



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:03 PM UTC

PDB ID : 7ABI / pdb_00007abi
EMDB ID : EMD-11697
Title : Human pre-Bact-2 spliceosome
Authors : Townsend, C.; Kastner, B.; Leelaram, M.N.; Bertram, K.; Stark, H.;
Luehrmann, R.
Deposited on : 2020-09-07
Resolution : 8.00 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

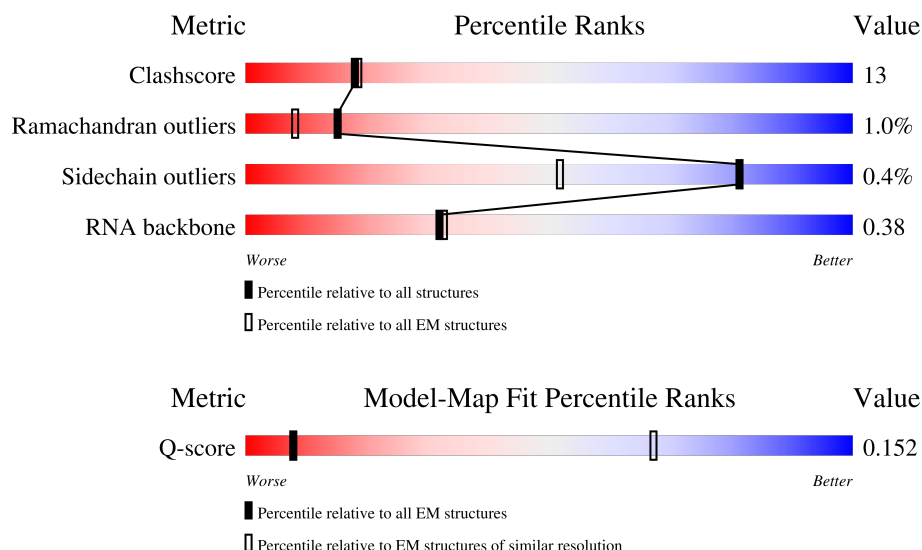
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.00 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	361 (7.50 - 8.50)

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	D	357	
2	E	1217	
3	b	86	

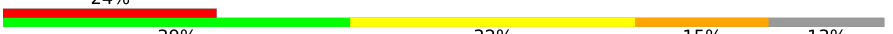
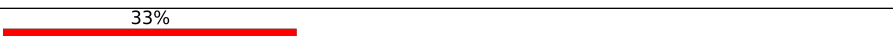
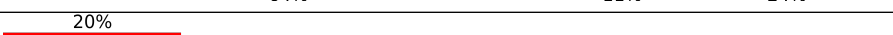
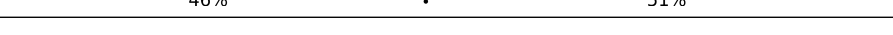
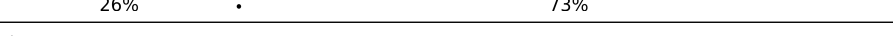
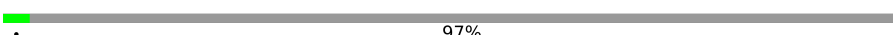
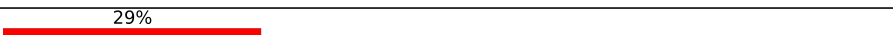
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	i	86	
4	W	255	
5	w	424	
6	d	76	
6	k	76	
7	U	1485	
8	x	86	
9	6	106	
10	B	225	
11	z	125	
12	q	73	
13	s	2136	
14	v	536	
15	3	619	
16	0	396	
17	Q	144	
18	1	322	
19	L	802	
20	N	199	
21	S	563	
22	r	972	
23	R	229	
24	Y	904	
25	7	393	
26	M	855	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	K	439	
28	O	848	
29	y	110	
30	2	188	
31	G	514	
32	a	118	
32	h	118	
33	o	301	
34	t	520	
35	f	240	
35	m	240	
36	Z	324	
37	e	126	
37	l	126	
38	A	2335	
39	8	579	
40	c	92	
40	j	92	
41	I	312	
42	g	119	
42	n	119	
43	P	420	
44	5	116	
45	p	793	
46	F	464	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
47	4	501	49% 79% 5% 16%
48	u	1304	65% 7% 28%
49	T	895	18% 80%

2 Entry composition [i](#)

There are 52 unique types of molecules in this entry. The entry contains 85564 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 U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	D	302	Total	C	N	O	0	0
			1506	902	302	302		

- Molecule 2 is a protein called Splicing factor 3B subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	E	1177	Total	C	N	O	0	0
			5926	3572	1177	1177		

- Molecule 3 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	b	73	Total	C	N	O	0	0
			364	218	73	73		
3	i	72	Total	C	N	O	0	0
			359	215	72	72		

- Molecule 4 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	W	162	Total	C	N	O	0	0
			816	492	162	162		

- Molecule 5 is a protein called Splicing factor 3B subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	w	78	Total	C	N	O	0	0
			391	235	78	78		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	d	69	Total	C	N	O	0	0
			344	206	69	69		
6	k	73	Total	C	N	O	0	0
			364	218	73	73		

- Molecule 7 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	U	1329	Total	C	N	O	0	0
			6730	4072	1329	1329		

- Molecule 8 is a protein called Splicing factor 3B subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	x	79	Total	C	N	O	0	0
			397	239	79	79		

- Molecule 9 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	6	91	Total	C	N	O	P	0	0
			1947	871	359	626	91		

- Molecule 10 is a protein called U2 small nuclear ribonucleoprotein B”.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	B	169	Total	C	N	O	0	0
			851	513	169	169		

- Molecule 11 is a protein called Splicing factor 3B subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	z	108	Total	C	N	O	0	0
			544	328	108	108		

- Molecule 12 is a protein called Ubiquitin-like protein 5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	q	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 13 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	s	1722	Total	C	N	O	0	0
			8688	5244	1722	1722		

- Molecule 14 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	v	206	Total	C	N	O	0	0
			1053	641	206	206		

- Molecule 15 is a protein called BUD13 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	3	55	Total	C	N	O	0	0
			283	173	55	55		

- Molecule 16 is a protein called Smad nuclear-interacting protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	0	150	Total	C	N	O	0	0
			761	461	150	150		

- Molecule 17 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	138	Total	C	N	O	0	0
			695	419	138	138		

- Molecule 18 is a protein called RNA-binding motif protein, X-linked 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	1	122	Total	C	N	O	0	0
			607	363	122	122		

- Molecule 19 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	L	116	Total	C	N	O	0	0
			582	350	116	116		

- Molecule 20 is a protein called Zinc finger matrin-type protein 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	N	56	Total	C	N	O	0	0
			277	165	56	56		

- Molecule 21 is a protein called Beta-catenin-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	S	355	Total	C	N	O	0	0
			1771	1061	355	355		

- Molecule 22 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	r	895	Total	C	N	O	0	0
			4531	2741	895	895		

- Molecule 23 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	R	44	Total	C	N	O	0	0
			219	131	44	44		

- Molecule 24 is a protein called Serine/arginine repetitive matrix protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	Y	95	Total	C	N	O	0	0
			478	288	95	95		

- Molecule 25 is a protein called DNA/RNA-binding protein KIN17.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	7	236	Total	C	N	O	0	0
			1178	706	236	236		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M	706	Total	C	N	O	0	0
			3553	2141	706	706		

- Molecule 27 is a protein called Microfibrillar-associated protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	K	123	Total	C	N	O	0	0
			614	368	123	123		

- Molecule 28 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	O	248	Total	C	N	O	0	0
			1243	747	248	248		

- Molecule 29 is a protein called PHD finger-like domain-containing protein 5A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	y	100	Total	C	N	O	0	0
			498	298	100	100		

- Molecule 30 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	2	164	Total	C	N	O	P	0	0
			3479	1554	600	1161	164		

- Molecule 31 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	G	320	Total	C	N	O	0	0
			1604	964	320	320		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	h	95	Total	C	N	O	0	0
			482	292	95	95		
32	a	78	Total	C	N	O	0	0
			393	237	78	78		

- Molecule 33 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	o	229	Total	C	N	O	0	0
			1135	677	229	229		

- Molecule 34 is a protein called RING-type E3 ubiquitin-protein ligase PPIL2.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	t	253	Total	C	N	O	0	0
			1272	766	253	253		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	m	82	Total	C	N	O	0	0
			413	249	82	82		
35	f	64	Total	C	N	O	0	0
			319	191	64	64		

- Molecule 36 is a RNA chain called MINX M3 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Z	57	Total	C	N	O	P	0	0
			1201	538	203	403	57		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	l	83	Total	C	N	O	0	0
			415	249	83	83		
37	e	78	Total	C	N	O	0	0
			390	234	78	78		

- Molecule 38 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	A	2163	Total	C	N	O	0	0
			10968	6642	2163	2163		

- Molecule 39 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	8	18	Total	C	N	O	0	0
			92	56	18	18		

- Molecule 40 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	j	81	Total	C	N	O	0	0
			403	241	81	81		
40	c	78	Total	C	N	O	0	0
			388	232	78	78		

- Molecule 41 is a protein called Pre-mRNA-splicing factor 38A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	I	176	Total	C	N	O	0	0
			883	531	176	176		

- Molecule 42 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	n	80	Total	C	N	O	0	0
			402	242	80	80		
42	g	93	Total	C	N	O	0	0
			469	283	93	93		

- Molecule 43 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	P	237	Total	C	N	O	0	0
			1194	720	237	237		

- Molecule 44 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	5	114	Total	C	N	O	P	0	0
			2397	1074	399	810	114		

- Molecule 45 is a protein called Splicing factor 3A subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	p	124	Total	C	N	O	0	0
			631	383	124	124		

- Molecule 46 is a protein called Splicing factor 3A subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	F	165	Total	C	N	O	0	0
			835	505	165	165		

- Molecule 47 is a protein called Splicing factor 3A subunit 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	4	421	Total	C	N	O	0	0
			2110	1268	421	421		

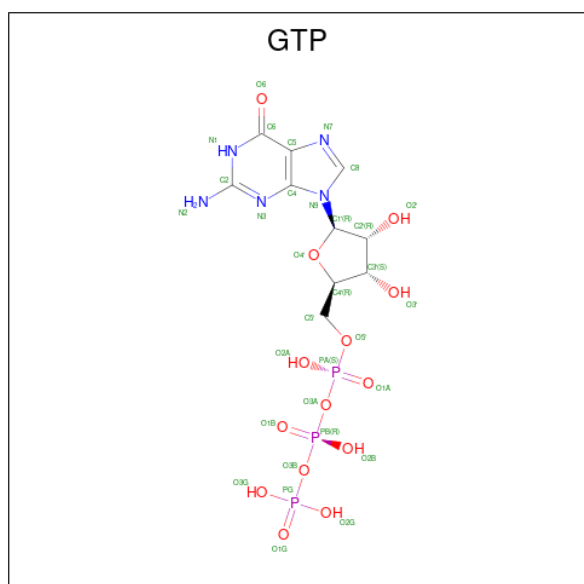
- Molecule 48 is a protein called Splicing factor 3B subunit 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	u	941	Total	C	N	O	0	0
			4748	2866	941	941		

- Molecule 49 is a protein called Splicing factor 3B subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	T	183	Total	C	N	O	0	0
			942	576	183	183		

- Molecule 50 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

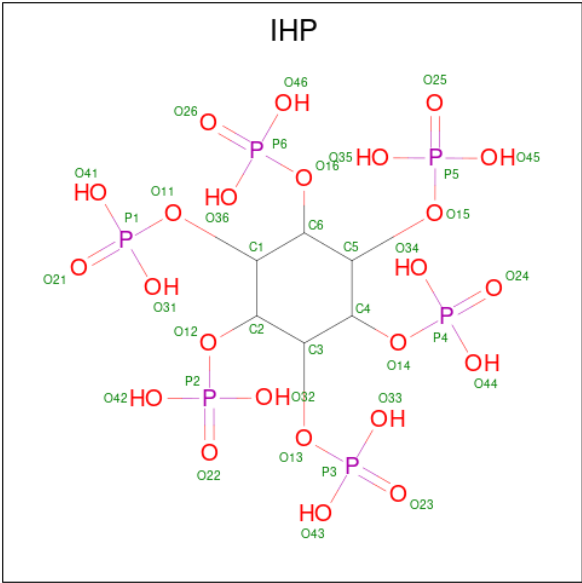


Mol	Chain	Residues	Atoms					AltConf
50	r	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 51 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
51	r	1	Total	Mg	0
			1	1	

- Molecule 52 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$).

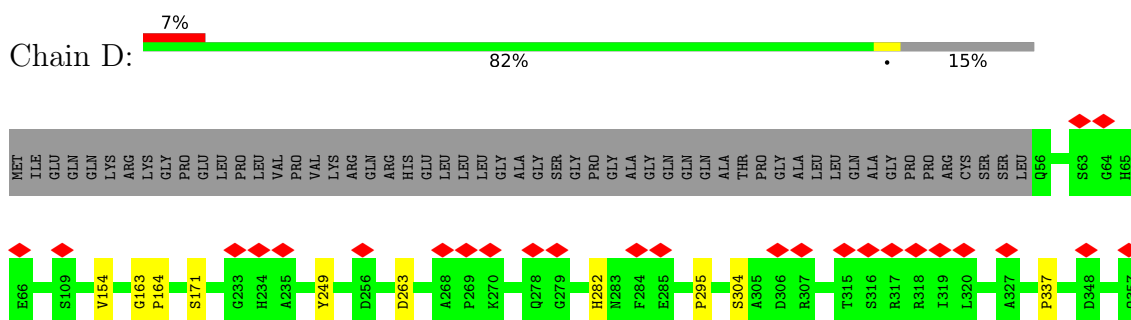


Mol	Chain	Residues	Atoms				AltConf
52	A	1	Total	C	O	P	0
			36	6	24	6	

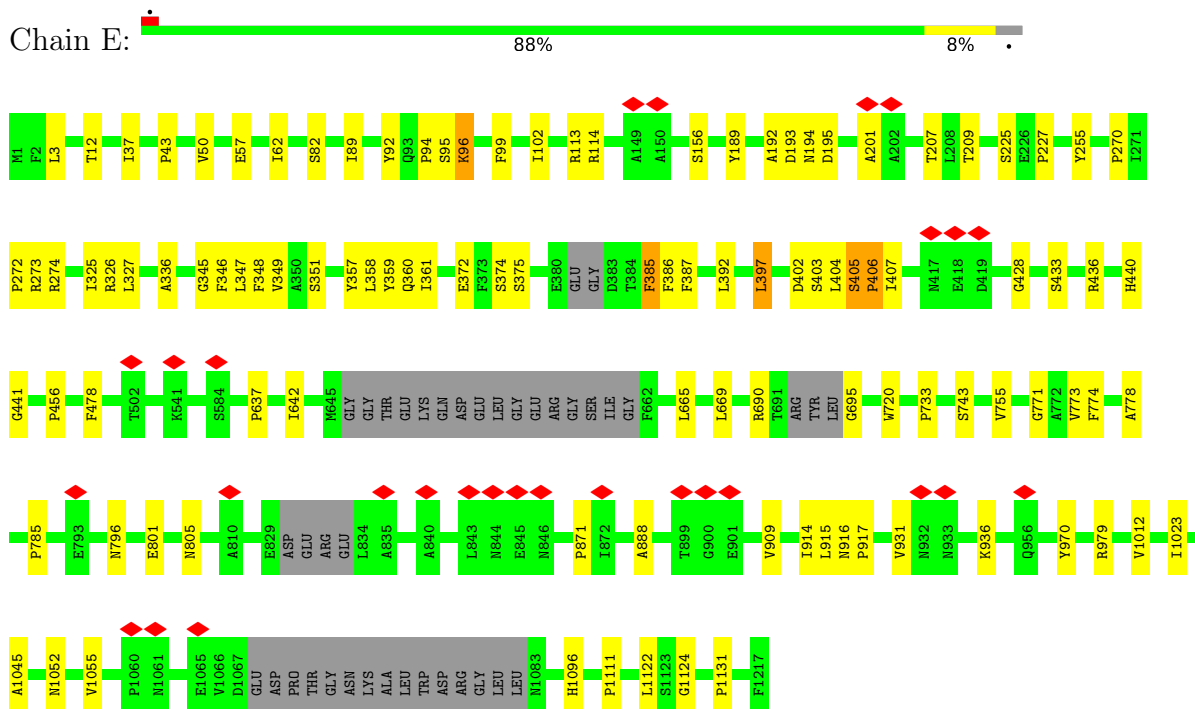
3 Residue-property plots

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

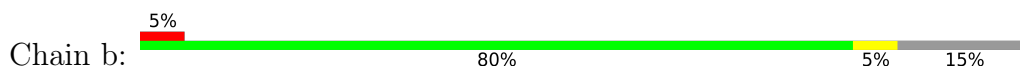
- Molecule 1: U5 small nuclear ribonucleoprotein 40 kDa protein

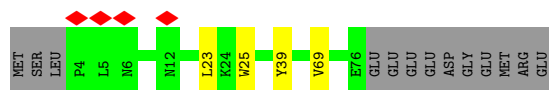


- Molecule 2: Splicing factor 3B subunit 3

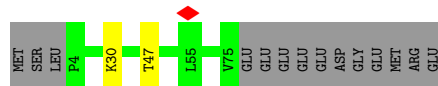
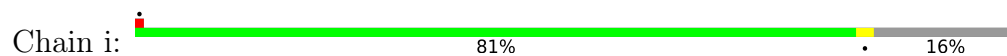


- Molecule 3: Small nuclear ribonucleoprotein F

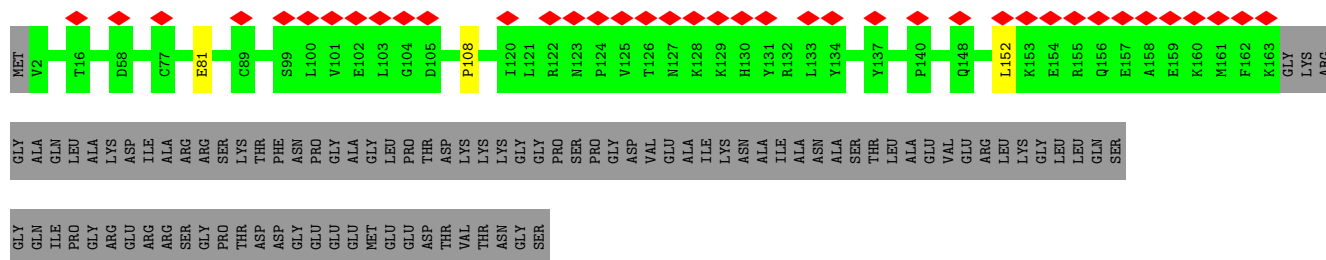




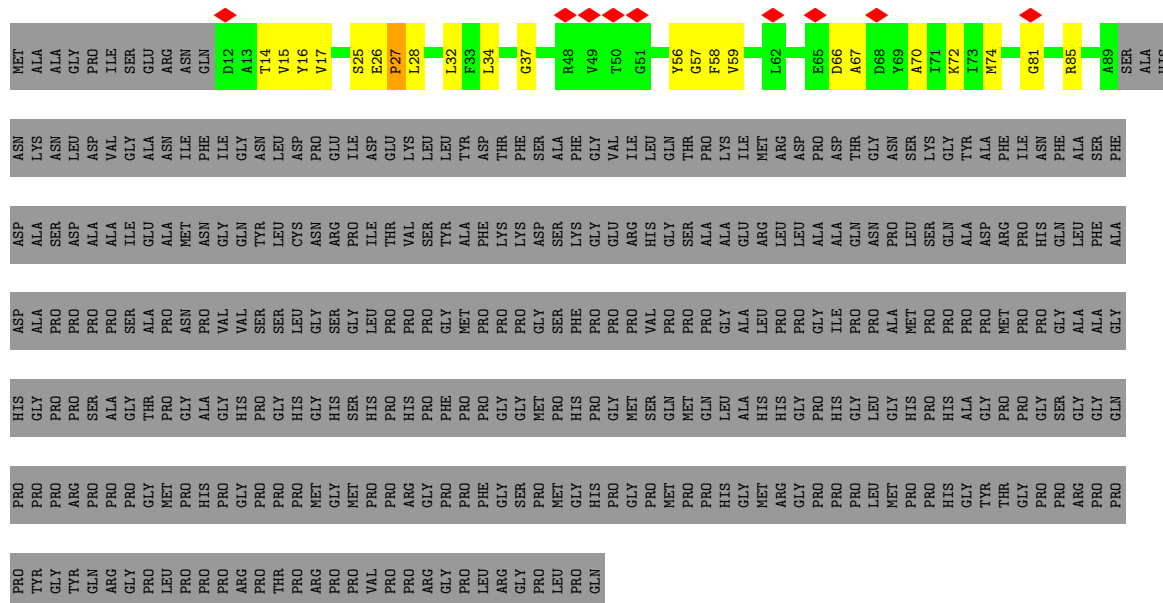
- Molecule 3: Small nuclear ribonucleoprotein F



