



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary 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:

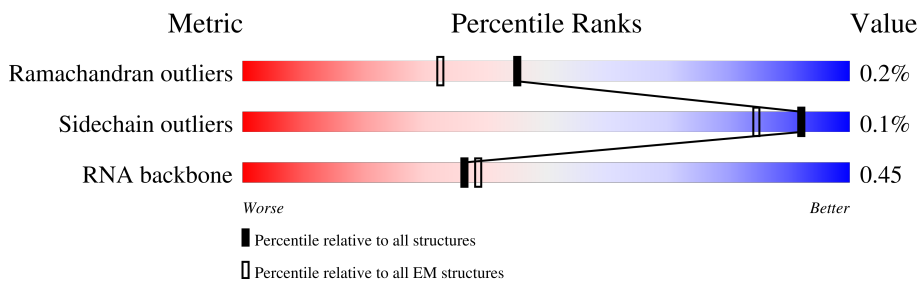
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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
			Total	C	N	O	S		
34	y	200	1606	1000	279	323	4	0	0

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

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

- Molecule 36 is a protein called UNK1.

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

- Molecule 37 is a protein called UNK2.

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

- Molecule 38 is a RNA chain called U6snRNA.

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

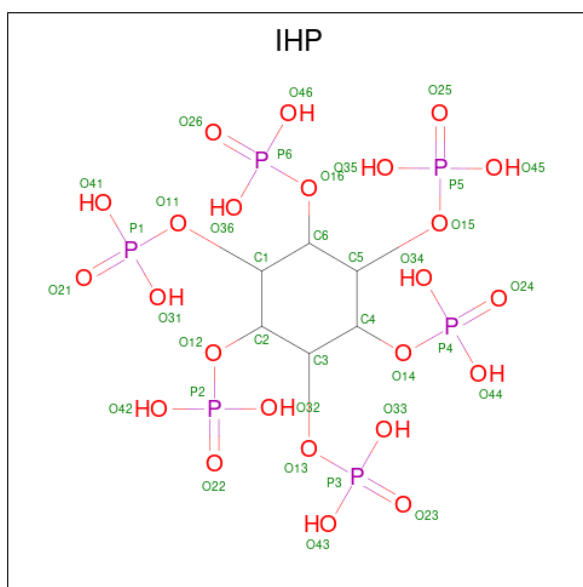
- Molecule 39 is a RNA chain called pre-mRNA.

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

- Molecule 40 is a protein called UNK3.

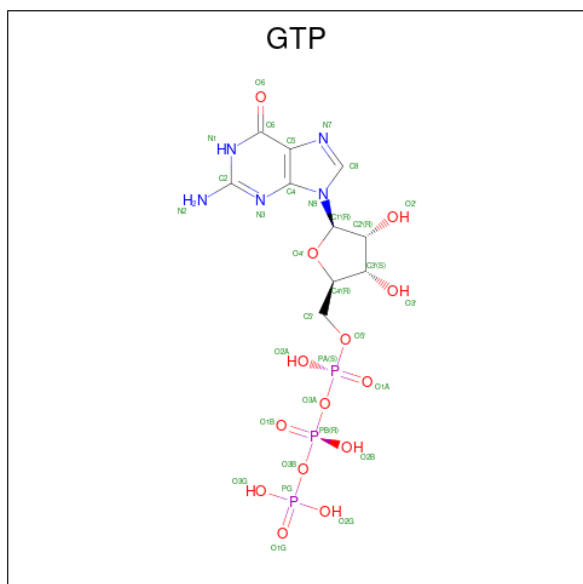
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
40	f	22	110	66	22	22	0	0

- 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).

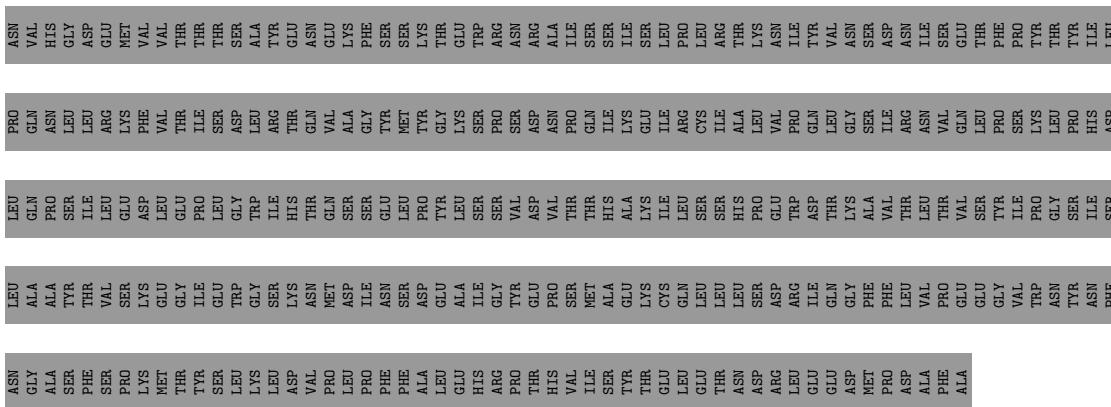
Mol	Chain	Residues	Atoms	AltConf
43	B	1	Total Mg 1 1	0
43	6	3	Total Mg 3 3	0

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

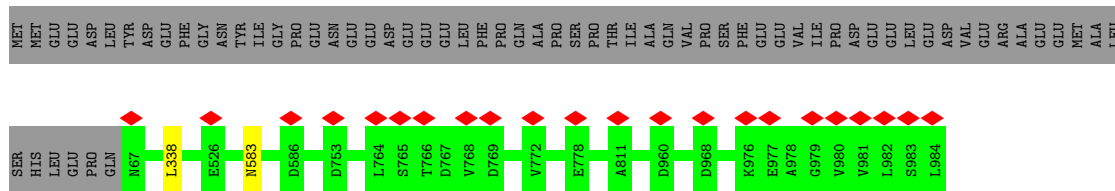
Mol	Chain	Residues	Atoms	AltConf
44	M	2	Total Zn 2 2	0
44	O	3	Total Zn 3 3	0
44	P	1	Total Zn 1 1	0

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

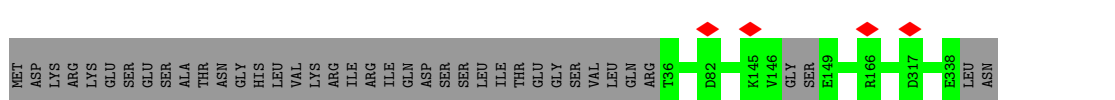
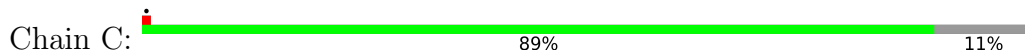
Mol	Chain	Residues	Atoms	AltConf
45	6	1	Total K 1 1	0



- Molecule 6: Pre-mRNA-splicing factor cwf10



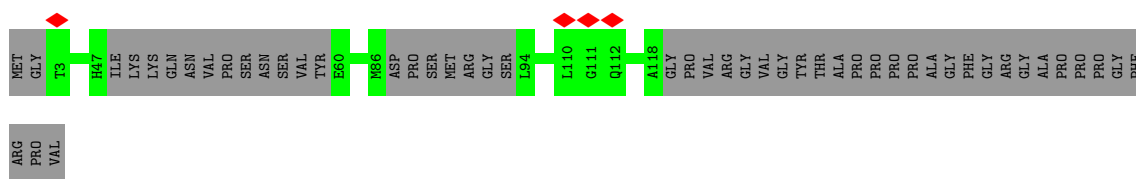
- Molecule 7: Pre-mRNA-splicing factor cwf17



- Molecule 8: Small nuclear ribonucleoprotein Sm D3

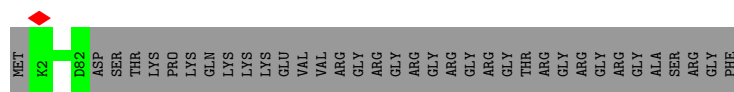


- Molecule 9: Small nuclear ribonucleoprotein-associated protein B

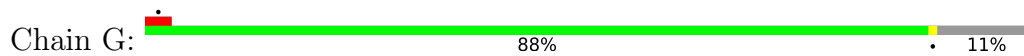


- Molecule 10: Small nuclear ribonucleoprotein Sm D1

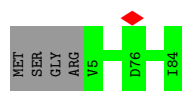




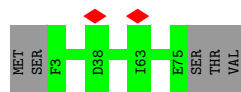
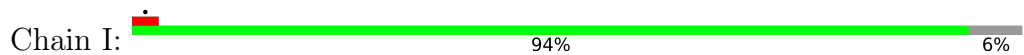
• Molecule 11: Small nuclear ribonucleoprotein Sm D2



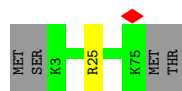
• Molecule 12: Small nuclear ribonucleoprotein E



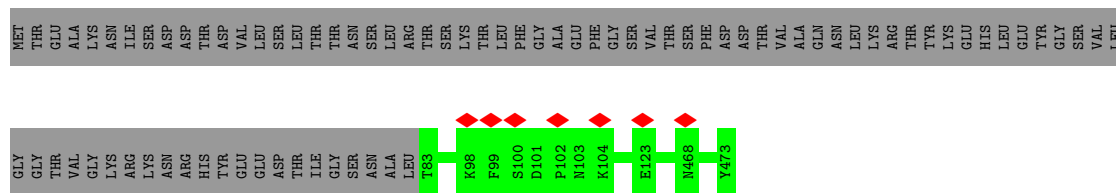
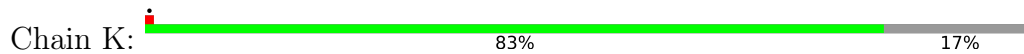
• Molecule 13: Small nuclear ribonucleoprotein F



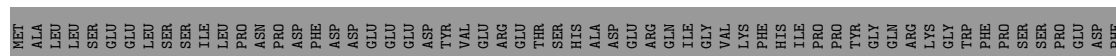
• Molecule 14: Small nuclear ribonucleoprotein G



