



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 04:58 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

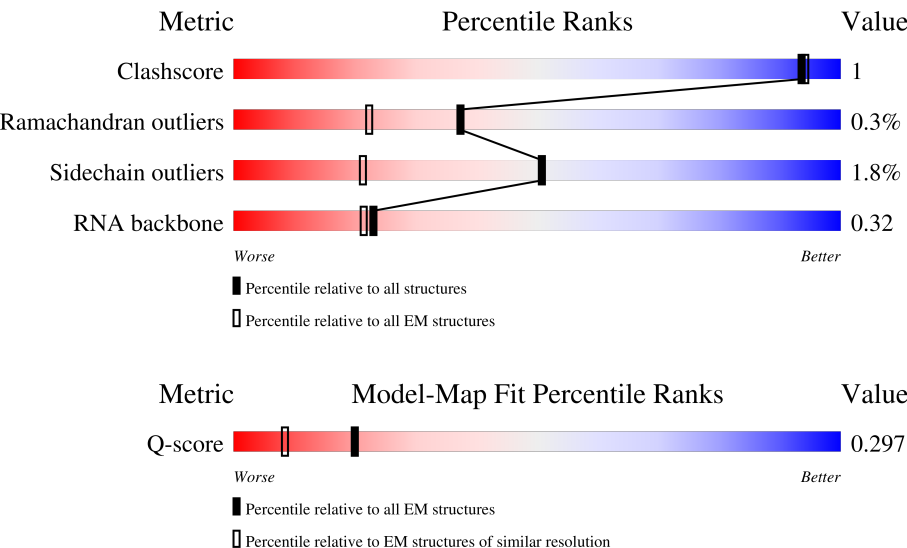
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

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	18% 10% 10% . 79%
2	6	106	80% 42% 42% 5% . 8%
3	C	972	5% 88% 5% 7%

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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

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
1	2	39	Total	C	N	O	P	0	0
			823	368	137	279	39		

- Molecule 2 is a RNA chain called U6 snRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Protein BUD31 homolog.

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

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

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

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

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

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

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

- 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
27	A	1981	Total	C	N	O	S	0	0
			16477	10621	2883	2902	71		

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

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

- Molecule 29 is a RNA chain called INTRON.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 35 is a protein called Pleiotropic regulator 1.

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

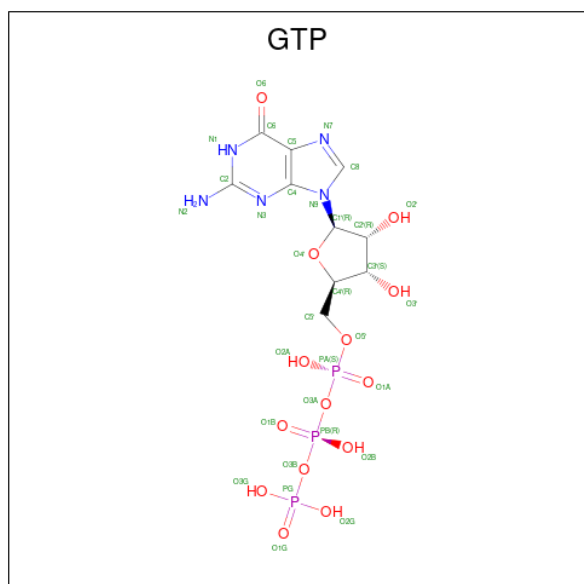
- Molecule 36 is a protein called Tuftelin-interacting protein 11.

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

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

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

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

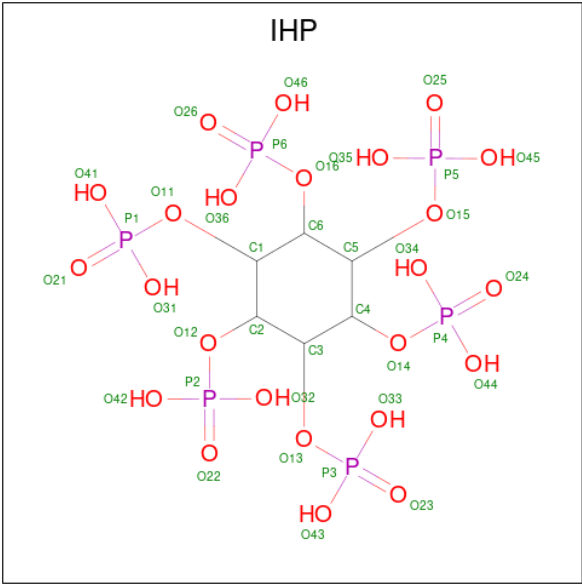


Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- 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).

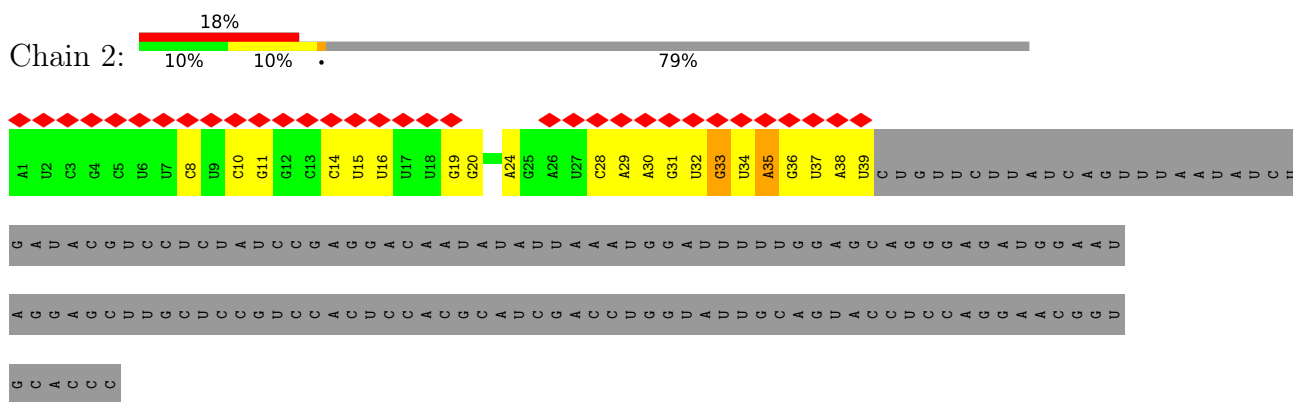


Mol	Chain	Residues	Atoms				AltConf
40	A	1	Total	C	O	P	0
			36	6	24	6	

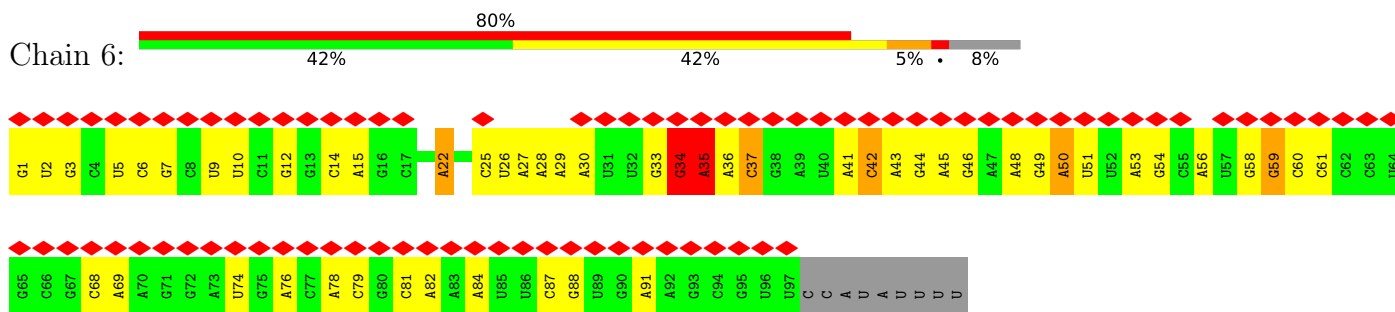
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

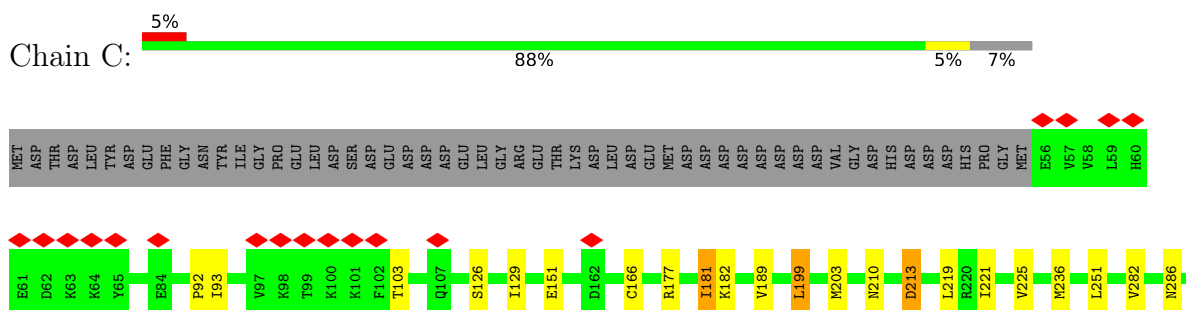
• Molecule 1: U2 snRNA

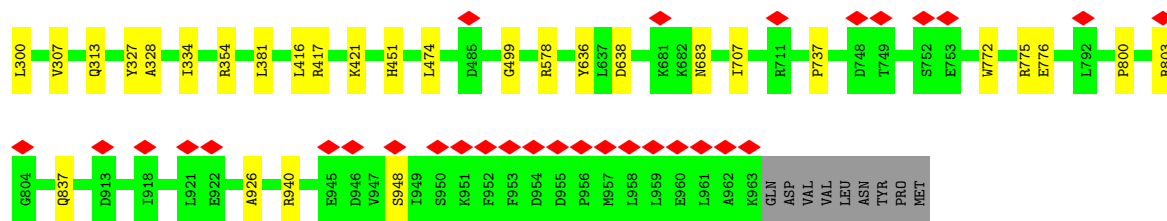


• Molecule 2: U6 snRNA

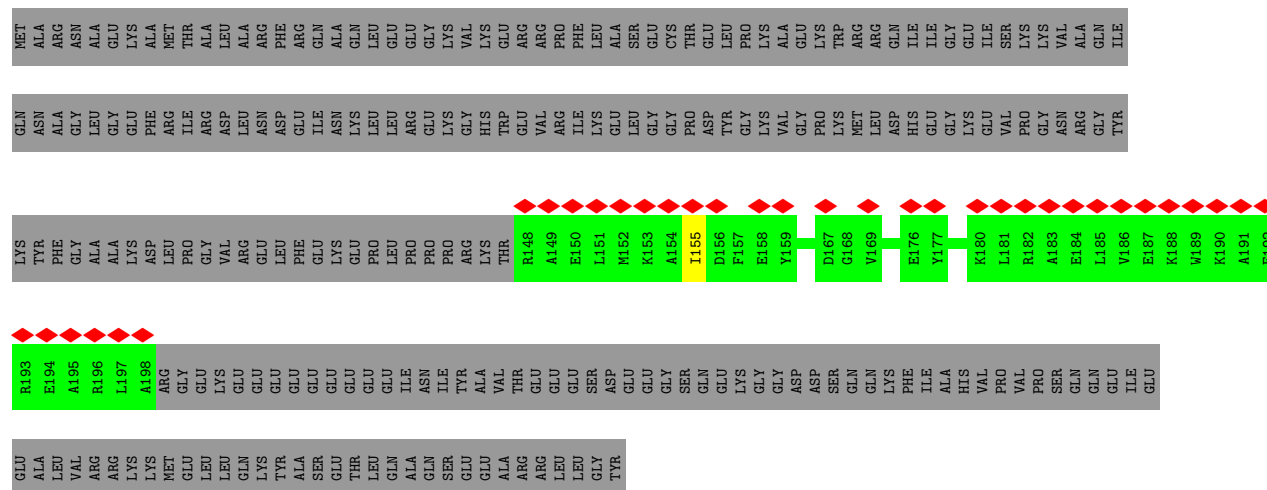


• Molecule 3: 116 kDa U5 small nuclear ribonucleoprotein component

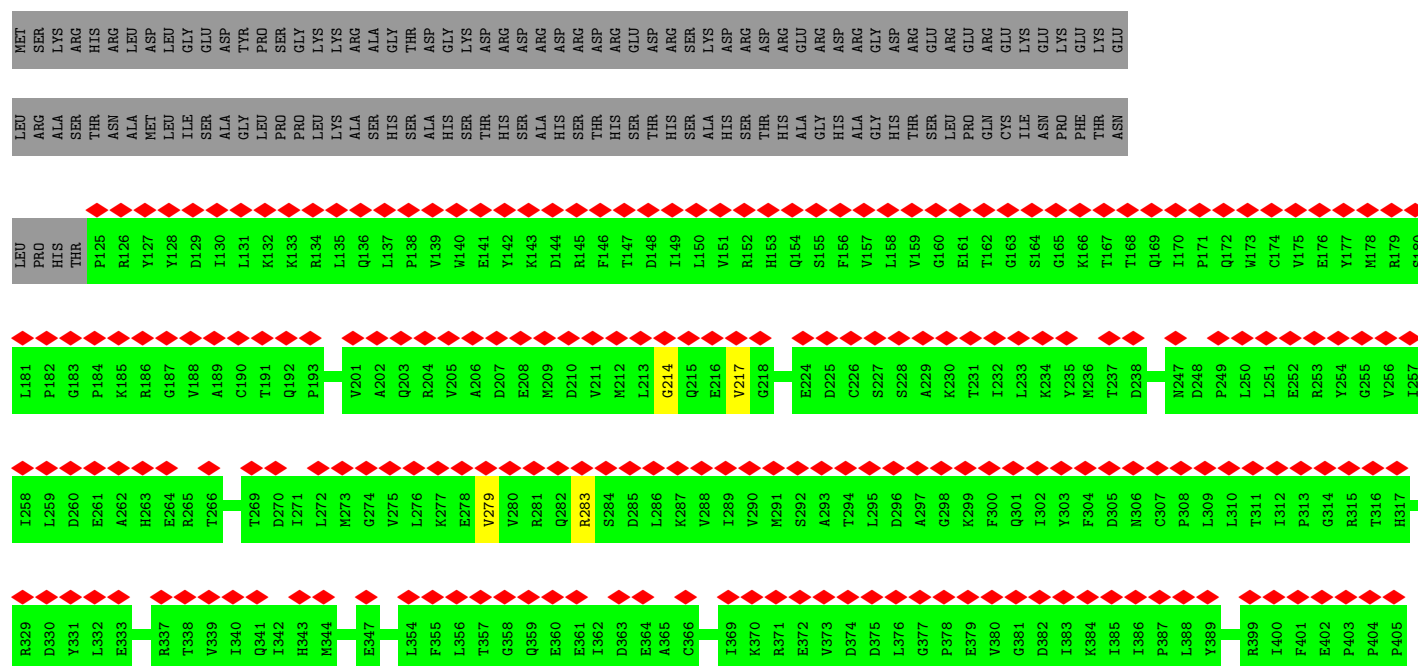
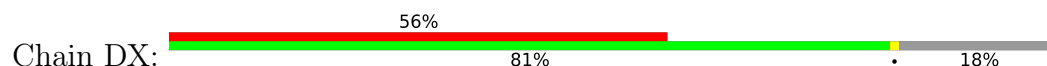


