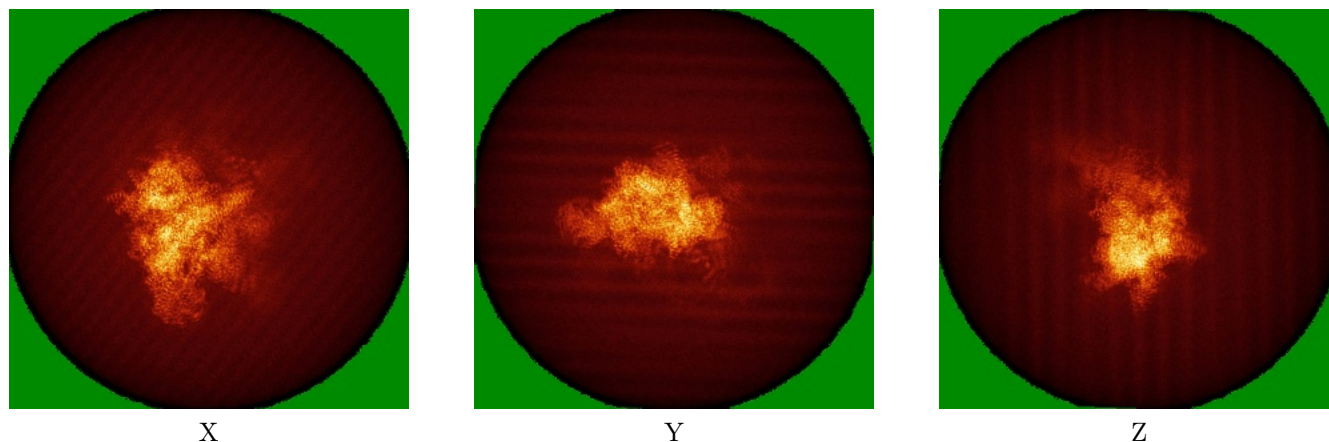


Z Index: 282

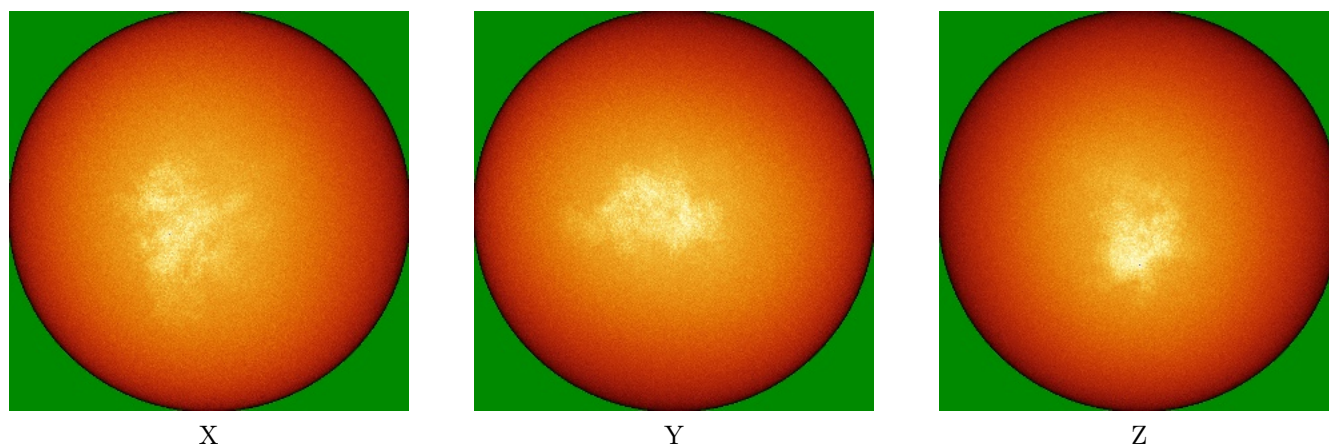
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



