



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 10:53 PM UTC

PDB ID : 6ID0 / pdb_00006id0
EMDB ID : EMD-9646
Title : Cryo-EM structure of a human intron lariat spliceosome prior to Prp43 loaded (ILS1 complex) at 2.9 angstrom resolution
Authors : Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on : 2018-09-07
Resolution : 2.90 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

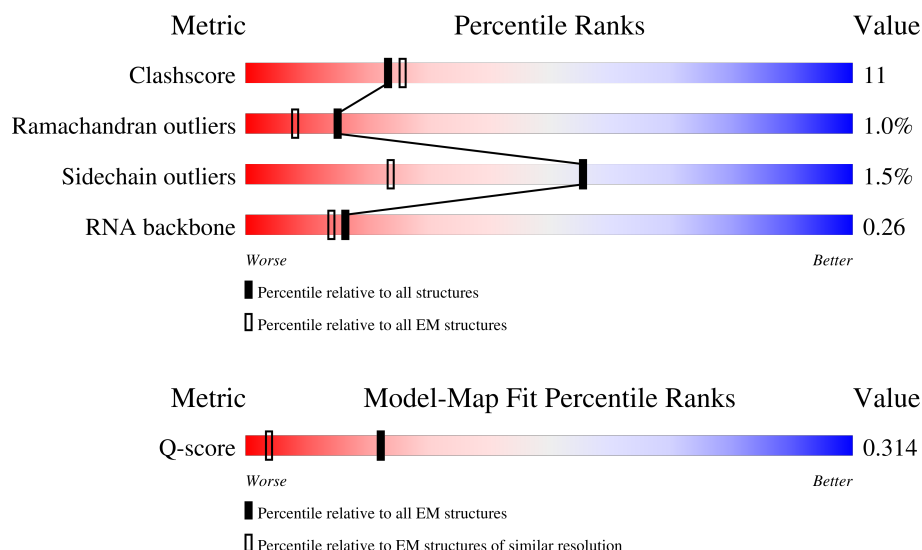
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2335	
2	B	117	
3	C	972	

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Mol	Chain	Length	Quality of chain
4	E	357	
5	F	107	
6	J	848	
7	L	802	
8	M	243	
9	N	144	
10	O	420	
11	P	229	
12	R	536	
13	S	166	
14	T	514	
15	W	579	
16	G	272	
17	H	188	
18	U	894	
19	I	855	
20	a	126	
20	h	126	
21	b	231	
21	i	231	
22	c	119	
22	j	119	
23	d	118	
23	k	118	
24	f	86	

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Mol	Chain	Length	Quality of chain
24	m	86	
25	e	92	
25	l	92	
26	g	76	
26	n	76	
27	q	504	
27	r	504	
27	s	504	
27	t	504	
28	K	225	
29	o	255	
30	p	225	
31	Q	1485	
32	y	301	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	GTP	C	1500	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 78004 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

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

- Molecule 2 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	98	Total	C	N	O	P	0	0
			2060	923	341	698	98		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	888	Total	C	N	O	S	0	0
			7022	4494	1172	1322	34		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 5 is a RNA chain called U6snRNA.

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

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	556	Total	C	N	O	S	0	0
			3758	2344	705	703	6		

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	475	Total	C	N	O	S	0	0
			3237	1985	627	619	6		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 9 is a protein called Protein BUD31 homolog.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	290	Total	C	N	O	S	0	0
			2340	1469	415	436	20		

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	118	Total	C	N	O	S	0	0
			985	601	194	188	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	272	Total	C	N	O	P	S	0	0
			2165	1357	393	401	2	12		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	317	Total	C	N	O	S	0	0
			2496	1574	453	461	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	509	Total	C	N	O	S	0	0
			3008	1833	568	603	4		

- Molecule 16 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	70	Total	C	N	O	P	0	0
			1246	549	158	469	70		

- Molecule 17 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	H	140	Total	C	N	O	P	0	0
			2968	1327	511	990	140		

- Molecule 18 is a protein called CWF19-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	347	Total	C	N	O	S	0	0
			2864	1817	496	529	22		

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	I	568	Total	C	N	O	S	0	0
			2822	1683	569	569	1		

- Molecule 20 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	a	81	Total	C	N	O	0	0
			399	237	81	81		
20	h	81	Total	C	N	O	0	0
			398	236	81	81		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	b	86	Total	C	N	O	0	0
			424	252	86	86		
21	i	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	c	82	Total	C	N	O	0	0
			406	242	82	82		
22	j	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	d	97	Total	C	N	O	0	0
			480	286	97	97		
23	k	85	Total	C	N	O	0	0
			422	252	85	85		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	f	74	Total	C	N	O	0	0
			361	213	74	74		
24	m	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	e	79	Total	C	N	O	0	0
			391	233	79	79		
25	l	79	Total	C	N	O	0	0
			391	233	79	79		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	g	74	Total	C	N	O	0	0
			363	215	74	74		

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Mol	Chain	Residues	Atoms				AltConf	Trace
26	n	67	Total	C	N	O	0	0
			329	195	67	67		

- Molecule 27 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	q	132	Total	C	N	O	0	0
			659	395	132	132		
27	r	131	Total	C	N	O	0	0
			654	392	131	131		
27	s	67	Total	C	N	O	0	0
			335	201	67	67		
27	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 28 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	K	152	Total	C	N	O	0	0
			757	453	152	152		

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	o	162	Total	C	N	O	0	0
			804	480	162	162		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	p	94	Total	C	N	O	0	0
			464	276	94	94		

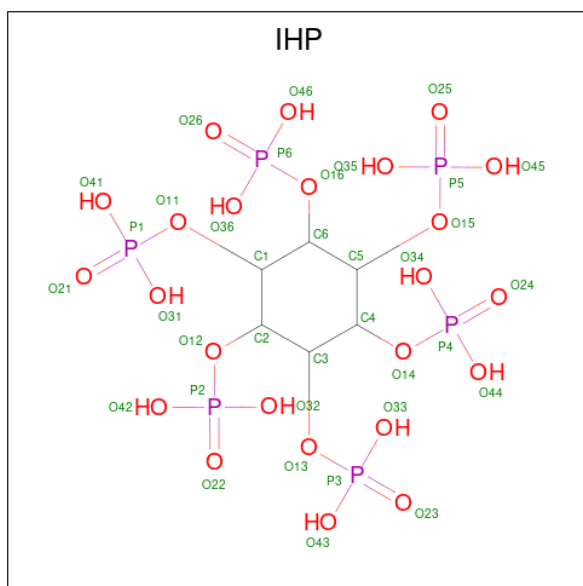
- Molecule 31 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Q	1322	Total	C	N	O	4	0
			6562	3918	1322	1322		

- Molecule 32 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 33 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	C	1	Total	Mg	0
			1	1	
35	F	6	Total	Mg	0
			6	6	

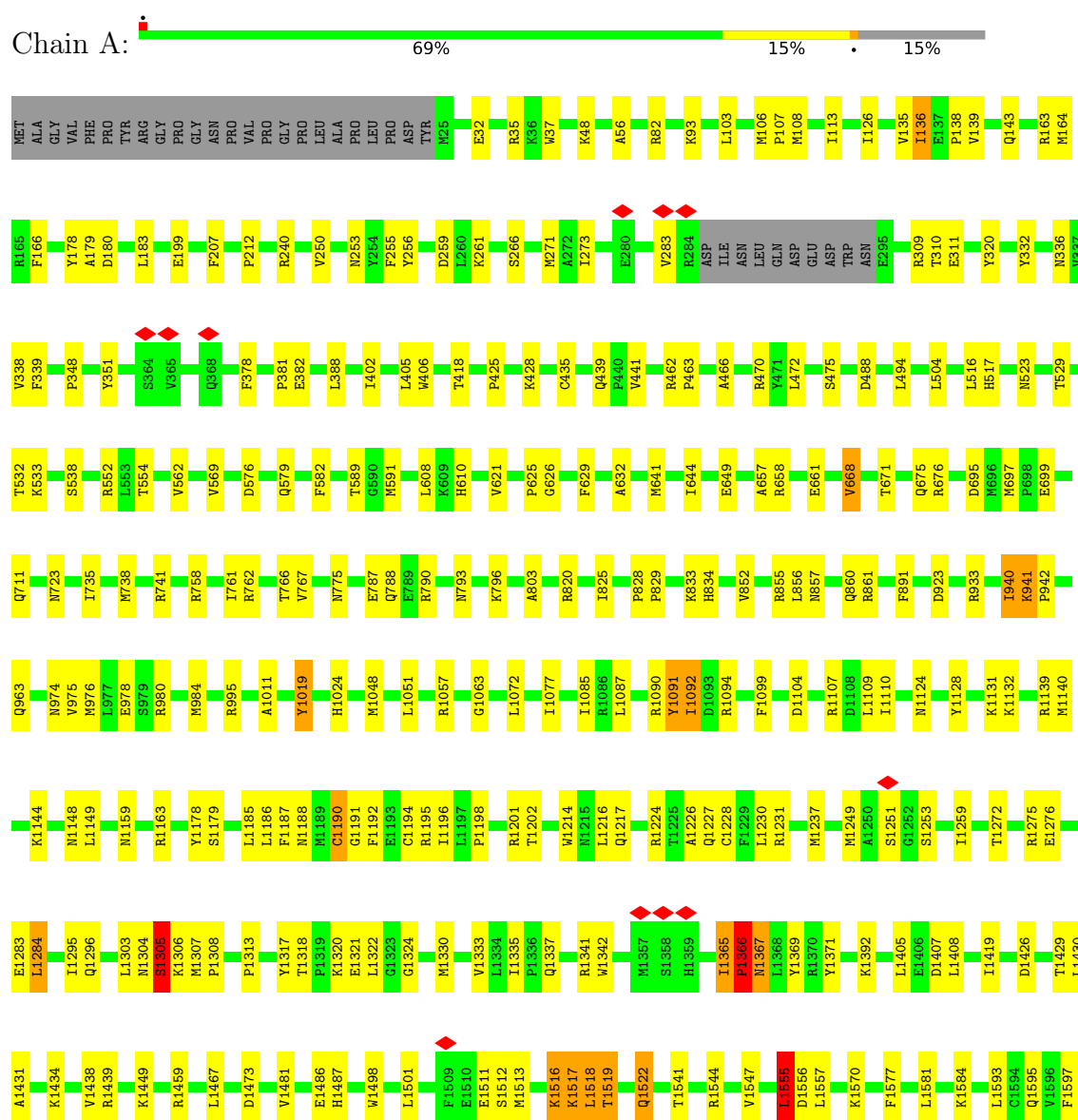
- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
36	N	3	Total	Zn	0
			3	3	
36	O	3	Total	Zn	0
			3	3	
36	U	1	Total	Zn	0
			1	1	

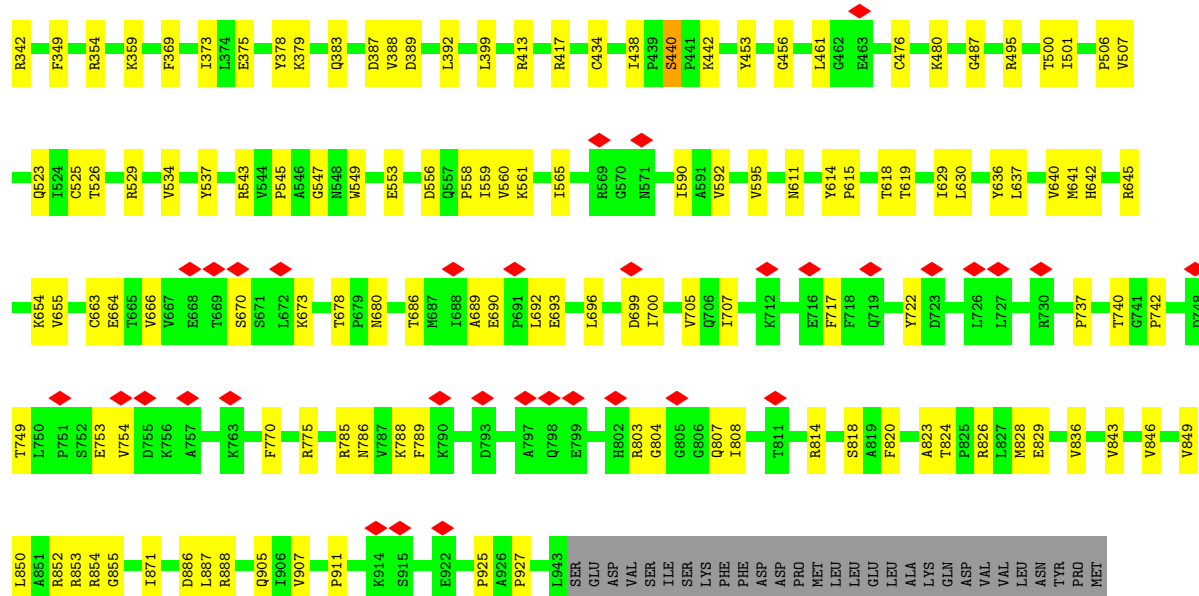
3 Residue-property plots

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.

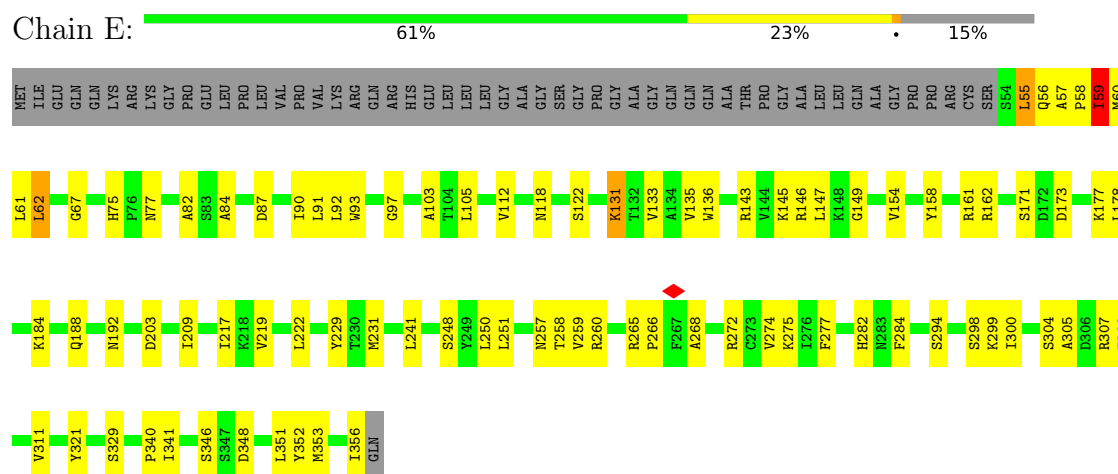
• Molecule 1: Pre-mRNA-processing-splicing factor 8



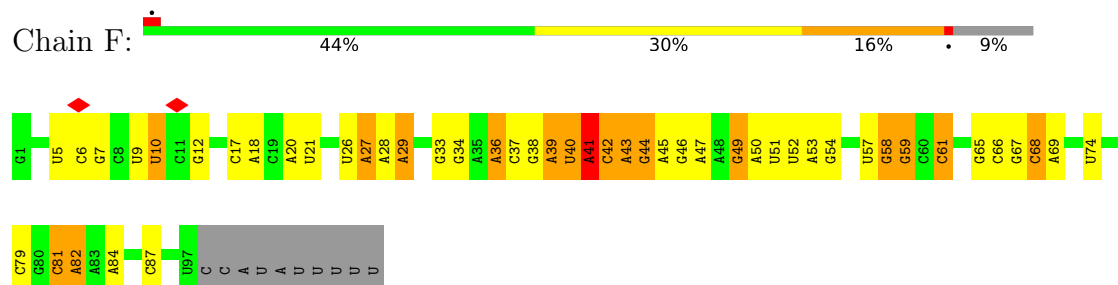




- Molecule 4: U5 small nuclear ribonucleoprotein 40 kDa protein

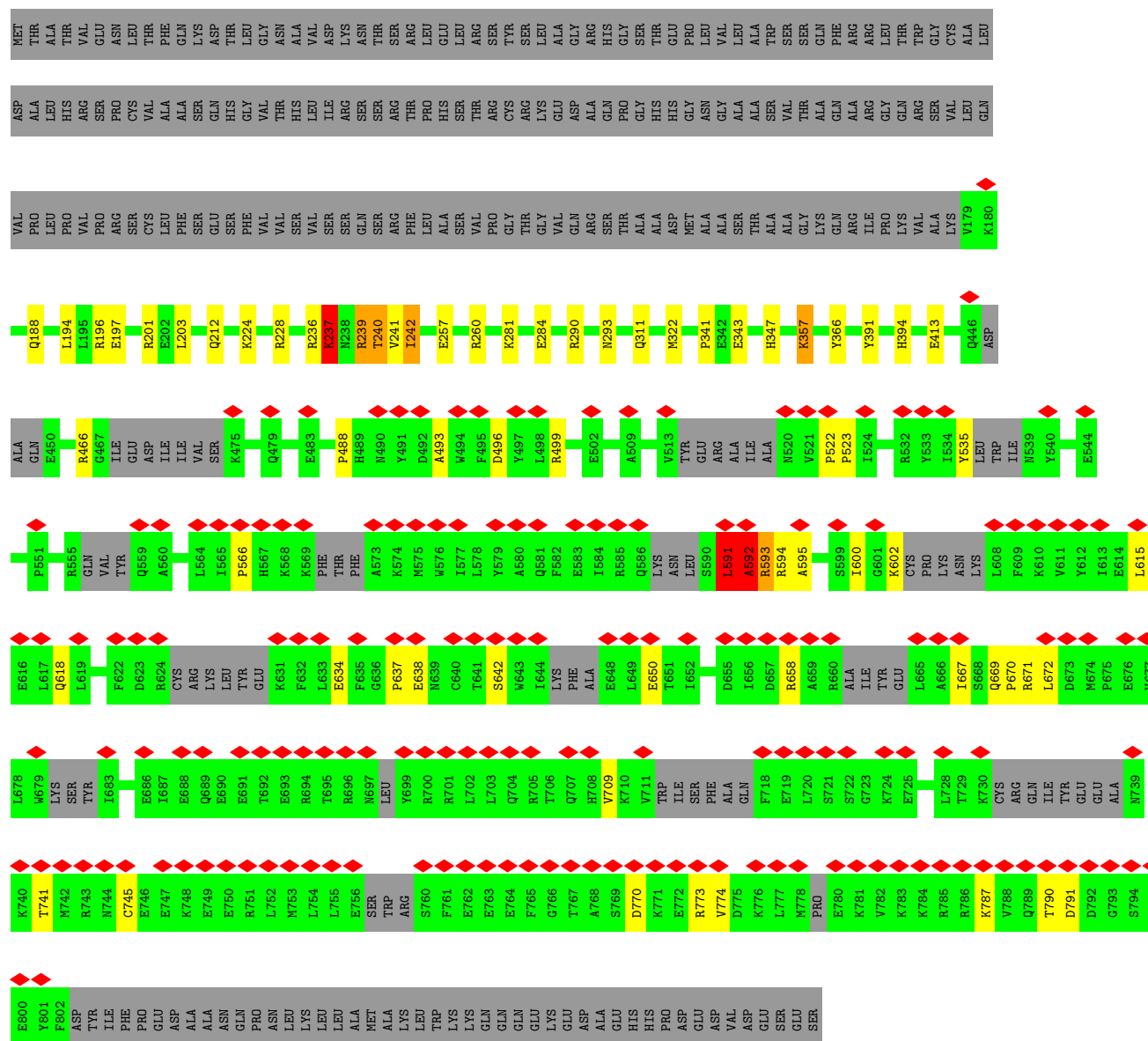


- Molecule 5: U6snRNA

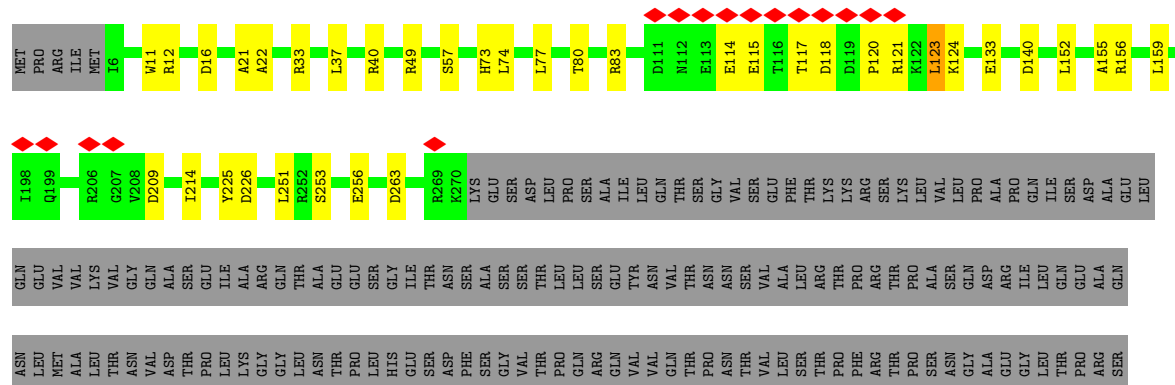


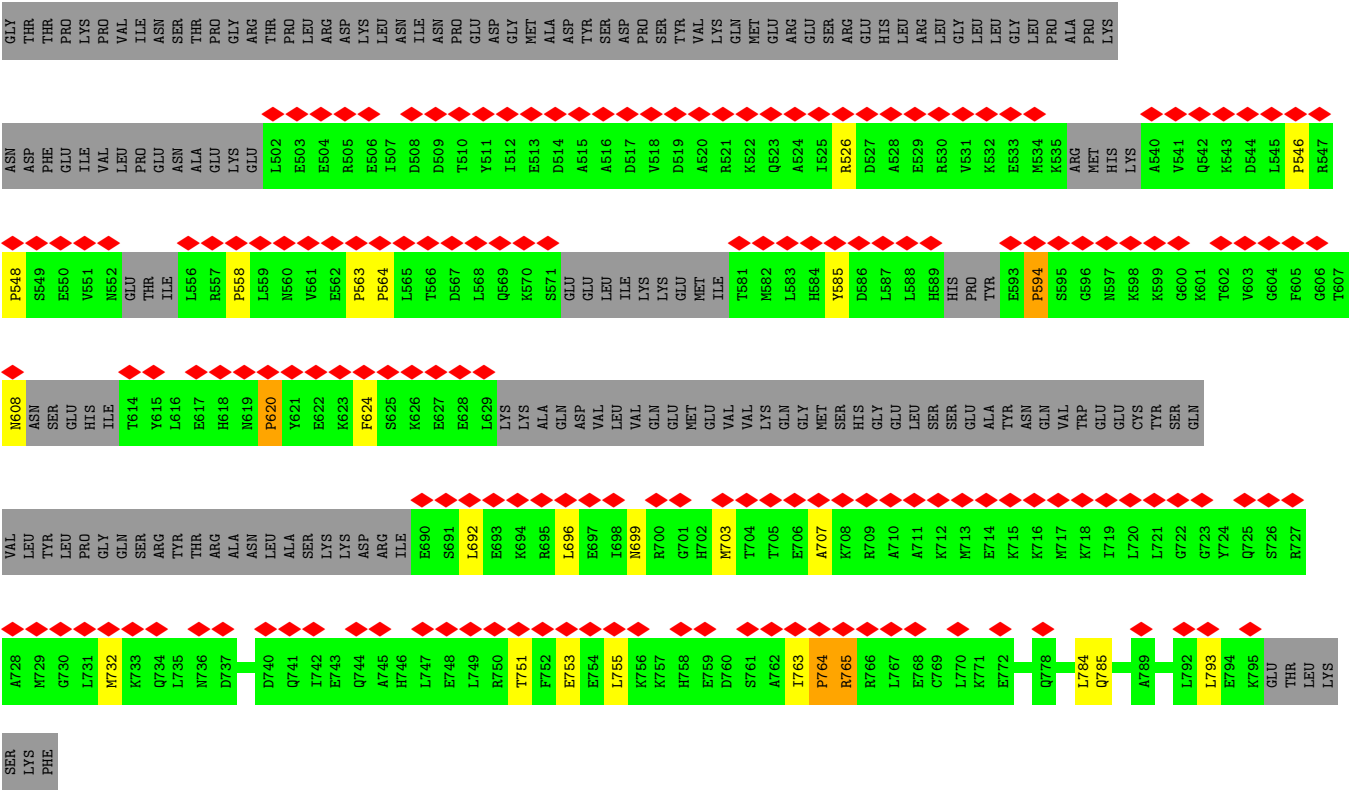
- Molecule 6: Crooked neck-like protein 1



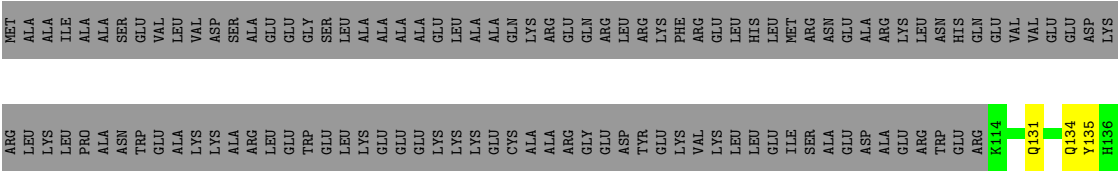


• Molecule 7: Cell division cycle 5-like protein

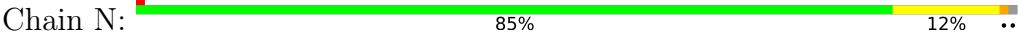




• Molecule 8: Pre-mRNA-splicing factor SYF2

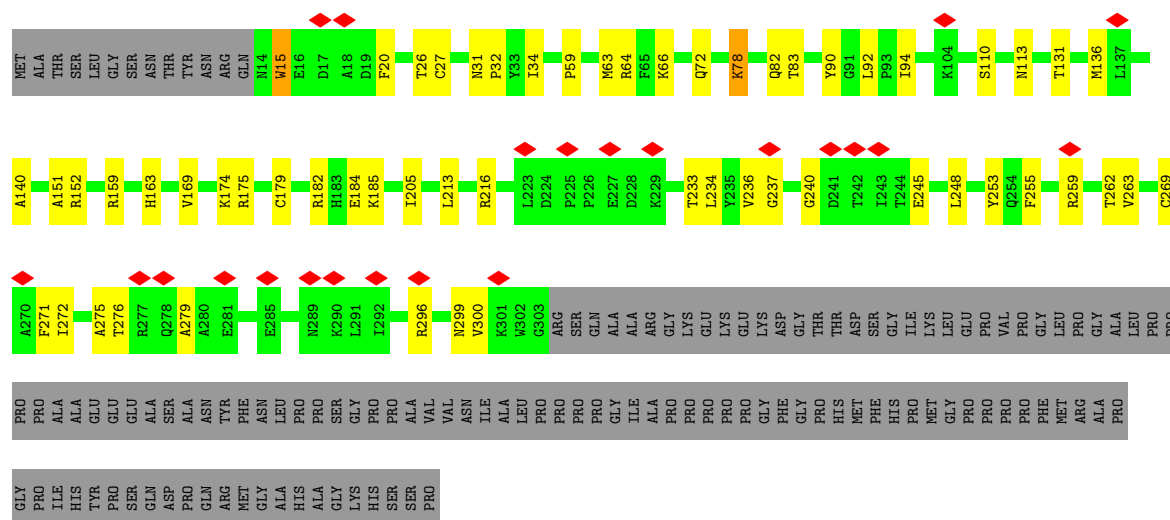


• Molecule 9: Protein BUD31 homolog

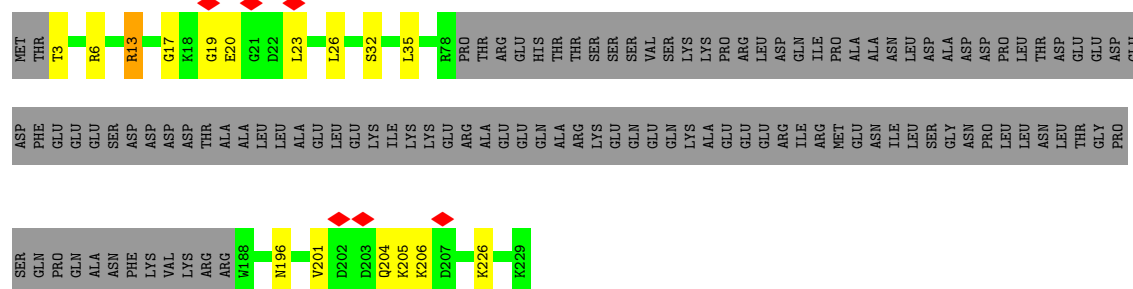


• Molecule 10: Pre-mRNA-splicing factor RBM22

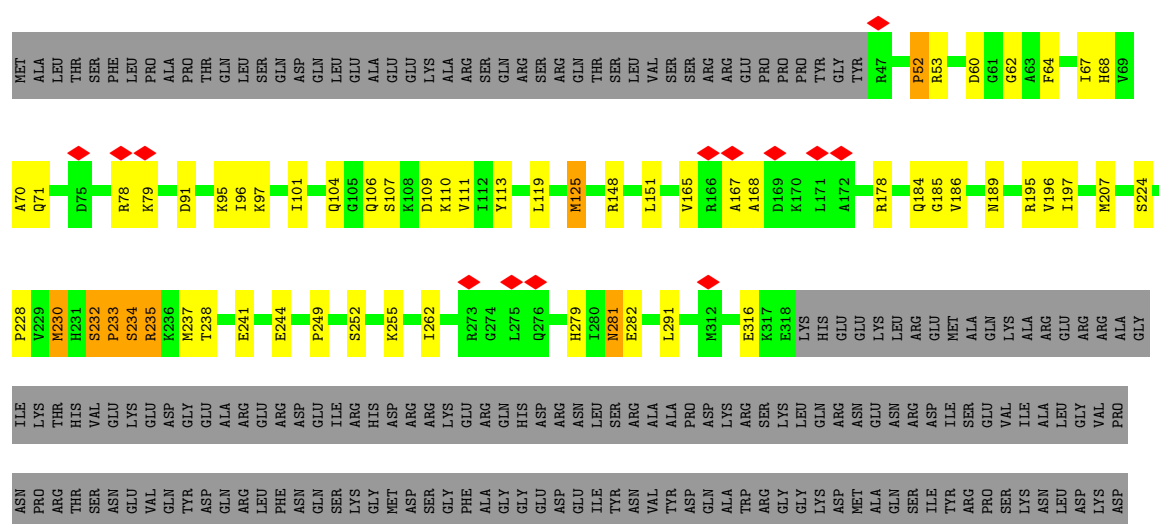
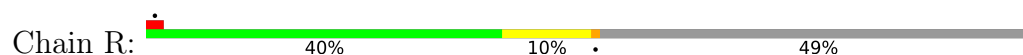




• Molecule 11: Spliceosome-associated protein CWC15 homolog



• Molecule 12: SNW domain-containing protein 1



[illegible]

- Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1



R131	R141	R152	R163	R174	R185	R196	R207	R218	R229	R240	R251	R262	R273	R284	R295	R306	R317	R328	R339	R350	R361	R372	R383	R394	R405	R416	R427	R438	R449	R460	R471	R482	R493	R504	R515	R526	R537	R548	R559	R570	R581	R592	R603	R614	R625	R636	R647	R658	R669	R680	R691	R702	R713	R724	R735	R746	R757	R768	R779	R790	R801	R812	R823	R834	R845	R856	R867	R878	R889	R900	R911	R922	R933	R944	R955	R966	R977	R988	R999	R1010	R1021	R1032	R1043	R1054	R1065	R1076	R1087	R1098	R1109	R1120	R1131	R1142	R1153	R1164	R1175	R1186	R1197	R1208	R1219	R1230	R1241	R1252	R1263	R1274	R1285	R1296	R1307	R1318	R1329	R1340	R1351	R1362	R1373	R1384	R1395	R1406	R1417	R1428	R1439	R1450	R1461	R1472	R1483	R1494	R1505	R1516	R1527	R1538	R1549	R1560	R1571	R1582	R1593	R1604	R1615	R1626	R1637	R1648	R1659	R1670	R1681	R1692	R1703	R1714	R1725	R1736	R1747	R1758	R1769	R1780	R1791	R1802	R1813	R1824	R1835	R1846	R1857	R1868	R1879	R1890	R1901	R1912	R1923	R1934	R1945	R1956	R1967	R1978	R1989	R2000	R2011	R2022	R2033	R2044	R2055	R2066	R2077	R2088	R2099	R2110	R2121	R2132	R2143	R2154	R2165	R2176	R2187	R2198	R2209	R2220	R2231	R2242	R2253	R2264	R2275	R2286	R2297	R2308	R2319	R2330	R2341	R2352	R2363	R2374	R2385	R2396	R2407	R2418	R2429	R2440	R2451	R2462	R2473	R2484	R2495	R2506	R2517	R2528	R2539	R2550	R2561	R2572	R2583	R2594	R2605	R2616	R2627	R2638	R2649	R2660	R2671	R2682	R2693	R2704	R2715	R2726	R2737	R2748	R2759	R2770	R2781	R2792	R2803	R2814	R2825	R2836	R2847	R2858	R2869	R2880	R2891	R2902	R2913	R2924	R2935	R2946	R2957	R2968	R2979	R2990	R3001	R3012	R3023	R3034	R3045	R3056	R3067	R3078	R3089	R3100	R3111	R3122	R3133	R3144	R3155	R3166	R3177	R3188	R3199	R3210	R3221	R3232	R3243	R3254	R3265	R3276	R3287	R3298	R3309	R3320	R3331	R3342	R3353	R3364	R3375	R3386	R3397	R3408	R3419	R3430	R3441	R3452	R3463	R3474	R3485	R3496	R3507	R3518	R3529	R3540	R3551	R3562	R3573	R3584	R3595	R3606	R3617	R3628	R3639	R3650	R3661	R3672	R3683	R3694	R3705	R3716	R3727	R3738	R3749	R3760	R3771	R3782	R3793	R3804	R3815	R3826	R3837	R3848	R3859	R3870	R3881	R3892	R3903	R3914	R3925	R3936	R3947	R3958	R3969	R3980	R3991	R4002	R4013	R4024	R4035	R4046	R4057	R4068	R4079	R4090	R4101	R4112	R4123	R4134	R4145	R4156	R4167	R4178	R4189	R4200	R4211	R4222	R4233	R4244	R4255	R4266	R4277	R4288	R4299	R4310	R4321	R4332	R4343	R4354	R4365	R4376	R4387	R4398	R4409	R4420	R4431	R4442	R4453	R4464	R4475	R4486	R4497	R4508	R4519	R4530	R4541	R4552	R4563	R4574	R4585	R4596	R4607	R4618	R4629	R4640	R4651	R4662	R4673	R4684	R4695	R4706	R4717	R4728	R4739	R4750	R4761	R4772	R4783	R4794	R4805	R4816	R4827	R4838	R4849	R4860	R4871	R4882	R4893	R4904	R4915	R4926	R4937	R4948	R4959	R4970	R4981	R4992	R5003	R5014	R5025	R5036	R5047	R5058	R5069	R5080	R5091	R5102	R5113	R5124	R5135	R5146	R5157	R5168	R5179	R5190	R5201	R5212	R5223	R5234	R5245	R5256	R5267	R5278	R5289	R5300	R5311	R5322	R5333	R5344	R5355	R5366	R5377	R5388	R5399	R5410	R5421	R5432	R5443	R5454	R5465	R5476	R5487	R5498	R5509	R5520	R5531	R5542	R5553	R5564	R5575	R5586	R5597	R5608	R5619	R5630	R5641	R5652	R5663	R5674	R5685	R5696	R5707	R5718	R5729	R5740	R5751	R5762	R5773	R5784	R5795	R5806	R5817	R5828	R5839	R5850	R5861	R5872	R5883	R5894	R5905	R5916	R5927	R5938	R5949	R5960	R5971	R5982	R5993	R6004	R6015	R6026	R6037	R6048	R6059	R6070	R6081	R6092	R6103	R6114	R6125	R6136	R6147	R6158	R6169	R6180	R6191	R6202	R6213	R6224	R6235	R6246	R6257	R6268	R6279	R6290	R6301	R6312	R6323	R6334	R6345	R6356	R6367	R6378	R6389	R6400	R6411	R6422	R6433	R6444	R6455	R6466	R6477	R6488	R6499	R6510	R6521	R6532	R6543	R6554	R6565	R6576	R6587	R6598	R6609	R6620	R6631	R6642	R6653	R6664	R6675	R6686	R6697	R6708	R6719	R6730	R6741	R6752	R6763	R6774	R6785	R6796	R6807	R6818	R6829	R6840	R6851	R6862	R6873	R6884	R6895	R6906	R6917	R6928	R6939	R6950	R6961	R6972	R6983	R6994	R7005	R7016	R7027	R7038	R7049	R7060	R7071	R7082	R7093	R7104	R7115	R7126	R7137	R7148	R7159	R7170	R7181	R7192	R7203	R7214	R7225	R7236	R7247	R7258	R7269	R7280	R7291	R7302	R7313	R7324	R7335	R7346	R7357	R7368	R7379	R7390	R7401	R7412	R7423	R7434	R7445	R7456	R7467	R7478	R7489	R7500	R7511	R7522	R7533	R7544	R7555	R7566	R7577	R7588	R7599	R7610	R7621	R7632	R7643	R7654	R7665	R7676	R7687	R7698	R7709	R7720	R7731	R7742	R7753	R7764	R7775	R7786	R7797	R7808	R7819	R7830	R7841	R7852	R7863	R7874	R7885	R7896	R7907	R7918	R7929	R7940	R7951	R7962	R7973	R7984	R7995	R8006	R8017	R8028	R8039	R8050	R8061	R8072	R8083	R8094	R8105	R8116	R8127	R8138	R8149	R8160	R8171	R8182	R8193	R8204	R8215	R8226	R8237	R8248	R8259	R8270	R8281	R8292	R8303	R8314	R8325	R8336	R8347	R8358	R8369	R8380	R8391	R8402	R8413	R8424	R8435	R8446	R8457	R8468	R8479	R8490	R8501	R8512	R8523	R8534	R8545	R8556	R8567	R8578	R8589	R8600	R8611	R8622	R8633	R8644	R8655	R8666	R8677	R8688	R8699	R8710	R8721	R8732	R8743	R8754	R8765	R8776	R8787	R8798	R8809	R8820	R8831	R8842	R8853	R8864	R8875	R8886	R8897	R8908	R8919	R8930	R8941	R8952	R8963	R8974	R8985	R8996	R9007	R9018	R9029	R9040	R9051	R9062	R9073	R9084	R9095	R9106	R9117	R9128	R9139	R9150	R9161	R9172	R9183	R9194	R9205	R9216	R9227	R9238	R9249	R9260	R9271	R9282	R9293	R9304	R9315	R9326	R9337	R9348	R9359	R9370	R9381	R9392	R9403	R9414	R9425	R943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- Molecule 14: Pleiotropic regulator 1