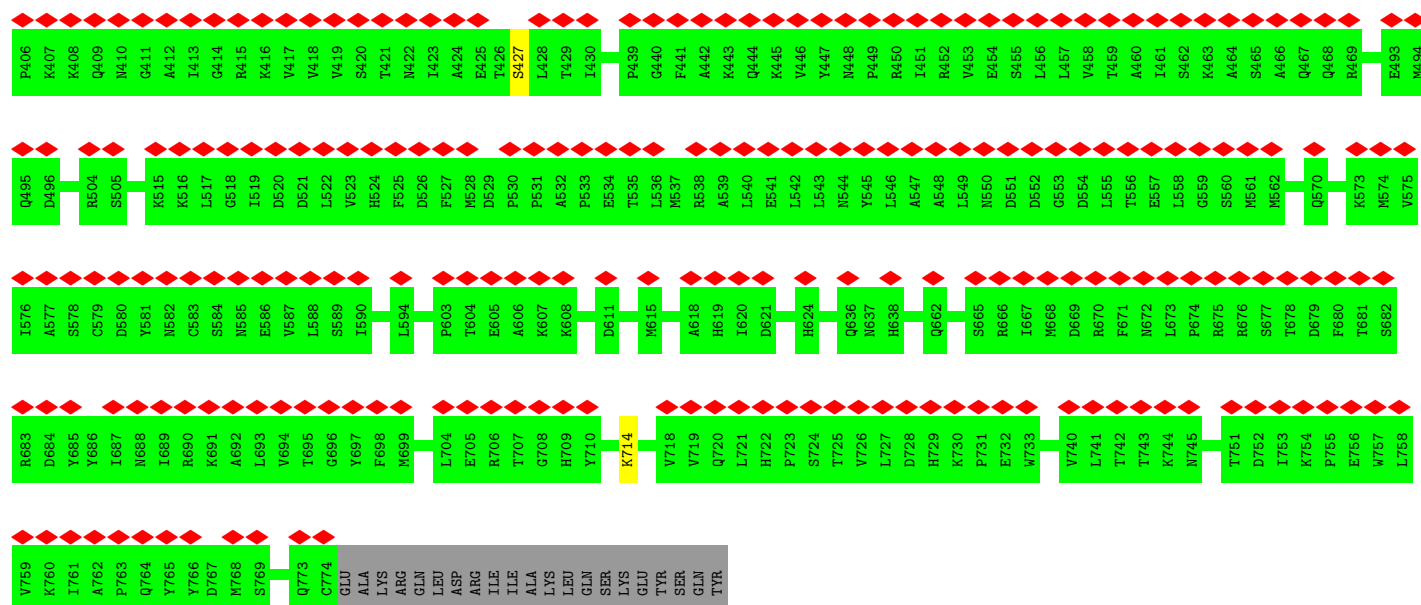


• Molecule 4: Pre-mRNA-splicing factor ISY1 homolog

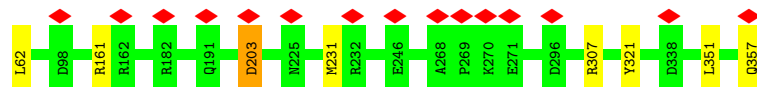
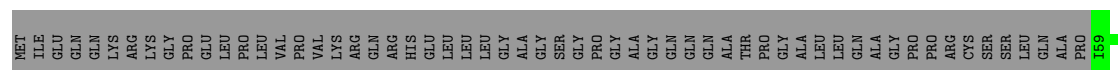
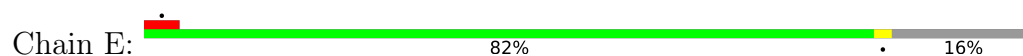


• Molecule 5: ATP-dependent RNA helicase DHX15

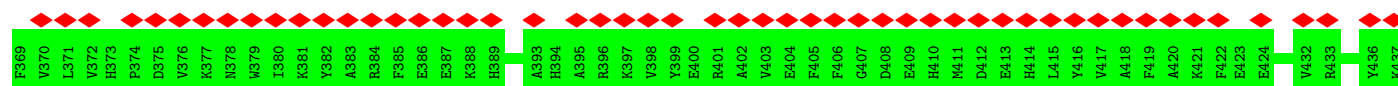
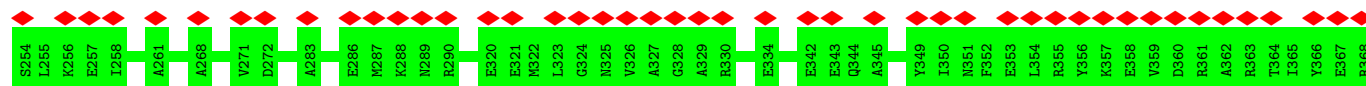
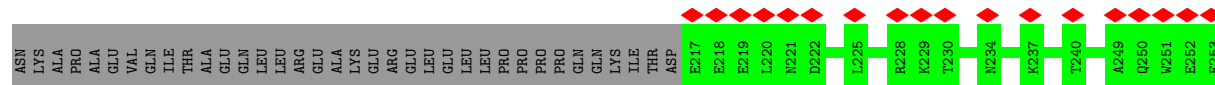
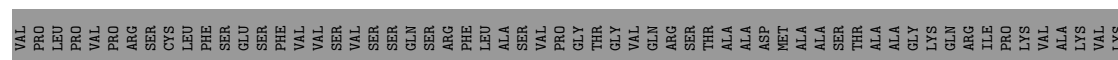


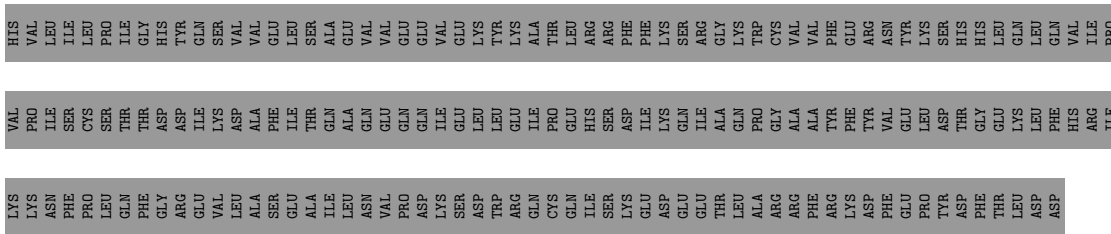


- Molecule 6: U5 small nuclear ribonucleoprotein 40 kDa protein

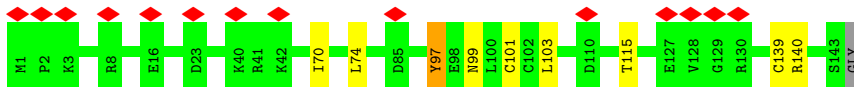
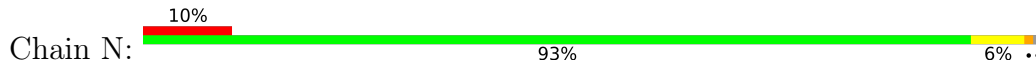


- Molecule 7: Crooked neck-like protein 1

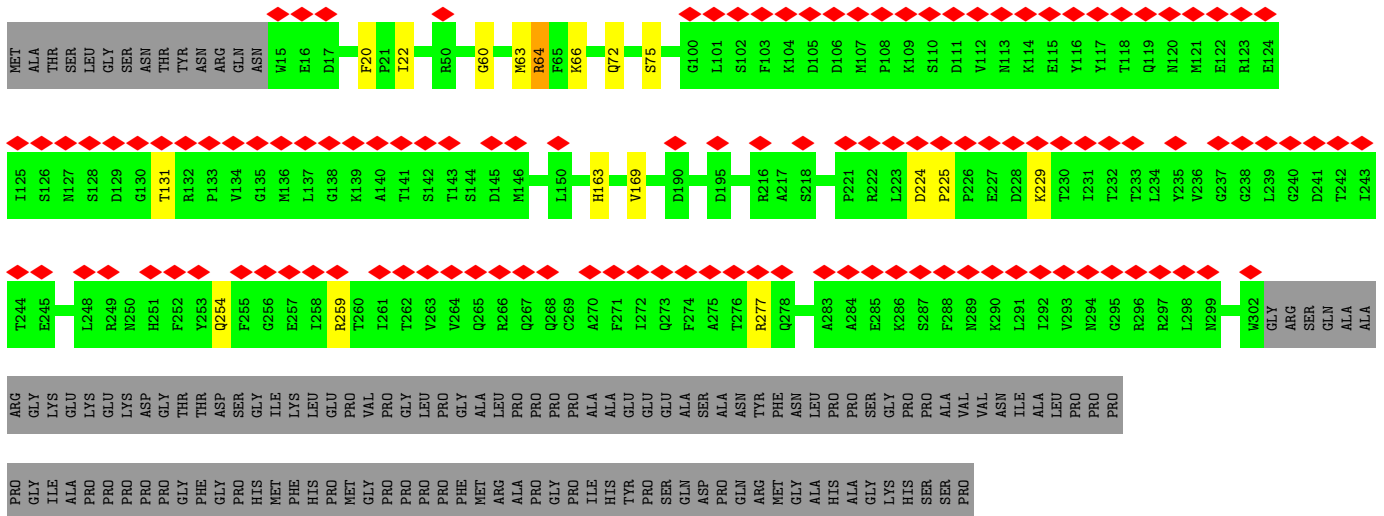




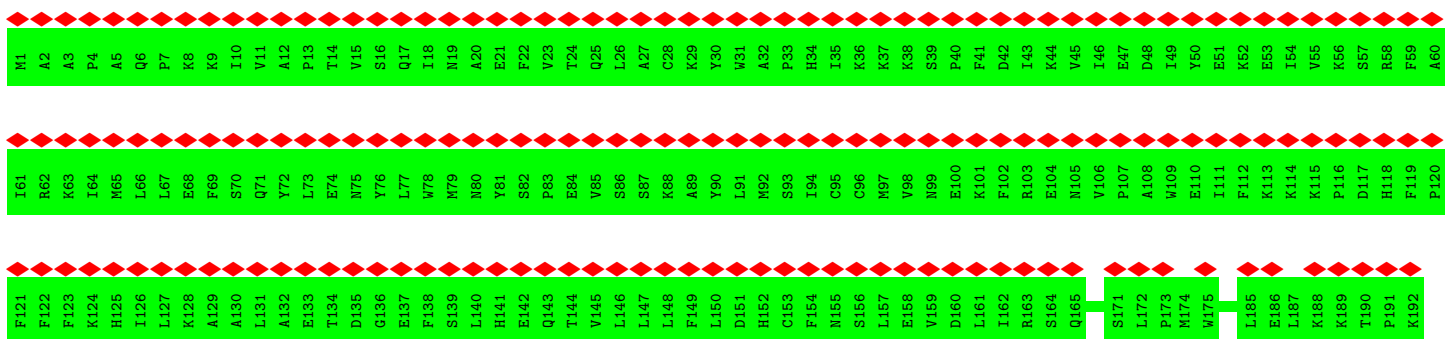
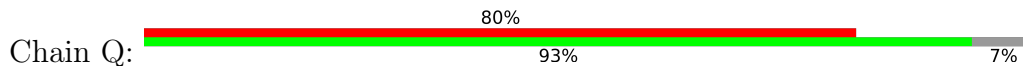
- Molecule 10: Protein BUD31 homolog



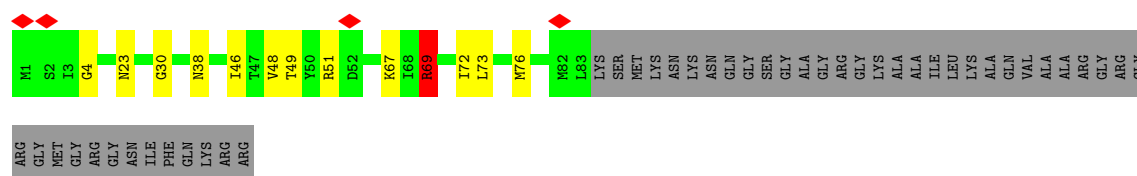
- Molecule 11: Pre-mRNA-splicing factor RBM22



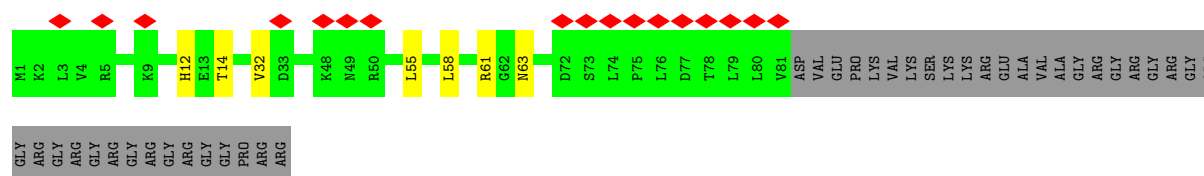
- Molecule 12: Intron-binding protein aquarius