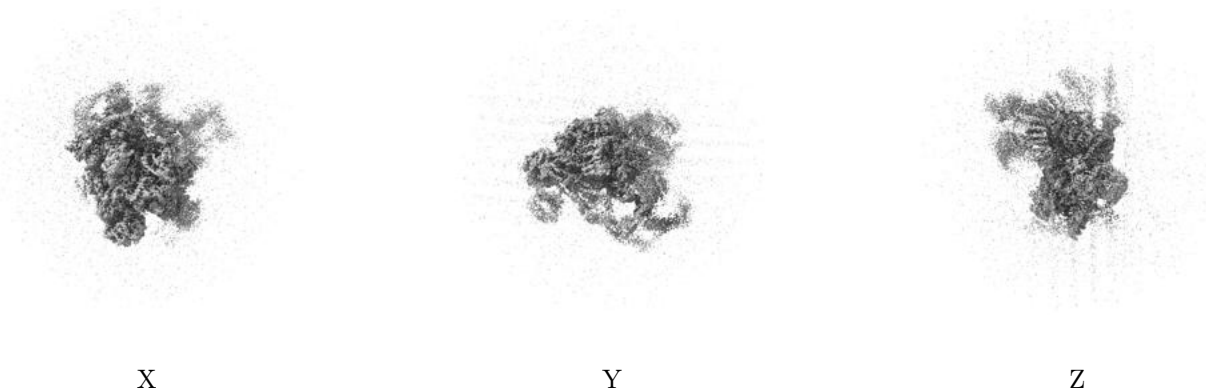
6.4.2 Raw map



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.

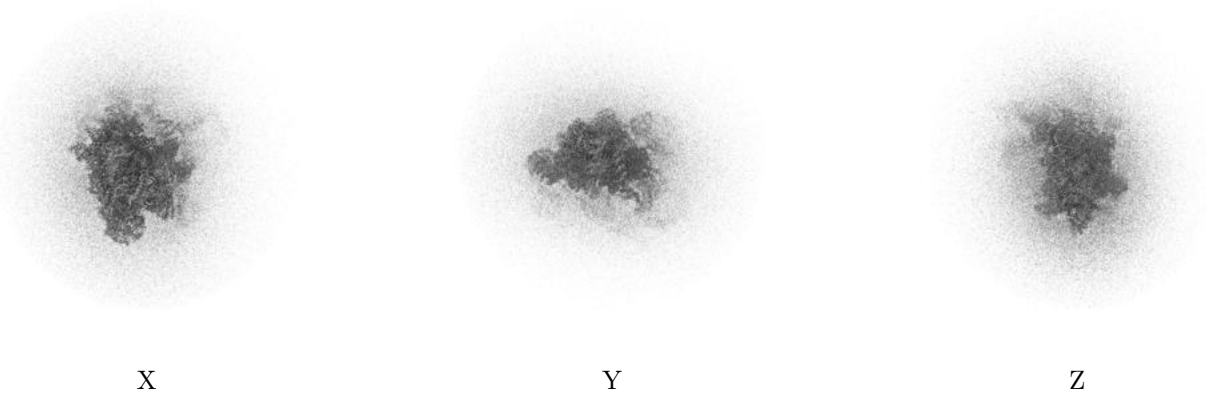
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.2. 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.

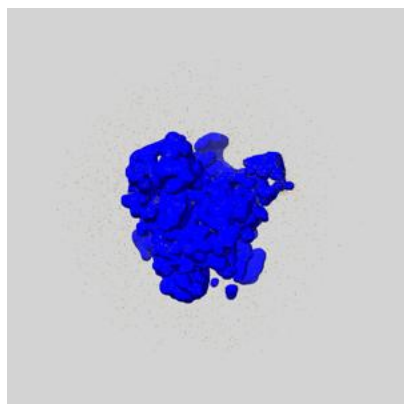
6.6 Mask visualisation [i](#)

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

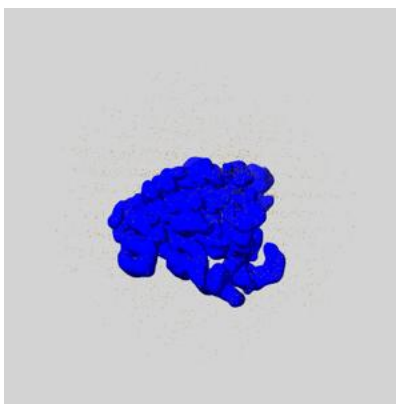
A mask typically either:

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

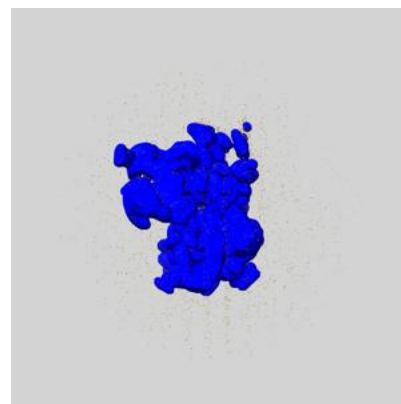
6.6.1 emd_19942_msk_1.map [i](#)



