



wwPDB EM Validation Summary Report ⓘ

Mar 28, 2026 – 04:57 AM UTC

PDB ID : 8RO2 / pdb_00008ro2
EMDB ID : EMD-19399
Title : Integrative Structure of the human intron lariat Spliceosome (ILS")
Authors : Rothe, P.; Vorlaender, M.K.; Plaschka, C.
Deposited on : 2024-01-11
Resolution : 3.50 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:

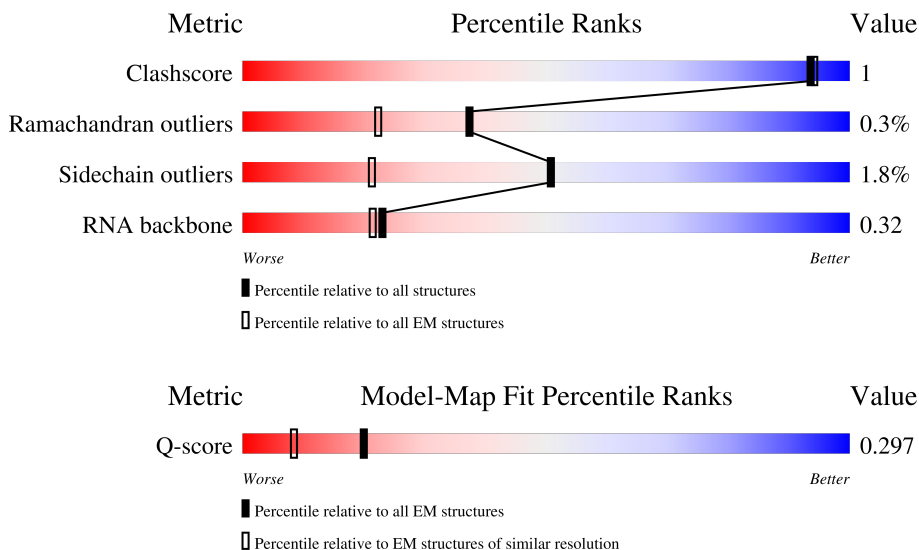
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	2	188	
2	6	106	
3	C	972	



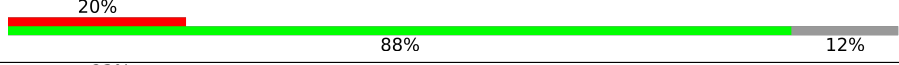



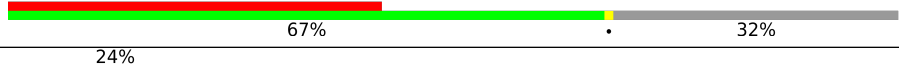




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Mol	Chain	Length	Quality of chain
4	D	285	
5	DX	795	
6	E	357	
7	J	848	
8	K	225	
9	L1	538	
10	N	144	
11	O	420	
12	Q	1485	
13	R	536	
14	S	166	
15	W	579	
16	Z	166	
17	a	126	
18	c	119	
19	d	118	
20	e	92	
21	f	86	
22	g	76	
23	q	504	
23	r	504	
23	s	504	
23	t	504	
24	z	451	
25	3	476	

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Mol	Chain	Length	Quality of chain
26	5	116	
27	A	2335	
28	I	855	
29	IN	154	
30	L	802	
31	L2	894	
32	M	243	
33	P	229	
34	PX	917	
35	T	514	
36	TF	837	
37	b	240	

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 81753 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 RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	39	823	368	137	279	39	0	0

- Molecule 2 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	6	97	2075	928	381	669	97	0	0

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	908	7184	4598	1194	1357	35	0	0

- Molecule 4 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	51	253	151	51	51	0	0

- Molecule 5 is a protein called ATP-dependent RNA helicase DHX15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	DX	650	3220	1920	650	650	0	0

- Molecule 6 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	E	299	2341	1470	411	447	13	0	0

- Molecule 7 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	J	561	2793	1671	561	561	0	0

- Molecule 8 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
8	K	189	941	563	189	189	0	0

- Molecule 9 is a protein called CWF19-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	L1	275	1353	803	275	275	0	0

- Molecule 10 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	N	143	1184	746	217	209	12	0	0

- Molecule 11 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	O	288	2328	1463	412	433	20	0	0

- Molecule 12 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	Q	1384	6859	4091	1384	1384	0	0

- Molecule 13 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	R	317	1571	937	317	317	0	0

- Molecule 14 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 15 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	158	Total	C	N	O	S	0	0
			1276	803	217	252	4		

- Molecule 16 is a protein called Coiled-coil domain-containing protein 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Z	92	Total	C	N	O	0	0
			459	275	92	92		

- Molecule 17 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	a	83	Total	C	N	O	S	0	0
			651	408	114	122	7		

- Molecule 18 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	c	81	Total	C	N	O	S	0	0
			641	409	112	116	4		

- Molecule 19 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	96	Total	C	N	O	S	0	0
			775	485	146	139	5		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	e	79	Total	C	N	O	S	0	0
			653	412	116	120	5		

- Molecule 21 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	72	Total	C	N	O	S	0	0
			564	364	93	102	5		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	73	Total	C	N	O	S	0	0
			568	358	102	102	6		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	132	Total	C	N	O	0	0
			659	395	132	132		
23	q	103	Total	C	N	O	0	0
			514	308	103	103		
23	r	119	Total	C	N	O	0	0
			594	356	119	119		
23	t	103	Total	C	N	O	0	0
			514	308	103	103		

- Molecule 24 is a protein called Splicing regulator SDE2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	z	25	Total	C	N	O	S	0	0
			198	119	35	41	3		

- Molecule 25 is a protein called Splicing factor ESS-2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	60	Total	C	N	O	S	0	0
			499	311	85	102	1		

- Molecule 26 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	5	92	Total	C	N	O	P	0	0
			1936	867	322	655	92		

- Molecule 27 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	A	1981	16477	10621	2883	2902	71	0	0

- Molecule 28 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	I	753	3739	2233	753	753	0	0

- Molecule 29 is a RNA chain called INTRON.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	O	P		
29	IN	41	492	205	246	41	0	0

- Molecule 30 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	L	555	3623	2216	695	705	7	0	0

- Molecule 31 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L2	369	3049	1930	527	569	23	0	0

- Molecule 32 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	M	166	827	495	166	166	0	0

- Molecule 33 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	P	112	942	575	184	181	2	0	0

- Molecule 34 is a protein called PAX3- and PAX7-binding protein 1.

Mol	Chain	Residues	Atoms			AltConf	Trace	
			Total	C	N			O
34	PX	295	1465	875	295	295	0	0

- Molecule 35 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	T	360	2854	1800	521	523	10	0	0

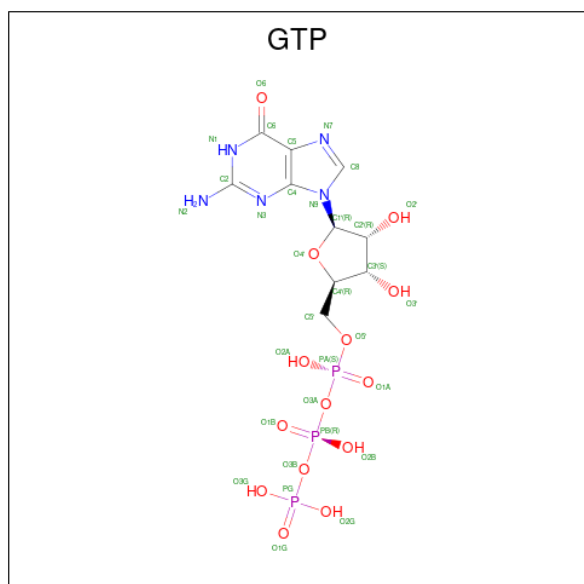
- Molecule 36 is a protein called Tuftelin-interacting protein 11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
36	TF	572	2835	1690	572	573	0	0

- Molecule 37 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	b	94	717	449	135	126	7	0	0

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

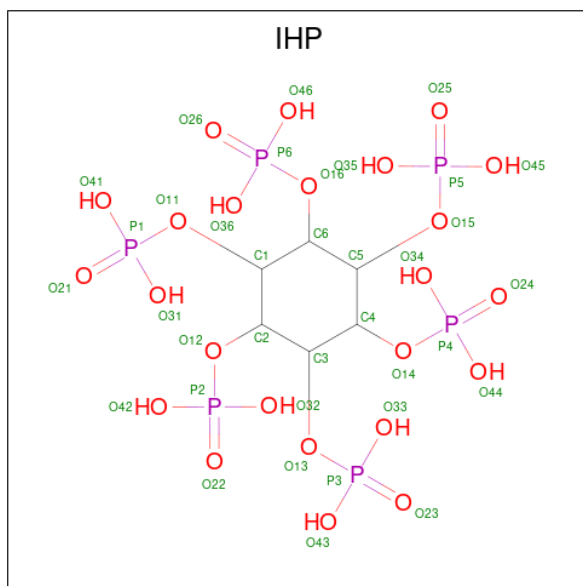


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	C	1	32	10	5	14	3	0

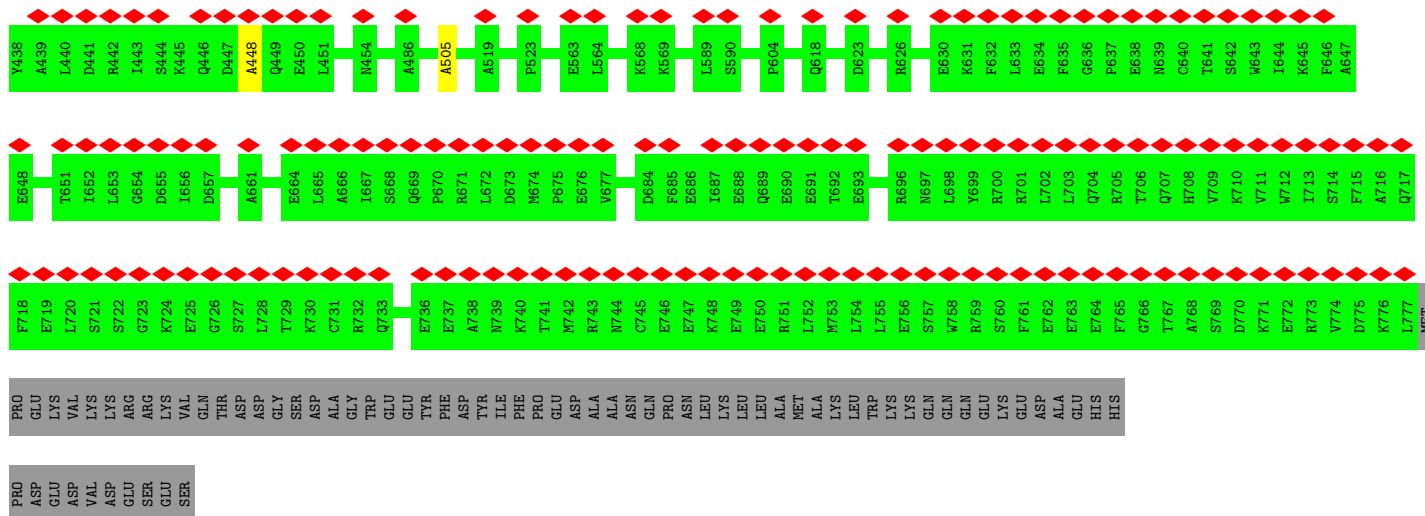
- Molecule 39 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
39	N	3	Total	Zn	0
			3	3	

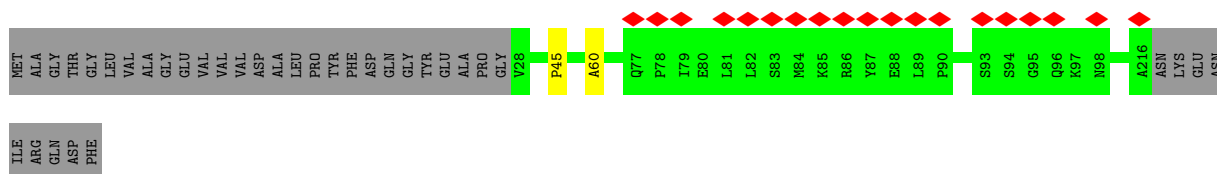
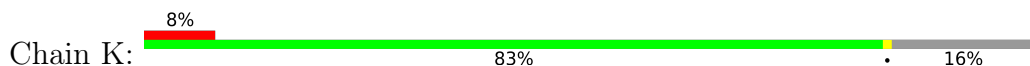
- Molecule 40 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