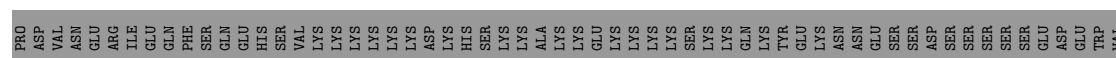


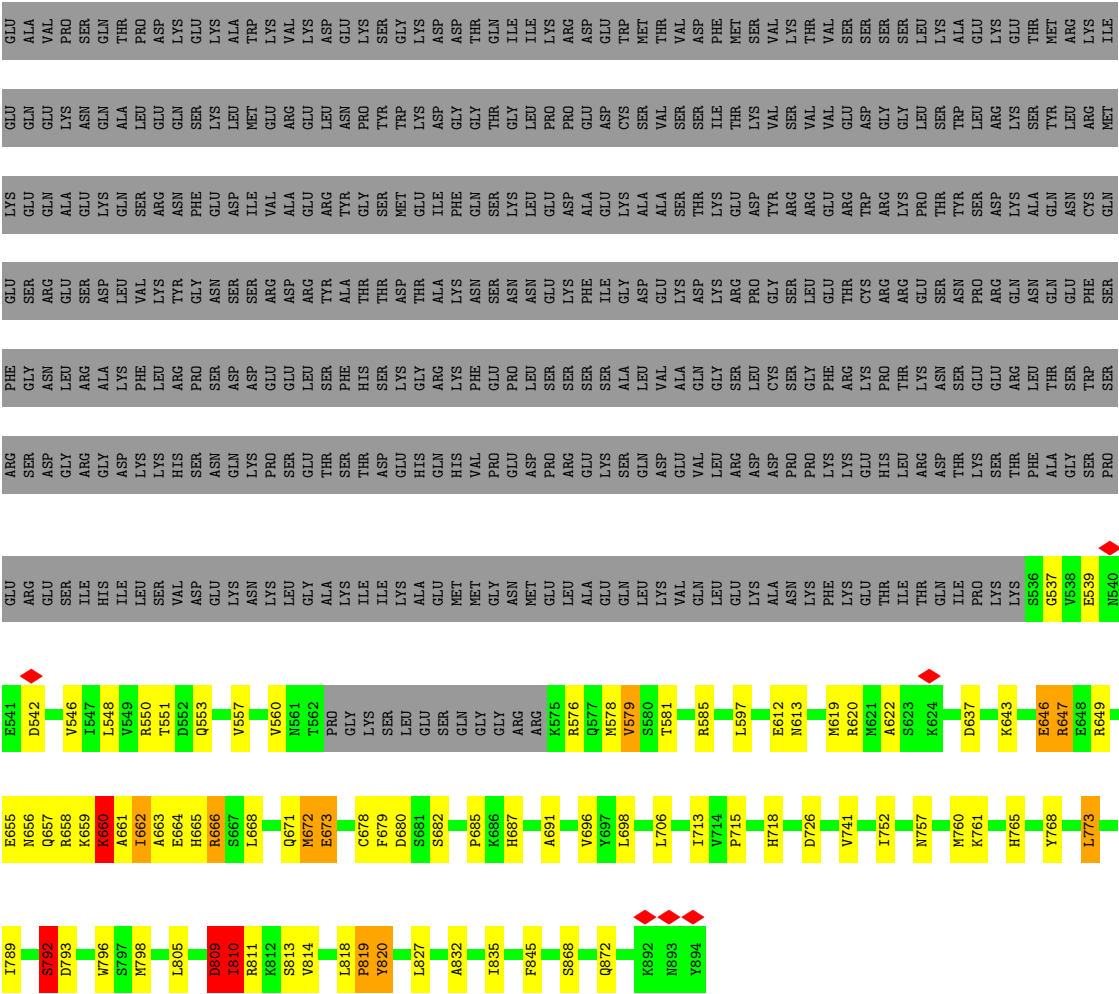
D471 Q472 L478 I486 K487 V488 Y489 A496 T496 E497 E498 T499 H500	P343 Q344 T346 T347 G348 S349 H350 D351 L356 L359 R365 H371 K372 K373 S374 V375 R376 L380 H381 P382 R383 G390 S391 P392 D393 V398 F399 F400 F401 D402 G403 S404 F405 I406 Q407 I415 I416 H417 T418 A431 N446 R449 V450 S463 A467 C468	LYS ALA PRO T184 W190 I200 ALA E213 N216 Q217 W218 F219 V220 S223 A224 L238 T248 L261 V270 W273 N278 Y284 H287 L294 T299 L303 V304 T306 C306 A312 R313 I314 V323 H324 T325 L326 T330 V335 T336 F340	SER ALA ALA GLN SER LEU ALA VAL ALA PRO LEU GLN LEU GLN THR THR LYS ASP ALA VAL ASN LEU ALA THR LYS ASP SER THR VAL LEU HIS LYS ARG GLY ASP GLN GLY THR HIS PRO SER VAL PHE VAL LEU LEU ASP GLY THR HIS PRO SER VAL PHE VAL GLY THR PRO GLY ARG MET LYS GLY ILE GLN ARG MET MET PRO SER THR LYS	
				MET VAL GLU GLU VAL GLN GLY HIS VAL HIS VAL HIS GLN LEU LEU PHE SER ARG SER LEU LEU LYS ARG GLN THR HIS ASP MET PHE VAL ALA ASP GLN GLY ASN VAL GLY HIS LYS PRO PRO VAL PRO LEU LEU ASP GLY GLU GLU SER SER HIS LYS ARG LYS MET MET ILE ALA LEU VAL PRO GLY GLY PRO HIS MET HIS MET PRO THR PRO
				THR THR

- Molecule 15: Pre-mRNA-processing factor 17

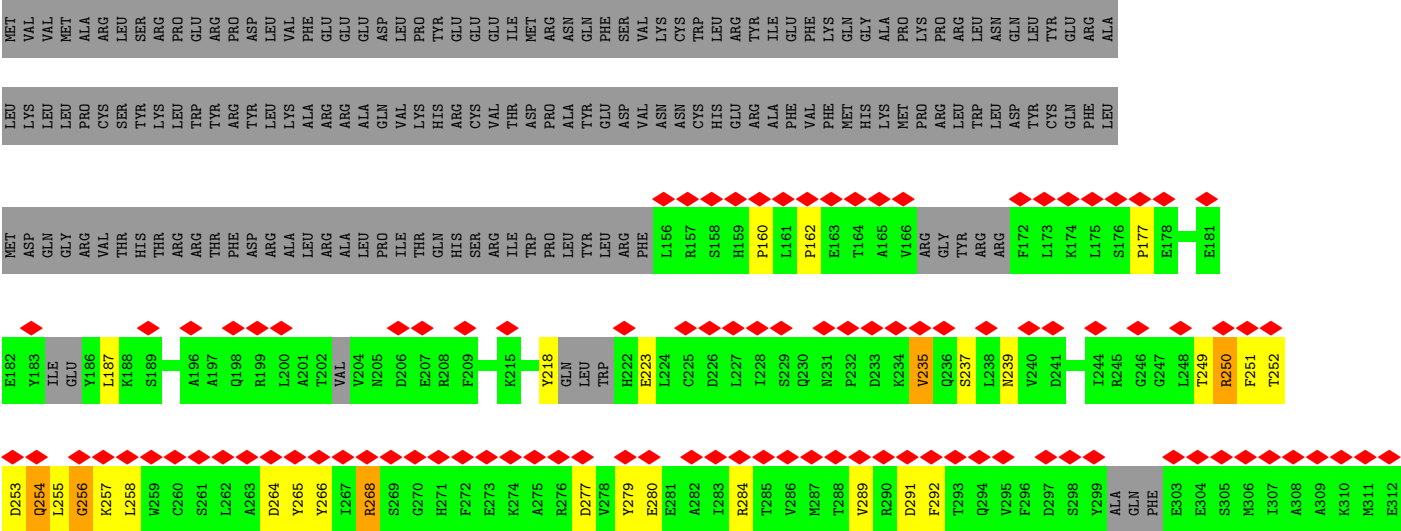


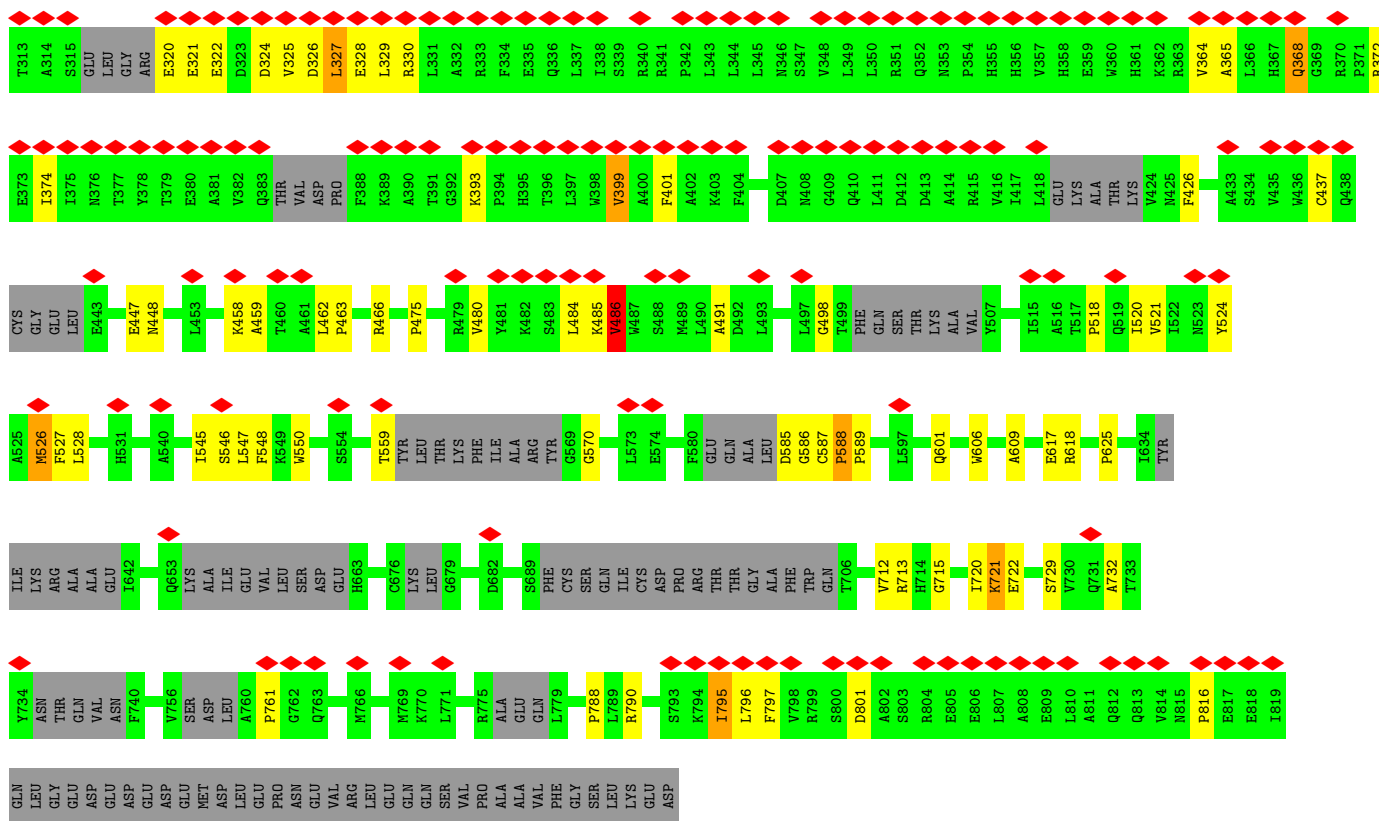
P208	L216	G227	K228	Q229	E230	E231	E232	K233	G234	G235	E236	I240	L241	H242	V243	M246	G251	I257	P258	Q259	D260	V261	G262	V263	M264	L265	G266	S267	T268	M269	P270	P271	E272	K273	C274	P277	K278	K279	Q280	I281	S285	G290	F297						
ALA	VAL	LYS	GLU	ASP	LEU	GLU	THR	GLY	V70	P74	A75	R76	K77	E78	P83	M88	N97	P98	F99	R100	Q103	R108	L111	I120	P141	S142	L143	D144	N145	V148	S149	I153	G154	S155	E158	M162	L165	Q172	L193	D204									
MET	SER	ILE	ALA	ALA	LEU	ALA	SER	TVR	GLY	GLY	SER	GLY	SER	GLY	SER	GLU	SER	ASP	SER	ASP	SER	GLU	SER	ARG	CYS	PRO	LEU	PRO	ALA	ALA	ASP	SER	SER	LEU	MET	HIS	LEU	THR	LYS	SER	PRO	SER	SER	LYS	PRO	ALA	PRO	GLU	VAL



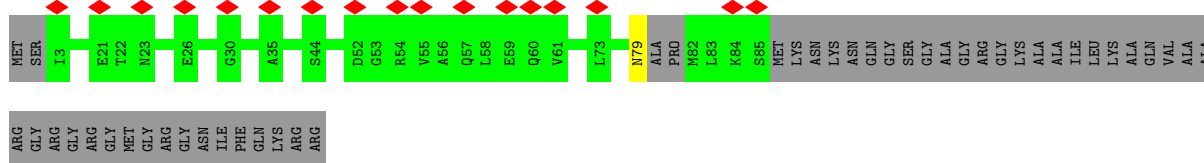


● Molecule 19: Pre-mRNA-splicing factor SYF1

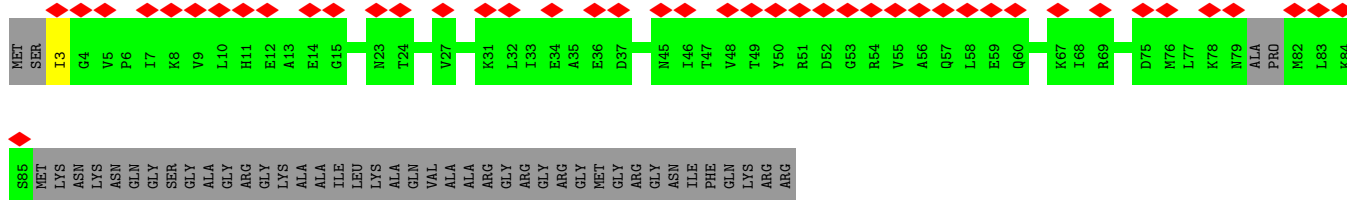




- Molecule 20: Small nuclear ribonucleoprotein Sm D3

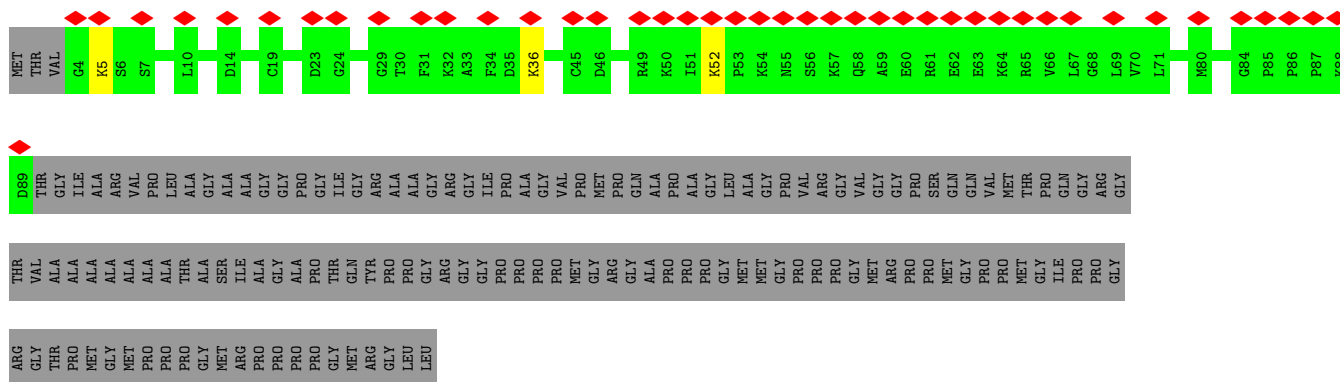


- Molecule 20: Small nuclear ribonucleoprotein Sm D3

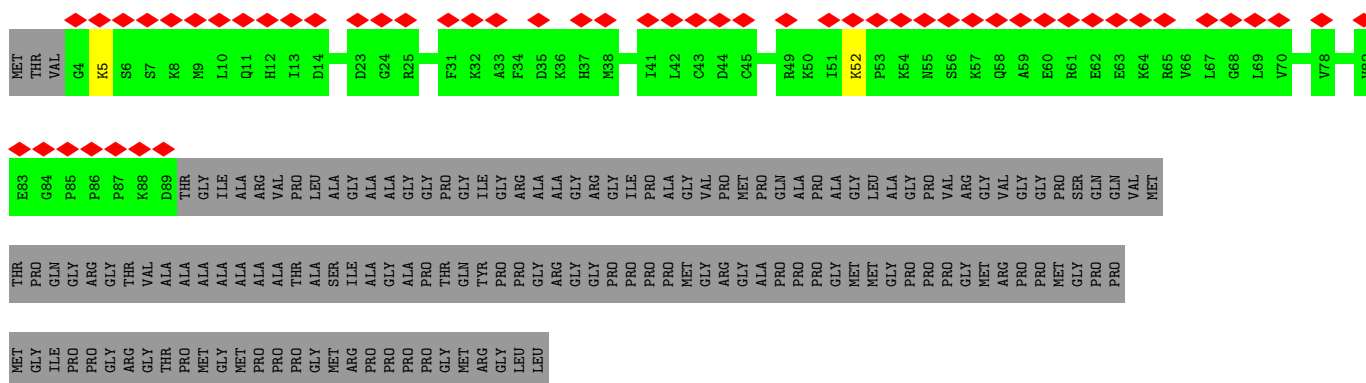


- Molecule 21: Small nuclear ribonucleoprotein-associated protein

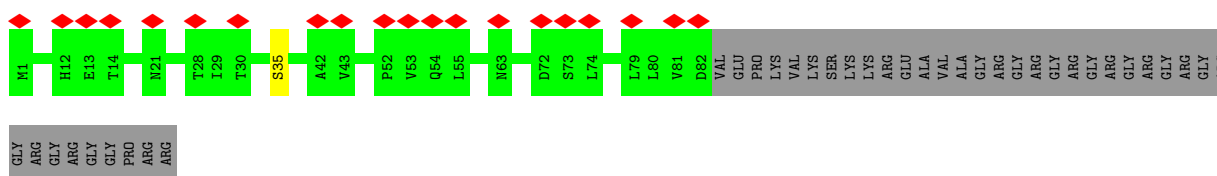




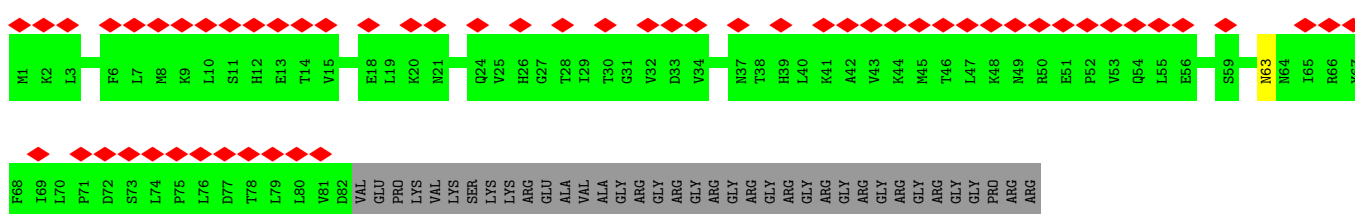
- Molecule 21: Small nuclear ribonucleoprotein-associated protein.



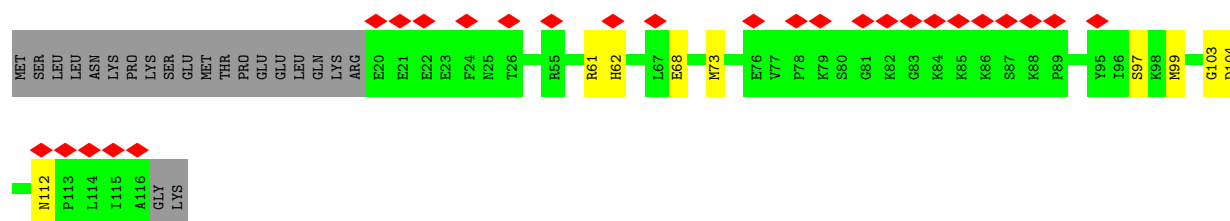
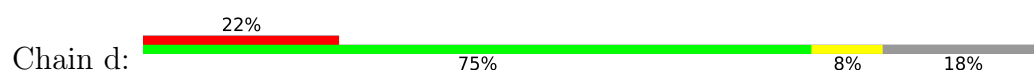
- Molecule 22: Small nuclear ribonucleoprotein Sm D1



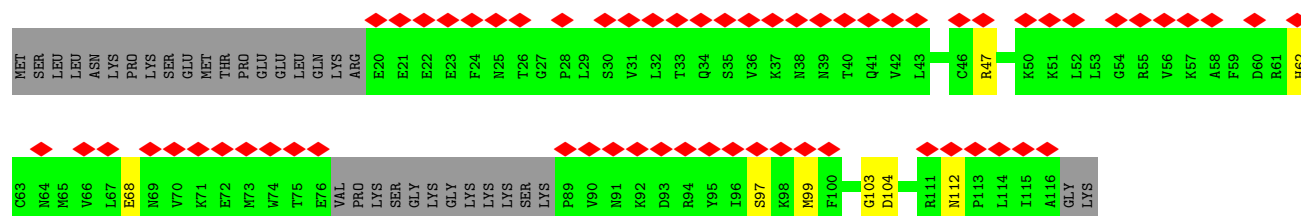
- Molecule 22: Small nuclear ribonucleoprotein Sm D1



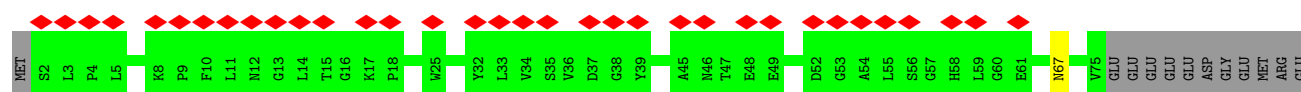
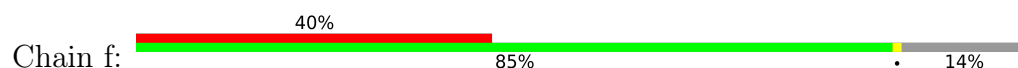
- Molecule 23: Small nuclear ribonucleoprotein Sm D2



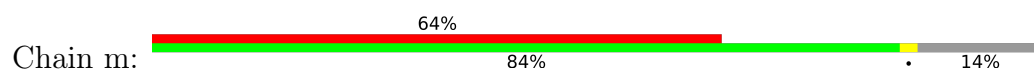
• Molecule 23: Small nuclear ribonucleoprotein Sm D2



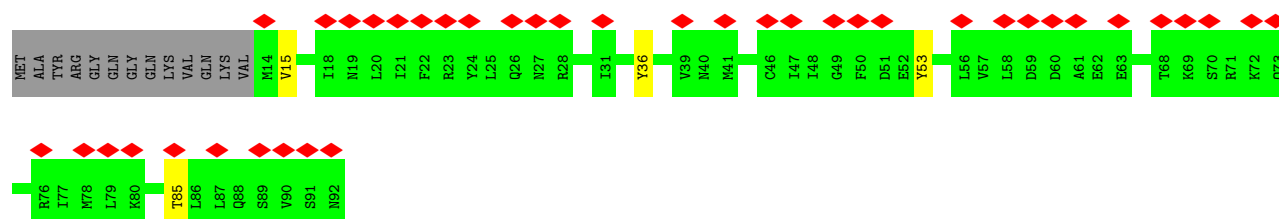
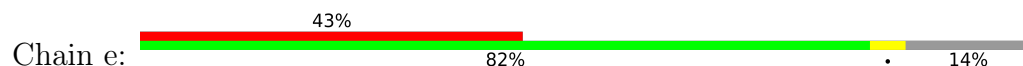
• Molecule 24: Small nuclear ribonucleoprotein F



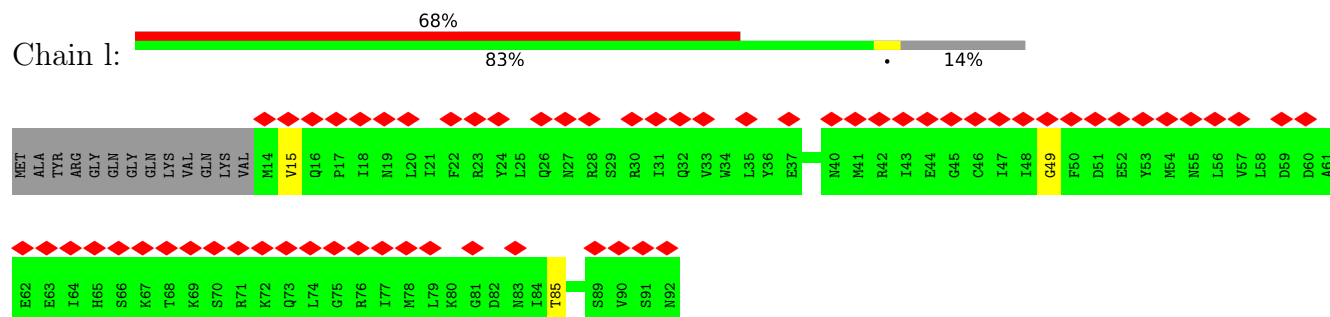
• Molecule 24: Small nuclear ribonucleoprotein F



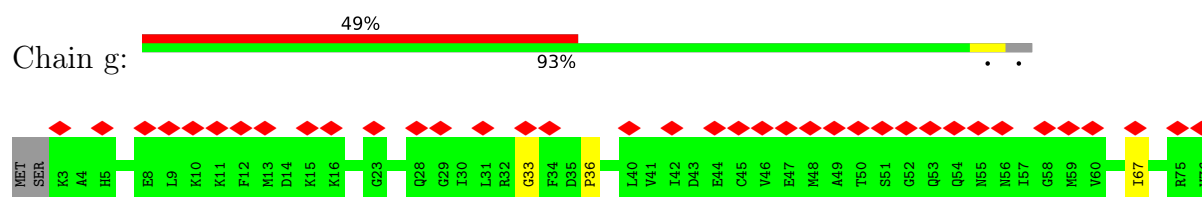
• Molecule 25: Small nuclear ribonucleoprotein E



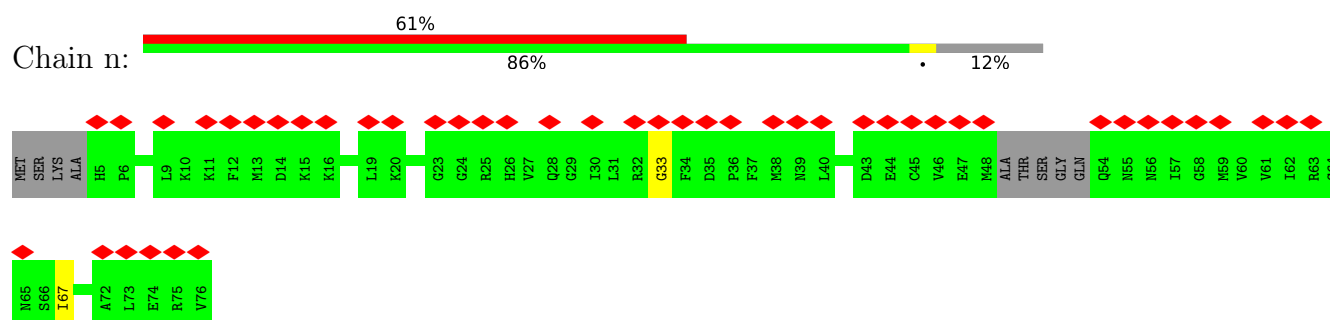
- Molecule 25: Small nuclear ribonucleoprotein E



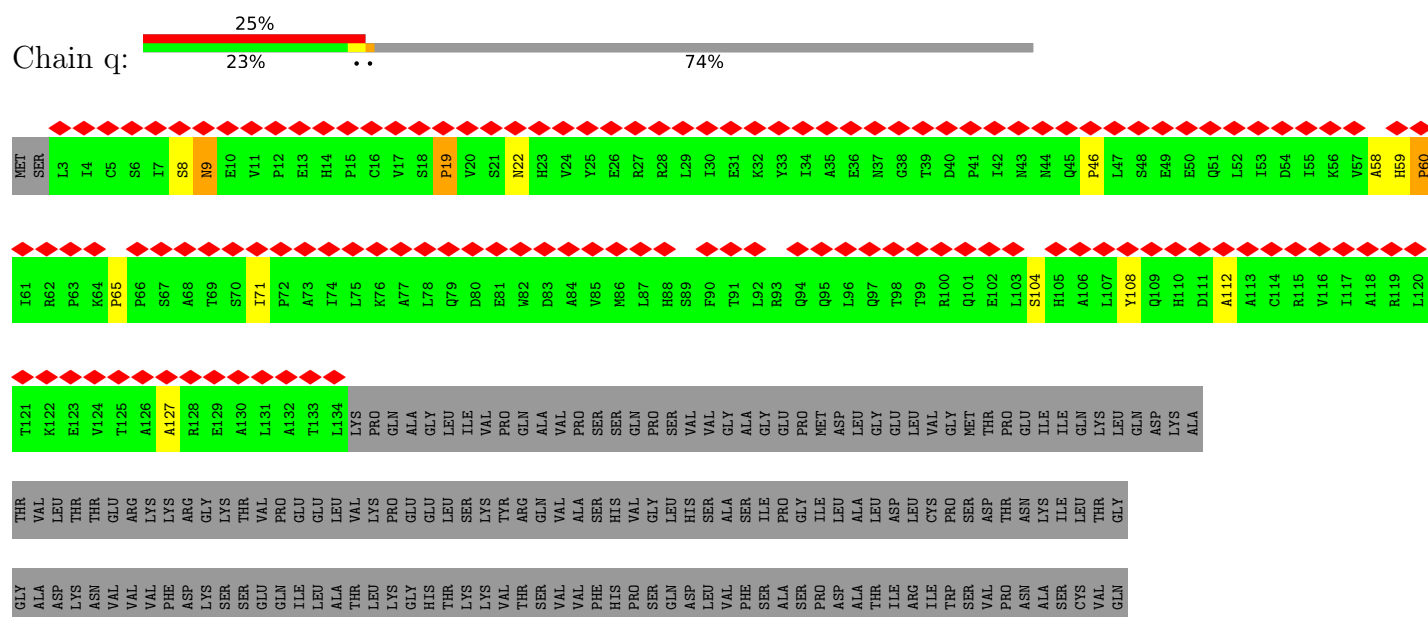
- Molecule 26: Small nuclear ribonucleoprotein G



- Molecule 26: Small nuclear ribonucleoprotein G

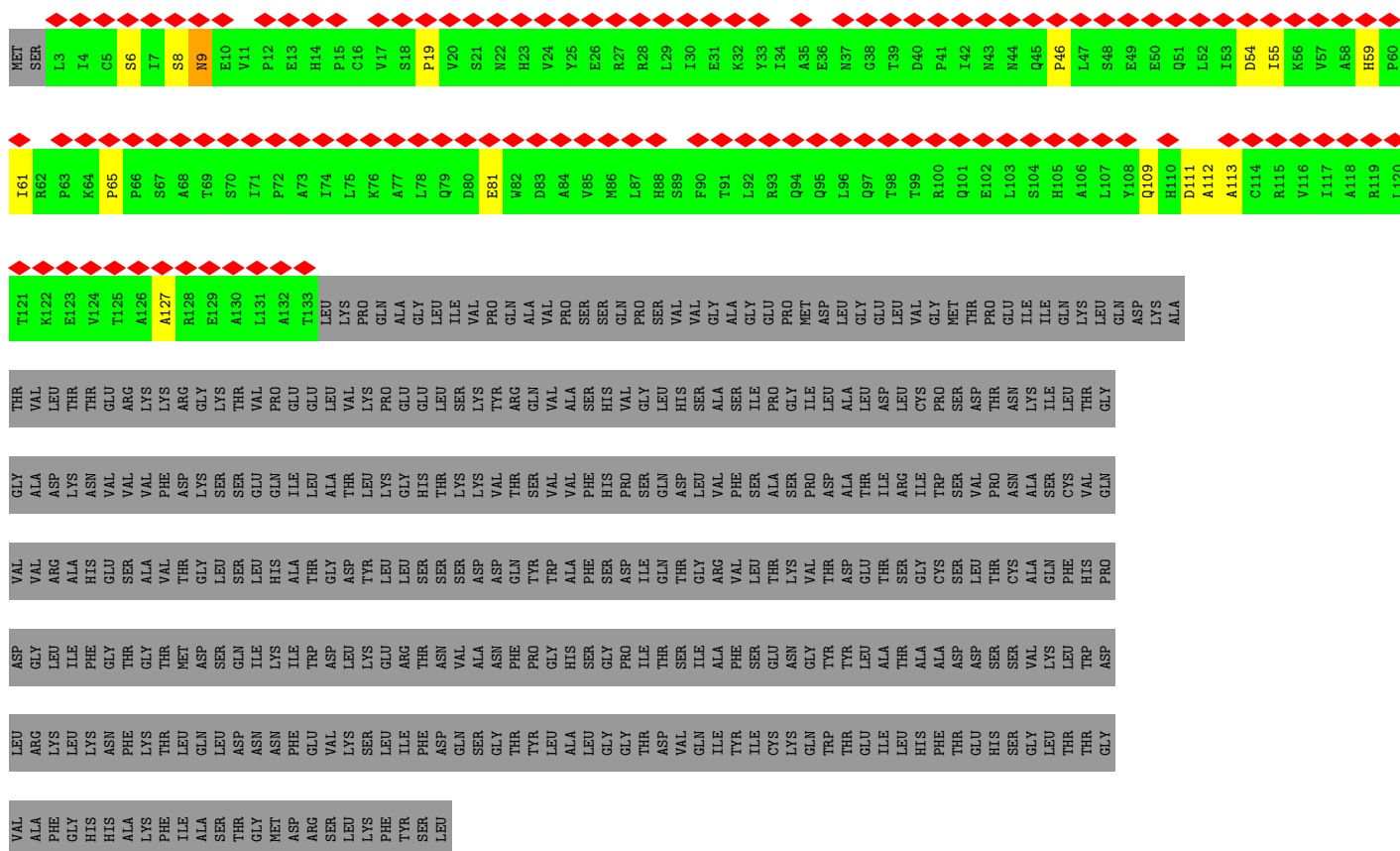


- Molecule 27: Pre-mRNA-processing factor 19

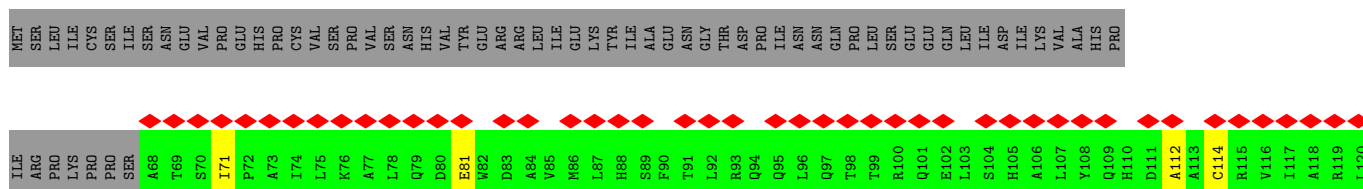


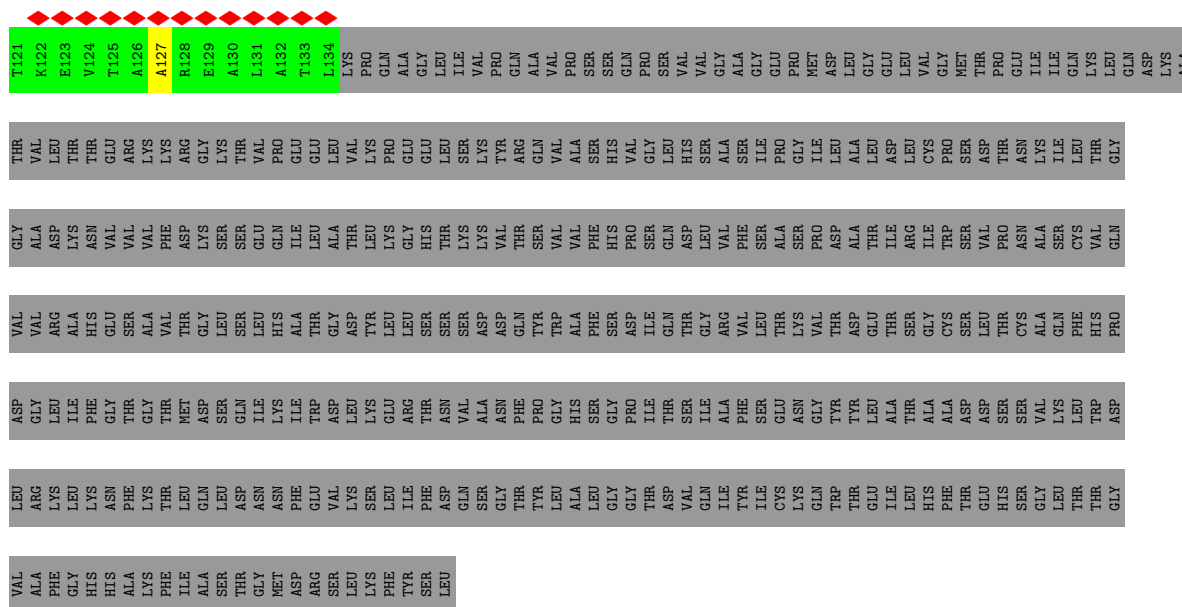
[illegible]