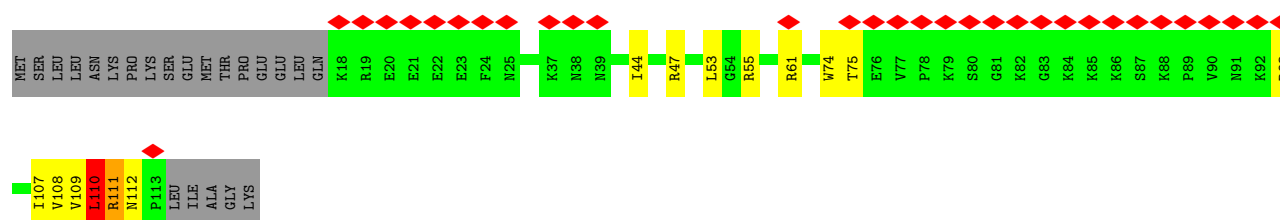
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R1012	G333	E873	T799	D739	N675	E813	W553	K493	T429	V359	R194
A1013	F335	R874	I800	P740	L676	P814	E554	P494	E430	D360	K195
S1014	F936	H875	Q801	A741	M677	R615	G555	W495	K431	T361	F196
E1015	L337	L876	F802	L742	N678	P616	L556	Q496	I432	E363	L199
L1016	L938	L877	T803	Q743	T679	N617	R557	S497	I433	L273	I200
L1017	Q939	R878	H804	I744	D680	L618	K558	E498	W434	L274	K201
R1018		L879	T805	P745	C681	R619	H559	Y499	D435	L365	K202
S1019	K954	G880	Q806	P746	W686	G820	D560	G500	E436	V366	
G1020	G955	H881	I807	F747	L687	E821	V561	G501	N437	K367	N203
L1021	S956	G882	E808	R748	H688	S822	C562	V502	L438	F368	D204
D1022		E883	A809	T749	D689	R623	F563	V503	V439	F369	E205
R1023	T957	E884	I810	T750	I690	T624	L564	F504	P440	G370	K206
S1024	L958	E885	R811	F751	I691	F625	I565	G505	T441	P371	M207
K1025	P959	L886	A812	P752	L692	R626	T566	G506	E442	L372	D208
	D960	E887	G813	V753	G693	W627	V567	W507	Y443	S373	P209
E1031	V961	T888	H814	R754	G694	F628	R568	A508	Y444	S374	E210
A1032	T962	E889	D815	S755	G695	L629	P569	R509	S445	N375	A211
K1033	V964	K890		G756	D696	D630	K571	M510	G446	T376	
I1035	S965	D891	V821	K757	P697	Q533	P572	A511	E447	L377	Q214
A1036	T966	F892	W822	G758	S698	Y634	Y573	Q512	G448		A215
M1037	F967	S893	G823	K759	S699	Q635	G574	P513	C449	V380	
		R894	P824	K760	A700	Q636	T575	I514	L450	A381	E218
		Y895	P825	R761		D637	K576	V515	A451		
H1047	H971	G896	G826	K762	S703	M638	F577	A516	L452	L384	F221
D1048	E972	R897	T827	D763	K704	T639	D578	F517	P453	C385	L222
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V1050	F974	N899	K829	D765	P706	N640	R579	V519	L455	L387	Q224
K1051	A975		T830	V766	N707	T641	R580	V520	N456	P388	L225
L1052	N976	Y900	D831	E767	Q708	I642	R681	E521	L457	T398	I226
G1053	A977	L902	W832	D768	L709	Q643	P582	V522		F298	
F1054	R978	A903	A833	E769	A710	N644	F583	K524	L462	L390	K234
	Q979	R904	V834	D770	T711	G645	I584	K524		Q300	S235
M1058	P980	R905	Q835	T771	L712	A646	E585	P525	Y465	L301	V236
I1059	L981	R906	T836	E772	D713	E547	Q586	N526	L466	L302	P237
L1060	F982	E907	T837	E773	F714	D648	V587	I527	L467	D303	L238
M1061	E907	L908	S838	A774	N715	V649	G588	G528	R468	K304	S239
E1062	G984	L909		K775	D716	Y650	L589	E529	N469	L305	E240
A1063	R985	E910	T849	K776	L717	E851	V590	E529	F470	K306	P241
A1064	S986	E911	L850	T776	F718	T652	Y591	N530	N471	F307	V242
A1065	Y987	E912	T851	L777	L719	F953	V592	W531	K400	V308	T243
Q1066	E987	E913	W852	L778	S720	N654	R593	P532	F473	T309	M244
L1067	E988	R913		V779	I721	I655	T533	T533	R474	G310	D245
E1068	D990	R914	S855	E780	E722	I656	G594	R534	L475	F311	K246
I1070	M991	L915	N856	P781	H723	M657	C595	V535	E476	E312	V247
E1071	E992	Q916	Q857	H782	L724	R658	E596	R536	S477	I313	H248
T1072	I993	K917	L858	V783	K725	R659	Q598	D538	T478	N314	Y249
F1073	A994	S918	L859	I784	A726	K660	Q599	V539	Y479	D315	C250
I1074	E995	L919	N860	P785	K725	G560	G599	V539	E480	L406	E251
P1075	G996	G920	Q861	N786	S727	P661	M600	T540	S409	V408	R252
L1076	C997	V921	L862	R787	F728	K662	L601	I541	I481	R410	F253
		P922	F863	G788	P729	N665	D602	N542	R482	H411	I254
P1081	F998	G923	E864	P789	G730	F666	D603	L543	Q483	E412	E255
Q1082	H1000	D924	K865	Y790	H731	K667	K604	N544	D484	R413	L256
D1083		A925	I866	P791	N732	A668	G605	V545	I485	E323	M257
G1084	T1006	S926	H867	Y792	V733	V669	R606	R546	E486	N324	
F1085	Q1007	Y927	T867	N793	K734	L670	V607	D547	S488		
	L1008	Q929	A868	Q794	V735	T670	H548	E609	V489		
	E1009	C929	L869	T795	T736	E871	I608	I549	S490	A341	
I1094	E1010	T931	D870	K796	V737	L672	D610	K550	R491	A357	
			L871	R797		I673	G611	D551			



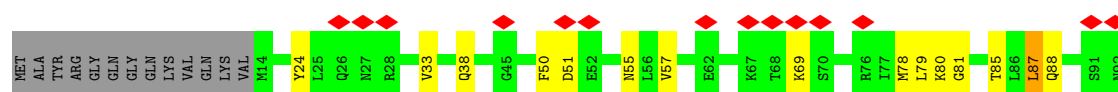
• Molecule 18: Small nuclear ribonucleoprotein Sm D1



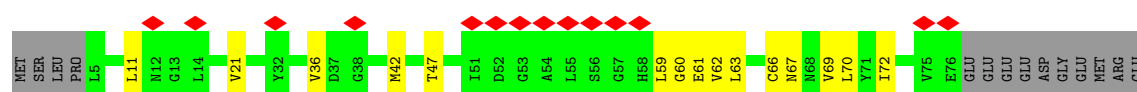
• Molecule 19: Small nuclear ribonucleoprotein Sm D2



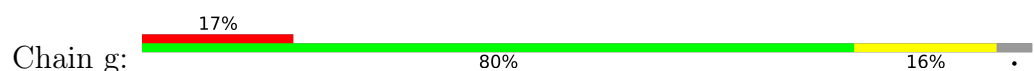
• Molecule 20: Small nuclear ribonucleoprotein E

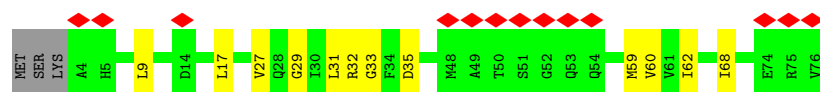


• Molecule 21: Small nuclear ribonucleoprotein F

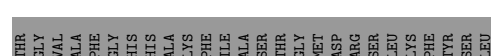
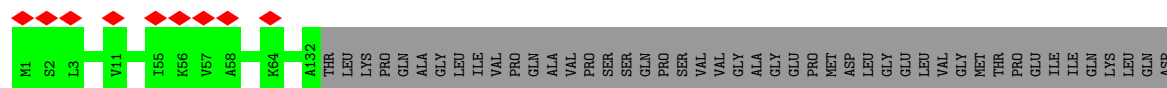


• Molecule 22: Small nuclear ribonucleoprotein G

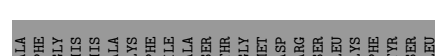
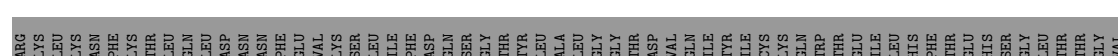
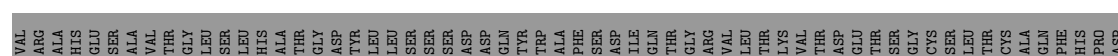
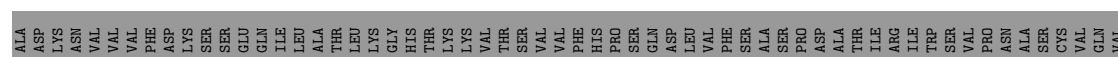
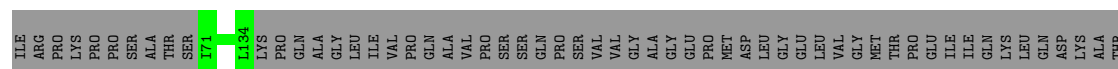
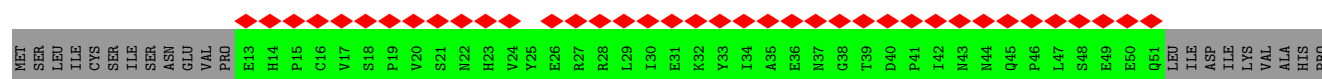




• Molecule 23: Pre-mRNA-processing factor 19



• Molecule 23: Pre-mRNA-processing factor 19



Chain r:



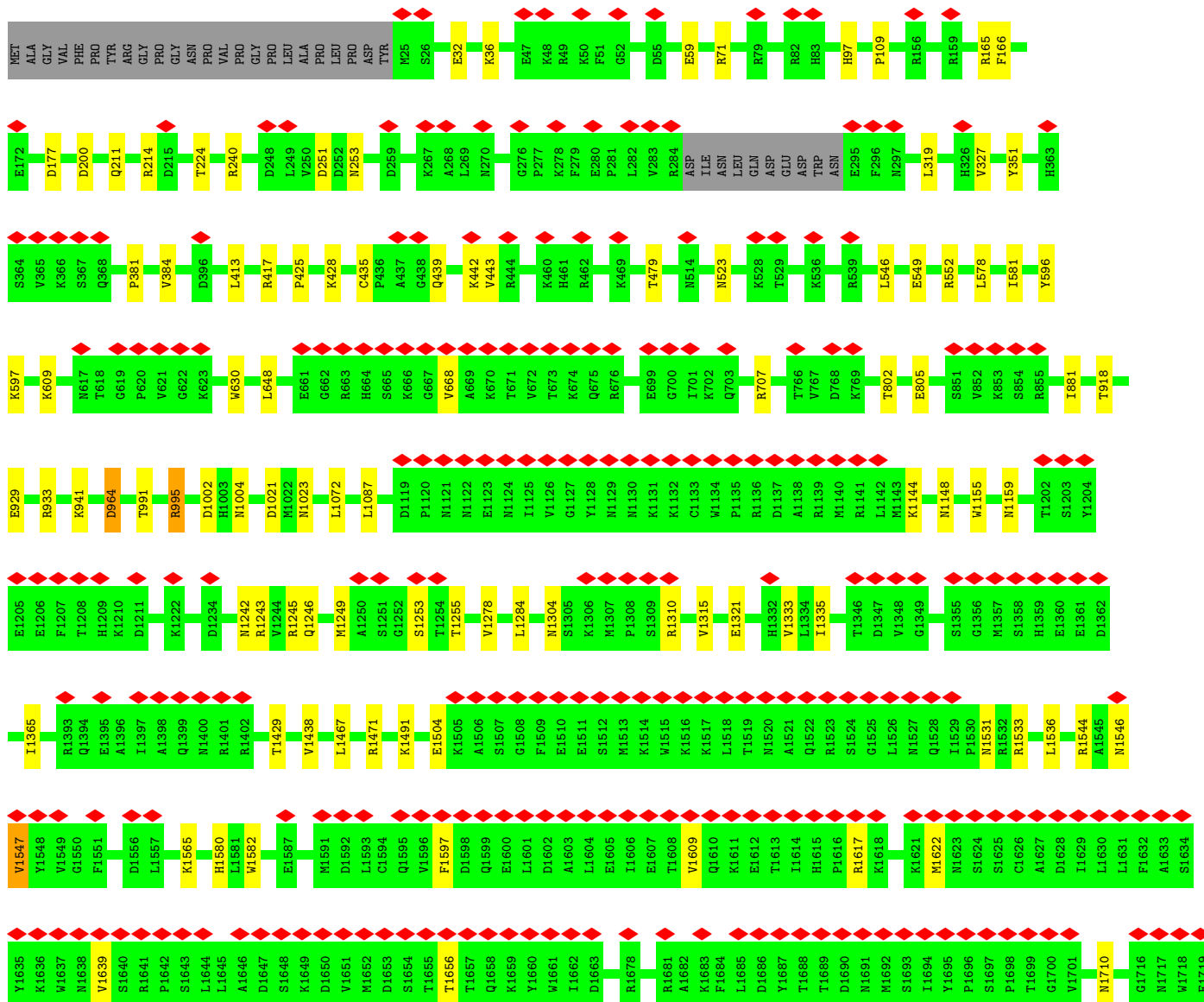
Chain z:

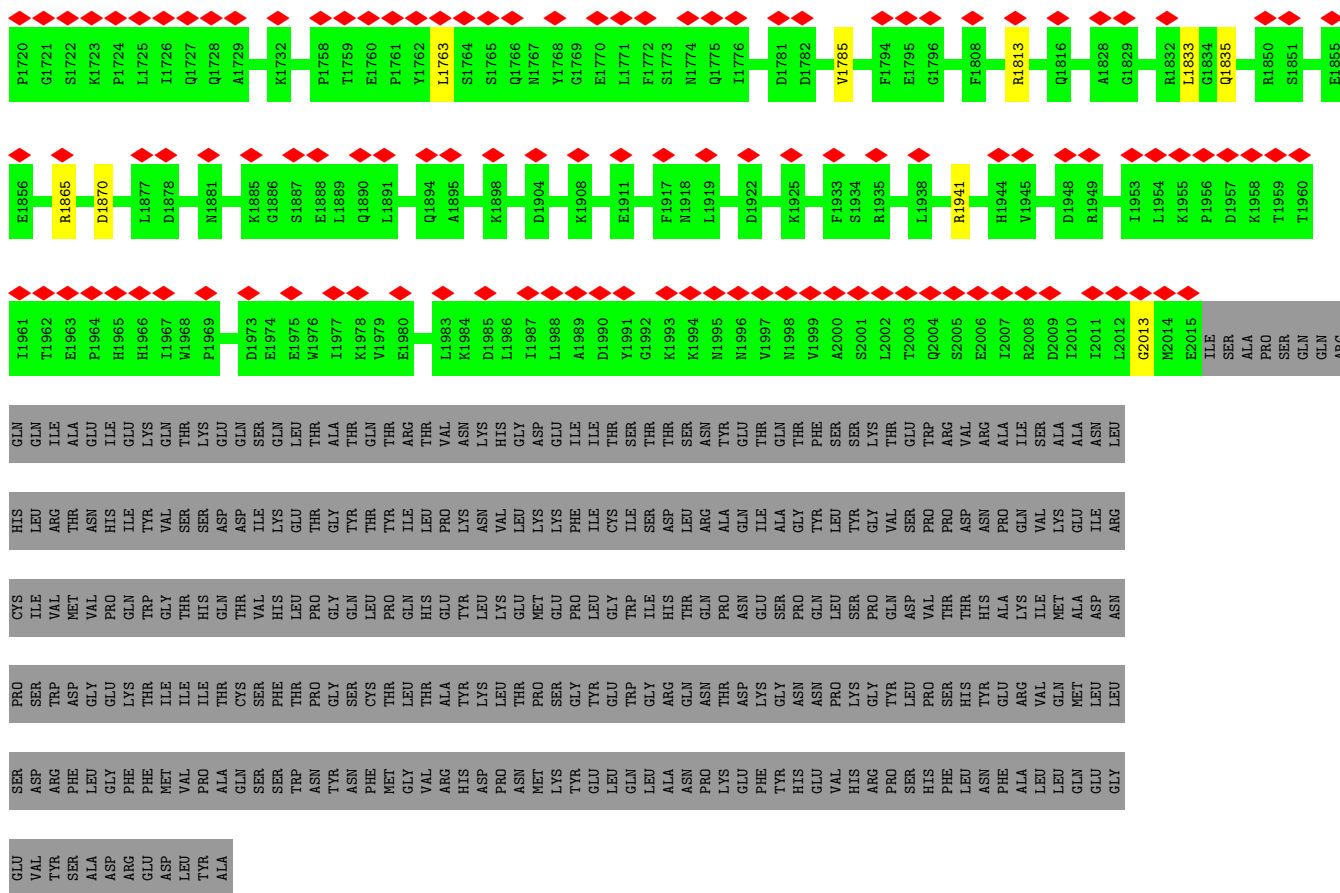


- Molecule 26: U5 snRNA

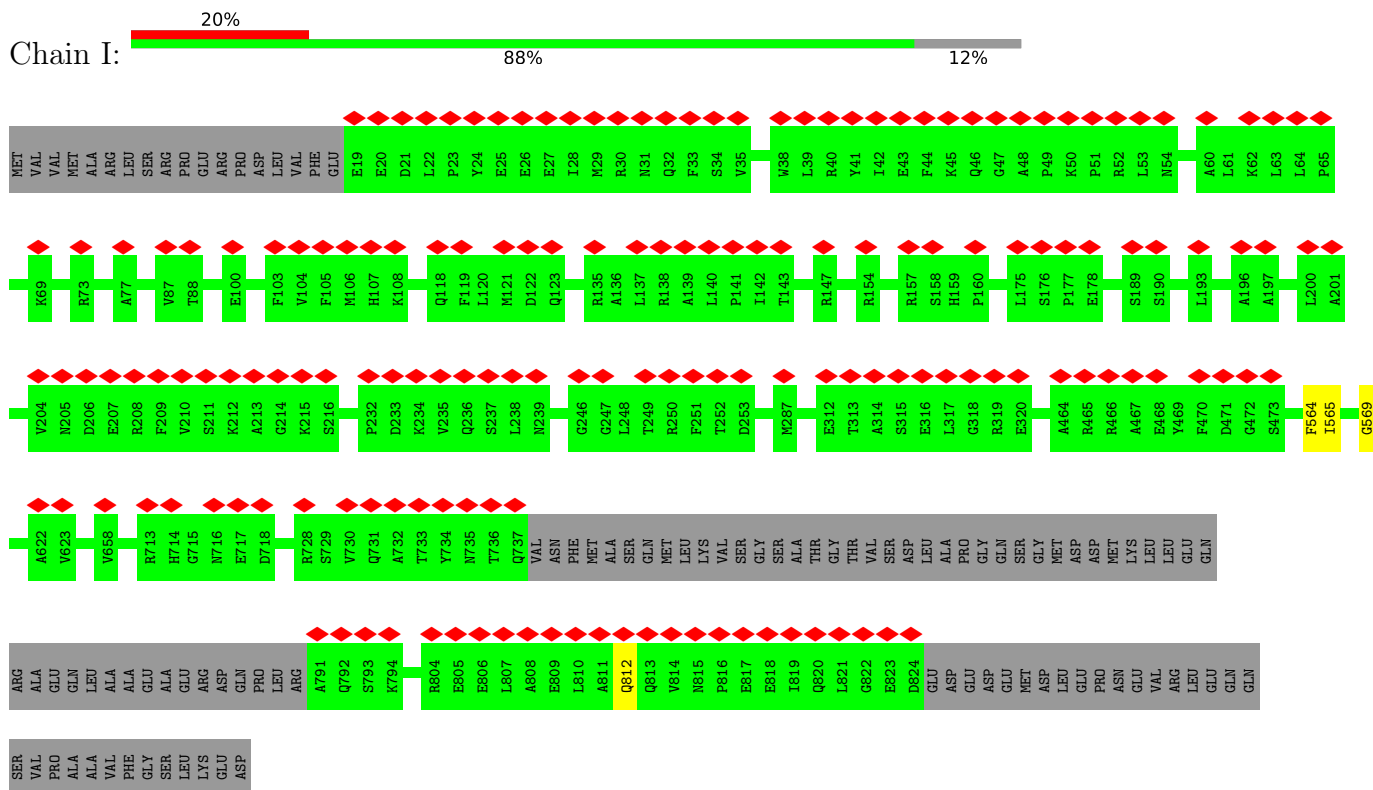
- Molecule 27: Pre-mRNA-processing-splicing factor 8

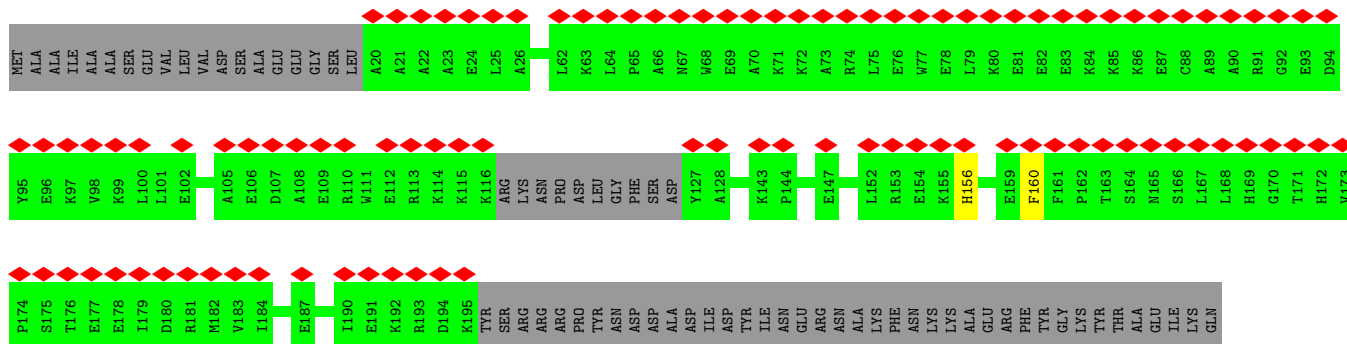
Chain A:  17% 80% 5% 15%

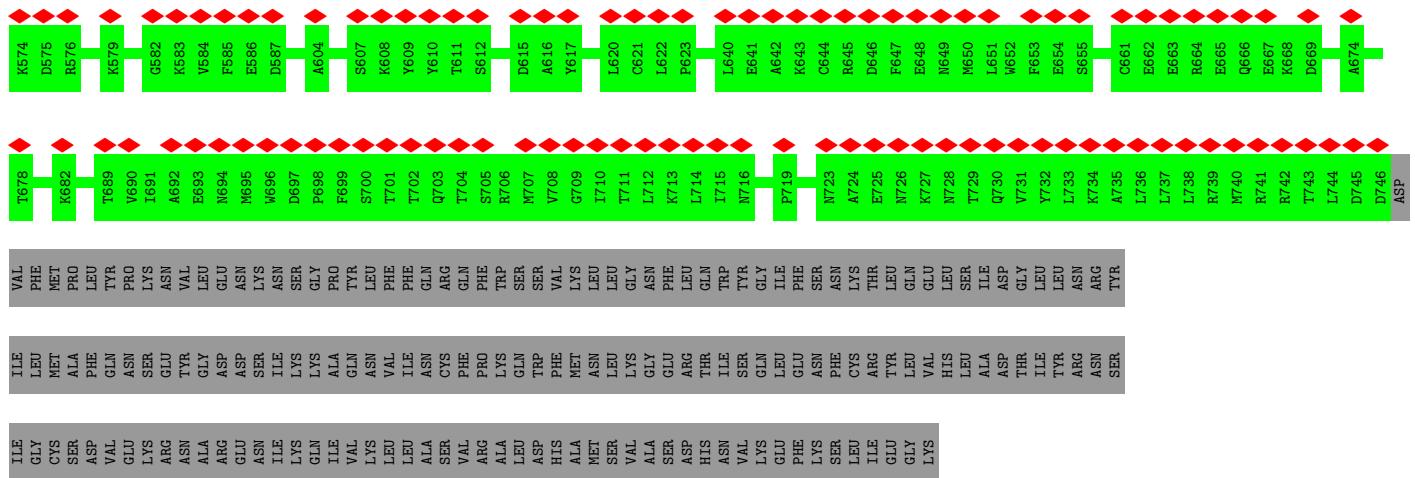




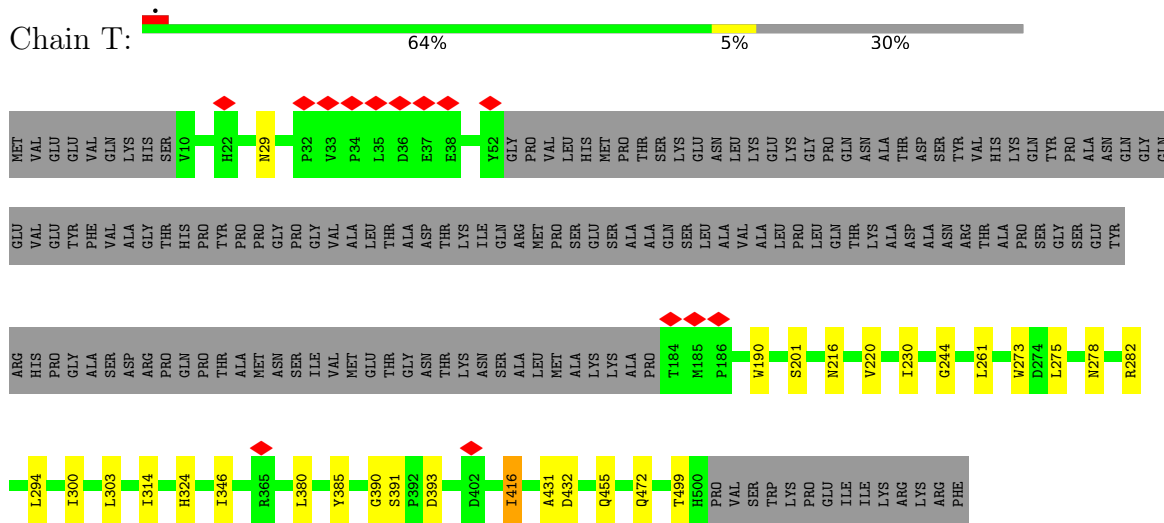
- Molecule 28: Pre-mRNA-splicing factor SYF1



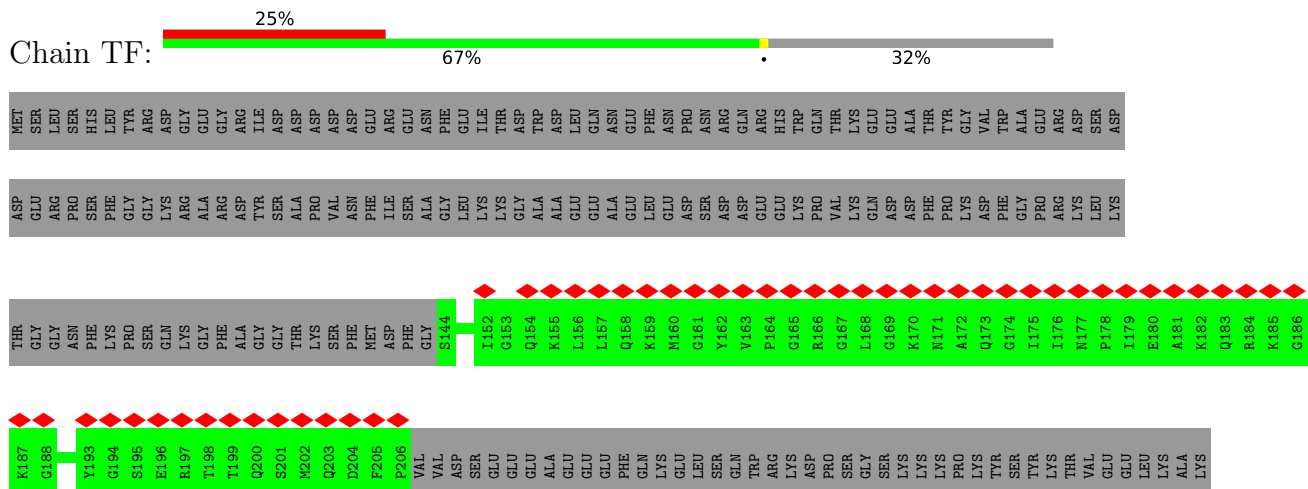




- Molecule 35: Pleiotropic regulator 1



- 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 ⓘ

5.1 Standard geometry ⓘ

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

All (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
13	R	136	ASP	N-CA-CB	-6.30	101.79	111.56
26	5	24	G	O4'-C1'-N9	-6.28	98.78	108.20
2	6	34	G	P-O3'-C3'	6.15	129.42	120.20
13	R	46	TYR	CA-C-N	5.87	132.76	121.54
13	R	46	TYR	C-N-CA	5.87	132.76	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	c	32	VAL	CG1-CB-CG2	-5.81	98.01	110.80
21	f	66	CYS	N-CA-C	5.76	118.33	111.71
2	6	42	C	P-O3'-C3'	5.73	128.80	120.20
2	6	37	C	O3'-P-O5'	5.69	112.53	104.00
11	O	64	ARG	CG-CD-NE	5.61	124.34	112.00
2	6	42	C	O3'-P-O5'	5.56	112.34	104.00
30	L	77	LEU	CA-CB-CG	5.43	135.29	116.30
20	e	85	THR	N-CA-C	-5.42	99.26	110.80
9	L1	196	ALA	CA-C-N	5.39	131.84	121.54
9	L1	196	ALA	C-N-CA	5.39	131.84	121.54
27	A	1639	VAL	CA-CB-CG1	5.37	119.53	110.40
35	T	300	ILE	CG1-CB-CG2	-5.36	94.64	110.70
17	a	69	ARG	CA-C-N	5.33	131.73	121.54
17	a	69	ARG	C-N-CA	5.33	131.73	121.54
17	a	38	ASN	CA-C-N	5.24	131.49	123.47
17	a	38	ASN	C-N-CA	5.24	131.49	123.47
33	P	57	ARG	N-CA-C	5.19	117.56	110.24
2	6	35	A	C4'-C3'-O3'	5.18	120.77	113.00
21	f	70	LEU	CA-CB-CG	5.17	134.38	116.30
2	6	50	A	C2'-C3'-O3'	5.17	121.45	113.70
10	N	97	TYR	CA-CB-CG	5.16	123.19	113.90
22	g	35	ASP	CB-CA-C	5.12	120.26	110.17
21	f	69	VAL	CA-C-N	5.11	131.30	121.54
21	f	69	VAL	C-N-CA	5.11	131.30	121.54
37	b	32	LYS	CA-C-N	5.07	131.22	121.54
37	b	32	LYS	C-N-CA	5.07	131.22	121.54
27	A	1547	VAL	CA-CB-CG1	5.06	119.01	110.40
11	O	224	ASP	N-CA-C	5.04	120.95	109.81
21	f	60	GLY	CA-C-N	5.03	129.96	122.82
21	f	60	GLY	C-N-CA	5.03	129.96	122.82
1	2	35	A	O4'-C1'-N9	-5.02	100.66	108.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	A	165	ARG	Peptide
27	A	707	ARG	Sidechain
27	A	995	ARG	Sidechain
3	C	940	ARG	Sidechain
17	a	51	ARG	Sidechain
17	a	69	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	d	110	LEU	Peptide
19	d	55	ARG	Sidechain
19	d	61	ARG	Sidechain
20	e	50	PHE	Peptide
22	g	33	GLY	Peptide

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	5	1936	0	982	13	0
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.