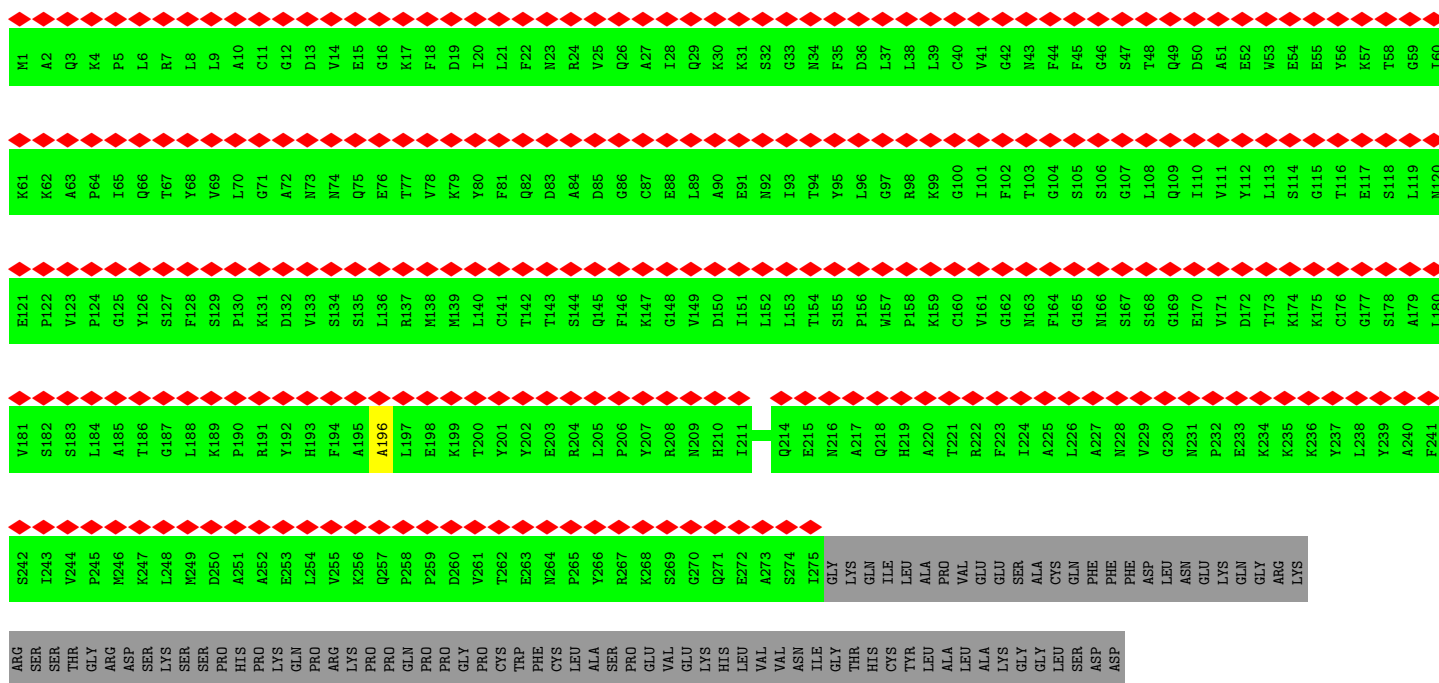
Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	C	O	P	0
			36	6	24	6	



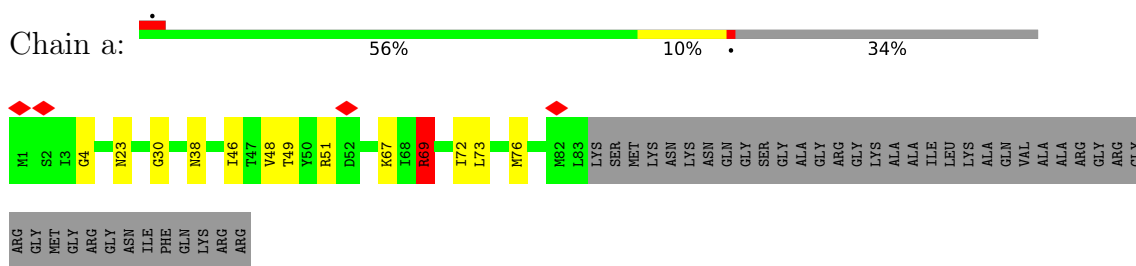
• Molecule 8: Pre-mRNA-splicing factor SPF27



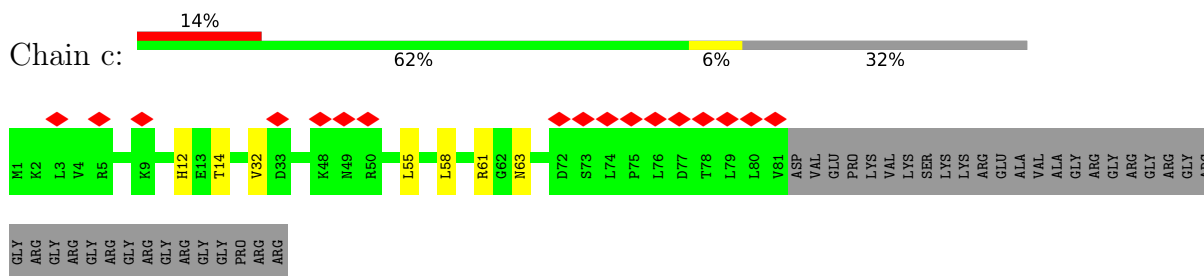
• Molecule 9: CWF19-like protein 1



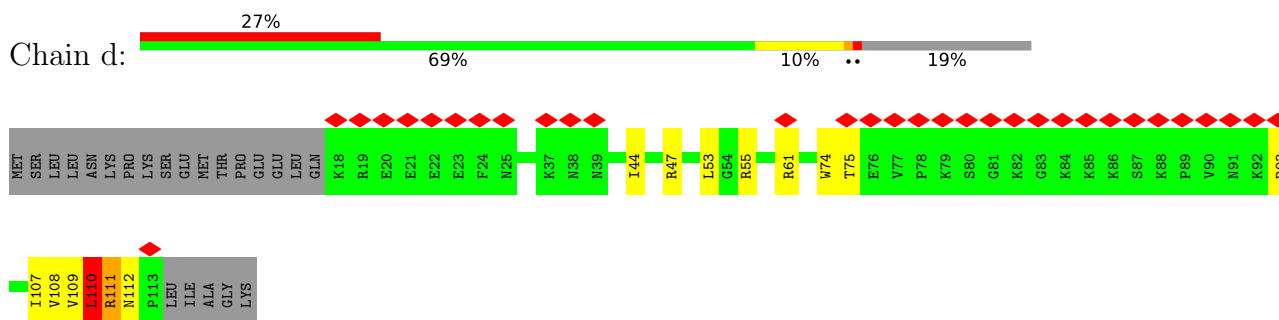
L193	R194	K195	F196	L199	I200	K201	K202	N203	D204	E205	K206	M207	D208	P209	E210	A211	Q214	A215	E218	F221	L222	S223	Q224	L225	I226	K234	S235	V236	P237	L238	S239	E240	P241	V242	T243	M244	D245	K246	V247	H248	Y249	C250	E251	R252	F253	I254	E255	M257	I258	D259	E261	A262							
L264	L264	P265	T272	I273	L274	D275	H278	L279	F368	L280	V281	H282	C283	L284	Y285	L286	S286	N287	L288	V289	R290	R291	E292	E293	D294	G295	H296	L297	F298	S299	Q300	L301	L302	D303	M304	L305	T306	F307	S308	T309	G310	F311	E312	I313	N314	D315	Q316	T317	G318	N319	A320	L321	E322	E323	N324	A341	A357		
E358	V359	D360	T361	R362	E363	S364	L365	S366	K367	F368	F369	G370	P371	L372	S373	S374	S375	T376	L377	V380	A381	L384	C385	L386	L387	P388	T389	L390	P391	K392	N393	E394	D395	T396	T397	F398	D399	K400	E401	F402	L403	L404	E405	L406	L407	V408	S409	R410	H411	E412	R413	R414	I415	S416	L426	Y427			
P428	T429	E430	K431	I432	I433	W434	D435	E436	N437	I438	V439	P440	T441	E442	Y443	Y444	S445	G446	E447	G448	C449	L450	A451	L452	P453	K454	L455	N456	L457	L462	Y465	L466	L467	R468	N469	F470	N471	L472	F473	R474	L475	E476	S477	T478	Y479	E480	I481	R482	Q483	D484	I485	I486	R487	S488	V489	S490	R491		
M492	K493	P494	W495	Q496	S497	E498	Y499	G500	G501	V502	V503	F504	G505	G506	M507	A508	R509	M510	A511	Q512	P513	I514	V515	A516	F517	T518	V519	V520	E521	V522	A523	K524	P525	M526	I527	G528	E529	M530	N531	P532	T533	R534	V535	R536	E537	D538	V539	T540	I541	M542	L543	M544	V545	R546	D547	H548	I549	K550	D551
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R674	H675	L676	M677	N678	D680	C681	W686	L687	H688	D689	L690	L691	L692	G693	Y694	G695	D696	S703	K704	R705	F706	R707	Q708	L709	A710	T711	L712	D713	F714	N715	D716	T717	F718	L719	S720	L721	E722	H723	L724	K725	A726	S727	F728	F729	G730	H731	N732	W733	K734	W735	T736	W737							
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M798	T799	I800	Q801	F802	T803	H804	T805	Q806	L807	E808	A809	I810	R811	A812	G813	M814	O815	V821	V822	G823	P824	P825	G826	T827	G828	K829	T830	D831	V832	A833	V834	Q835	I836	I837	S838	T849	L850	L851	V852	S855	M856	O857	A858	L859	M860	O861	L862	F863	E864	K865	I866	M867	A868	L869	D870	I871			
D872	E873	R874	H875	L876	L877	R878	L879	G880	H881	G882	E883	E884	E885	L886	E887	T888	K889	D891	F892	S893	R894	Y895	G896	R897	W898	N899	Y900	V901	L902	A903	R904	R905	I906	E907	K983	G984	R985	A1064	Y987	E988	K913	R914	L915	Q916	K917	S918	L919	G920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931
A932	G933	Y934	F935	F936	L937	Y938	Q939	K954	G955	S956	T957	L958	P959	D960	V961	E963	I1033	Y964	S965	T966	F967	H971	E972	F973	F974	A975	N976	A977	P978	Q979	P980	I981	L1060	M1061	K983	G984	R985	A1064	Y987	E988	K913	R914	L915	Q916	K917	S918	L919	G920	V921	P922	G923	D924	A925	S926	Y927	T928	C929	E930	T931
F1011	R1012	A1013	S1014	E1015	L1016	L1017	R1018	S1019	G1020	L1021	D1022	R1023	S1024	K1025	E1031	A1032	K1033	I1034	I1035	A1036	M1037	H1047	D1048	L1049	V1050	K1051	L1052	G1053	F1054	M1058	I1059	L1060	M1061	E1062	E1063	A1064	A1065	Q1066	I1067	L1068	E1069	I1070	E1071	T1072	F1073	I1074	P1075	L1076	F1081	Q1082	D1083	G1084	F1085	I1094					



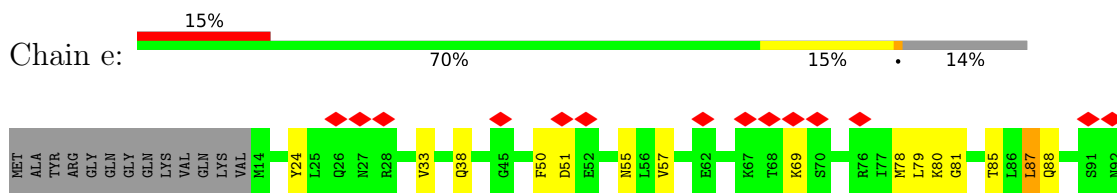
• Molecule 18: Small nuclear ribonucleoprotein Sm D1