- Molecule 27: Pre-mRNA-processing factor 19

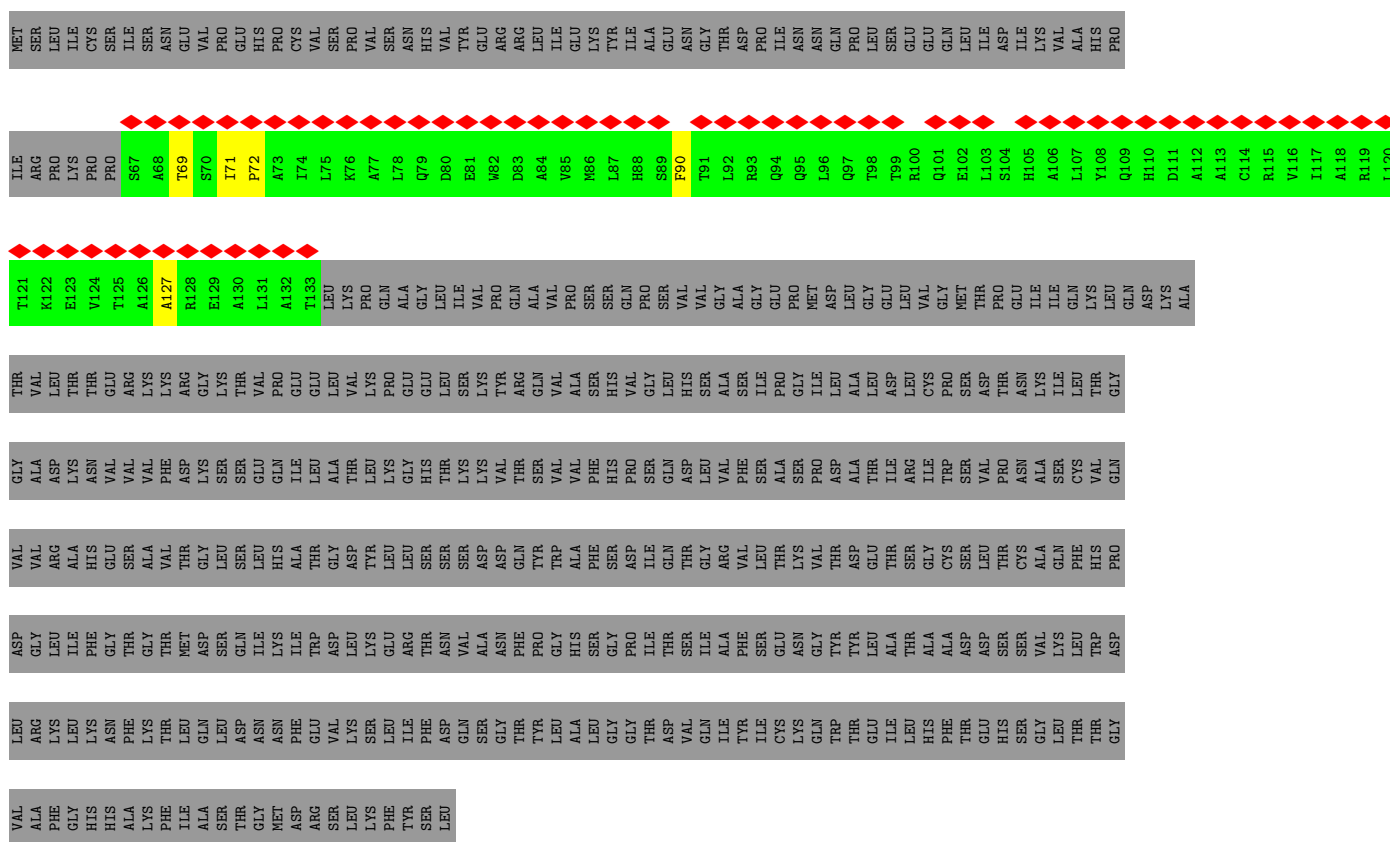


- Molecule 27: Pre-mRNA-processing factor 19





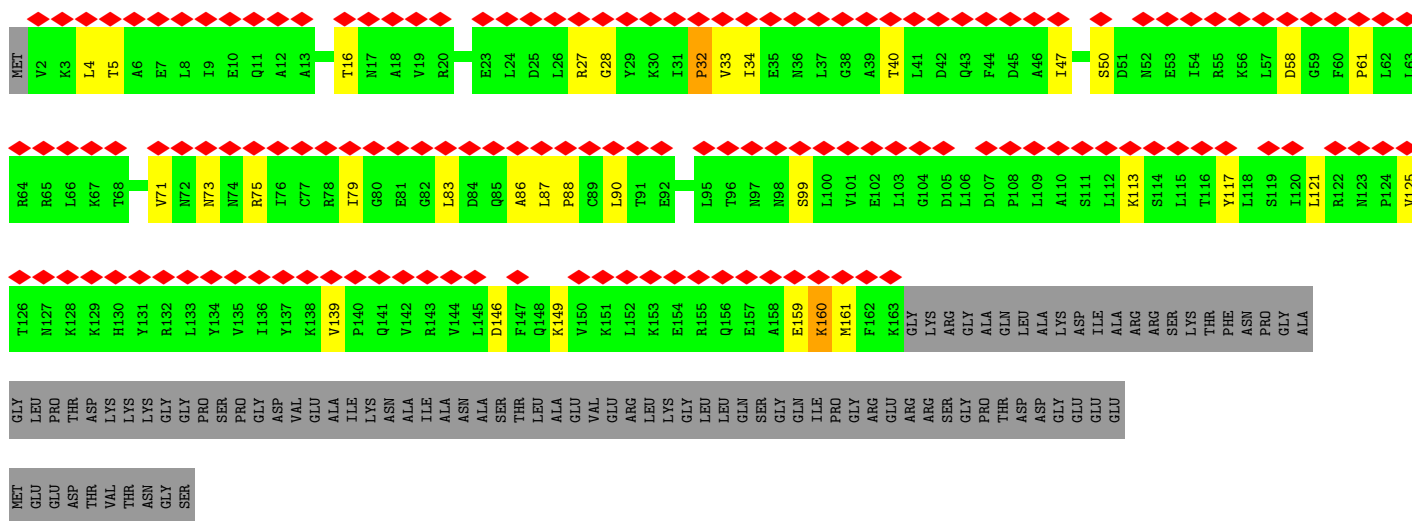
- Molecule 27: Pre-mRNA-processing factor 19



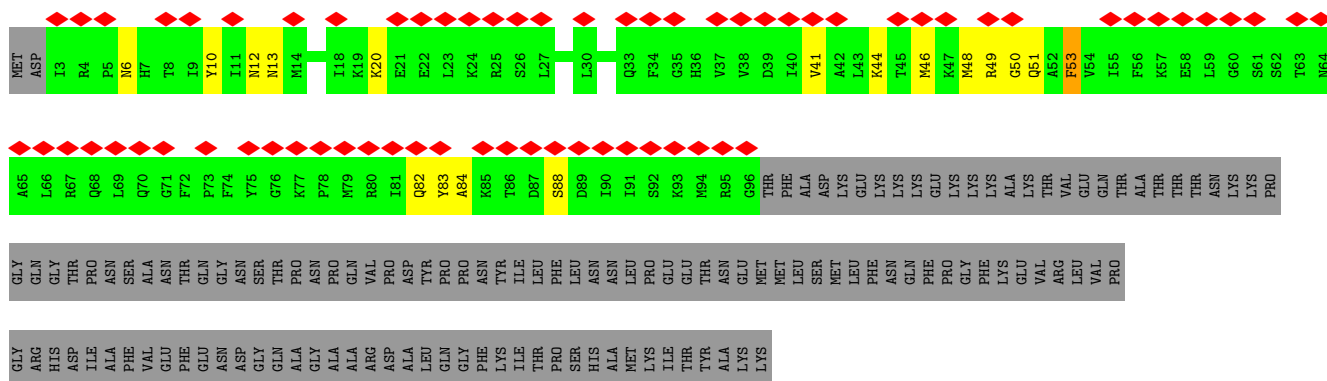
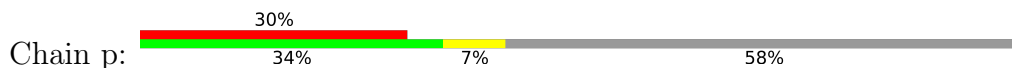
- Molecule 28: Pre-mRNA-splicing factor SPF27



- Molecule 29: U2 small nuclear ribonucleoprotein A'

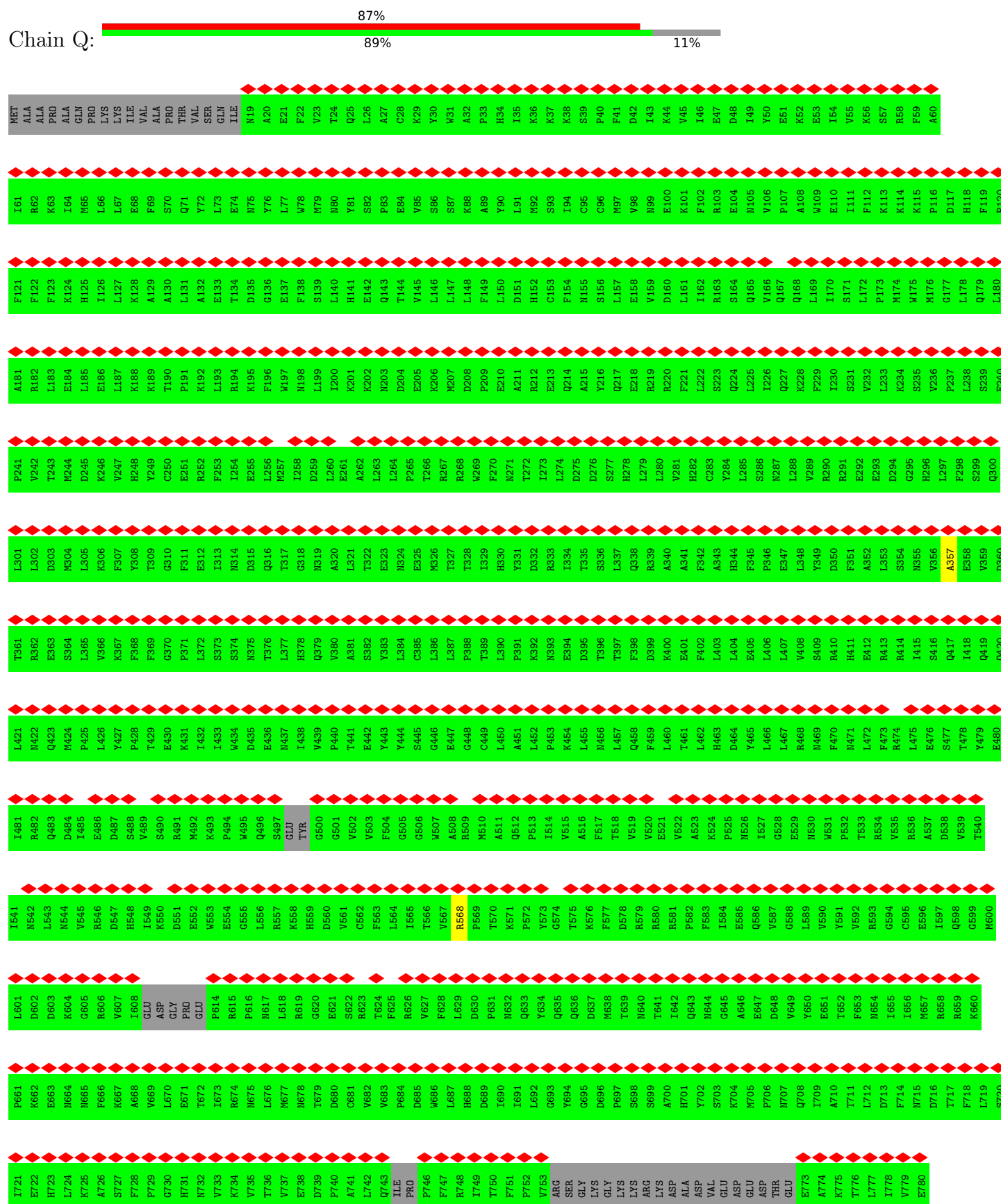


- Molecule 30: U2 small nuclear ribonucleoprotein B''

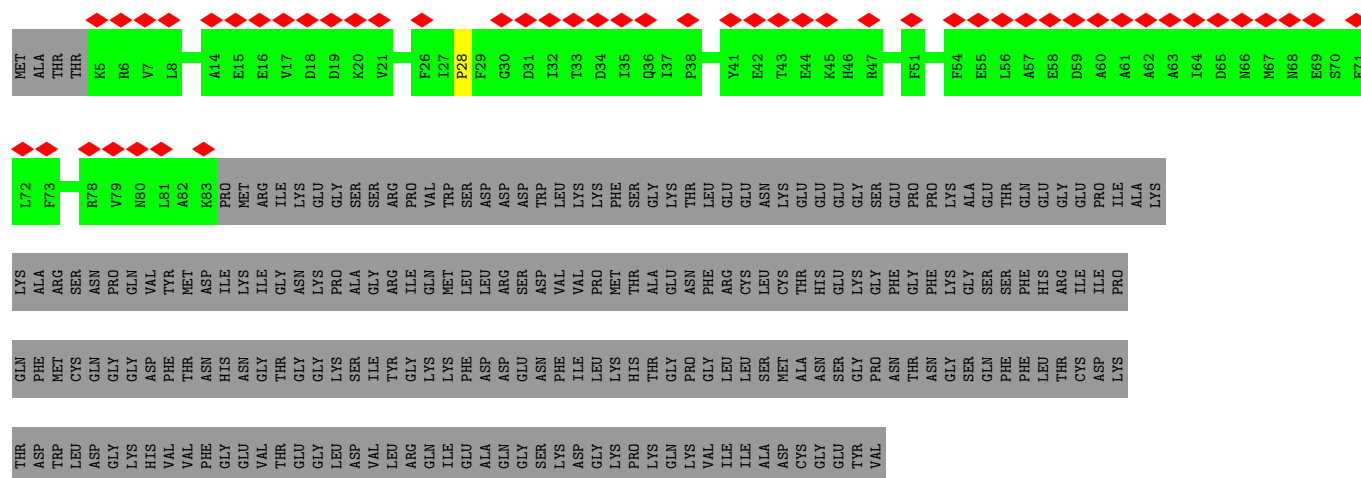


• Molecule 31: RNA helicase aquarius

Chain Q:







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	390072	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.543	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.025	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.38	1/16926 (0.0%)	0.76	30/22947 (0.1%)
2	B	0.41	1/2296 (0.0%)	0.62	2/3569 (0.1%)
3	C	0.31	0/7181	0.81	7/9758 (0.1%)
4	E	0.27	0/2420	0.70	3/3281 (0.1%)
5	F	0.34	0/2323	0.54	0/3619
6	J	0.49	2/3802 (0.1%)	0.88	17/5162 (0.3%)
7	L	0.41	1/3267 (0.0%)	0.86	11/4418 (0.2%)
8	M	0.28	0/1119	0.66	0/1497
9	N	0.79	1/1210 (0.1%)	0.80	1/1622 (0.1%)
10	O	0.33	0/2390	0.72	3/3227 (0.1%)
11	P	0.33	0/1000	0.72	0/1330
12	R	0.36	0/2186	0.85	7/2937 (0.2%)
13	S	0.28	0/1268	0.70	0/1714
14	T	0.49	0/2562	0.83	1/3492 (0.0%)
15	W	0.70	1/3038 (0.0%)	1.16	30/4171 (0.7%)
16	G	0.65	5/1378 (0.4%)	1.12	13/2133 (0.6%)
17	H	0.72	22/3308 (0.7%)	1.17	34/5135 (0.7%)
18	U	0.37	0/2928	0.89	10/3928 (0.3%)
19	I	0.52	0/2803	1.09	28/3870 (0.7%)
20	a	0.78	0/397	0.99	0/549
20	h	0.78	0/396	0.99	0/547
21	b	0.85	0/423	1.14	3/587 (0.5%)
21	i	0.84	0/423	1.15	3/587 (0.5%)
22	c	0.88	0/405	1.12	0/563
22	j	0.87	0/405	1.11	0/563
23	d	1.12	1/479 (0.2%)	1.25	1/666 (0.2%)
23	k	1.14	0/420	1.24	1/583 (0.2%)
24	f	1.20	0/360	1.25	0/497
24	m	1.21	1/360 (0.3%)	1.24	0/497
25	e	1.04	0/390	1.24	1/542 (0.2%)
25	l	1.03	0/390	1.24	1/542 (0.2%)
26	g	0.86	0/362	1.09	1/501 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	n	0.83	0/327	1.08	1/451 (0.2%)
27	q	0.63	0/658	0.97	3/919 (0.3%)
27	r	0.57	0/653	1.06	6/912 (0.7%)
27	s	0.50	0/334	0.91	0/466
27	t	0.55	0/334	0.83	0/466
28	K	0.60	1/753 (0.1%)	1.01	4/1046 (0.4%)
29	o	0.97	0/803	2.25	43/1119 (3.8%)
30	p	0.95	0/463	1.88	7/643 (1.1%)
31	Q	0.38	0/6565	0.86	3/9143 (0.0%)
32	y	0.43	0/389	1.01	0/540
All	All	0.51	37/79894 (0.0%)	0.91	275/110739 (0.2%)

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
1	A	0	16
3	C	0	6
4	E	0	1
5	F	0	1
6	J	0	1
9	N	0	1
12	R	0	8
14	T	0	5
15	W	0	3
16	G	0	5
17	H	0	1
18	U	0	6
23	d	0	1
23	k	0	1
All	All	0	56

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	77	C	C1'-N1	7.54	1.59	1.48
15	W	278	LYS	CA-C	-7.39	1.44	1.53
28	K	186	VAL	CA-CB	-7.32	1.44	1.54
2	B	103	G	C1'-N9	-7.15	1.37	1.48
17	H	74	U	C1'-N1	7.12	1.59	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	91	U	C1'-N1	7.10	1.59	1.48
17	H	92	U	C1'-N1	7.08	1.59	1.48
17	H	60	U	C1'-N1	7.07	1.59	1.48
17	H	72	U	C1'-N1	7.06	1.59	1.48
17	H	58	U	C1'-N1	7.04	1.59	1.48
17	H	89	U	C1'-N1	6.97	1.58	1.48
16	G	137	C	C1'-N1	6.83	1.57	1.47
17	H	97	G	C1'-N9	-6.75	1.37	1.48
17	H	84	C	C1'-N1	6.52	1.58	1.48
17	H	73	C	C1'-N1	6.52	1.58	1.48
17	H	78	C	C1'-N1	6.49	1.58	1.48
17	H	71	C	C1'-N1	6.40	1.58	1.48
17	H	148	C	C1'-N1	6.40	1.58	1.48
1	A	1307	MET	C-N	6.37	1.41	1.33
17	H	67	C	C1'-N1	6.32	1.57	1.48
16	G	139	U	C1'-N1	6.28	1.56	1.47
17	H	41	U	C1'-N1	6.27	1.56	1.47
17	H	37	U	C1'-N1	6.25	1.56	1.47
16	G	134	U	C1'-N1	6.24	1.56	1.47
16	G	136	U	C1'-N1	6.23	1.56	1.47
17	H	39	U	C1'-N1	6.23	1.56	1.47
17	H	43	U	C1'-N1	6.21	1.56	1.47
17	H	40	C	C1'-N1	5.65	1.55	1.47
9	N	137	CYS	CB-SG	-5.39	1.63	1.81
7	L	793	LEU	CA-CB	-5.32	1.44	1.53
17	H	110	A	C1'-N9	-5.27	1.40	1.48
16	G	147	C	O5'-C5'	5.24	1.50	1.42
17	H	35	A	O3'-P	-5.21	1.53	1.61
24	m	14	LEU	CA-C	5.11	1.59	1.52
6	J	591	LEU	C-O	-5.10	1.17	1.24
6	J	592	ALA	CA-C	5.08	1.59	1.52
23	d	73	MET	CA-C	-5.00	1.46	1.52

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	32	U	C1'-C2'-O2'	11.22	128.62	111.80
2	B	104	C	C2'-C3'-O3'	-10.04	94.44	109.50
19	I	327	LEU	N-CA-C	-10.00	100.38	111.28
15	W	278	LYS	CB-CA-C	-9.99	95.78	111.17
16	G	142	U	C4'-C3'-O3'	9.97	124.35	109.40
6	J	594	ARG	N-CA-C	-9.78	100.76	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	H	32	U	C3'-C2'-O2'	-9.68	100.08	114.60
18	U	792	SER	CA-C-N	9.61	139.89	121.54
18	U	792	SER	C-N-CA	9.61	139.89	121.54
15	W	382	ASN	CA-C-N	8.95	128.67	119.19
15	W	382	ASN	C-N-CA	8.95	128.67	119.19
16	G	141	C	C1'-C2'-O2'	8.69	124.84	111.80
17	H	88	A	O3'-P-O5'	-8.67	91.00	104.00
17	H	82	G	O3'-P-O5'	-8.66	91.01	104.00
17	H	30	A	C4'-C3'-O3'	-8.66	96.41	109.40
27	r	46	PRO	N-CA-CB	8.65	111.05	103.27
17	H	73	C	O3'-P-O5'	-8.64	91.03	104.00
17	H	78	C	O3'-P-O5'	-8.64	91.04	104.00
17	H	72	U	O3'-P-O5'	-8.63	91.05	104.00
17	H	71	C	O3'-P-O5'	-8.62	91.08	104.00
17	H	84	C	O3'-P-O5'	-8.61	91.08	104.00
17	H	80	A	O3'-P-O5'	-8.61	91.08	104.00
17	H	83	A	O3'-P-O5'	-8.61	91.09	104.00
17	H	113	G	O3'-P-O5'	-8.61	91.09	104.00
17	H	57	A	O3'-P-O5'	-8.60	91.10	104.00
17	H	79	G	O3'-P-O5'	-8.59	91.11	104.00
17	H	77	C	O3'-P-O5'	-8.58	91.12	104.00
17	H	59	A	O3'-P-O5'	-8.58	91.13	104.00
17	H	89	U	O3'-P-O5'	-8.57	91.14	104.00
17	H	74	U	O3'-P-O5'	-8.57	91.15	104.00
17	H	81	G	O3'-P-O5'	-8.56	91.16	104.00
17	H	90	A	O3'-P-O5'	-8.55	91.18	104.00
17	H	114	A	O3'-P-O5'	-8.55	91.18	104.00
17	H	56	A	O3'-P-O5'	-8.53	91.20	104.00
17	H	91	U	O3'-P-O5'	-8.53	91.21	104.00
27	q	46	PRO	N-CA-CB	8.52	111.26	103.34
17	H	58	U	O3'-P-O5'	-8.50	91.25	104.00
29	o	5	THR	N-CA-CB	-8.47	98.34	111.05
16	G	3	A	C2'-C3'-O3'	8.45	122.17	109.50
6	J	593	ARG	N-CA-C	-8.32	101.24	111.40
15	W	279	LYS	N-CA-C	-8.27	93.19	110.80
2	B	80	U	C2'-C3'-O3'	8.21	121.81	109.50
16	G	2	U	N1-C1'-C2'	8.00	126.00	114.00
29	o	16	THR	CA-C-O	-7.99	111.81	120.36
29	o	99	SER	N-CA-C	7.95	122.76	112.26
6	J	240	THR	N-CA-C	-7.95	102.27	108.78
19	I	235	VAL	N-CA-C	7.89	118.47	110.82
29	o	47	ILE	N-CA-CB	7.89	123.03	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	G	148	U	C2'-C3'-O3'	7.73	121.09	109.50
29	o	117	TYR	CA-C-O	7.67	128.45	120.40
16	G	147	C	C2'-C3'-O3'	7.65	125.17	113.70
1	A	941	LYS	N-CA-C	7.63	126.68	109.81
15	W	260	ASP	N-CA-C	7.58	119.54	111.28
28	K	90	PRO	N-CA-CB	7.56	111.19	103.25
7	L	563	PRO	N-CA-CB	7.55	110.40	103.08
31	Q	1379	TYR	N-CA-C	7.55	122.56	112.30
27	q	60	PRO	N-CA-CB	7.36	110.98	103.25
6	J	522	PRO	N-CA-CB	7.34	110.20	103.08
28	K	78	PRO	N-CA-CB	7.30	110.91	103.25
29	o	71	VAL	CA-C-N	7.20	131.62	120.75
29	o	71	VAL	C-N-CA	7.20	131.62	120.75
19	I	588	PRO	N-CA-CB	7.12	109.99	103.08
1	A	1756	SER	CA-C-N	7.07	128.93	120.09
1	A	1756	SER	C-N-CA	7.07	128.93	120.09
3	C	168	THR	N-CA-C	-7.03	105.89	114.75
16	G	1	G	C4'-C3'-O3'	7.02	119.94	109.40
15	W	269	MET	CA-C-N	-6.96	113.21	120.38
15	W	269	MET	C-N-CA	-6.96	113.21	120.38
19	I	589	PRO	N-CA-CB	6.96	110.90	103.39
19	I	237	SER	N-CA-C	6.95	118.86	111.28
1	A	1305	SER	CA-C-N	6.92	134.77	121.54
1	A	1305	SER	C-N-CA	6.92	134.77	121.54
19	I	291	ASP	N-CA-C	-6.92	103.74	111.28
29	o	121	LEU	CA-C-O	6.92	128.91	121.44
19	I	160	PRO	N-CA-CB	6.90	110.50	103.25
29	o	4	LEU	N-CA-C	-6.90	97.98	108.67
17	H	35	A	C4'-C3'-O3'	-6.85	99.13	109.40
19	I	475	PRO	N-CA-CB	6.85	110.78	103.52
15	W	257	ILE	CA-C-N	6.84	126.30	118.85
15	W	257	ILE	C-N-CA	6.84	126.30	118.85
15	W	439	ASP	N-CA-C	-6.83	100.17	110.28
27	r	19	PRO	N-CA-CB	6.82	110.40	102.76
19	I	162	PRO	N-CA-CB	6.80	110.73	103.52
30	p	53	PHE	CA-C-O	-6.80	112.84	120.32
7	L	594	PRO	N-CA-CB	6.80	110.39	103.25
1	A	1304	ASN	CA-C-N	6.77	134.47	121.54
1	A	1304	ASN	C-N-CA	6.77	134.47	121.54
27	q	19	PRO	N-CA-CB	6.77	110.36	103.25
7	L	558	PRO	N-CA-CB	6.75	110.68	103.52
29	o	58	ASP	N-CA-CB	-6.74	100.59	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	488	PRO	N-CA-CB	6.73	110.32	103.25
16	G	146	C	O3'-P-O5'	6.65	113.98	104.00
1	A	1303	LEU	CA-C-N	6.63	134.21	121.54
1	A	1303	LEU	C-N-CA	6.63	134.21	121.54
15	W	565	LYS	N-CA-C	6.61	118.91	108.79
4	E	58	PRO	CA-C-N	6.60	133.85	121.97
4	E	58	PRO	C-N-CA	6.60	133.85	121.97
19	I	722	GLU	N-CA-C	6.60	118.47	111.28
6	J	523	PRO	N-CA-CB	6.58	110.50	103.52
7	L	620	PRO	N-CA-CB	6.57	110.15	103.25
7	L	117	THR	CA-C-N	6.54	134.04	121.54
7	L	117	THR	C-N-CA	6.54	134.04	121.54
6	J	637	PRO	N-CA-CB	6.54	110.45	103.52
19	I	177	PRO	N-CA-CB	6.46	110.67	103.44
1	A	1653	ASP	CA-C-N	6.43	133.82	121.54
1	A	1653	ASP	C-N-CA	6.43	133.82	121.54
19	I	816	PRO	N-CA-CB	6.43	110.33	103.52
15	W	259	GLN	N-CA-C	6.38	124.40	110.80
7	L	546	PRO	N-CA-CB	6.37	110.57	103.44
19	I	518	PRO	N-CA-CB	6.37	110.27	103.52
7	L	564	PRO	N-CA-CB	6.35	110.25	103.52
19	I	788	PRO	N-CA-CB	6.33	110.53	103.44
15	W	460	SER	N-CA-C	6.33	118.18	111.28
1	A	1091	TYR	N-CA-C	-6.32	100.00	110.17
15	W	76	VAL	CA-C-N	6.30	133.58	121.54
15	W	76	VAL	C-N-CA	6.30	133.58	121.54
29	o	87	LEU	CA-C-N	6.30	126.21	119.28
29	o	87	LEU	C-N-CA	6.30	126.21	119.28
15	W	261	VAL	N-CA-C	6.29	118.69	109.63
1	A	37	TRP	N-CA-C	-6.28	107.46	114.62
3	C	87	GLN	CA-CB-CG	6.27	126.64	114.10
29	o	40	THR	CA-C-N	6.27	131.49	122.40
29	o	40	THR	C-N-CA	6.27	131.49	122.40
16	G	145	U	C4'-C3'-O3'	6.27	118.80	109.40
1	A	1019	TYR	N-CA-C	-6.26	99.55	109.07
15	W	281	ILE	N-CA-C	6.21	117.57	111.67
1	A	1652	MET	CA-C-N	6.19	133.37	121.54
1	A	1652	MET	C-N-CA	6.19	133.37	121.54
6	J	237	LYS	N-CA-C	6.16	117.79	111.14
7	L	548	PRO	N-CA-CB	6.12	110.29	103.44
29	o	73	ASN	N-CA-C	6.11	119.79	111.17
6	J	566	PRO	N-CA-CB	6.06	110.22	103.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	U	612	GLU	CA-C-N	6.06	133.11	121.54
18	U	612	GLU	C-N-CA	6.06	133.11	121.54
7	L	753	GLU	N-CA-C	-6.05	104.32	111.03
19	I	761	PRO	N-CA-CB	6.05	109.93	103.52
29	o	75	ARG	N-CA-CB	-6.00	102.62	111.51
27	r	59	HIS	CA-C-N	5.99	127.33	119.84
27	r	59	HIS	C-N-CA	5.99	127.33	119.84
16	G	6	A	N9-C1'-C2'	5.96	120.95	112.00
30	p	46	MET	N-CA-C	-5.94	104.72	111.07
18	U	660	LYS	N-CA-C	5.93	117.54	111.14
29	o	79	ILE	CA-C-N	5.92	125.73	120.10
29	o	79	ILE	C-N-CA	5.92	125.73	120.10
19	I	625	PRO	N-CA-CB	5.92	109.84	103.33
1	A	283	VAL	N-CA-C	-5.91	107.36	113.10
12	R	125	MET	CA-C-N	5.90	129.66	120.82
12	R	125	MET	C-N-CA	5.90	129.66	120.82
16	G	1	G	C2'-C3'-O3'	5.89	118.33	109.50
26	n	67	ILE	CB-CA-C	-5.88	104.88	111.23
29	o	27	ARG	CB-CA-C	-5.87	98.73	109.54
1	A	1649	LYS	N-CA-C	5.86	115.75	108.19
29	o	113	LYS	N-CA-C	5.84	118.40	111.33
26	g	67	ILE	CB-CA-C	-5.82	104.94	111.23
15	W	285	SER	CB-CA-C	-5.82	109.88	116.63
15	W	464	MET	CA-C-N	-5.81	113.03	119.19
15	W	464	MET	C-N-CA	-5.81	113.03	119.19
29	o	50	SER	CA-C-O	5.81	127.70	121.55
6	J	242	ILE	N-CA-C	5.75	119.10	111.17
18	U	820	TYR	CA-CB-CG	5.74	124.23	113.90
18	U	819	PRO	N-CA-C	5.72	123.06	113.78
1	A	1366	PRO	N-CA-C	5.70	124.22	112.47
4	E	59	ILE	N-CA-CB	5.69	120.61	111.23
29	o	149	LYS	CB-CA-C	-5.68	101.98	110.16
12	R	230	MET	N-CA-C	5.67	119.25	111.54
29	o	71	VAL	O-C-N	-5.64	115.52	122.57
12	R	91	ASP	CA-C-N	5.63	128.62	120.79
12	R	91	ASP	C-N-CA	5.63	128.62	120.79
19	I	268	ARG	N-CA-C	5.62	120.16	112.68
29	o	27	ARG	CA-C-N	5.61	128.59	120.11
29	o	27	ARG	C-N-CA	5.61	128.59	120.11
19	I	252	THR	N-CA-C	5.59	117.37	111.28
29	o	159	GLU	N-CA-C	-5.57	104.84	111.69
1	A	1367	ASN	N-CA-C	5.55	122.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	400	PHE	N-CA-C	5.54	122.06	109.81
17	H	157	G	P-O5'-C5'	-5.53	112.60	120.90
19	I	279	TYR	CA-C-N	5.53	128.45	120.38
19	I	279	TYR	C-N-CA	5.53	128.45	120.38
17	H	160	A	P-O5'-C5'	-5.53	112.61	120.90
6	J	593	ARG	CA-C-N	-5.52	111.47	121.14
6	J	593	ARG	C-N-CA	-5.52	111.47	121.14
21	b	52	LYS	CA-C-N	-5.52	114.24	119.76
21	b	52	LYS	C-N-CA	-5.52	114.24	119.76
21	i	52	LYS	CA-C-N	-5.50	114.26	119.76
21	i	52	LYS	C-N-CA	-5.50	114.26	119.76
19	I	250	ARG	N-CA-C	5.49	122.50	110.80
21	i	5	LYS	N-CA-C	5.49	118.18	111.82
16	G	3	A	N9-C1'-C2'	5.48	122.22	114.00
19	I	322	GLU	N-CA-C	-5.48	105.41	111.71
29	o	34	ILE	CA-C-O	-5.43	114.34	120.74
29	o	32	PRO	CA-C-N	5.42	130.52	122.99
29	o	32	PRO	C-N-CA	5.42	130.52	122.99
29	o	16	THR	O-C-N	5.41	129.39	123.22
7	L	57	SER	N-CA-C	-5.41	106.42	114.64
15	W	279	LYS	N-CA-CB	5.39	119.61	110.49
19	I	239	ASN	CB-CA-C	-5.39	109.90	117.23
21	b	5	LYS	N-CA-C	5.34	118.01	111.82
29	o	40	THR	N-CA-C	-5.34	106.27	112.89
6	J	594	ARG	CA-C-N	-5.34	111.34	121.54
6	J	594	ARG	C-N-CA	-5.34	111.34	121.54
29	o	125	VAL	CA-C-N	5.34	127.97	120.28
29	o	125	VAL	C-N-CA	5.34	127.97	120.28
6	J	413	GLU	CA-C-N	5.31	127.65	120.38
6	J	413	GLU	C-N-CA	5.31	127.65	120.38
29	o	33	VAL	N-CA-CB	-5.30	103.78	111.52
1	A	1640	SER	CA-C-N	5.30	134.73	121.80
1	A	1640	SER	C-N-CA	5.30	134.73	121.80
30	p	6	ASN	N-CA-CB	-5.28	101.71	111.53
27	r	111	ASP	CA-C-N	5.27	127.34	120.28
27	r	111	ASP	C-N-CA	5.27	127.34	120.28
29	o	88	PRO	CB-CA-C	-5.27	103.99	112.21
29	o	146	ASP	CA-C-N	5.26	130.02	122.40
29	o	146	ASP	C-N-CA	5.26	130.02	122.40
17	H	171	U	C2'-C3'-O3'	-5.25	105.83	113.70
30	p	20	LYS	N-CA-C	5.24	117.40	111.11
3	C	160	ARG	N-CA-C	5.24	117.62	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	W	274	CYS	N-CA-C	5.24	117.45	110.53
15	W	143	LEU	CA-C-N	-5.22	115.33	121.90
15	W	143	LEU	C-N-CA	-5.22	115.33	121.90
3	C	905	GLN	CA-C-N	5.21	127.55	120.63
3	C	905	GLN	C-N-CA	5.21	127.55	120.63
15	W	470	SER	CA-C-N	5.19	124.86	119.56
15	W	470	SER	C-N-CA	5.19	124.86	119.56
1	A	1653	ASP	N-CA-C	5.19	121.85	110.80
30	p	48	MET	N-CA-C	5.19	119.61	113.28
12	R	233	PRO	CA-C-N	5.19	131.45	121.54
12	R	233	PRO	C-N-CA	5.19	131.45	121.54
17	H	156	U	C4'-C3'-C2'	5.18	107.78	102.60
6	J	592	ALA	N-CA-C	5.18	121.83	110.80
1	A	441	VAL	CA-C-N	5.18	127.99	120.79
1	A	441	VAL	C-N-CA	5.18	127.99	120.79
1	A	1759	THR	CA-C-N	-5.17	113.14	120.49
1	A	1759	THR	C-N-CA	-5.17	113.14	120.49
15	W	462	HIS	N-CA-C	5.16	116.98	111.36
1	A	1308	PRO	N-CA-C	5.16	119.30	111.15
16	G	143	U	O4'-C4'-C3'	-5.16	100.94	106.10
30	p	51	GLN	N-CA-C	5.15	117.50	109.52
17	H	29	A	C4'-C3'-O3'	5.14	117.12	109.40
3	C	754	VAL	N-CA-C	-5.14	106.03	113.07
18	U	646	GLU	CA-C-N	5.13	128.37	120.82
18	U	646	GLU	C-N-CA	5.13	128.37	120.82
15	W	297	PHE	CA-C-N	5.13	125.42	119.93
15	W	297	PHE	C-N-CA	5.13	125.42	119.93
30	p	83	TYR	CA-C-O	-5.13	115.20	121.05
19	I	550	TRP	CA-C-N	5.13	124.74	119.05
19	I	550	TRP	C-N-CA	5.13	124.74	119.05
29	o	90	LEU	O-C-N	5.12	129.40	122.59
23	k	99	MET	N-CA-C	5.11	116.83	108.76
29	o	90	LEU	CA-C-O	-5.10	113.22	120.51
3	C	487	GLY	N-CA-C	5.10	117.32	111.36
18	U	649	ARG	CA-CB-CG	5.08	124.27	114.10
17	H	160	A	C4'-C3'-C2'	-5.08	97.52	102.60
29	o	83	LEU	N-CA-C	5.07	117.47	111.33
31	Q	568	ARG	CA-C-N	5.07	125.07	119.90
31	Q	568	ARG	C-N-CA	5.07	125.07	119.90
10	O	15	TRP	CA-CB-CG	5.06	123.21	113.60
23	d	99	MET	N-CA-C	5.06	116.75	108.76
19	I	393	LYS	CA-C-N	5.05	124.66	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	I	393	LYS	C-N-CA	5.05	124.66	119.05
29	o	139	VAL	CA-C-N	5.05	124.71	119.56
29	o	139	VAL	C-N-CA	5.05	124.71	119.56
9	N	19	GLU	N-CA-C	5.04	120.96	109.81
19	I	401	PHE	N-CA-C	5.04	117.28	108.76
15	W	399	LYS	N-CA-C	5.04	117.61	110.50
25	e	85	THR	N-CA-C	-5.04	105.98	112.68
25	l	85	THR	N-CA-C	-5.03	105.99	112.68
17	H	31	G	C1'-C2'-O2'	5.02	119.33	111.80
17	H	155	C	P-O3'-C3'	5.02	127.73	120.20
28	K	127	MET	CA-C-N	-5.02	113.92	120.44
28	K	127	MET	C-N-CA	-5.02	113.92	120.44
29	o	28	GLY	N-CA-C	5.01	120.80	113.48
10	O	205	ILE	CA-C-N	5.01	129.53	122.46
10	O	205	ILE	C-N-CA	5.01	129.53	122.46
1	A	504	LEU	CA-C-N	-5.01	112.75	122.06
1	A	504	LEU	C-N-CA	-5.01	112.75	122.06