All (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
26:5:12:U:H3	26:5:65:G:H1	1.48	0.61
27:A:435:CYS:SG	27:A:439:GLN:NE2	2.73	0.61
21:f:47:THR:OG1	21:f:59:LEU:O	2.20	0.59
6:E:62:LEU:HB2	6:E:351:LEU:HB2	1.85	0.58
21:f:67:ASN:ND2	26:5:94:U:OP2	2.34	0.58
27:A:1304:ASN:ND2	27:A:1565:LYS:O	2.36	0.58
27:A:929:GLU:OE1	27:A:933:ARG:NH1	2.38	0.57
35:T:390:GLY:HA3	35:T:416:ILE:HD11	1.87	0.56
33:P:57:ARG:NH1	35:T:472:GLN:O	2.38	0.56
35:T:314:ILE:HD12	35:T:324:HIS:HB2	1.87	0.56
26:5:36:C:N4	26:5:37:G:O6	2.39	0.55
27:A:1335:ILE:HG23	27:A:1365:ILE:HD11	1.88	0.55
1:2:10:C:H2'	1:2:11:G:H8	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1255:THR:HA	27:A:1531:ASN:HD21	1.72	0.55
26:5:59:G:OP1	27:A:417:ARG:NH2	2.40	0.54
27:A:549:GLU:OE1	27:A:552:ARG:NH1	2.40	0.54
3:C:451:HIS:O	3:C:578:ARG:NH1	2.41	0.54
27:A:71:ARG:NH1	27:A:177:ASP:OD2	2.41	0.54
31:L2:844:TYR:OH	31:L2:862:ARG:NH2	2.41	0.54
11:O:169:VAL:HG13	15:W:216:LEU:HD22	1.90	0.54
19:d:107:ILE:HG13	19:d:108:VAL:HG12	1.89	0.54
27:A:1333:VAL:HG13	27:A:1365:ILE:HD13	1.90	0.54
11:O:20:PHE:O	11:O:72:GLN:NE2	2.41	0.54
27:A:32:GLU:OE2	27:A:36:LYS:NZ	2.42	0.53
27:A:1310:ARG:NH1	27:A:1546:ASN:O	2.42	0.53
18:c:55:LEU:HD13	37:b:81:THR:HG21	1.90	0.52
26:5:46:U:OP2	27:A:597:LYS:NZ	2.42	0.52
27:A:881:ILE:HG23	27:A:918:THR:HG23	1.90	0.52
31:L2:685:PRO:O	31:L2:687:HIS:ND1	2.43	0.52
3:C:93:ILE:HD12	35:T:275:LEU:HD22	1.91	0.51
3:C:213:ASP:OD1	3:C:213:ASP:N	2.44	0.51
20:e:88:GLN:HA	22:g:60:VAL:HG22	1.92	0.51
35:T:190:TRP:CD1	35:T:499:THR:HG1	2.29	0.51
2:6:49:G:OP1	30:L:33:ARG:NH2	2.44	0.51
36:TF:790:PRO:HA	36:TF:802:TYR:HA	1.92	0.51
27:A:1155:TRP:O	27:A:1159:ASN:ND2	2.43	0.51
27:A:1617:ARG:NH1	31:L2:586:GLU:OE2	2.44	0.51
3:C:313:GLN:O	3:C:417:ARG:NH1	2.44	0.50
18:c:58:LEU:HD11	37:b:79:SER:HB2	1.91	0.50
21:f:11:LEU:HD13	21:f:36:VAL:HG21	1.94	0.50
10:N:139:CYS:SG	10:N:140:ARG:N	2.85	0.50
36:TF:617:GLY:O	36:TF:621:GLY:N	2.44	0.50
6:E:161:ARG:HD2	6:E:203:ASP:HA	1.93	0.49
11:O:66:LYS:NZ	29:IN:19:N:OP1	2.45	0.49
19:d:47:ARG:NH2	26:5:95:G:OP2	2.44	0.49
3:C:92:PRO:HA	35:T:278:ASN:HD21	1.77	0.49
3:C:236:MET:SD	3:C:837:GLN:NE2	2.83	0.49
30:L:376:ASP:OD1	30:L:376:ASP:N	2.46	0.49
35:T:346:ILE:HD13	35:T:380:LEU:HD11	1.94	0.49
20:e:51:ASP:OD1	20:e:51:ASP:N	2.43	0.49
3:C:772:TRP:NE1	3:C:776:GLU:OE2	2.44	0.49
19:d:111:ARG:NE	21:f:61:GLU:OE1	2.45	0.49
27:A:211:GLN:OE1	27:A:214:ARG:NH1	2.44	0.49
36:TF:789:MET:O	36:TF:803:THR:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:1580:HIS:NE2	31:L2:595:ASP:OD1	2.45	0.49
11:O:229:LYS:O	11:O:277:ARG:NH1	2.45	0.49
32:M:156:HIS:O	32:M:160:PHE:N	2.43	0.49
19:d:44:ILE:HG12	19:d:109:VAL:HG22	1.96	0.48
27:A:425:PRO:HB2	27:A:428:LYS:HB2	1.95	0.48
27:A:442:LYS:NZ	40:A:3000:IHP:O45	2.45	0.48
3:C:381:LEU:HG	3:C:416:LEU:HD21	1.95	0.48
15:W:126:GLU:HG3	15:W:130:ARG:HE	1.78	0.48
27:A:109:PRO:HG3	27:A:630:TRP:HE1	1.77	0.48
27:A:991:THR:HG22	30:L:81:GLN:HE22	1.76	0.48
30:L:37:LEU:HD11	30:L:155:ALA:HA	1.96	0.48
22:g:17:LEU:HD11	22:g:31:LEU:HD22	1.96	0.48
2:6:14:C:H2'	2:6:15:A:H8	1.77	0.48
30:L:119:ASP:OD2	30:L:122:LYS:NZ	2.46	0.48
35:T:244:GLY:H	35:T:273:TRP:HH2	1.62	0.48
26:5:97:G:N2	26:5:115:U:O2	2.47	0.48
27:A:1870:ASP:OD2	31:L2:556:ARG:NH1	2.43	0.47
6:E:321:TYR:OH	6:E:357:GLN:O	2.31	0.47
31:L2:550:ARG:HB3	31:L2:660:LYS:HB3	1.95	0.47
27:A:523:ASN:OD1	27:A:552:ARG:NH2	2.47	0.47
17:a:67:LYS:HB3	22:g:68:ILE:HG23	1.96	0.47
27:A:1865:ARG:NH2	31:L2:726:ASP:OD2	2.43	0.47
35:T:391:SER:OG	35:T:393:ASP:OD1	2.32	0.47
27:A:1243:ARG:NH1	27:A:1246:GLN:OE1	2.46	0.47
27:A:1242:ASN:OD1	27:A:1245:ARG:NH1	2.47	0.47
14:S:51:THR:HB	14:S:66:ASP:H	1.80	0.47
26:5:12:U:H5'	27:A:224:THR:HG23	1.97	0.47
35:T:416:ILE:HA	35:T:431:ALA:HA	1.95	0.46
20:e:24:TYR:OH	22:g:59:MET:O	2.34	0.46
13:R:134:ARG:HA	35:T:385:TYR:HB2	1.97	0.46
36:TF:452:ILE:O	36:TF:456:LYS:N	2.47	0.46
10:N:101:CYS:SG	10:N:139:CYS:HB2	2.56	0.46
11:O:64:ARG:NH1	29:IN:19:N:OP2	2.49	0.46
27:A:1504:GLU:O	27:A:1533:ARG:NH1	2.48	0.46
31:L2:60:LEU:HD11	31:L2:876:ALA:HB1	1.97	0.46
20:e:55:ASN:OD1	20:e:81:GLY:N	2.44	0.46
31:L2:677:TYR:HB3	31:L2:714:VAL:HG11	1.97	0.46
22:g:17:LEU:N	22:g:29:GLY:O	2.48	0.45
27:A:251:ASP:OD2	27:A:253:ASN:ND2	2.49	0.45
3:C:203:MET:HE2	3:C:221:ILE:HD11	1.98	0.45
31:L2:695:LYS:NZ	31:L2:728:ASP:OD2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:e:87:LEU:H	22:g:60:VAL:HG13	1.81	0.45
35:T:201:SER:OG	35:T:455:GLN:NE2	2.49	0.45
3:C:800:PRO:HA	3:C:803:ARG:HE	1.82	0.45
26:5:45:C:H4'	27:A:596:TYR:HB3	1.98	0.45
31:L2:548:LEU:HD22	31:L2:661:ALA:HB1	1.98	0.45
2:6:2:U:H2'	2:6:3:G:H8	1.82	0.45
11:O:60:GLY:HA3	11:O:63:MET:HE2	1.98	0.45
31:L2:675:CYS:SG	31:L2:678:CYS:N	2.86	0.45
33:P:38:HIS:HB2	35:T:282:ARG:HD3	1.99	0.44
15:W:180:LYS:HD3	15:W:197:ALA:HB3	1.99	0.44
27:A:609:LYS:NZ	40:A:3000:IHP:O12	2.50	0.44
27:A:1144:LYS:HE2	27:A:1148:ASN:HD21	1.82	0.44
31:L2:805:LEU:HD11	31:L2:832:ALA:HB2	1.99	0.44
2:6:34:G:H2'	2:6:35:A:H8	1.82	0.44
19:d:110:LEU:HD22	21:f:62:VAL:HG22	1.99	0.44
28:I:565:ILE:HA	28:I:569:GLY:HA3	1.99	0.44
3:C:354:ARG:NH1	27:A:381:PRO:O	2.50	0.44
35:T:393:ASP:OD1	35:T:393:ASP:N	2.51	0.44
20:e:33:VAL:HG11	20:e:79:LEU:HD21	2.00	0.44
27:A:1278:VAL:HG13	27:A:1284:LEU:HD12	2.00	0.44
10:N:103:LEU:HD13	27:A:59:GLU:HB2	2.00	0.44
14:S:52:LYS:HA	14:S:158:LYS:HA	2.00	0.44
13:R:9:ALA:O	13:R:11:THR:N	2.45	0.43
14:S:60:PHE:HB2	15:W:99:PHE:HE2	1.83	0.43
17:a:30:GLY:HA3	17:a:46:ILE:HG12	2.00	0.43
26:5:23:C:H5'	26:5:24:G:H5''	1.99	0.43
27:A:1491:LYS:O	27:A:1710:ASN:ND2	2.49	0.43
3:C:737:PRO:HB2	3:C:775:ARG:HE	1.82	0.43
27:A:578:LEU:HA	27:A:581:ILE:HD12	2.00	0.43
6:E:307:ARG:NH1	15:W:116:GLU:OE1	2.51	0.43
27:A:1544:ARG:HB2	27:A:1547:VAL:HG12	2.00	0.43
31:L2:810:ILE:H	31:L2:810:ILE:HG13	1.56	0.43
2:6:30:A:O2'	15:W:223:ARG:NH1	2.51	0.43
10:N:70:ILE:HG23	10:N:74:LEU:HB3	2.01	0.43
26:5:12:U:O2	26:5:65:G:N2	2.41	0.43
35:T:220:VAL:HG11	35:T:261:LEU:HD21	1.99	0.43
14:S:83:GLU:HA	14:S:106:ASP:HB2	1.99	0.43
17:a:67:LYS:HG3	22:g:68:ILE:HA	2.00	0.43
31:L2:580:SER:O	31:L2:589:ARG:NH1	2.52	0.43
27:A:1321:GLU:OE1	27:A:1471:ARG:NH1	2.51	0.43
3:C:189:VAL:HG12	3:C:199:LEU:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:L2:868:SER:HB2	31:L2:872:GLN:H	1.84	0.43
31:L2:56:ASP:OD1	31:L2:56:ASP:N	2.52	0.42
18:c:61:ARG:NH1	18:c:63:ASN:OD1	2.49	0.42
1:2:33:G:OP1	31:L2:666:ARG:NH2	2.49	0.42
19:d:110:LEU:HD11	21:f:59:LEU:HD22	2.02	0.42
27:A:1941:ARG:HH22	27:A:2013:GLY:HA2	1.84	0.42
3:C:181:ILE:HG13	3:C:182:LYS:HG2	2.02	0.42
3:C:282:VAL:O	3:C:286:ASN:ND2	2.44	0.42
20:e:57:VAL:HG22	20:e:78:MET:HG3	2.02	0.42
27:A:1072:LEU:HD22	27:A:1087:LEU:HD22	2.02	0.42
3:C:151:GLU:OE1	3:C:421:LYS:NZ	2.52	0.42
3:C:225:VAL:HG23	3:C:251:LEU:HD12	2.02	0.42
27:A:546:LEU:HD13	27:A:648:LEU:HD21	2.02	0.42
29:IN:149:N:H3'	31:L2:839:HIS:HE1	1.85	0.42
31:L2:757:ASN:HD21	31:L2:760:MET:HE2	1.85	0.42
2:6:22:A:H62	15:W:167:VAL:HG11	1.84	0.42
3:C:210:ASN:HB3	3:C:636:TYR:HB2	2.01	0.42
5:DX:279:VAL:O	5:DX:283:ARG:N	2.44	0.42
27:A:802:THR:HB	27:A:805:GLU:HG3	2.02	0.42
13:R:61:GLY:HA3	14:S:136:ILE:HG21	2.02	0.41
17:a:23:ASN:HA	17:a:69:ARG:HD2	2.02	0.41
35:T:294:LEU:HD12	35:T:303:LEU:HD11	2.02	0.41
27:A:200:ASP:OD1	27:A:240:ARG:NH2	2.53	0.41
31:L2:805:LEU:HD13	31:L2:810:ILE:HG12	2.03	0.41
27:A:1002:ASP:OD1	27:A:1004:ASN:ND2	2.49	0.41
2:6:14:C:H2'	2:6:15:A:C8	2.55	0.41
21:f:42:MET:HE1	21:f:72:ILE:HG21	2.03	0.41
27:A:1597:PHE:HB3	27:A:1609:VAL:HG11	2.03	0.41
2:6:2:U:H2'	2:6:3:G:C8	2.56	0.41
3:C:474:LEU:HA	3:C:499:GLY:HA3	2.03	0.41
20:e:38:GLN:NE2	26:5:95:G:O6	2.43	0.41
28:I:564:PHE:O	28:I:569:GLY:N	2.53	0.41
3:C:177:ARG:NH2	3:C:638:ASP:OD2	2.49	0.41
5:DX:214:GLY:N	5:DX:217:VAL:O	2.53	0.41
26:5:100:U:H2'	26:5:101:U:H6	1.85	0.41
27:A:964:ASP:OD1	27:A:964:ASP:N	2.52	0.41
27:A:1835:GLN:HB3	31:L2:557:VAL:HG11	2.02	0.41
31:L2:752:ILE:HD12	31:L2:773:LEU:HD21	2.03	0.41
29:IN:145:N:H1'2	29:IN:146:N:H5'	2.02	0.41
11:O:72:GLN:HA	11:O:75:SER:HB3	2.02	0.41
15:W:116:GLU:HA	15:W:117:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:73:LEU:HD11	37:b:71:LEU:HD22	2.02	0.41
37:b:10:LEU:HD23	37:b:13:ILE:HG13	2.03	0.41
30:L:236:ASP:OD1	30:L:236:ASP:N	2.49	0.40
21:f:21:VAL:HG13	21:f:72:ILE:HG22	2.02	0.40
11:O:22:ILE:HG21	15:W:111:LEU:HD23	2.03	0.40
15:W:209:SER:HB2	15:W:212:GLU:HB2	2.03	0.40
27:A:1249:MET:O	27:A:1253:SER:OG	2.37	0.40
3:C:328:ALA:HA	3:C:334:ILE:HD12	2.04	0.40
11:O:64:ARG:HH21	11:O:163:HIS:CE1	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
3	C	948	SER