X



Y

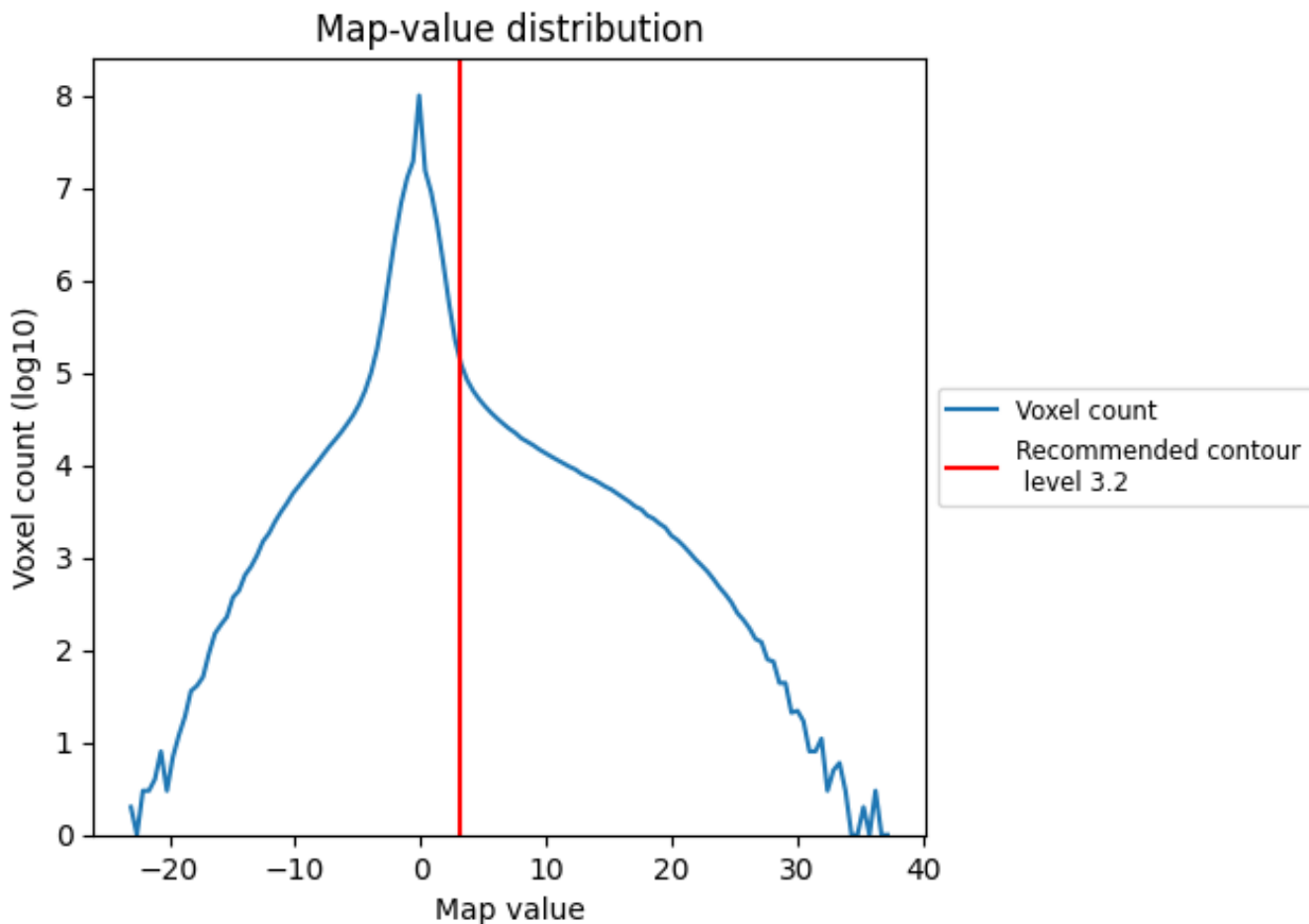


Z

7 Map analysis [i](#)

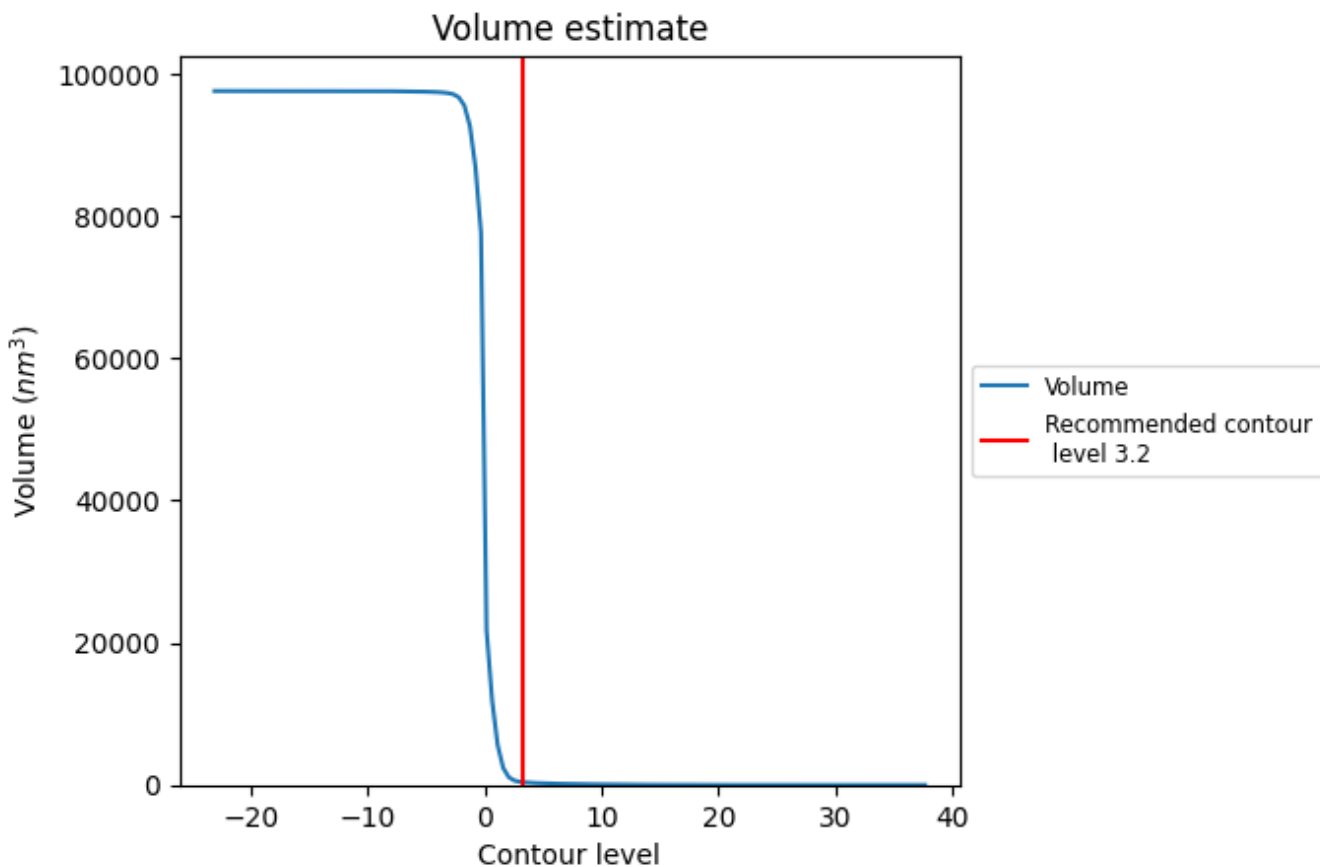
This section contains the results of statistical analysis of the map.

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.