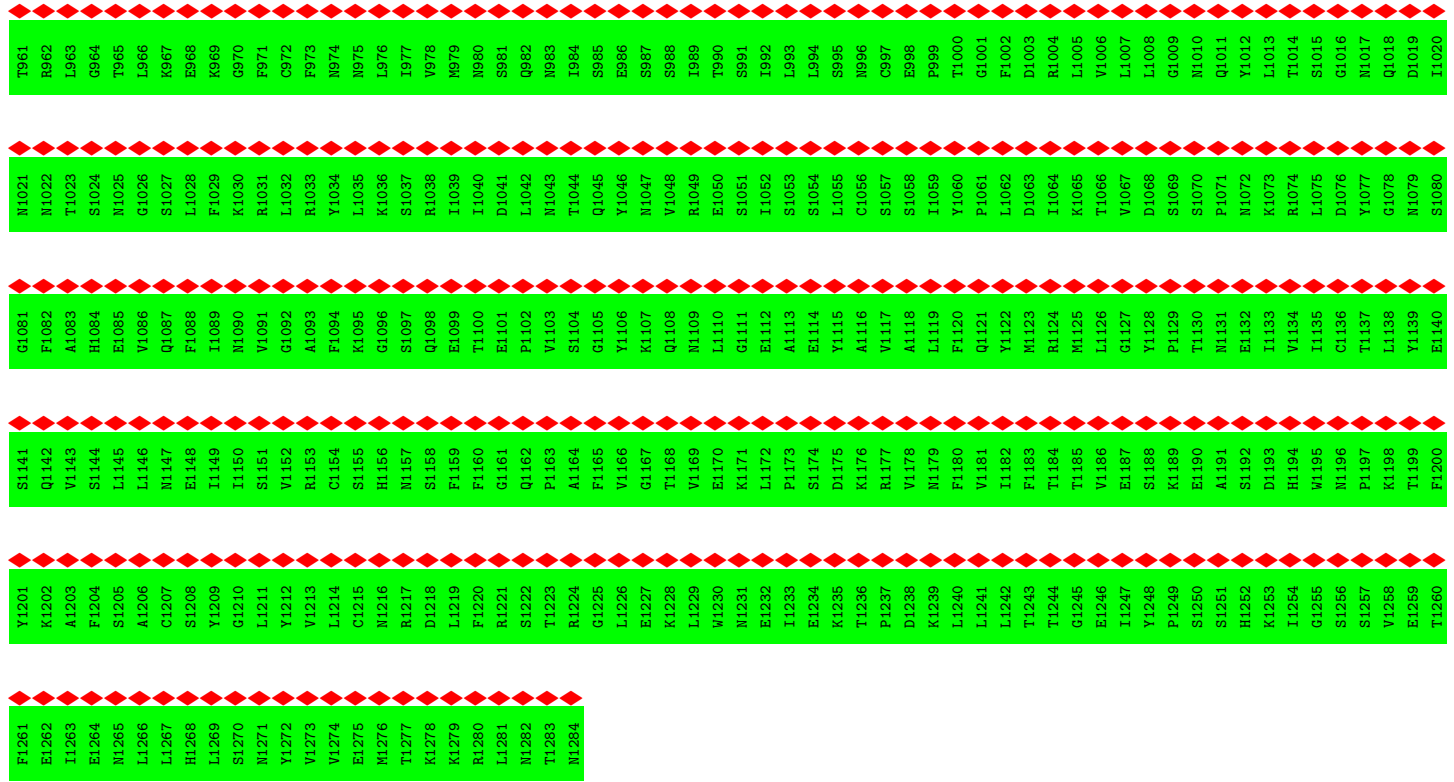
• Molecule 15: Pre-mRNA-splicing factor prp5



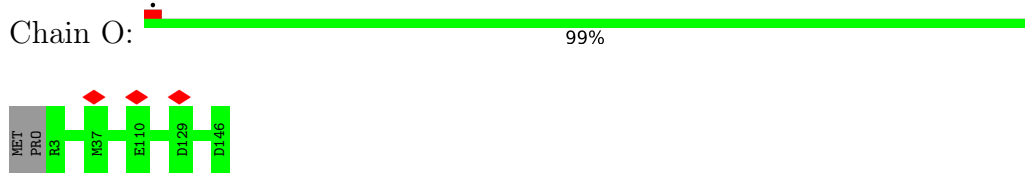
• Molecule 16: Pre-mRNA-processing protein 45



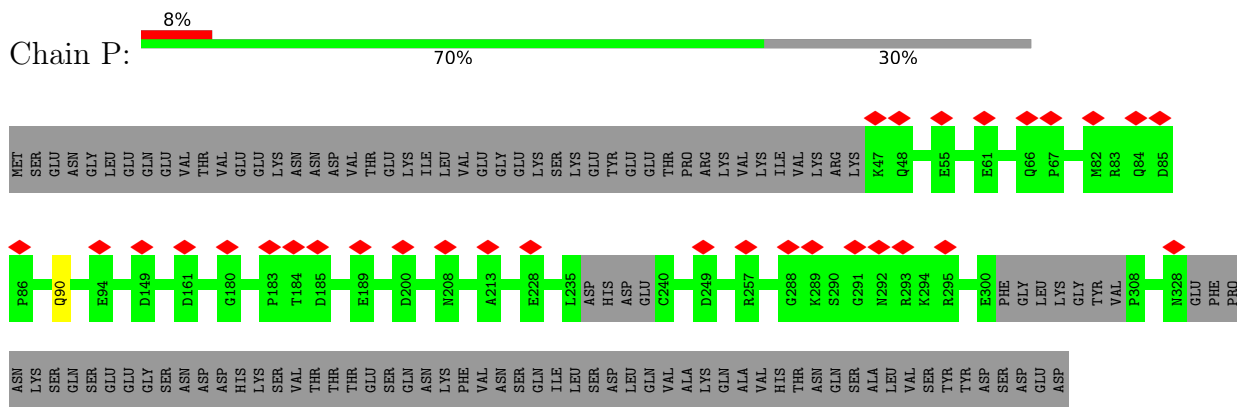
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V121	Y122	M123	I124	Q125	F126	I127	T128	L129	C130	F131	Q132	F133	L134	N135	I136	E137	K138	L139	R140	K141	L142	V143	Y144	Q145	L146	T147	M148	I149	S150	I151	L152	N153	S154	L155	D156	M157	L158	D159	K160	V161	Y162	Y163	L164	L165	H166	D167	S168	S169	S170	L171	T172	K173	A174	F175	D176	S177	Y178	K179	E180	
K181	R182	P183	S184	I185	V186	E187	K188	F189	P190	L191	H192	N193	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	R230	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	L262	S263	N264	E265	L266	F267	K268	C269	M270	T271	D272	D273	L274	N275	Y276	Z277	L278	K279	F280	P281	L282	D283	N284	L285	I286	G287	N288	E289	Y290	E291	K292	E293	Q294	K295	I296	R297	N298	D299	E300	
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P361	E362	K363	Y364	A365	I366	K367	V368	D369	F370	E371	F372	L373	K374	N375	V376	F377	I378	N379	T380	Y381	D382	R383	T384	R385	L386	V387	N388	D389	Y390	D391	E392	I393	I394	N395	F396	T397	L398	K399	D400	L401	L402	G403	E404	R405	S406	V407	M408	D409	Q410	E411	M412	S413	L414	T415	M416	Y417	F418	L419	L420	
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	S458	Q459	Y460	R461	L462	L463	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	O504	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	Y540	
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	Y567	G568	M569	F570	Q571	S572	D573	H574	Q575	S576	D577	S578	D579	N580	K581	S582	L583	N584	V585	S586	L587	S588	P589	L590	G591	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	G622	L623	D624	L625	N626	L627	L628	V629	S630	L631	L632	N633	R634	A635	K636	E637	F638	P639	K640	M641	F642	E643	D644	L645	V646	L647	G648	F649	G650	T651	P652	D653	L654	C655	A656	F657	P658	N659	A660	
G661	L662	N663	S664	I665	V666	A667	R668	N669	L670	F671	N672	T673	V674	E675	Q676	L677	Q678	S679	V680	L681	P682	N683	C684	H685	V686	P687	S688	N689	L690	S691	T692	E693	S694	L695	L696	L697	K698	F699	Y700	L701	N702	Q703	E704	N704	K705	L706	T707	A708	D709	P710	T711	A712	S713	D714	R715	V716	L717	S718	L719	P720
S721	N722	R723	L724	T725	V726	Y727	N728	D729	K730	Q731	L732	E733	S734	L735	L736	R737	G738	S739	Q740	F741	G742	L743	T744	M745	V746	M747	G748	P749	L750	R751	C752	G753	K754	H755	L756	L757	V758	C759	K760	L761	E762	E763	L764	V765	L766	D767	T768	S769	P770	M771	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	S822	W823	I824	S825	K826	L827	R828	G829	L830	L831	R832	E833	I834	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	N871	T872	G873	D874	D875	K876	D877	S878	R879	D880	A881	S882	M883	R884	F885	P886	F887	H888	S889	R890	F891	C892	D893	K894	S895	K896	R897	P898	L899	E900	



● Molecule 19: Pre-mRNA-splicing factor cwf14

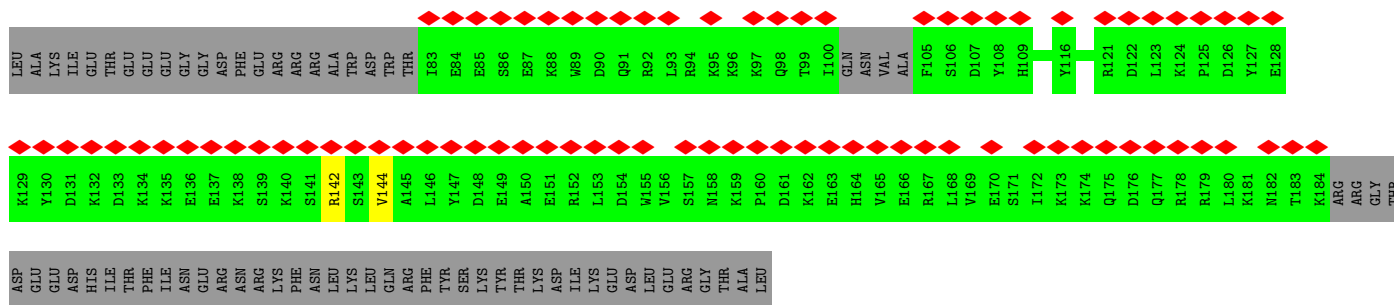


● Molecule 20: Pre-mRNA-splicing factor cwf2

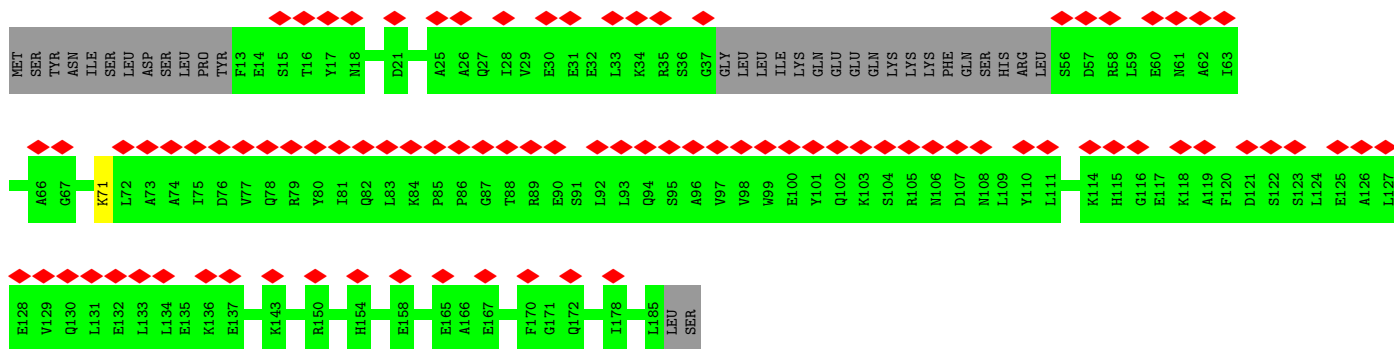
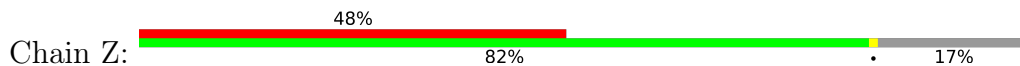