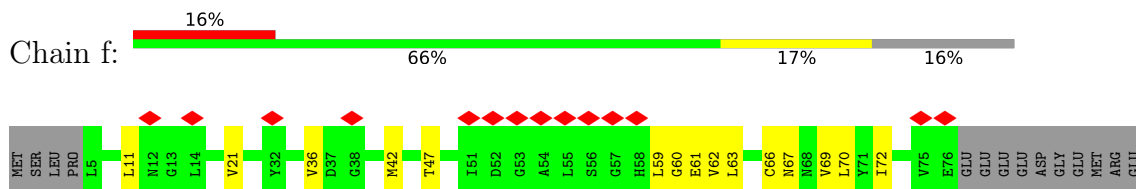
• Molecule 19: Small nuclear ribonucleoprotein Sm D2



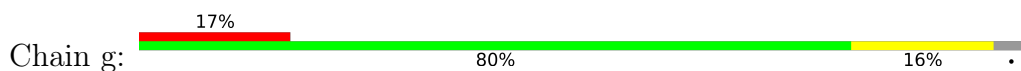
• Molecule 20: Small nuclear ribonucleoprotein E

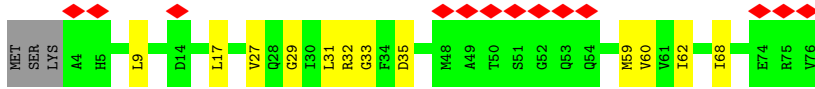


• Molecule 21: Small nuclear ribonucleoprotein F



• Molecule 22: Small nuclear ribonucleoprotein G

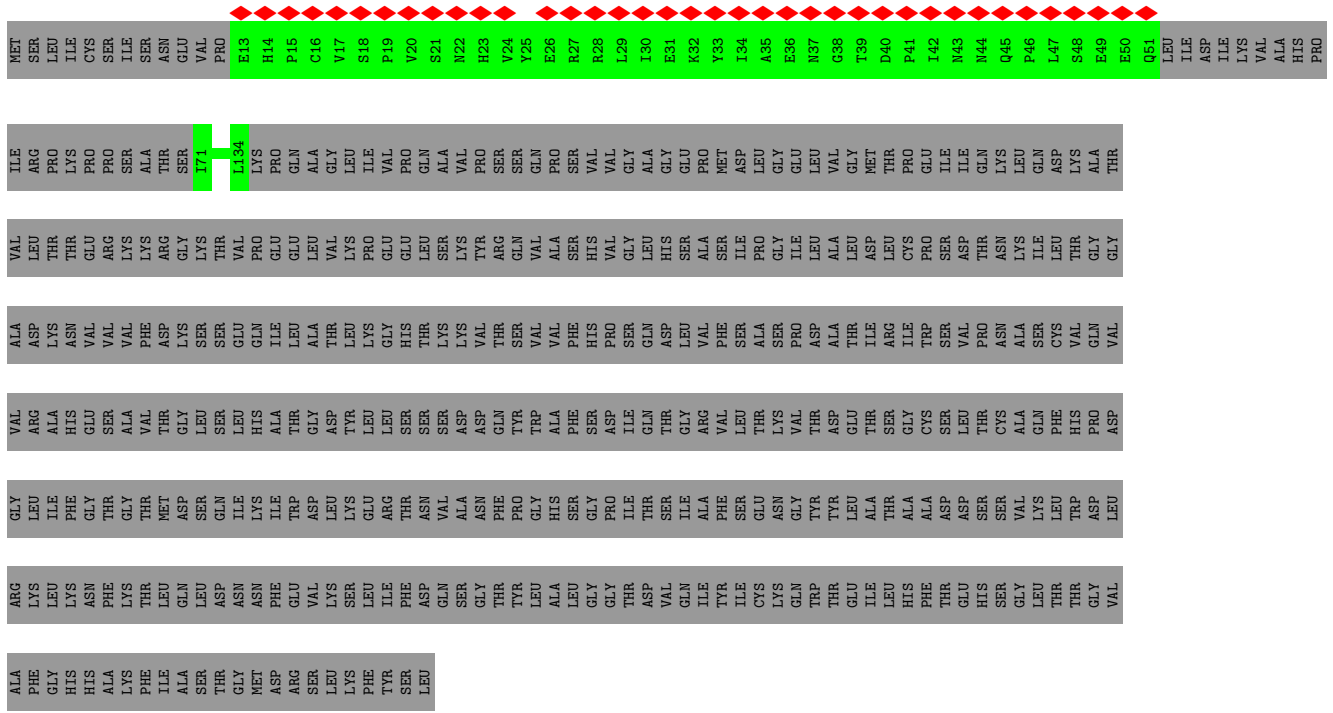




• Molecule 23: Pre-mRNA-processing factor 19

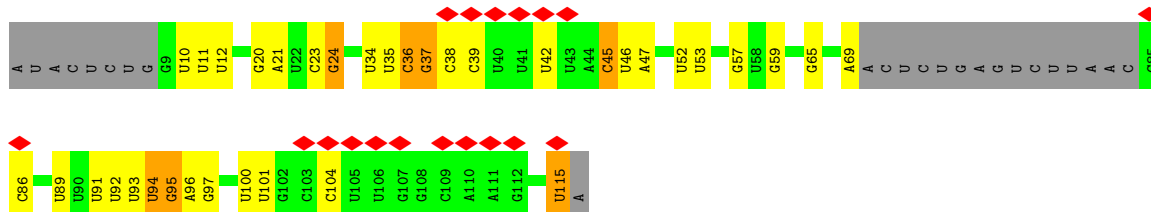


• Molecule 23: Pre-mRNA-processing factor 19

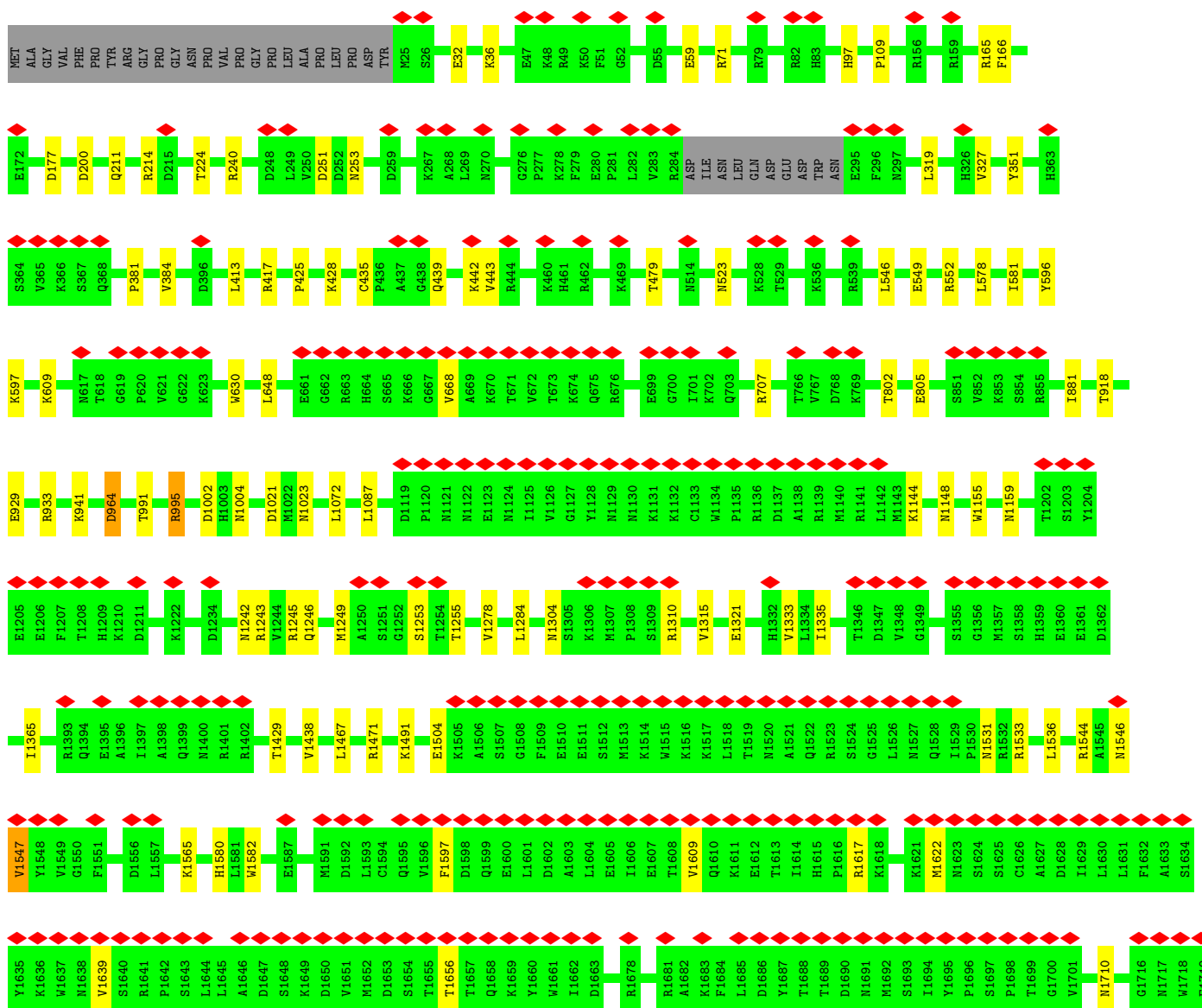
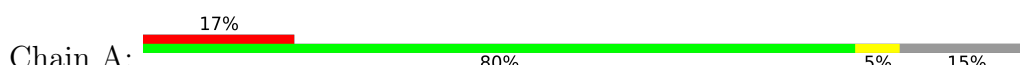


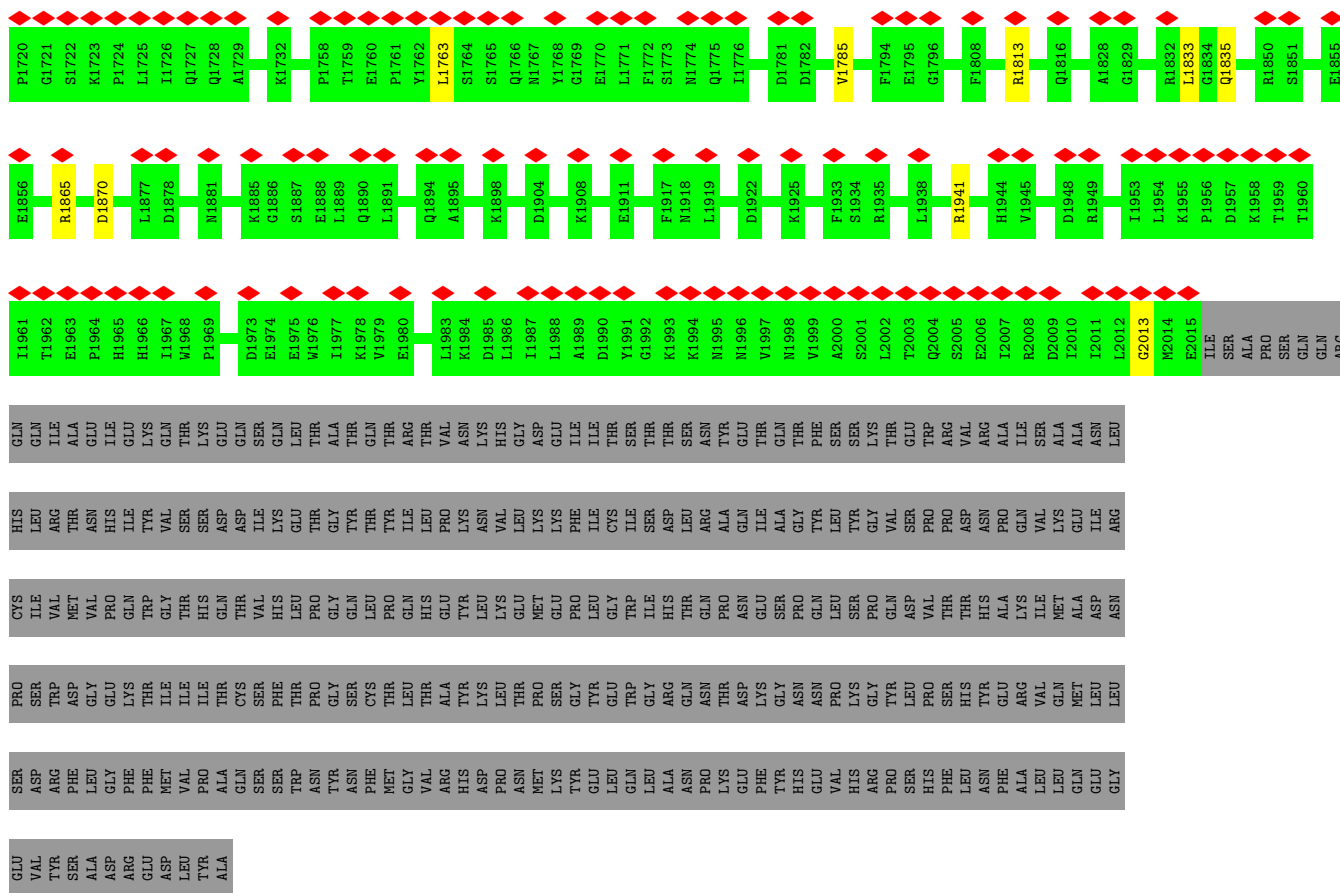
SER	THR	HIS	LEU	LYS	THR	PRO	ALA	SER	GLY	LEU	GLN	THR	PRO	THR	THR	THR	THR	PRO	ALA	ALA	PRO	GLY	SER	ALA	THR	ARG	THR	PRO	LEU	LEU	GLN	GLN	ASP	PRO	ALA	ALA	SER	ILE	THR	THR	ASP	ASN	LEU	LEU	LEU	GLN	LEU	LEU	ALA	ALA	ARG	ARG	ARG	LYS	ALA	ALA	SER	ASP	ASP	PHE	PHE
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 26: U5 snRNA