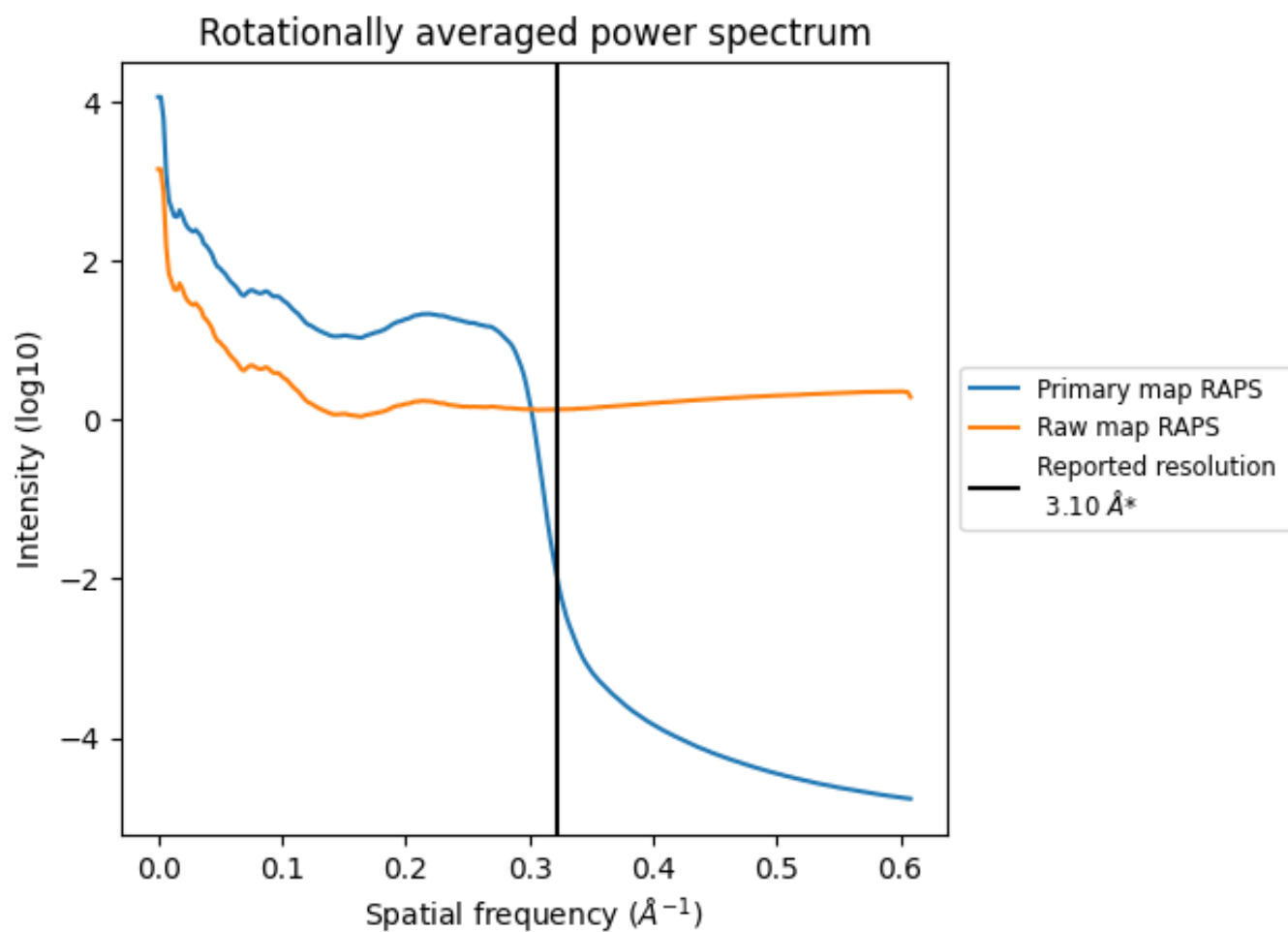
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 415 nm³; this corresponds to an approximate mass of 375 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