● Molecule 21: Pre-mRNA-splicing factor cwf15

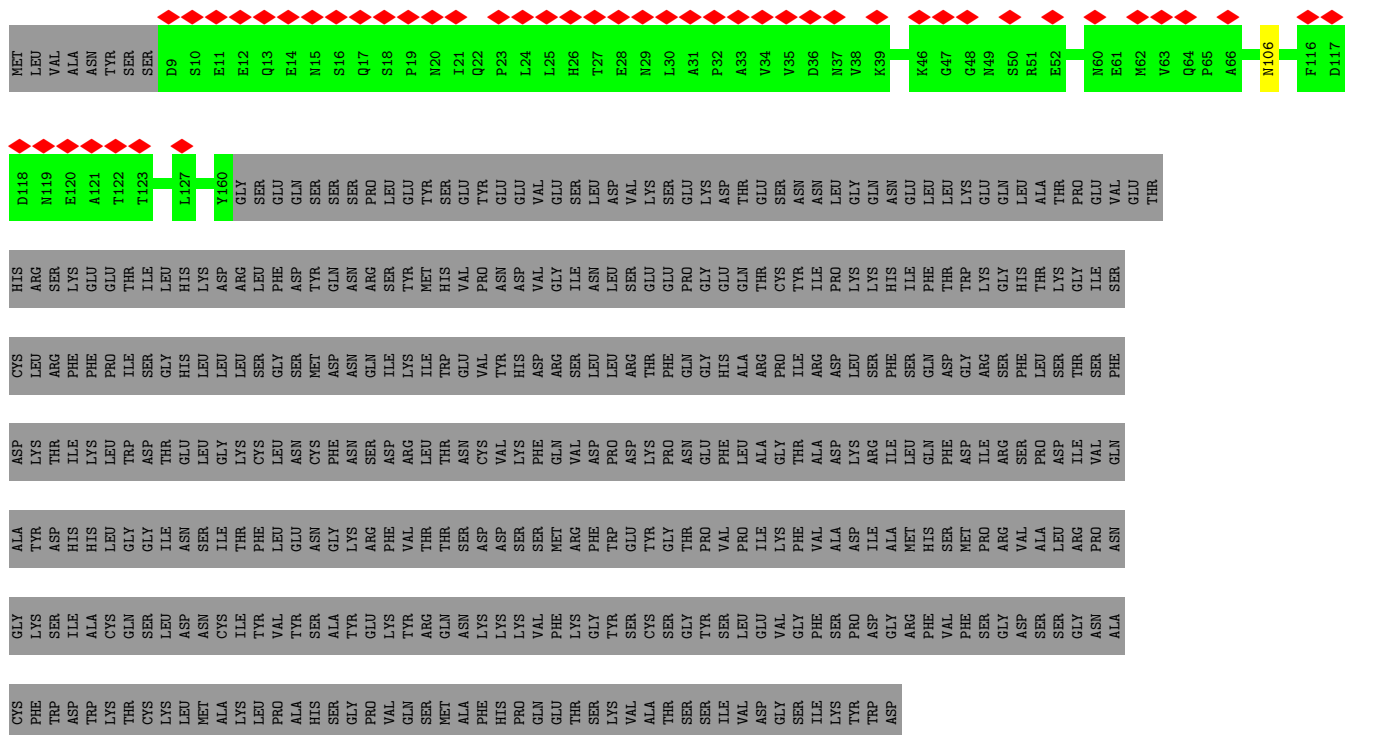




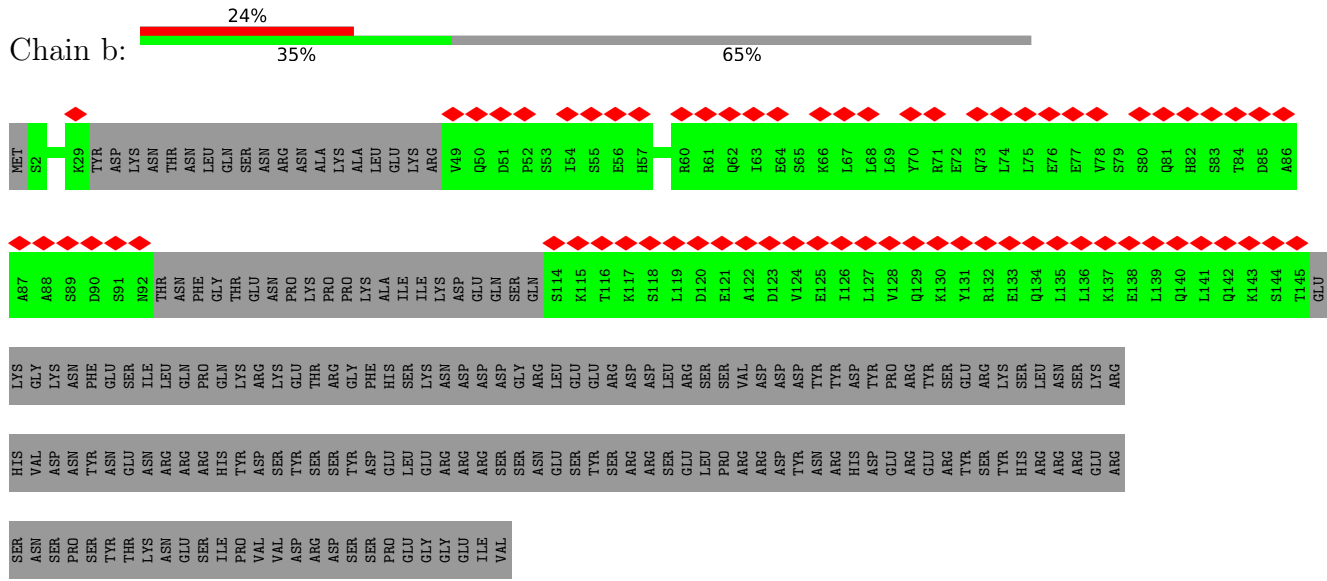
• Molecule 27: Pre-mRNA-splicing factor cwf7



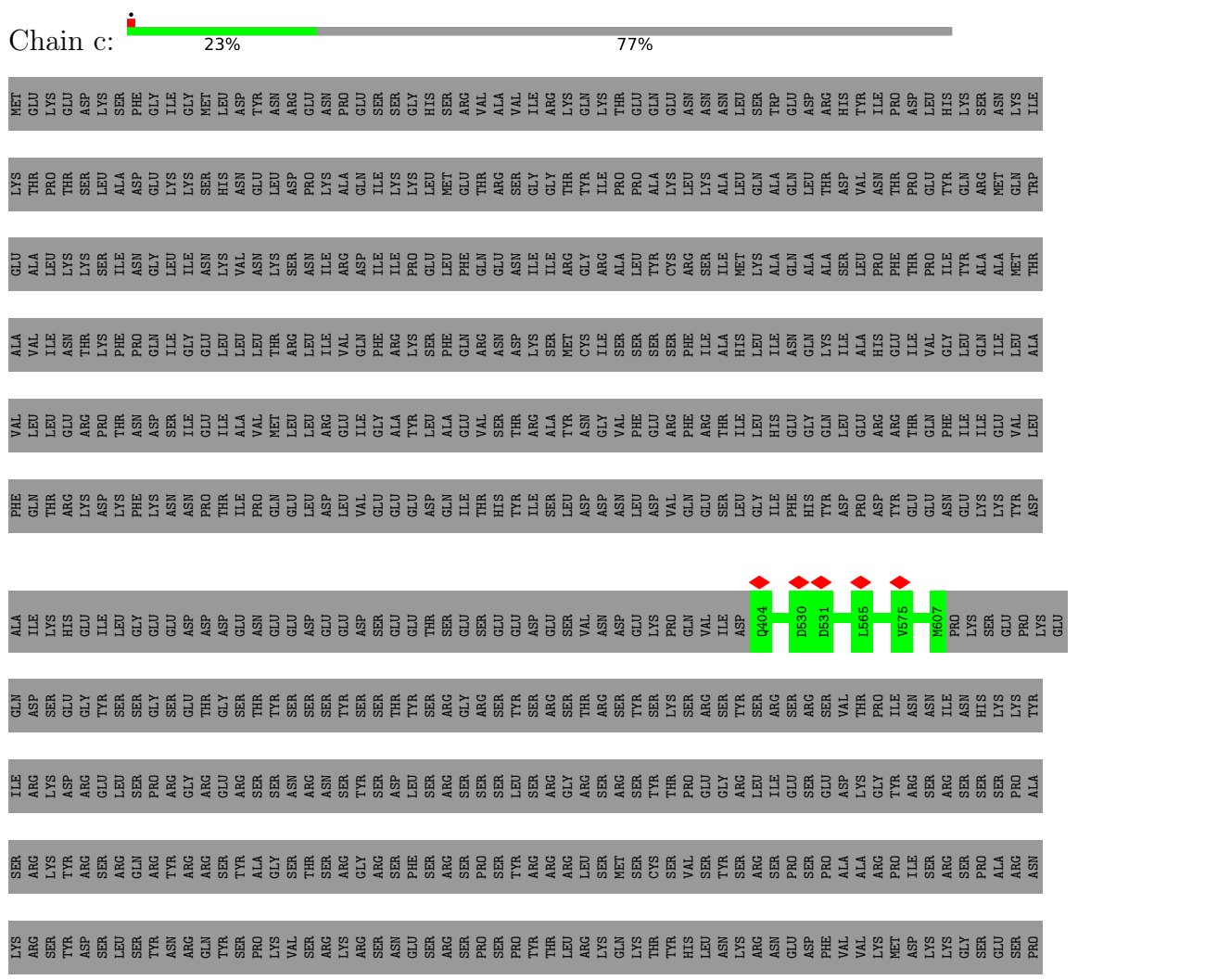
• Molecule 28: Pre-mRNA-processing factor 17