- Molecule 4: U2 small nuclear ribonucleoprotein A'

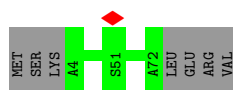


- Molecule 5: Splicing factor 3B subunit 4

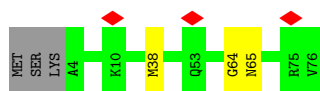
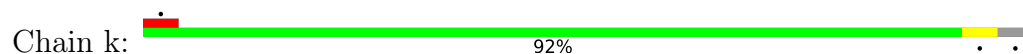


- Molecule 6: Small nuclear ribonucleoprotein G

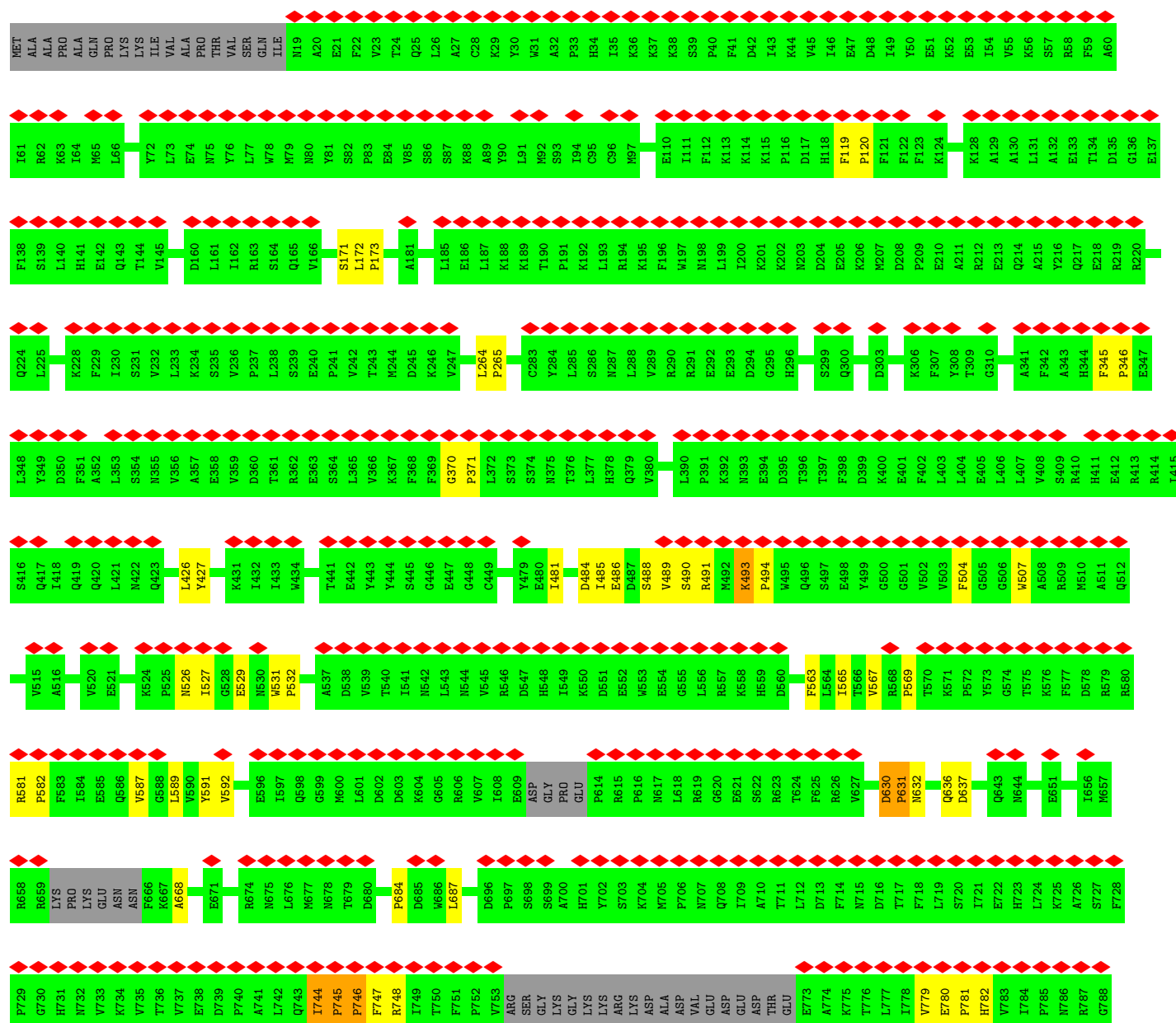
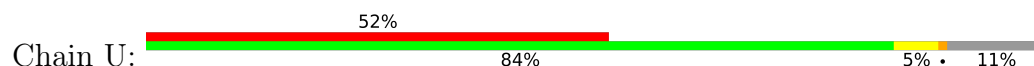


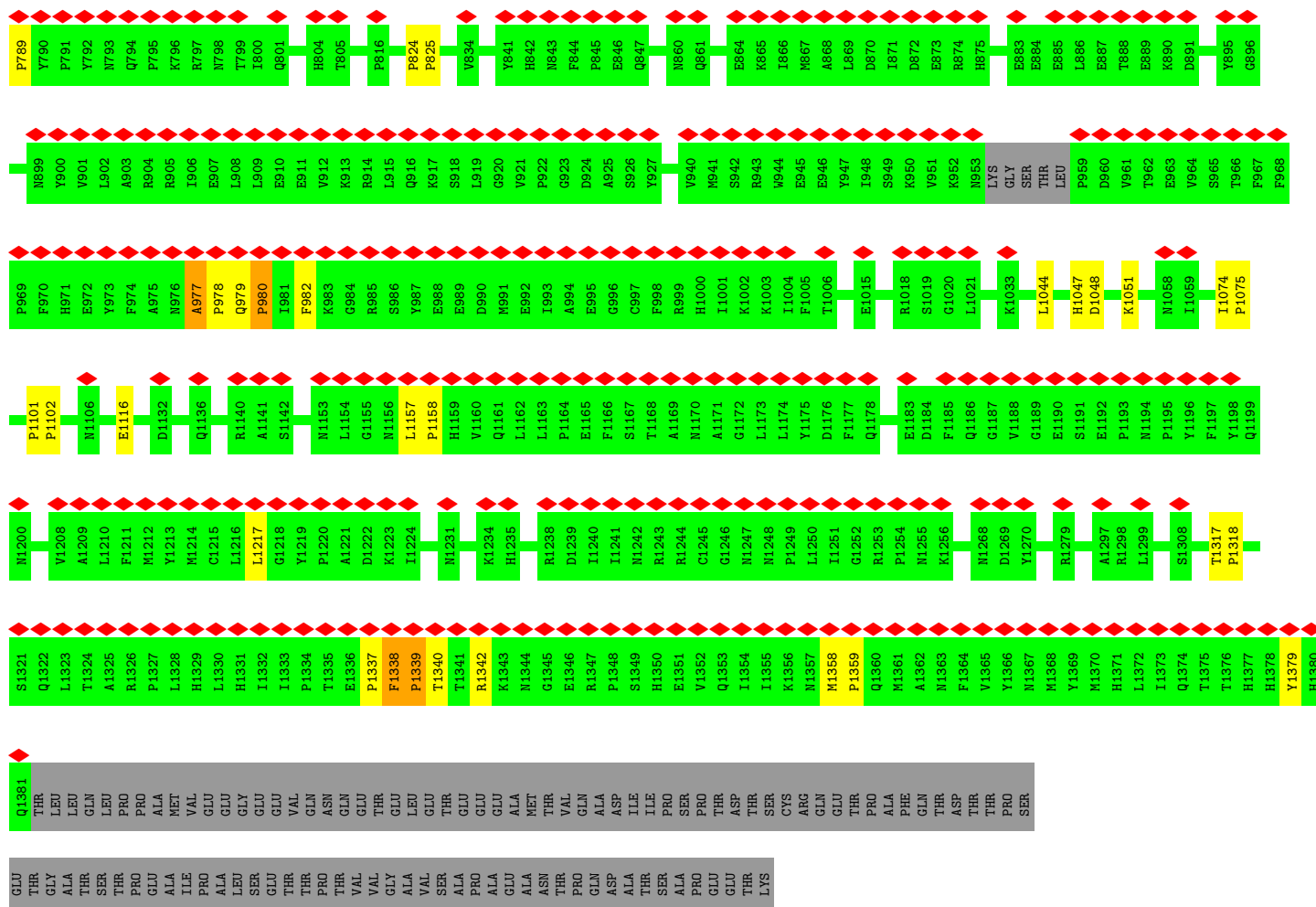


- Molecule 6: Small nuclear ribonucleoprotein G



- Molecule 7: Intron-binding protein aquarius





• Molecule 8: Splicing factor 3B subunit 5

Chain x: 76% 15% 8%



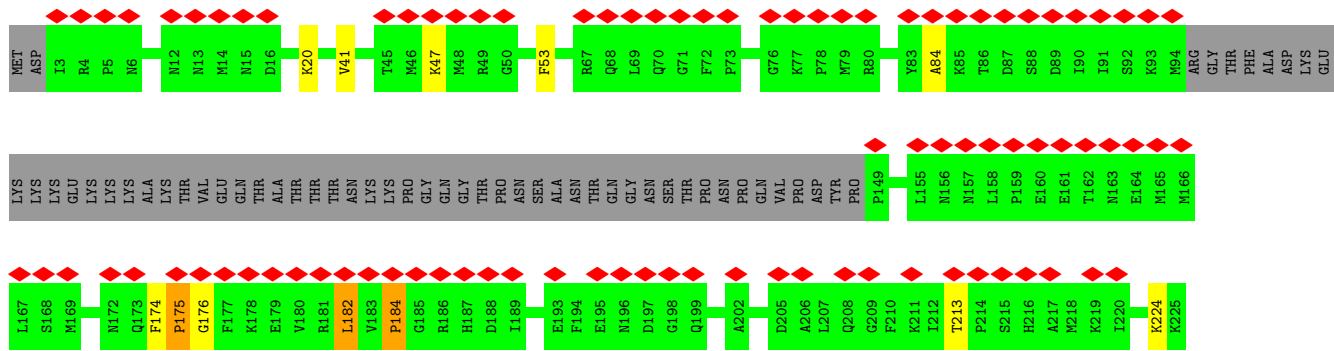
• Molecule 9: U6 snRNA

Chain 6: 5% 30% 24% 25% 7% 14%



• Molecule 10: U2 small nuclear ribonucleoprotein B''

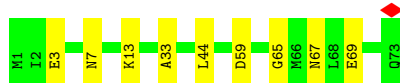
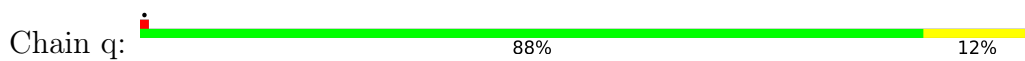
Chain B: 40% 70% 25%



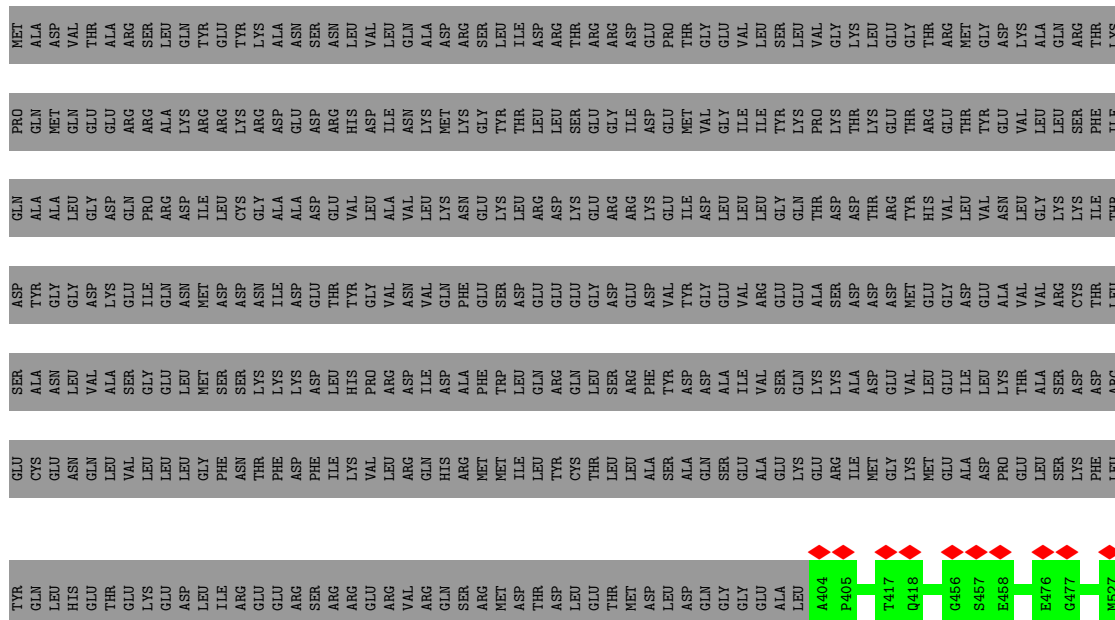
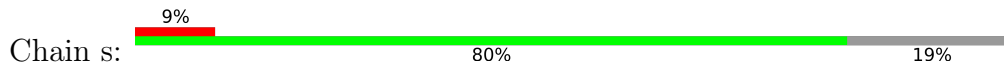
- Molecule 11: Splicing factor 3B subunit 6