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	107	PRO	Peptide
1	A	1091	TYR	Peptide
1	A	1190	CYS	Peptide
1	A	1305	SER	Peptide
1	A	135	VAL	Peptide
1	A	1366	PRO	Peptide
1	A	1555	LEU	Peptide
1	A	1606	ILE	Peptide
1	A	1638	ASN	Peptide
1	A	1639	VAL	Peptide
1	A	1653	ASP	Peptide
1	A	1763	LEU	Peptide
1	A	1920	TYR	Peptide
1	A	320	TYR	Peptide
1	A	940	ILE	Peptide
3	C	359	LYS	Peptide
3	C	440	SER	Peptide
3	C	559	ILE	Peptide
3	C	560	VAL	Peptide

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Mol	Chain	Res	Type	Group
3	C	823	ALA	Peptide
3	C	93	ILE	Peptide
4	E	192	ASN	Peptide
5	F	41	A	Sidechain
16	G	142	U	Sidechain
16	G	2	U	Sidechain
16	G	5	G	Sidechain
16	G	6	A	Sidechain
16	G	7	G	Sidechain
17	H	33	G	Sidechain
6	J	357	LYS	Peptide
9	N	3	LYS	Peptide
12	R	125	MET	Peptide
12	R	167	ALA	Peptide
12	R	168	ALA	Peptide
12	R	184	GLN	Peptide
12	R	185	GLY	Peptide
12	R	186	VAL	Peptide
12	R	189	ASN	Peptide
12	R	316	GLU	Peptide
14	T	342	GLU	Peptide
14	T	404	SER	Peptide
14	T	405	PHE	Peptide
14	T	495	ALA	Peptide
14	T	497	GLU	Peptide
18	U	542	ASP	Peptide
18	U	578	MET	Peptide
18	U	647	ARG	Peptide
18	U	792	SER	Peptide
18	U	809	ASP	Peptide
18	U	818	LEU	Peptide
15	W	148	VAL	Peptide
15	W	204	ASP	Peptide
15	W	76	VAL	Peptide
23	d	112	ASN	Peptide
23	k	112	ASN	Peptide

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16477	0	16462	244	0
2	B	2060	0	1044	93	0
3	C	7022	0	7047	167	0
4	E	2366	0	2303	70	0
5	F	2075	0	1048	43	0
6	J	3758	0	2888	47	0
7	L	3237	0	2680	49	0
8	M	1098	0	1082	16	0
9	N	1184	0	1189	11	0
10	O	2340	0	2316	46	0
11	P	985	0	965	14	0
12	R	2165	0	2214	40	0
13	S	1236	0	1210	27	0
14	T	2496	0	2446	48	0
15	W	3008	0	1977	66	0
16	G	1246	0	631	210	0
17	H	2968	0	1504	301	0
18	U	2864	0	2814	83	0
19	I	2822	0	1319	70	0
20	a	399	0	173	3	0
20	h	398	0	172	6	0
21	b	424	0	179	1	0
21	i	424	0	179	0	0
22	c	406	0	170	1	0
22	j	406	0	170	1	0
23	d	480	0	200	6	0
23	k	422	0	175	6	0
24	f	361	0	158	1	0
24	m	361	0	158	1	0
25	e	391	0	163	5	0
25	l	391	0	163	2	0
26	g	363	0	160	4	0
26	n	329	0	138	1	0
27	q	659	0	296	23	0
27	r	654	0	294	30	0
27	s	335	0	168	6	0
27	t	335	0	168	8	0
28	K	757	0	338	49	0
29	o	804	0	350	2	0
30	p	464	0	205	31	0
31	Q	6562	0	2836	2	0
32	y	390	0	190	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A	36	0	6	1	0
34	C	32	0	12	22	0
35	C	1	0	0	0	0
35	F	6	0	0	0	0
36	N	3	0	0	0	0
36	O	3	0	0	0	0
36	U	1	0	0	0	0
All	All	78004	0	60360	1514	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 11.