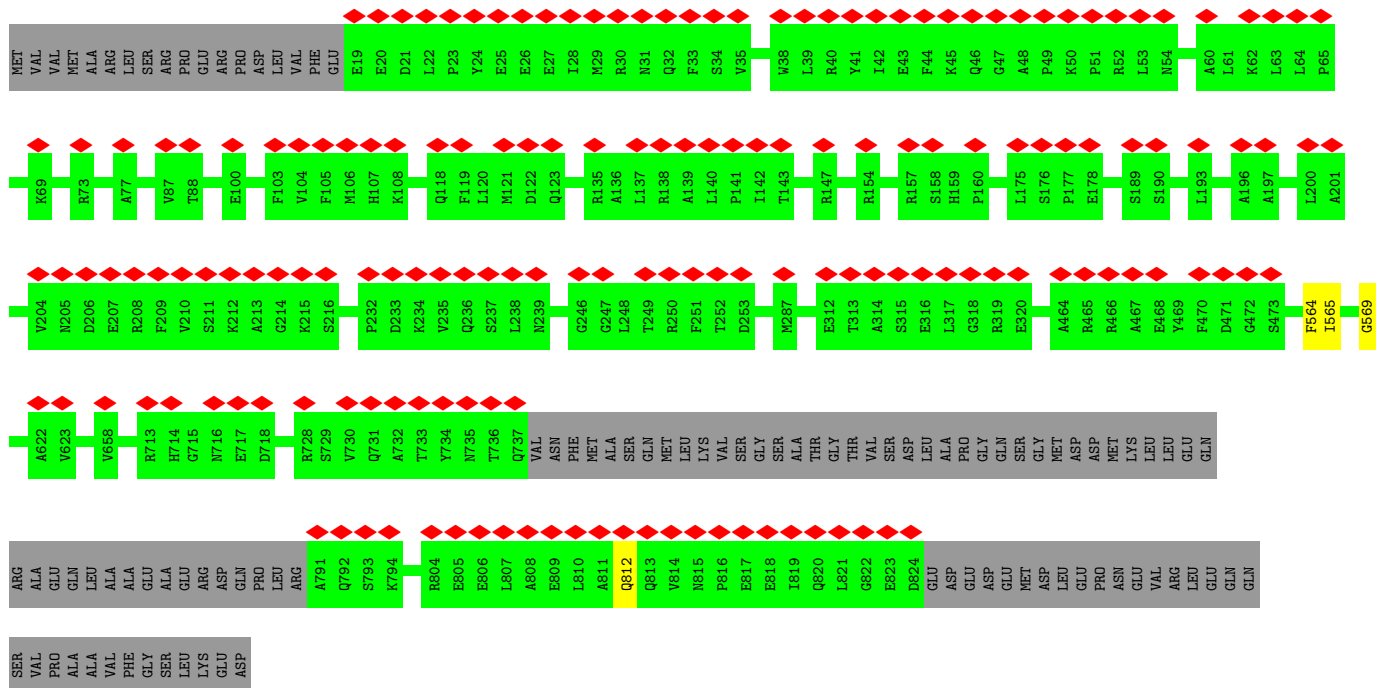
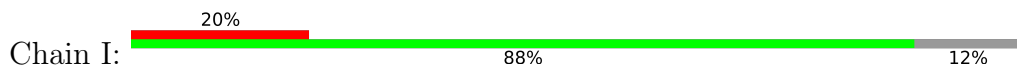


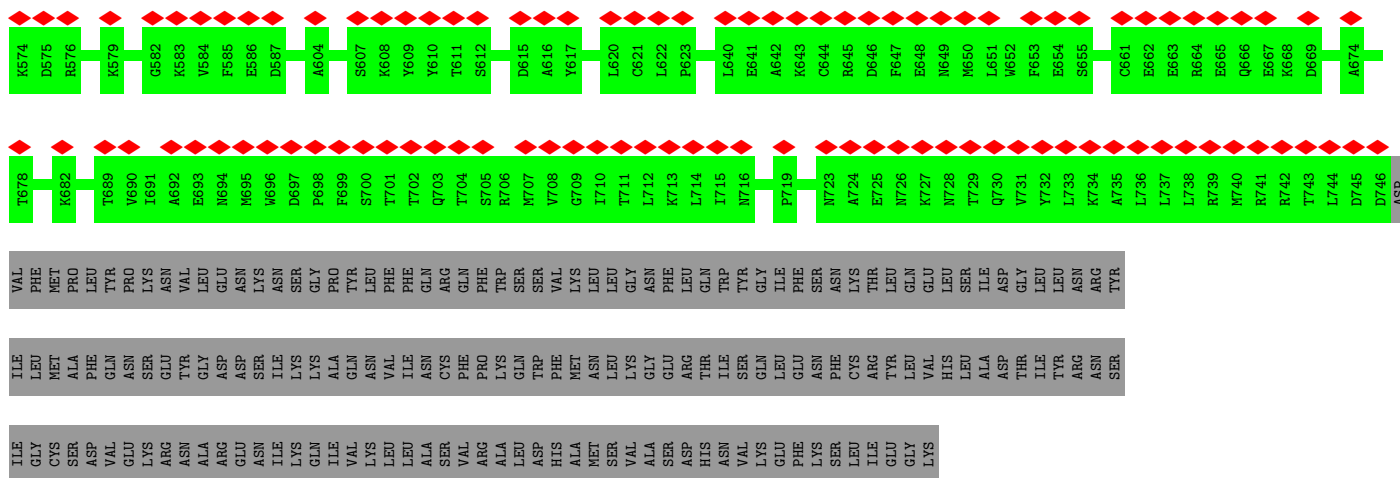
• Molecule 27: Pre-mRNA-processing-splicing factor 8



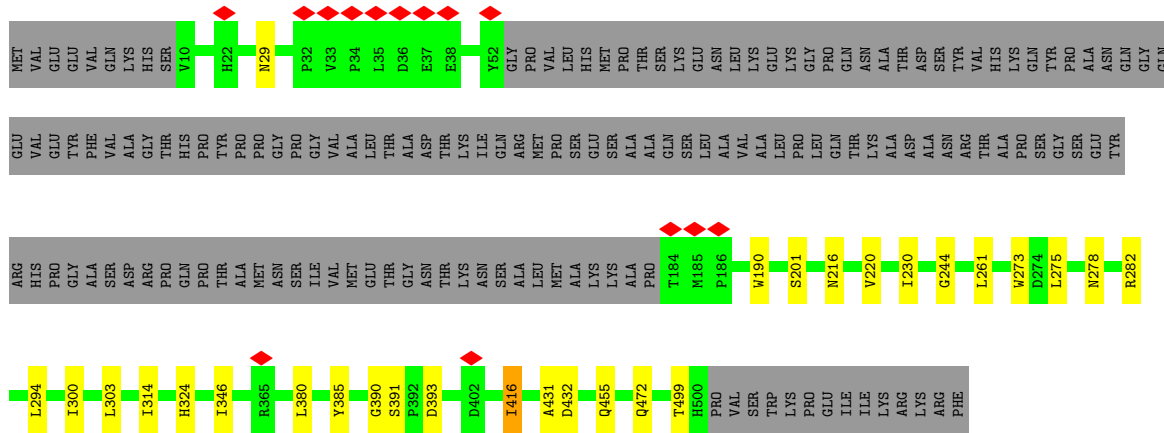


● Molecule 28: Pre-mRNA-splicing factor SYF1

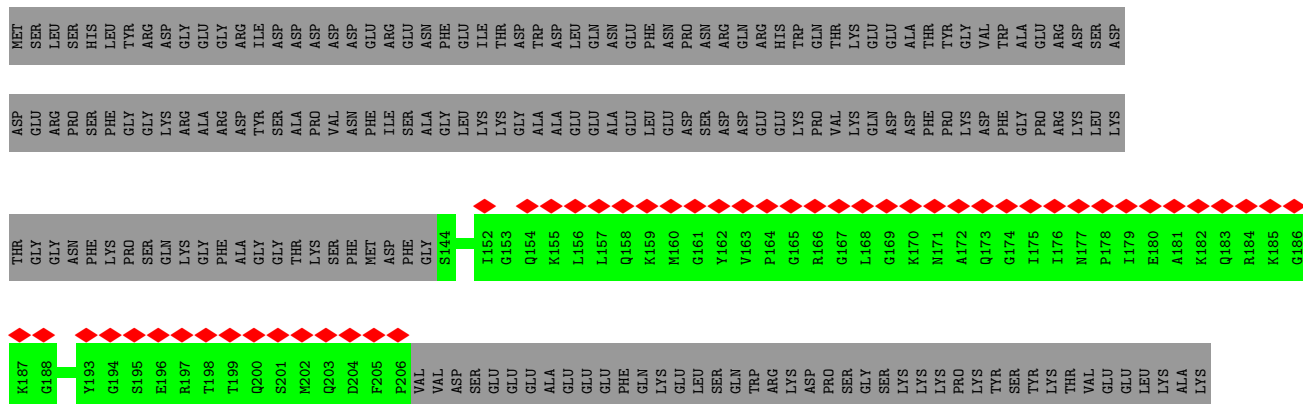




• Molecule 35: Pleiotropic regulator 1



• Molecule 36: Tuftelin-interacting protein 11



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87951	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	5.823	Depositor
Minimum map value	0.000	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.127	Depositor
Recommended contour level	0.975	Depositor
Map size (Å)	519.75, 519.75, 519.75	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	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: ZN, IHP, GTP, SEP

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	2	0.38	0/917	0.83	1/1425 (0.1%)
2	6	0.34	0/2323	0.72	6/3619 (0.2%)
3	C	0.34	1/7346 (0.0%)	0.79	0/9980
4	D	0.45	0/252	0.93	0/350
5	DX	0.36	0/3219	0.89	0/4487
6	E	0.31	0/2394	0.72	0/3243
7	J	0.36	0/2792	0.94	0/3900
8	K	0.38	0/940	0.93	0/1312
9	L1	0.32	0/1352	0.81	2/1878 (0.1%)
10	N	0.33	0/1210	0.82	1/1622 (0.1%)
11	O	0.41	1/2378 (0.0%)	0.92	3/3211 (0.1%)
12	Q	0.35	0/6858	0.82	0/9563
13	R	0.41	0/1558	1.01	3/2168 (0.1%)
14	S	0.30	0/1268	0.76	0/1714
15	W	0.33	0/1306	0.84	0/1760
16	Z	0.38	0/458	0.84	0/639
17	a	0.44	0/659	1.15	6/888 (0.7%)
18	c	0.43	0/649	1.11	1/877 (0.1%)
19	d	0.45	0/785	1.09	0/1049
20	e	0.43	0/661	1.12	1/886 (0.1%)
21	f	0.45	0/575	1.12	6/776 (0.8%)
22	g	0.48	0/575	1.06	1/768 (0.1%)
23	q	0.42	0/512	0.89	0/713
23	r	0.45	0/592	0.88	0/825
23	s	0.39	0/658	0.91	0/919
23	t	0.42	0/512	0.89	0/713
24	z	0.25	0/200	0.64	0/266
25	3	0.32	0/504	0.86	0/675
26	5	0.31	0/2157	0.70	2/3351 (0.1%)
27	A	0.34	0/16926	0.82	3/22947 (0.0%)
28	I	0.38	0/3737	0.94	0/5213
30	L	0.32	0/3657	0.81	1/4979 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	L2	0.33	0/3117	0.86	0/4183
32	M	0.39	0/825	0.91	0/1150
33	P	0.36	0/957	0.84	1/1276 (0.1%)
34	PX	0.40	0/1463	0.86	0/2039
35	T	0.33	0/2927	0.82	1/3980 (0.0%)
36	TF	0.38	0/2830	0.84	0/3937
37	b	0.38	0/726	0.95	2/966 (0.2%)
All	All	0.36	2/82775 (0.0%)	0.85	41/114247 (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
3	C	0	1
17	a	0	2
19	d	0	3
20	e	0	1
22	g	0	1
27	A	0	3
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	926	ALA	C-N	7.23	1.42	1.33
11	O	225	PRO	C-N	5.43	1.46	1.33