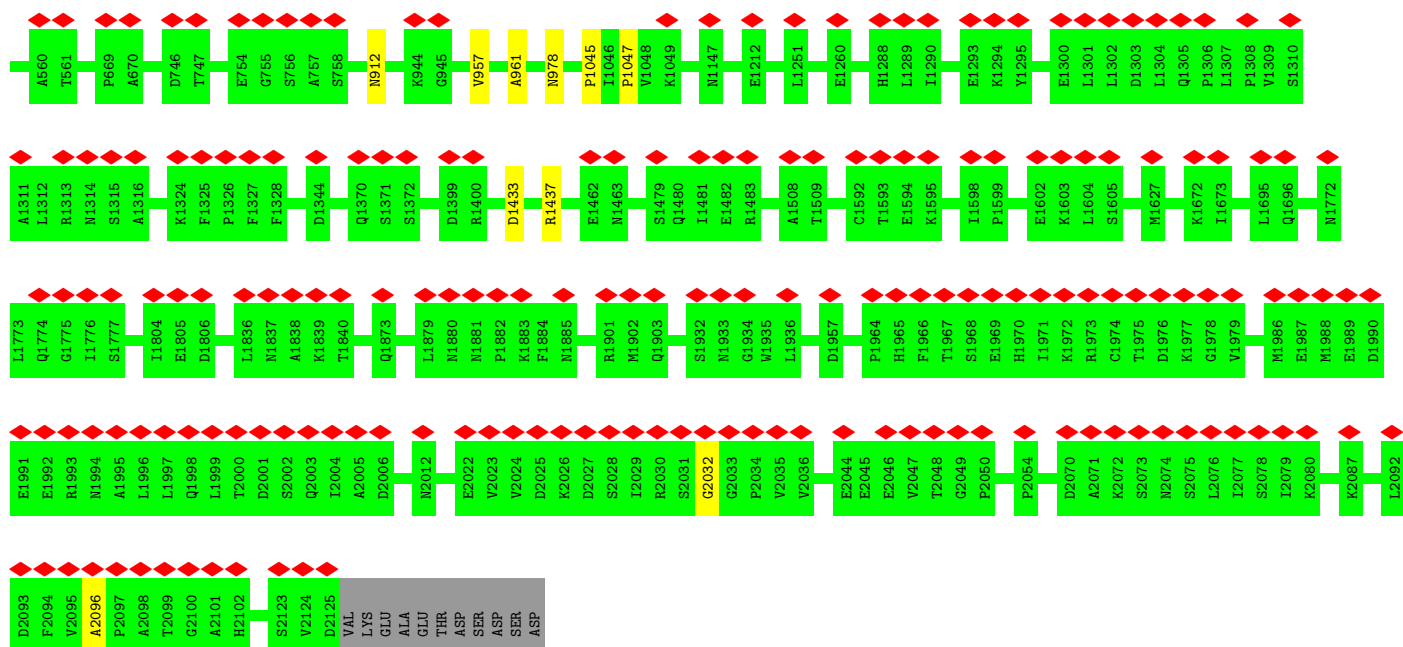


- Molecule 12: Ubiquitin-like protein 5

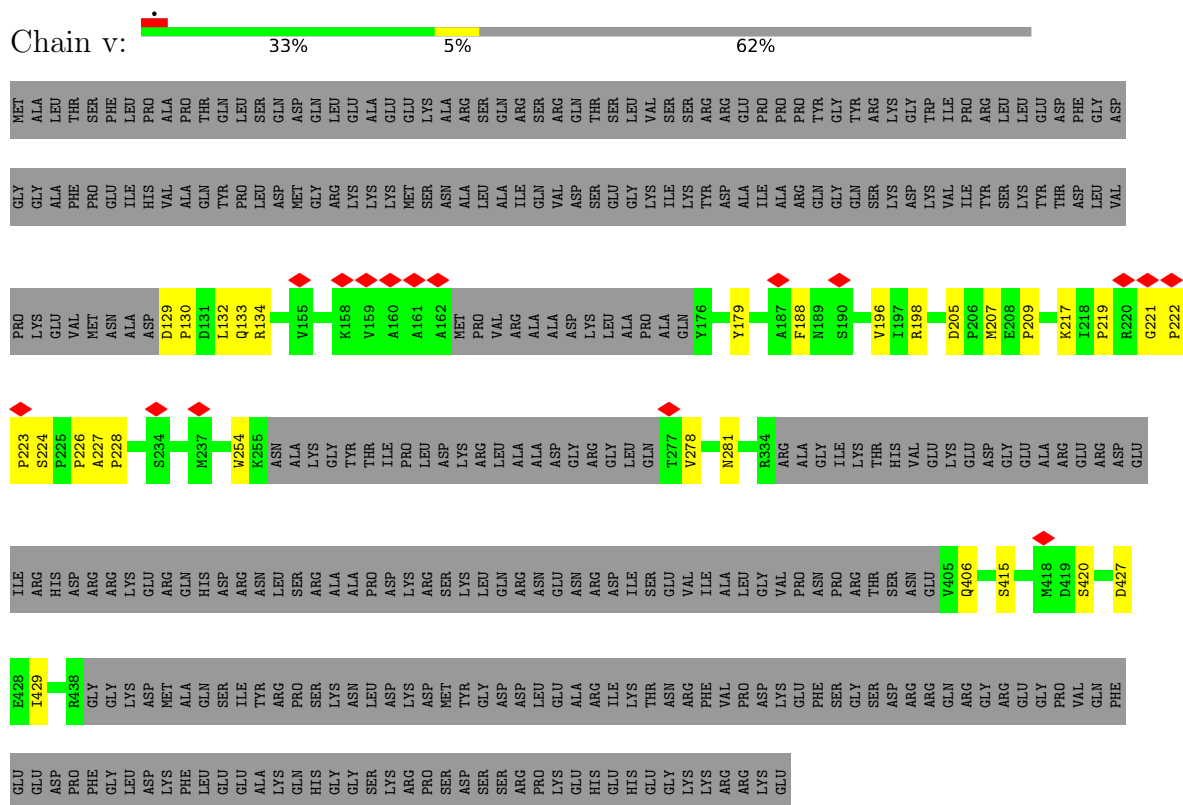


- Molecule 13: U5 small nuclear ribonucleoprotein 200 kDa helicase

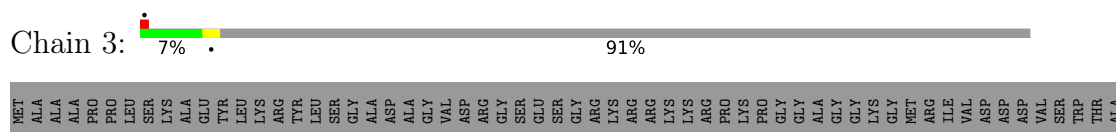


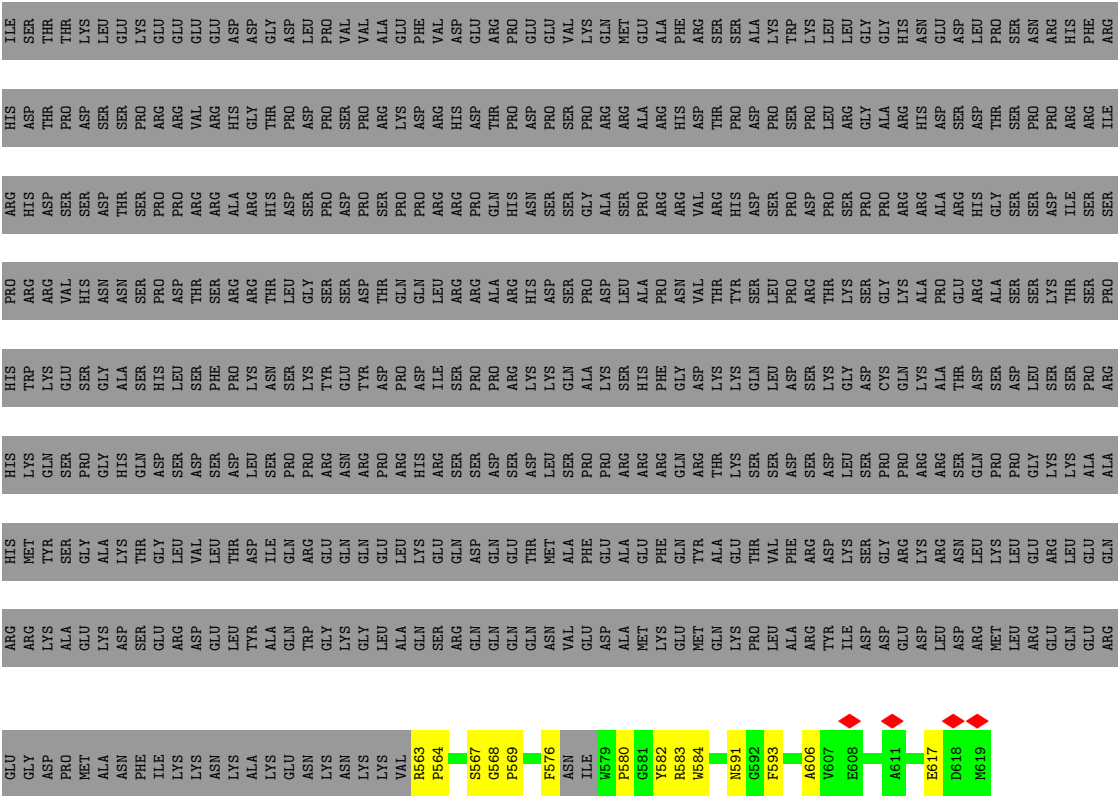


• Molecule 14: SNW domain-containing protein 1

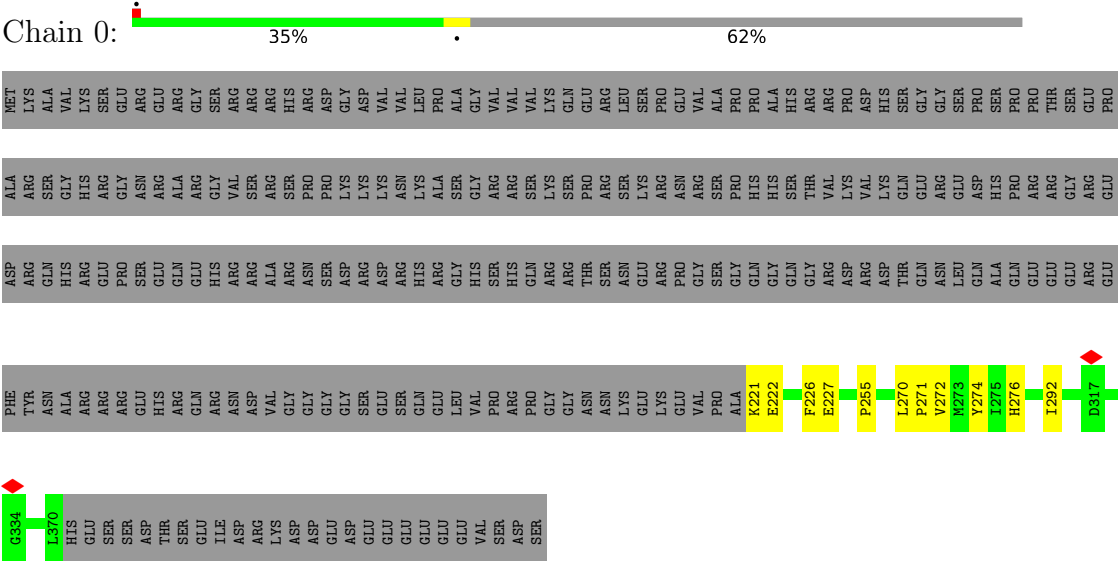


• Molecule 15: BUD13 homolog

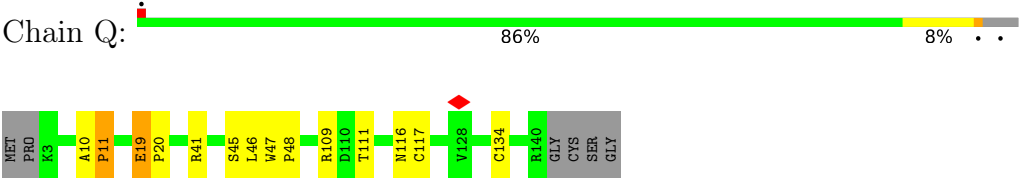




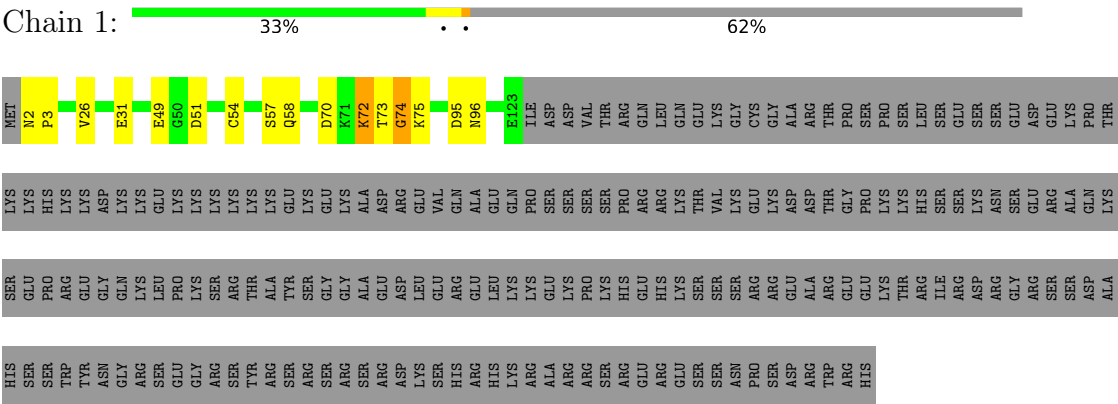
• Molecule 16: Smad nuclear-interacting protein 1



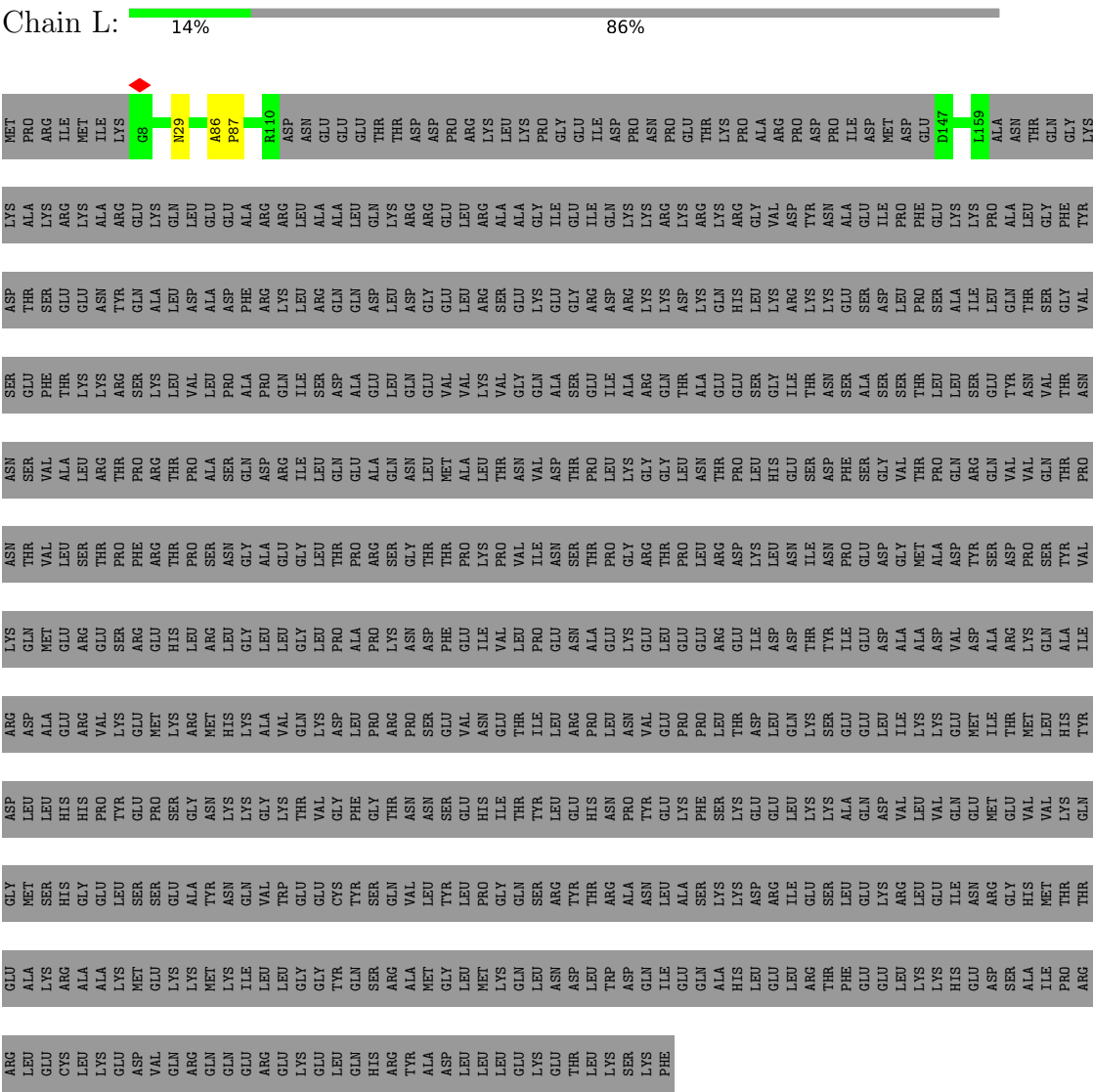
• Molecule 17: Protein BUD31 homolog



• Molecule 18: RNA-binding motif protein, X-linked 2



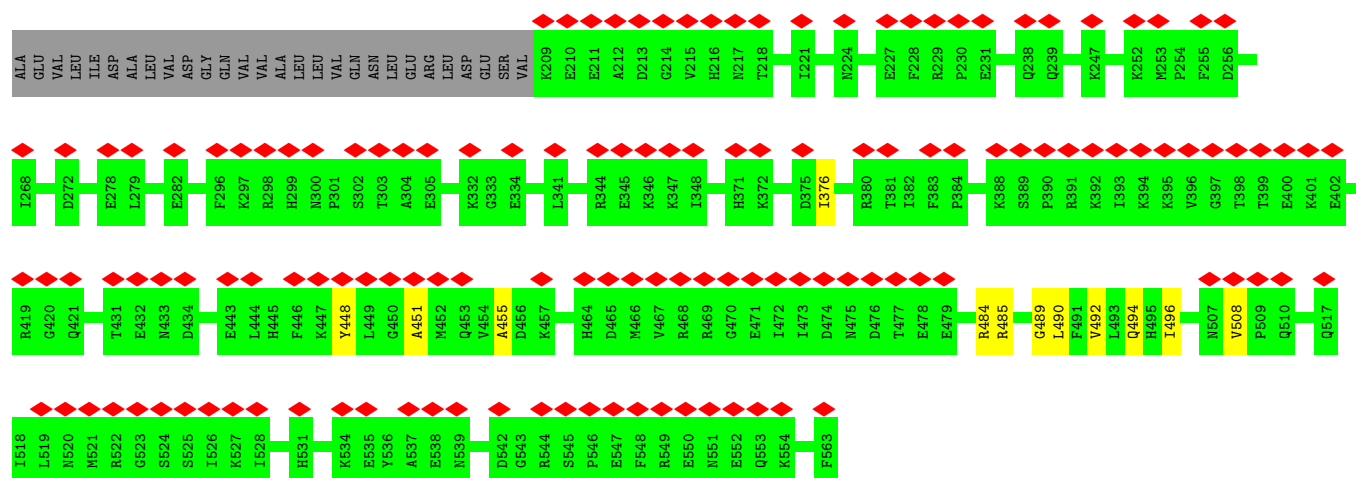
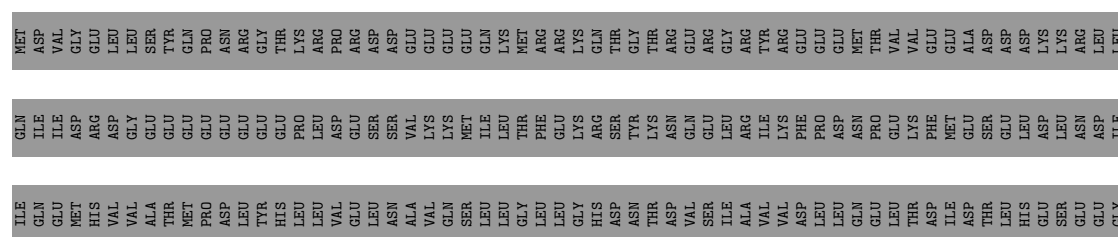
• Molecule 19: Cell division cycle 5-like protein



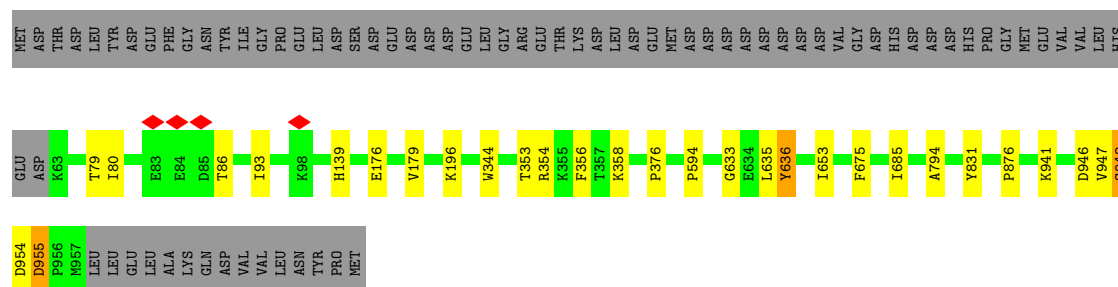
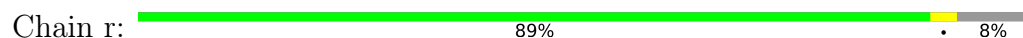
• Molecule 20: Zinc finger matrin-type protein 2



- Molecule 21: Beta-catenin-like protein 1



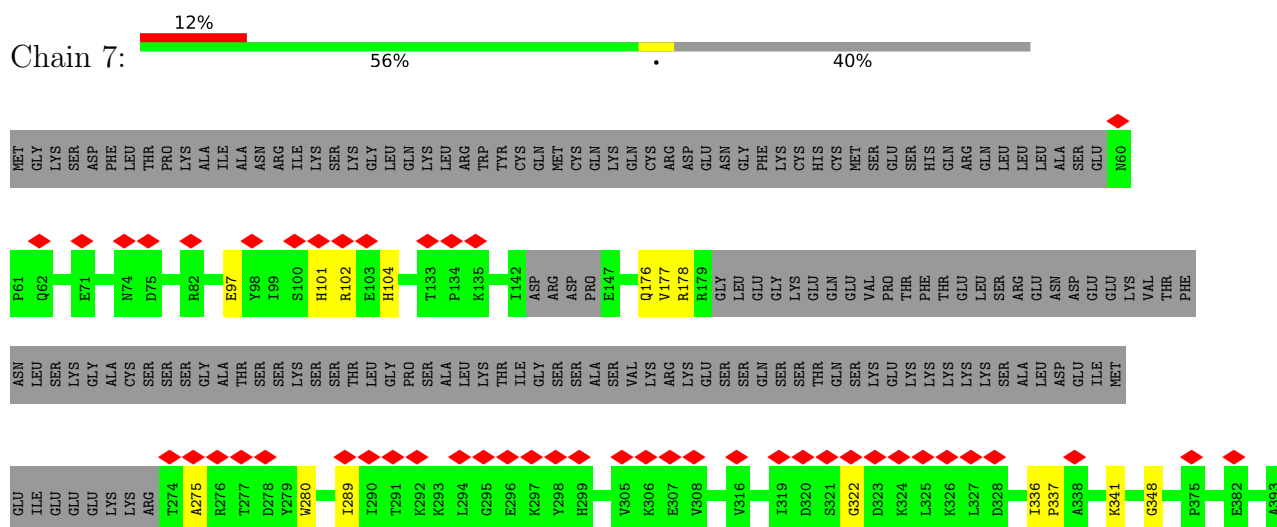
- Molecule 22: 116 kDa U5 small nuclear ribonucleoprotein component