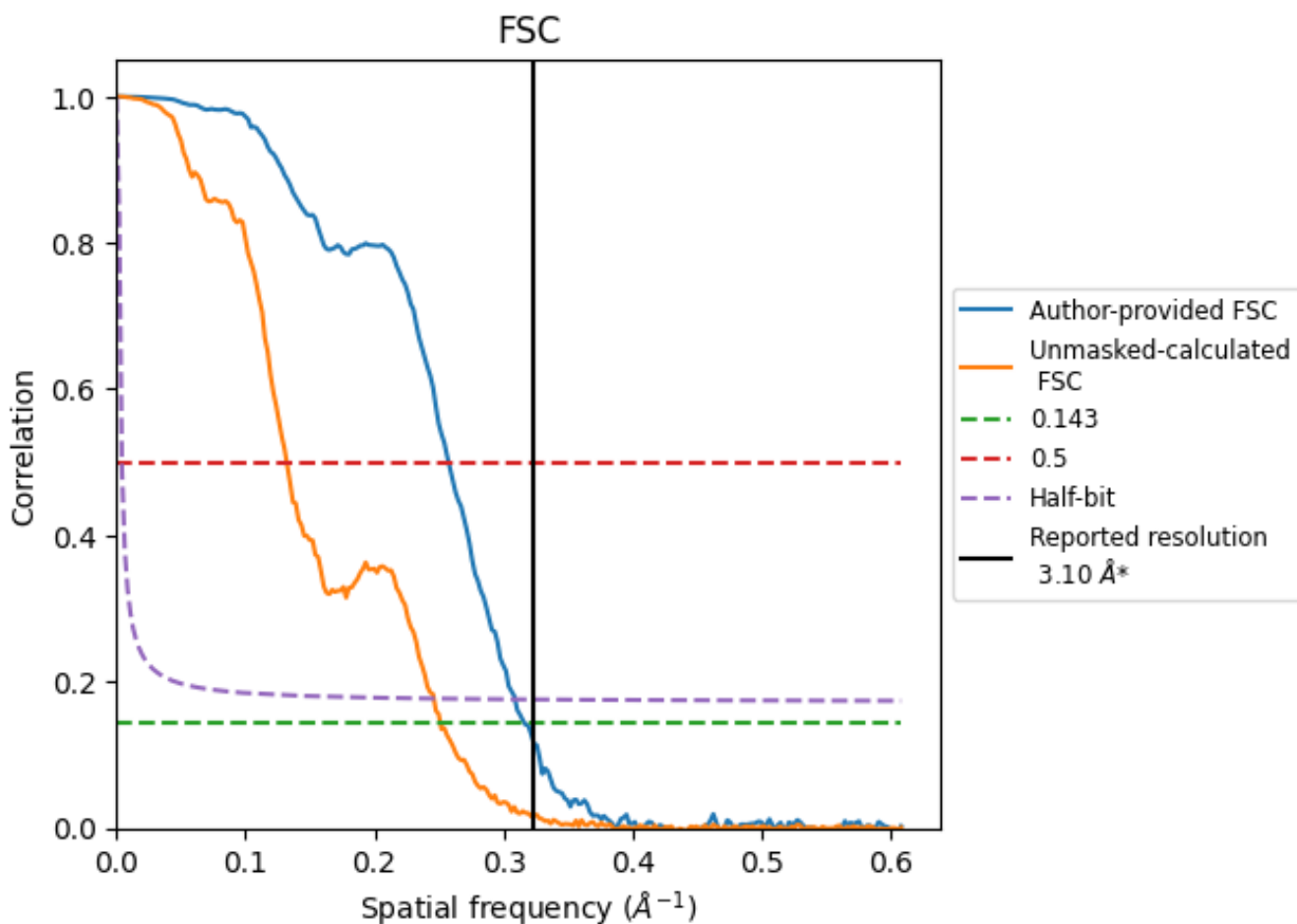


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

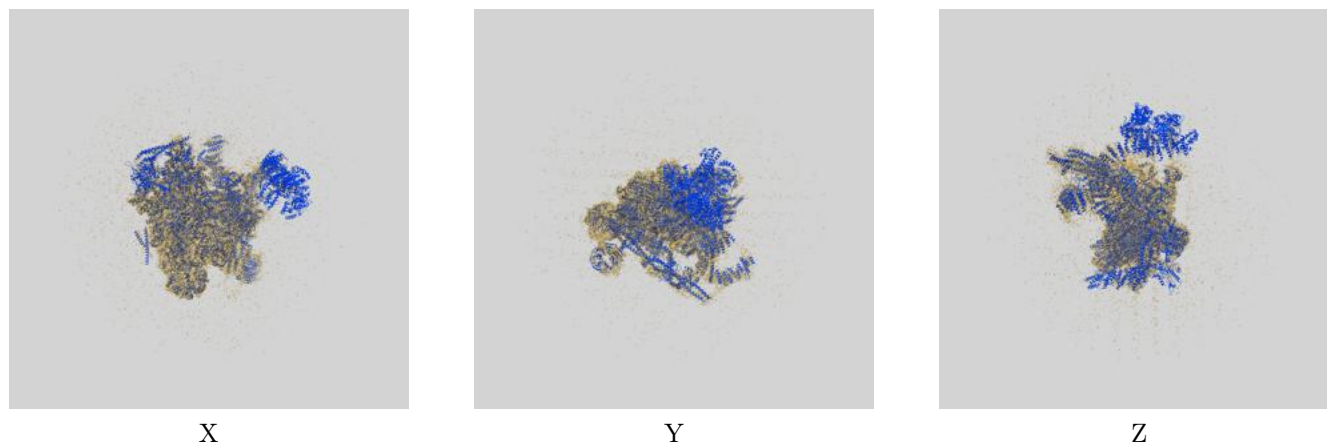
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.98 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