All (1514) 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)
19:I:437:CYS:CB	19:I:447:GLU:CB	1.98	1.42
5:F:44:G:N2	16:G:3:A:C2	1.84	1.38
18:U:546:VAL:HG21	18:U:665:HIS:CE1	1.56	1.38
5:F:44:G:N2	16:G:3:A:H2	1.14	1.36
5:F:41:A:N6	16:G:6:A:H61	1.17	1.34
17:H:34:U:H2'	17:H:35:A:C8	1.66	1.28
4:E:55:LEU:HD11	4:E:341:ILE:CD1	1.62	1.27
16:G:148:U:N3	17:H:30:A:N1	1.79	1.27
5:F:41:A:H61	16:G:6:A:N6	1.31	1.26
1:A:532:THR:OG1	16:G:3:A:C5'	1.84	1.25
27:t:72:PRO:HA	28:K:81:LEU:CB	1.67	1.23
27:r:112:ALA:HB1	28:K:39:GLU:CB	1.67	1.22
17:H:153:A:H2'	17:H:154:C:C5'	1.70	1.21
16:G:151:C:H2'	16:G:152:C:C6	1.74	1.21
3:C:114:TYR:HE2	20:a:79:ASN:O	1.23	1.21
16:G:133:A:O2'	16:G:134:U:C6	1.86	1.21
17:H:165:A:C4	30:p:53:PHE:CB	2.24	1.20
19:I:364:VAL:C	19:I:372:ARG:CB	2.16	1.19
17:H:109:C:H4'	23:k:47:ARG:CB	1.72	1.19
27:q:22:ASN:CB	27:r:55:ILE:HA	1.72	1.19
17:H:179:C:O2'	17:H:180:G:H5'	1.44	1.18
19:I:462:LEU:CB	19:I:466:ARG:CB	2.21	1.17
17:H:164:C:O2	30:p:84:ALA:HA	1.45	1.16
19:I:790:ARG:CB	19:I:801:ASP:CB	2.23	1.16
16:G:143:U:O4	17:H:34:U:N3	1.77	1.15
1:A:861:ARG:NH1	17:H:29:A:H5'	1.59	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:608:ASN:HA	27:q:112:ALA:CB	1.77	1.14
1:A:532:THR:HB	16:G:3:A:H3'	1.14	1.13
6:J:773:ARG:CB	6:J:790:THR:CB	2.26	1.13
3:C:139:HIS:HA	34:C:1500:GTP:O3B	1.45	1.13
4:E:61:LEU:HD13	4:E:352:TYR:CZ	1.83	1.13
1:A:532:THR:OG1	16:G:3:A:H5'	1.41	1.12
1:A:532:THR:HB	16:G:3:A:C3'	1.78	1.12
17:H:156:U:H6	17:H:156:U:H5''	1.10	1.12
17:H:179:C:C2'	17:H:180:G:H5'	1.80	1.11
27:r:112:ALA:CB	28:K:39:GLU:C	2.23	1.11
1:A:1512:SER:OG	16:G:148:U:OP2	1.68	1.11
5:F:44:G:N1	16:G:3:A:N1	1.99	1.10
16:G:151:C:C2	16:G:152:C:C5	2.38	1.10
2:B:74:U:H5	2:B:76:A:N6	1.49	1.10
17:H:179:C:H2'	17:H:180:G:H8	1.13	1.10
3:C:142:LYS:HG3	3:C:228:PHE:CD2	1.86	1.10
17:H:153:A:H2'	17:H:154:C:H5'	1.15	1.09
17:H:35:A:O2'	17:H:36:G:C8	2.04	1.08
5:F:43:A:H2	16:G:4:A:N1	1.48	1.08
16:G:132:G:P	16:G:133:A:OP1	2.12	1.08
18:U:550:ARG:HB3	18:U:660:LYS:HD3	1.29	1.08
17:H:153:A:C2'	17:H:154:C:H5'	1.83	1.07
27:r:112:ALA:HB1	28:K:39:GLU:CA	1.84	1.07
1:A:855:ARG:HH22	1:A:1518:LEU:CD1	1.66	1.07
3:C:114:TYR:CE2	20:a:79:ASN:O	2.07	1.07
17:H:108:G:H4'	23:k:104:ASP:CB	1.85	1.06
6:J:658:ARG:HA	6:J:667:ILE:CB	1.85	1.05
16:G:129:G:H4'	16:G:130:A:OP1	1.52	1.05
16:G:145:U:H3	17:H:33:G:N2	1.55	1.05
17:H:102:U:C2	20:h:3:ILE:N	2.23	1.05
2:B:11:U:H6	2:B:11:U:H5'	1.18	1.05
17:H:165:A:N3	30:p:53:PHE:CB	2.20	1.04
27:r:113:ALA:HB2	28:K:36:VAL:CB	1.86	1.04
4:E:55:LEU:CD1	4:E:341:ILE:CD1	2.35	1.04
1:A:533:LYS:NZ	16:G:5:G:OP2	1.90	1.04
27:r:112:ALA:HB2	28:K:39:GLU:C	1.80	1.03
16:G:148:U:O4	17:H:30:A:N6	1.92	1.03
1:A:532:THR:OG1	16:G:3:A:H5''	1.56	1.02
17:H:163:G:O6	30:p:50:GLY:HA3	1.60	1.02
27:r:112:ALA:CB	28:K:39:GLU:CB	2.38	1.01
4:E:55:LEU:CD1	4:E:341:ILE:HD13	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:ARG:C	3:C:159:LYS:HD2	1.85	1.00
1:A:1517:LYS:HE2	1:A:1517:LYS:HA	1.44	1.00
17:H:54:U:H2'	17:H:55:U:H6	1.24	0.99
19:I:374:ILE:CB	31:Q:357:ALA:HB3	1.91	0.99
17:H:165:A:H61	30:p:88:SER:CB	1.75	0.99
18:U:546:VAL:CG2	18:U:665:HIS:CE1	2.45	0.99
6:J:773:ARG:CB	6:J:787:LYS:HA	1.93	0.99
10:O:236:VAL:O	10:O:269:CYS:HA	1.62	0.99
17:H:92:U:H2'	17:H:93:A:C8	1.98	0.98
2:B:74:U:C5	2:B:76:A:N6	2.31	0.98
2:B:66:A:H5''	2:B:67:A:OP2	1.62	0.98
1:A:1522:GLN:HE22	18:U:622:ALA:HB1	1.27	0.97
16:G:151:C:H3'	16:G:152:C:C5	2.00	0.97
17:H:34:U:C2'	17:H:35:A:C8	2.47	0.96
17:H:54:U:O2'	17:H:55:U:H5'	1.66	0.96
7:L:608:ASN:HA	27:q:112:ALA:HB1	1.48	0.96
16:G:151:C:C2'	16:G:152:C:C5	2.49	0.96
4:E:55:LEU:HD11	4:E:341:ILE:HD13	0.97	0.95
3:C:139:HIS:HB2	34:C:1500:GTP:H5''	1.48	0.95
6:J:212:GLN:HG2	15:W:508:ALA:HB1	1.49	0.95
17:H:156:U:H5''	17:H:156:U:C6	2.02	0.95
27:s:112:ALA:O	28:K:15:ALA:CB	2.14	0.95
16:G:151:C:C4	16:G:152:C:N4	2.34	0.95
5:F:43:A:C2	16:G:4:A:N1	2.35	0.94
17:H:56:A:N6	17:H:92:U:C4	2.35	0.94
11:P:13:ARG:HH21	11:P:13:ARG:HG3	1.32	0.94
16:G:27:U:O2'	16:G:28:A:O5'	1.86	0.94
3:C:143:THR:CG2	34:C:1500:GTP:O1A	2.16	0.94
3:C:143:THR:HG22	34:C:1500:GTP:O1B	1.68	0.93
5:F:41:A:N6	16:G:6:A:N6	1.98	0.93
16:G:151:C:C5	16:G:152:C:N4	2.37	0.93
27:r:112:ALA:HB1	28:K:39:GLU:C	1.91	0.93
17:H:70:C:H2'	17:H:71:C:H6	1.33	0.93
17:H:164:C:C2	30:p:84:ALA:HA	2.03	0.93
27:t:72:PRO:CA	28:K:81:LEU:CB	2.46	0.92
16:G:151:C:H2'	16:G:152:C:C5	2.03	0.92
17:H:30:A:O2'	17:H:31:G:OP2	1.86	0.92
16:G:145:U:H3	17:H:33:G:H22	1.09	0.92
1:A:532:THR:CB	16:G:3:A:H3'	1.99	0.92
16:G:132:G:O2'	16:G:133:A:C8	2.22	0.91
17:H:27:U:O2'	17:H:28:C:H5'	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:34:U:O2'	17:H:35:A:O4'	1.89	0.91
3:C:139:HIS:HB2	34:C:1500:GTP:C5'	2.00	0.91
17:H:165:A:H2'	30:p:41:VAL:CB	2.01	0.90
17:H:179:C:H2'	17:H:180:G:C8	2.05	0.90
3:C:142:LYS:HG3	3:C:228:PHE:HD2	1.31	0.90
17:H:33:G:OP1	18:U:666:ARG:NE	2.04	0.90
16:G:5:G:C2	16:G:6:A:N7	2.40	0.90
17:H:54:U:H2'	17:H:55:U:C6	2.06	0.90
3:C:143:THR:HG22	34:C:1500:GTP:O1A	1.71	0.90
1:A:855:ARG:HH22	1:A:1518:LEU:HD11	1.35	0.90
16:G:27:U:C2'	16:G:28:A:O5'	2.19	0.90
27:q:22:ASN:CB	27:r:55:ILE:CA	2.49	0.90
28:K:127:MET:O	28:K:131:GLY:N	2.03	0.90
16:G:151:C:H2'	16:G:152:C:H6	1.32	0.89
19:I:485:LYS:O	19:I:486:VAL:HG13	1.73	0.89
17:H:35:A:O2'	17:H:36:G:H8	1.52	0.89
17:H:164:C:C2	30:p:10:TYR:CB	2.56	0.89
1:A:861:ARG:HH11	17:H:29:A:H5'	1.38	0.89
1:A:855:ARG:NH2	1:A:1518:LEU:HD11	1.87	0.88
16:G:143:U:O4	17:H:34:U:C4	2.25	0.88
17:H:33:G:P	18:U:666:ARG:HE	1.96	0.88
19:I:448:ASN:CB	19:I:491:ALA:HB1	2.04	0.88
12:R:232:SEP:HB2	12:R:233:PRO:CD	2.02	0.88
16:G:151:C:C2'	16:G:152:C:C6	2.55	0.88
19:I:364:VAL:O	19:I:372:ARG:CB	2.22	0.88
3:C:158:ARG:O	3:C:159:LYS:HD2	1.73	0.88
27:r:112:ALA:CA	28:K:39:GLU:CB	2.51	0.88
17:H:109:C:O2'	17:H:110:A:H5'	1.74	0.88
19:I:325:VAL:O	19:I:328:GLU:CB	2.22	0.88
2:B:11:U:H5'	2:B:11:U:C6	2.07	0.87
7:L:732:MET:CB	27:q:65:PRO:CB	2.52	0.87
19:I:459:ALA:HB1	19:I:498:GLY:O	1.73	0.87
17:H:179:C:C2	17:H:180:G:N7	2.43	0.87
2:B:93:U:O2	23:d:104:ASP:CB	2.22	0.87
12:R:232:SEP:HB2	12:R:233:PRO:HD2	1.56	0.87
16:G:147:C:N3	17:H:31:G:N1	2.20	0.87
17:H:154:C:O2	17:H:176:G:N2	2.07	0.87
3:C:143:THR:CG2	34:C:1500:GTP:PA	2.63	0.87
19:I:520:ILE:O	19:I:524:TYR:CB	2.23	0.87
1:A:1517:LYS:HA	1:A:1517:LYS:CE	2.00	0.86
17:H:162:U:C6	30:p:13:ASN:HA	2.10	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:520:ILE:O	19:I:524:TYR:N	2.06	0.86
27:r:112:ALA:HB2	28:K:40:THR:N	1.91	0.86
4:E:62:LEU:HB3	4:E:93:TRP:HZ3	1.41	0.86
16:G:151:C:C2	16:G:152:C:C4	2.63	0.85
16:G:5:G:C5	16:G:6:A:C8	2.64	0.85
1:A:533:LYS:HD2	16:G:4:A:H5''	1.57	0.85
16:G:5:G:C4	16:G:6:A:C8	2.64	0.85
16:G:151:C:C3'	16:G:152:C:C5	2.58	0.85
17:H:156:U:H6	17:H:156:U:C5'	1.88	0.85
17:H:163:G:C6	30:p:50:GLY:HA3	2.10	0.85
1:A:1833:LEU:HD12	18:U:672:MET:HE1	1.58	0.85
16:G:140:A:O2'	16:G:141:C:OP2	1.94	0.85
16:G:151:C:C3'	16:G:152:C:H5	1.89	0.85
17:H:164:C:O2	30:p:84:ALA:CA	2.25	0.85
3:C:144:CYS:SG	3:C:165:LEU:HD12	2.17	0.84
18:U:550:ARG:CB	18:U:660:LYS:HD3	2.07	0.84
2:B:80:U:H2'	2:B:80:U:OP1	1.77	0.84
15:W:277:PRO:CB	15:W:578:TRP:C	2.51	0.84
19:I:365:ALA:N	19:I:372:ARG:CB	2.40	0.84
27:r:112:ALA:CB	28:K:40:THR:N	2.41	0.84
18:U:551:THR:HG22	18:U:664:GLU:OE1	1.78	0.83
19:I:448:ASN:CB	19:I:491:ALA:CB	2.55	0.83
16:G:129:G:C4'	16:G:130:A:OP1	2.25	0.83
3:C:144:CYS:CB	3:C:165:LEU:HD12	2.08	0.83
16:G:133:A:N6	17:H:43:U:O4	2.12	0.83
5:F:41:A:N1	16:G:6:A:N1	2.27	0.83
2:B:66:A:H2'	2:B:67:A:O4'	1.78	0.83
4:E:55:LEU:CD1	4:E:341:ILE:HD11	2.06	0.83
5:F:44:G:C2	16:G:3:A:N1	2.46	0.83
17:H:42:G:H2'	17:H:43:U:C6	2.14	0.82
17:H:153:A:C2'	17:H:154:C:C5'	2.51	0.82
17:H:56:A:N6	17:H:91:U:H3	1.77	0.82
19:I:255:LEU:O	19:I:258:LEU:N	2.12	0.82
1:A:855:ARG:HH22	1:A:1518:LEU:HD12	1.44	0.82
1:A:861:ARG:NH1	17:H:29:A:C5'	2.42	0.82
17:H:179:C:O2'	17:H:180:G:C5'	2.26	0.82
17:H:165:A:N6	30:p:88:SER:CB	2.42	0.82
17:H:153:A:H2'	17:H:154:C:H5''	1.62	0.82
19:I:521:VAL:O	19:I:527:PHE:CB	2.27	0.82
1:A:861:ARG:HH11	17:H:29:A:C5'	1.93	0.82
3:C:137:HIS:HA	3:C:238:ASN:HB3	1.61	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:546:VAL:HG21	18:U:665:HIS:NE2	1.93	0.82
16:G:133:A:O2'	16:G:134:U:H6	1.59	0.81
17:H:102:U:N1	20:h:3:ILE:N	2.28	0.81
1:A:1513:MET:CE	1:A:1517:LYS:HD2	2.11	0.81
3:C:139:HIS:HA	34:C:1500:GTP:PB	2.19	0.81
6:J:669:GLN:O	6:J:670:PRO:C	2.21	0.81
17:H:70:C:H2'	17:H:71:C:C6	2.15	0.81
17:H:165:A:N3	30:p:41:VAL:CB	2.44	0.80
16:G:151:C:N1	16:G:152:C:C5	2.49	0.80
1:A:855:ARG:NH2	1:A:1518:LEU:CD1	2.44	0.80
17:H:179:C:C2	17:H:180:G:C8	2.69	0.79
3:C:160:ARG:O	3:C:160:ARG:NH1	2.15	0.79
17:H:27:U:C2'	17:H:28:C:H5'	2.12	0.79
18:U:560:VAL:HG11	18:U:660:LYS:HZ3	1.47	0.79
16:G:147:C:O2	17:H:31:G:N2	2.15	0.79
17:H:163:G:O6	30:p:50:GLY:CA	2.31	0.79
17:H:50:C:H5''	17:H:50:C:H6	1.48	0.78
17:H:102:U:C6	20:h:3:ILE:N	2.51	0.78
1:A:532:THR:CB	16:G:3:A:C5'	2.61	0.78
16:G:5:G:N3	16:G:6:A:C8	2.50	0.78
16:G:132:G:OP2	16:G:133:A:OP1	2.00	0.78
16:G:147:C:N4	17:H:31:G:O6	2.15	0.78
16:G:151:C:H3'	16:G:152:C:H5	1.41	0.78
18:U:550:ARG:HB3	18:U:660:LYS:CD	2.12	0.78
17:H:108:G:OP1	22:j:63:ASN:CB	2.31	0.78
2:B:11:U:H6	2:B:11:U:C5'	1.96	0.78
4:E:61:LEU:CD1	4:E:352:TYR:CE2	2.66	0.78
10:O:159:ARG:HD3	16:G:20:A:OP1	1.84	0.78
4:E:62:LEU:HB3	4:E:93:TRP:CZ3	2.19	0.77
17:H:179:C:O2	17:H:180:G:C8	2.37	0.77
19:I:545:ILE:C	19:I:547:LEU:H	1.91	0.77
16:G:6:A:N6	16:G:7:G:C6	2.53	0.77
17:H:34:U:H2'	17:H:35:A:N7	2.00	0.77
28:K:126:LEU:O	28:K:130:HIS:N	2.16	0.77
4:E:61:LEU:CD1	4:E:352:TYR:CZ	2.67	0.77
18:U:546:VAL:HG11	18:U:665:HIS:CE1	2.20	0.77
17:H:177:A:H5''	17:H:178:A:OP1	1.84	0.76
2:B:66:A:H3'	2:B:67:A:H5''	1.66	0.76
16:G:145:U:H3	17:H:33:G:H1	1.18	0.76
16:G:132:G:OP1	16:G:133:A:OP1	2.02	0.76
17:H:56:A:H61	17:H:91:U:H3	1.33	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:132:G:O2'	16:G:133:A:N7	2.19	0.75
12:R:235:ARG:HG2	12:R:235:ARG:HH11	1.48	0.75
17:H:56:A:N6	17:H:92:U:N3	2.35	0.75
27:q:8:SER:O	27:q:9:ASN:CB	2.34	0.75
1:A:532:THR:CB	16:G:3:A:H5'	2.16	0.75
2:B:8:G:N3	2:B:8:G:H2'	2.00	0.75
2:B:66:A:C5'	2:B:67:A:OP2	2.34	0.75
27:r:112:ALA:HB3	28:K:36:VAL:O	1.87	0.75
2:B:94:U:OP2	24:f:67:ASN:CB	2.35	0.74
5:F:20:A:O2'	9:N:120:ARG:NH2	2.21	0.74
3:C:143:THR:HG23	34:C:1500:GTP:O1A	1.86	0.74
17:H:102:U:N3	20:h:3:ILE:N	2.35	0.74
28:K:131:GLY:O	28:K:135:TRP:N	2.21	0.74
16:G:150:U:O2'	16:G:151:C:H5''	1.87	0.74
27:t:90:PHE:CB	28:K:111:MET:O	2.35	0.74
2:B:87:A:N7	23:d:61:ARG:CB	2.50	0.74
5:F:41:A:H61	16:G:6:A:H61	0.75	0.74
19:I:720:ILE:O	19:I:721:LYS:CB	2.34	0.74
16:G:145:U:C2	17:H:33:G:N2	2.54	0.74
19:I:545:ILE:O	19:I:547:LEU:N	2.20	0.74
6:J:493:ALA:HB1	6:J:499:ARG:CB	2.18	0.74
17:H:179:C:H2'	17:H:180:G:H5'	1.66	0.74
1:A:1833:LEU:HD13	18:U:668:LEU:HD21	1.70	0.74
27:s:112:ALA:O	28:K:15:ALA:HB3	1.88	0.73
4:E:55:LEU:N	4:E:55:LEU:HD13	2.03	0.73
16:G:132:G:OP1	16:G:132:G:H4'	1.88	0.73
6:J:642:SER:CB	6:J:650:GLU:HA	2.17	0.73
1:A:179:ALA:O	1:A:183:LEU:HB2	1.89	0.73
16:G:151:C:N3	16:G:152:C:C4	2.57	0.73
28:K:126:LEU:O	28:K:130:HIS:CB	2.36	0.73
17:H:92:U:H2'	17:H:93:A:H8	1.52	0.73
5:F:41:A:H62	16:G:6:A:H61	1.35	0.73
4:E:55:LEU:HD13	4:E:55:LEU:H	1.54	0.72
3:C:137:HIS:O	3:C:207:GLY:O	2.05	0.72
5:F:44:G:C2	16:G:3:A:C2	2.76	0.72
1:A:1513:MET:HE2	1:A:1517:LYS:HD2	1.70	0.72
3:C:690:GLU:O	3:C:788:LYS:HB3	1.88	0.72
15:W:491:GLN:O	15:W:493:ARG:N	2.21	0.72
10:O:26:THR:HG21	10:O:159:ARG:HH21	1.55	0.71
2:B:74:U:C5	2:B:76:A:C6	2.77	0.71
17:H:43:U:O2'	17:H:44:U:C6	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:A:N3	2:B:87:A:H3'	2.06	0.71
2:B:96:A:C6	2:B:97:G:C5	2.78	0.71
16:G:145:U:N3	17:H:33:G:N1	2.29	0.71
16:G:146:C:O2'	16:G:147:C:P	2.48	0.71
15:W:277:PRO:CB	15:W:578:TRP:O	2.39	0.71
28:K:120:ARG:O	28:K:124:LEU:N	2.21	0.71
16:G:145:U:O2	17:H:33:G:N2	2.23	0.71
2:B:92:U:O4	21:b:36:LYS:O	2.09	0.70
3:C:143:THR:HG22	34:C:1500:GTP:PA	2.27	0.70
17:H:154:C:H2'	17:H:155:C:C6	2.26	0.70
28:K:135:TRP:O	28:K:136:LYS:CB	2.38	0.70
3:C:141:GLY:N	34:C:1500:GTP:O2B	2.24	0.70
16:G:27:U:H2'	16:G:28:A:O5'	1.91	0.70
10:O:159:ARG:CG	16:G:20:A:OP1	2.39	0.70
16:G:143:U:C6	16:G:143:U:H5''	2.27	0.70
16:G:147:C:C2	17:H:31:G:N2	2.56	0.70
19:I:585:ASP:O	19:I:588:PRO:N	2.25	0.70
4:E:61:LEU:HD13	4:E:352:TYR:CE2	2.24	0.70
1:A:1811:ASN:HD22	1:A:1816:GLN:HB3	1.55	0.70
4:E:162:ARG:HH21	4:E:203:ASP:HB3	1.56	0.70
6:J:496:ASP:CB	6:J:535:TYR:HA	2.21	0.70
1:A:1522:GLN:NE2	18:U:622:ALA:HB1	2.04	0.70
3:C:139:HIS:CA	34:C:1500:GTP:O3B	2.33	0.70
4:E:259:VAL:HB	4:E:277:PHE:HB2	1.74	0.70
16:G:145:U:N3	17:H:33:G:N2	2.23	0.70
2:B:93:U:H1'	23:d:104:ASP:CB	2.21	0.69
27:t:71:ILE:CB	28:K:70:PHE:CB	2.70	0.69
1:A:1570:LYS:HE2	18:U:637:ASP:HB3	1.74	0.69
4:E:266:PRO:HG2	7:L:785:GLN:CB	2.22	0.69
11:P:13:ARG:HG3	11:P:13:ARG:NH2	2.00	0.69
17:H:165:A:C2	30:p:53:PHE:CB	2.75	0.69
18:U:548:LEU:HD22	18:U:661:ALA:HB1	1.74	0.69
18:U:678:CYS:SG	18:U:765:HIS:HE1	2.15	0.69
1:A:980:ARG:HG2	1:A:1094:ARG:HG2	1.75	0.69
19:I:485:LYS:C	19:I:486:VAL:HG22	2.18	0.69
3:C:173:THR:HG1	3:C:642:HIS:HE2	1.41	0.69
15:W:466:ALA:CB	15:W:512:CYS:O	2.41	0.69
28:K:127:MET:O	28:K:131:GLY:CA	2.41	0.69
7:L:620:PRO:CB	27:q:108:TYR:CB	2.70	0.68
10:O:159:ARG:CD	16:G:20:A:OP1	2.41	0.68
1:A:942:PRO:HB2	1:A:1438:VAL:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:U:O2'	2:B:82:A:OP2	2.11	0.68
17:H:164:C:N4	30:p:82:GLN:CB	2.57	0.68
16:G:5:G:H4'	16:G:5:G:OP1	1.94	0.68
4:E:55:LEU:O	4:E:55:LEU:HD22	1.94	0.68
6:J:669:GLN:O	6:J:672:LEU:N	2.26	0.68
27:q:71:ILE:HA	27:r:81:GLU:CB	2.22	0.68
17:H:55:U:C4	17:H:93:A:N1	2.62	0.68
27:r:112:ALA:O	28:K:39:GLU:CB	2.41	0.67
2:B:10:U:OP2	2:B:10:U:H6	1.78	0.67
5:F:40:U:H3	16:G:7:G:H22	1.42	0.67
10:O:262:THR:HB	10:O:271:PHE:HB2	1.76	0.67
16:G:6:A:C4	16:G:7:G:C8	2.83	0.67
16:G:147:C:N4	17:H:31:G:N1	2.42	0.67
19:I:484:LEU:O	19:I:486:VAL:HG22	1.93	0.67
16:G:147:C:N4	17:H:31:G:H1	1.92	0.67
17:H:166:G:H2'	17:H:166:G:N3	2.09	0.67
19:I:790:ARG:CB	19:I:797:PHE:O	2.42	0.67
15:W:474:LYS:HA	15:W:490:ALA:HB3	1.75	0.67
18:U:673:GLU:OE2	18:U:682:SER:HB3	1.95	0.67
3:C:140:HIS:N	34:C:1500:GTP:O2B	2.27	0.67
17:H:34:U:HO2'	17:H:35:A:C1'	2.09	0.67
1:A:1662:ILE:HA	1:A:1701:VAL:O	1.94	0.66
17:H:109:C:C4'	23:k:47:ARG:CB	2.63	0.66
17:H:156:U:C6	17:H:156:U:C5'	2.72	0.66
19:I:790:ARG:CB	19:I:801:ASP:CA	2.74	0.66
18:U:673:GLU:OE1	18:U:673:GLU:HA	1.93	0.66
3:C:144:CYS:SG	3:C:165:LEU:CD1	2.83	0.66
2:B:96:A:O2'	2:B:97:G:H5'	1.95	0.66
3:C:159:LYS:HD2	3:C:159:LYS:N	1.96	0.66
17:H:75:A:H61	17:H:77:C:H42	1.43	0.66
18:U:656:ASN:O	18:U:660:LYS:HE3	1.96	0.66
4:E:90:ILE:HB	4:E:105:LEU:HB2	1.78	0.66
27:r:112:ALA:C	28:K:39:GLU:CB	2.69	0.66
2:B:96:A:C6	2:B:97:G:C6	2.84	0.66
17:H:153:A:C3'	17:H:154:C:H5'	2.24	0.66
17:H:150:U:H6	17:H:150:U:O5'	1.77	0.65
17:H:102:U:C4	20:h:3:ILE:N	2.64	0.65
18:U:868:SER:HB2	18:U:872:GLN:H	1.61	0.65
16:G:147:C:N3	17:H:31:G:C2	2.63	0.65
17:H:34:U:O2'	17:H:35:A:C5'	2.44	0.65
17:H:165:A:C2'	30:p:41:VAL:CB	2.75	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:656:ASN:O	18:U:660:LYS:HB3	1.95	0.65
17:H:151:C:H2'	17:H:152:G:C8	2.31	0.65
2:B:90:U:N3	26:g:36:PRO:O	2.29	0.65
13:S:56:ILE:HG12	13:S:62:ILE:HG23	1.79	0.65
17:H:57:A:N6	17:H:91:U:N3	2.45	0.65
19:I:448:ASN:CB	19:I:491:ALA:HB2	2.26	0.65
1:A:761:ILE:HD12	1:A:775:ASN:HD22	1.61	0.65
17:H:43:U:O2'	17:H:44:U:C5	2.48	0.65
17:H:67:C:H42	17:H:85:A:H61	1.44	0.65
18:U:551:THR:HG22	18:U:664:GLU:CD	2.21	0.65
1:A:1214:TRP:HB2	1:A:1228:CYS:HB3	1.78	0.64
16:G:145:U:O4	17:H:33:G:O6	2.16	0.64
1:A:1629:ILE:HG22	1:A:1662:ILE:HG12	1.79	0.64
15:W:97:ASN:HD21	15:W:100:ARG:HH21	1.45	0.64
16:G:19:G:O2'	16:G:20:A:H5'	1.98	0.64
2:B:74:U:H5	2:B:76:A:H61	1.45	0.64
2:B:76:A:O2'	2:B:77:G:H5''	1.97	0.64
7:L:608:ASN:CA	27:q:112:ALA:CB	2.68	0.64
3:C:144:CYS:CA	3:C:165:LEU:HD12	2.27	0.64
16:G:125:C:O2'	16:G:126:C:H2'	1.98	0.64
3:C:678:THR:HG21	3:C:807:GLN:HB3	1.80	0.64
1:A:533:LYS:HD2	16:G:4:A:C5'	2.27	0.63
1:A:855:ARG:CZ	1:A:1518:LEU:HD11	2.28	0.63
8:M:165:ASN:HD22	12:R:95:LYS:HA	1.63	0.63
14:T:216:ASN:HD21	14:T:472:GLN:H	1.46	0.63
2:B:9:G:H4'	2:B:9:G:OP1	1.97	0.63
17:H:33:G:OP1	18:U:666:ARG:NH2	2.31	0.63
1:A:1513:MET:HE3	1:A:1517:LYS:HD2	1.79	0.63
18:U:560:VAL:HG11	18:U:660:LYS:NZ	2.13	0.63
28:K:127:MET:O	28:K:131:GLY:HA3	1.97	0.63
15:W:264:ASN:O	15:W:267:SER:CB	2.46	0.63
17:H:33:G:P	18:U:666:ARG:NE	2.68	0.63
17:H:163:G:O6	30:p:50:GLY:C	2.42	0.63
3:C:160:ARG:HH11	3:C:160:ARG:CG	2.11	0.63
1:A:1839:TRP:NE1	18:U:557:VAL:O	2.31	0.63
3:C:210:ASN:HB3	3:C:636:TYR:HB2	1.80	0.63
14:T:314:ILE:HD12	14:T:324:HIS:HB2	1.80	0.63
17:H:50:C:H5''	17:H:50:C:C6	2.33	0.63
17:H:67:C:H2'	17:H:68:G:H8	1.63	0.63
17:H:154:C:H2'	17:H:155:C:H6	1.62	0.63
1:A:1313:PRO:HG2	1:A:1335:ILE:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:15:TRP:HE1	11:P:26:LEU:HB2	1.64	0.63
4:E:219:VAL:HB	4:E:229:TYR:HB2	1.81	0.62
13:S:15:TYR:HB2	13:S:163:TYR:HB2	1.79	0.62
16:G:151:C:C4	16:G:152:C:C4	2.86	0.62
17:H:55:U:H2'	17:H:56:A:H8	1.63	0.62
18:U:539:GLU:OE2	18:U:662:ILE:CG1	2.47	0.62
4:E:158:TYR:OH	4:E:161:ARG:NH1	2.32	0.62
6:J:239:ARG:CG	6:J:239:ARG:HH11	2.12	0.62
12:R:235:ARG:HH11	12:R:235:ARG:CG	2.12	0.62
15:W:463:SER:O	15:W:480:SER:HA	1.98	0.62
27:r:112:ALA:HA	28:K:39:GLU:CB	2.27	0.62
1:A:1144:LYS:HE2	1:A:1148:ASN:HD21	1.64	0.62
4:E:274:VAL:HG12	4:E:275:LYS:HG3	1.81	0.62
10:O:233:THR:HA	10:O:272:ILE:O	1.99	0.62
16:G:151:C:C2'	16:G:152:C:H5	2.00	0.62
18:U:620:ARG:NH2	18:U:643:LYS:O	2.33	0.62
27:r:8:SER:O	27:r:9:ASN:CB	2.47	0.62
6:J:741:THR:O	6:J:745:CYS:CB	2.47	0.62
17:H:163:G:N7	30:p:12:ASN:CB	2.63	0.62
6:J:228:ARG:NH2	6:J:257:GLU:OE1	2.32	0.62
7:L:764:PRO:O	7:L:765:ARG:CB	2.48	0.62
16:G:143:U:C4	17:H:34:U:N3	2.49	0.62
19:I:559:THR:CB	19:I:570:GLY:HA3	2.30	0.62
1:A:610:HIS:NE2	33:A:3000:IHP:O33	2.31	0.62
3:C:523:GLN:NE2	3:C:525:CYS:SG	2.73	0.62
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.80	0.62
1:A:1838:LYS:HG2	1:A:1871:PRO:HG2	1.82	0.62
10:O:27:CYS:SG	10:O:66:LYS:NZ	2.71	0.62
16:G:145:U:O4	17:H:33:G:C6	2.53	0.62
18:U:663:ALA:HA	18:U:666:ARG:NH1	2.14	0.62
10:O:240:GLY:HA3	10:O:296:ARG:HH12	1.63	0.62
10:O:34:ILE:HB	12:R:197:ILE:HG12	1.81	0.61
17:H:102:U:C5	20:h:3:ILE:N	2.68	0.61
18:U:576:ARG:HH22	18:U:647:ARG:HD3	1.65	0.61
18:U:658:ARG:O	18:U:662:ILE:HB	1.99	0.61
16:G:144:A:H4'	16:G:145:U:H3'	1.82	0.61
19:I:526:MET:HE2	19:I:526:MET:O	2.00	0.61
17:H:112:G:H2'	17:H:113:G:H8	1.65	0.61
6:J:658:ARG:CA	6:J:667:ILE:CB	2.71	0.61
16:G:4:A:H8	16:G:4:A:OP1	1.84	0.61
16:G:6:A:C5	16:G:7:G:N7	2.69	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:399:VAL:HG13	19:I:399:VAL:O	2.00	0.61
19:I:795:ILE:HG22	19:I:795:ILE:O	1.99	0.61
17:H:54:U:C4	17:H:93:A:N1	2.69	0.61
3:C:157:ILE:HG23	3:C:158:ARG:HG2	1.83	0.61
17:H:148:C:C2'	17:H:149:A:H5'	2.30	0.61
19:I:365:ALA:HA	19:I:372:ARG:CB	2.31	0.61
1:A:113:ILE:HG21	9:N:6:ARG:HE	1.66	0.61
1:A:199:GLU:O	1:A:240:ARG:NH2	2.33	0.61
1:A:532:THR:HB	16:G:3:A:C4'	2.30	0.61
10:O:92:LEU:HD11	10:O:151:ALA:HA	1.82	0.61
10:O:182:ARG:NH1	10:O:184:GLU:OE2	2.34	0.61
15:W:280:GLN:HA	15:W:577:LEU:O	2.00	0.61
15:W:290:GLY:CA	15:W:571:TRP:O	2.49	0.61
6:J:241:VAL:HG12	6:J:241:VAL:O	2.00	0.61
13:S:83:GLU:HA	13:S:106:ASP:HB2	1.82	0.61
16:G:6:A:C6	16:G:7:G:C4	2.89	0.61
16:G:147:C:N4	17:H:31:G:C6	2.56	0.61
19:I:365:ALA:CA	19:I:372:ARG:CB	2.79	0.61
27:s:112:ALA:O	28:K:15:ALA:HB1	1.99	0.60
1:A:382:GLU:HA	3:C:354:ARG:HH12	1.65	0.60
6:J:293:ASN:ND2	7:L:226:ASP:O	2.34	0.60
8:M:166:SER:O	13:S:141:ARG:NH2	2.34	0.60
15:W:491:GLN:CB	16:G:136:U:OP2	2.49	0.60
16:G:143:U:O4	17:H:34:U:O4	2.19	0.60
17:H:179:C:N3	17:H:180:G:N7	2.49	0.60
3:C:160:ARG:HH11	3:C:160:ARG:CB	2.14	0.60
3:C:160:ARG:HB3	3:C:164:ASP:HB2	1.83	0.60
3:C:618:THR:HB	3:C:630:LEU:HB2	1.82	0.60
7:L:732:MET:HA	27:q:65:PRO:CB	2.31	0.60
5:F:49:G:OP1	7:L:33:ARG:NH2	2.34	0.60
10:O:72:GLN:OE1	10:O:82:GLN:NE2	2.34	0.60
14:T:393:ASP:OD1	14:T:393:ASP:N	2.34	0.60
15:W:531:LYS:CB	15:W:546:PHE:O	2.50	0.60
17:H:157:G:H8	17:H:157:G:H5''	1.65	0.60
3:C:165:LEU:O	3:C:165:LEU:HD23	2.01	0.60
4:E:340:PRO:HB2	4:E:356:ILE:HB	1.84	0.60
17:H:34:U:O2'	17:H:35:A:C1'	2.48	0.60
19:I:374:ILE:CB	31:Q:357:ALA:CB	2.75	0.60
2:B:11:U:H2'	2:B:12:U:O4'	2.02	0.60
16:G:26:U:H2'	16:G:27:U:H5''	1.82	0.60
6:J:669:GLN:O	6:J:671:ARG:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1371:TYR:OH	1:A:1473:ASP:OD2	2.17	0.59
1:A:82:ARG:NH2	16:G:14:A:OP2	2.35	0.59
1:A:695:ASP:OD2	14:T:376:ARG:NH2	2.35	0.59
2:B:88:A:N3	25:e:53:TYR:CB	2.65	0.59
7:L:123:LEU:HD13	7:L:124:LYS:H	1.67	0.59
15:W:290:GLY:HA3	15:W:571:TRP:HA	1.84	0.59
2:B:10:U:OP2	2:B:10:U:H2'	2.03	0.59
3:C:147:ASP:OD1	3:C:158:ARG:NH1	2.35	0.59
10:O:253:TYR:OH	13:S:123:ASP:OD2	2.19	0.59
10:O:234:LEU:HB2	10:O:272:ILE:HB	1.85	0.59
16:G:4:A:C6	16:G:5:G:N2	2.71	0.59
17:H:34:U:O2'	17:H:35:A:N9	2.35	0.59
17:H:54:U:HO2'	17:H:55:U:H5'	1.64	0.59
10:O:185:LYS:HZ3	15:W:216:LEU:HG	1.68	0.59
11:P:20:GLU:OE2	14:T:313:ARG:NH2	2.36	0.59
16:G:1:G:H1'	16:G:2:U:OP1	2.03	0.59
17:H:55:U:O4	17:H:93:A:N6	2.36	0.59
1:A:1631:LEU:HB2	1:A:1660:TYR:HB3	1.83	0.59
3:C:139:HIS:HB2	34:C:1500:GTP:H5'	1.82	0.59
3:C:678:THR:OG1	3:C:680:ASN:O	2.21	0.59
12:R:101:ILE:O	12:R:104:GLN:NE2	2.36	0.59
12:R:196:VAL:HG11	15:W:120:ILE:HD12	1.85	0.59
18:U:657:GLN:HA	18:U:660:LYS:HZ1	1.68	0.59
1:A:163:ARG:NE	1:A:576:ASP:OD2	2.34	0.59
3:C:308:CYS:SG	3:C:309:PHE:N	2.76	0.59
6:J:600:ILE:C	6:J:602:LYS:H	2.10	0.59
2:B:96:A:N6	2:B:97:G:C6	2.71	0.58
4:E:143:ARG:HD3	4:E:146:ARG:HB2	1.85	0.58
18:U:678:CYS:SG	18:U:718:HIS:HD2	2.26	0.58
2:B:9:G:O6	2:B:69:A:C2	2.56	0.58
8:M:236:ASN:ND2	8:M:242:ALA:O	2.35	0.58
1:A:1813:ARG:HD3	1:A:1814:THR:HG23	1.83	0.58
4:E:178:LEU:HD12	4:E:188:GLN:HB2	1.84	0.58
17:H:107:A:O2'	17:H:108:G:H5'	2.03	0.58
16:G:145:U:C4	17:H:33:G:N1	2.58	0.58
1:A:48:LYS:NZ	5:F:21:U:OP2	2.36	0.58
17:H:50:C:H6	17:H:50:C:C5'	2.17	0.58
1:A:255:PHE:HB3	1:A:259:ASP:HB3	1.86	0.58
11:P:13:ARG:NH1	14:T:330:THR:O	2.37	0.58
1:A:1194:CYS:HB3	1:A:1230:LEU:HD23	1.85	0.58
14:T:342:GLU:OE1	14:T:365:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:350:HIS:HA	14:T:374:SER:HB2	1.86	0.58
17:H:33:G:OP1	18:U:666:ARG:CZ	2.50	0.58
18:U:671:GLN:OE1	18:U:671:GLN:HA	2.02	0.58
1:A:163:ARG:HD2	1:A:166:PHE:HZ	1.69	0.58
4:E:67:GLY:N	4:E:87:ASP:OD1	2.37	0.58
4:E:268:ALA:HB2	4:E:272:ARG:HH21	1.67	0.58
7:L:608:ASN:CA	27:q:112:ALA:HB1	2.28	0.58
16:G:143:U:C6	16:G:143:U:C5'	2.87	0.58
17:H:164:C:N3	30:p:84:ALA:HA	2.19	0.58
1:A:1321:GLU:HG3	1:A:1322:LEU:HD22	1.85	0.57
1:A:1833:LEU:CD1	18:U:668:LEU:HD21	2.33	0.57
2:B:69:A:H2'	2:B:69:A:N3	2.18	0.57
2:B:74:U:O4	2:B:76:A:N1	2.37	0.57
3:C:663:CYS:HB2	3:C:828:MET:HB2	1.85	0.57
3:C:742:PRO:HG3	3:C:785:ARG:HD2	1.85	0.57
1:A:164:MET:HE2	1:A:569:VAL:HG11	1.85	0.57
2:B:96:A:C5	2:B:97:G:N7	2.73	0.57
19:I:327:LEU:O	19:I:330:ARG:N	2.37	0.57
27:q:22:ASN:CB	27:r:55:ILE:CB	2.81	0.57
12:R:64:PHE:O	12:R:71:GLN:NE2	2.38	0.57
13:S:57:ILE:HD13	15:W:97:ASN:HB3	1.87	0.57
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.38	0.57
3:C:166:CYS:HA	3:C:169:ASP:HB3	1.86	0.57
5:F:41:A:C6	16:G:7:G:N2	2.73	0.57
5:F:59:G:O2'	5:F:61:C:OP1	2.22	0.57
16:G:26:U:H2'	16:G:27:U:C5'	2.34	0.57
17:H:154:C:O2'	17:H:155:C:H5'	2.04	0.57
1:A:466:ALA:HA	2:B:20:G:H21	1.69	0.57
1:A:1606:ILE:O	1:A:1634:SER:OG	2.23	0.57
3:C:224:GLY:HA3	3:C:438:ILE:HD12	1.84	0.57
16:G:5:G:N3	16:G:6:A:N7	2.48	0.57
16:G:141:C:OP2	16:G:141:C:H6	1.88	0.57
1:A:1555:LEU:HD21	1:A:1570:LYS:HG3	1.87	0.57
3:C:174:GLU:HG3	3:C:181:ILE:H	1.69	0.57
5:F:41:A:N6	16:G:7:G:C2	2.73	0.57
10:O:159:ARG:NH1	16:G:20:A:OP1	2.30	0.57
17:H:57:A:N6	17:H:90:A:C2	2.72	0.57
1:A:975:VAL:HB	1:A:1099:PHE:HB2	1.87	0.57
2:B:96:A:C2'	2:B:97:G:H5'	2.34	0.57
17:H:109:C:O2'	17:H:110:A:C5'	2.51	0.57
1:A:1624:SER:HB2	1:A:1693:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:G:O6	2:B:69:A:H2	1.88	0.56
2:B:66:A:C2'	2:B:67:A:O4'	2.50	0.56
7:L:37:LEU:HD11	7:L:155:ALA:HA	1.87	0.56
12:R:148:ARG:NH2	14:T:299:THR:O	2.36	0.56
14:T:294:LEU:HD12	14:T:303:LEU:HD11	1.86	0.56
19:I:364:VAL:CB	19:I:372:ARG:CB	2.83	0.56
1:A:1186:LEU:HD23	1:A:1195:ARG:HB3	1.87	0.56
15:W:103:GLN:NE2	15:W:111:LEU:O	2.38	0.56
16:G:22:C:O2'	16:G:23:U:P	2.63	0.56
1:A:608:LEU:HD13	1:A:632:ALA:HB1	1.87	0.56
2:B:9:G:C5	2:B:70:A:C8	2.94	0.56
8:M:221:LYS:NZ	17:H:18:U:OP2	2.38	0.56
16:G:5:G:C2	16:G:6:A:C8	2.93	0.56
17:H:77:C:C2	17:H:78:C:C5	2.93	0.56
17:H:147:G:C2	17:H:148:C:C5	2.92	0.56
17:H:148:C:H2'	17:H:149:A:H8	1.70	0.56
17:H:163:G:O6	30:p:50:GLY:O	2.22	0.56
19:I:187:LEU:CB	32:y:28:PRO:O	2.53	0.56
27:q:58:ALA:HB1	27:r:6:SER:HA	1.87	0.56
4:E:346:SER:OG	4:E:348:ASP:OD1	2.23	0.56
13:S:52:LYS:HA	13:S:158:LYS:HA	1.88	0.56
16:G:136:U:O2'	16:G:137:C:C6	2.58	0.56
17:H:71:C:H2'	17:H:72:U:H6	1.70	0.56
17:H:73:C:H2'	17:H:74:U:H6	1.70	0.56
17:H:77:C:H2'	17:H:78:C:H6	1.70	0.56
1:A:143:GLN:NE2	1:A:207:PHE:O	2.32	0.56
1:A:855:ARG:NH1	1:A:1518:LEU:HD11	2.21	0.56
12:R:106:GLN:HG2	12:R:110:LYS:HG2	1.87	0.56
14:T:349:SER:OG	14:T:351:ASP:OD1	2.23	0.56
16:G:154:U:H2'	16:G:154:U:O2	2.05	0.56
17:H:72:U:C2	17:H:73:C:C5	2.94	0.56
17:H:90:A:H2'	17:H:91:U:H6	1.71	0.56
17:H:91:U:H2'	17:H:92:U:H6	1.71	0.56
1:A:405:LEU:HD22	3:C:413:ARG:HE	1.68	0.56
1:A:891:PHE:O	7:L:83:ARG:NH1	2.38	0.56
2:B:96:A:C4	2:B:97:G:C8	2.93	0.56
16:G:149:G:H8	16:G:149:G:OP2	1.89	0.56
17:H:71:C:C2	17:H:72:U:C5	2.94	0.56
17:H:88:A:H2'	17:H:89:U:H6	1.70	0.56
4:E:178:LEU:HD11	4:E:222:LEU:HD22	1.86	0.56
16:G:138:A:O2'	16:G:139:U:C6	2.59	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:73:C:C2	17:H:74:U:C5	2.94	0.56
14:T:190:TRP:HE1	14:T:498:GLU:HB3	1.71	0.56
27:q:71:ILE:CA	27:r:81:GLU:CB	2.84	0.56
1:A:1342:TRP:HB2	1:A:1486:GLU:HG3	1.88	0.56
3:C:375:GLU:OE2	3:C:379:LYS:NZ	2.33	0.56
4:E:62:LEU:HB2	4:E:351:LEU:HB2	1.88	0.56
14:T:312:ALA:HB3	14:T:326:LEU:HB2	1.88	0.56
17:H:39:U:O2'	17:H:40:C:C6	2.59	0.56
17:H:151:C:H2'	17:H:152:G:H8	1.68	0.56
27:q:71:ILE:CB	27:r:81:GLU:CB	2.84	0.56
27:s:81:GLU:CB	28:K:67:ARG:CB	2.84	0.56
3:C:205:THR:HB	3:C:215:VAL:HG22	1.87	0.56
4:E:257:ASN:HD22	15:W:149:SER:HA	1.71	0.56
13:S:25:LEU:HD22	13:S:98:LEU:HD22	1.88	0.56
17:H:59:A:H2'	17:H:60:U:H6	1.70	0.56
17:H:72:U:H2'	17:H:73:C:H6	1.71	0.56
1:A:1330:MET:HE1	1:A:1369:TYR:HB2	1.88	0.55
3:C:135:CYS:HB2	3:C:242:LEU:HD13	1.87	0.55
17:H:33:G:O5'	18:U:666:ARG:NE	2.39	0.55
18:U:678:CYS:SG	18:U:718:HIS:CD2	2.98	0.55
1:A:1865:ARG:NH1	18:U:726:ASP:OD2	2.39	0.55
2:B:9:G:H5''	2:B:10:U:C5	2.41	0.55
12:R:78:ARG:HG3	12:R:79:LYS:HG2	1.86	0.55
17:H:108:G:C4'	23:k:104:ASP:CB	2.74	0.55
17:H:161:U:O2'	17:H:163:G:N2	2.39	0.55
1:A:1392:LYS:HD3	1:A:1407:ASP:HB3	1.87	0.55
13:S:26:GLU:OE1	13:S:131:ARG:NH1	2.40	0.55
15:W:474:LYS:C	15:W:490:ALA:CB	2.80	0.55
18:U:666:ARG:CZ	18:U:666:ARG:HB3	2.36	0.55
3:C:139:HIS:CA	34:C:1500:GTP:PB	2.93	0.55
6:J:618:GLN:O	6:J:634:GLU:CB	2.55	0.55
8:M:178:GLU:OE1	8:M:181:ARG:NH1	2.37	0.55
14:T:261:LEU:HB3	14:T:273:TRP:HB2	1.86	0.55
17:H:55:U:O2	17:H:56:A:C8	2.59	0.55
17:H:57:A:H2'	17:H:58:U:H6	1.71	0.55
17:H:83:A:H2'	17:H:84:C:H6	1.71	0.55
3:C:803:ARG:O	3:C:807:GLN:HB2	2.07	0.55
4:E:266:PRO:HG2	7:L:785:GLN:CA	2.37	0.55
10:O:236:VAL:HG22	10:O:300:VAL:HG22	1.87	0.55
12:R:232:SEP:CB	12:R:233:PRO:CD	2.77	0.55
16:G:6:A:C6	16:G:7:G:C6	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:148:U:C4	17:H:30:A:N1	2.70	0.55
14:T:418:THR:HG21	14:T:467:ALA:HA	1.88	0.55
18:U:546:VAL:CB	18:U:665:HIS:CE1	2.88	0.55
19:I:265:TYR:O	19:I:266:TYR:C	2.50	0.55
1:A:425:PRO:HB2	1:A:428:LYS:HB2	1.88	0.55
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.88	0.55
17:H:108:G:H2'	17:H:109:C:C6	2.41	0.55
2:B:71:C:H3'	2:B:71:C:H6	1.72	0.55
3:C:523:GLN:HE21	3:C:558:PRO:HG3	1.72	0.55
5:F:82:A:N6	17:H:19:G:OP1	2.34	0.55
6:J:770:ASP:CB	6:J:791:ASP:CB	2.85	0.55
17:H:88:A:C4	17:H:89:U:C5	2.95	0.55
3:C:692:LEU:O	3:C:786:ASN:ND2	2.39	0.55
4:E:90:ILE:HD11	4:E:112:VAL:HG11	1.87	0.55
6:J:260:ARG:HD3	7:L:214:ILE:HG12	1.88	0.55
3:C:637:LEU:HA	3:C:640:VAL:HG12	1.88	0.55
16:G:22:C:O2'	16:G:23:U:OP1	2.25	0.55
17:H:34:U:O2'	17:H:35:A:C8	2.60	0.55
18:U:546:VAL:CB	18:U:665:HIS:HE1	2.20	0.55
1:A:1132:LYS:HA	1:A:1139:ARG:HH12	1.72	0.54
1:A:1431:ALA:O	1:A:1434:LYS:NZ	2.40	0.54
4:E:118:ASN:ND2	4:E:122:SER:OG	2.37	0.54
15:W:531:LYS:HA	15:W:546:PHE:O	2.07	0.54
17:H:57:A:C4	17:H:58:U:C5	2.95	0.54
18:U:666:ARG:CZ	18:U:666:ARG:CB	2.85	0.54
1:A:1335:ILE:HG23	1:A:1365:ILE:HD11	1.88	0.54
1:A:1609:VAL:HG12	1:A:1631:LEU:HG	1.89	0.54
14:T:270:VAL:HB	14:T:284:TYR:HB2	1.89	0.54
17:H:91:U:C2	17:H:92:U:C5	2.94	0.54
17:H:148:C:H2'	17:H:149:A:C8	2.43	0.54
18:U:546:VAL:CG1	18:U:665:HIS:CE1	2.90	0.54
2:B:85:C:H3'	2:B:85:C:OP1	2.07	0.54
2:B:100:C:H2'	2:B:101:U:C6	2.42	0.54
3:C:219:LEU:HD13	3:C:245:HIS:HD2	1.72	0.54
7:L:732:MET:CA	27:q:65:PRO:CB	2.86	0.54
17:H:50:C:H2'	17:H:51:A:C8	2.42	0.54
17:H:102:U:HO2'	17:H:103:U:H6	1.55	0.54
1:A:470:ARG:NH1	2:B:56:C:OP2	2.41	0.54
16:G:151:C:C2'	16:G:152:C:H6	2.09	0.54
17:H:83:A:C4	17:H:84:C:C5	2.95	0.54
1:A:657:ALA:O	1:A:661:GLU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:43:A:O5'	5:F:43:A:H8	1.89	0.54
12:R:68:HIS:NE2	13:S:89:ASP:O	2.36	0.54
17:H:32:U:N3	17:H:33:G:C6	2.76	0.54
2:B:66:A:H3'	2:B:67:A:C5'	2.36	0.54
3:C:529:ARG:H	3:C:553:GLU:HB3	1.71	0.54
15:W:474:LYS:C	15:W:490:ALA:HB3	2.33	0.54
16:G:135:G:O2'	16:G:136:U:C6	2.59	0.54
17:H:90:A:C4	17:H:91:U:C5	2.95	0.54
19:I:585:ASP:O	19:I:586:GLY:C	2.50	0.54
13:S:11:PRO:O	13:S:29:TRP:NE1	2.40	0.54
14:T:392:PRO:HG3	14:T:415:ILE:HA	1.90	0.54
17:H:59:A:C4	17:H:60:U:C5	2.95	0.54
17:H:153:A:C3'	17:H:154:C:C5'	2.85	0.54
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.90	0.54
2:B:10:U:O2'	2:B:11:U:OP2	2.17	0.54
5:F:29:A:N6	16:G:17:U:OP2	2.39	0.54
6:J:311:GLN:HG3	8:M:131:GLN:HG2	1.90	0.54
7:L:624:PHE:CB	27:q:104:SER:HA	2.38	0.54
16:G:151:C:O2	16:G:152:C:C6	2.61	0.54
18:U:539:GLU:OE2	18:U:662:ILE:HG13	2.07	0.54
1:A:1614:ILE:HD13	1:A:1626:CYS:HB2	1.89	0.54
16:G:147:C:H6	16:G:147:C:OP1	1.90	0.54
17:H:166:G:O6	30:p:88:SER:CB	2.56	0.54
19:I:797:PHE:O	19:I:801:ASP:CB	2.56	0.54
3:C:693:GLU:H	3:C:696:LEU:HD12	1.73	0.54
6:J:466:ARG:CB	19:I:606:TRP:CB	2.86	0.54
17:H:54:U:C2'	17:H:55:U:H5'	2.38	0.54
27:q:22:ASN:CB	27:r:54:ASP:O	2.56	0.54
28:K:131:GLY:O	28:K:135:TRP:CB	2.56	0.54
1:A:658:ARG:NH2	5:F:65:G:OP2	2.41	0.53
2:B:79:C:H2'	2:B:79:C:O2	2.07	0.53
17:H:30:A:C2'	17:H:31:G:OP2	2.56	0.53
16:G:151:C:C3'	16:G:152:C:C6	2.89	0.53
17:H:36:G:O2'	17:H:37:U:C6	2.59	0.53
1:A:761:ILE:HG12	1:A:767:VAL:HG21	1.90	0.53
1:A:1104:ASP:OD1	1:A:1107:ARG:NH2	2.42	0.53
3:C:139:HIS:CD2	3:C:139:HIS:H	2.26	0.53
6:J:239:ARG:HG3	6:J:239:ARG:NH1	2.22	0.53
10:O:78:LYS:HD3	10:O:94:ILE:HG21	1.91	0.53
15:W:474:LYS:CA	15:W:490:ALA:HB3	2.37	0.53
16:G:6:A:C6	16:G:7:G:C5	2.97	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:THR:OG1	2:B:39:C:N4	2.41	0.53
7:L:608:ASN:HA	27:q:112:ALA:HB3	1.84	0.53
9:N:139:CYS:SG	9:N:140:ARG:N	2.81	0.53
15:W:481:MET:O	15:W:483:ASN:N	2.41	0.53
16:G:22:C:H2'	16:G:22:C:O2	2.08	0.53
17:H:182:U:H2'	17:H:183:G:C8	2.44	0.53
18:U:814:VAL:HG11	18:U:820:TYR:HB3	1.90	0.53
1:A:253:ASN:ND2	1:A:336:ASN:OD1	2.42	0.53
17:H:163:G:C6	30:p:50:GLY:CA	2.86	0.53
17:H:170:C:H2'	30:p:44:LYS:CB	2.38	0.53
27:t:72:PRO:CB	28:K:81:LEU:CB	2.87	0.53
1:A:1090:ARG:NH1	1:A:1092:ILE:O	2.41	0.53
1:A:1544:ARG:HB2	1:A:1547:VAL:HG12	1.91	0.53
14:T:371:HIS:ND1	14:T:391:SER:OG	2.40	0.53
15:W:227:GLY:O	15:W:228:LYS:O	2.25	0.53
18:U:539:GLU:OE2	18:U:662:ILE:HG12	2.07	0.53
7:L:608:ASN:HA	27:q:112:ALA:HB2	1.83	0.53
13:S:84:ASP:OD1	13:S:108:ASN:ND2	2.41	0.53
17:H:107:A:H8	17:H:107:A:H5''	1.72	0.53
3:C:148:CYS:SG	3:C:417:ARG:NH2	2.82	0.53
14:T:390:GLY:HA3	14:T:416:ILE:HD11	1.89	0.53
18:U:809:ASP:O	18:U:811:ARG:N	2.42	0.53
2:B:9:G:H5''	2:B:10:U:H5	1.73	0.53
3:C:92:PRO:HA	14:T:278:ASN:HD21	1.74	0.53
3:C:139:HIS:CB	34:C:1500:GTP:O3A	2.57	0.53
3:C:534:VAL:HB	3:C:537:TYR:HB2	1.90	0.53
13:S:41:GLU:OE2	13:S:44:ARG:NH2	2.38	0.53
19:I:249:THR:O	19:I:250:ARG:CB	2.57	0.53
2:B:68:C:O2	2:B:68:C:H2'	2.09	0.52
3:C:134:LEU:HD13	3:C:202:ILE:HG23	1.89	0.52
4:E:75:HIS:ND1	4:E:77:ASN:OD1	2.42	0.52
5:F:29:A:H62	16:G:16:G:H1'	1.74	0.52
10:O:32:PRO:HG2	15:W:153:ILE:HD12	1.91	0.52
12:R:70:ALA:HA	13:S:93:THR:HG21	1.91	0.52
16:G:151:C:C6	16:G:152:C:N4	2.74	0.52
19:I:264:ASP:O	19:I:268:ARG:CB	2.58	0.52
1:A:261:LYS:NZ	3:C:176:GLU:OE2	2.42	0.52
2:B:96:A:N6	2:B:97:G:O6	2.42	0.52
4:E:84:ALA:HB2	4:E:90:ILE:HD13	1.91	0.52
10:O:110:SER:OG	10:O:113:ASN:ND2	2.42	0.52
15:W:491:GLN:O	15:W:492:ASN:C	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:W:536:ASP:O	15:W:540:THR:N	2.41	0.52
1:A:963:GLN:HG3	1:A:1077:ILE:HG23	1.91	0.52
2:B:87:A:C5	23:d:61:ARG:CB	2.92	0.52
10:O:31:ASN:O	12:R:195:ARG:NH1	2.40	0.52
16:G:7:G:H2'	16:G:8:C:C6	2.44	0.52
16:G:22:C:HO2'	16:G:23:U:P	2.31	0.52
16:G:151:C:C2	16:G:152:C:C6	2.96	0.52
17:H:147:G:C2	17:H:148:C:C6	2.97	0.52
1:A:1820:LYS:NZ	1:A:1844:GLU:OE1	2.42	0.52
2:B:9:G:C6	2:B:70:A:N7	2.77	0.52
17:H:40:C:O2'	17:H:41:U:C6	2.59	0.52
17:H:182:U:H2'	17:H:183:G:H8	1.74	0.52
3:C:143:THR:HG23	34:C:1500:GTP:PA	2.48	0.52
7:L:263:ASP:OD2	8:M:199:ARG:NH1	2.37	0.52
16:G:146:C:O2'	16:G:147:C:OP2	2.27	0.52
17:H:67:C:H2'	17:H:68:G:C8	2.42	0.52
16:G:2:U:H2'	16:G:3:A:C4	2.45	0.52
16:G:143:U:N3	17:H:34:U:N3	2.57	0.52
27:r:112:ALA:HB2	28:K:39:GLU:O	2.08	0.52
1:A:532:THR:CB	16:G:3:A:C3'	2.69	0.52
1:A:1320:LYS:HG2	18:U:798:MET:HG2	1.90	0.52
3:C:369:PHE:O	3:C:373:ILE:HB	2.10	0.52
4:E:171:SER:OG	4:E:173:ASP:OD1	2.25	0.52
6:J:774:VAL:CA	6:J:787:LYS:CB	2.86	0.52