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Mol	Chain	Res	Type
7	J	448	ALA
7	J	505	ALA
14	S	12	PRO
14	S	80	LYS
27	A	1656	THR
28	I	812	GLN
31	L2	644	ALA
31	L2	776	GLU
14	S	86	LEU
20	e	69	LYS
5	DX	427	SER
8	K	45	PRO
13	R	82	MET
13	R	97	LYS
31	L2	584	GLU
36	TF	560	GLN
23	r	52	LEU
5	DX	714	LYS
8	K	60	ALA
12	Q	956	SER
31	L2	684	PHE
37	b	87	PRO
13	R	10	PRO
27	A	1785	VAL
30	L	208	VAL
4	D	155	ILE
37	b	113	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	103	THR
3	C	129	ILE
3	C	181	ILE
3	C	199	LEU
3	C	213	ASP
3	C	219	LEU
3	C	300	LEU
3	C	307	VAL
3	C	327	TYR
3	C	683	ASN
3	C	707	ILE
6	E	203	ASP
6	E	231	MET
10	N	97	TYR

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Mol	Chain	Res	Type
10	N	115	THR
11	O	131	THR
11	O	254	GLN
11	O	259	ARG
14	S	102	ASN
14	S	152	ARG
14	S	157	VAL
15	W	87	THR
15	W	129	ARG
15	W	212	GLU
17	a	48	VAL
17	a	49	THR
17	a	72	ILE
17	a	76	MET
18	c	12	HIS
18	c	14	THR
19	d	53	LEU
19	d	74	TRP
19	d	75	THR
19	d	93	ASP
19	d	110	LEU
19	d	111	ARG
19	d	112	ASN
20	e	80	LYS
20	e	87	LEU
21	f	63	LEU
22	g	9	LEU
22	g	27	VAL
22	g	32	ARG
22	g	62	ILE
24	z	172	LEU
27	A	97	HIS
27	A	166	PHE
27	A	319	LEU
27	A	327	VAL
27	A	351	TYR
27	A	384	VAL
27	A	413	LEU
27	A	443	VAL
27	A	479	THR
27	A	668	VAL
27	A	964	ASP

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Mol	Chain	Res	Type
27	A	995	ARG
27	A	1021	ASP
27	A	1023	ASN
27	A	1315	VAL
27	A	1429	THR
27	A	1438	VAL
27	A	1467	LEU
27	A	1536	LEU
27	A	1582	TRP
27	A	1622	MET
27	A	1763	LEU
27	A	1813	ARG
27	A	1833	LEU
30	L	89	ILE
30	L	213	GLU
30	L	222	LEU
30	L	250	GLU
31	L2	539	GLU
31	L2	589	ARG
31	L2	657	GLN
31	L2	658	ARG
31	L2	676	LEU
31	L2	686	LYS
31	L2	810	ILE
33	P	83	HIS
35	T	29	ASN
35	T	216	ASN
35	T	230	ILE
35	T	416	ILE
35	T	432	ASP
37	b	10	LEU
37	b	25	ARG
37	b	81	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	280	HIS
3	C	491	HIS
3	C	743	ASN
10	N	99	ASN
11	O	163	HIS

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Mol	Chain	Res	Type
14	S	10	GLN
14	S	102	ASN
15	W	82	ASN
15	W	102	GLN
15	W	213	GLN
17	a	60	GLN
20	e	32	GLN
27	A	368	GLN
27	A	579	GLN
27	A	659	GLN
27	A	703	GLN
27	A	1014	ASN
27	A	1023	ASN
27	A	1035	GLN
27	A	1096	HIS
27	A	1121	ASN
27	A	1215	ASN
27	A	1227	GLN
27	A	1282	GLN
27	A	1293	ASN
27	A	1367	ASN
27	A	1468	ASN
27	A	1531	ASN
27	A	1658	GLN
27	A	1712	HIS
27	A	1717	ASN
27	A	1830	GLN
27	A	1918	ASN
27	A	1944	HIS
27	A	1946	ASN
27	A	1965	HIS
30	L	13	ASN
30	L	81	GLN
30	L	245	GLN
31	L2	64	ASN
31	L2	710	HIS
31	L2	717	GLN
31	L2	719	HIS
31	L2	757	ASN
31	L2	828	HIS
31	L2	838	GLN
31	L2	839	HIS

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Mol	Chain	Res	Type
35	T	11	HIS
35	T	50	ASN
35	T	278	ASN
35	T	283	HIS
35	T	324	HIS
35	T	384	HIS
35	T	394	ASN
35	T	417	ASN
35	T	433	ASN
35	T	446	ASN
35	T	455	GLN
37	b	11	GLN

5.3.3 RNA ⓘ

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%)

All (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
1	2	20	G
1	2	24	A
1	2	28	C
1	2	29	A
1	2	30	A
1	2	31	G
1	2	32	U
1	2	33	G
1	2	34	U
1	2	35	A
1	2	36	G

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Mol	Chain	Res	Type
1	2	37	U
1	2	38	A
1	2	39	U
2	6	5	U
2	6	6	C
2	6	7	G
2	6	9	U
2	6	10	U
2	6	12	G
2	6	22	A
2	6	25	C
2	6	26	U
2	6	27	A
2	6	28	A
2	6	29	A
2	6	33	G
2	6	34	G
2	6	35	A
2	6	36	A
2	6	37	C
2	6	41	A
2	6	42	C
2	6	43	A
2	6	44	G
2	6	45	A
2	6	46	G
2	6	48	A
2	6	51	U
2	6	53	A
2	6	54	G
2	6	56	A
2	6	59	G
2	6	60	C
2	6	61	C
2	6	68	C
2	6	69	A
2	6	74	U
2	6	78	A
2	6	79	C
2	6	81	C
2	6	82	A
2	6	84	A

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Mol	Chain	Res	Type
2	6	87	C
2	6	88	G
2	6	91	A
26	5	10	U
26	5	11	U
26	5	20	G
26	5	21	A
26	5	34	U
26	5	35	U
26	5	36	C
26	5	38	C
26	5	39	C
26	5	42	U
26	5	45	C
26	5	47	A
26	5	52	U
26	5	53	U
26	5	57	G
26	5	69	A
26	5	86	C
26	5	89	U
26	5	91	U
26	5	92	U
26	5	93	U
26	5	94	U
26	5	95	G
26	5	96	A
26	5	104	C
26	5	115	U

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	28	C
2	6	5	U
2	6	33	G
2	6	35	A
2	6	50	A
2	6	58	G
2	6	81	C
2	6	82	A
26	5	92	U

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Mol	Chain	Res	Type
26	5	95	G

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

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

All (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
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
40	A	3000	IHP	P4-O14	3.16	1.65	1.59
38	C	1500	GTP	C2-N3	2.16	1.38	1.33
38	C	1500	GTP	PB-O3A	2.11	1.61	1.59
38	C	1500	GTP	PB-O3B	2.06	1.61	1.59
38	C	1500	GTP	C5-N7	-2.00	1.35	1.39

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
40	A	3000	IHP	O11-C1-C6	-2.37	103.72	108.76
38	C	1500	GTP	O6-C6-C5	-2.36	120.30	126.53
38	C	1500	GTP	C5-C6-N1	2.33	119.18	113.25
38	C	1500	GTP	N9-C8-N7	-2.18	109.37	113.40
40	A	3000	IHP	P6-O16-C6	-2.14	117.71	123.43
40	A	3000	IHP	P4-O14-C4	-2.10	117.83	123.43
40	A	3000	IHP	C6-C1-C2	2.09	115.02	110.43
38	C	1500	GTP	C8-N7-C5	2.09	107.98	104.26
38	C	1500	GTP	O5'-C5'-C4'	2.05	115.96	108.99

There are no chirality outliers.

All (3) torsion outliers are listed below:

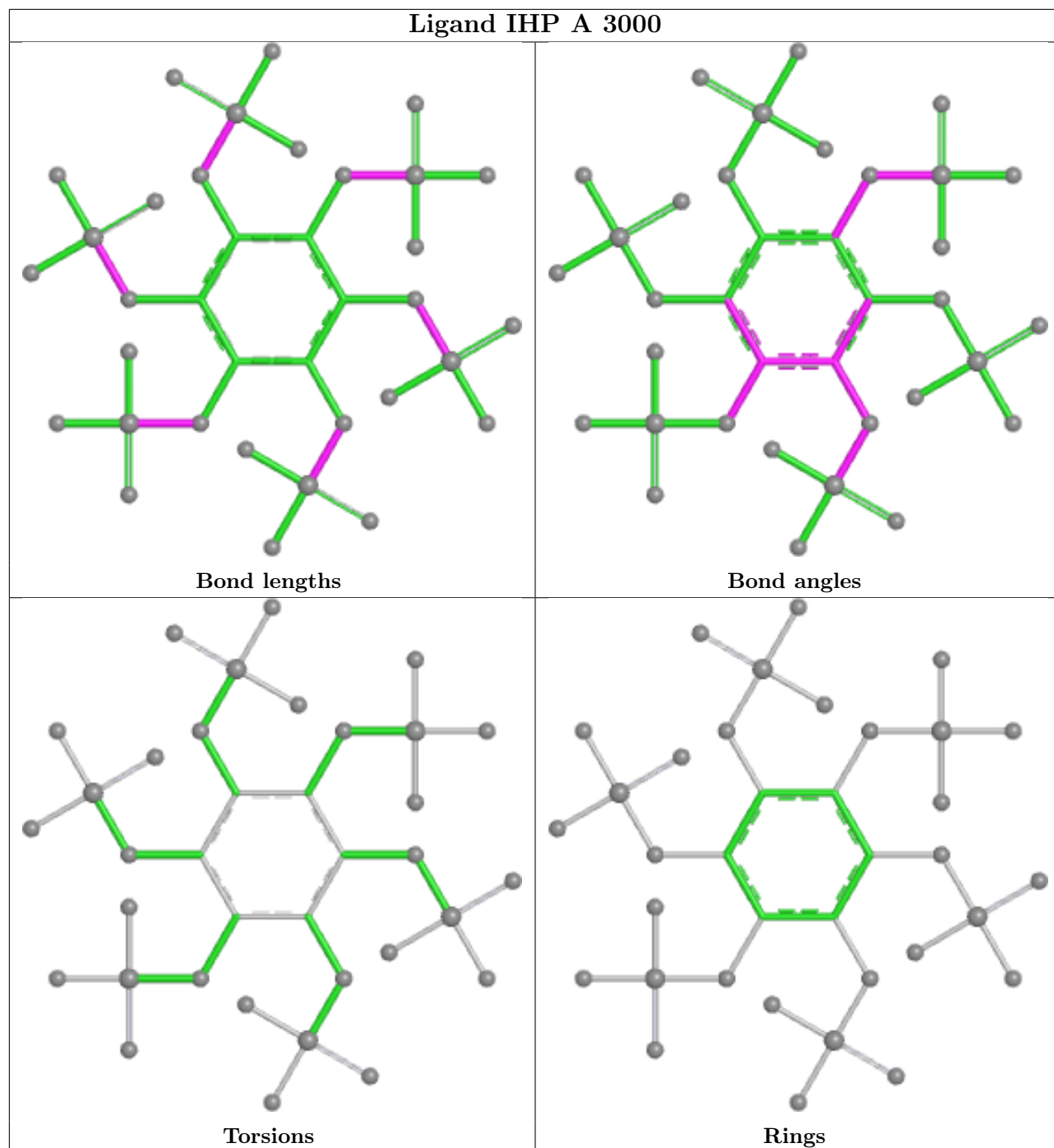
Mol	Chain	Res	Type	Atoms
38	C	1500	GTP	C5'-O5'-PA-O2A
38	C	1500	GTP	C5'-O5'-PA-O3A
38	C	1500	GTP	C5'-O5'-PA-O1A

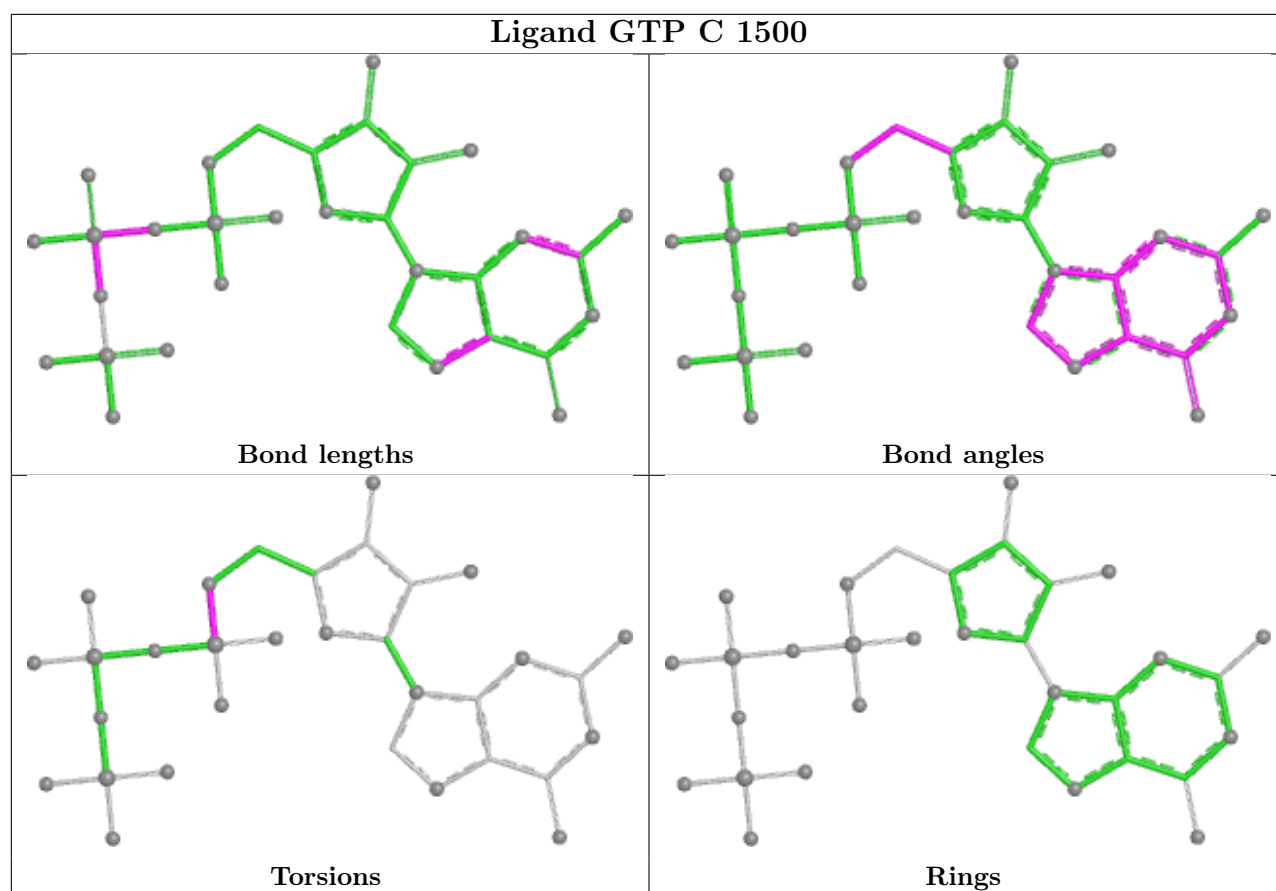
There are no ring outliers.