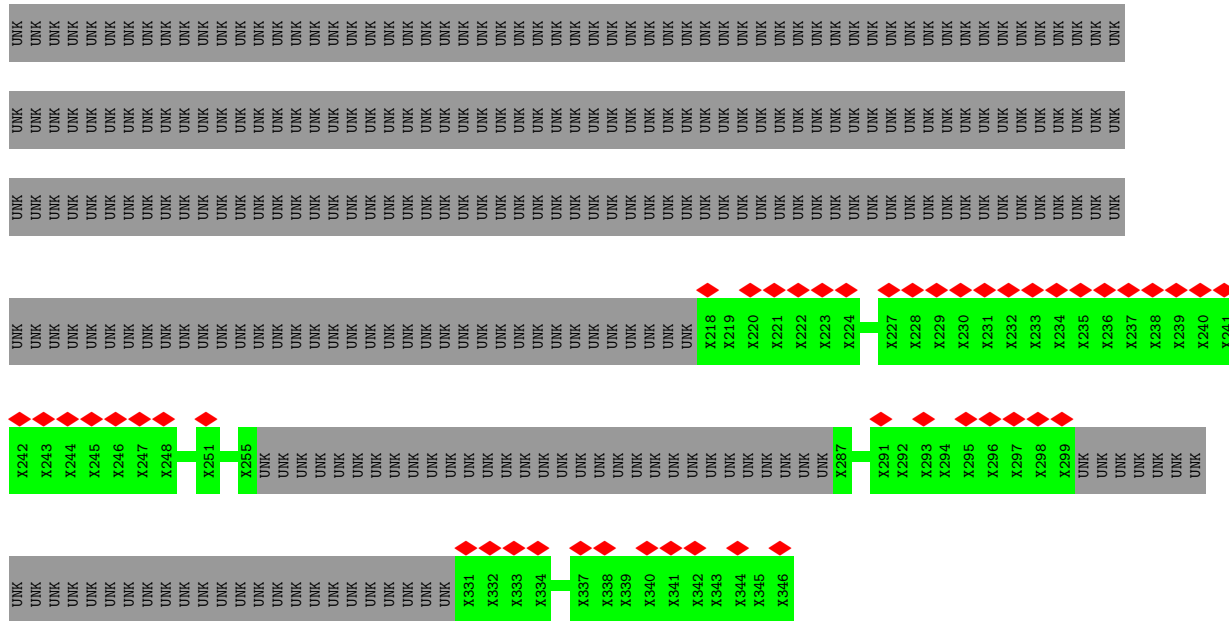


• Molecule 29: Pre-mRNA-splicing factor cwf21

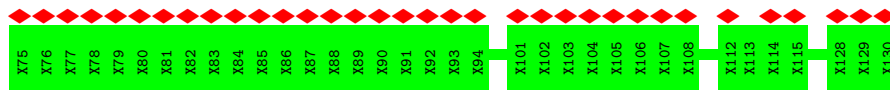


• Molecule 30: Pre-mRNA-splicing factor cwf22

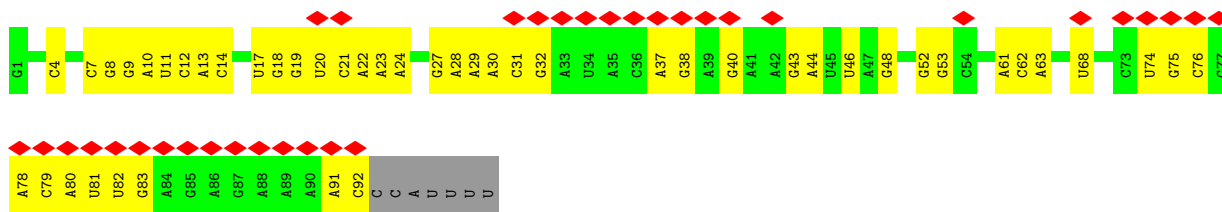




• Molecule 37: UNK2



• Molecule 38: U6snRNA

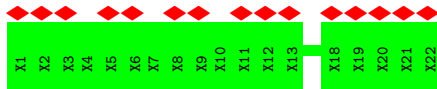


• Molecule 39: pre-mRNA



• 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.

The worst 5 of 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

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	U	415	PRO
26	Y	142	ARG
35	z	358	MET
28	a	106	ASN
14	J	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
27	Z	108	ASN
34	y	208	ASN
27	Z	156	GLN
31	d	101	GLN
35	z	384	ASN

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%)

5 of 90 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	11	U

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Mol	Chain	Res	Type
3	2	12	G
3	2	13	C
3	2	24	A
3	2	29	A

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
38	6	52	G
38	6	74	U
39	1	1	G
39	1	0	G
38	6	29	A

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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

All (4) torsion outliers are listed below:

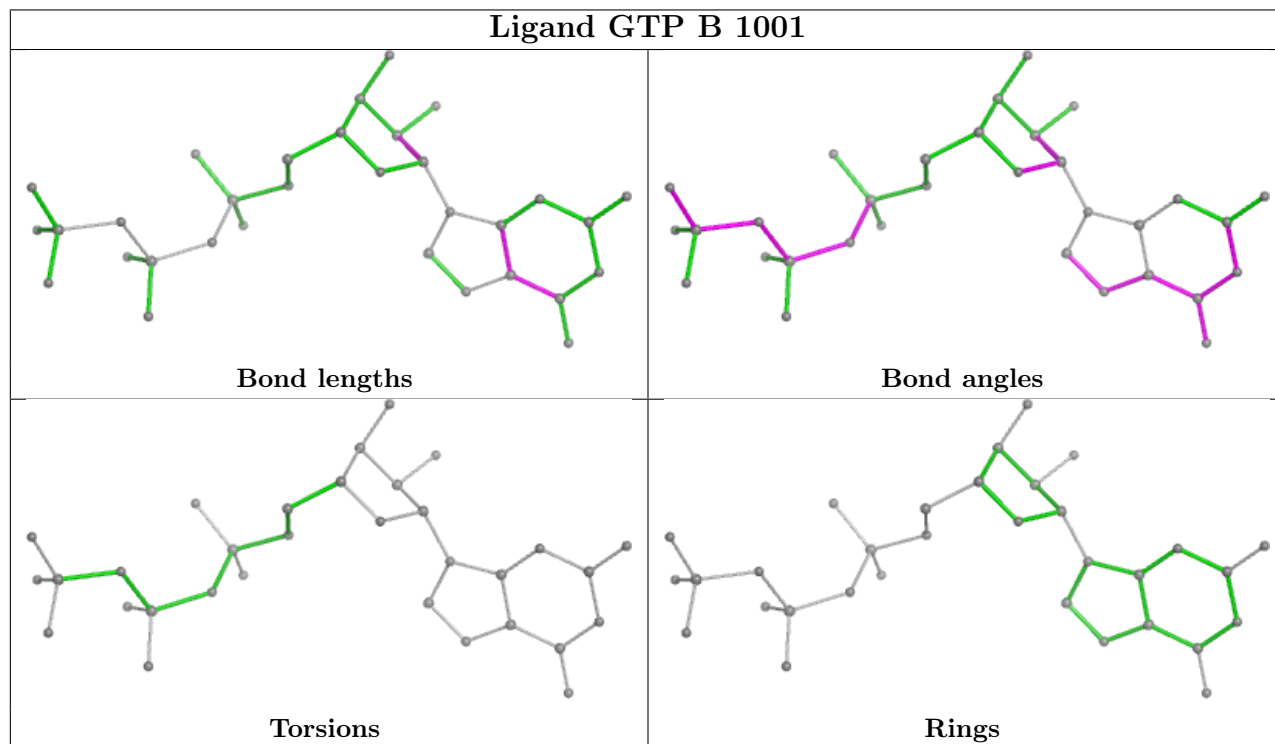
Mol	Chain	Res	Type	Atoms
41	A	2401	IHP	C6-O16-P6-O26
41	A	2401	IHP	C1-O11-P1-O41
41	A	2401	IHP	C6-O16-P6-O36
41	A	2401	IHP	C5-O15-P5-O35

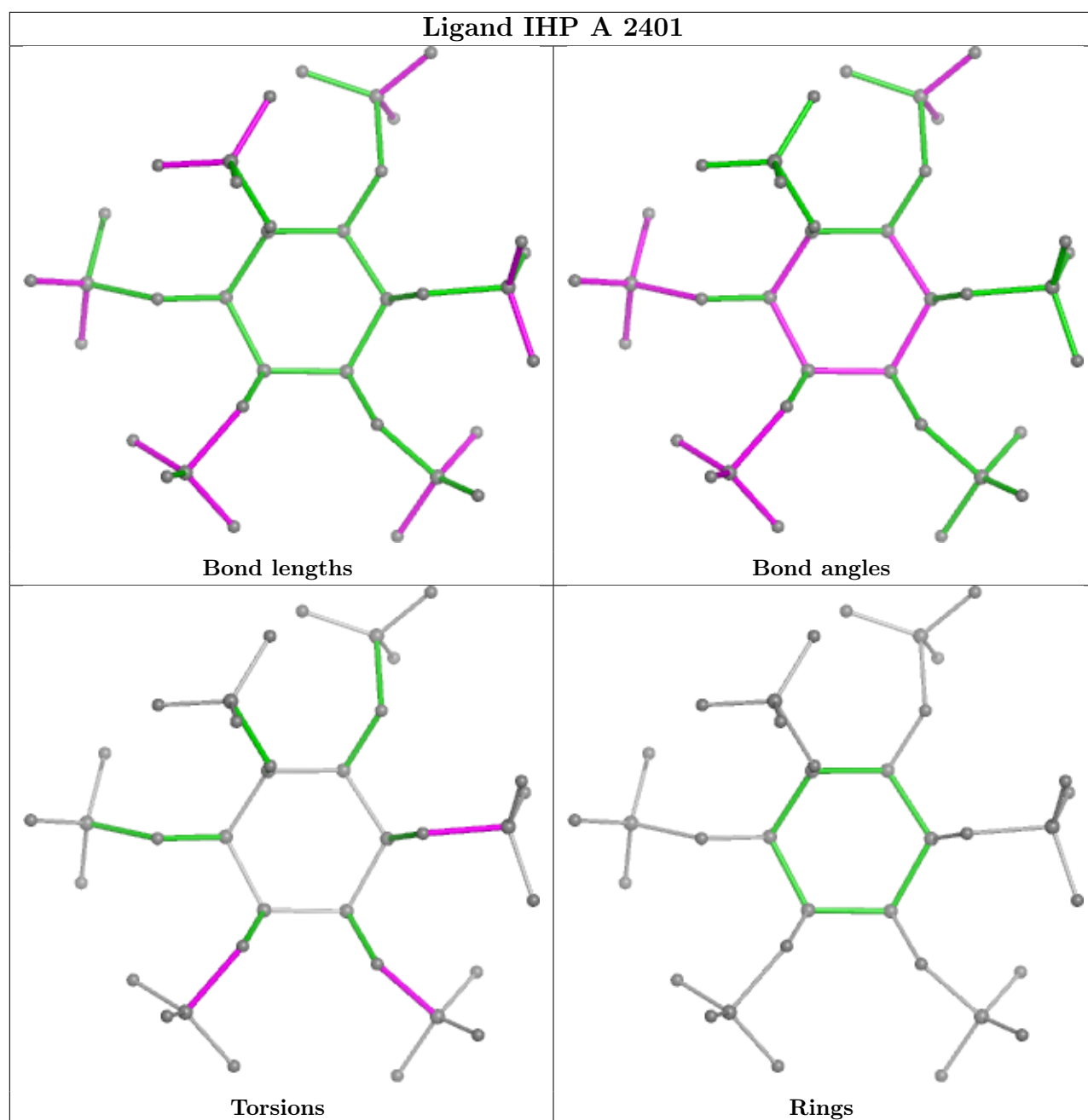
There are no ring outliers.