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	37	G	N9-C1'-C2'	7.93	123.90	112.00
27	A	941	LYS	N-CA-C	7.40	126.17	109.81
11	O	225	PRO	N-CA-C	7.18	119.47	110.70
17	a	4	GLY	CA-C-N	6.50	124.34	120.24
17	a	4	GLY	C-N-CA	6.50	124.34	120.24

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	940	ARG	Sidechain
17	a	51	ARG	Sidechain
17	a	69	ARG	Sidechain
19	d	55	ARG	Sidechain
19	d	61	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	823	0	416	2	0
2	6	2075	0	1048	11	0
3	C	7184	0	7206	21	0
4	D	253	0	120	0	0
5	DX	3220	0	1416	2	0
6	E	2341	0	2275	4	0
7	J	2793	0	1241	0	0
8	K	941	0	424	0	0
9	L1	1353	0	620	0	0
10	N	1184	0	1189	5	0
11	O	2328	0	2317	9	0
12	Q	6859	0	2971	0	0
13	R	1571	0	725	3	0
14	S	1236	0	1210	7	0
15	W	1276	0	1221	11	0
16	Z	459	0	204	0	0
17	a	651	0	669	5	0
18	c	641	0	689	3	0
19	d	775	0	818	6	0
20	e	653	0	668	8	0
21	f	564	0	572	8	0
22	g	568	0	590	7	0
23	q	514	0	236	0	0
23	r	594	0	270	0	0
23	s	659	0	299	0	0
23	t	514	0	236	0	0
24	z	198	0	184	0	0
25	3	499	0	479	0	0
26	5	1936	0	982	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	A	16477	0	16462	49	0
28	I	3739	0	1699	2	0
29	IN	492	0	330	4	0
30	L	3623	0	2842	6	0
31	L2	3049	0	2973	23	0
32	M	827	0	380	1	0
33	P	942	0	929	2	0
34	PX	1465	0	620	0	0
35	T	2854	0	2812	16	0
36	TF	2835	0	1200	4	0
37	b	717	0	736	4	0
38	C	32	0	12	0	0
39	N	3	0	0	0	0
40	A	36	0	6	2	0
All	All	81753	0	62296	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

The worst 5 of 191 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:6:59:G:H1	2:6:76:A:H61	1.01	0.96
2:6:59:G:H1	2:6:76:A:N6	1.75	0.84
14:S:56:ILE:HG12	14:S:62:ILE:HG23	1.78	0.65
14:S:57:ILE:HD13	15:W:97:ASN:HB3	1.80	0.63
2:6:1:G:O2'	10:N:99:ASN:ND2	2.33	0.62

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	906/972 (93%)	868 (96%)	35 (4%)	3 (0%)	36	67
4	D	49/285 (17%)	48 (98%)	0	1 (2%)	6	32
5	DX	648/795 (82%)	631 (97%)	15 (2%)	2 (0%)	36	67
6	E	297/357 (83%)	285 (96%)	12 (4%)	0	100	100
7	J	559/848 (66%)	548 (98%)	9 (2%)	2 (0%)	30	62
8	K	187/225 (83%)	182 (97%)	3 (2%)	2 (1%)	11	43
9	L1	273/538 (51%)	264 (97%)	9 (3%)	0	100	100
10	N	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
11	O	286/420 (68%)	265 (93%)	21 (7%)	0	100	100
12	Q	1382/1485 (93%)	1346 (97%)	35 (2%)	1 (0%)	48	79
13	R	313/536 (58%)	281 (90%)	27 (9%)	5 (2%)	7	36
14	S	157/166 (95%)	143 (91%)	11 (7%)	3 (2%)	6	33
15	W	156/579 (27%)	137 (88%)	19 (12%)	0	100	100
16	Z	90/166 (54%)	83 (92%)	7 (8%)	0	100	100
17	a	81/126 (64%)	71 (88%)	10 (12%)	0	100	100
18	c	79/119 (66%)	69 (87%)	10 (13%)	0	100	100
19	d	94/118 (80%)	82 (87%)	12 (13%)	0	100	100
20	e	77/92 (84%)	63 (82%)	13 (17%)	1 (1%)	9	39
21	f	70/86 (81%)	64 (91%)	6 (9%)	0	100	100
22	g	71/76 (93%)	65 (92%)	6 (8%)	0	100	100
23	q	99/504 (20%)	97 (98%)	2 (2%)	0	100	100
23	r	115/504 (23%)	112 (97%)	2 (2%)	1 (1%)	14	47
23	s	130/504 (26%)	126 (97%)	4 (3%)	0	100	100
23	t	99/504 (20%)	97 (98%)	2 (2%)	0	100	100
24	z	23/451 (5%)	23 (100%)	0	0	100	100
25	3	56/476 (12%)	56 (100%)	0	0	100	100
27	A	1977/2335 (85%)	1863 (94%)	112 (6%)	2 (0%)	48	79
28	I	749/855 (88%)	728 (97%)	20 (3%)	1 (0%)	48	79
30	L	547/802 (68%)	514 (94%)	32 (6%)	1 (0%)	43	74
31	L2	363/894 (41%)	321 (88%)	37 (10%)	5 (1%)	9	38
32	M	162/243 (67%)	159 (98%)	3 (2%)	0	100	100
33	P	108/229 (47%)	103 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	PX	291/917 (32%)	286 (98%)	5 (2%)	0	100	100
35	T	356/514 (69%)	337 (95%)	19 (5%)	0	100	100
36	TF	562/837 (67%)	549 (98%)	12 (2%)	1 (0%)	43	74
37	b	88/240 (37%)	78 (89%)	8 (9%)	2 (2%)	5	30
All	All	11641/18942 (62%)	11069 (95%)	539 (5%)	33 (0%)	37	67

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	L2	579	VAL
3	C	166	CYS
13	R	47	ARG
13	R	277	THR
3	C	126	SER

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	
3	C	807/866 (93%)	796 (99%)	11 (1%)	59	71
6	E	256/300 (85%)	254 (99%)	2 (1%)	73	77
10	N	130/130 (100%)	128 (98%)	2 (2%)	57	71
11	O	258/361 (72%)	255 (99%)	3 (1%)	63	73
14	S	129/134 (96%)	126 (98%)	3 (2%)	44	64
15	W	135/502 (27%)	132 (98%)	3 (2%)	45	65
17	a	73/101 (72%)	69 (94%)	4 (6%)	19	46
18	c	76/101 (75%)	74 (97%)	2 (3%)	40	62
19	d	90/110 (82%)	83 (92%)	7 (8%)	11	36
20	e	74/84 (88%)	72 (97%)	2 (3%)	39	62
21	f	61/74 (82%)	60 (98%)	1 (2%)	55	70
22	g	63/66 (96%)	59 (94%)	4 (6%)	16	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	z	21/371 (6%)	20 (95%)	1 (5%)	23	49
25	3	55/395 (14%)	55 (100%)	0	100	100
27	A	1792/2108 (85%)	1768 (99%)	24 (1%)	61	72
30	L	231/709 (33%)	227 (98%)	4 (2%)	53	70
31	L2	334/806 (41%)	327 (98%)	7 (2%)	47	66
33	P	103/203 (51%)	102 (99%)	1 (1%)	68	75
35	T	313/441 (71%)	308 (98%)	5 (2%)	55	70
37	b	74/177 (42%)	71 (96%)	3 (4%)	27	53
All	All	5075/8039 (63%)	4986 (98%)	89 (2%)	51	69

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	A	1021	ASP
30	L	222	LEU
27	A	1315	VAL
27	A	1622	MET
31	L2	657	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
27	A	1658	GLN
35	T	433	ASN
27	A	1965	HIS
35	T	417	ASN
35	T	278	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	38/188 (20%)	19 (50%)	1 (2%)
2	6	96/106 (90%)	42 (43%)	7 (7%)
26	5	90/116 (77%)	26 (28%)	2 (2%)
29	IN	0/154	-	-
All	All	224/564 (39%)	87 (38%)	10 (4%)

5 of 87 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	8	C
1	2	14	C
1	2	15	U
1	2	16	U
1	2	19	G

5 of 10 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	6	82	A
26	5	92	U
26	5	95	G
2	6	35	A
2	6	50	A

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
13	SEP	R	224	13	3,4,10	0.71	0	2,4,14	1.27	0
13	SEP	R	232	13	3,4,10	0.74	0	2,4,14	1.35	0

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
13	SEP	R	224	13	-	0/1/2/10	-
13	SEP	R	232	13	-	0/1/2/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 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
40	IHP	A	3000	-	36,36,36	1.55	6 (16%)	60,60,60	0.96	5 (8%)
38	GTP	C	1500	-	33,34,34	1.03	4 (12%)	50,54,54	1.57	9 (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
40	IHP	A	3000	-	-	0/30/54/54	0/1/1/1
38	GTP	C	1500	-	-	3/22/38/38	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	3000	IHP	P1-O11	3.34	1.65	1.59
40	A	3000	IHP	P3-O13	3.33	1.65	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	A	3000	IHP	P6-O16	3.30	1.65	1.59
40	A	3000	IHP	P2-O12	3.27	1.65	1.59
40	A	3000	IHP	P5-O15	3.22	1.65	1.59

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	C	1500	GTP	C5-C4-N3	-4.94	120.53	128.39
38	C	1500	GTP	C2-N3-C4	4.36	119.80	112.30
38	C	1500	GTP	N9-C4-N3	3.27	132.50	125.95
40	A	3000	IHP	C5-C6-C1	2.85	116.68	110.43
38	C	1500	GTP	C2-N1-C6	-2.82	120.00	125.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