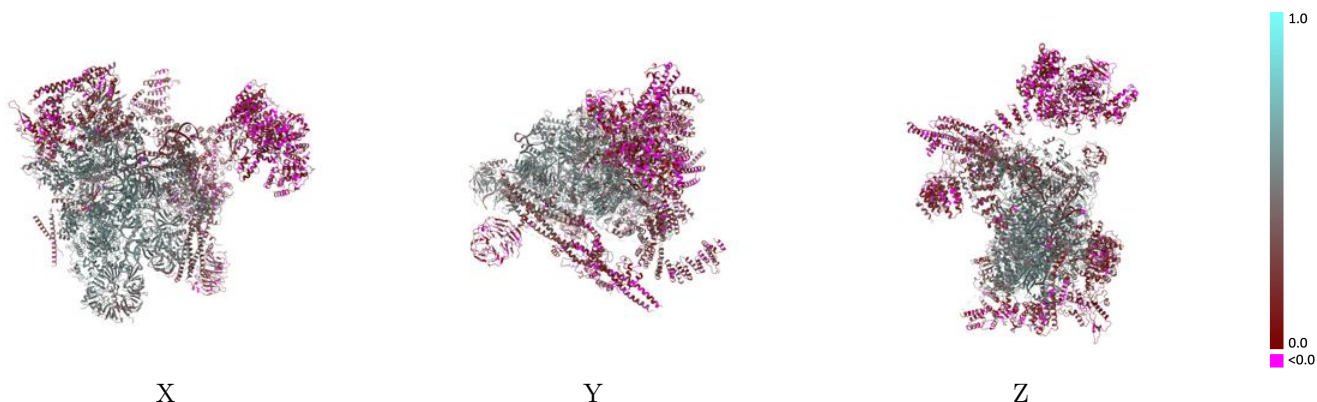
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



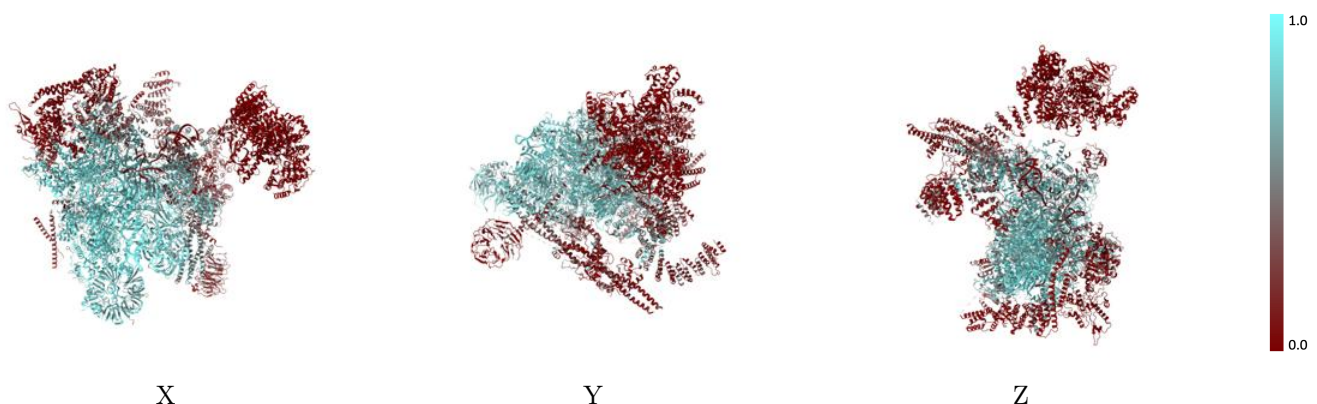
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