7:L:526:ARG:CB	7:L:594:PRO:CB	2.88	0.52
16:G:147:C:N4	16:G:148:U:O4	2.42	0.52
1:A:378:PHE:HB3	3:C:342:ARG:HH11	1.75	0.52
16:G:143:U:N3	17:H:34:U:C2	2.70	0.52
1:A:1555:LEU:HD13	1:A:1556:ASP:H	1.74	0.52
2:B:70:A:N3	2:B:70:A:C5'	2.73	0.52
16:G:140:A:O2'	16:G:141:C:C6	2.61	0.52
17:H:54:U:N3	17:H:93:A:C2	2.77	0.52
17:H:183:G:H2'	17:H:184:C:C6	2.45	0.52
27:t:90:PHE:CB	28:K:111:MET:C	2.83	0.52
2:B:99:C:H2'	2:B:100:C:C6	2.45	0.52
10:O:276:THR:HG23	10:O:279:ALA:H	1.75	0.52
15:W:531:LYS:CA	15:W:546:PHE:O	2.57	0.52
27:r:61:ILE:CB	28:K:138:TYR:CB	2.88	0.52
3:C:158:ARG:C	3:C:159:LYS:CD	2.73	0.51
3:C:203:MET:HG2	3:C:218:GLY:HA3	1.91	0.51
15:W:518:PRO:O	15:W:519:ASP:CB	2.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:38:A:O2'	17:H:39:U:C6	2.59	0.51
27:r:112:ALA:CB	28:K:36:VAL:O	2.58	0.51
1:A:1249:MET:O	1:A:1253:SER:OG	2.22	0.51
3:C:160:ARG:NH1	3:C:160:ARG:CG	2.73	0.51
3:C:507:VAL:HG13	3:C:565:ILE:HG23	1.92	0.51
7:L:21:ALA:HB1	7:L:159:LEU:HD21	1.92	0.51
10:O:169:VAL:HA	15:W:216:LEU:HD13	1.92	0.51
19:I:795:ILE:CD1	19:I:795:ILE:N	2.73	0.51
1:A:82:ARG:HH22	16:G:14:A:H5''	1.74	0.51
3:C:434:CYS:O	3:C:438:ILE:N	2.43	0.51
4:E:266:PRO:HG2	7:L:785:GLN:C	2.35	0.51
6:J:201:ARG:HB3	6:J:203:LEU:HD23	1.91	0.51
16:G:151:C:O2	16:G:152:C:C5	2.63	0.51
17:H:50:C:C6	17:H:50:C:C5'	2.94	0.51
17:H:70:C:C2	17:H:71:C:C5	2.98	0.51
28:K:128:SER:O	28:K:132:CYS:N	2.37	0.51
3:C:476:CYS:HB2	3:C:565:ILE:HB	1.92	0.51
15:W:425:VAL:O	15:W:433:PHE:CB	2.59	0.51
27:q:127:ALA:HB1	27:t:127:ALA:HB1	1.93	0.51
1:A:1190:CYS:O	1:A:1192:PHE:N	2.41	0.51
1:A:1518:LEU:O	1:A:1519:THR:C	2.52	0.51
1:A:1605:GLU:HB3	1:A:1637:TRP:HE1	1.75	0.51
2:B:90:U:O4	26:g:36:PRO:O	2.28	0.51
3:C:137:HIS:ND1	3:C:138:LEU:HB2	2.25	0.51
3:C:160:ARG:HH11	3:C:160:ARG:C	2.18	0.51
5:F:36:A:N6	5:F:38:G:O6	2.44	0.51
12:R:235:ARG:CG	12:R:235:ARG:NH1	2.73	0.51
16:G:148:U:C2	17:H:30:A:N1	2.70	0.51
1:A:103:LEU:HD11	1:A:554:THR:HG22	1.92	0.51
2:B:87:A:N3	2:B:87:A:C3'	2.73	0.51
17:H:67:C:C2'	17:H:68:G:H5'	2.41	0.51
2:B:78:U:H4'	2:B:79:C:OP2	2.10	0.51
4:E:60:MET:HB2	4:E:353:MET:HB2	1.91	0.51
16:G:147:C:P	16:G:147:C:O4'	2.69	0.51
16:G:151:C:H2'	16:G:151:C:O2	2.10	0.51
3:C:115:GLU:HB2	3:C:118:PHE:HB3	1.93	0.51
3:C:849:VAL:HG22	3:C:852:ARG:HH21	1.75	0.51
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.93	0.51
3:C:666:VAL:HG13	3:C:824:THR:HG23	1.92	0.51
12:R:241:GLU:HA	12:R:244:GLU:HG2	1.93	0.51
16:G:133:A:C2'	16:G:134:U:C6	2.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:151:C:C1'	16:G:152:C:C5	2.93	0.51
19:I:729:SER:O	19:I:732:ALA:HB3	2.09	0.51
17:H:68:G:H2'	17:H:69:U:C6	2.46	0.51
19:I:187:LEU:H	32:y:28:PRO:CB	2.23	0.51
1:A:711:GLN:HE22	17:H:18:U:H3'	1.77	0.50
1:A:1217:GLN:HA	1:A:1224:ARG:HA	1.92	0.50
6:J:188:GLN:NE2	7:L:140:ASP:OD1	2.44	0.50
15:W:481:MET:C	15:W:483:ASN:H	2.18	0.50
18:U:819:PRO:HB2	18:U:835:ILE:HB	1.93	0.50
1:A:381:PRO:O	3:C:354:ARG:NH2	2.45	0.50
1:A:1628:ASP:OD2	1:A:1664:ILE:N	2.44	0.50
14:T:468:CYS:HA	14:T:478:LEU:O	2.12	0.50
17:H:180:G:H2'	17:H:181:G:C8	2.45	0.50
16:G:5:G:C6	16:G:6:A:C4	2.99	0.50
17:H:34:U:O2'	17:H:35:A:C4'	2.59	0.50
17:H:165:A:C5	30:p:53:PHE:CB	2.92	0.50
19:I:545:ILE:C	19:I:547:LEU:N	2.51	0.50
1:A:388:LEU:HD11	3:C:399:LEU:HD11	1.94	0.50
1:A:857:ASN:OD1	1:A:860:GLN:NE2	2.44	0.50
3:C:160:ARG:NH1	3:C:160:ARG:HG3	2.26	0.50
3:C:749:THR:HG23	3:C:753:GLU:HB3	1.93	0.50
7:L:696:LEU:HA	28:K:110:SER:CB	2.40	0.50
14:T:200:ILE:HB	14:T:486:ILE:HB	1.93	0.50
19:I:795:ILE:N	19:I:795:ILE:HD12	2.26	0.50
12:R:235:ARG:HB2	12:R:235:ARG:CZ	2.40	0.50
17:H:111:G:O3'	17:H:112:G:O4'	2.28	0.50
1:A:136:ILE:HG22	1:A:138:PRO:HD2	1.93	0.50
1:A:1467:LEU:HD11	18:U:796:TRP:HH2	1.77	0.50
2:B:90:U:C4	26:g:36:PRO:O	2.64	0.50
3:C:641:MET:HE2	3:C:645:ARG:HH12	1.75	0.50
6:J:615:LEU:CB	6:J:638:GLU:CB	2.89	0.50
7:L:751:THR:O	7:L:755:LEU:N	2.38	0.50
10:O:259:ARG:HE	10:O:275:ALA:HA	1.77	0.50
15:W:430:ASN:O	15:W:447:TRP:CB	2.60	0.50
16:G:148:U:O2	17:H:30:A:C2	2.64	0.50
17:H:32:U:C2	17:H:33:G:C5	2.99	0.50
3:C:165:LEU:HD21	34:C:1500:GTP:O2A	2.12	0.50
3:C:260:ILE:HG13	3:C:311:SER:HB2	1.93	0.50
4:E:136:TRP:CD1	4:E:143:ARG:HA	2.46	0.50
1:A:1405:LEU:HD12	1:A:1408:LEU:HD23	1.94	0.50
3:C:699:ASP:OD2	3:C:722:TYR:OH	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:55:LEU:CD1	4:E:55:LEU:N	2.73	0.50
16:G:5:G:N1	16:G:6:A:C5	2.80	0.50
16:G:151:C:N1	16:G:152:C:H5	2.05	0.50
17:H:93:A:C2'	17:H:94:A:H5'	2.42	0.50
19:I:218:TYR:CB	19:I:223:GLU:CB	2.90	0.50
3:C:143:THR:HG22	34:C:1500:GTP:PB	2.52	0.50
3:C:673:LYS:HG3	3:C:686:THR:HG23	1.93	0.50
25:e:15:VAL:O	26:g:33:GLY:HA3	2.12	0.50
4:E:311:VAL:HB	4:E:321:TYR:HB2	1.93	0.49
6:J:239:ARG:HH11	6:J:239:ARG:HG3	1.77	0.49
17:H:106:G:H1'	17:H:107:A:C8	2.47	0.49
1:A:309:ARG:HE	1:A:310:THR:H	1.60	0.49
1:A:1782:ASP:HB3	1:A:1841:THR:HG21	1.93	0.49
3:C:117:ASP:OD2	20:a:79:ASN:CB	2.60	0.49
1:A:641:MET:HA	1:A:644:ILE:HG22	1.93	0.49
1:A:825:ILE:HA	1:A:933:ARG:HH12	1.78	0.49
1:A:1663:ASP:HB3	1:A:1702:LEU:HB2	1.93	0.49
1:A:1863:VAL:HG11	1:A:1868:MET:HB2	1.93	0.49
6:J:290:ARG:NH1	8:M:180:ASP:OD1	2.40	0.49
17:H:93:A:H2'	17:H:94:A:H5'	1.94	0.49
17:H:149:A:H2'	17:H:150:U:C6	2.47	0.49
1:A:552:ARG:NH1	1:A:589:THR:O	2.45	0.49
1:A:1430:LEU:HD21	1:A:1459:ARG:HE	1.78	0.49
1:A:1518:LEU:HD13	1:A:1518:LEU:N	2.27	0.49
12:R:252:SER:OG	12:R:255:LYS:O	2.30	0.49
18:U:691:ALA:HB3	18:U:698:LEU:H	1.78	0.49
1:A:1131:LYS:O	1:A:1139:ARG:NH1	2.45	0.49
1:A:1231:ARG:NH2	1:A:1283:GLU:OE1	2.45	0.49
2:B:79:C:C6	2:B:79:C:C5'	2.95	0.49
16:G:144:A:H4'	16:G:145:U:H2'	1.95	0.49
19:I:320:GLU:O	19:I:324:ASP:CB	2.60	0.49
1:A:820:ARG:NH1	1:A:1063:GLY:O	2.43	0.49
1:A:1781:ASP:HB3	1:A:1808:PHE:HB3	1.94	0.49
14:T:287:HIS:NE2	14:T:305:THR:OG1	2.40	0.49
15:W:155:SER:OG	15:W:158:GLU:OE1	2.29	0.49
15:W:290:GLY:HA2	15:W:573:GLY:HA2	1.94	0.49
16:G:125:C:O2'	16:G:126:C:C2'	2.61	0.49
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.94	0.49
1:A:1337:GLN:O	1:A:1341:ARG:NH2	2.46	0.49
5:F:41:A:C6	16:G:7:G:C2	2.99	0.49
17:H:168:A:H3'	17:H:169:C:H6	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:591:LEU:O	6:J:593:ARG:N	2.44	0.49
7:L:784:LEU:CB	28:K:195:ILE:CB	2.90	0.49
1:A:978:GLU:OE2	1:A:1188:ASN:N	2.45	0.49
15:W:144:ASP:OD1	15:W:144:ASP:N	2.44	0.49
1:A:1511:GLU:OE2	18:U:761:LYS:NZ	2.36	0.49
2:B:87:A:N3	2:B:87:A:C2'	2.75	0.49
9:N:70:ILE:HG12	9:N:74:LEU:HD23	1.95	0.49
12:R:107:SER:OG	12:R:109:ASP:OD1	2.28	0.49
17:H:93:A:O2'	17:H:94:A:H5'	2.13	0.49
1:A:271:MET:HE1	1:A:311:GLU:HA	1.95	0.48
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.46	0.48
4:E:61:LEU:HD13	4:E:352:TYR:CE1	2.43	0.48
19:I:326:ASP:O	19:I:329:LEU:CB	2.60	0.48
1:A:529:THR:OG1	18:U:581:THR:OG1	2.22	0.48
16:G:148:U:O2	17:H:30:A:H2	1.95	0.48
16:G:151:C:C1'	16:G:152:C:H5	2.25	0.48
18:U:579:VAL:HG22	18:U:646:GLU:HB2	1.94	0.48
3:C:139:HIS:HB2	34:C:1500:GTP:O3A	2.13	0.48
3:C:183:SER:HB2	3:C:214:GLU:HB3	1.94	0.48
18:U:663:ALA:HA	18:U:666:ARG:HH12	1.76	0.48
18:U:666:ARG:NH1	18:U:666:ARG:HB2	2.28	0.48
19:I:485:LYS:O	19:I:486:VAL:CG1	2.53	0.48
25:l:15:VAL:O	26:n:33:GLY:HA3	2.12	0.48
1:A:741:ARG:NH2	14:T:463:SER:O	2.47	0.48
1:A:1639:VAL:HG12	1:A:1719:PHE:HB3	1.94	0.48
2:B:70:A:H2	2:B:70:A:OP2	1.97	0.48
2:B:96:A:C2	2:B:97:G:C4	3.02	0.48
17:H:104:U:H4'	17:H:105:G:H5''	1.95	0.48
3:C:159:LYS:N	3:C:159:LYS:CD	2.74	0.48
3:C:814:ARG:NH1	3:C:818:SER:OG	2.46	0.48
17:H:51:A:H8	17:H:51:A:OP2	1.96	0.48
18:U:752:ILE:HD12	18:U:773:LEU:HD21	1.94	0.48
1:A:940:ILE:HD12	1:A:1090:ARG:HH21	1.78	0.48
1:A:1501:LEU:HD13	1:A:1753:LEU:HD11	1.96	0.48
1:A:1522:GLN:NE2	18:U:622:ALA:O	2.47	0.48
1:A:1957:ASP:HB3	1:A:1960:THR:HG23	1.96	0.48
3:C:700:ILE:O	3:C:740:THR:OG1	2.32	0.48
15:W:528:GLY:O	15:W:552:VAL:CB	2.62	0.48
17:H:181:G:H2'	17:H:182:U:C6	2.49	0.48
18:U:713:ILE:HB	18:U:768:TYR:HB3	1.95	0.48
3:C:737:PRO:HB3	3:C:775:ARG:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:41:A:C6	16:G:6:A:N1	2.81	0.48
10:O:136:MET:O	10:O:140:ALA:HB2	2.13	0.48
10:O:245:GLU:HG2	10:O:248:LEU:HD12	1.95	0.48
14:T:223:SER:OG	14:T:224:ALA:N	2.47	0.48
3:C:501:ILE:O	3:C:543:ARG:HA	2.14	0.48
14:T:343:PRO:HG2	14:T:356:LEU:HD23	1.95	0.48
17:H:34:U:C2'	17:H:35:A:N9	2.76	0.48
1:A:855:ARG:HH12	1:A:1518:LEU:HD11	1.78	0.48
3:C:641:MET:HE3	3:C:655:VAL:HG21	1.96	0.48
7:L:73:HIS:O	7:L:77:LEU:HB2	2.13	0.48
17:H:77:C:H2'	17:H:78:C:C6	2.49	0.48
1:A:1597:PHE:HB3	1:A:1609:VAL:HG11	1.96	0.48
1:A:1784:ASN:HD21	1:A:1894:GLN:HG2	1.78	0.48
3:C:826:ARG:HA	3:C:911:PRO:HG3	1.96	0.48
18:U:657:GLN:O	18:U:661:ALA:HB3	2.14	0.48
3:C:150:ILE:HD13	3:C:167:TYR:HD2	1.79	0.47
16:G:141:C:OP2	16:G:141:C:H2'	2.14	0.47
17:H:34:U:O2'	17:H:35:A:H5'	2.14	0.47
17:H:54:U:O4	17:H:93:A:N1	2.46	0.47
19:I:520:ILE:O	19:I:524:TYR:CA	2.61	0.47
1:A:136:ILE:HG12	1:A:418:THR:HG22	1.97	0.47
1:A:579:GLN:HG3	1:A:629:PHE:H	1.79	0.47
1:A:1214:TRP:NE1	1:A:1276:GLU:OE2	2.34	0.47
1:A:1577:PHE:HD1	1:A:1581:LEU:HB3	1.79	0.47
3:C:258:ASN:OD1	3:C:259:LYS:N	2.44	0.47
14:T:224:ALA:HA	14:T:248:THR:HG23	1.94	0.47
17:H:67:C:O2'	17:H:68:G:H5'	2.13	0.47
2:B:72:U:H3'	2:B:72:U:H6	1.78	0.47
12:R:52:PRO:HG3	12:R:67:ILE:HG21	1.97	0.47
17:H:104:U:H4'	17:H:105:G:C5'	2.44	0.47
18:U:741:VAL:HG11	18:U:827:LEU:HG	1.96	0.47
3:C:160:ARG:NH1	3:C:160:ARG:C	2.73	0.47
10:O:245:GLU:HG3	10:O:263:VAL:HG21	1.95	0.47
1:A:995:ARG:HG3	12:R:291:LEU:HD13	1.97	0.47
1:A:1636:LYS:HB2	1:A:1655:THR:HB	1.95	0.47
17:H:148:C:O2'	17:H:149:A:H5'	2.13	0.47
1:A:516:LEU:HD11	1:A:538:SER:HB2	1.97	0.47
6:J:197:GLU:OE1	7:L:156:ARG:NE	2.46	0.47
8:M:235:GLN:HB3	8:M:239:ARG:HH21	1.79	0.47
12:R:238:THR:HB	12:R:241:GLU:HG2	1.96	0.47
14:T:216:ASN:HD21	14:T:471:ASP:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:G:6:A:C5	16:G:7:G:C8	3.02	0.47
2:B:11:U:C6	2:B:11:U:C4'	2.97	0.47
3:C:829:GLU:HB2	3:C:907:VAL:HG22	1.97	0.47
17:H:50:C:C6	17:H:50:C:C3'	2.97	0.47
27:r:109:GLN:HA	28:K:40:THR:CB	2.45	0.47
27:r:127:ALA:O	27:s:127:ALA:HB1	2.13	0.47
1:A:1237:MET:HG2	1:A:1284:LEU:HD23	1.95	0.47
1:A:1899:VAL:HB	1:A:1902:PHE:HD2	1.80	0.47
2:B:77:G:C6	2:B:80:U:C5	3.03	0.47
2:B:88:A:C4	25:e:53:TYR:CB	2.97	0.47
3:C:137:HIS:CE1	3:C:138:LEU:HB2	2.50	0.47
3:C:349:PHE:HZ	3:C:354:ARG:HE	1.63	0.47
7:L:12:ARG:HH12	7:L:40:ARG:HH11	1.63	0.47
8:M:134:GLN:HG2	8:M:137:ARG:HH21	1.79	0.47
10:O:131:THR:O	15:W:108:ARG:NH1	2.37	0.47
12:R:60:ASP:HB2	13:S:134:GLN:HA	1.96	0.47
16:G:1:G:H5'	16:G:144:A:H1'	1.95	0.47
17:H:71:C:H2'	17:H:72:U:C6	2.50	0.47
1:A:32:GLU:OE1	1:A:35:ARG:NH1	2.48	0.47
1:A:532:THR:CB	16:G:3:A:C4'	2.93	0.47
14:T:398:TRP:CD1	14:T:405:PHE:HA	2.50	0.47
16:G:147:C:OP1	16:G:147:C:C6	2.67	0.47
17:H:69:U:H6	17:H:69:U:O5'	1.97	0.47
19:I:289:VAL:O	19:I:292:PHE:CB	2.63	0.47
19:I:326:ASP:O	19:I:329:LEU:N	2.48	0.47
1:A:723:ASN:ND2	1:A:788:GLN:OE1	2.48	0.47
12:R:119:LEU:HD21	12:R:230:MET:HB3	1.97	0.47
13:S:55:ARG:HB3	13:S:63:GLN:HB3	1.96	0.47
13:S:90:LEU:HB3	13:S:128:ILE:HD12	1.97	0.47
17:H:10:C:H2'	17:H:11:G:H8	1.80	0.47
1:A:1745:GLU:O	1:A:1749:LYS:HB2	2.15	0.46
17:H:147:G:N3	17:H:148:C:C6	2.84	0.46
17:H:164:C:O2	30:p:84:ALA:CB	2.63	0.46
2:B:78:U:O2'	2:B:79:C:OP1	2.28	0.46
6:J:224:LYS:NZ	6:J:257:GLU:OE2	2.42	0.46
6:J:774:VAL:HA	6:J:787:LYS:CB	2.45	0.46
7:L:209:ASP:HB2	10:O:113:ASN:HD21	1.80	0.46
8:M:207:ASP:N	8:M:207:ASP:OD1	2.48	0.46
14:T:213:GLU:HG3	14:T:218:TRP:CE2	2.50	0.46
17:H:51:A:N3	17:H:51:A:H2'	2.30	0.46
17:H:55:U:H2'	17:H:56:A:C8	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:659:LYS:O	18:U:663:ALA:CB	2.63	0.46
1:A:256:TYR:HE1	1:A:332:TYR:HB2	1.80	0.46
3:C:80:ILE:HG22	3:C:82:GLN:HG2	1.97	0.46
6:J:391:TYR:HB3	6:J:394:HIS:HB2	1.96	0.46
6:J:669:GLN:C	6:J:671:ARG:N	2.74	0.46
17:H:90:A:H2'	17:H:91:U:C6	2.50	0.46
19:I:712:VAL:O	19:I:713:ARG:C	2.57	0.46
1:A:1676:ILE:HD13	1:A:1706:ASP:HB2	1.96	0.46
5:F:39:A:C2'	5:F:40:U:H5'	2.45	0.46
5:F:43:A:O5'	5:F:43:A:C8	2.69	0.46
14:T:416:ILE:HA	14:T:431:ALA:HA	1.97	0.46
16:G:148:U:C2	17:H:30:A:C2	3.04	0.46
17:H:81:G:H2'	17:H:82:G:H8	1.81	0.46
17:H:88:A:H2'	17:H:89:U:C6	2.50	0.46
17:H:164:C:OP2	17:H:164:C:H6	1.99	0.46
18:U:537:GLY:HA3	18:U:548:LEU:HD12	1.95	0.46
18:U:673:GLU:O	18:U:682:SER:OG	2.26	0.46
1:A:1481:VAL:HG11	1:A:1498:TRP:CD2	2.51	0.46
2:B:29:A:H2'	2:B:30:A:H8	1.80	0.46
4:E:217:ILE:HB	4:E:231:MET:HB2	1.97	0.46
4:E:257:ASN:OD1	4:E:282:HIS:N	2.48	0.46
16:G:4:A:C2	16:G:5:G:C2	3.04	0.46
17:H:80:A:H2'	17:H:81:G:H8	1.81	0.46
1:A:1128:TYR:OH	1:A:1140:MET:SD	2.73	0.46
3:C:221:ILE:O	3:C:495:ARG:NH1	2.49	0.46
10:O:237:GLY:O	10:O:299:ASN:HB3	2.15	0.46
13:S:160:ILE:HG22	13:S:161:LYS:HG3	1.98	0.46
15:W:516:PHE:HA	15:W:522:TYR:O	2.16	0.46
19:I:521:VAL:O	19:I:527:PHE:N	2.48	0.46
4:E:56:GLN:HB3	4:E:57:ALA:H	1.47	0.46
4:E:266:PRO:HG2	7:L:785:GLN:O	2.16	0.46
10:O:255:PHE:O	12:R:78:ARG:NH1	2.48	0.46
12:R:151:LEU:HD22	14:T:323:VAL:HG11	1.96	0.46
16:G:5:G:C5	16:G:6:A:N9	2.84	0.46
17:H:78:C:H2'	17:H:79:G:H8	1.81	0.46
17:H:92:U:C2'	17:H:93:A:C8	2.85	0.46
17:H:114:A:H2'	17:H:115:G:H8	1.81	0.46
1:A:852:VAL:HG11	1:A:1449:LYS:HZ2	1.81	0.46
1:A:1163:ARG:HH12	11:P:201:VAL:HG11	1.81	0.46
2:B:11:U:C6	2:B:11:U:C3'	2.99	0.46
3:C:191:PRO:HA	3:C:197:SER:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:850:LEU:HD23	3:C:855:GLY:HA3	1.97	0.46
10:O:90:TYR:HB3	10:O:92:LEU:HD13	1.98	0.46
17:H:108:G:O5'	17:H:108:G:H8	1.99	0.46
4:E:56:GLN:HG2	4:E:97:GLY:O	2.16	0.46
16:G:5:G:C2	16:G:6:A:C5	3.04	0.46
1:A:1198:PRO:HA	1:A:1226:ALA:HA	1.98	0.46
1:A:1699:THR:HA	1:A:1717:ASN:HD22	1.81	0.46
1:A:1946:ASN:ND2	1:A:1990:ASP:OD2	2.46	0.46
17:H:148:C:H2'	17:H:149:A:H5'	1.98	0.46
19:I:712:VAL:O	19:I:715:GLY:N	2.49	0.46
27:q:71:ILE:CB	27:r:81:GLU:CA	2.94	0.46
1:A:762:ARG:HH12	11:P:226:LYS:HZ1	1.63	0.45
1:A:941:LYS:HA	1:A:941:LYS:HD2	1.72	0.45
2:B:92:U:C2	22:c:35:SER:CB	3.00	0.45
4:E:135:VAL:HB	4:E:145:LYS:HB3	1.97	0.45
5:F:41:A:C2'	5:F:42:C:H5'	2.46	0.45
8:M:135:TYR:O	8:M:139:THR:OG1	2.27	0.45
15:W:476:LEU:O	15:W:487:ILE:HA	2.17	0.45
16:G:23:U:C6	16:G:23:U:H5''	2.51	0.45
16:G:27:U:HO2'	16:G:28:A:C4'	2.29	0.45
16:G:133:A:N6	17:H:43:U:C4	2.79	0.45
17:H:82:G:H2'	17:H:83:A:H8	1.81	0.45
19:I:255:LEU:O	19:I:256:GLY:C	2.59	0.45
1:A:106:MET:HE1	1:A:582:PHE:HZ	1.82	0.45
2:B:74:U:C4	2:B:76:A:C6	3.04	0.45
3:C:85:ASP:OD1	3:C:85:ASP:N	2.47	0.45
4:E:251:LEU:HD21	4:E:300:ILE:HG23	1.97	0.45
7:L:74:LEU:HA	7:L:77:LEU:HB3	1.97	0.45
10:O:175:ARG:HB2	10:O:179:CYS:HB2	1.98	0.45
17:H:74:U:H2'	17:H:75:A:H8	1.81	0.45
1:A:787:GLU:OE2	1:A:790:ARG:NH2	2.44	0.45
3:C:82:GLN:HE21	14:T:238:LEU:H	1.64	0.45
16:G:145:U:C5	16:G:146:C:C5	3.04	0.45
27:t:90:PHE:CB	28:K:111:MET:CB	2.94	0.45
1:A:339:PHE:HE1	1:A:402:ILE:HG22	1.82	0.45
2:B:66:A:H2'	2:B:67:A:C1'	2.46	0.45
3:C:160:ARG:HH11	3:C:160:ARG:HB2	1.81	0.45
3:C:162:ASP:OD1	3:C:162:ASP:N	2.48	0.45
3:C:440:SER:O	3:C:442:LYS:N	2.46	0.45
7:L:16:ASP:OD2	7:L:49:ARG:NH2	2.39	0.45
17:H:73:C:H2'	17:H:74:U:C6	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1201:ARG:HG3	1:A:1202:THR:H	1.82	0.45
3:C:142:LYS:HE2	3:C:142:LYS:HB2	1.67	0.45
3:C:383:GLN:HA	3:C:387:ASP:HB2	1.98	0.45
3:C:670:SER:HB2	3:C:689:ALA:H	1.82	0.45
17:H:89:U:H2'	17:H:90:A:H8	1.82	0.45
17:H:107:A:H5''	17:H:107:A:C8	2.50	0.45
1:A:668:VAL:HB	5:F:68:C:H5''	1.99	0.45
1:A:1807:ILE:HB	1:A:1820:LYS:HB3	1.98	0.45
2:B:93:U:H4'	2:B:94:U:H5''	1.99	0.45
2:B:96:A:N1	2:B:97:G:C5	2.84	0.45
3:C:595:VAL:HG22	3:C:654:LYS:HG3	1.99	0.45
16:G:7:G:H2'	16:G:8:C:H6	1.80	0.45
18:U:546:VAL:HG11	18:U:665:HIS:ND1	2.31	0.45
19:I:277:ASP:O	19:I:280:GLU:CB	2.64	0.45
29:o:61:PRO:O	29:o:86:ALA:HB1	2.16	0.45
1:A:1296:GLN:NE2	1:A:1317:TYR:OH	2.50	0.45
10:O:152:ARG:HH12	16:G:22:C:H41	1.65	0.45
11:P:3:THR:O	11:P:6:ARG:NE	2.43	0.45
17:H:58:U:O4	17:H:90:A:N1	2.50	0.45
17:H:113:G:H2'	17:H:114:A:H8	1.82	0.45
1:A:1011:ALA:HB2	7:L:80:THR:HB	1.98	0.45
1:A:1701:VAL:HA	1:A:1716:GLY:HA3	1.99	0.45
2:B:70:A:OP2	2:B:70:A:C2	2.70	0.45
3:C:94:ILE:H	3:C:94:ILE:HG13	1.44	0.45
3:C:157:ILE:O	3:C:159:LYS:HD3	2.17	0.45
3:C:556:ASP:OD1	3:C:556:ASP:N	2.49	0.45
6:J:322:MET:O	8:M:181:ARG:NH1	2.48	0.45
12:R:62:GLY:HA2	13:S:96:GLY:HA3	1.99	0.45
13:S:99:ALA:HA	13:S:129:PHE:H	1.81	0.45
1:A:1892:PRO:HD3	1:A:1941:ARG:HH21	1.81	0.45
3:C:139:HIS:CB	34:C:1500:GTP:H5''	2.33	0.45
5:F:9:U:O2	5:F:10:U:N3	2.50	0.45
7:L:699:ASN:CB	28:K:114:LEU:CB	2.95	0.45
15:W:466:ALA:HB2	15:W:512:CYS:O	2.17	0.45
16:G:2:U:H2'	16:G:3:A:N3	2.32	0.45
2:B:66:A:C3'	2:B:67:A:O4'	2.65	0.45
3:C:770:PHE:HE1	3:C:789:PHE:HD2	1.64	0.45
16:G:144:A:H4'	16:G:145:U:C3'	2.46	0.45
1:A:435:CYS:SG	1:A:439:GLN:NE2	2.67	0.44
2:B:11:U:C6	2:B:11:U:C5'	2.85	0.44
3:C:144:CYS:HA	3:C:165:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:619:THR:HG22	3:C:629:ILE:HG13	1.99	0.44
4:E:149:GLY:O	4:E:177:LYS:NZ	2.50	0.44
9:N:119:CYS:SG	9:N:139:CYS:HB3	2.57	0.44
10:O:83:THR:O	16:G:18:A:O2'	2.32	0.44
17:H:83:A:H2'	17:H:84:C:C6	2.49	0.44
18:U:655:GLU:O	18:U:659:LYS:HB3	2.16	0.44
18:U:805:LEU:HD11	18:U:832:ALA:HB2	1.99	0.44
1:A:126:ILE:HG21	12:R:207:MET:HE2	1.98	0.44
2:B:8:G:N3	2:B:8:G:C2'	2.73	0.44
4:E:300:ILE:O	4:E:311:VAL:HA	2.18	0.44
17:H:34:U:C6	17:H:34:U:OP2	2.70	0.44
1:A:1426:ASP:OD1	1:A:1426:ASP:N	2.49	0.44
6:J:600:ILE:C	6:J:602:LYS:N	2.74	0.44
8:M:165:ASN:HB3	12:R:96:ILE:H	1.82	0.44
15:W:266:ARG:O	15:W:267:SER:O	2.35	0.44
17:H:50:C:H2'	17:H:51:A:C1'	2.48	0.44
17:H:51:A:C8	17:H:51:A:OP2	2.70	0.44
1:A:675:GLN:HG3	1:A:676:ARG:HD3	1.99	0.44
1:A:1831:LYS:HD2	1:A:1831:LYS:HA	1.76	0.44
4:E:61:LEU:HD13	4:E:352:TYR:OH	2.15	0.44
4:E:307:ARG:HH11	15:W:143:LEU:HD12	1.83	0.44
5:F:58:G:H2'	5:F:59:G:C8	2.52	0.44
9:N:70:ILE:HG23	9:N:74:LEU:HB3	1.98	0.44
10:O:174:LYS:HA	15:W:205:VAL:HG22	2.00	0.44
16:G:149:G:OP2	16:G:149:G:C8	2.70	0.44
17:H:79:G:H2'	17:H:80:A:H8	1.81	0.44
19:I:368:GLN:OE1	19:I:368:GLN:HA	2.18	0.44
4:E:92:LEU:HB2	4:E:103:ALA:HB3	1.99	0.44
5:F:44:G:OP2	5:F:44:G:C8	2.70	0.44
17:H:58:U:H2'	17:H:59:A:H8	1.82	0.44
17:H:84:C:H2'	17:H:85:A:H8	1.82	0.44
17:H:109:C:C5	17:H:109:C:OP2	2.71	0.44
17:H:166:G:O6	30:p:88:SER:CA	2.66	0.44
1:A:139:VAL:HG11	1:A:212:PRO:HG2	1.99	0.44
1:A:671:THR:O	1:A:676:ARG:NH2	2.50	0.44
1:A:1426:ASP:HB2	1:A:1429:THR:HG22	1.98	0.44
3:C:614:TYR:HA	3:C:615:PRO:HD3	1.87	0.44
8:M:221:LYS:HE3	12:R:249:PRO:HB3	1.98	0.44
16:G:141:C:H2'	16:G:141:C:O5'	2.18	0.44
19:I:253:ASP:O	19:I:254:GLN:CB	2.64	0.44
1:A:179:ALA:HA	1:A:183:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1754:TYR:OH	18:U:553:GLN:OE1	2.35	0.44
3:C:144:CYS:CB	3:C:165:LEU:CD1	2.89	0.44
4:E:90:ILE:HG13	4:E:136:TRP:CZ3	2.53	0.44
10:O:64:ARG:HD2	10:O:163:HIS:CE1	2.53	0.44
17:H:56:A:H2'	17:H:57:A:H8	1.82	0.44
17:H:57:A:H2'	17:H:58:U:C6	2.50	0.44
17:H:154:C:O2'	17:H:155:C:C5'	2.66	0.44
17:H:163:G:N1	30:p:49:ARG:O	2.51	0.44
18:U:546:VAL:HG11	18:U:665:HIS:HE1	1.75	0.44
19:I:251:PHE:CB	19:I:254:GLN:CB	2.95	0.44
1:A:1110:ILE:HD11	1:A:1149:LEU:HB2	2.00	0.44
3:C:122:LEU:HD22	3:C:128:LEU:HD12	1.98	0.44
3:C:300:LEU:HA	3:C:306:ASN:HD21	1.83	0.44
4:E:241:LEU:HD22	4:E:250:LEU:HD21	2.00	0.44
11:P:23:LEU:HD23	11:P:26:LEU:HD13	2.00	0.44
16:G:5:G:C4	16:G:6:A:H8	2.31	0.44
17:H:168:A:N3	17:H:168:A:H2'	2.33	0.44
1:A:348:PRO:HG2	1:A:351:TYR:HB3	1.99	0.44
1:A:517:HIS:CD2	18:U:585:ARG:HD3	2.53	0.44
1:A:1779:PHE:O	1:A:1809:ILE:HA	2.18	0.44
2:B:77:G:O6	2:B:80:U:C5	2.71	0.44
3:C:705:VAL:HG22	3:C:717:PHE:HE2	1.83	0.44
4:E:294:SER:HB3	4:E:299:LYS:HB2	2.00	0.44
7:L:703:MET:O	7:L:707:ALA:HB3	2.18	0.44
14:T:406:ILE:HG22	14:T:407:GLN:HB2	2.00	0.44
15:W:309:MET:HA	15:W:334:ALA:HB1	1.99	0.44
16:G:153:C:O5'	16:G:153:C:C6	2.70	0.44
1:A:266:SER:OG	1:A:271:MET:O	2.32	0.43
2:B:11:U:O2'	2:B:12:U:H5'	2.18	0.43
2:B:77:G:C6	2:B:80:U:H5	2.35	0.43
10:O:59:PRO:HB2	10:O:63:MET:HG3	1.99	0.43
12:R:97:LYS:NZ	13:S:146:GLU:OE1	2.50	0.43
16:G:146:C:C2'	16:G:147:C:OP1	2.66	0.43
1:A:1365:ILE:HA	1:A:1366:PRO:HD3	1.82	0.43
3:C:561:LYS:NZ	3:C:611:ASN:OD1	2.36	0.43
3:C:692:LEU:HD12	3:C:696:LEU:HB3	1.99	0.43
4:E:82:ALA:HA	4:E:91:LEU:O	2.19	0.43
9:N:128:VAL:HG13	9:N:130:ARG:H	1.82	0.43
10:O:213:LEU:CD1	16:G:21:A:H2'	2.48	0.43
15:W:162:ASN:HB3	15:W:165:LEU:HD22	2.00	0.43
17:H:59:A:H2'	17:H:60:U:C6	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:72:U:H2'	17:H:73:C:C6	2.50	0.43
17:H:162:U:N1	30:p:13:ASN:HA	2.31	0.43
1:A:1196:ILE:HA	1:A:1227:GLN:O	2.18	0.43
1:A:1595:GLN:HA	1:A:1598:ASP:HB2	2.01	0.43
3:C:925:PRO:HB2	3:C:927:PRO:HD2	1.99	0.43
4:E:284:PHE:HZ	15:W:120:ILE:HD13	1.83	0.43
4:E:294:SER:OG	4:E:298:SER:N	2.51	0.43
15:W:426:PHE:HA	15:W:433:PHE:HA	1.99	0.43
16:G:134:U:O2'	16:G:135:G:C8	2.66	0.43
16:G:153:C:H3'	16:G:153:C:H6	1.83	0.43
1:A:178:TYR:OH	1:A:488:ASP:OD2	2.32	0.43
1:A:923:ASP:OD2	1:A:1439:ARG:NE	2.49	0.43
1:A:1622:MET:O	1:A:1687:TYR:OH	2.35	0.43
3:C:223:ASP:HA	3:C:251:LEU:HD22	2.00	0.43
6:J:196:ARG:HA	8:M:208:ILE:HD11	2.00	0.43
6:J:496:ASP:CB	6:J:535:TYR:CA	2.95	0.43
14:T:306:CYS:SG	14:T:336:VAL:HB	2.58	0.43
17:H:157:G:H5''	17:H:157:G:C8	2.50	0.43
1:A:793:ASN:HD22	3:C:60:HIS:CE1	2.37	0.43
15:W:381:PHE:O	15:W:382:ASN:C	2.60	0.43
16:G:27:U:HO2'	16:G:28:A:C5'	2.28	0.43
17:H:165:A:O2'	30:p:41:VAL:C	2.62	0.43
17:H:178:A:N3	17:H:178:A:H2'	2.33	0.43
1:A:494:LEU:HD21	1:A:562:VAL:HG21	2.00	0.43
1:A:856:LEU:HD23	1:A:860:GLN:HB3	2.00	0.43
1:A:1745:GLU:OE2	1:A:1748:ARG:NH1	2.51	0.43
2:B:71:C:C3'	2:B:71:C:C6	3.01	0.43
16:G:141:C:OP2	16:G:141:C:C6	2.70	0.43
17:H:45:C:O2'	17:H:46:U:O5'	2.33	0.43
17:H:50:C:C6	17:H:50:C:C4'	3.02	0.43
18:U:680:ASP:OD1	18:U:680:ASP:N	2.44	0.43
3:C:590:ILE:HG22	3:C:592:VAL:HG23	2.01	0.43
3:C:707:ILE:H	3:C:707:ILE:HG13	1.67	0.43
13:S:122:LEU:O	13:S:126:HIS:N	2.52	0.43
15:W:458:GLU:O	15:W:459:PRO:C	2.58	0.43
15:W:517:SER:O	15:W:518:PRO:C	2.61	0.43
17:H:157:G:H2'	17:H:158:G:O4'	2.19	0.43
28:K:134:ALA:O	28:K:136:LYS:N	2.52	0.43
1:A:180:ASP:OD1	1:A:180:ASP:N	2.49	0.43
1:A:828:PRO:HA	1:A:829:PRO:HD3	1.82	0.43
3:C:495:ARG:HB3	3:C:549:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:843:VAL:HG13	3:C:871:ILE:HD11	2.00	0.43
11:P:17:GLY:N	11:P:20:GLU:OE1	2.48	0.43
17:H:91:U:H2'	17:H:92:U:C6	2.50	0.43
19:I:526:MET:HE2	19:I:528:LEU:H	1.82	0.43
2:B:11:U:H6	2:B:11:U:C4'	2.32	0.43
3:C:259:LYS:HG2	34:C:1500:GTP:C2	2.54	0.43
3:C:592:VAL:HG22	3:C:655:VAL:HG22	2.00	0.43
5:F:41:A:N6	5:F:42:C:N4	2.66	0.43
10:O:234:LEU:O	10:O:271:PHE:HA	2.19	0.43
12:R:178:ARG:NH1	15:W:141:PRO:O	2.52	0.43
13:S:25:LEU:HD23	13:S:132:VAL:HG12	2.00	0.43
15:W:474:LYS:C	15:W:490:ALA:HB2	2.44	0.43
16:G:22:C:C2'	16:G:23:U:O5'	2.66	0.43
17:H:37:U:O2'	17:H:38:A:C8	2.67	0.43
17:H:168:A:H3'	17:H:169:C:C6	2.53	0.43
2:B:46:U:O4	2:B:47:A:N6	2.46	0.43
3:C:453:TYR:HD2	3:C:456:GLY:H	1.67	0.43
3:C:829:GLU:OE2	3:C:854:ARG:NH2	2.52	0.43
6:J:194:LEU:HD21	7:L:152:LEU:HD22	2.01	0.43
16:G:21:A:H3'	16:G:21:A:H8	1.84	0.43
17:H:98:G:H5'	17:H:104:U:OP2	2.19	0.43
1:A:1516:LYS:HB3	1:A:1516:LYS:HE2	1.57	0.42
4:E:75:HIS:HD1	4:E:77:ASN:H	1.66	0.42
4:E:258:THR:HG21	4:E:260:ARG:HH21	1.84	0.42
6:J:343:GLU:HG2	6:J:347:HIS:CD2	2.54	0.42
13:S:152:ARG:HH22	15:W:74:PRO:HG2	1.84	0.42
15:W:571:TRP:O	15:W:573:GLY:N	2.52	0.42
16:G:6:A:N1	16:G:7:G:C4	2.87	0.42
19:I:545:ILE:O	19:I:548:PHE:N	2.51	0.42
1:A:1272:THR:HA	1:A:1275:ARG:HD3	2.00	0.42
16:G:137:C:O2'	16:G:138:A:C8	2.67	0.42
16:G:140:A:O2'	16:G:141:C:C5	2.72	0.42
19:I:790:ARG:CB	19:I:801:ASP:HA	2.48	0.42
1:A:833:LYS:HG3	1:A:834:HIS:CD2	2.54	0.42
9:N:105:CYS:HB3	9:N:117:CYS:SG	2.59	0.42
10:O:159:ARG:HG2	16:G:20:A:P	2.59	0.42
15:W:571:TRP:C	15:W:573:GLY:N	2.77	0.42
16:G:125:C:O2'	16:G:126:C:C1'	2.67	0.42
18:U:685:PRO:O	18:U:687:HIS:ND1	2.50	0.42
23:k:68:GLU:HA	23:k:97:SER:O	2.19	0.42
1:A:472:LEU:O	1:A:475:SER:OG	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:305:ALA:HA	4:E:329:SER:HB2	2.01	0.42
13:S:26:GLU:N	13:S:131:ARG:O	2.50	0.42
17:H:32:U:H6	17:H:32:U:H2'	1.57	0.42
17:H:42:G:C2	17:H:43:U:O4	2.72	0.42
23:d:68:GLU:HA	23:d:97:SER:O	2.19	0.42
1:A:1259:ILE:HD13	1:A:1259:ILE:HA	1.89	0.42
3:C:388:VAL:HA	3:C:392:LEU:HB2	2.00	0.42
5:F:17:C:H2'	5:F:18:A:C8	2.54	0.42
14:T:478:LEU:HD13	14:T:488:VAL:HG22	2.02	0.42
15:W:431:ARG:O	15:W:446:GLU:HA	2.19	0.42
15:W:528:GLY:HA2	15:W:552:VAL:CB	2.49	0.42
16:G:6:A:N6	16:G:7:G:N1	2.68	0.42
17:H:69:U:C2'	17:H:70:C:H5'	2.49	0.42
28:K:18:TYR:CB	28:K:168:LYS:HA	2.50	0.42
1:A:462:ARG:HA	1:A:463:PRO:HD3	1.94	0.42
1:A:984:MET:HG3	1:A:1048:MET:HE1	2.00	0.42
5:F:38:G:H2'	5:F:39:A:C8	2.55	0.42
16:G:1:G:C1'	16:G:2:U:OP1	2.67	0.42
16:G:6:A:C5	16:G:7:G:C5	3.07	0.42
1:A:1333:VAL:HG13	1:A:1365:ILE:HD13	2.02	0.42
1:A:1584:LYS:NZ	18:U:597:LEU:O	2.48	0.42
1:A:1666:LEU:HD23	1:A:1705:ILE:HB	2.00	0.42
3:C:369:PHE:CD1	3:C:373:ILE:HG13	2.54	0.42
15:W:290:GLY:HA2	15:W:571:TRP:O	2.19	0.42
16:G:4:A:OP1	16:G:4:A:C8	2.70	0.42
16:G:12:G:H2'	16:G:13:C:C6	2.55	0.42
1:A:1048:MET:HE3	1:A:1048:MET:HB2	1.89	0.42
1:A:1057:ARG:NH2	1:A:1085:ILE:O	2.50	0.42
3:C:500:THR:HG22	3:C:545:PRO:HA	2.02	0.42
14:T:382:PRO:HB2	14:T:383:ARG:HD2	2.02	0.42
17:H:155:C:H2'	17:H:156:U:H5''	2.01	0.42
17:H:180:G:H2'	17:H:181:G:H8	1.83	0.42
3:C:129:ILE:HG22	3:C:199:LEU:HB3	2.02	0.42
3:C:853:ARG:NH2	3:C:886:ASP:OD2	2.52	0.42
5:F:57:U:H2'	5:F:58:G:C8	2.55	0.42
16:G:152:C:O2	16:G:152:C:H2'	2.19	0.42
19:I:585:ASP:C	19:I:587:CYS:N	2.78	0.42
1:A:1318:THR:HB	1:A:1324:GLY:HA3	2.01	0.42
4:E:131:LYS:HA	4:E:154:VAL:HG23	2.01	0.42
4:E:209:ILE:HG12	4:E:219:VAL:HG22	2.02	0.42
7:L:11:TRP:HE1	7:L:133:GLU:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:253:SER:HA	7:L:256:GLU:HG2	2.02	0.42
17:H:147:G:N1	17:H:148:C:C4	2.88	0.42
17:H:163:G:C2	30:p:49:ARG:O	2.73	0.42
1:A:738:MET:HB3	1:A:738:MET:HE2	1.74	0.41
1:A:758:ARG:HD2	1:A:758:ARG:HA	1.69	0.41
3:C:144:CYS:HB2	3:C:165:LEU:HD12	1.98	0.41
4:E:133:VAL:HB	4:E:147:LEU:HG	2.02	0.41
4:E:145:LYS:HE2	4:E:184:LYS:HG2	2.02	0.41
7:L:120:PRO:O	7:L:121:ARG:NE	2.53	0.41
12:R:228:PRO:HB2	12:R:230:MET:HE3	2.02	0.41
17:H:112:G:H2'	17:H:113:G:C8	2.50	0.41
1:A:93:LYS:O	1:A:649:GLU:HG2	2.20	0.41
3:C:506:PRO:HA	3:C:526:THR:HA	2.01	0.41
3:C:664:GLU:HB3	3:C:820:PHE:HZ	1.85	0.41
1:A:788:GLN:HG2	1:A:1024:HIS:HB3	2.02	0.41
3:C:263:LEU:HD23	3:C:267:LEU:HD12	2.02	0.41
3:C:389:ASP:OD1	3:C:389:ASP:N	2.54	0.41
4:E:59:ILE:HD12	4:E:59:ILE:HA	1.88	0.41
4:E:248:SER:HB3	4:E:265:ARG:HH21	1.85	0.41
11:P:19:GLY:HA2	11:P:23:LEU:HD12	2.02	0.41
13:S:92:PHE:CD2	13:S:122:LEU:HB3	2.55	0.41
16:G:21:A:H3'	16:G:21:A:C8	2.55	0.41
17:H:103:U:C3'	17:H:104:U:H5'	2.51	0.41
17:H:150:U:C2'	17:H:151:C:H5'	2.50	0.41
28:K:128:SER:O	28:K:132:CYS:CB	2.68	0.41
1:A:1159:ASN:HB3	11:P:196:ASN:HA	2.02	0.41
2:B:70:A:N3	2:B:70:A:H5''	2.34	0.41
7:L:209:ASP:OD1	7:L:209:ASP:N	2.52	0.41
7:L:699:ASN:HA	28:K:114:LEU:CB	2.50	0.41
10:O:213:LEU:HD12	16:G:21:A:H2'	2.02	0.41
14:T:380:LEU:HG	14:T:400:PHE:HZ	1.85	0.41
15:W:371:THR:O	15:W:372:ASN:CB	2.68	0.41
16:G:21:A:C8	16:G:21:A:C3'	3.03	0.41
18:U:789:ILE:O	18:U:792:SER:OG	2.30	0.41
18:U:810:ILE:HA	18:U:813:SER:HB2	2.01	0.41
27:q:71:ILE:CB	27:r:81:GLU:HA	2.51	0.41
1:A:1048:MET:HG2	1:A:1051:LEU:HD12	2.03	0.41
2:B:88:A:C2	25:e:53:TYR:CB	3.02	0.41
3:C:163:GLN:HB3	3:C:164:ASP:H	1.60	0.41
3:C:375:GLU:O	3:C:379:LYS:HG2	2.21	0.41
18:U:696:VAL:HG12	18:U:715:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:I:255:LEU:O	19:I:257:LYS:N	2.53	0.41
1:A:250:VAL:HG13	1:A:406:TRP:HB3	2.02	0.41
1:A:697:MET:O	14:T:373:LYS:NZ	2.48	0.41
1:A:796:LYS:HG3	12:R:279:HIS:HE1	1.84	0.41
1:A:1513:MET:SD	18:U:619:MET:HG2	2.60	0.41
3:C:836:VAL:HG11	3:C:846:VAL:HG21	2.03	0.41
5:F:27:A:OP1	10:O:175:ARG:NH1	2.46	0.41
10:O:216:ARG:HD2	16:G:22:C:H5''	2.03	0.41
11:P:32:SER:HA	11:P:35:LEU:HD13	2.02	0.41
11:P:204:GLN:O	11:P:206:LYS:N	2.53	0.41
14:T:380:LEU:HG	14:T:400:PHE:CZ	2.55	0.41
15:W:491:GLN:CB	16:G:136:U:P	3.09	0.41
17:H:168:A:H5''	17:H:169:C:H5	1.86	0.41
18:U:560:VAL:CG1	18:U:660:LYS:HZ3	2.26	0.41
18:U:757:ASN:HD21	18:U:760:MET:HE2	1.84	0.41
19:I:526:MET:O	19:I:526:MET:SD	2.78	0.41
1:A:332:TYR:O	3:C:888:ARG:NH2	2.48	0.41
1:A:591:MET:HE2	1:A:591:MET:HB3	1.92	0.41
12:R:237:MET:HE3	12:R:241:GLU:HG3	2.02	0.41
17:H:153:A:H3'	17:H:154:C:H5'	2.00	0.41
18:U:620:ARG:NH1	18:U:647:ARG:HE	2.19	0.41
3:C:214:GLU:OE1	3:C:480:LYS:NZ	2.39	0.41
9:N:22:LEU:HD21	9:N:60:ILE:HD11	2.02	0.41
14:T:450:VAL:HG11	14:T:489:TYR:HE2	1.86	0.41
17:H:171:U:H2'	17:H:172:C:O4'	2.21	0.41
29:o:160:LYS:O	29:o:161:MET:C	2.63	0.41
1:A:199:GLU:OE2	1:A:240:ARG:NH1	2.51	0.41
1:A:699:GLU:OE2	12:R:235:ARG:HB3	2.21	0.41
1:A:1178:TYR:HB2	1:A:1185:LEU:HB3	2.02	0.41
1:A:1487:HIS:HD2	1:A:1541:THR:HG21	1.85	0.41
1:A:1556:ASP:OD1	1:A:1557:LEU:N	2.50	0.41
1:A:1648:SER:HB2	1:A:1649:LYS:HD2	2.03	0.41
1:A:1971:LEU:HB2	1:A:1976:TRP:CE2	2.55	0.41
3:C:92:PRO:HA	14:T:278:ASN:ND2	2.36	0.41
3:C:804:GLY:O	3:C:808:ILE:HB	2.21	0.41
12:R:113:TYR:OH	14:T:402:ASP:O	2.25	0.41
13:S:121:TRP:CZ2	15:W:98:PRO:HG3	2.56	0.41
14:T:345:ILE:HD11	14:T:359:LEU:HD13	2.03	0.41
16:G:6:A:N9	16:G:7:G:C8	2.89	0.41
16:G:147:C:C4	17:H:31:G:N1	2.69	0.41
17:H:35:A:H8	17:H:35:A:OP2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:H:51:A:H5'	17:H:99:A:O2'	2.21	0.41
17:H:112:G:H8	17:H:112:G:O5'	2.04	0.41
17:H:147:G:C4	17:H:148:C:C5	3.09	0.41
1:A:1971:LEU:O	1:A:1976:TRP:NE1	2.53	0.41
2:B:72:U:C3'	2:B:72:U:C6	3.04	0.41
14:T:335:THR:O	14:T:347:THR:OG1	2.38	0.41
17:H:88:A:C6	17:H:89:U:C4	3.09	0.41
17:H:92:U:C2'	17:H:93:A:H8	2.28	0.41
1:A:56:ALA:O	9:N:109:ARG:NH1	2.35	0.40
2:B:73:C:O2	2:B:73:C:O2'	2.35	0.40
3:C:637:LEU:HA	3:C:637:LEU:HD23	1.90	0.40
5:F:17:C:H2'	5:F:18:A:H8	1.87	0.40
6:J:281:LYS:HA	6:J:284:GLU:HG2	2.02	0.40
6:J:774:VAL:CB	6:J:787:LYS:CB	2.99	0.40
7:L:114:GLU:HG2	7:L:115:GLU:H	1.86	0.40
14:T:213:GLU:HG3	14:T:218:TRP:CZ2	2.57	0.40
15:W:83:PRO:HG3	15:W:88:MET:HE3	2.03	0.40
27:s:114:CYS:CB	28:K:32:ALA:CB	2.99	0.40
23:k:62:HIS:O	23:k:103:GLY:HA3	2.21	0.40
3:C:134:LEU:O	3:C:205:THR:OG1	2.29	0.40
6:J:293:ASN:OD1	7:L:225:TYR:HB3	2.21	0.40
7:L:22:ALA:HB2	7:L:37:LEU:HD23	2.04	0.40
15:W:298:PRO:O	15:W:299:LEU:CB	2.68	0.40
16:G:22:C:O2	16:G:22:C:C2'	2.69	0.40
16:G:141:C:O5'	16:G:141:C:C2'	2.70	0.40
17:H:38:A:O2'	17:H:39:U:C5	2.74	0.40
17:H:59:A:C6	17:H:60:U:C4	3.09	0.40
1:A:1179:SER:O	1:A:1201:ARG:NH2	2.37	0.40
3:C:495:ARG:HH21	3:C:547:GLY:HA2	1.86	0.40
5:F:78:A:H4'	6:J:237:LYS:HE2	2.03	0.40
7:L:140:ASP:OD1	7:L:140:ASP:N	2.55	0.40
15:W:77:LYS:HA	15:W:77:LYS:HD3	1.86	0.40
17:H:102:U:O2'	17:H:103:U:C6	2.74	0.40
19:I:426:PHE:CB	19:I:458:LYS:CB	2.99	0.40
23:d:62:HIS:O	23:d:103:GLY:HA3	2.21	0.40
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	2.04	0.40
2:B:85:C:H3'	2:B:85:C:P	2.61	0.40
2:B:95:G:C5	25:e:36:TYR:O	2.74	0.40
5:F:81:C:H5''	5:F:82:A:H5''	2.03	0.40
6:J:493:ALA:CB	6:J:499:ARG:CB	2.96	0.40
6:J:592:ALA:N	6:J:595:ALA:HB3	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:3:LYS:HA	9:N:3:LYS:HD2	1.91	0.40
12:R:281:ASN:ND2	12:R:282:GLU:OE1	2.54	0.40
14:T:216:ASN:ND2	14:T:471:ASP:HB2	2.37	0.40
17:H:181:G:C4	17:H:182:U:C5	3.10	0.40
28:K:92:PRO:O	28:K:93:SER:C	2.64	0.40
24:m:5:LEU:O	25:l:49:GLY:HA3	2.21	0.40
3:C:264:ILE:HG12	3:C:378:TYR:CE1	2.57	0.40
4:E:304:SER:OG	4:E:308:PHE:O	2.39	0.40
7:L:692:LEU:CB	28:K:107:VAL:CB	3.00	0.40
14:T:446:ASN:ND2	14:T:449:ARG:HE	2.19	0.40
19:I:326:ASP:C	19:I:329:LEU:H	2.28	0.40
19:I:606:TRP:O	19:I:609:ALA:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1977/2335 (85%)	1793 (91%)	165 (8%)	19 (1%)	12	39
3	C	886/972 (91%)	788 (89%)	96 (11%)	2 (0%)	43	72
4	E	301/357 (84%)	280 (93%)	20 (7%)	1 (0%)	36	65
6	J	520/848 (61%)	473 (91%)	42 (8%)	5 (1%)	12	39
7	L	459/802 (57%)	423 (92%)	31 (7%)	5 (1%)	11	36
8	M	128/243 (53%)	116 (91%)	12 (9%)	0	100	100
9	N	141/144 (98%)	128 (91%)	12 (8%)	1 (1%)	18	48
10	O	288/420 (69%)	262 (91%)	25 (9%)	1 (0%)	36	65
11	P	114/229 (50%)	98 (86%)	15 (13%)	1 (1%)	14	41
12	R	268/536 (50%)	227 (85%)	38 (14%)	3 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	S	157/166 (95%)	141 (90%)	16 (10%)	0	100	100
14	T	315/514 (61%)	292 (93%)	21 (7%)	2 (1%)	21	51
15	W	507/579 (88%)	433 (85%)	46 (9%)	28 (6%)	1	4
18	U	343/894 (38%)	277 (81%)	58 (17%)	8 (2%)	5	19
19	I	528/855 (62%)	491 (93%)	23 (4%)	14 (3%)	4	16
20	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
20	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
21	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
21	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
22	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
22	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
23	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
23	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
24	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
24	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
25	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
25	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
26	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
26	n	63/76 (83%)	61 (97%)	2 (3%)	0	100	100
27	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	14
27	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	7	27
27	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	8	28
27	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	28
28	K	144/225 (64%)	130 (90%)	8 (6%)	6 (4%)	2	9
29	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	32
30	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
31	Q	1308/1485 (88%)	1283 (98%)	25 (2%)	0	100	100
32	y	77/301 (26%)	75 (97%)	2 (3%)	0	100	100
All	All	10193/16097 (63%)	9369 (92%)	718 (7%)	106 (1%)	15	39