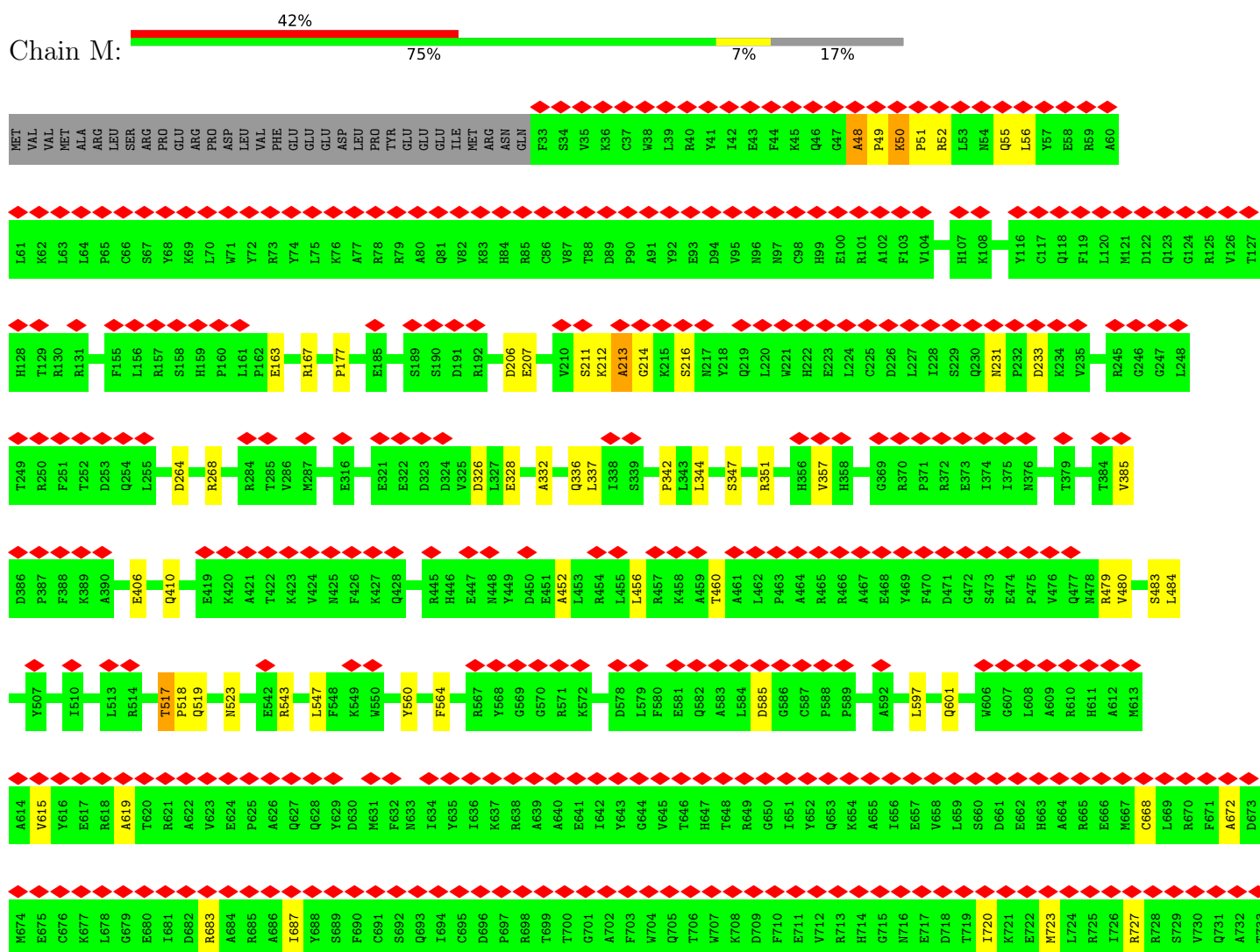
- Molecule 23: Spliceosome-associated protein CWC15 homolog



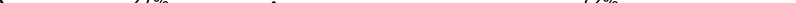
• Molecule 25: DNA/RNA-binding protein KIN17

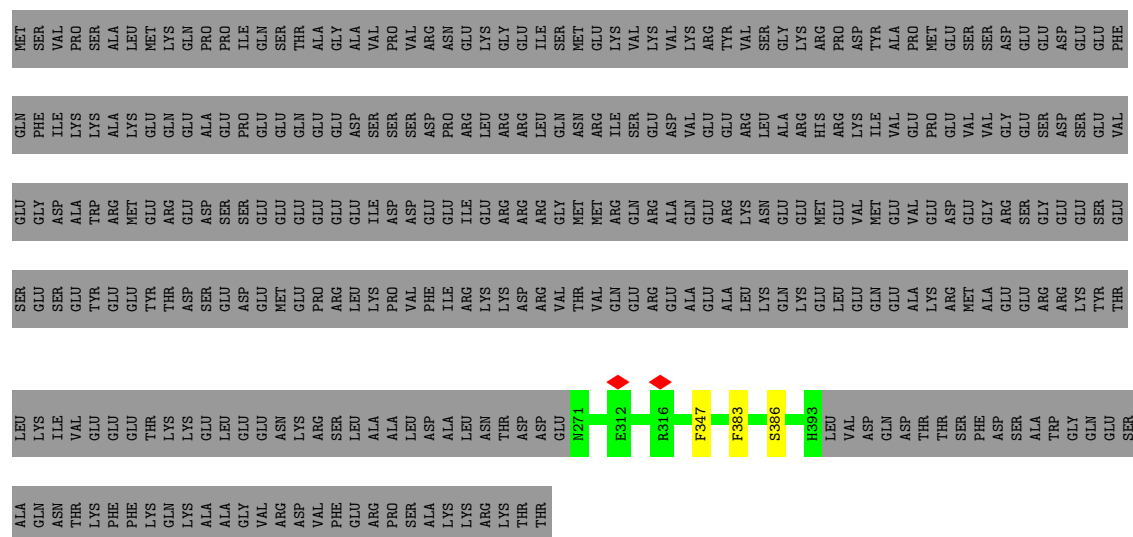


• Molecule 26: Pre-mRNA-splicing factor SYF1

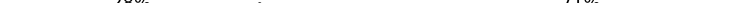


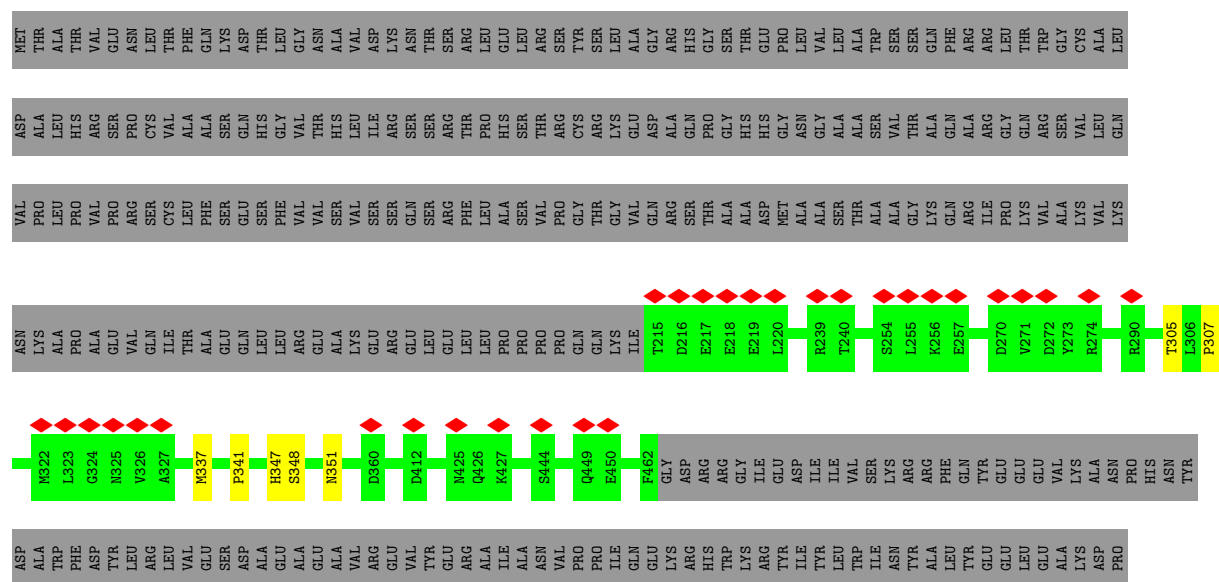
- Molecule 27: Microfibrillar-associated protein 1

Chain K:  27% : 72%



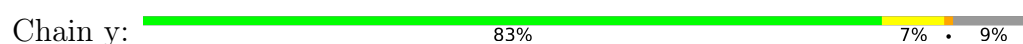
- Molecule 28: Crooked neck-like protein 1

Chain O:  28% 71%

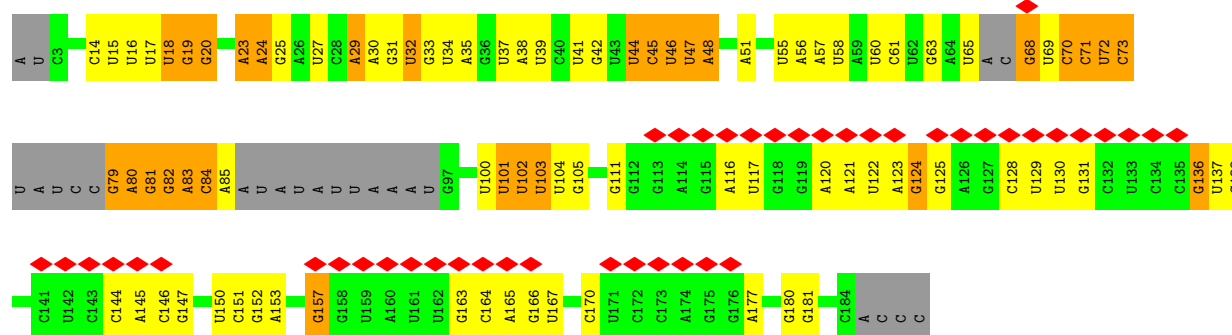




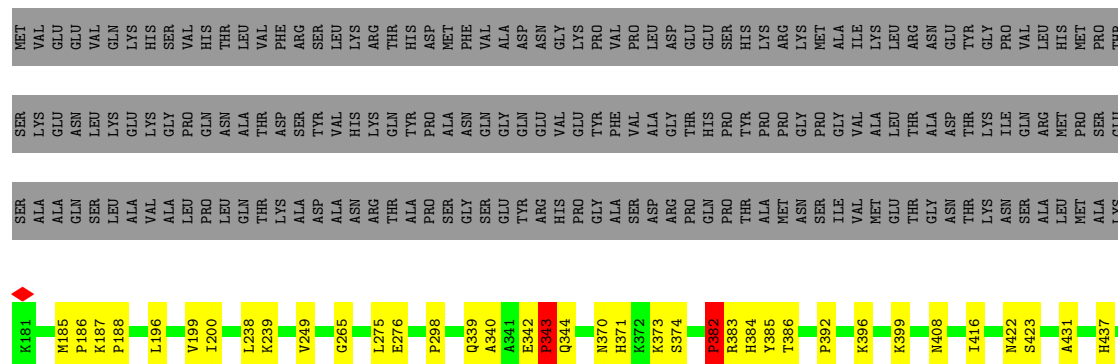
- Molecule 29: PHD finger-like domain-containing protein 5A



- Molecule 30: U2 snRNA

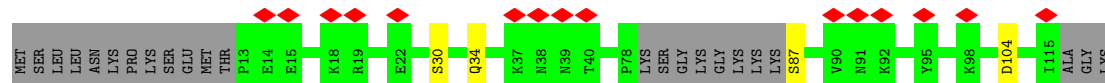
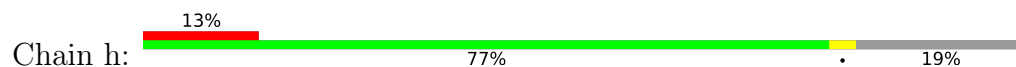


- Molecule 31: Pleiotropic regulator 1

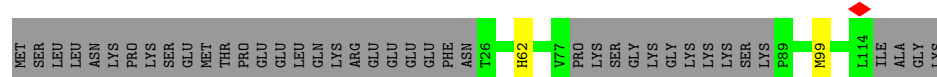




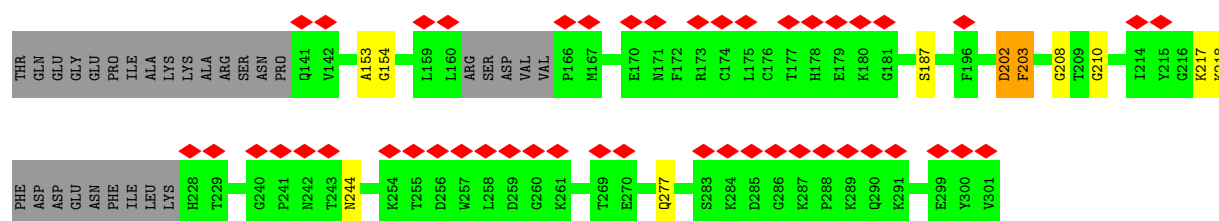
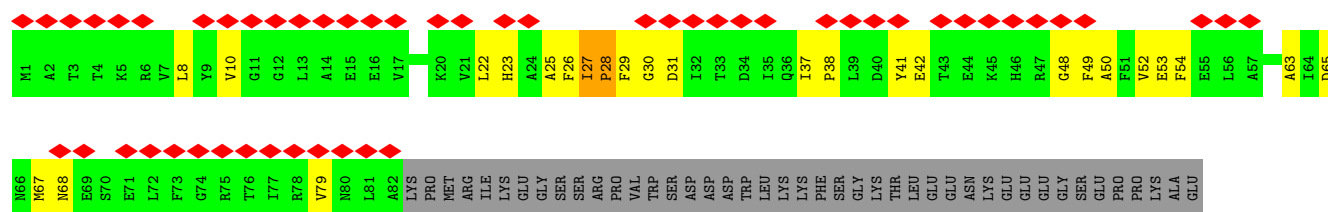
• Molecule 32: Small nuclear ribonucleoprotein Sm D2



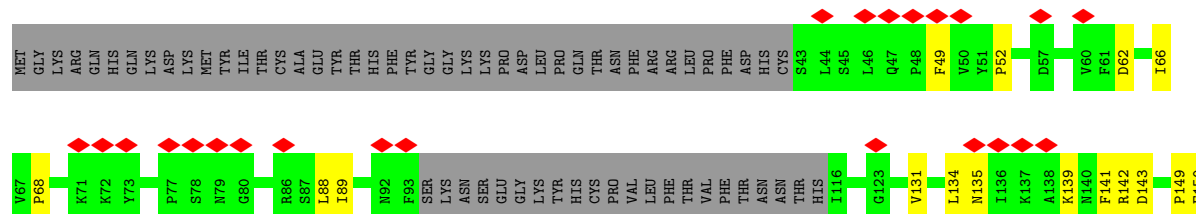
• Molecule 32: Small nuclear ribonucleoprotein Sm D2

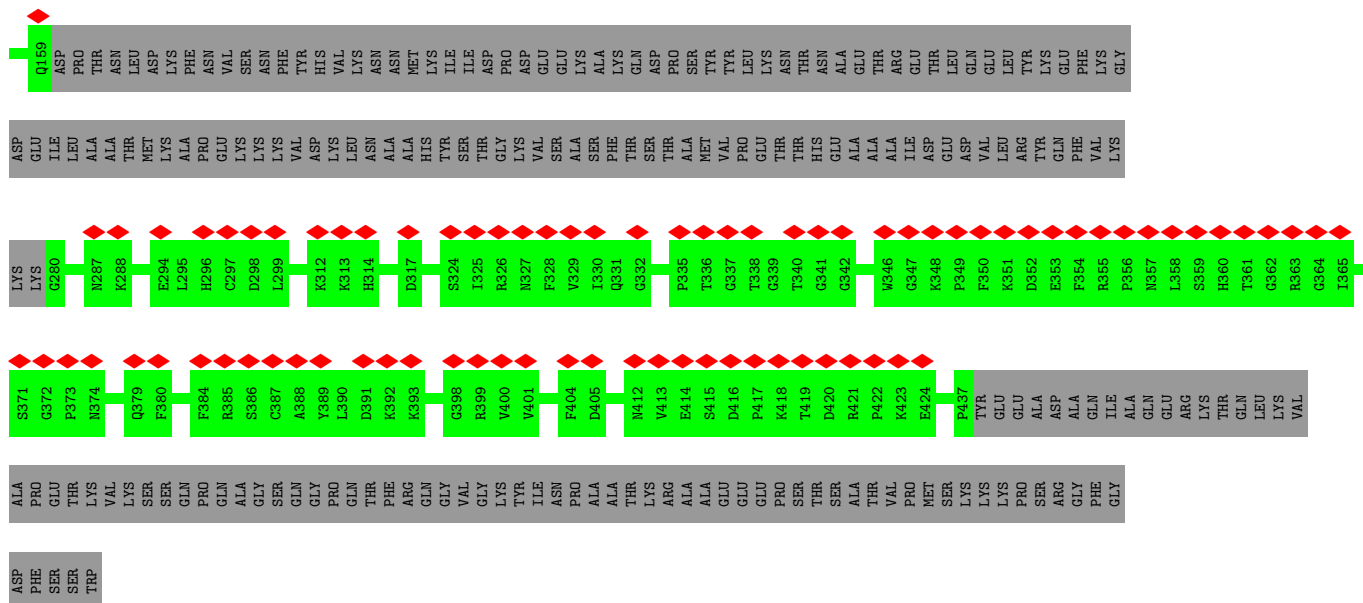


• Molecule 33: Peptidyl-prolyl cis-trans isomerase E

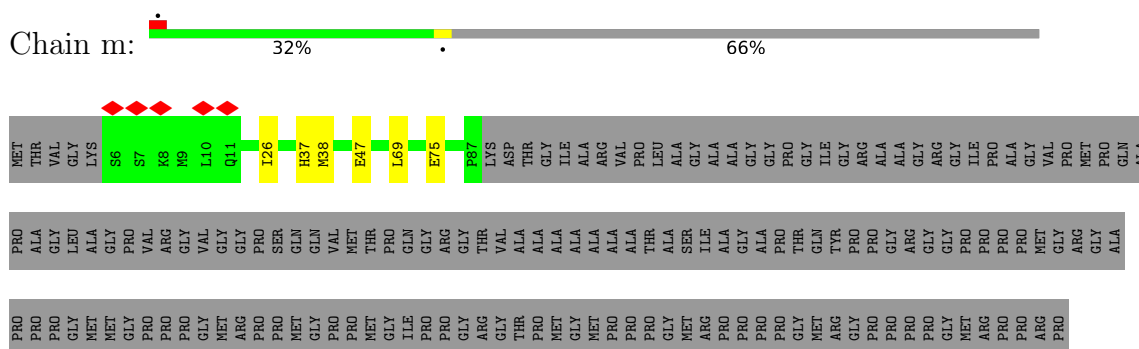


• Molecule 34: RING-type E3 ubiquitin-protein ligase PPIL2

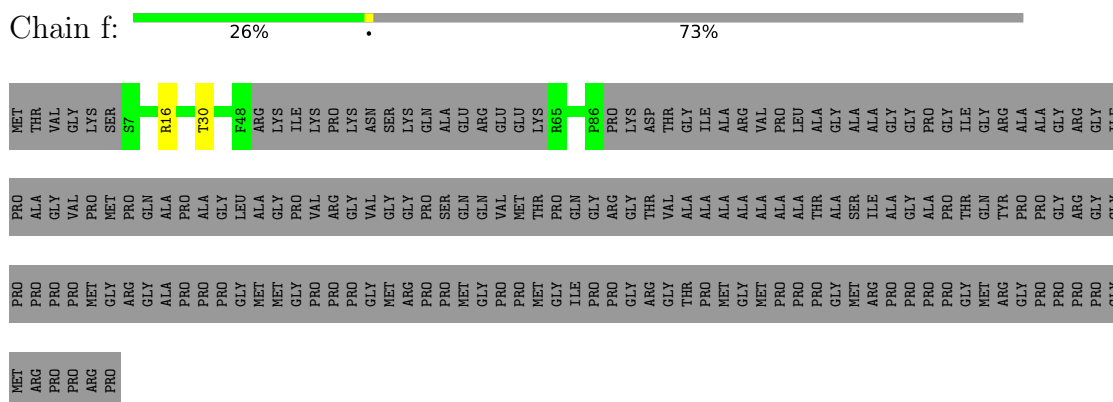




- Molecule 35: Small nuclear ribonucleoprotein-associated proteins B and B'