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.

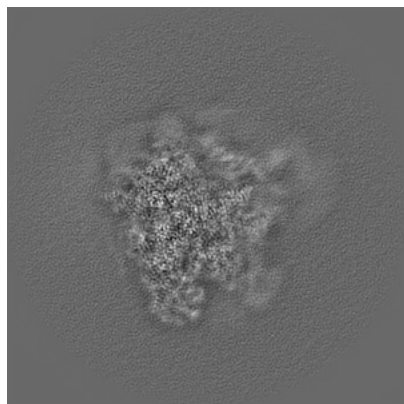
6 Map visualisation [i](#)

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.

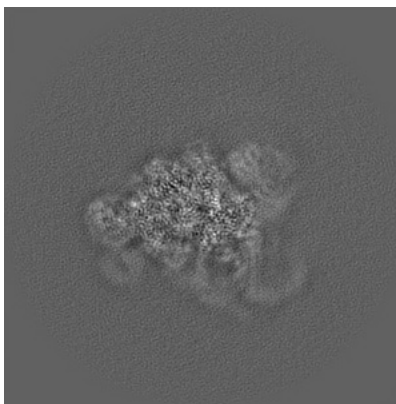
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

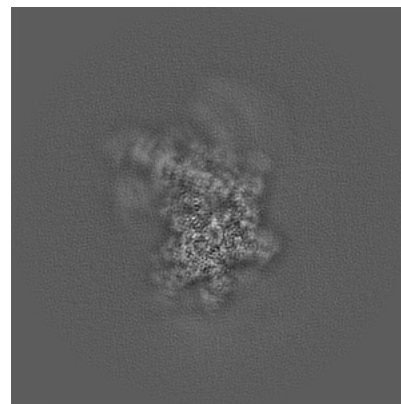
6.1.1 Primary map



X

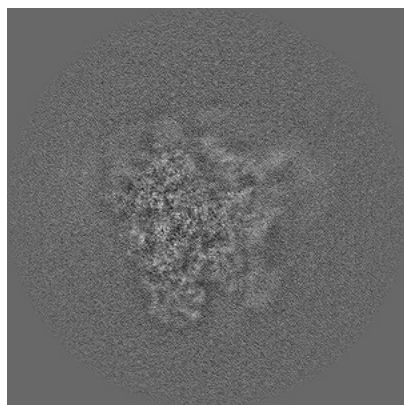


Y

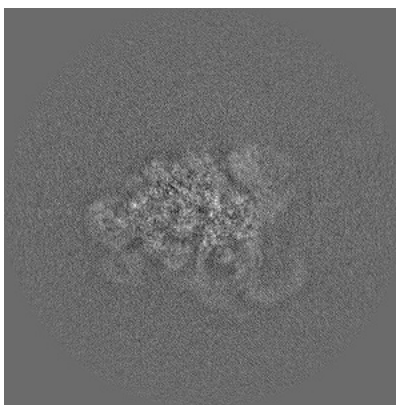


Z

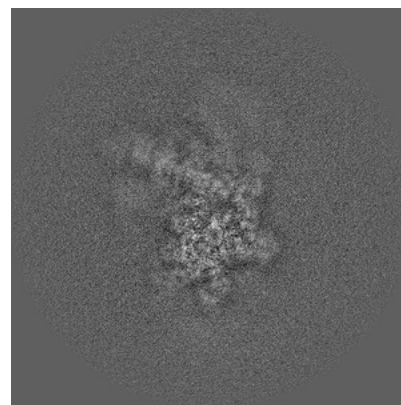
6.1.2 Raw map



X



Y

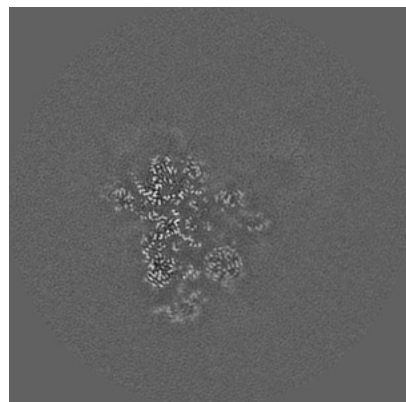


Z

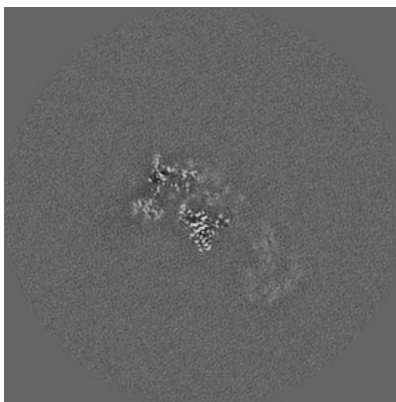
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

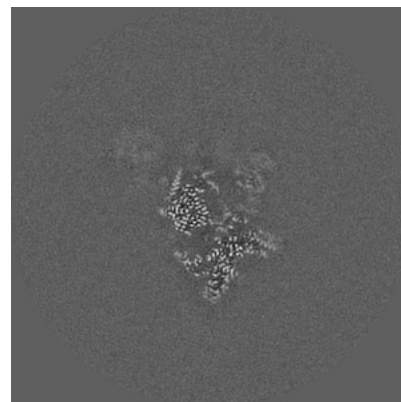
6.2.1 Primary map



X Index: 280

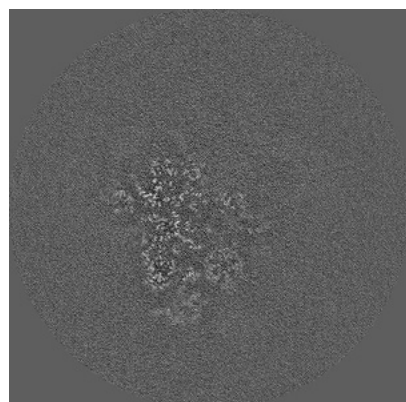


Y Index: 280

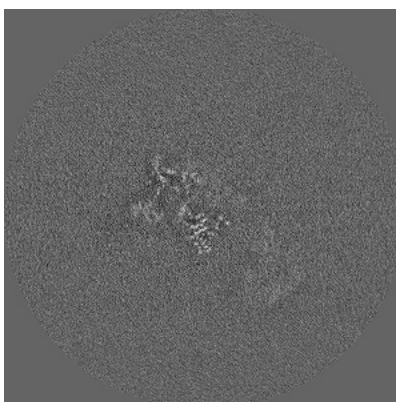


Z Index: 280

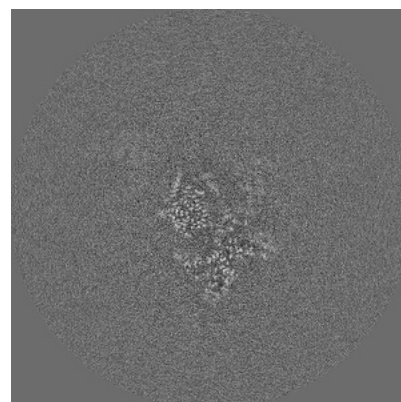
6.2.2 Raw map



X Index: 280



Y Index: 280

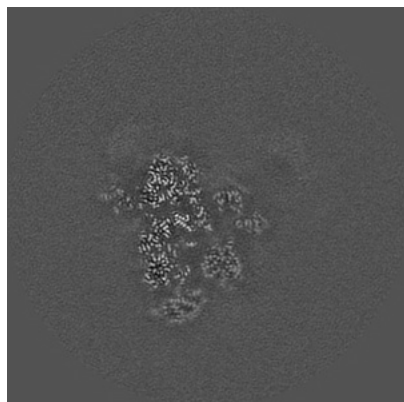


Z Index: 280

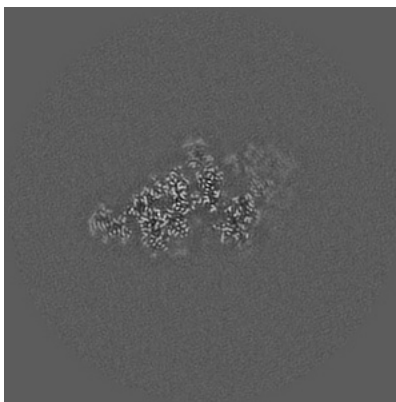
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

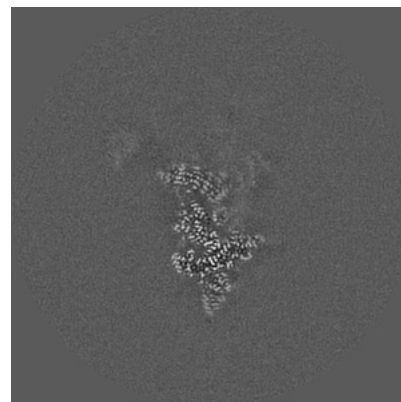
6.3.1 Primary map



X Index: 276

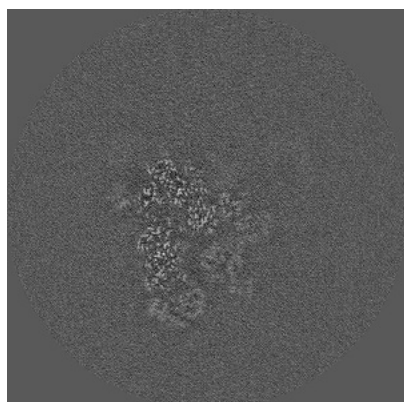


Y Index: 219

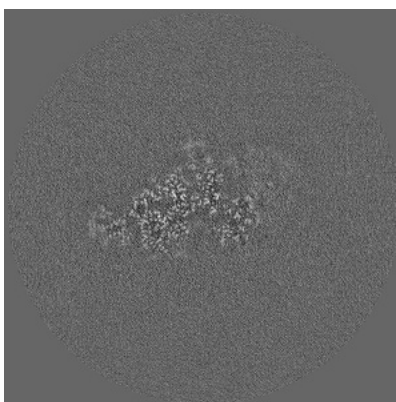


Z Index: 295

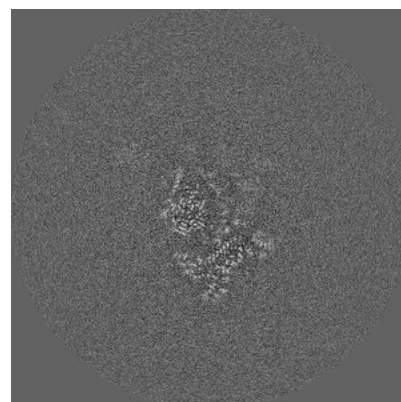
6.3.2 Raw map



X Index: 269



Y Index: 219

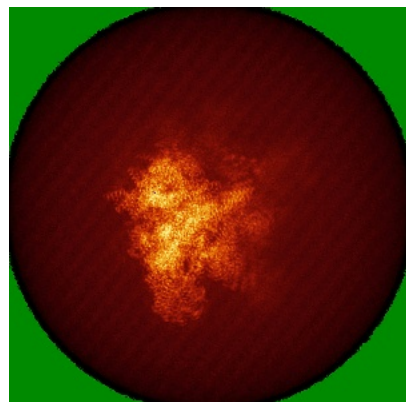


Z Index: 282

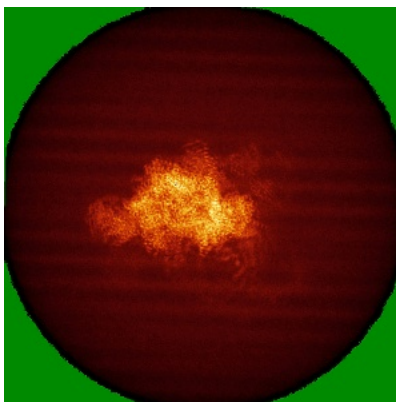
The images above show the largest variance slices of the map in three orthogonal directions.