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1306	LYS
1	A	1367	ASN
1	A	1639	VAL
1	A	1653	ASP
1	A	1654	SER
4	E	59	ILE
6	J	592	ALA
15	W	228	LYS
15	W	240	ILE
15	W	259	GLN
15	W	263	VAL
15	W	267	SER
15	W	279	LYS
15	W	299	LEU
15	W	372	ASN
15	W	492	ASN
18	U	579	VAL
18	U	613	ASN
18	U	706	LEU
18	U	793	ASP
18	U	810	ILE
19	I	463	PRO
19	I	486	VAL
19	I	721	LYS
27	q	59	HIS
27	q	60	PRO
27	s	71	ILE
27	t	69	THR
28	K	78	PRO
28	K	90	PRO
1	A	136	ILE
1	A	626	GLY
1	A	1191	GLY
1	A	1305	SER
1	A	1366	PRO
1	A	1419	ILE
6	J	709	VAL
7	L	765	ARG
9	N	4	VAL
11	P	205	LYS
12	R	52	PRO
12	R	234	SER
14	T	406	ILE

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Mol	Chain	Res	Type
15	W	318	VAL
15	W	325	LEU
15	W	482	ASP
19	I	368	GLN
19	I	546	SER
19	I	618	ARG
27	q	9	ASN
28	K	136	LYS
28	K	172	LEU
29	o	160	LYS
1	A	625	PRO
1	A	803	ALA
1	A	1092	ILE
3	C	94	ILE
7	L	118	ASP
12	R	53	ARG
14	T	343	PRO
15	W	77	LYS
15	W	149	SER
15	W	243	VAL
15	W	246	MET
18	U	679	PHE
18	U	809	ASP
19	I	284	ARG
19	I	480	VAL
19	I	601	GLN
27	q	19	PRO
27	r	9	ASN
1	A	1519	THR
6	J	341	PRO
6	J	591	LEU
7	L	585	TYR
15	W	204	ASP
15	W	272	GLU
15	W	554	ILE
18	U	845	PHE
19	I	617	GLU
28	K	65	ILE
29	o	32	PRO
1	A	108	MET
1	A	1365	ILE
1	A	1652	MET

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Mol	Chain	Res	Type
6	J	357	LYS
15	W	301	GLY
15	W	330	GLY
19	I	254	GLN
19	I	256	GLY
19	I	321	GLU
19	I	796	LEU
1	A	1251	SER
7	L	763	ILE
10	O	20	PHE
15	W	229	GLN
15	W	376	PRO
15	W	549	HIS
7	L	764	PRO
15	W	205	VAL
15	W	208	PRO
3	C	87	GLN
15	W	251	GLY
27	r	65	PRO
28	K	17	PRO
15	W	270	PRO

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	
1	A	1792/2108 (85%)	1774 (99%)	18 (1%)	68	89
3	C	787/866 (91%)	773 (98%)	14 (2%)	51	80
4	E	259/300 (86%)	255 (98%)	4 (2%)	57	84
6	J	242/751 (32%)	236 (98%)	6 (2%)	42	74
7	L	228/709 (32%)	226 (99%)	2 (1%)	70	90
8	M	117/209 (56%)	116 (99%)	1 (1%)	70	90
9	N	130/130 (100%)	127 (98%)	3 (2%)	44	76
10	O	259/361 (72%)	258 (100%)	1 (0%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	104/203 (51%)	103 (99%)	1 (1%)	68	89
12	R	227/457 (50%)	221 (97%)	6 (3%)	40	73
13	S	129/134 (96%)	128 (99%)	1 (1%)	73	90
14	T	273/441 (62%)	271 (99%)	2 (1%)	76	92
15	W	135/502 (27%)	133 (98%)	2 (2%)	57	84
18	U	313/806 (39%)	306 (98%)	7 (2%)	45	77
19	I	7/749 (1%)	2 (29%)	5 (71%)	0	0
All	All	5002/8726 (57%)	4929 (98%)	73 (2%)	55	84

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	273	ILE
1	A	338	VAL
1	A	621	VAL
1	A	668	VAL
1	A	735	ILE
1	A	1109	LEU
1	A	1216	LEU
1	A	1284	LEU
1	A	1295	ILE
1	A	1516	LYS
1	A	1517	LYS
1	A	1518	LEU
1	A	1522	GLN
1	A	1555	LEU
1	A	1593	LEU
1	A	1639	VAL
1	A	1649	LYS
1	A	1838	LYS
3	C	100	LYS
3	C	128	LEU
3	C	138	LEU
3	C	139	HIS
3	C	142	LYS
3	C	144	CYS
3	C	159	LYS
3	C	160	ARG
3	C	161	TYR
3	C	162	ASP

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Mol	Chain	Res	Type
3	C	190	LEU
3	C	221	ILE
3	C	307	VAL
3	C	461	LEU
4	E	55	LEU
4	E	59	ILE
4	E	62	LEU
4	E	131	LYS
6	J	236	ARG
6	J	237	LYS
6	J	239	ARG
6	J	240	THR
6	J	242	ILE
6	J	366	TYR
7	L	123	LEU
7	L	251	LEU
8	M	212	ASN
9	N	49	ILE
9	N	60	ILE
9	N	101	CYS
10	O	78	LYS
11	P	13	ARG
12	R	111	VAL
12	R	165	VAL
12	R	234	SER
12	R	235	ARG
12	R	262	ILE
12	R	281	ASN
13	S	102	ASN
14	T	220	VAL
14	T	489	TYR
15	W	76	VAL
15	W	193	LEU
18	U	660	LYS
18	U	662	ILE
18	U	666	ARG
18	U	672	MET
18	U	673	GLU
18	U	773	LEU
18	U	810	ILE
19	I	235	VAL
19	I	399	VAL

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Mol	Chain	Res	Type
19	I	486	VAL
19	I	526	MET
19	I	795	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	HIS
1	A	517	HIS
1	A	711	GLN
1	A	723	ASN
1	A	775	ASN
1	A	860	GLN
1	A	1023	ASN
1	A	1238	GLN
1	A	1293	ASN
1	A	1296	GLN
1	A	1373	GLN
1	A	1394	GLN
1	A	1487	HIS
1	A	1522	GLN
1	A	1580	HIS
1	A	1658	GLN
1	A	1717	ASN
1	A	1767	ASN
1	A	1791	HIS
1	A	1811	ASN
1	A	1918	ASN
3	C	60	HIS
3	C	82	GLN
3	C	139	HIS
3	C	238	ASN
3	C	245	HIS
3	C	366	GLN
3	C	437	HIS
3	C	513	ASN
3	C	523	GLN
3	C	538	HIS
3	C	903	HIS
4	E	253	ASN
6	J	188	GLN
6	J	212	GLN

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Mol	Chain	Res	Type
6	J	311	GLN
6	J	347	HIS
6	J	389	HIS
6	J	394	HIS
6	J	410	HIS
7	L	175	GLN
7	L	233	GLN
7	L	244	GLN
8	M	212	ASN
9	N	37	HIS
9	N	136	HIS
10	O	14	ASN
10	O	25	GLN
10	O	79	ASN
10	O	113	ASN
11	P	75	ASN
11	P	212	ASN
12	R	133	GLN
12	R	189	ASN
12	R	242	GLN
12	R	276	GLN
12	R	279	HIS
12	R	281	ASN
13	S	63	GLN
13	S	102	ASN
14	T	216	ASN
14	T	283	HIS
14	T	285	HIS
14	T	324	HIS
14	T	446	ASN
15	W	102	GLN
15	W	103	GLN
15	W	127	GLN
15	W	145	ASN
18	U	605	ASN
18	U	665	HIS
18	U	717	GLN
18	U	718	HIS
18	U	757	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	G	69/272 (25%)	55 (79%)	12 (17%)
17	H	133/188 (70%)	53 (39%)	8 (6%)
2	B	97/117 (82%)	44 (45%)	5 (5%)
5	F	96/107 (89%)	41 (42%)	6 (6%)
All	All	395/684 (57%)	193 (48%)	31 (7%)

All (193) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	G
2	B	9	G
2	B	10	U
2	B	11	U
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	25	C
2	B	26	A
2	B	28	A
2	B	35	U
2	B	36	C
2	B	38	C
2	B	45	C
2	B	47	A
2	B	48	A
2	B	57	G
2	B	67	A
2	B	69	A
2	B	70	A
2	B	71	C
2	B	73	C
2	B	74	U
2	B	75	G
2	B	77	G
2	B	78	U
2	B	79	C
2	B	80	U
2	B	81	U
2	B	82	A
2	B	83	A
2	B	84	C
2	B	85	C

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Mol	Chain	Res	Type
2	B	86	C
2	B	87	A
2	B	88	A
2	B	89	U
2	B	90	U
2	B	91	U
2	B	92	U
2	B	94	U
2	B	95	G
2	B	96	A
5	F	5	U
5	F	6	C
5	F	7	G
5	F	10	U
5	F	12	G
5	F	26	U
5	F	27	A
5	F	28	A
5	F	29	A
5	F	33	G
5	F	34	G
5	F	36	A
5	F	37	C
5	F	39	A
5	F	40	U
5	F	41	A
5	F	42	C
5	F	43	A
5	F	44	G
5	F	45	A
5	F	46	G
5	F	47	A
5	F	49	G
5	F	51	U
5	F	52	U
5	F	53	A
5	F	54	G
5	F	58	G
5	F	59	G
5	F	61	C
5	F	66	C
5	F	67	G

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Mol	Chain	Res	Type
5	F	68	C
5	F	69	A
5	F	74	U
5	F	78	A
5	F	79	C
5	F	81	C
5	F	82	A
5	F	84	A
5	F	87	C
16	G	2	U
16	G	3	A
16	G	4	A
16	G	5	G
16	G	7	G
16	G	11	A
16	G	13	C
16	G	15	U
16	G	17	U
16	G	20	A
16	G	21	A
16	G	22	C
16	G	23	U
16	G	24	G
16	G	25	G
16	G	26	U
16	G	27	U
16	G	28	A
16	G	29	C
16	G	30	C
16	G	31	U
16	G	119	G
16	G	121	G
16	G	122	U
16	G	123	U
16	G	124	U
16	G	125	C
16	G	126	C
16	G	127	U
16	G	128	U
16	G	129	G
16	G	130	A
16	G	131	U

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Mol	Chain	Res	Type
16	G	132	G
16	G	133	A
16	G	134	U
16	G	135	G
16	G	136	U
16	G	137	C
16	G	138	A
16	G	139	U
16	G	140	A
16	G	141	C
16	G	142	U
16	G	143	U
16	G	144	A
16	G	145	U
16	G	146	C
16	G	147	C
16	G	148	U
16	G	149	G
16	G	150	U
16	G	151	C
16	G	153	C
16	G	154	U
17	H	15	U
17	H	16	U
17	H	17	U
17	H	19	G
17	H	20	G
17	H	23	A
17	H	25	G
17	H	28	C
17	H	29	A
17	H	30	A
17	H	31	G
17	H	32	U
17	H	34	U
17	H	35	A
17	H	36	G
17	H	37	U
17	H	38	A
17	H	39	U
17	H	40	C
17	H	41	U

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Mol	Chain	Res	Type
17	H	43	U
17	H	44	U
17	H	45	C
17	H	46	U
17	H	47	U
17	H	48	A
17	H	49	U
17	H	50	C
17	H	51	A
17	H	68	G
17	H	70	C
17	H	94	A
17	H	101	U
17	H	102	U
17	H	105	G
17	H	106	G
17	H	107	A
17	H	109	C
17	H	112	G
17	H	149	A
17	H	151	C
17	H	154	C
17	H	156	U
17	H	157	G
17	H	164	C
17	H	166	G
17	H	167	U
17	H	168	A
17	H	177	A
17	H	178	A
17	H	179	C
17	H	180	G
17	H	182	U

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	78	U
2	B	79	C
2	B	80	U
2	B	92	U
2	B	95	G

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Mol	Chain	Res	Type
5	F	5	U
5	F	33	G
5	F	43	A
5	F	45	A
5	F	50	A
5	F	58	G
16	G	1	G
16	G	2	U
16	G	3	A
16	G	16	G
16	G	21	A
16	G	22	C
16	G	133	A
16	G	141	C
16	G	143	U
16	G	145	U
16	G	147	C
16	G	148	U
17	H	29	A
17	H	30	A
17	H	31	G
17	H	34	U
17	H	46	U
17	H	49	U
17	H	50	C
17	H	156	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	$\# Z > 2$
12	SEP	R	224	12	8,9,10	0.88	0	7,12,14	2.11	1 (14%)
12	SEP	R	232	12	8,9,10	0.94	0	7,12,14	2.19	1 (14%)

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
12	SEP	R	224	12	-	2/6/8/10	-
12	SEP	R	232	12	-	3/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	232	SEP	OG-CB-CA	5.17	113.17	108.14
12	R	224	SEP	OG-CB-CA	4.66	112.67	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	224	SEP	N-CA-CB-OG
12	R	224	SEP	C-CA-CB-OG
12	R	232	SEP	CB-OG-P-O1P
12	R	232	SEP	CB-OG-P-O2P
12	R	232	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	232	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 14 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
34	GTP	C	1500	35	33,34,34	1.15	3 (9%)	50,54,54	1.72	6 (12%)
33	IHP	A	3000	-	36,36,36	0.71	0	60,60,60	0.97	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
34	GTP	C	1500	35	-	5/22/38/38	0/3/3/3
33	IHP	A	3000	-	-	8/30/54/54	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1500	GTP	C5-C4	2.85	1.46	1.38
34	C	1500	GTP	C6-N1	-2.70	1.33	1.38
34	C	1500	GTP	C5-N7	-2.37	1.34	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1500	GTP	C5-C4-N3	-6.20	118.52	128.39
34	C	1500	GTP	C2-N3-C4	5.07	121.04	112.30
34	C	1500	GTP	N9-C4-N3	4.58	135.11	125.95
34	C	1500	GTP	C6-C5-N7	3.26	136.22	130.29
34	C	1500	GTP	C4-C5-N7	-2.59	106.56	110.67
34	C	1500	GTP	O6-C6-C5	-2.24	120.61	126.53

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C6-C1-O11-P1
34	C	1500	GTP	C5'-O5'-PA-O2A