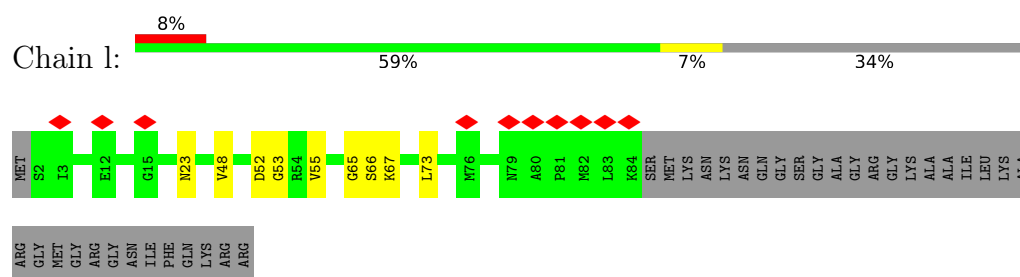
- Molecule 35: Small nuclear ribonucleoprotein-associated proteins B and B'



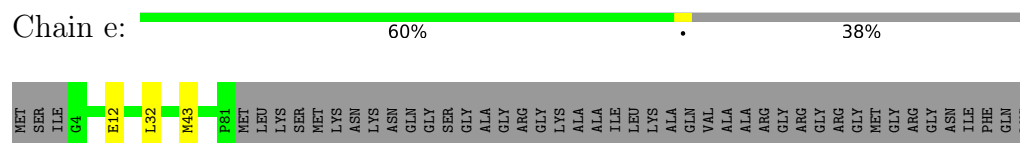
- Molecule 36: MINX M3 pre-mRNA



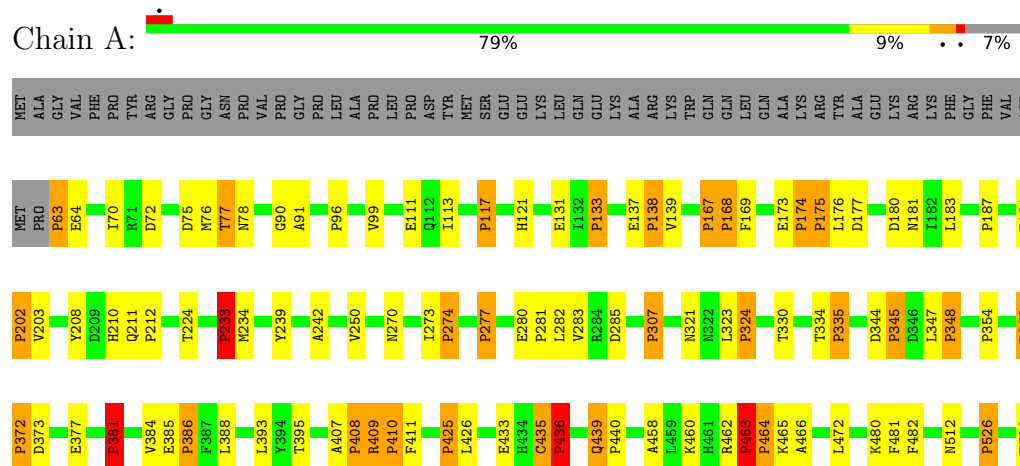
- Molecule 37: Small nuclear ribonucleoprotein Sm D3

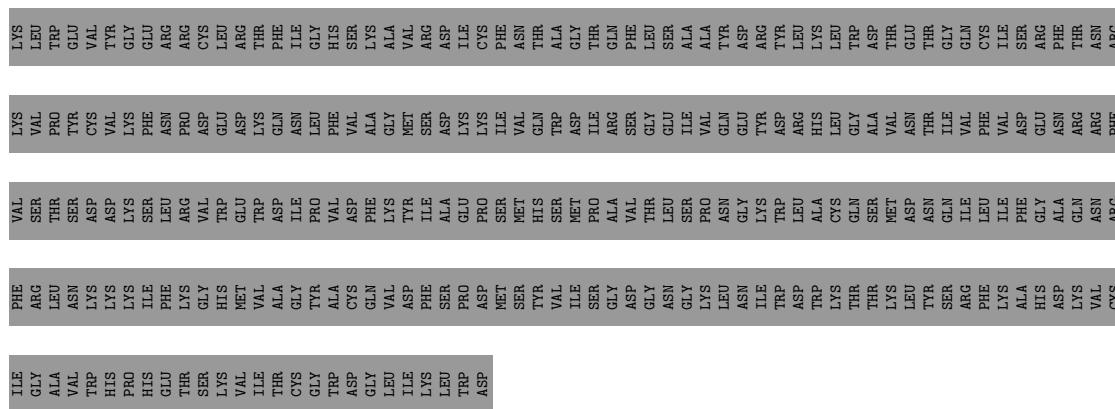


- Molecule 37: Small nuclear ribonucleoprotein Sm D3

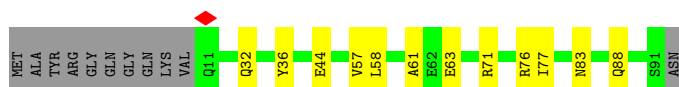
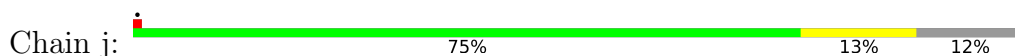


- Molecule 38: Pre-mRNA-processing-splicing factor 8

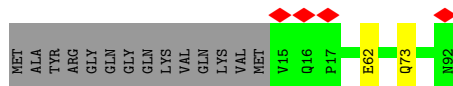
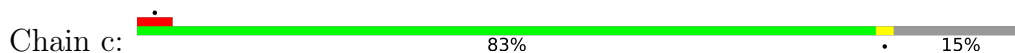




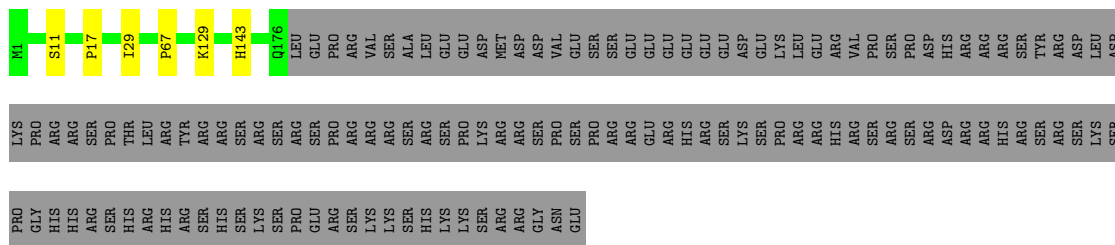
- Molecule 40: Small nuclear ribonucleoprotein E



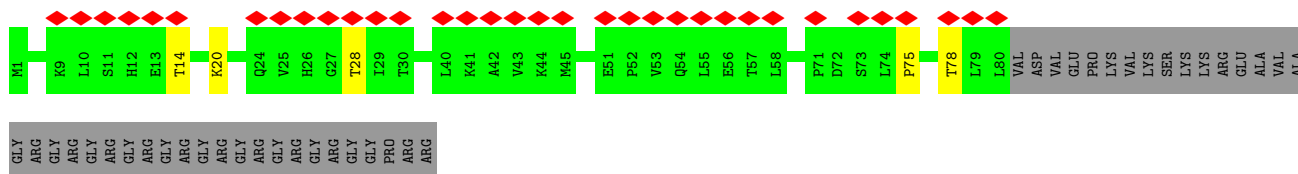
- Molecule 40: Small nuclear ribonucleoprotein E



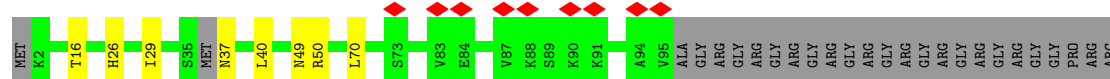
- Molecule 41: Pre-mRNA-splicing factor 38A



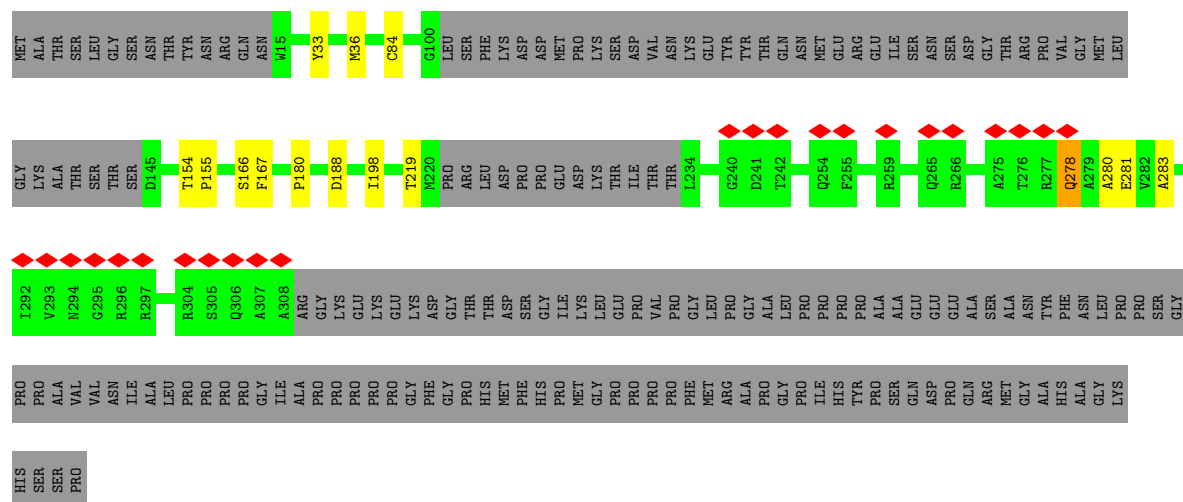
- Molecule 42: Small nuclear ribonucleoprotein Sm D1



- Molecule 42: Small nuclear ribonucleoprotein Sm D1



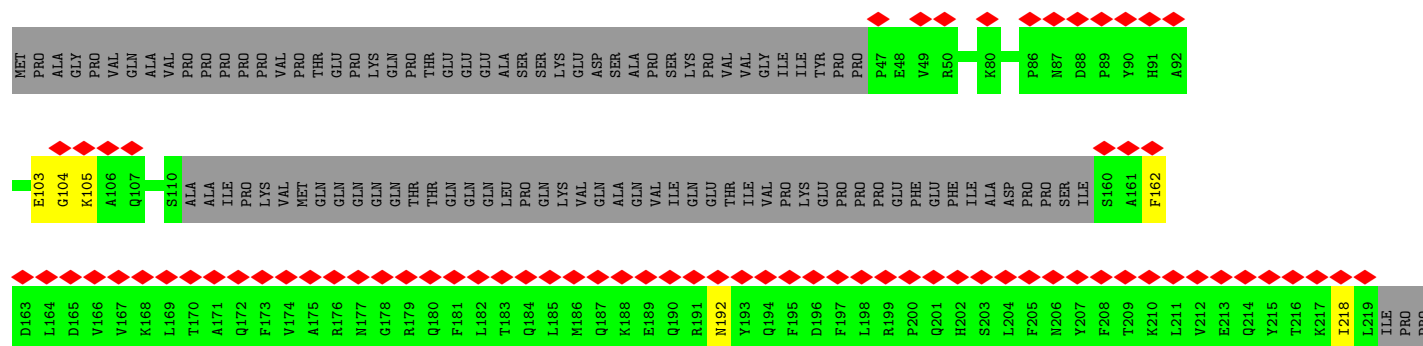
• Molecule 43: Pre-mRNA-splicing factor RBM22

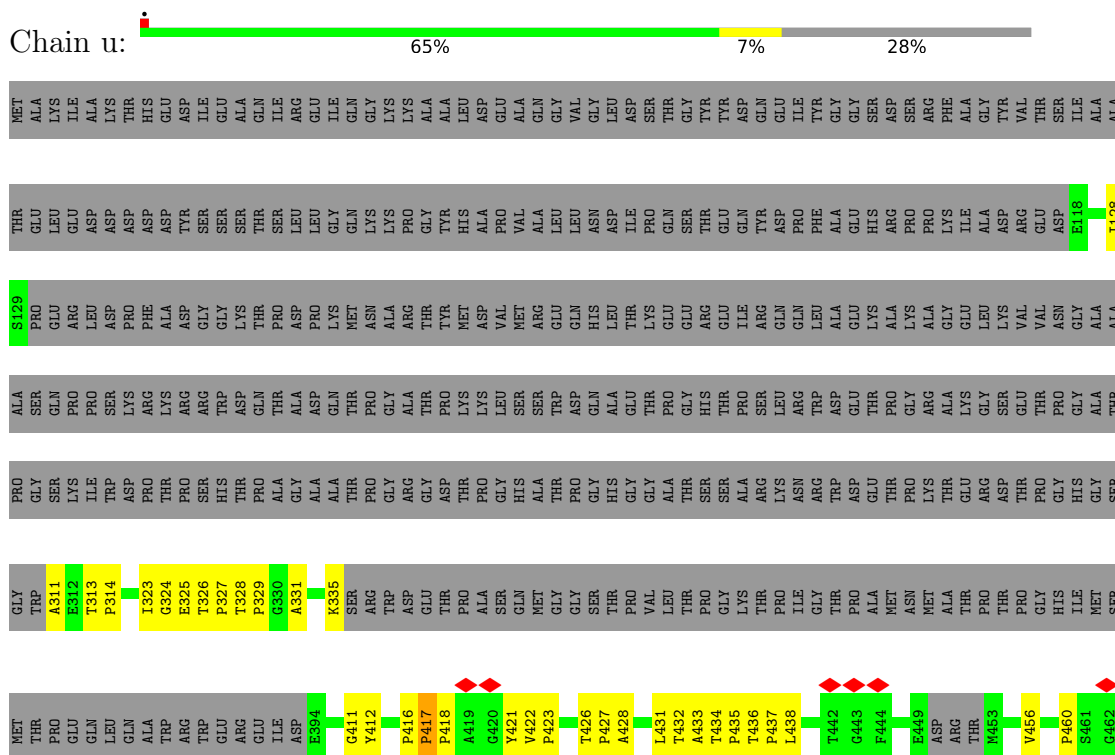


• Molecule 44: U5 snRNA



• Molecule 45: Splicing factor 3A subunit 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	39336	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2.27	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.055	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.013	Depositor
Map size ($\text{\AA}$)	445.44, 445.44, 445.44	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.16, 1.16, 1.16	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	D	0.16	0/1515	0.52	0/2113
2	E	0.34	0/5980	0.52	0/8363
3	b	0.22	0/367	0.53	0/509
3	i	0.40	0/362	0.71	0/502
4	W	0.28	0/821	0.69	0/1149
5	w	1.01	0/394	1.13	1/549 (0.2%)
6	d	0.24	0/346	0.60	0/481
6	k	0.45	0/366	0.72	0/509
7	U	0.47	1/6796 (0.0%)	0.95	7/9527 (0.1%)
8	x	0.71	0/399	0.88	2/557 (0.4%)
9	6	0.44	0/2178	0.87	15/3388 (0.4%)
10	B	1.05	0/857	1.23	6/1196 (0.5%)
11	z	0.21	0/548	0.60	1/766 (0.1%)
12	q	0.51	0/359	0.77	0/498
13	s	0.17	0/8766	0.50	0/12286
14	v	0.19	0/1064	0.62	1/1491 (0.1%)
15	3	0.20	0/288	0.67	0/404
16	0	0.25	0/770	0.56	0/1079
17	Q	0.64	1/700 (0.1%)	1.08	5/979 (0.5%)
18	1	0.33	0/609	0.57	0/848
19	L	0.22	0/583	0.62	0/813
20	N	0.17	0/276	0.67	0/383
21	S	0.45	0/1778	0.91	2/2482 (0.1%)
22	r	0.34	0/4585	0.59	7/6429 (0.1%)
23	R	0.21	0/218	0.64	0/303
24	Y	0.13	0/481	0.94	2/672 (0.3%)
25	7	1.42	0/1181	1.66	10/1645 (0.6%)
26	M	0.27	0/3576	0.56	3/5009 (0.1%)
27	K	0.16	0/615	0.35	0/858
28	O	0.18	0/1245	0.55	0/1742
29	y	0.23	0/501	0.72	2/697 (0.3%)
30	2	0.34	5/3882 (0.1%)	0.61	9/6040 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	G	0.36	0/1616	0.67	3/2258 (0.1%)
32	a	0.16	0/394	0.48	0/548
32	h	0.38	0/485	0.71	0/677
33	o	0.79	0/1139	0.89	1/1578 (0.1%)
34	t	0.80	0/1283	1.35	12/1790 (0.7%)
35	f	0.16	0/319	0.40	0/442
35	m	0.40	0/416	0.65	0/581
36	Z	0.39	3/1338 (0.2%)	0.51	0/2077
37	e	0.19	0/392	0.47	0/546
37	l	0.47	0/417	0.78	0/581
38	A	0.64	3/11086 (0.0%)	1.11	103/15554 (0.7%)
39	8	0.26	0/92	0.57	0/128
40	c	0.18	0/388	0.58	0/540
40	j	0.42	0/403	0.76	0/561
41	I	0.18	0/888	0.55	0/1241
42	g	0.19	0/471	0.47	0/657
42	n	0.39	0/404	0.66	0/564
43	P	0.56	1/1203 (0.1%)	1.04	4/1680 (0.2%)
44	5	0.17	0/2672	0.31	0/4154
45	p	0.74	0/636	1.54	2/890 (0.2%)
46	F	0.64	0/840	1.12	2/1174 (0.2%)
47	4	0.86	0/2119	1.62	12/2960 (0.4%)
48	u	0.36	0/4792	0.71	4/6707 (0.1%)
49	T	0.81	4/957 (0.4%)	1.08	6/1341 (0.4%)
All	All	0.48	18/87156 (0.0%)	0.83	222/123496 (0.2%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A	1366	PRO	N-CA	18.14	1.70	1.47
49	T	605	LYS	C-N	14.93	1.50	1.33
43	P	188	ASP	C-N	14.01	1.50	1.33
17	Q	19	GLU	C-N	13.52	1.50	1.34
7	U	493	LYS	C-N	12.85	1.50	1.33
30	2	72	U	C1'-N1	7.25	1.59	1.48
38	A	1416	ILE	C-N	7.05	1.50	1.33
30	2	73	C	C1'-N1	6.55	1.58	1.48
30	2	84	C	C1'-N1	6.43	1.58	1.48
49	T	619	MET	C-N	6.35	1.41	1.33
30	2	70	C	C1'-N1	6.32	1.57	1.48
30	2	71	C	C1'-N1	6.27	1.57	1.48
36	Z	154	U	C1'-N1	5.58	1.56	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	T	620	PRO	N-CD	5.53	1.55	1.47
36	Z	144	A	C1'-N9	-5.39	1.39	1.48
49	T	643	PRO	N-CD	5.33	1.55	1.47
36	Z	141	A	C1'-N9	-5.29	1.40	1.48
38	A	1365	ILE	C-N	5.10	1.45	1.33