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

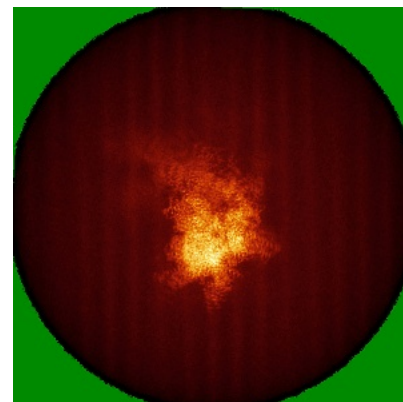
6.4.1 Primary map



X

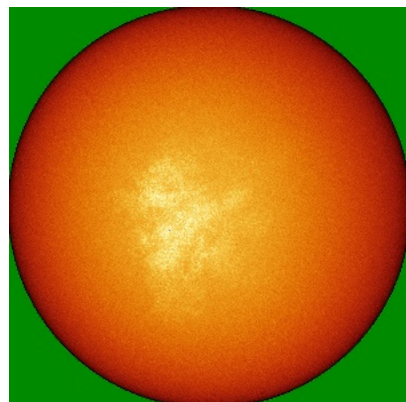


Y

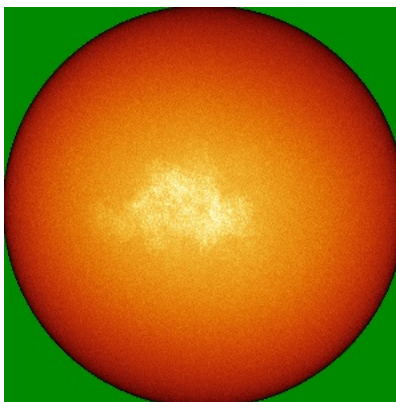


Z

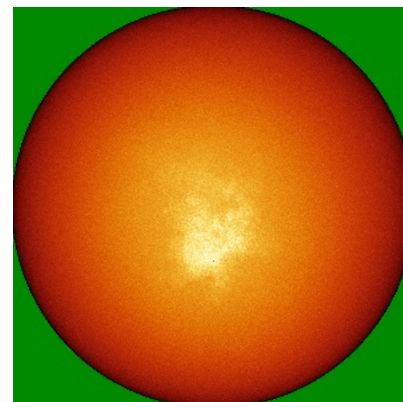
6.4.2 Raw map



X



Y

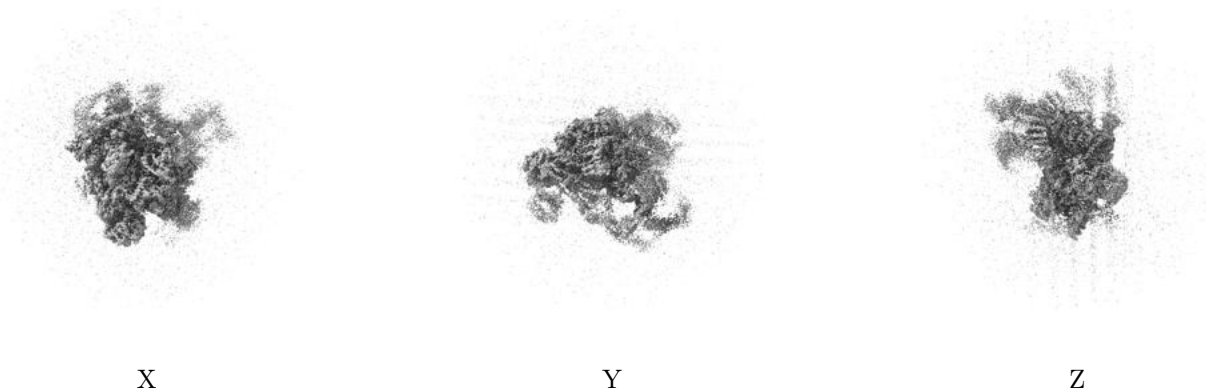


Z

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.

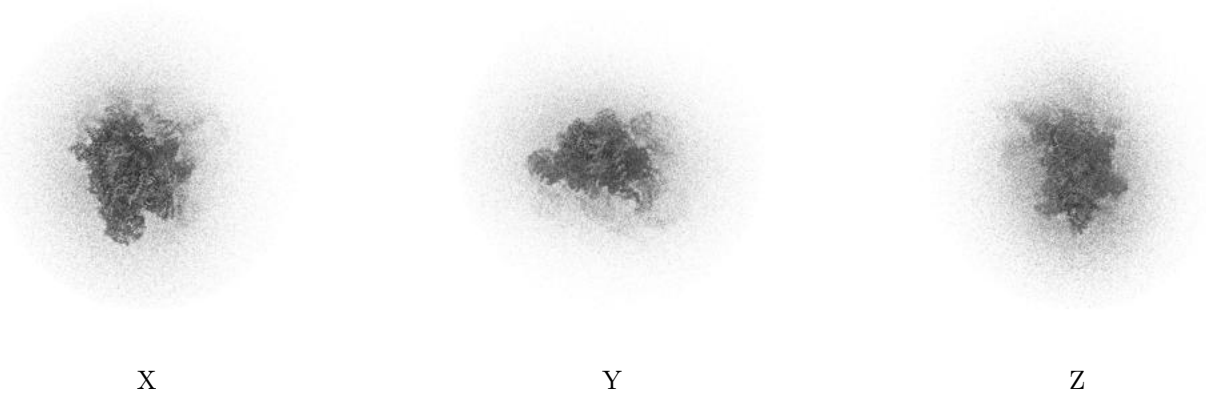
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

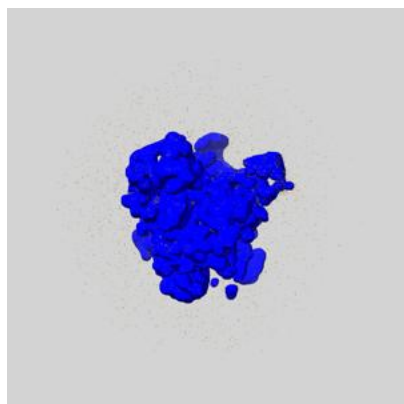
6.6 Mask visualisation [i](#)

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

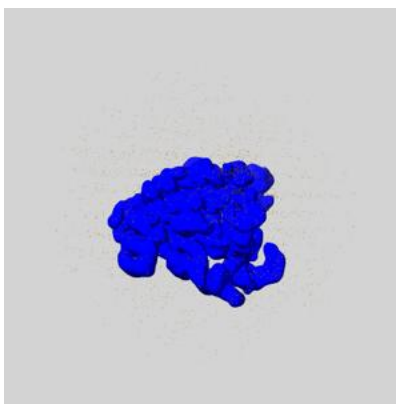
A mask typically either:

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

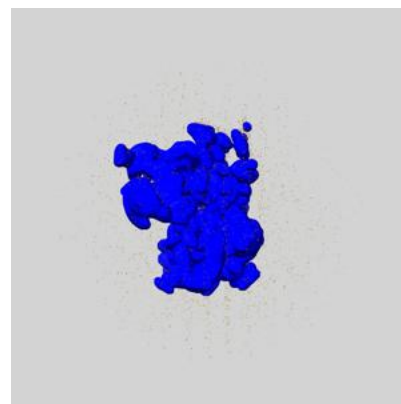
6.6.1 emd_19942_msk_1.map [i](#)