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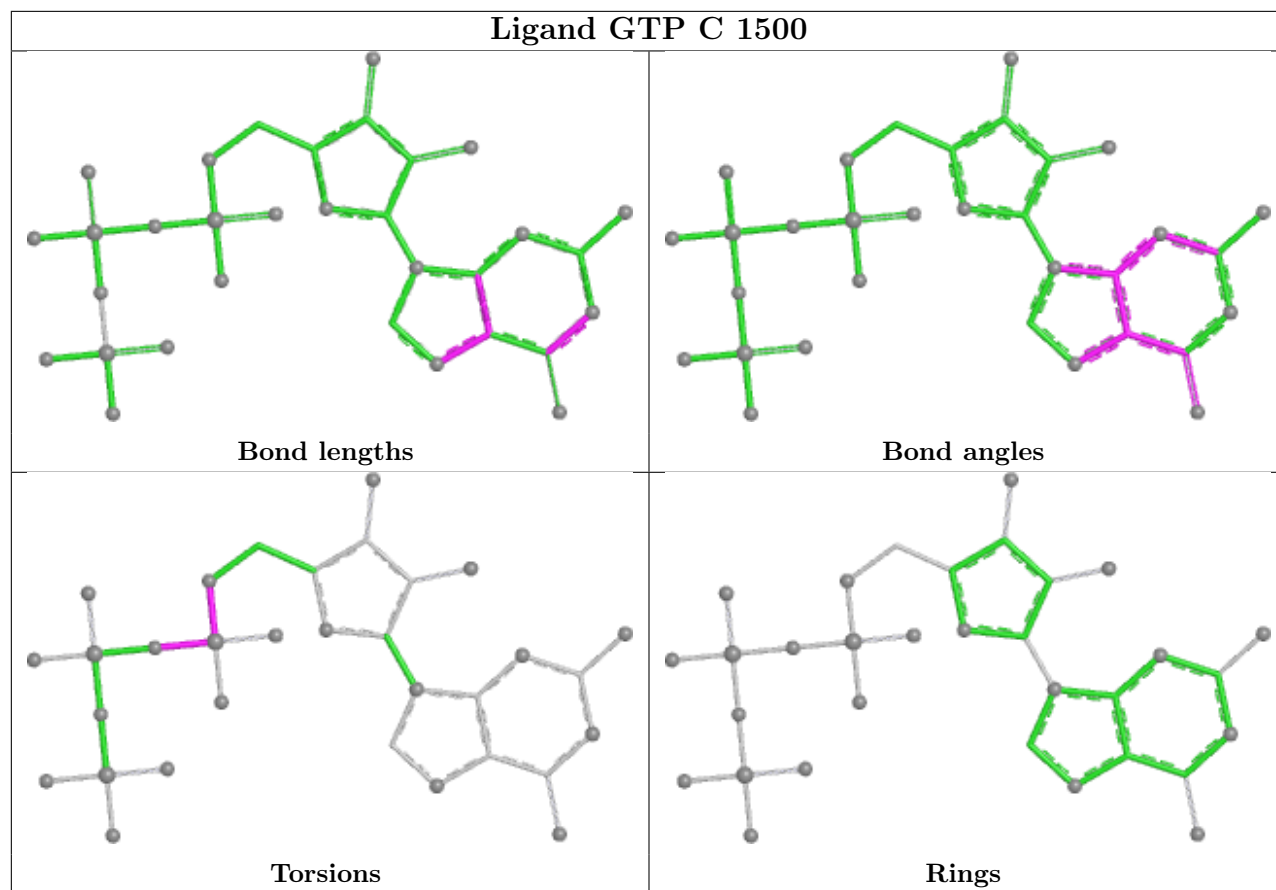
Mol	Chain	Res	Type	Atoms
33	A	3000	IHP	C2-C1-O11-P1
33	A	3000	IHP	C1-C2-O12-P2
33	A	3000	IHP	C3-C2-O12-P2
34	C	1500	GTP	C5'-O5'-PA-O3A
34	C	1500	GTP	C5'-O5'-PA-O1A
33	A	3000	IHP	C4-O14-P4-O44
33	A	3000	IHP	C6-O16-P6-O36
33	A	3000	IHP	C6-O16-P6-O26
34	C	1500	GTP	PB-O3A-PA-O2A
33	A	3000	IHP	C6-O16-P6-O46
34	C	1500	GTP	PB-O3A-PA-O1A

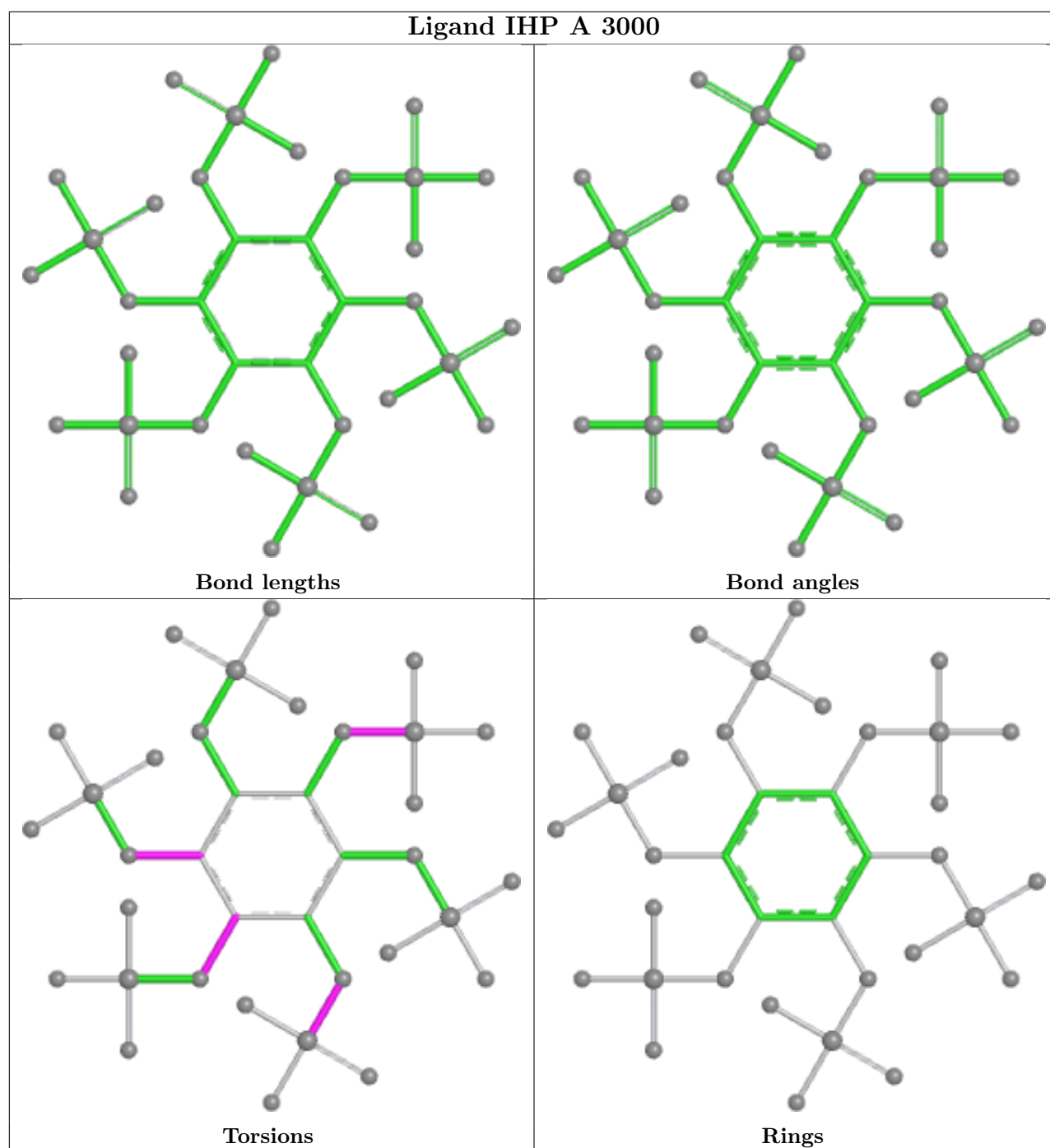
There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	C	1500	GTP	22	0
33	A	3000	IHP	1	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.

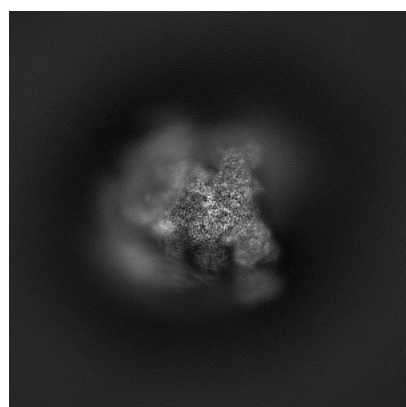
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9646. These allow visual inspection of the internal detail of the map and identification of artifacts.

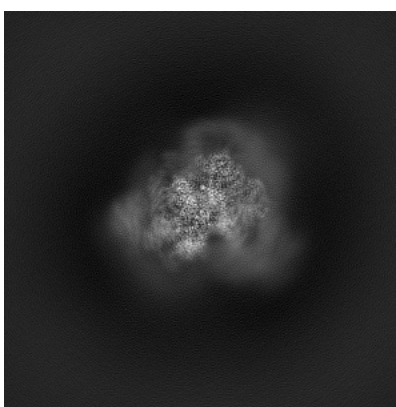
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

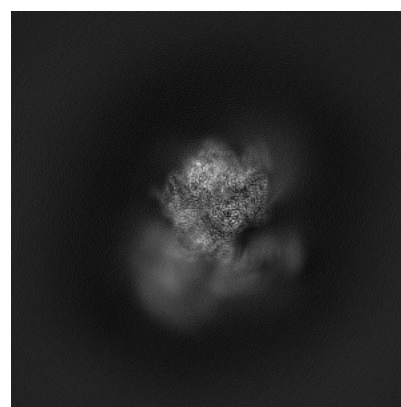
6.1.1 Primary map



X



Y

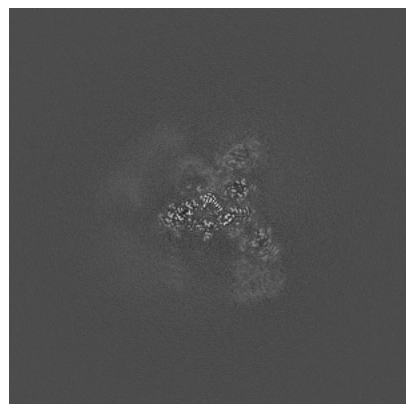


Z

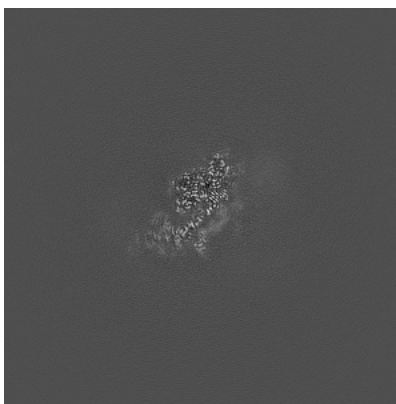
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

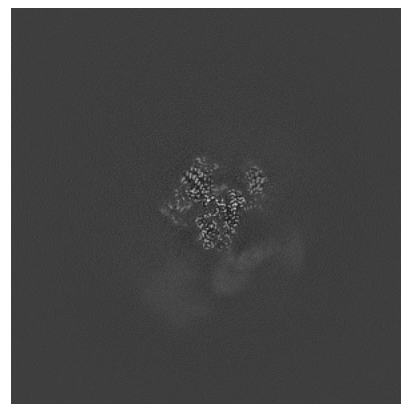
6.2.1 Primary map



X Index: 200



Y Index: 200

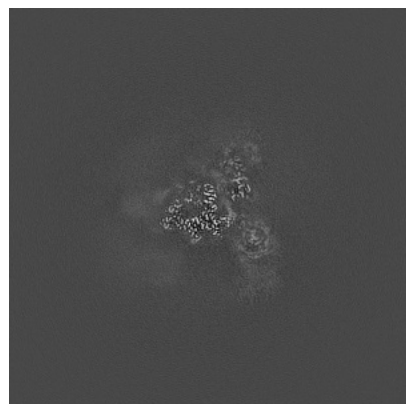


Z Index: 200

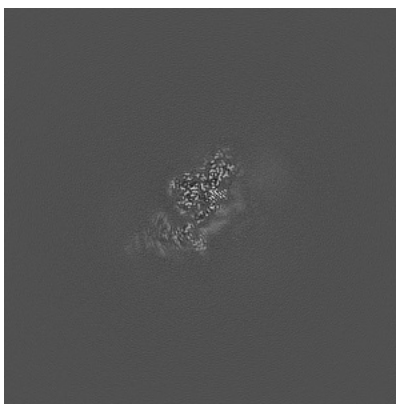
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

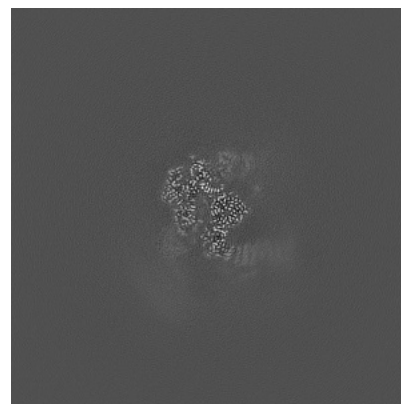
6.3.1 Primary map



X Index: 210



Y Index: 201

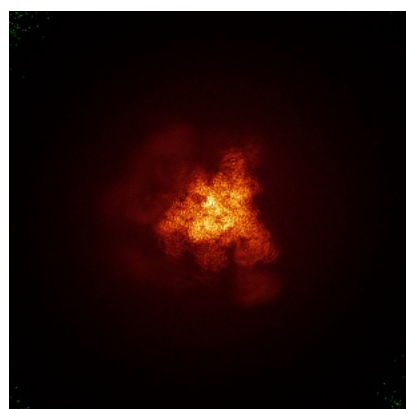


Z Index: 185

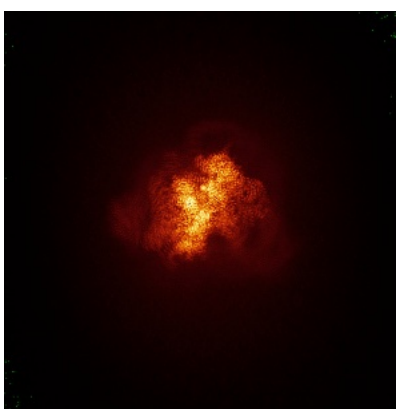
The images above show the largest variance slices of the map in three orthogonal directions.

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

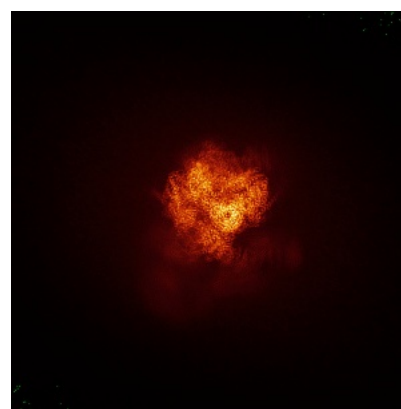
6.4.1 Primary map



X



Y



Z

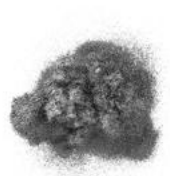
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

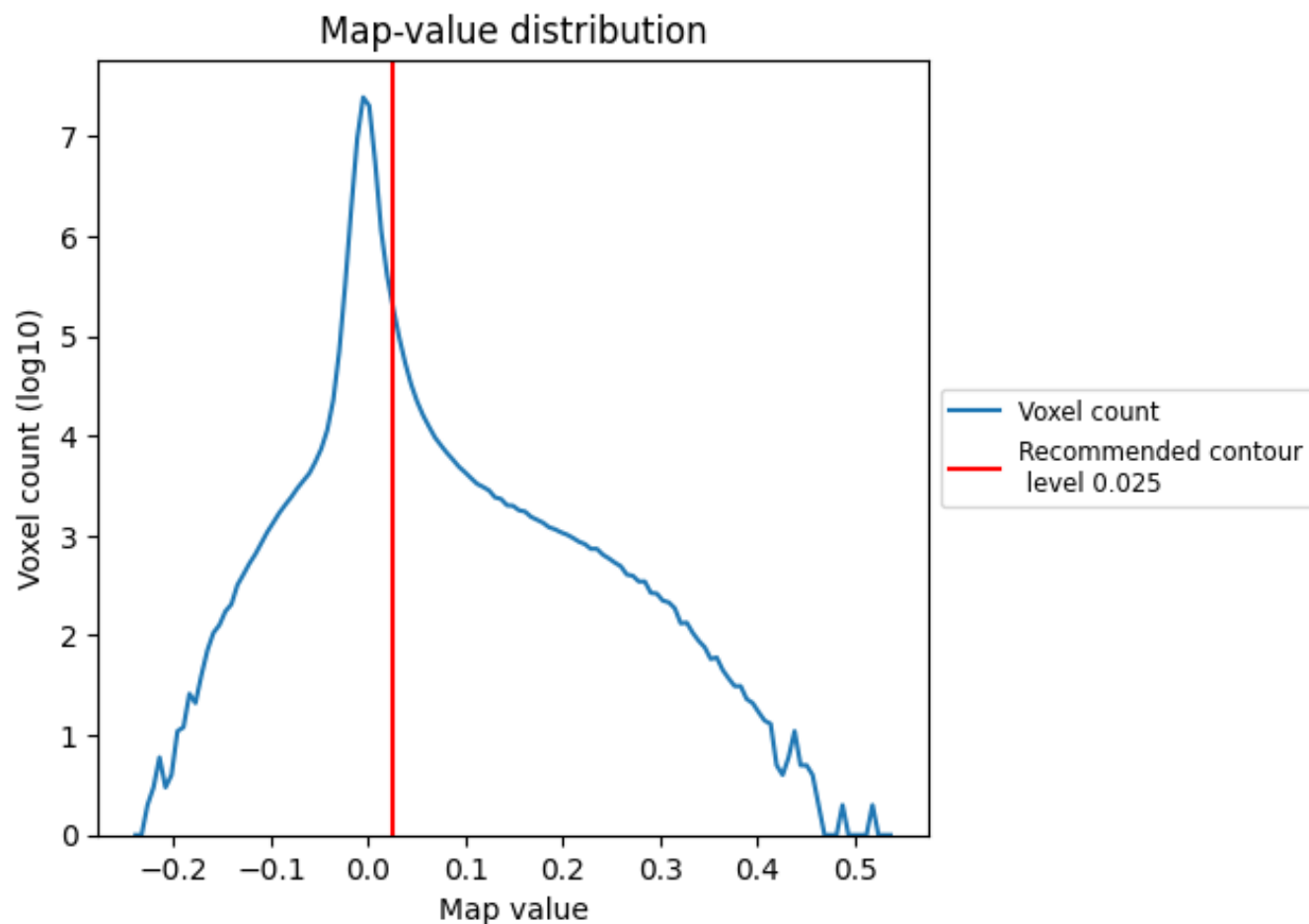
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

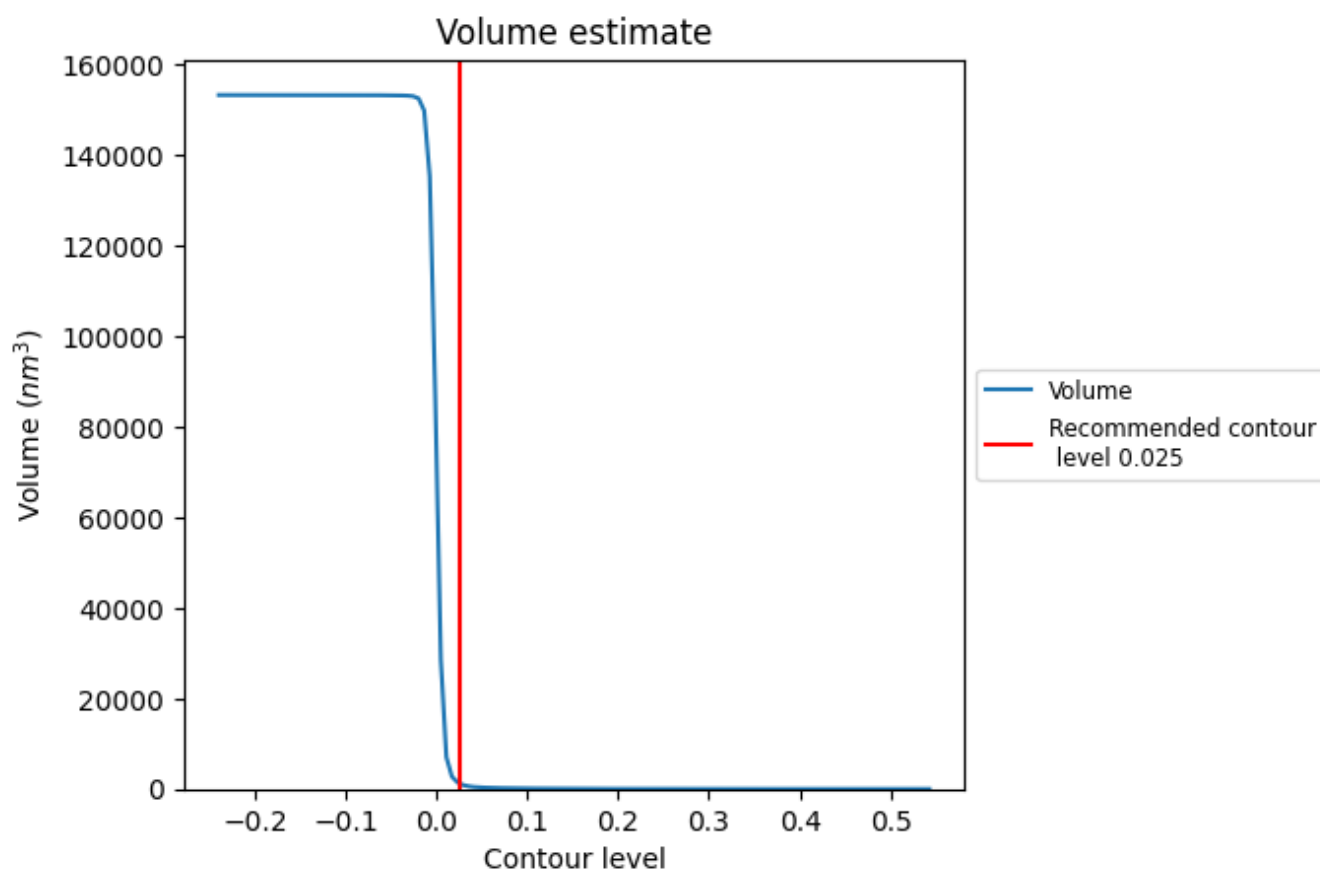
This section contains the results of statistical analysis of the map.

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.

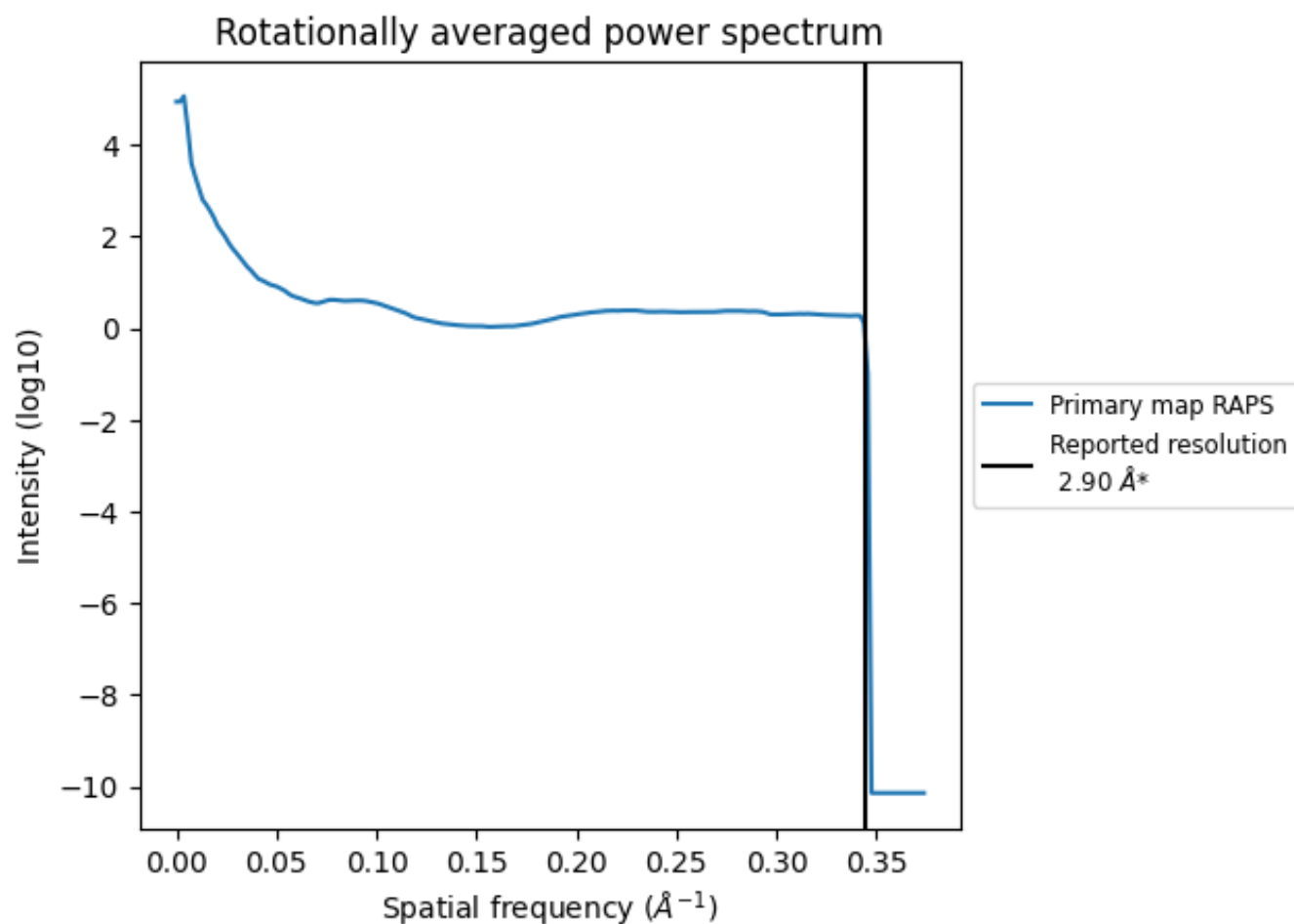
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1297 nm^3 ; this corresponds to an approximate mass of 1172 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 0.345 Å⁻¹

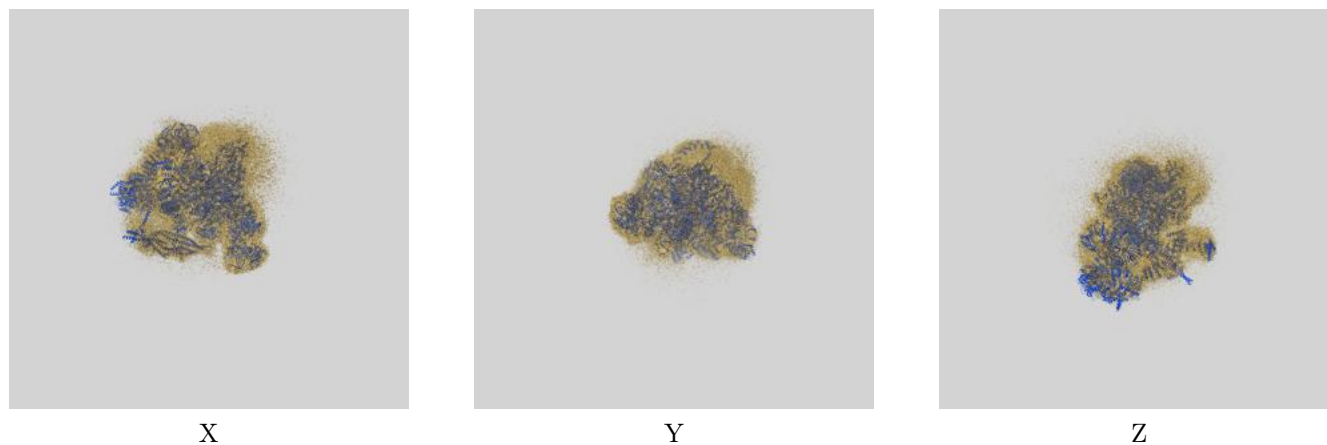
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

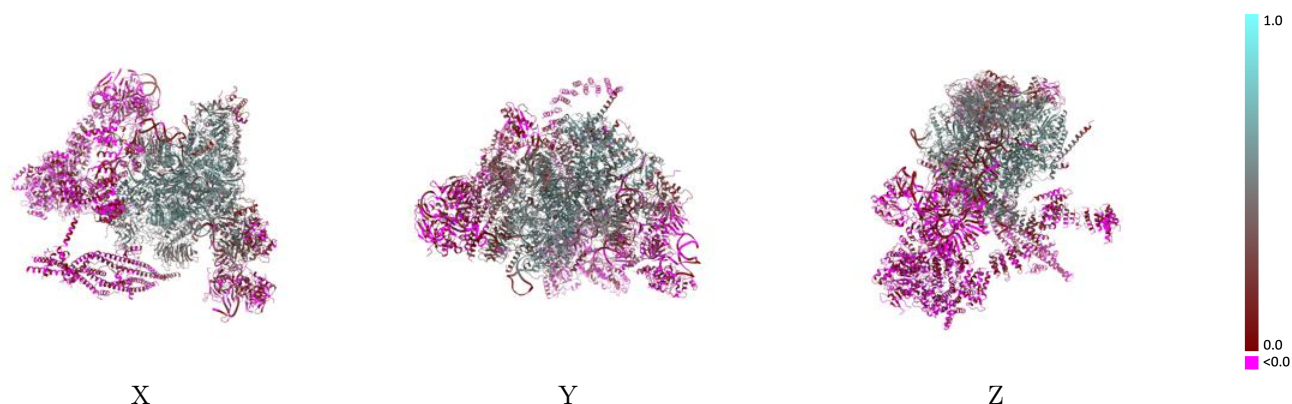
This section contains information regarding the fit between EMDB map EMD-9646 and PDB model 6ID0. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



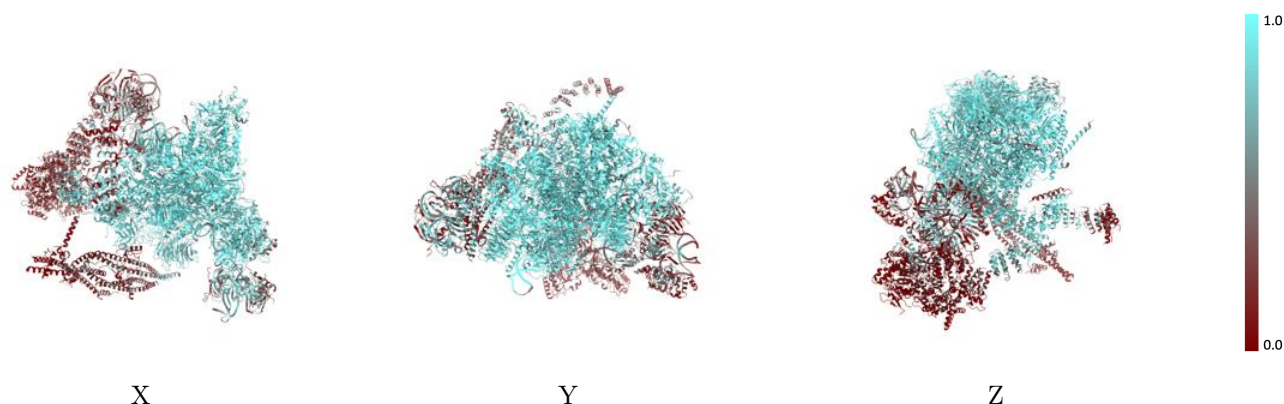
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



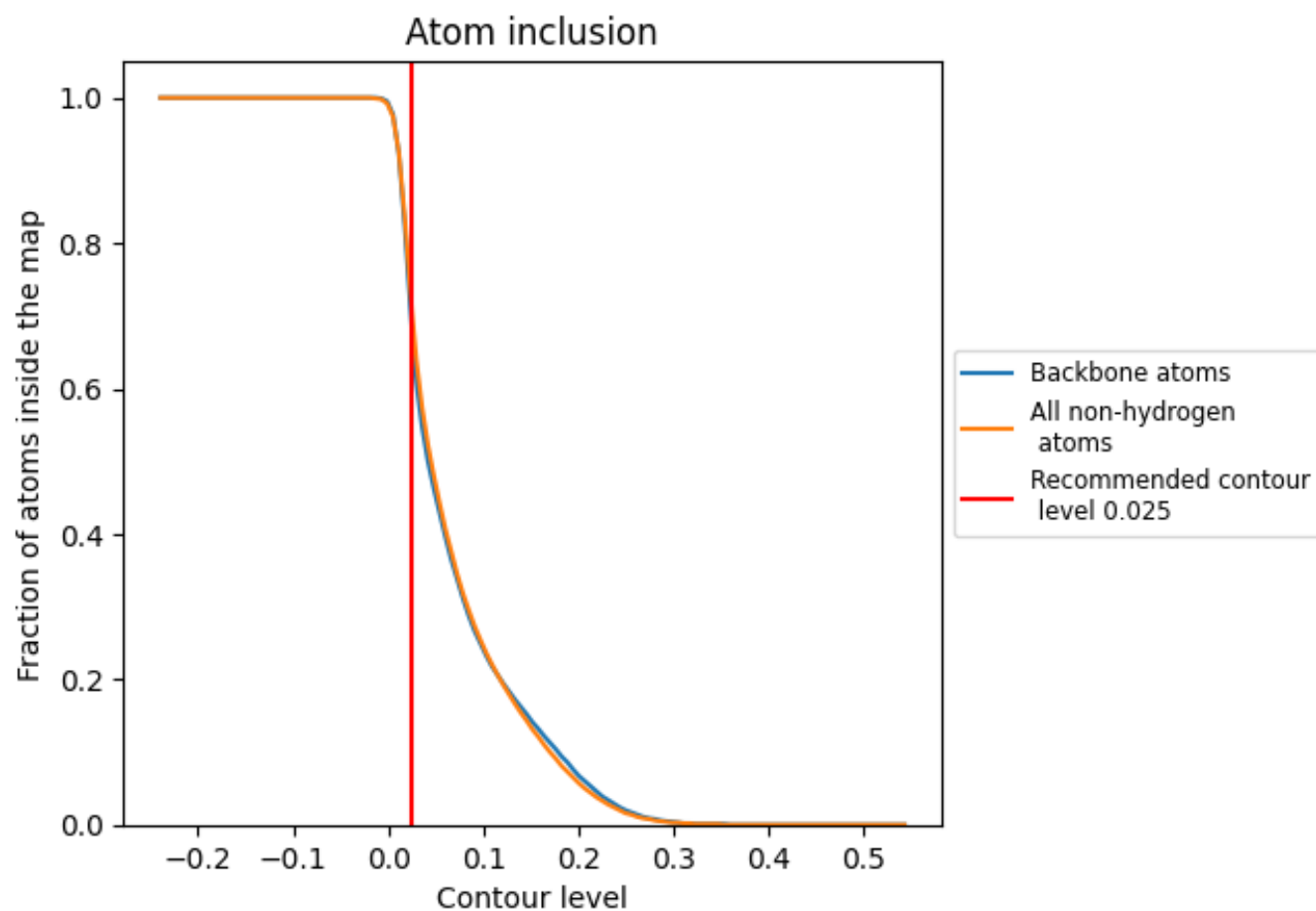
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 70% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7050	 0.3140
A	 0.9230	 0.5020
B	 0.8300	 0.3370
C	 0.8520	 0.3270
E	 0.8910	 0.4110
F	 0.9420	 0.4650
G	 0.6680	 0.1420
H	 0.5130	 0.1100
I	 0.5350	 0.0560
J	 0.7370	 0.3250
K	 0.2560	 0.0580
L	 0.6480	 0.3380
M	 0.8870	 0.4960
N	 0.9570	 0.5500
O	 0.8310	 0.3930
P	 0.8380	 0.4610
Q	 0.0690	 -0.0050
R	 0.8700	 0.4660
S	 0.9190	 0.4670
T	 0.9760	 0.5980
U	 0.8780	 0.4540
W	 0.8620	 0.3360
a	 0.6670	 0.1900
b	 0.4910	 0.0340
c	 0.6480	 0.0540
d	 0.6400	 0.0330
e	 0.4810	 0.0550
f	 0.4930	 -0.0020
g	 0.4850	 0.0500
h	 0.4700	 0.0160
i	 0.3660	 0.0240
j	 0.3520	 -0.0110
k	 0.3010	 -0.0100
l	 0.2530	 -0.0090
m	 0.3130	 0.0350



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Chain	Atom inclusion	Q-score
n	 0.3830	 0.0330
o	 0.1870	 -0.0010
p	 0.3730	 0.0250
q	 0.1150	 0.0380
r	 0.1850	 0.0200
s	 0.2330	 0.0550
t	 0.1400	 0.0050
y	 0.3920	 0.0170