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.

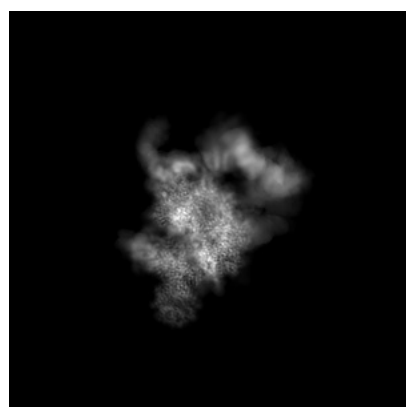
6 Map visualisation [i](#)

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.

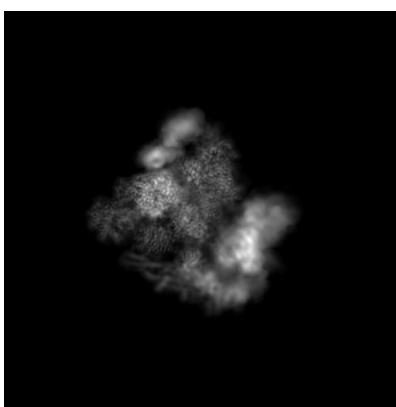
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

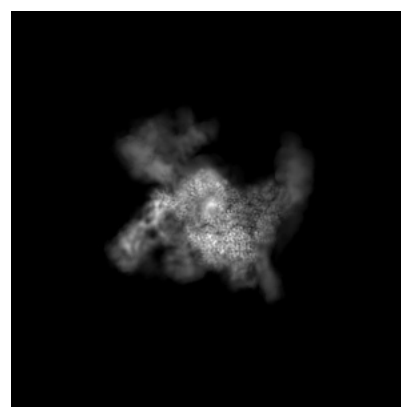
6.1.1 Primary map



X



Y

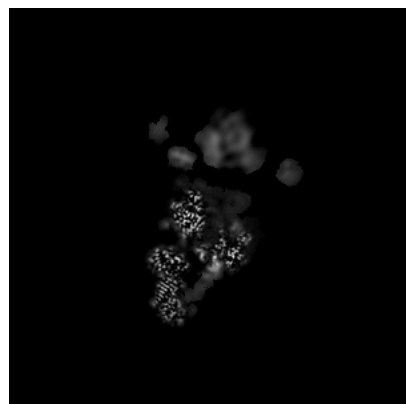


Z

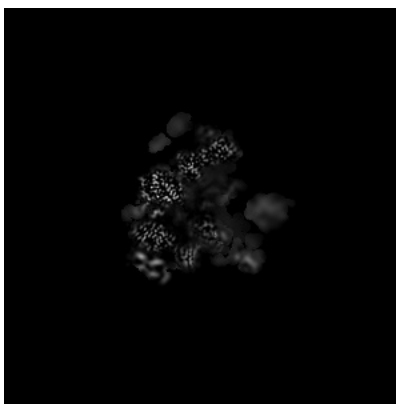
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

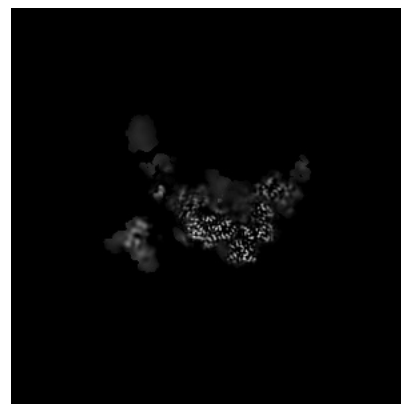
6.2.1 Primary map



X Index: 210



Y Index: 210

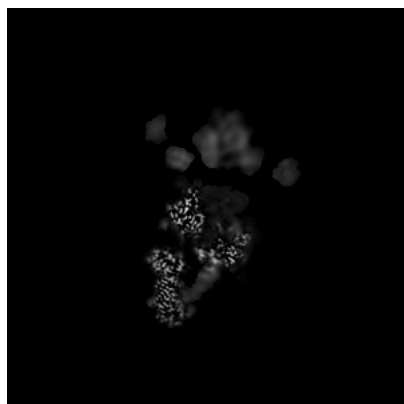


Z Index: 210

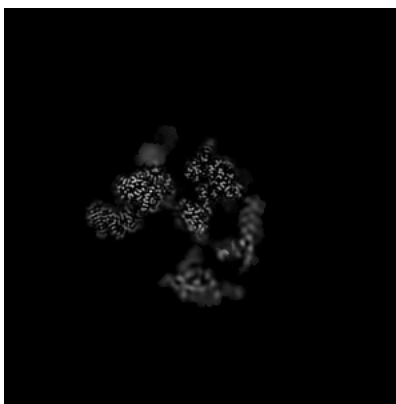
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

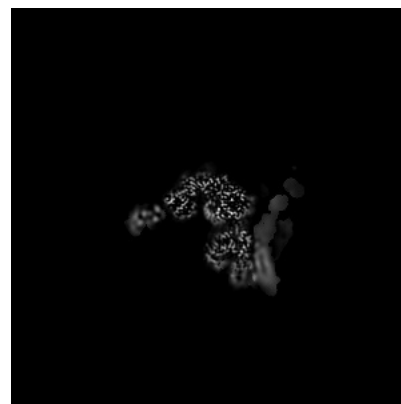
6.3.1 Primary map



X Index: 208



Y Index: 181

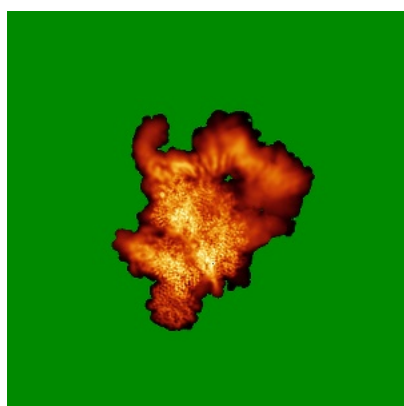


Z Index: 164

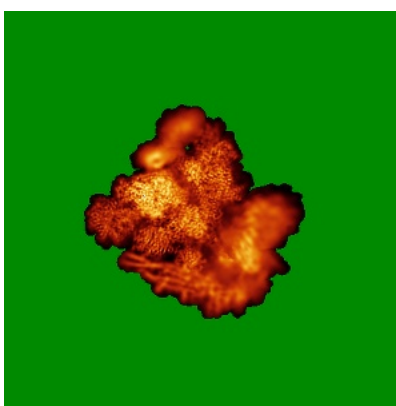
The images above show the largest variance slices of the map in three orthogonal directions.

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

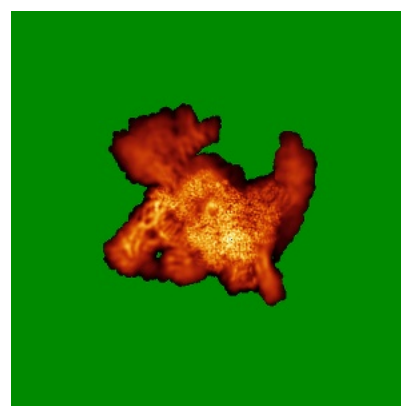
6.4.1 Primary map



X



Y

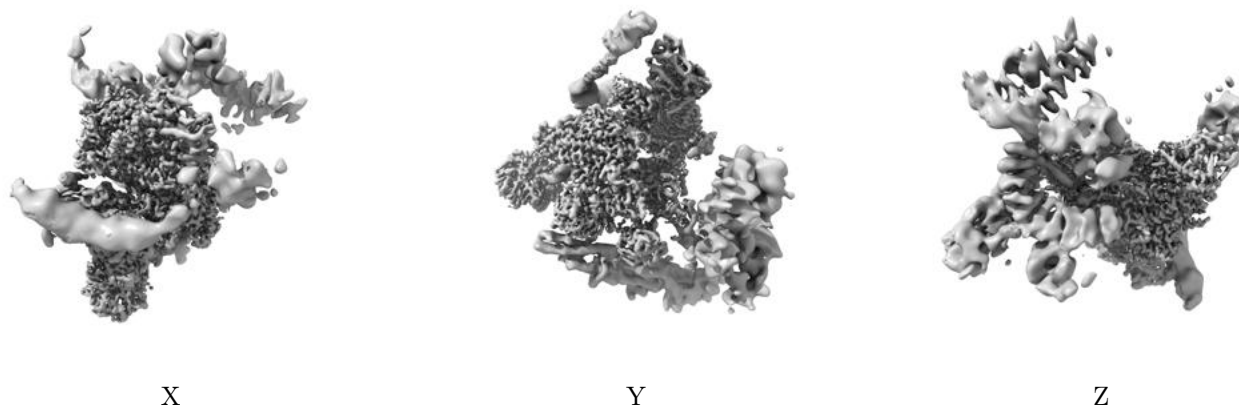


Z

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.

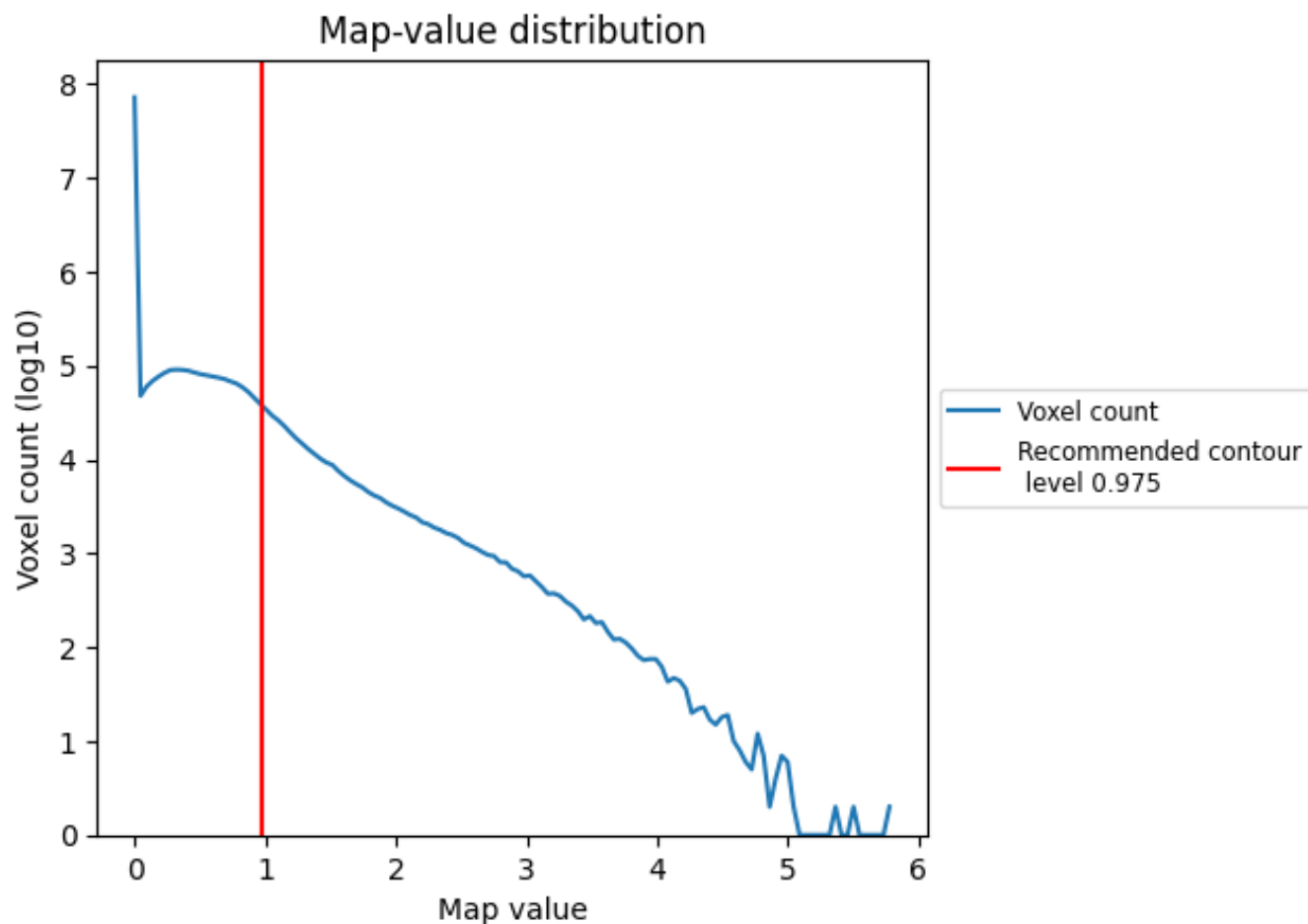
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

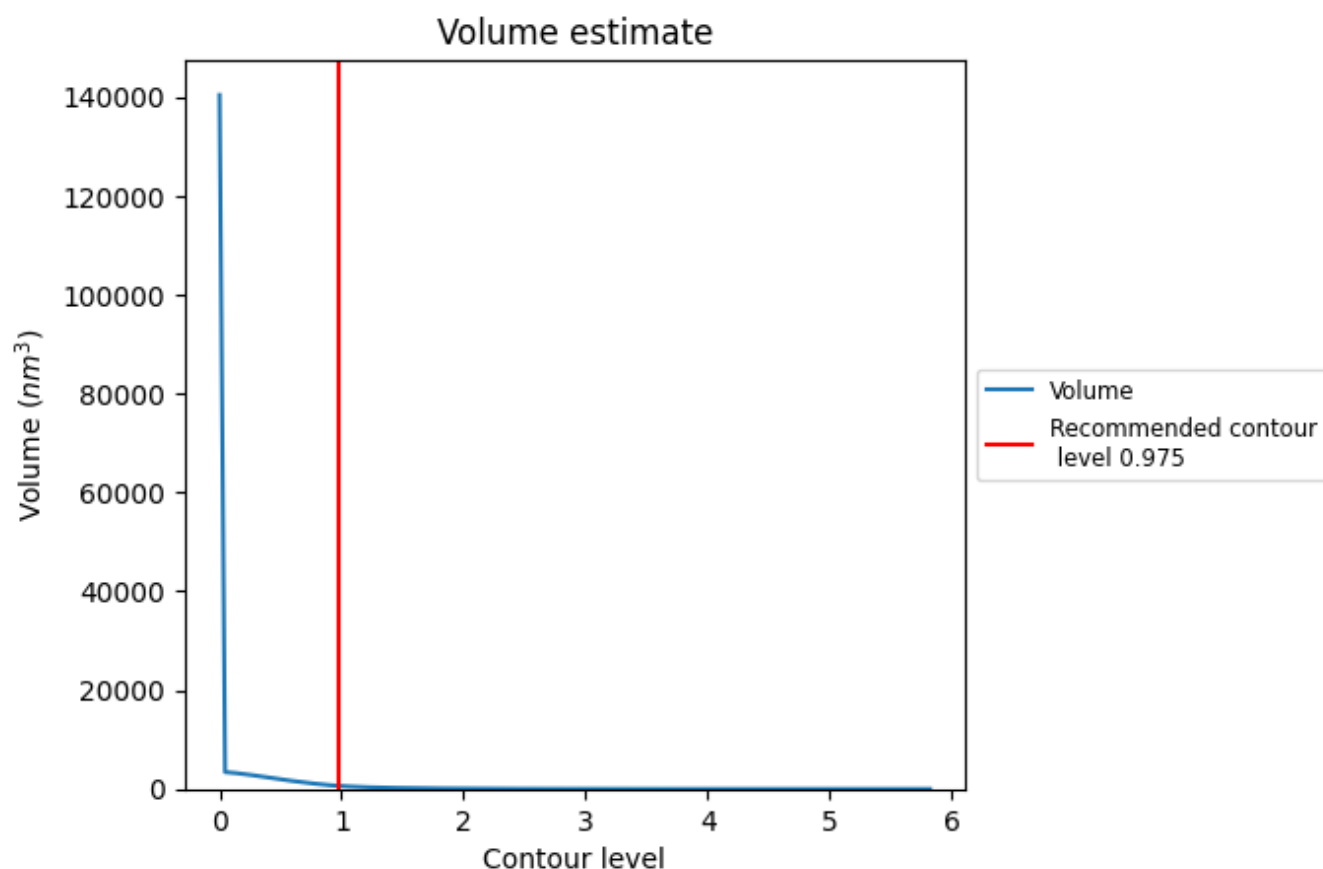
This section contains the results of statistical analysis of the map.