X



Y

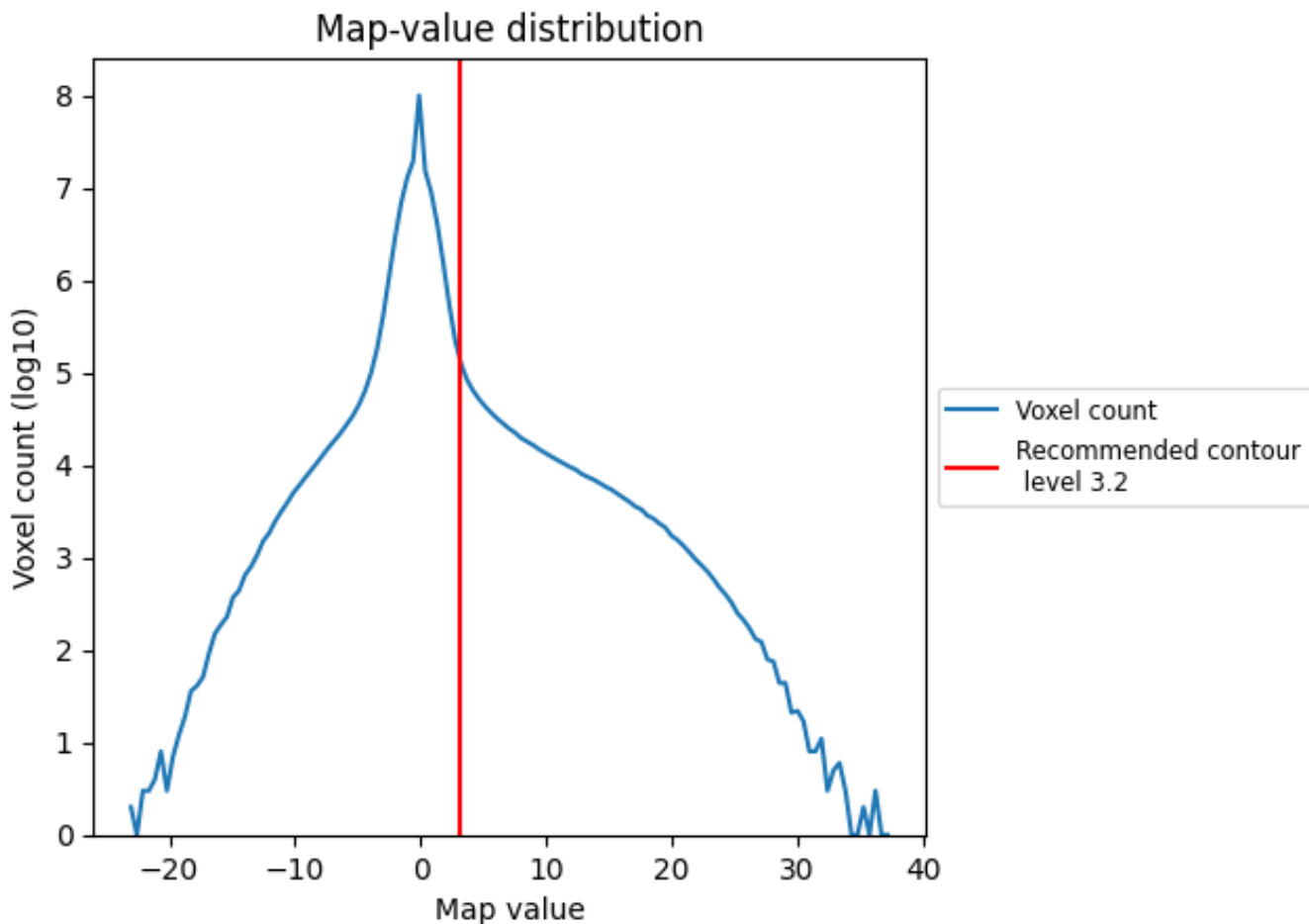


Z

7 Map analysis [i](#)

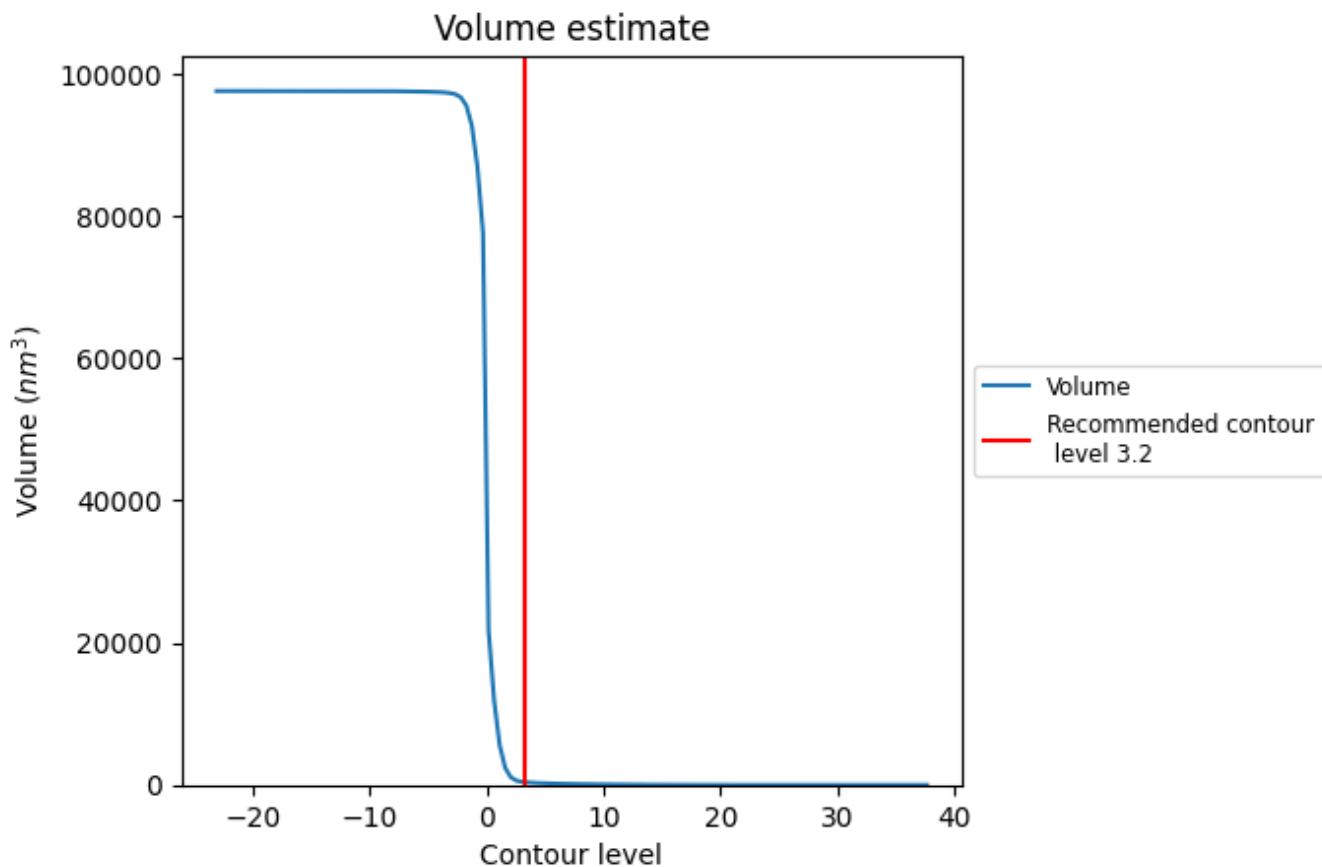
This section contains the results of statistical analysis of the map.

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.

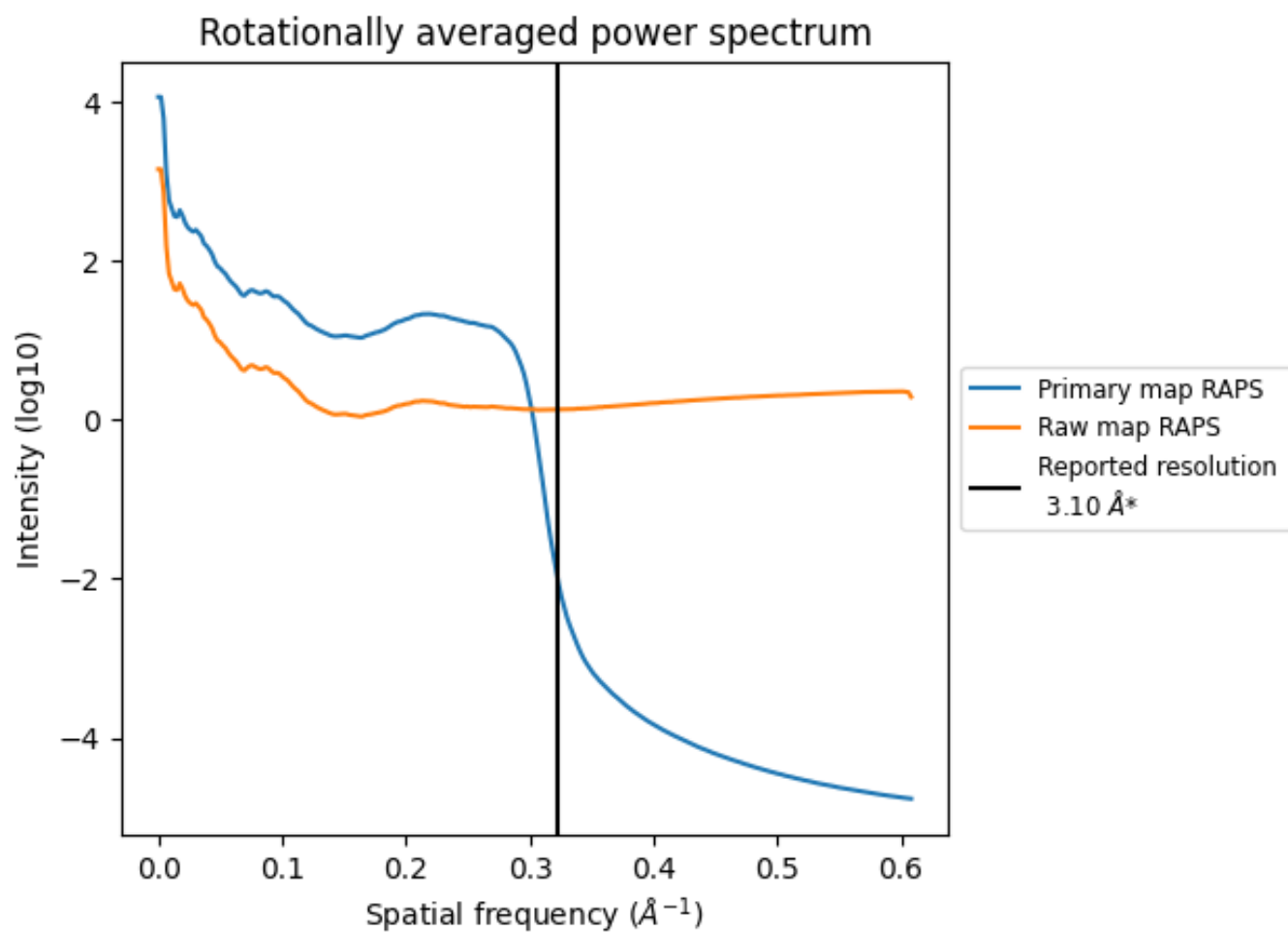
7.2 Volume estimate [i](#)



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](#)

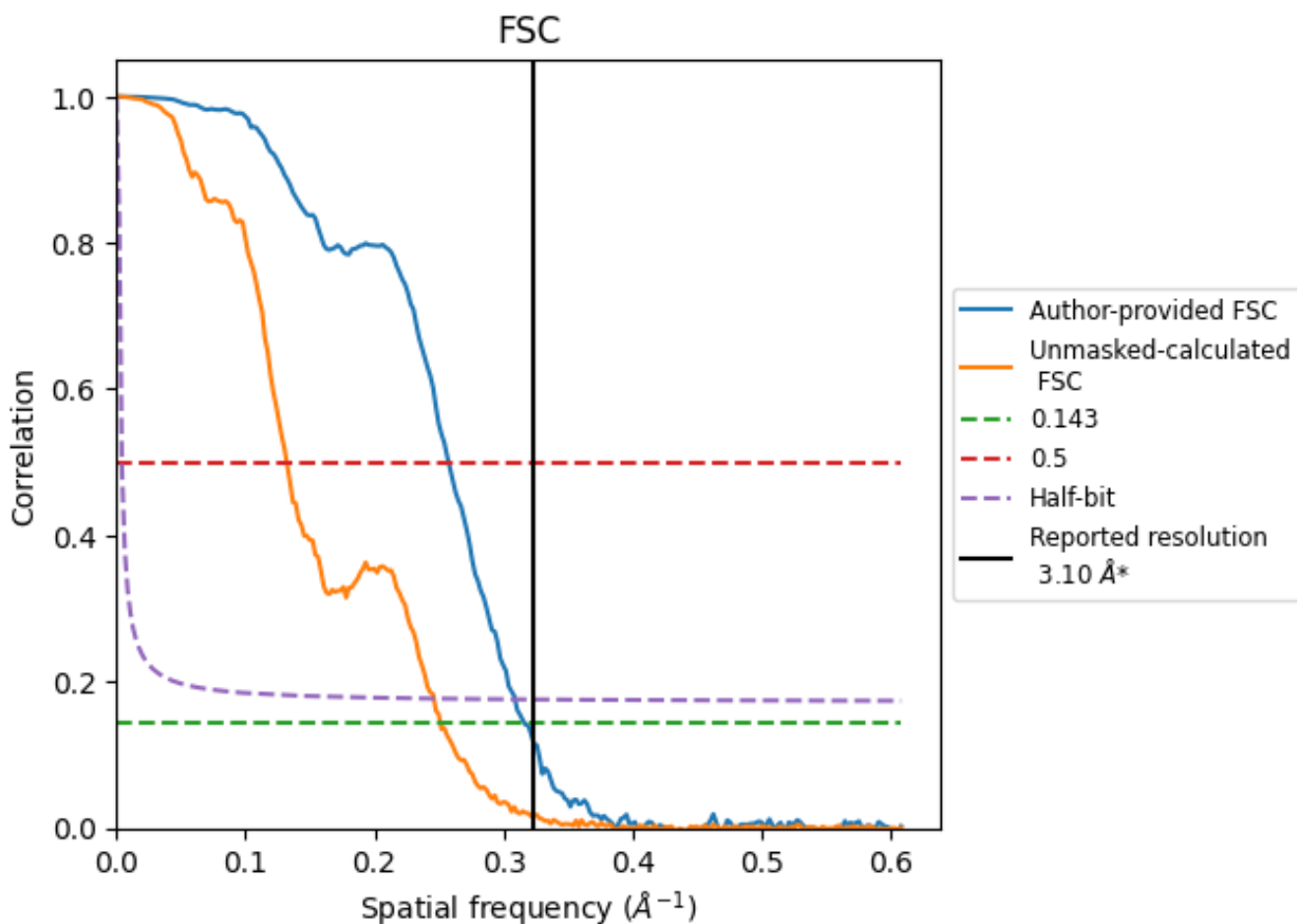


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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](#)