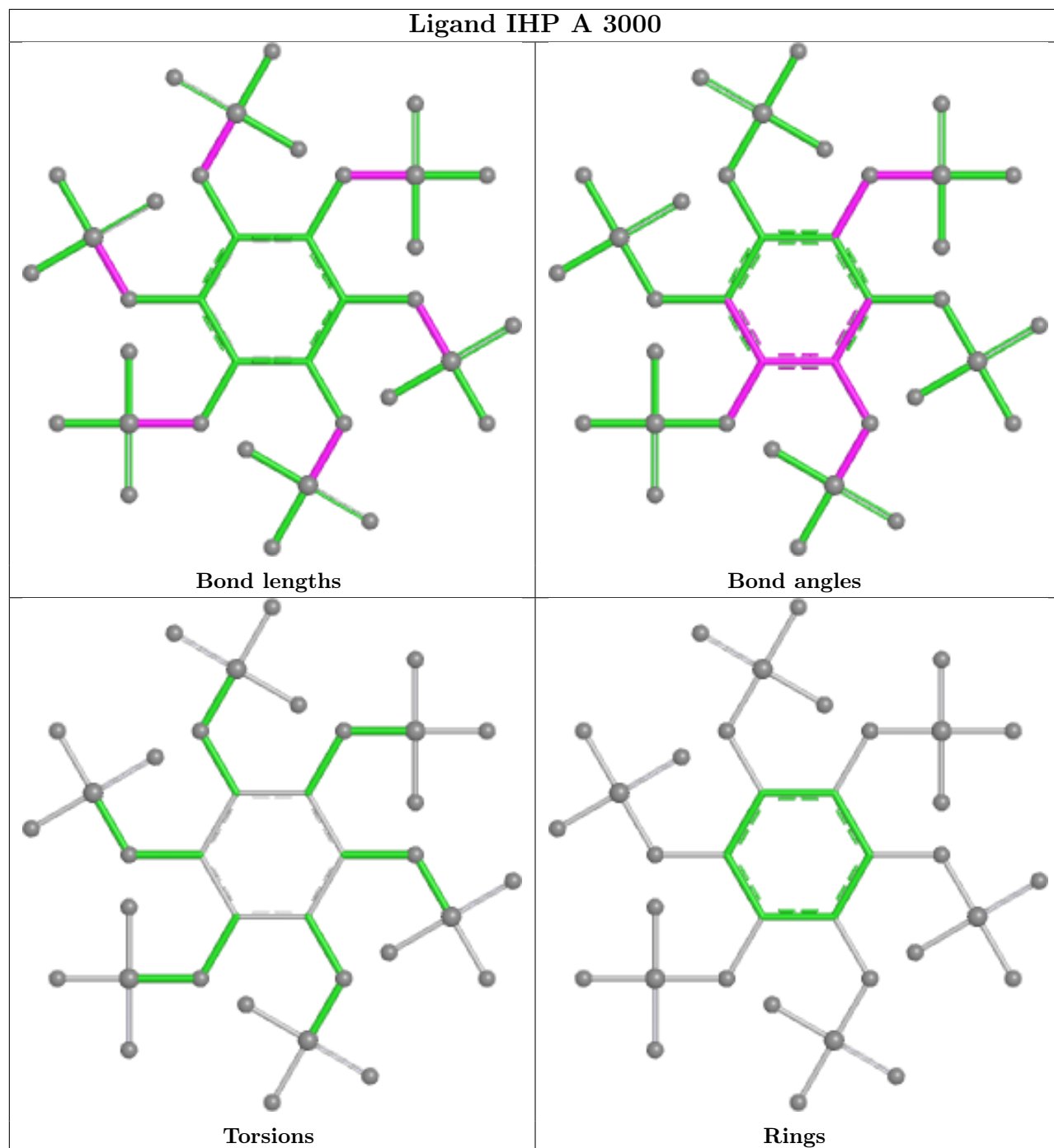
Mol	Chain	Res	Type	Atoms
38	C	1500	GTP	C5'-O5'-PA-O2A
38	C	1500	GTP	C5'-O5'-PA-O3A
38	C	1500	GTP	C5'-O5'-PA-O1A

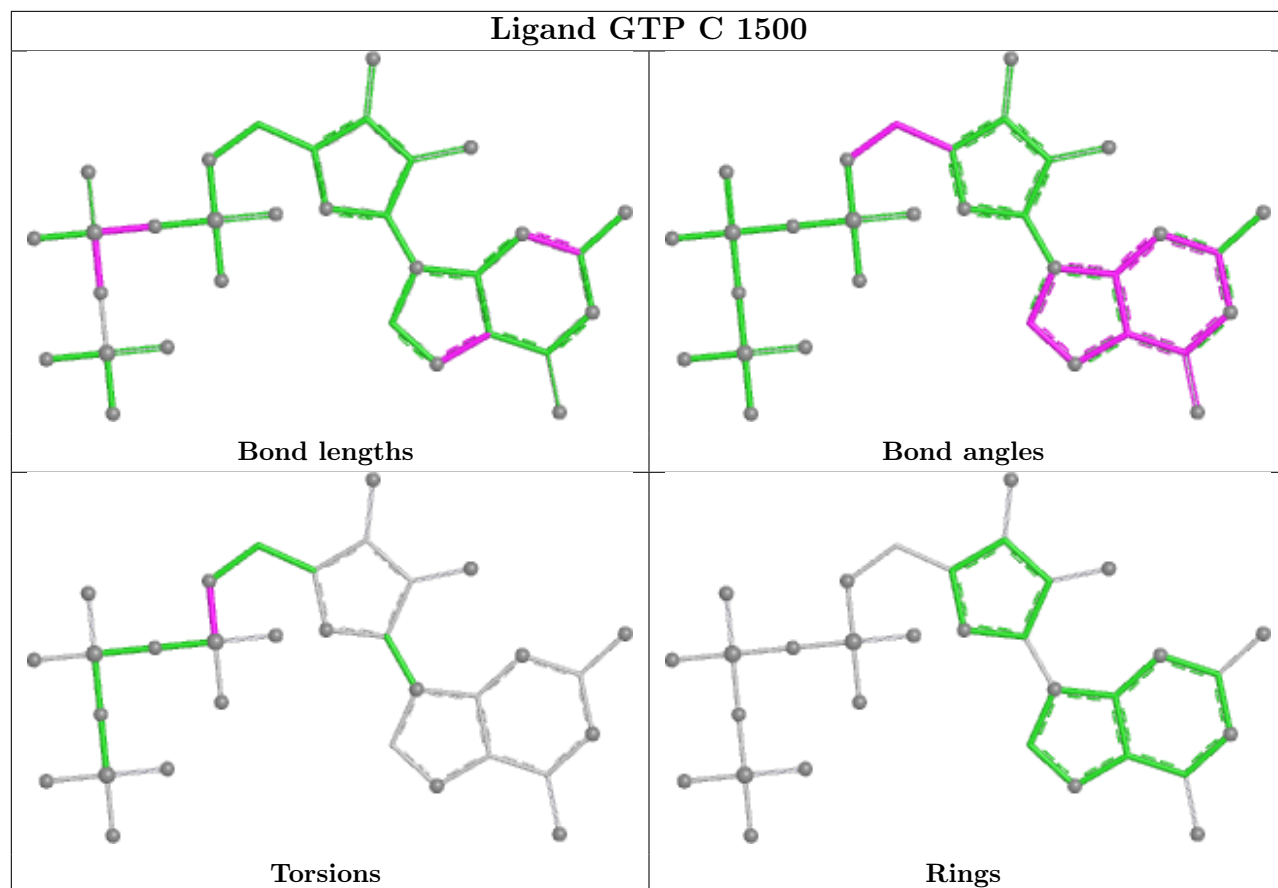
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	A	3000	IHP	2	0

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.

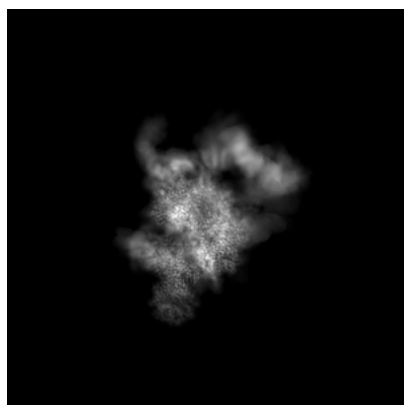
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19399. These allow visual inspection of the internal detail of the map and identification of artifacts.

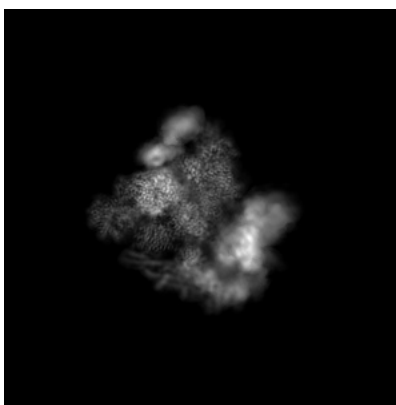
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

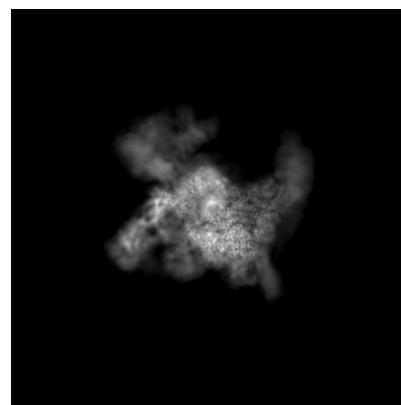
6.1.1 Primary map



X



Y

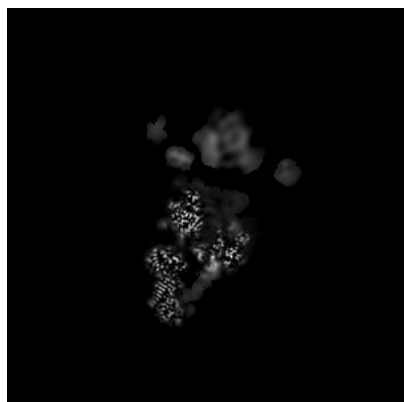


Z

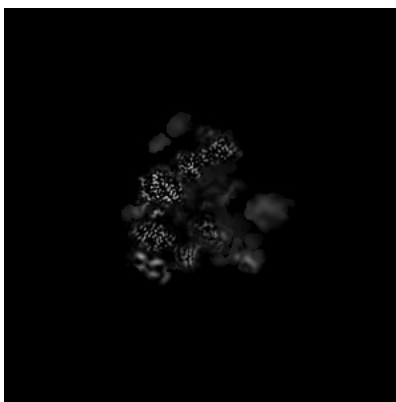
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

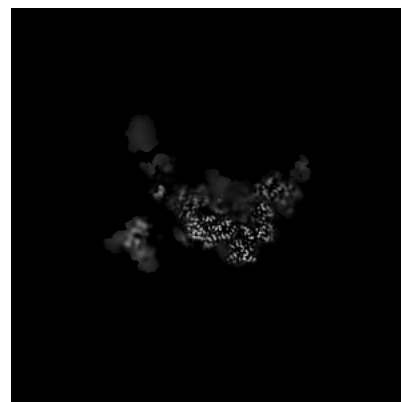
6.2.1 Primary map



X Index: 210



Y Index: 210

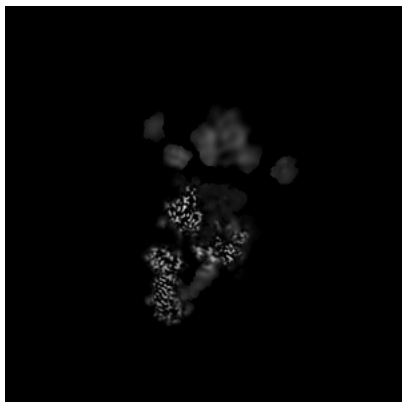


Z Index: 210

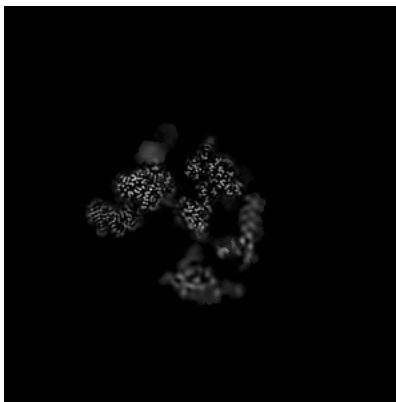
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [\(i\)](#)

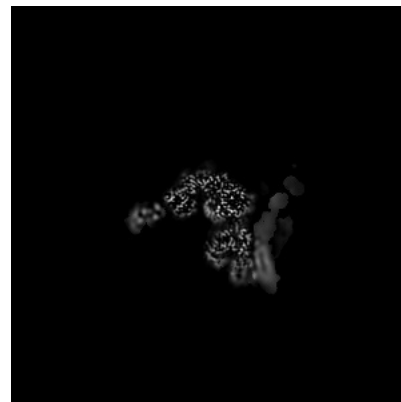
6.3.1 Primary map



X Index: 208



Y Index: 181

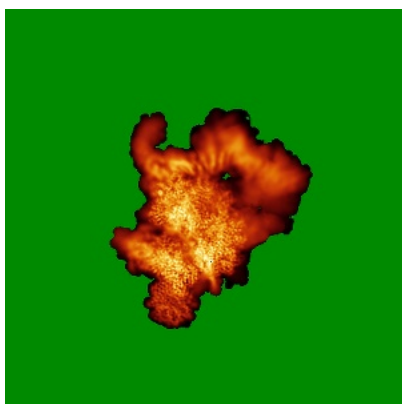


Z Index: 164

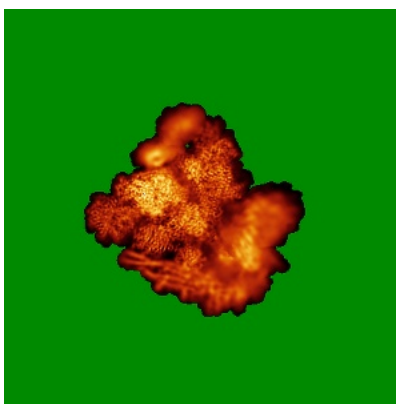
The images above show the largest variance slices of the map in three orthogonal directions.