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	75	LEU	N-CA-CB	-18.70	82.37	110.61
7	U	493	LYS	CA-C-N	18.11	138.41	119.76
7	U	493	LYS	C-N-CA	18.11	138.41	119.76
47	4	422	PHE	N-CA-CB	-18.04	82.32	110.28
43	P	188	ASP	CA-C-N	17.78	137.69	119.56
43	P	188	ASP	C-N-CA	17.78	137.69	119.56
17	Q	19	GLU	CA-C-N	17.42	137.84	118.85
17	Q	19	GLU	C-N-CA	17.42	137.84	118.85
49	T	605	LYS	CA-C-N	17.35	140.11	119.98
49	T	605	LYS	C-N-CA	17.35	140.11	119.98
38	A	1365	ILE	CA-C-N	15.83	139.63	119.84
38	A	1365	ILE	C-N-CA	15.83	139.63	119.84
38	A	1416	ILE	CA-C-N	15.45	139.15	119.84
38	A	1416	ILE	C-N-CA	15.45	139.15	119.84
9	6	46	G	C2'-C3'-O3'	13.47	129.70	109.50
9	6	52	U	C2'-C3'-O3'	12.78	132.86	113.70
24	Y	75	LEU	CB-CA-C	10.48	127.89	110.17
34	t	89	ILE	N-CA-CB	-10.02	97.59	111.41
38	A	372	PRO	CA-N-CD	-9.80	98.27	112.00
47	4	472	GLN	C-N-CD	-9.72	85.13	125.00
34	t	89	ILE	CB-CA-C	9.59	124.81	110.63
26	M	213	ALA	CA-C-N	-9.47	105.68	119.98
26	M	213	ALA	C-N-CA	-9.47	105.68	119.98
38	A	874	PRO	CA-N-CD	-9.31	98.97	112.00
31	G	382	PRO	CA-N-CD	-9.30	98.97	112.00
38	A	1530	PRO	CA-N-CD	-9.31	98.97	112.00
38	A	277	PRO	CA-N-CD	-9.26	99.04	112.00
38	A	1308	PRO	CA-N-CD	-9.21	99.11	112.00
7	U	746	PRO	CA-N-CD	-9.18	99.16	112.00
38	A	828	PRO	CA-N-CD	-9.16	99.17	112.00
38	A	913	PRO	CA-N-CD	-9.15	99.19	112.00
31	G	343	PRO	CA-N-CD	-9.13	99.21	112.00
7	U	1339	PRO	CA-N-CD	-9.12	99.23	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1065	PRO	CA-N-CD	-9.11	99.25	112.00
38	A	1567	PRO	CA-N-CD	-9.11	99.25	112.00
38	A	1319	PRO	CA-N-CD	-9.09	99.28	112.00
38	A	1313	PRO	CA-N-CD	-9.06	99.31	112.00
38	A	133	PRO	CA-N-CD	-9.05	99.32	112.00
38	A	335	PRO	CA-N-CD	-9.02	99.37	112.00
38	A	947	PRO	CA-N-CD	-9.01	99.39	112.00
38	A	1496	PRO	CA-N-CD	-8.99	99.41	112.00
38	A	370	PRO	CA-N-CD	-8.99	99.41	112.00
38	A	734	PRO	CA-N-CD	-8.99	99.42	112.00
38	A	646	PRO	CA-N-CD	-8.97	99.44	112.00
38	A	1135	PRO	CA-N-CD	-8.95	99.47	112.00
38	A	1738	PRO	CA-N-CD	-8.95	99.47	112.00
38	A	1120	PRO	CA-N-CD	-8.91	99.53	112.00
38	A	197	PRO	CA-N-CD	-8.90	99.53	112.00
38	A	175	PRO	CA-N-CD	-8.90	99.54	112.00
38	A	1183	PRO	CA-N-CD	-8.89	99.55	112.00
46	F	115	PRO	CA-N-CD	-8.87	99.58	112.00
38	A	938	PRO	CA-N-CD	-8.85	99.60	112.00
38	A	425	PRO	CA-N-CD	-8.85	99.62	112.00
38	A	732	PRO	CA-N-CD	-8.84	99.62	112.00
38	A	63	PRO	CA-N-CD	-8.83	99.64	112.00
38	A	233	PRO	CA-N-CD	-8.83	99.64	112.00
38	A	1118	PRO	CA-N-CD	-8.83	99.64	112.00
38	A	937	PRO	CA-N-CD	-8.82	99.65	112.00
38	A	1198	PRO	CA-N-CD	-8.82	99.66	112.00
38	A	942	PRO	CA-N-CD	-8.78	99.71	112.00
38	A	345	PRO	CA-N-CD	-8.77	99.72	112.00
38	A	354	PRO	CA-N-CD	-8.76	99.74	112.00
38	A	948	PRO	CA-N-CD	-8.76	99.74	112.00
38	A	1724	PRO	CA-N-CD	-8.76	99.74	112.00
38	A	138	PRO	CA-N-CD	-8.75	99.75	112.00
38	A	168	PRO	CA-N-CD	-8.74	99.76	112.00
38	A	949	PRO	CA-N-CD	-8.73	99.77	112.00
30	2	84	C	O3'-P-O5'	-8.73	90.90	104.00
38	A	799	PRO	CA-N-CD	-8.73	99.78	112.00
26	M	213	ALA	CA-C-O	-8.73	109.17	119.03
38	A	187	PRO	CA-N-CD	-8.72	99.79	112.00
38	A	1540	PRO	CA-N-CD	-8.72	99.80	112.00
30	2	72	U	O3'-P-O5'	-8.70	90.95	104.00
38	A	274	PRO	CA-N-CD	-8.69	99.83	112.00
38	A	202	PRO	CA-N-CD	-8.68	99.85	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1616	PRO	CA-N-CD	-8.67	99.87	112.00
38	A	381	PRO	CA-N-CD	-8.65	99.89	112.00
30	2	81	G	O3'-P-O5'	-8.65	91.03	104.00
30	2	82	G	O3'-P-O5'	-8.65	91.03	104.00
38	A	1084	PRO	CA-N-CD	-8.65	99.90	112.00
38	A	464	PRO	CA-N-CD	-8.63	99.92	112.00
30	2	71	C	O3'-P-O5'	-8.62	91.06	104.00
38	A	463	PRO	CA-N-CD	-8.62	99.93	112.00
38	A	307	PRO	CA-N-CD	-8.62	99.93	112.00
38	A	907	PRO	CA-N-CD	-8.62	99.94	112.00
30	2	79	G	O3'-P-O5'	-8.61	91.08	104.00
38	A	826	PRO	CA-N-CD	-8.61	99.95	112.00
38	A	1068	PRO	CA-N-CD	-8.61	99.95	112.00
38	A	408	PRO	CA-N-CD	-8.59	99.98	112.00
38	A	386	PRO	CA-N-CD	-8.58	99.98	112.00
38	A	729	PRO	CA-N-CD	-8.57	100.00	112.00
30	2	80	A	O3'-P-O5'	-8.57	91.15	104.00
38	A	348	PRO	CA-N-CD	-8.55	100.03	112.00
48	u	1108	ASN	CA-C-N	8.55	132.61	122.44
48	u	1108	ASN	C-N-CA	8.55	132.61	122.44
30	2	70	C	O3'-P-O5'	-8.54	91.19	104.00
38	A	358	PRO	CA-N-CD	-8.54	100.04	112.00
38	A	324	PRO	CA-N-CD	-8.53	100.06	112.00
38	A	1162	PRO	CA-N-CD	-8.52	100.07	112.00
38	A	1312	PRO	CA-N-CD	-8.52	100.07	112.00
38	A	410	PRO	CA-N-CD	-8.48	100.13	112.00
22	r	635	LEU	CA-C-N	8.46	131.95	120.44
22	r	635	LEU	C-N-CA	8.46	131.95	120.44
38	A	1698	PRO	CA-N-CD	-8.46	100.16	112.00
30	2	83	A	O3'-P-O5'	-8.45	91.32	104.00
38	A	829	PRO	CA-N-CD	-8.45	100.18	112.00
38	A	1642	PRO	CA-N-CD	-8.43	100.20	112.00
38	A	526	PRO	CA-N-CD	-8.39	100.26	112.00
38	A	1696	PRO	CA-N-CD	-8.38	100.27	112.00
38	A	824	PRO	CA-N-CD	-8.38	100.27	112.00
38	A	625	PRO	CA-N-CD	-8.35	100.31	112.00
38	A	1452	PRO	CA-N-CD	-8.33	100.34	112.00
38	A	174	PRO	CA-N-CD	-8.27	100.42	112.00
38	A	725	PRO	CA-N-CD	-8.26	100.44	112.00
38	A	1720	PRO	CA-N-CD	-8.25	100.45	112.00
38	A	1336	PRO	CA-N-CD	-8.21	100.51	112.00
38	A	167	PRO	CA-N-CD	-8.17	100.57	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	117	PRO	CA-N-CD	-8.16	100.58	112.00
38	A	1366	PRO	CA-N-CD	-8.13	100.61	112.00
38	A	1064	PRO	CA-N-CD	-8.02	100.78	112.00
7	U	1379	TYR	N-CA-C	7.72	122.80	112.30
17	Q	11	PRO	N-CA-C	7.67	120.06	110.70
9	6	49	G	C2'-C3'-O3'	7.57	120.86	109.50
9	6	28	A	C2'-C3'-O3'	7.49	124.94	113.70
34	t	68	PRO	CA-N-CD	-7.45	101.57	112.00
47	4	77	GLY	CA-C-N	7.38	129.07	119.84
47	4	77	GLY	C-N-CA	7.38	129.07	119.84
9	6	79	C	C2'-C3'-O3'	7.21	120.31	109.50
38	A	1307	MET	CA-C-N	7.20	128.84	119.84
38	A	1307	MET	C-N-CA	7.20	128.84	119.84
10	B	175	PRO	N-CA-C	7.04	126.97	112.47
47	4	281	ARG	N-CA-C	6.94	119.44	111.11
29	y	2	ALA	CA-C-N	6.92	134.75	121.54
29	y	2	ALA	C-N-CA	6.92	134.75	121.54
9	6	33	G	C2'-C3'-O3'	-6.67	103.69	113.70
9	6	79	C	C4'-C3'-O3'	6.63	119.34	109.40
49	T	619	MET	CA-C-N	-6.51	113.59	120.03
49	T	619	MET	C-N-CA	-6.51	113.59	120.03
25	7	97	GLU	CA-C-N	6.36	128.70	120.44
25	7	97	GLU	C-N-CA	6.36	128.70	120.44
25	7	102	ARG	CA-C-N	6.25	133.48	121.54
25	7	102	ARG	C-N-CA	6.25	133.48	121.54
34	t	134	LEU	N-CA-CB	6.25	119.41	110.16
10	B	174	PHE	CA-C-N	6.23	127.63	119.84
10	B	174	PHE	C-N-CA	6.23	127.63	119.84
9	6	34	G	C2'-C3'-O3'	-6.18	104.42	113.70
38	A	1028	TYR	N-CA-C	-6.15	105.80	113.55
9	6	56	A	C2'-C3'-O3'	-6.12	104.53	113.70
47	4	351	ARG	N-CA-C	6.09	118.63	110.35
22	r	344	TRP	N-CA-CB	6.05	120.64	110.79
34	t	131	VAL	N-CA-CB	6.03	118.74	110.54
22	r	954	ASP	CA-C-N	6.00	136.44	121.80
22	r	954	ASP	C-N-CA	6.00	136.44	121.80
9	6	28	A	C3'-C2'-O2'	6.00	119.69	110.70
38	A	1307	MET	C-N-CD	-5.96	100.56	125.00
8	x	73	LEU	CA-C-O	-5.96	113.58	120.49
10	B	182	LEU	CA-C-N	-5.93	116.86	123.02
10	B	182	LEU	C-N-CA	-5.93	116.86	123.02
34	t	88	LEU	CA-C-N	-5.88	115.44	123.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	t	88	LEU	C-N-CA	-5.88	115.44	123.14
38	A	1581	LEU	N-CA-C	-5.88	106.03	113.43
22	r	636	TYR	O-C-N	5.86	128.42	122.09
46	F	140	GLU	N-CA-C	5.83	118.79	110.10
9	6	83	A	O4'-C4'-C3'	-5.81	100.29	106.10
47	4	291	LYS	CA-C-N	5.78	132.57	121.54
47	4	291	LYS	C-N-CA	5.78	132.57	121.54
43	P	219	THR	CA-C-N	5.77	132.09	121.70
43	P	219	THR	C-N-CA	5.77	132.09	121.70
17	Q	10	ALA	CA-C-N	5.77	126.32	120.38
17	Q	10	ALA	C-N-CA	5.77	126.32	120.38
22	r	636	TYR	CA-C-O	5.75	126.62	120.70
38	A	725	PRO	N-CA-C	-5.71	106.69	114.80
9	6	33	G	C4'-C3'-O3'	5.68	121.52	113.00
34	t	139	LYS	CA-C-N	-5.60	114.29	122.86
34	t	139	LYS	C-N-CA	-5.60	114.29	122.86
47	4	78	PRO	N-CA-C	5.60	124.01	112.47
33	o	202	ASP	N-CA-C	-5.59	103.75	111.81
7	U	979	GLN	CA-C-N	5.58	126.81	119.84
7	U	979	GLN	C-N-CA	5.58	126.81	119.84
5	w	81	GLY	N-CA-C	-5.53	108.23	115.47
38	A	371	LEU	CA-C-N	5.49	125.20	119.82
38	A	371	LEU	C-N-CA	5.49	125.20	119.82
47	4	104	VAL	CA-C-O	-5.48	115.02	118.69
38	A	436	PRO	N-CA-CB	-5.42	97.56	103.25
49	T	642	PRO	CA-C-N	-5.40	113.05	119.05
49	T	642	PRO	C-N-CA	-5.40	113.05	119.05
25	7	336	ILE	CA-C-N	5.40	125.40	120.21
25	7	336	ILE	C-N-CA	5.40	125.40	120.21
9	6	56	A	C1'-C2'-O2'	-5.34	100.38	108.40
10	B	184	PRO	N-CA-C	-5.34	106.76	114.18
48	u	1125	PRO	CA-C-N	5.32	128.14	120.38
48	u	1125	PRO	C-N-CA	5.32	128.14	120.38
38	A	1577	PHE	CA-C-N	5.30	127.65	120.65
38	A	1577	PHE	C-N-CA	5.30	127.65	120.65
25	7	289	ILE	CA-C-N	5.30	129.33	120.64
25	7	289	ILE	C-N-CA	5.30	129.33	120.64
38	A	1411	SER	O-C-N	5.30	125.90	122.03
38	A	985	TYR	N-CA-C	-5.27	106.63	114.64
25	7	280	TRP	N-CA-C	5.25	119.78	112.90
34	t	66	ILE	CA-C-N	-5.25	116.13	120.33
34	t	66	ILE	C-N-CA	-5.25	116.13	120.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	1015	VAL	N-CA-C	5.25	120.25	109.34
25	7	322	GLY	N-CA-C	-5.24	108.10	115.32
21	S	508	VAL	CA-C-N	5.23	124.85	119.05
21	S	508	VAL	C-N-CA	5.23	124.85	119.05
31	G	370	ASN	CA-C-O	-5.19	115.68	121.23
9	6	34	G	C4'-C3'-O3'	5.18	120.77	113.00
9	6	48	A	O4'-C4'-C3'	-5.09	101.01	106.10
8	x	73	LEU	N-CA-C	-5.09	101.47	109.25
38	A	873	ASN	CA-C-N	5.08	124.69	119.05
38	A	873	ASN	C-N-CA	5.08	124.69	119.05
45	p	162	PHE	CA-C-N	5.08	127.04	120.44
45	p	162	PHE	C-N-CA	5.08	127.04	120.44
47	4	312	ARG	CA-C-N	5.06	131.21	121.54
47	4	312	ARG	C-N-CA	5.06	131.21	121.54
34	t	131	VAL	CB-CA-C	-5.06	105.30	112.14
14	v	278	VAL	N-CA-C	-5.06	108.90	113.71
38	A	1315	VAL	CA-C-N	-5.05	113.32	120.89
38	A	1315	VAL	C-N-CA	-5.05	113.32	120.89
38	A	1468	ASN	CA-C-N	5.01	131.11	121.54
38	A	1468	ASN	C-N-CA	5.01	131.11	121.54
11	z	96	ARG	CB-CA-C	-5.00	110.42	117.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1506	0	737	5	0
2	E	5926	0	2964	116	0
3	b	364	0	181	6	0
3	i	359	0	179	1	0
4	W	816	0	386	2	0
5	w	391	0	197	20	0
6	d	344	0	168	0	0
6	k	364	0	176	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	U	6730	0	3268	111	0
8	x	397	0	191	40	0
9	6	1947	0	984	174	0
10	B	851	0	423	10	0
11	z	544	0	264	13	0
12	q	360	0	159	6	0
13	s	8688	0	4221	7	0
14	v	1053	0	550	54	0
15	3	283	0	158	27	0
16	0	761	0	375	20	0
17	Q	695	0	327	31	0
18	1	607	0	277	25	0
19	L	582	0	288	7	0
20	N	277	0	114	3	0
21	S	1771	0	820	8	0
22	r	4531	0	2256	32	0
23	R	219	0	91	3	0
24	Y	478	0	226	15	0
25	7	1178	0	537	10	0
26	M	3553	0	1739	49	0
27	K	614	0	284	6	0
28	O	1243	0	570	15	0
29	y	498	0	241	6	0
30	2	3479	0	1754	139	0
31	G	1604	0	795	54	0
32	a	393	0	176	4	0
32	h	482	0	220	6	0
33	o	1135	0	572	57	0
34	t	1272	0	618	5	0
35	f	319	0	144	1	0
35	m	413	0	193	8	0
36	Z	1201	0	607	113	0
37	e	390	0	188	7	0
37	l	415	0	198	17	0
38	A	10968	0	5356	462	0
39	8	92	0	46	4	0
40	c	388	0	167	1	0
40	j	403	0	173	6	0
41	I	883	0	414	3	0
42	g	469	0	214	6	0
42	n	402	0	184	18	0
43	P	1194	0	589	19	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	5	2397	0	1214	118	0
45	p	631	0	309	7	0
46	F	835	0	412	32	0
47	4	2110	0	987	41	0
48	u	4748	0	2402	159	0
49	T	942	0	490	26	0
50	r	32	0	12	2	0
51	r	1	0	0	0	0
52	A	36	0	6	0	0
All	All	85564	0	41791	1682	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 13.