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.

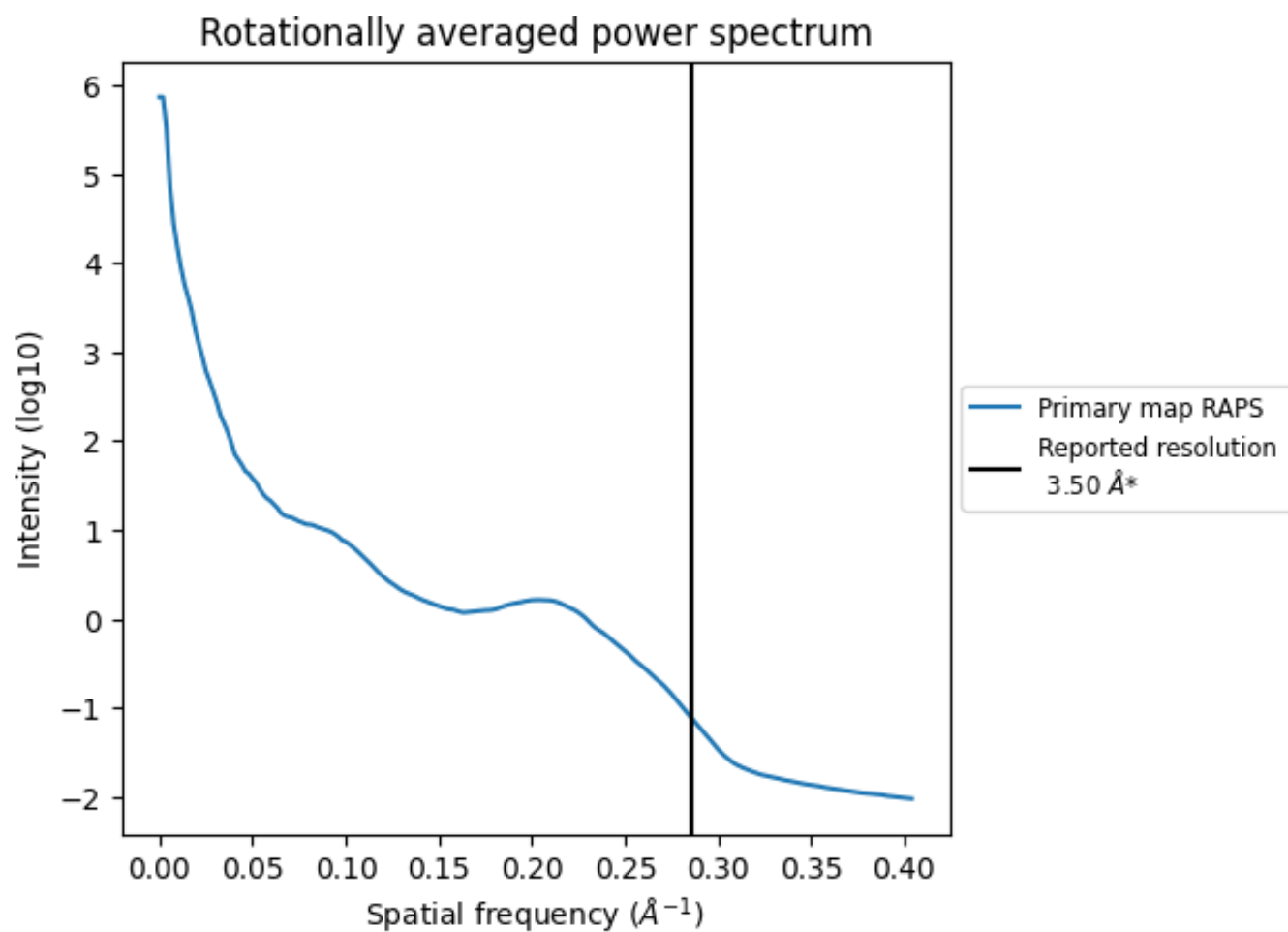
7.2 Volume estimate [i](#)



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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

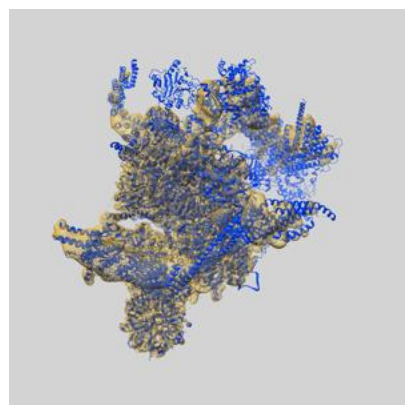
8 Fourier-Shell correlation

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

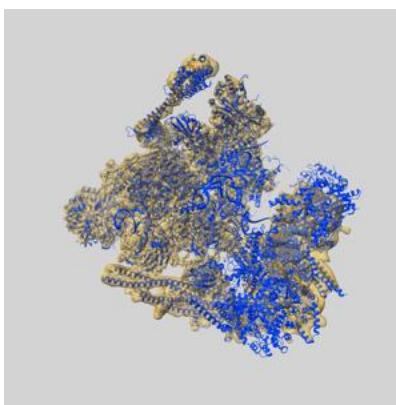
9 Map-model fit [i](#)

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](#).

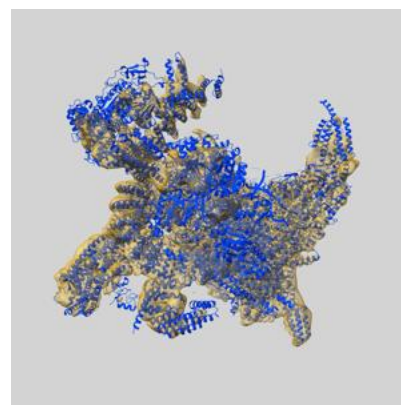
9.1 Map-model overlay [i](#)



X



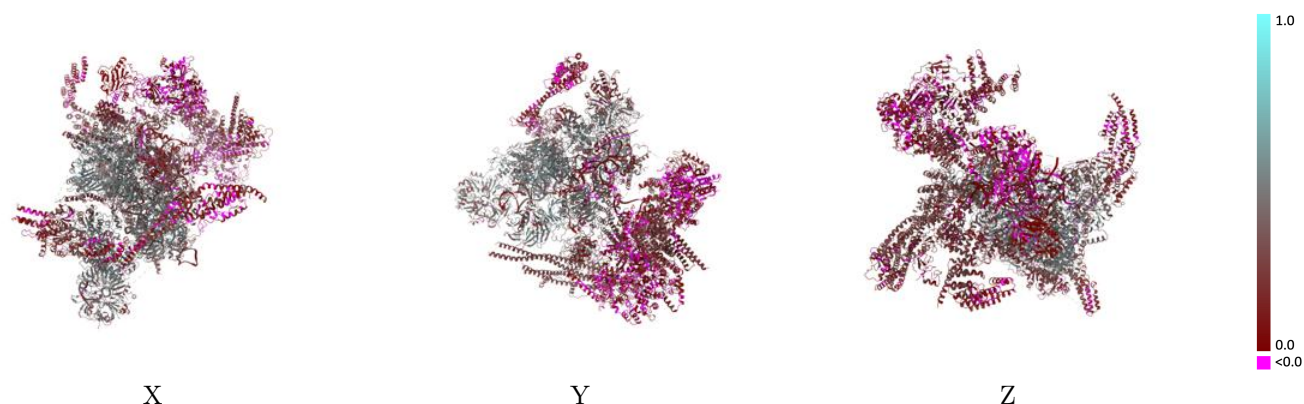
Y



Z

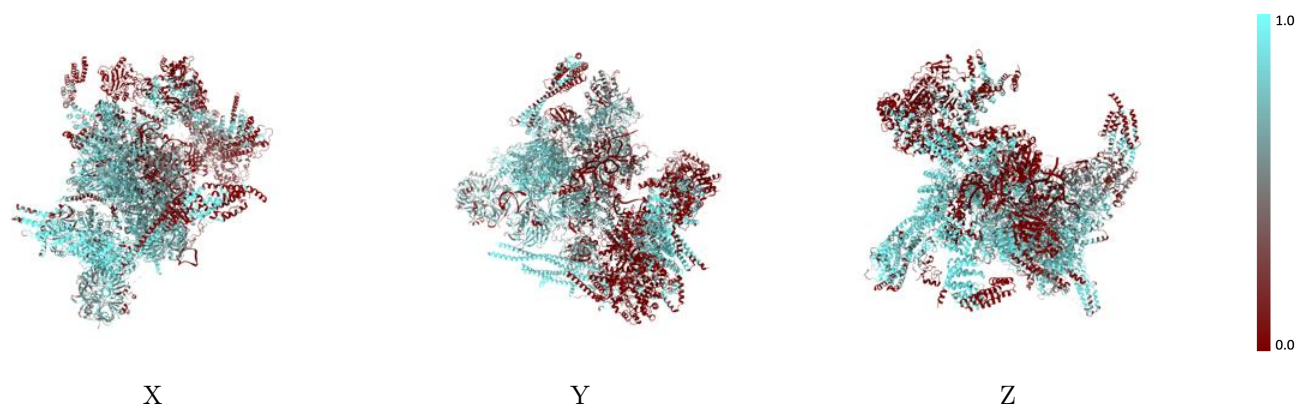
The images above show the 3D surface view of the map at the recommended contour level 0.975 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



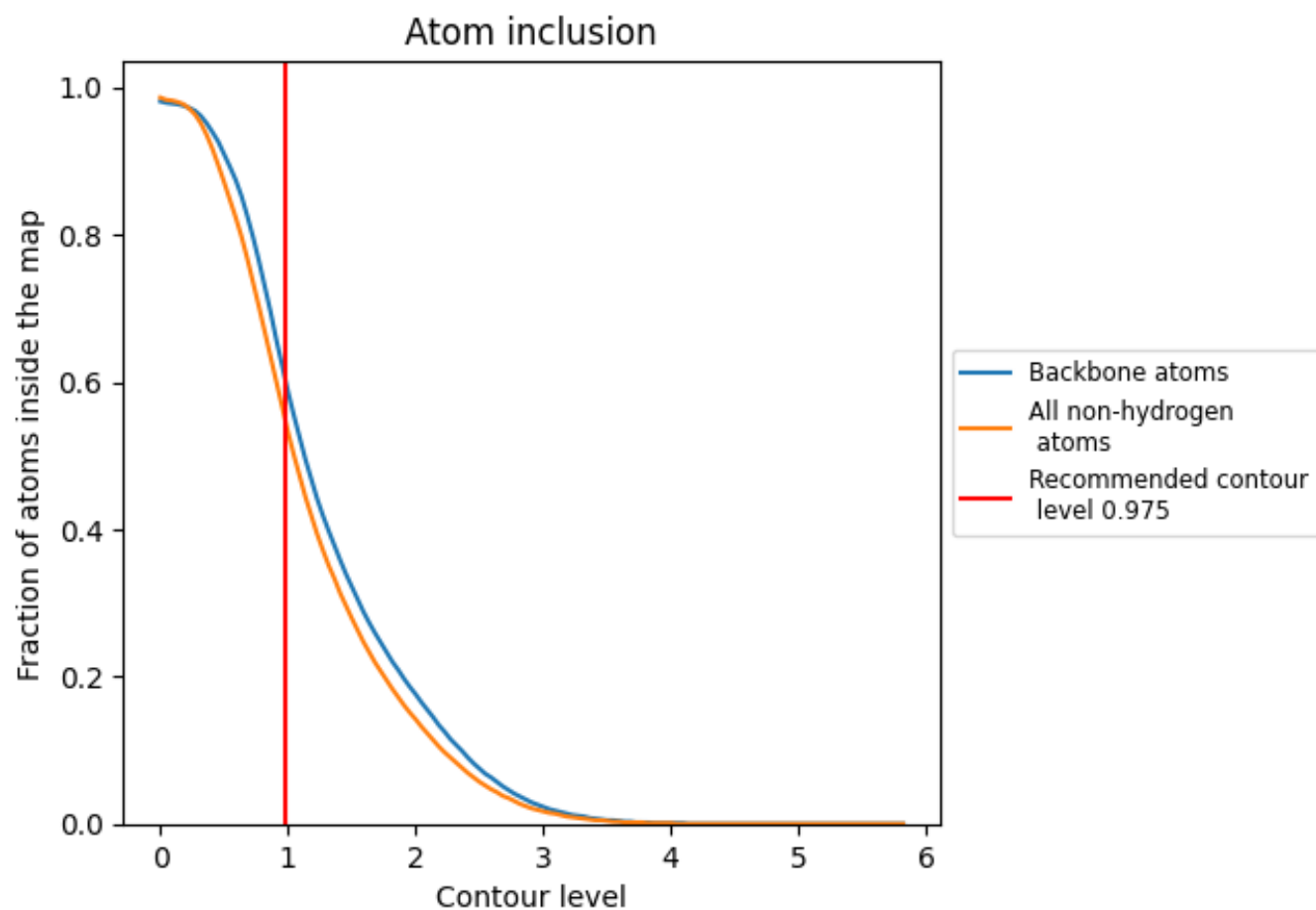
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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