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

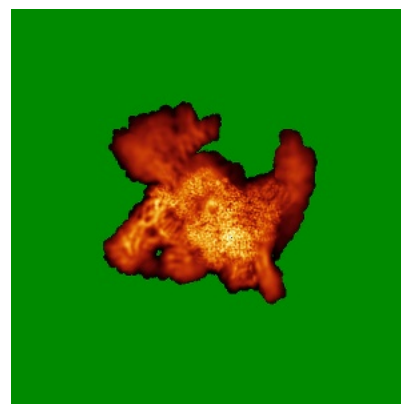
6.4.1 Primary map



X



Y

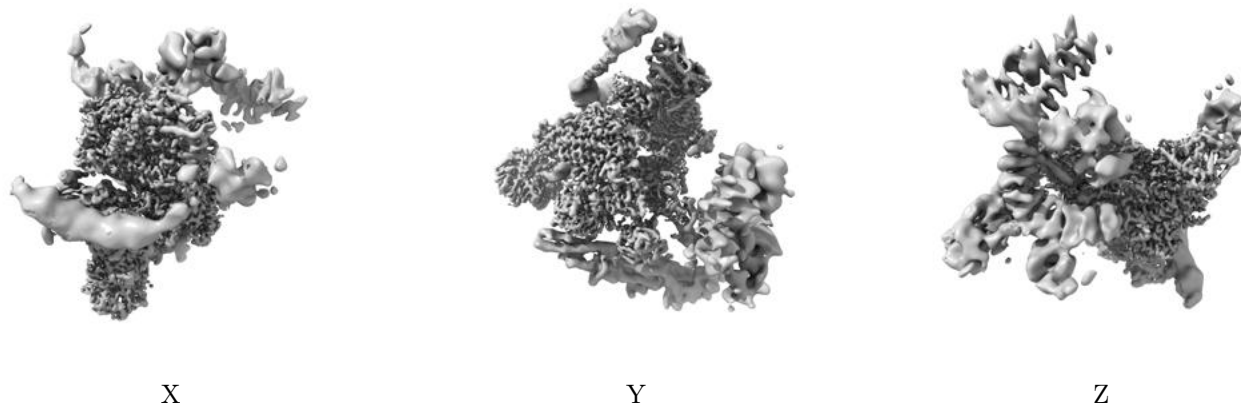


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.975. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

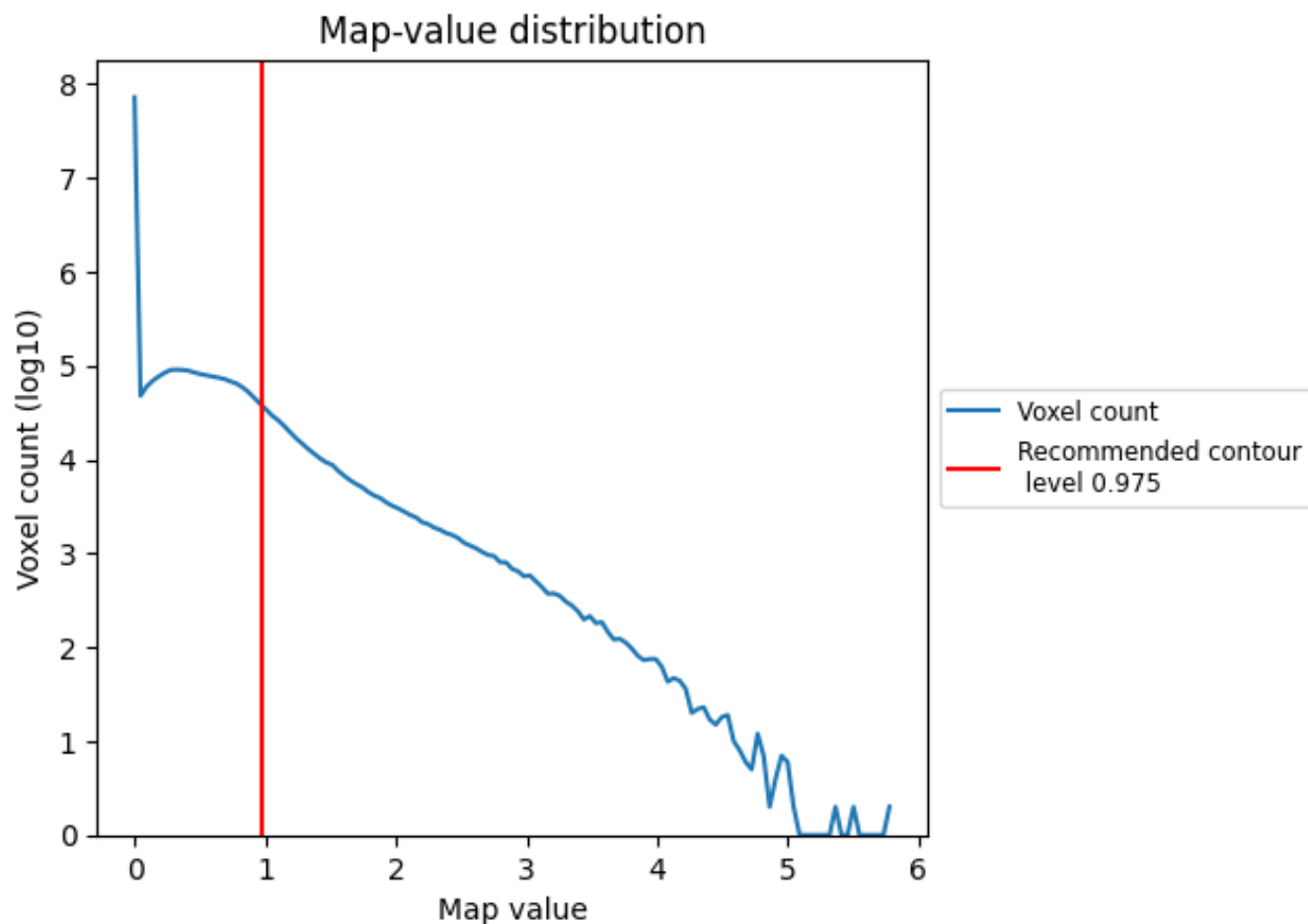
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

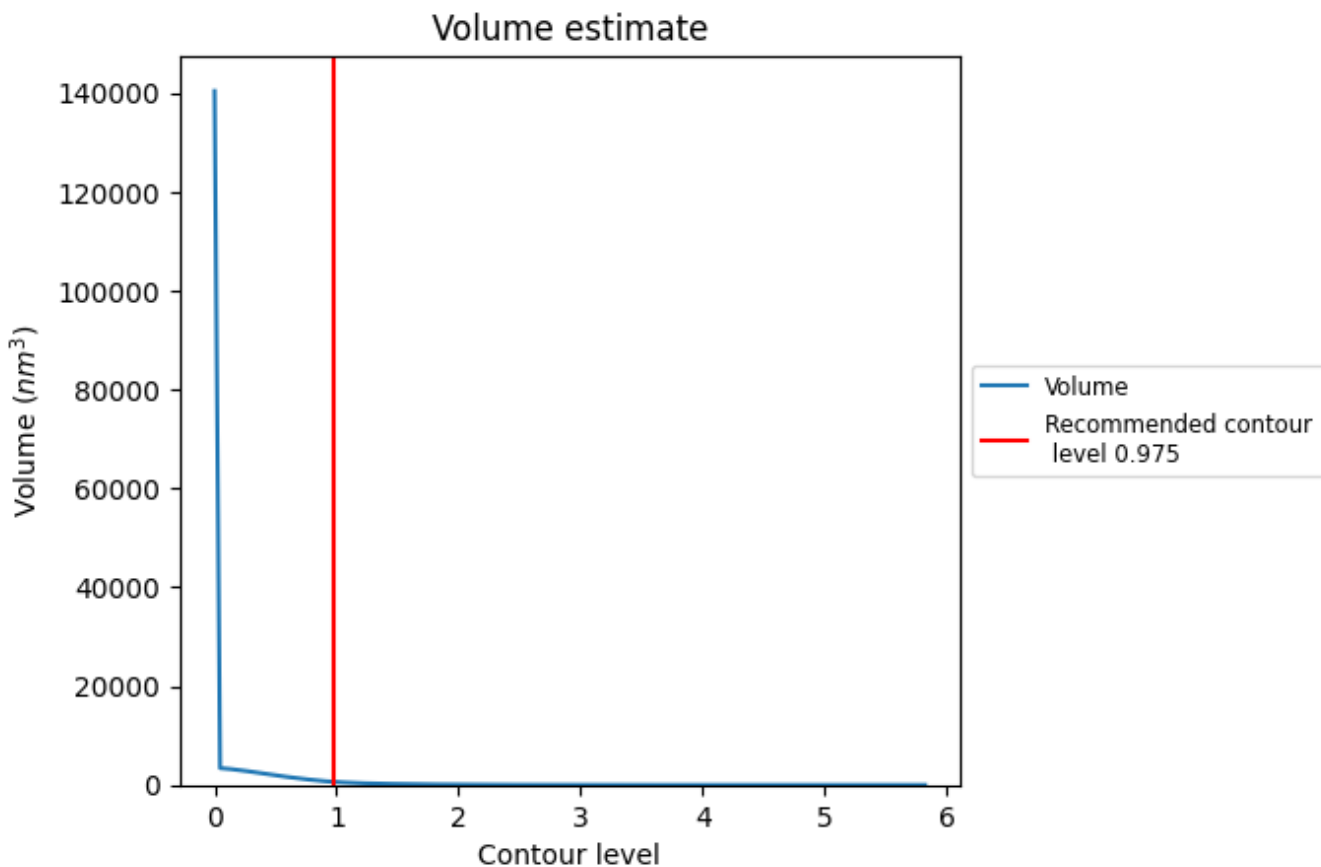
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

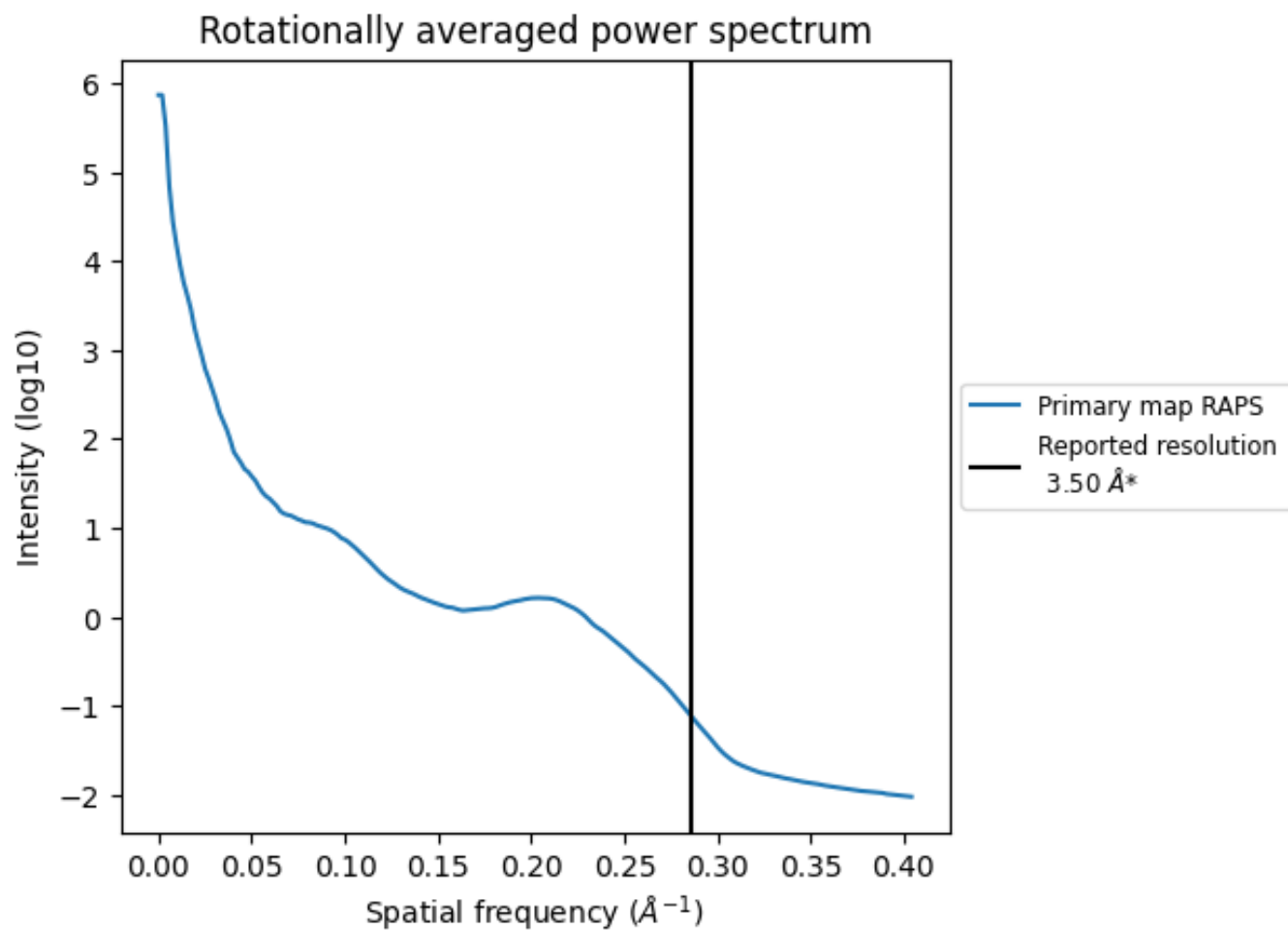
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 632 nm³; this corresponds to an approximate mass of 571 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 0.286 Å⁻¹