All (1682) 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)
18:1:26:VAL:CB	48:u:861:ALA:HB2	1.14	1.60
8:x:29:TRP:CB	8:x:79:PRO:CB	1.75	1.58
38:A:270:ASN:CB	38:A:282:LEU:HA	1.33	1.57
45:p:103:GLU:CB	46:F:115:PRO:HB2	1.34	1.57
9:6:28:A:H5''	17:Q:41:ARG:CA	1.36	1.54
2:E:407:ILE:CB	2:E:1122:LEU:CB	1.81	1.53
8:x:29:TRP:CB	8:x:79:PRO:CG	1.86	1.53
38:A:466:ALA:CB	44:5:20:G:C6	1.93	1.50
38:A:948:PRO:HD2	38:A:949:PRO:CD	1.40	1.50
38:A:466:ALA:HB2	44:5:20:G:N1	1.18	1.50
2:E:193:ASP:C	8:x:78:PRO:CB	1.81	1.49
33:o:28:PRO:HA	33:o:63:ALA:CB	1.04	1.48
33:o:28:PRO:CA	33:o:63:ALA:CB	1.91	1.48
2:E:193:ASP:C	8:x:78:PRO:HB3	1.05	1.46
38:A:464:PRO:HB2	44:5:20:G:C2	1.25	1.45
38:A:224:THR:CB	44:5:12:U:H5''	1.44	1.45
2:E:12:THR:CB	2:E:403:SER:CB	1.93	1.45
30:2:181:G:H21	37:l:52:ASP:CB	1.30	1.45
33:o:28:PRO:CA	33:o:63:ALA:HB1	1.49	1.43
38:A:224:THR:CB	44:5:12:U:C5'	1.95	1.42
7:U:529:GLU:CB	7:U:1047:HIS:CB	1.97	1.42
16:0:274:TYR:N	48:u:437:PRO:CA	1.71	1.40
9:6:36:A:C8	36:Z:69:A:C2	2.10	1.40
2:E:407:ILE:CB	2:E:1122:LEU:CA	1.98	1.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:404:LEU:CB	2:E:1124:GLY:CA	1.98	1.40
38:A:948:PRO:CD	38:A:949:PRO:HD3	1.52	1.38
2:E:114:ARG:CB	8:x:41:CYS:CB	2.01	1.37
48:u:323:ILE:O	48:u:327:PRO:CD	1.69	1.36
8:x:29:TRP:CB	8:x:79:PRO:HG3	1.44	1.35
9:6:28:A:C5'	17:Q:41:ARG:HA	1.52	1.35
7:U:484:ASP:O	7:U:565:ILE:CB	1.74	1.35
9:6:28:A:C6	43:P:167:PHE:CB	2.07	1.35
30:2:181:G:N3	37:l:52:ASP:CB	1.88	1.34
33:o:23:HIS:O	33:o:31:ASP:CB	1.75	1.34
48:u:433:ALA:O	48:u:437:PRO:HD2	1.20	1.34
30:2:181:G:N2	37:l:52:ASP:CB	1.87	1.34
23:R:191:ASP:CB	38:A:1054:GLY:HA3	1.57	1.33
30:2:32:U:O2	36:Z:158:C:N4	1.59	1.32
9:6:36:A:N6	36:Z:68:U:O2	1.58	1.32
23:R:191:ASP:CB	38:A:1054:GLY:CA	2.06	1.31
38:A:617:ASN:CB	38:A:622:GLY:HA3	1.59	1.31
38:A:1366:PRO:N	38:A:1366:PRO:CA	1.70	1.31
9:6:24:A:H2	9:6:26:U:N3	1.28	1.31
15:3:591:ASN:CB	18:1:96:ASN:O	1.79	1.31
14:v:228:PRO:HB3	28:O:305:THR:O	1.15	1.31
30:2:181:G:C2	37:l:52:ASP:CB	2.15	1.30
38:A:466:ALA:CB	44:5:20:G:N1	1.86	1.30
9:6:42:C:H5''	38:A:2055:ILE:CB	1.59	1.29
38:A:1608:THR:CB	38:A:2065:GLN:HA	1.61	1.29
38:A:1608:THR:CB	38:A:2065:GLN:CA	2.10	1.29
38:A:947:PRO:CG	38:A:948:PRO:HD3	1.62	1.29
2:E:325:ILE:H	2:E:375:SER:CB	1.44	1.28
48:u:460:PRO:HG3	48:u:479:LEU:O	1.15	1.28
38:A:1214:TRP:O	38:A:1228:CYS:CB	1.81	1.28
18:1:26:VAL:CB	48:u:861:ALA:CB	2.09	1.28
48:u:417:PRO:HB2	48:u:418:PRO:CD	1.63	1.28
49:T:605:LYS:CB	49:T:606:PRO:HD2	1.56	1.28
2:E:404:LEU:CB	2:E:1124:GLY:HA3	1.57	1.28
30:2:42:G:OP1	46:F:75:GLY:CA	1.83	1.26
33:o:23:HIS:C	33:o:31:ASP:CB	2.09	1.26
27:K:383:PHE:CB	44:5:39:C:O2'	1.84	1.25
38:A:1416:ILE:CB	38:A:1417:PRO:HD3	1.64	1.25
5:w:14:THR:HA	5:w:59:VAL:O	1.32	1.25
33:o:42:GLU:CB	33:o:277:GLN:CB	2.14	1.25
48:u:431:LEU:C	48:u:435:PRO:HD2	1.59	1.25