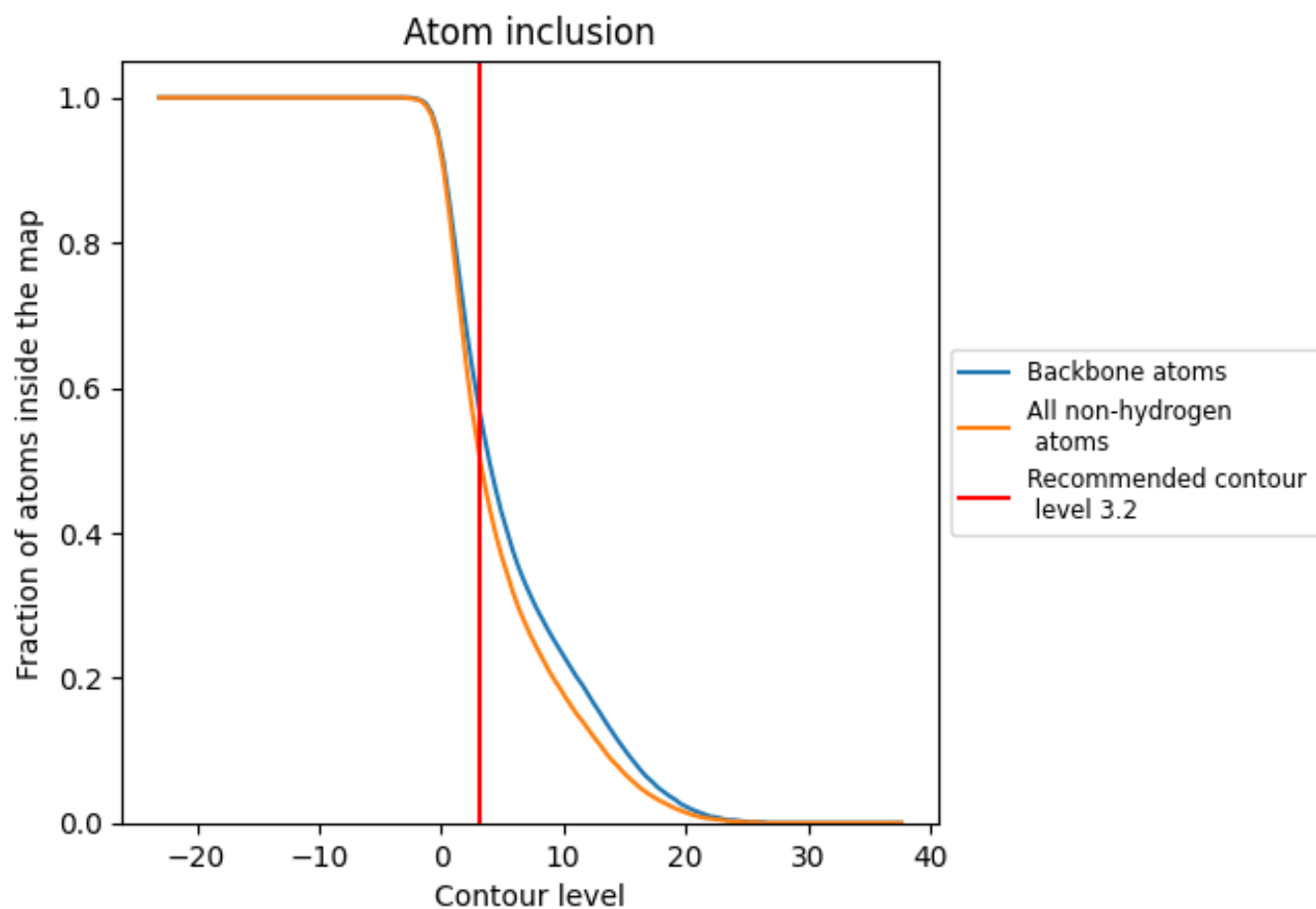
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 50% 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 (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4990	 0.3640
1	 0.5170	 0.4200
2	 0.4320	 0.3200
5	 0.9380	 0.5360
6	 0.5180	 0.4060
A	 0.7590	 0.4960
B	 0.8490	 0.5310
C	 0.7990	 0.5030
D	 0.8680	 0.5490
E	 0.7970	 0.5080
F	 0.7330	 0.4680
G	 0.7130	 0.4240
H	 0.7930	 0.5050
I	 0.7390	 0.4490
J	 0.8260	 0.5340
K	 0.8780	 0.5480
L	 0.7030	 0.4700
M	 0.4680	 0.3830
N	 0.0050	 0.1040
O	 0.8500	 0.5400
P	 0.6750	 0.4450
Q	 0.7790	 0.5310
R	 0.4450	 0.3280
S	 0.0530	 0.1340
T	 0.2000	 0.2100
U	 0.1300	 0.1600
V	 0.0770	 0.1340
W	 0.4690	 0.3200
X	 0.1770	 0.1980
Y	 0.1780	 0.3150
Z	 0.3780	 0.2660
a	 0.6470	 0.4370
b	 0.3050	 0.3220
c	 0.8220	 0.5050
d	 0.7110	 0.4720



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Chain	Atom inclusion	Q-score
e	 0.4730	 0.4550
f	 0.3910	 0.3230
m	 0.0830	 0.1860
n	 0.0210	 0.1600
p	 0.3440	 0.3510
q	 0.3880	 0.4780
r	 0.3490	 0.2780
y	 0.4500	 0.3500
z	 0.2880	 0.2760