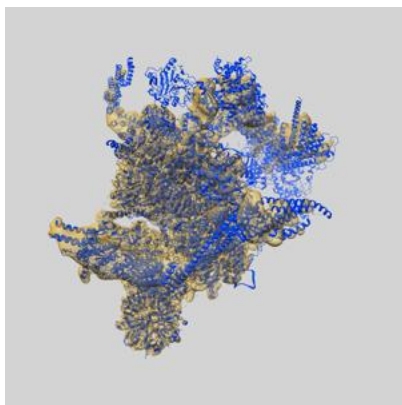
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

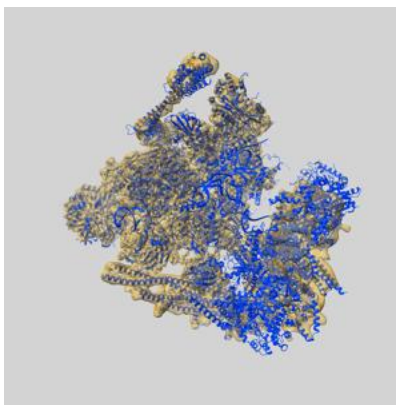
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19399 and PDB model 8RO2. Per-residue inclusion information can be found in section 3 on page 12.

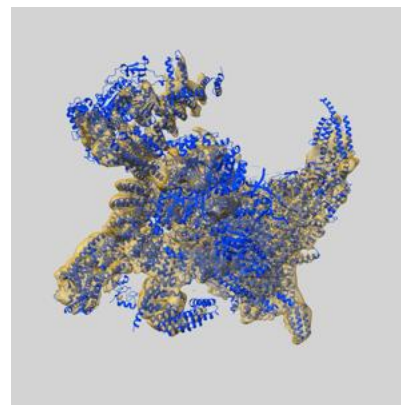
9.1 Map-model overlay [i](#)



X



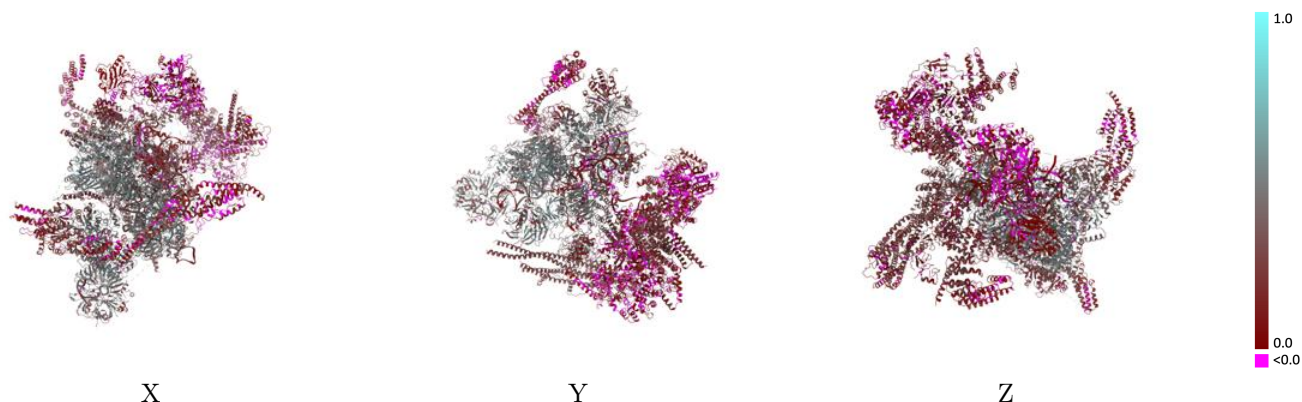
Y



Z

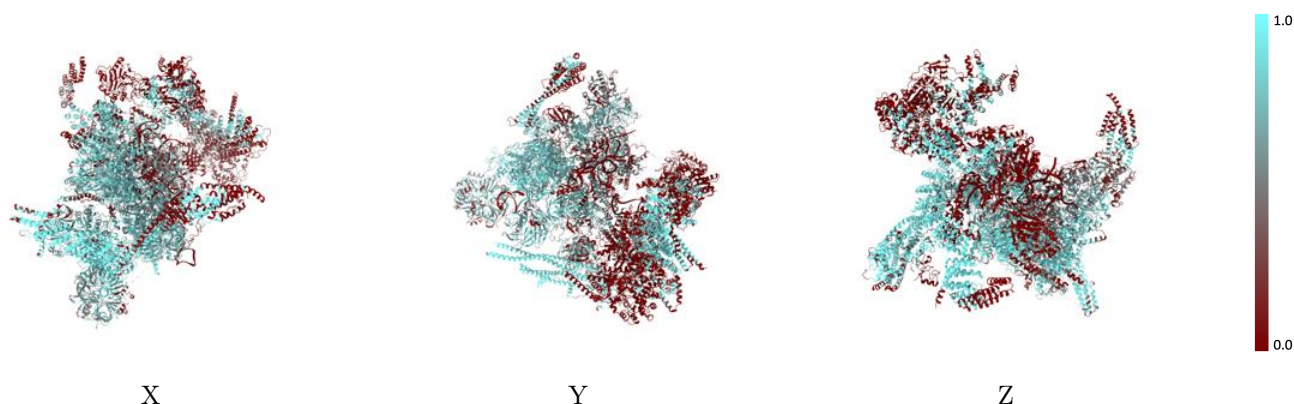
The images above show the 3D surface view of the map at the recommended contour level 0.975 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



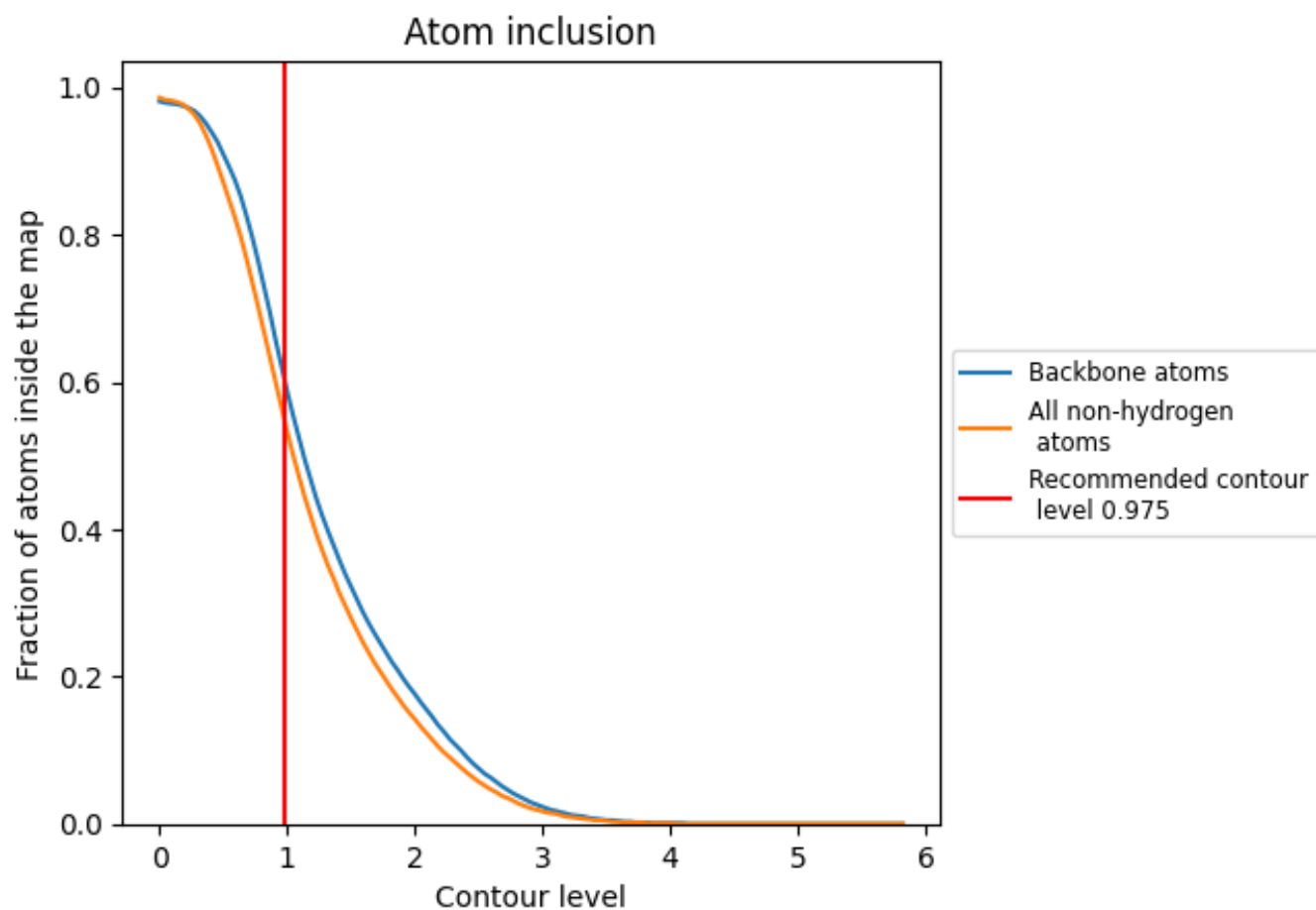
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.975).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary













The table lists the average atom inclusion at the recommended contour level (0.975) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5500	 0.2970
2	 0.1030	 0.1420
3	 0.1130	 0.2610
5	 0.7420	 0.3420
6	 0.1140	 0.1380
A	 0.6610	 0.4410
C	 0.7990	 0.4230
D	 0.3200	 0.1480
DX	 0.3170	 0.0420
E	 0.7530	 0.4590
I	 0.7640	 0.2170
IN	 0.1340	 0.1400
J	 0.4970	 0.2040
K	 0.8930	 0.2380
L	 0.5120	 0.2490
L1	 0.0050	 -0.0160
L2	 0.5040	 0.3570
M	 0.3880	 0.2140
N	 0.7100	 0.4570
O	 0.4830	 0.3360
P	 0.3950	 0.3060
PX	 0.3900	 0.0850
Q	 0.1440	 0.0730
R	 0.5260	 0.3470
S	 0.6770	 0.3700
T	 0.8480	 0.4350
TF	 0.6370	 0.1070
W	 0.4190	 0.3350
Z	 0.5930	 0.1980
a	 0.7150	 0.4790
b	 0.5820	 0.4170
c	 0.5730	 0.4140
d	 0.4780	 0.3430
e	 0.5900	 0.4110
f	 0.6080	 0.4210



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Chain	Atom inclusion	Q-score
g	 0.5840	 0.4440
q	 0.6130	 0.2030
r	 0.5660	 0.1850
s	 0.9060	 0.2290
t	 0.5800	 0.1830
z	 0.0260	 -0.0320