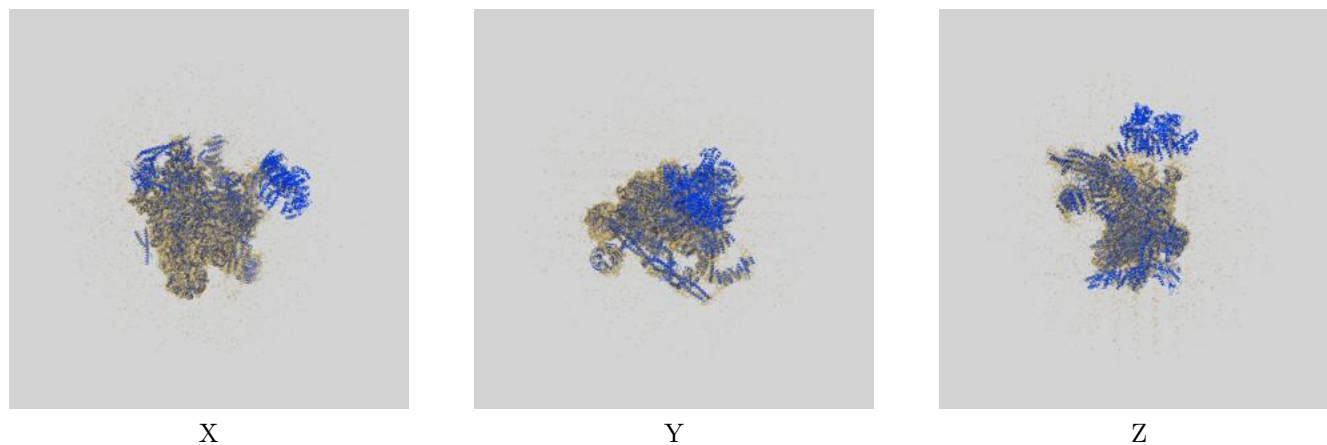
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.16	3.88	3.24
Unmasked-calculated*	3.98	7.58	4.06

*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](#)

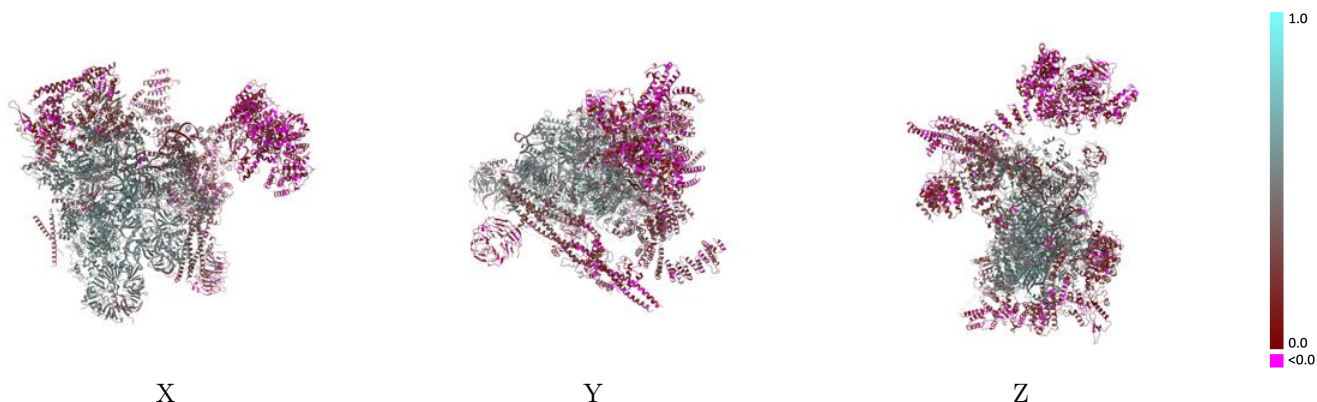
This section contains information regarding the fit between EMDB map EMD-19942 and PDB model 9ESI. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



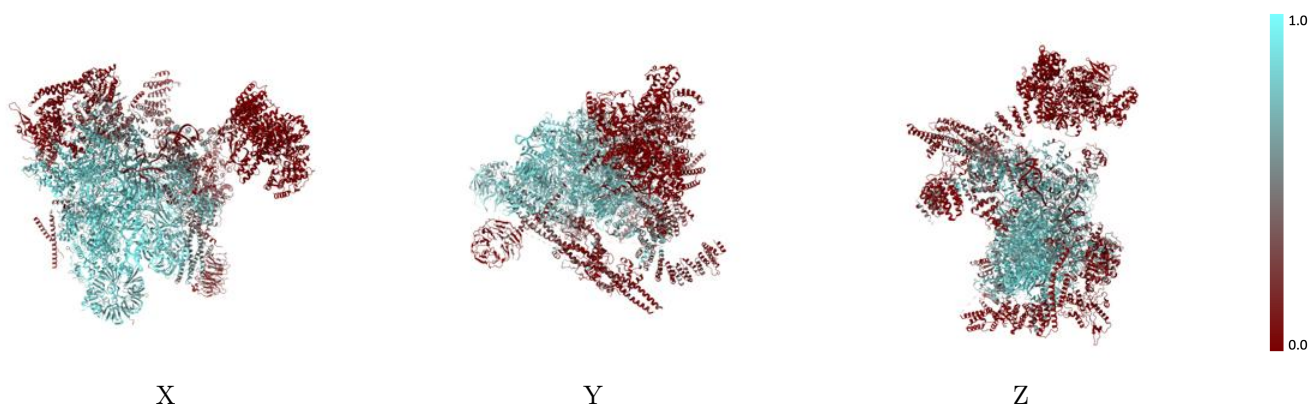
The images above show the 3D surface view of the map at the recommended contour level 3.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



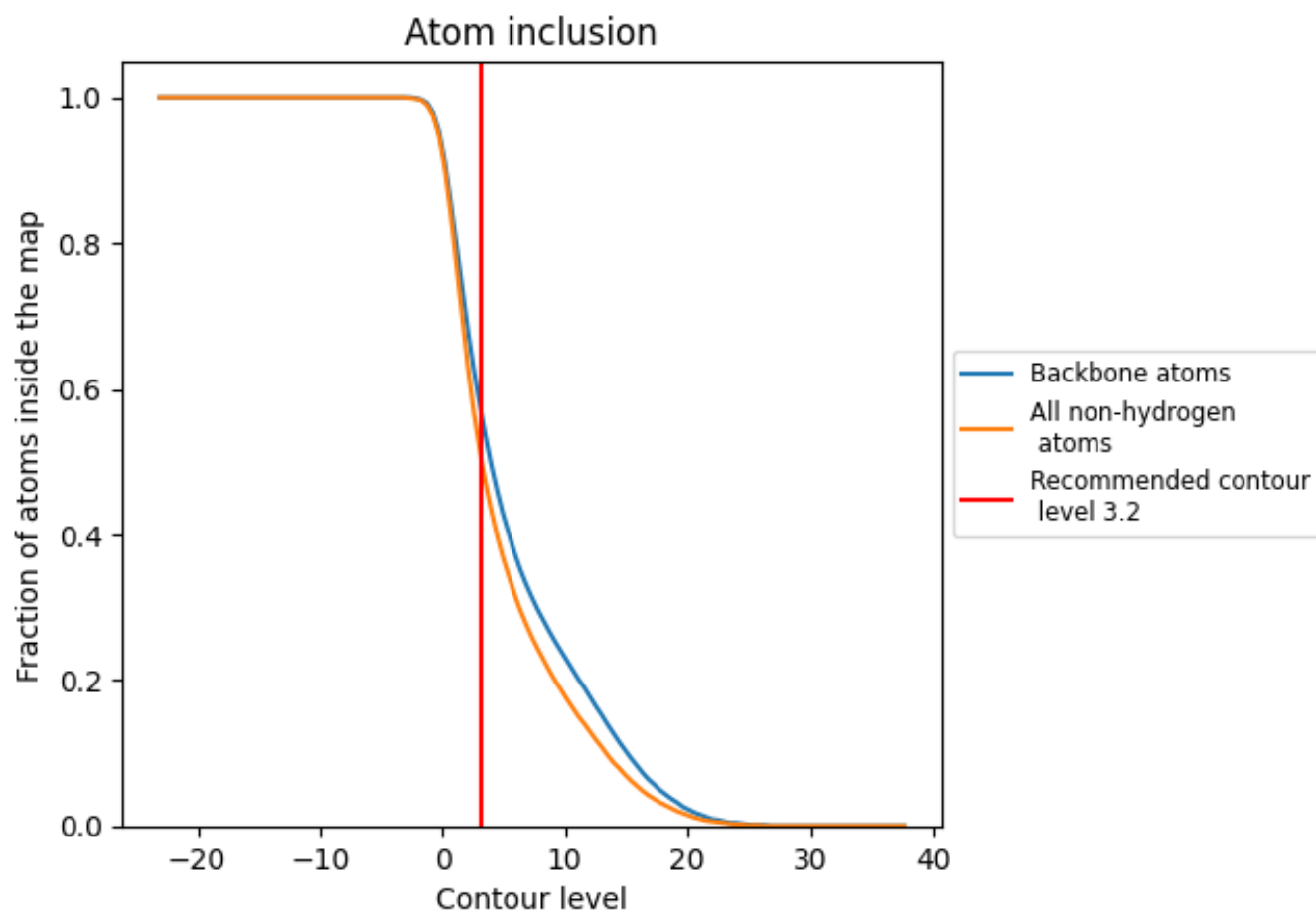
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



Continued on next page...

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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