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:n:75:PRO:HB3	47:4:356:ARG:CB	1.66	1.25
14:v:406:GLN:O	38:A:1402:ARG:CB	1.85	1.24
38:A:466:ALA:HB2	44:5:20:G:C6	1.61	1.24
7:U:481:ILE:HA	7:U:592:VAL:CB	1.64	1.24
7:U:529:GLU:CA	7:U:1047:HIS:CB	2.15	1.24
9:6:36:A:N7	36:Z:69:A:C2	2.04	1.24
48:u:311:ALA:C	48:u:314:PRO:HD2	1.59	1.24
2:E:193:ASP:O	8:x:78:PRO:HB3	1.11	1.23
2:E:189:TYR:CB	8:x:73:LEU:HA	1.68	1.22
7:U:489:VAL:CB	7:U:504:PHE:CB	2.16	1.22
19:L:29:ASN:O	30:2:24:A:N1	1.73	1.22
38:A:464:PRO:CB	44:5:20:G:C2	2.19	1.22
38:A:617:ASN:CB	38:A:622:GLY:CA	2.18	1.21
15:3:576:PHE:O	15:3:580:PRO:HD3	1.36	1.21
48:u:431:LEU:O	48:u:435:PRO:HD2	1.10	1.21
26:M:213:ALA:HB3	26:M:216:SER:O	1.39	1.20
9:6:28:A:N6	43:P:167:PHE:CB	2.02	1.20
8:x:29:TRP:CB	8:x:79:PRO:HB3	1.44	1.20
33:o:8:LEU:CB	33:o:28:PRO:HG3	1.70	1.20
33:o:28:PRO:HA	33:o:63:ALA:HB2	1.25	1.19
38:A:1608:THR:CB	38:A:2065:GLN:CB	2.21	1.19
38:A:270:ASN:CB	38:A:282:LEU:CA	2.20	1.18
38:A:466:ALA:CB	44:5:20:G:O6	1.90	1.18
38:A:617:ASN:CA	38:A:622:GLY:HA3	1.73	1.18
38:A:1608:THR:CA	38:A:2066:THR:H	1.56	1.17
24:Y:91:GLY:HA3	48:u:607:ALA:HB1	1.24	1.17
2:E:407:ILE:CB	2:E:1122:LEU:HA	1.65	1.17
7:U:744:ILE:H	7:U:745:PRO:CD	1.57	1.17
9:6:93:G:OP1	28:O:348:SER:HA	1.45	1.17
30:2:103:U:O4	35:m:38:MET:CB	1.91	1.17
38:A:949:PRO:HD2	38:A:950:LEU:H	1.09	1.17
2:E:405:SER:H	2:E:406:PRO:HD3	1.07	1.16
24:Y:73:ASN:CB	48:u:646:PRO:CB	2.24	1.16
7:U:481:ILE:C	7:U:592:VAL:CB	2.18	1.16
9:6:36:A:N6	36:Z:68:U:C2	2.13	1.16
33:o:23:HIS:CA	33:o:31:ASP:CB	2.23	1.15
38:A:1214:TRP:CB	38:A:1228:CYS:CB	2.23	1.15
38:A:1609:VAL:CB	38:A:2064:THR:O	1.95	1.15
7:U:481:ILE:CA	7:U:592:VAL:CB	2.23	1.15
9:6:34:G:H8	36:Z:71:C:N4	1.46	1.14
38:A:1567:PRO:HD2	38:A:1568:THR:H	1.10	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:v:224:SER:O	14:v:226:PRO:HD3	1.47	1.13
33:o:23:HIS:HA	33:o:31:ASP:CA	1.78	1.13
48:u:433:ALA:O	48:u:437:PRO:CD	1.96	1.13
8:x:71:LYS:O	8:x:75:PRO:HB3	1.44	1.13
33:o:29:PHE:O	33:o:53:GLU:O	1.66	1.13
2:E:405:SER:N	2:E:406:PRO:HD3	1.64	1.12
38:A:1330:MET:CB	38:A:1367:ASN:CB	2.27	1.13
14:v:228:PRO:CB	28:O:305:THR:O	1.96	1.12
45:p:103:GLU:CB	46:F:115:PRO:CB	2.26	1.12
38:A:646:PRO:HD2	38:A:647:LEU:H	1.16	1.11
48:u:324:GLY:O	48:u:327:PRO:HG2	1.51	1.11
38:A:466:ALA:HB3	44:5:20:G:O6	1.43	1.11
42:n:75:PRO:HG3	47:4:356:ARG:C	1.76	1.11
48:u:324:GLY:HA2	48:u:327:PRO:HG3	1.18	1.11
2:E:347:LEU:CB	2:E:359:TYR:O	1.97	1.10
48:u:324:GLY:C	48:u:327:PRO:HD2	1.76	1.10
15:3:567:SER:C	15:3:569:PRO:HD2	1.76	1.10
9:6:78:A:N7	30:2:19:G:O6	1.83	1.10
38:A:1724:PRO:HD2	38:A:1725:LEU:H	1.03	1.10
2:E:272:PRO:HB3	2:E:385:PHE:O	1.52	1.10
30:2:42:G:OP1	46:F:75:GLY:HA2	1.44	1.10
2:E:193:ASP:CA	8:x:78:PRO:HB3	1.81	1.09
38:A:464:PRO:HB2	44:5:20:G:N1	1.64	1.09
48:u:431:LEU:O	48:u:435:PRO:CD	1.99	1.09
9:6:28:A:N1	43:P:167:PHE:CB	2.15	1.09
2:E:193:ASP:CA	8:x:78:PRO:CB	2.18	1.08
9:6:24:A:C2	9:6:26:U:N3	2.19	1.08
48:u:417:PRO:HB2	48:u:418:PRO:HD3	1.14	1.08
38:A:874:PRO:HD2	38:A:875:HIS:H	1.18	1.08
5:w:17:VAL:HA	5:w:85:ARG:O	1.53	1.08
19:L:29:ASN:O	30:2:24:A:C2	2.05	1.08
31:G:298:PRO:HG3	31:G:340:ALA:N	1.68	1.08
38:A:940:ILE:O	38:A:942:PRO:HD3	1.54	1.08
48:u:324:GLY:HA2	48:u:327:PRO:CG	1.84	1.08
9:6:93:G:P	28:O:348:SER:HA	1.94	1.08
30:2:100:U:H1'	6:k:65:ASN:CB	1.84	1.07
14:v:196:VAL:O	43:P:33:TYR:HA	1.53	1.07
33:o:23:HIS:HA	33:o:31:ASP:CB	1.84	1.07
38:A:1382:SER:HA	38:A:1415:GLY:CA	1.76	1.07
5:w:25:SER:C	5:w:27:PRO:HD2	1.77	1.07
38:A:168:PRO:HD2	38:A:169:PHE:H	1.10	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:408:PRO:O	38:A:410:PRO:HD2	1.55	1.07
24:Y:73:ASN:CB	48:u:646:PRO:HB2	1.85	1.07
38:A:1313:PRO:HD3	38:A:1336:PRO:HG3	1.34	1.07
7:U:746:PRO:CD	7:U:782:HIS:O	2.03	1.07
14:v:188:PHE:CB	43:P:155:PRO:HD3	1.85	1.07
38:A:947:PRO:HD2	38:A:949:PRO:HD3	1.24	1.07
38:A:1120:PRO:HD2	38:A:1121:ASN:H	1.18	1.07
38:A:1530:PRO:HD2	38:A:1531:ASN:H	1.18	1.07
24:Y:103:GLY:O	24:Y:107:PRO:CD	2.03	1.06
30:2:42:G:OP1	46:F:75:GLY:HA3	1.52	1.06
2:E:404:LEU:CB	2:E:1124:GLY:HA2	1.70	1.06
38:A:1738:PRO:HD2	38:A:1739:ALA:H	1.15	1.06
44:5:37:G:N2	44:5:45:C:N3	2.03	1.06
38:A:466:ALA:HB3	44:5:20:G:C6	1.82	1.06
38:A:1608:THR:HA	38:A:2066:THR:H	0.96	1.06
21:S:484:ARG:O	21:S:489:GLY:N	1.88	1.05
8:x:29:TRP:C	8:x:79:PRO:HG3	1.82	1.05
9:6:78:A:C5	30:2:19:G:O6	2.08	1.05
30:2:100:U:O2	6:k:65:ASN:N	1.89	1.05
48:u:323:ILE:O	48:u:327:PRO:HD3	0.87	1.05
38:A:732:PRO:HG2	38:A:735:ILE:CB	1.87	1.05
48:u:1257:PRO:HG3	49:T:482:ALA:HB2	1.38	1.05
7:U:745:PRO:HB2	7:U:746:PRO:HD3	1.32	1.05
2:E:189:TYR:CB	8:x:73:LEU:CA	2.35	1.04
31:G:373:LYS:CB	31:G:392:PRO:HG2	1.87	1.04
9:6:42:C:C5'	38:A:2055:ILE:CB	2.35	1.04
23:R:191:ASP:CB	38:A:1054:GLY:HA2	1.82	1.04
47:4:445:HIS:CB	49:T:472:PRO:O	2.05	1.04
9:6:34:G:C8	36:Z:71:C:N4	2.24	1.04
22:r:86:THR:O	31:G:239:LYS:O	1.76	1.04
38:A:410:PRO:HD2	38:A:411:PHE:H	1.21	1.04
5:w:70:ALA:O	5:w:74:MET:CB	2.06	1.04
14:v:406:GLN:O	38:A:1402:ARG:CA	2.06	1.04
30:2:104:U:O3'	32:h:104:ASP:CB	2.05	1.04
7:U:632:ASN:CB	7:U:668:ALA:HB2	1.87	1.03
26:M:48:ALA:HB1	26:M:49:PRO:HD2	1.39	1.03
29:y:93:SER:O	30:2:34:U:O2'	1.74	1.03
48:u:417:PRO:HG2	48:u:418:PRO:HD2	1.38	1.03
7:U:789:PRO:O	7:U:978:PRO:HG2	1.58	1.03
2:E:407:ILE:CA	2:E:1122:LEU:HA	1.87	1.03
33:o:30:GLY:HA2	33:o:52:VAL:CB	1.89	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:1084:PRO:HD2	38:A:1085:ILE:H	1.14	1.03
38:A:1608:THR:HA	38:A:2066:THR:N	1.72	1.03
48:u:311:ALA:O	48:u:314:PRO:HD2	1.57	1.03
7:U:746:PRO:HD3	7:U:782:HIS:O	1.58	1.03
24:Y:103:GLY:O	24:Y:107:PRO:HD3	1.57	1.03
38:A:947:PRO:HG2	38:A:948:PRO:HD3	1.03	1.02
38:A:1616:PRO:HD2	38:A:1617:ARG:H	1.24	1.02
38:A:425:PRO:HD2	38:A:426:LEU:H	1.24	1.02
26:M:48:ALA:HB1	26:M:49:PRO:CD	1.88	1.02
14:v:221:GLY:C	14:v:223:PRO:HD2	1.85	1.02
30:2:136:G:O3'	32:h:87:SER:N	1.92	1.02
14:v:207:MET:CB	38:A:91:ALA:CB	2.38	1.02
38:A:439:GLN:H	38:A:440:PRO:HD3	1.24	1.02
46:F:51:LEU:CA	48:u:1141:LEU:N	2.22	1.02
2:E:441:GLY:O	2:E:771:GLY:O	1.78	1.01
7:U:481:ILE:O	7:U:592:VAL:CB	2.08	1.01
22:r:80:ILE:N	31:G:199:VAL:O	1.92	1.01
16:0:274:TYR:N	48:u:437:PRO:HA	0.87	1.01
38:A:224:THR:CB	44:5:12:U:OP1	2.08	1.01
38:A:1382:SER:CA	38:A:1415:GLY:HA2	1.89	1.01
9:6:38:G:N2	36:Z:67:C:O2	1.93	1.00
36:Z:143:G:N3	47:4:399:LEU:CB	2.24	1.00
38:A:174:PRO:HB2	38:A:175:PRO:HD3	1.43	1.00
2:E:192:ALA:HB1	8:x:74:GLN:CB	1.91	1.00
15:3:582:TYR:CB	18:1:58:GLN:O	2.09	1.00
46:F:51:LEU:HA	48:u:1141:LEU:N	1.77	1.00
48:u:417:PRO:CB	48:u:418:PRO:CD	2.36	1.00
16:0:272:VAL:O	48:u:438:LEU:CB	2.10	0.99
33:o:28:PRO:CA	33:o:63:ALA:HB3	1.90	0.99
38:A:224:THR:CB	44:5:12:U:H5'	1.89	0.99
48:u:460:PRO:CG	48:u:479:LEU:O	2.11	0.99
30:2:101:U:H1'	37:l:66:SER:N	1.78	0.99
38:A:273:ILE:CB	38:A:277:PRO:HG3	1.92	0.99
7:U:427:TYR:CB	7:U:637:ASP:HA	1.93	0.99
38:A:1065:PRO:HD2	38:A:1066:GLN:H	1.26	0.98
38:A:1839:TRP:C	38:A:2220:PRO:HG2	1.85	0.98
8:x:29:TRP:CA	8:x:79:PRO:HG3	1.92	0.98
24:Y:73:ASN:CB	48:u:646:PRO:HB3	1.90	0.98
9:6:33:G:N2	36:Z:72:A:C2	2.31	0.98
14:v:205:ASP:CB	38:A:481:PHE:CB	2.40	0.98
38:A:408:PRO:C	38:A:410:PRO:HD3	1.88	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:q:67:ASN:CB	38:A:1549:VAL:O	2.10	0.98
48:u:431:LEU:CA	48:u:435:PRO:HD2	1.93	0.97
13:s:1047:PRO:HB3	38:A:2074:ARG:CB	1.94	0.97
38:A:138:PRO:HD2	38:A:139:VAL:H	1.27	0.97
3:b:25:TRP:O	44:5:116:A:C2	2.18	0.97
7:U:977:ALA:HB1	7:U:978:PRO:CD	1.94	0.97
22:r:86:THR:CB	31:G:238:LEU:O	2.13	0.96
30:2:29:A:OP2	38:A:858:GLN:CB	2.13	0.96
14:v:207:MET:C	38:A:91:ALA:HB2	1.90	0.96
33:o:29:PHE:CB	33:o:54:PHE:CB	2.43	0.96
38:A:174:PRO:HB2	38:A:175:PRO:CD	1.94	0.96
48:u:311:ALA:HA	48:u:314:PRO:HG2	1.48	0.96
38:A:224:THR:CB	44:5:12:U:P	2.54	0.96
30:2:181:G:N3	37:l:52:ASP:CA	2.29	0.96
7:U:485:ILE:HA	7:U:591:TYR:O	1.66	0.95
26:M:213:ALA:CB	26:M:216:SER:O	2.13	0.95
7:U:529:GLU:HA	7:U:1047:HIS:CB	1.96	0.95
38:A:464:PRO:HD2	38:A:465:LYS:H	1.31	0.95
9:6:24:A:H2	9:6:26:U:C2	1.85	0.95
2:E:325:ILE:N	2:E:375:SER:CB	2.30	0.95
3:b:25:TRP:O	44:5:116:A:N3	1.99	0.95
30:2:100:U:O2	6:k:64:GLY:N	1.99	0.95
33:o:28:PRO:CB	33:o:63:ALA:HB3	1.95	0.95
7:U:527:ILE:O	7:U:1051:LYS:CB	2.14	0.95
30:2:42:G:P	46:F:75:GLY:HA3	2.07	0.95
49:T:605:LYS:CB	49:T:606:PRO:CD	2.43	0.95
9:6:34:G:H8	36:Z:71:C:H42	1.02	0.94
48:u:431:LEU:HA	48:u:435:PRO:HD3	1.49	0.94
14:v:406:GLN:O	38:A:1402:ARG:HA	1.64	0.94
38:A:947:PRO:HD2	38:A:948:PRO:CD	1.97	0.94
48:u:431:LEU:CA	48:u:435:PRO:CD	2.44	0.94
7:U:745:PRO:HB2	7:U:746:PRO:CD	1.98	0.94
9:6:8:C:H5"	9:6:8:C:H6	1.31	0.94
38:A:200:ASP:C	38:A:202:PRO:HD3	1.92	0.94
11:z:50:VAL:O	48:u:412:TYR:HA	1.67	0.93
33:o:23:HIS:HA	33:o:31:ASP:HA	1.50	0.93
16:0:222:GLU:O	18:1:74:GLY:HA2	1.68	0.93
22:r:196:LYS:O	37:e:12:GLU:HA	1.68	0.93
38:A:408:PRO:C	38:A:410:PRO:CD	2.41	0.93
38:A:734:PRO:HD2	38:A:735:ILE:H	1.33	0.93
38:A:948:PRO:HD2	38:A:949:PRO:HD3	0.95	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:1382:SER:HA	38:A:1415:GLY:HA2	0.95	0.93
38:A:439:GLN:N	38:A:440:PRO:HD3	1.81	0.93
48:u:417:PRO:CG	48:u:418:PRO:HD2	1.99	0.93
24:Y:91:GLY:HA3	48:u:607:ALA:CB	1.97	0.93
2:E:405:SER:H	2:E:406:PRO:CD	1.82	0.93
7:U:632:ASN:H	7:U:668:ALA:HB2	1.33	0.92
9:6:28:A:C5'	17:Q:41:ARG:CA	2.28	0.92
10:B:20:LYS:CB	30:2:170:C:OP1	2.17	0.92
38:A:1724:PRO:HD2	38:A:1725:LEU:N	1.83	0.92
38:A:1214:TRP:O	38:A:1228:CYS:N	2.01	0.92
8:x:71:LYS:O	8:x:75:PRO:CB	2.17	0.92
31:G:382:PRO:HB2	31:G:423:SER:HA	1.50	0.92
36:Z:54:G:N1	44:5:44:A:N7	2.17	0.92
38:A:1540:PRO:HD2	38:A:1541:THR:H	1.34	0.92
7:U:744:ILE:H	7:U:745:PRO:HD3	1.32	0.91
38:A:408:PRO:O	38:A:410:PRO:CD	2.17	0.91
38:A:913:PRO:HD2	38:A:914:LEU:H	1.33	0.91
31:G:382:PRO:HG2	31:G:422:ASN:O	1.70	0.91
30:2:44:U:N3	36:Z:144:A:C2	2.39	0.91
48:u:324:GLY:C	48:u:327:PRO:CD	2.43	0.91
14:v:224:SER:O	14:v:226:PRO:CD	2.19	0.91
44:5:17:U:H3	44:5:60:G:H1	1.17	0.91
38:A:466:ALA:CB	44:5:20:G:H1	1.68	0.91
30:2:32:U:O2	36:Z:158:C:C4	2.24	0.90
34:t:49:PHE:CB	34:t:62:ASP:CB	2.49	0.90
47:4:472:GLN:N	47:4:473:PRO:HD2	1.85	0.90
9:6:24:A:C2	9:6:26:U:C2	2.59	0.90
38:A:273:ILE:H	38:A:277:PRO:HG2	1.36	0.90
47:4:472:GLN:N	47:4:473:PRO:CD	2.34	0.90
38:A:372:PRO:HD2	38:A:373:ASP:H	1.37	0.90
31:G:298:PRO:CG	31:G:340:ALA:N	2.35	0.90
42:n:75:PRO:CB	47:4:356:ARG:CB	2.49	0.90
9:6:28:A:C5'	17:Q:41:ARG:CB	2.50	0.90
8:x:29:TRP:CB	8:x:79:PRO:HB2	2.02	0.90
14:v:134:ARG:N	31:G:384:HIS:HA	1.87	0.90
38:A:948:PRO:HD2	38:A:949:PRO:N	1.86	0.90
22:r:93:ILE:O	31:G:275:LEU:O	1.89	0.90
30:2:44:U:N3	36:Z:144:A:N1	2.19	0.90
26:M:48:ALA:CB	26:M:49:PRO:HD2	2.02	0.89
48:u:324:GLY:O	48:u:327:PRO:CG	2.19	0.89
36:Z:54:G:N1	44:5:44:A:C8	2.40	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:w:26:GLU:N	5:w:27:PRO:HD2	1.88	0.89
36:Z:147:U:H5"	36:Z:147:U:H6	1.37	0.89
38:A:948:PRO:CD	38:A:949:PRO:CD	2.25	0.89
47:4:445:HIS:CB	49:T:472:PRO:C	2.45	0.89
48:u:324:GLY:CA	48:u:327:PRO:CG	2.50	0.89
48:u:431:LEU:HA	48:u:435:PRO:CD	2.02	0.89
9:6:38:G:N1	36:Z:67:C:N3	2.20	0.89
7:U:746:PRO:HD2	7:U:782:HIS:O	1.72	0.88
22:r:196:LYS:C	37:e:12:GLU:HA	1.98	0.88
38:A:947:PRO:CG	38:A:948:PRO:CD	2.51	0.88
9:6:36:A:C8	36:Z:69:A:H2	1.69	0.88
16:0:226:PHE:CB	18:1:49:GLU:CB	2.51	0.88
38:A:1567:PRO:HD2	38:A:1568:THR:N	1.88	0.88
9:6:28:A:H5"	17:Q:41:ARG:CB	2.03	0.88
7:U:747:PHE:HA	7:U:780:GLU:O	1.74	0.88
14:v:207:MET:CB	38:A:91:ALA:HB1	2.04	0.88
38:A:949:PRO:HD2	38:A:950:LEU:N	1.87	0.88
42:n:78:THR:CB	47:4:353:GLY:C	2.47	0.88
48:u:1257:PRO:HG2	49:T:478:HIS:O	1.73	0.88
15:3:576:PHE:O	15:3:580:PRO:CD	2.22	0.88
2:E:407:ILE:N	2:E:1122:LEU:HA	1.89	0.87
38:A:1724:PRO:CD	38:A:1725:LEU:H	1.87	0.87
16:0:255:PRO:HG2	16:0:276:HIS:CB	2.05	0.87
38:A:731:LEU:CB	38:A:732:PRO:HD3	2.05	0.87
44:5:9:G:H2'	44:5:9:G:OP2	1.74	0.87
14:v:207:MET:CA	38:A:91:ALA:HB2	2.05	0.87
38:A:1697:SER:CB	38:A:1698:PRO:HD3	2.04	0.87
2:E:189:TYR:HA	8:x:73:LEU:CB	2.05	0.87
38:A:466:ALA:HB2	44:5:20:G:C2	2.10	0.87
38:A:797:ASP:O	38:A:799:PRO:HD3	1.74	0.87
38:A:1214:TRP:O	38:A:1228:CYS:CA	2.23	0.87
7:U:491:ARG:HA	7:U:507:TRP:C	2.00	0.86
15:3:567:SER:C	15:3:569:PRO:CD	2.49	0.86
9:6:75:G:N2	9:6:75:G:OP2	2.08	0.86
14:v:133:GLN:C	31:G:385:TYR:H	1.82	0.86
38:A:385:GLU:CB	38:A:386:PRO:CD	2.53	0.86
9:6:36:A:C6	36:Z:68:U:N3	2.43	0.86
38:A:1738:PRO:HD2	38:A:1739:ALA:N	1.91	0.86
7:U:744:ILE:N	7:U:745:PRO:CD	2.37	0.86
7:U:494:PRO:CG	7:U:587:VAL:CB	2.54	0.86
7:U:744:ILE:H	7:U:745:PRO:HD2	1.41	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:z:96:ARG:CB	48:u:537:PRO:HG3	2.06	0.86
38:A:1496:PRO:HD2	38:A:1497:THR:H	1.40	0.86
38:A:947:PRO:HD2	38:A:949:PRO:CD	2.06	0.86
33:o:187:SER:CB	33:o:203:PHE:HA	2.06	0.85
33:o:42:GLU:HA	33:o:153:ALA:HB1	1.58	0.85
38:A:1839:TRP:O	38:A:2220:PRO:HG2	1.76	0.85
9:6:23:U:C4'	17:Q:117:CYS:HA	2.06	0.85
2:E:156:SER:CB	29:y:16:GLY:HA2	2.06	0.85
16:0:221:LYS:CB	18:1:72:LYS:CB	2.55	0.85
3:b:39:TYR:CB	44:5:93:U:C5	2.60	0.85
14:v:209:PRO:HD3	38:A:90:GLY:HA3	1.58	0.85
33:o:30:GLY:CA	33:o:52:VAL:CB	2.55	0.85
7:U:632:ASN:CB	7:U:668:ALA:CB	2.54	0.85
2:E:189:TYR:CB	8:x:73:LEU:CB	2.55	0.85
38:A:464:PRO:HD2	38:A:465:LYS:N	1.91	0.85
38:A:617:ASN:HA	38:A:622:GLY:HA3	1.57	0.85
42:n:75:PRO:HG2	47:4:357:GLU:CA	2.07	0.84
44:5:92:U:O2'	32:a:62:HIS:CB	2.25	0.84
46:F:51:LEU:HA	48:u:1140:GLU:C	2.01	0.84
33:o:28:PRO:HB3	33:o:63:ALA:HB3	1.59	0.84
38:A:617:ASN:CB	38:A:622:GLY:HA2	2.06	0.84
14:v:222:PRO:N	14:v:223:PRO:CD	2.40	0.84
26:M:177:PRO:HG3	33:o:65:ASP:CB	2.07	0.84
38:A:200:ASP:C	38:A:202:PRO:CD	2.51	0.84
38:A:425:PRO:HD2	38:A:426:LEU:N	1.90	0.84
38:A:1416:ILE:CB	38:A:1417:PRO:CD	2.52	0.84
7:U:494:PRO:HG3	7:U:587:VAL:CB	2.08	0.84
2:E:405:SER:N	2:E:406:PRO:CD	2.41	0.83
2:E:347:LEU:CA	2:E:359:TYR:O	2.25	0.83
38:A:1120:PRO:HD2	38:A:1121:ASN:N	1.93	0.83
38:A:1313:PRO:CD	38:A:1336:PRO:HG3	2.08	0.83
4:W:152:LEU:N	30:2:157:G:OP1	2.11	0.83
12:q:59:ASP:CB	38:A:1682:ALA:HB2	2.08	0.83
14:v:134:ARG:H	31:G:384:HIS:HA	1.42	0.83
38:A:947:PRO:CD	38:A:948:PRO:HD3	2.07	0.83
2:E:690:ARG:O	25:7:177:VAL:CB	2.26	0.83
14:v:281:ASN:CB	38:A:798:GLY:HA3	2.08	0.83
9:6:22:A:H5''	17:Q:116:ASN:O	1.79	0.83
48:u:324:GLY:C	48:u:327:PRO:CG	2.52	0.83
38:A:874:PRO:HD2	38:A:875:HIS:N	1.94	0.83
9:6:78:A:C5	30:2:19:G:C6	2.67	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:50:LYS:CB	26:M:51:PRO:HD3	2.09	0.82
38:A:385:GLU:CB	38:A:386:PRO:HD3	2.09	0.82
30:2:105:G:P	32:h:104:ASP:CB	2.67	0.82
42:n:75:PRO:CG	47:4:357:GLU:N	2.42	0.82
15:3:568:GLY:N	15:3:569:PRO:CD	2.42	0.82
38:A:410:PRO:HD2	38:A:411:PHE:N	1.91	0.82
5:w:28:LEU:O	5:w:32:LEU:CB	2.27	0.82
10:B:53:PHE:CB	30:2:165:A:H2	1.91	0.82
30:2:101:U:C1'	37:l:66:SER:N	2.39	0.82
5:w:26:GLU:N	5:w:27:PRO:CD	2.41	0.82
11:z:51:GLY:HA2	48:u:411:GLY:O	1.77	0.82
42:n:75:PRO:CG	47:4:356:ARG:C	2.53	0.82
48:u:1257:PRO:CG	49:T:482:ALA:HB2	2.10	0.82
38:A:466:ALA:HB3	44:5:20:G:N1	1.88	0.82
40:j:58:LEU:O	40:j:76:ARG:HA	1.80	0.82
2:E:193:ASP:O	8:x:78:PRO:CB	2.02	0.81
7:U:531:TRP:CB	7:U:632:ASN:CB	2.57	0.81
31:G:298:PRO:HG3	31:G:339:GLN:C	2.06	0.81
48:u:324:GLY:CA	48:u:327:PRO:HG3	2.06	0.81
2:E:113:ARG:CB	48:u:1278:ASP:CB	2.58	0.81
38:A:344:ASP:CB	38:A:345:PRO:HD3	2.09	0.81
38:A:466:ALA:HB1	44:5:20:G:C6	2.14	0.81
38:A:1719:PHE:CB	38:A:1720:PRO:CD	2.57	0.81
9:6:36:A:C8	36:Z:69:A:N1	2.46	0.81
38:A:1567:PRO:CD	38:A:1568:THR:H	1.93	0.81
38:A:168:PRO:HD2	38:A:169:PHE:N	1.88	0.81
38:A:1538:TRP:C	38:A:1540:PRO:HD3	2.04	0.81
38:A:211:GLN:H	38:A:212:PRO:HD3	1.45	0.81
36:Z:167:U:P	36:Z:167:U:H3'	2.21	0.81
38:A:1530:PRO:HD2	38:A:1531:ASN:N	1.92	0.81
38:A:270:ASN:CA	38:A:282:LEU:HA	2.11	0.81
7:U:789:PRO:O	7:U:978:PRO:CG	2.29	0.81
9:6:92:A:O3'	28:O:348:SER:HA	1.81	0.81
16:0:227:GLU:O	18:1:51:ASP:N	2.13	0.81
7:U:1338:PHE:CB	7:U:1339:PRO:HD3	2.12	0.80
26:M:517:THR:H	26:M:518:PRO:CD	1.93	0.80
38:A:1608:THR:CA	38:A:2066:THR:N	2.37	0.80
48:u:326:THR:N	48:u:327:PRO:HD2	1.94	0.80
15:3:582:TYR:CB	18:1:58:GLN:C	2.54	0.80
38:A:1064:PRO:HD2	38:A:1067:MET:O	1.81	0.80
14:v:134:ARG:N	31:G:384:HIS:CA	2.37	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:1698:PRO:HD2	38:A:1699:THR:H	1.46	0.80
9:6:93:G:OP1	28:O:351:ASN:CB	2.29	0.80
15:3:582:TYR:HA	18:1:57:SER:O	1.81	0.80
33:o:27:ILE:CB	33:o:28:PRO:HD3	2.11	0.80
38:A:949:PRO:CD	38:A:950:LEU:H	1.93	0.80
38:A:1065:PRO:HD2	38:A:1066:GLN:N	1.97	0.80
7:U:748:ARG:N	7:U:780:GLU:O	2.15	0.80
38:A:1616:PRO:HD2	38:A:1617:ARG:N	1.93	0.80
30:2:181:G:N3	37:l:52:ASP:HA	1.96	0.80
47:4:472:GLN:H	47:4:473:PRO:HD2	1.44	0.80
7:U:529:GLU:N	7:U:1047:HIS:CB	2.44	0.80
38:A:1539:SER:N	38:A:1540:PRO:HD3	1.97	0.80
38:A:617:ASN:CA	38:A:622:GLY:CA	2.53	0.79
38:A:1698:PRO:HD2	38:A:1699:THR:N	1.96	0.79
7:U:632:ASN:N	7:U:668:ALA:HB2	1.96	0.79
26:M:517:THR:N	26:M:518:PRO:CD	2.44	0.79
38:A:273:ILE:CB	38:A:274:PRO:HD3	2.12	0.79
38:A:646:PRO:HD2	38:A:647:LEU:N	1.90	0.79
48:u:431:LEU:CB	48:u:435:PRO:HG2	2.12	0.79
14:v:207:MET:CA	38:A:91:ALA:CB	2.61	0.79
26:M:214:GLY:CA	33:o:79:VAL:O	2.30	0.79
47:4:445:HIS:CB	49:T:473:ASP:HA	2.13	0.79
2:E:916:ASN:N	2:E:917:PRO:HD2	1.97	0.79
9:6:93:G:OP1	28:O:348:SER:CA	2.28	0.79
38:A:1183:PRO:HD2	38:A:1184:ASN:H	1.47	0.79
38:A:1609:VAL:CB	38:A:2063:GLU:O	2.30	0.79
16:0:222:GLU:O	18:1:74:GLY:CA	2.31	0.79
33:o:28:PRO:HA	33:o:63:ALA:HB1	0.79	0.79
9:6:23:U:H5'	17:Q:117:CYS:HA	1.65	0.79
9:6:31:U:H5''	9:6:31:U:C6	2.18	0.78
26:M:51:PRO:O	26:M:55:GLN:CB	2.31	0.78
36:Z:76:A:O2'	43:P:84:CYS:HA	1.81	0.78
38:A:168:PRO:CD	38:A:169:PHE:H	1.92	0.78
38:A:202:PRO:HD2	38:A:203:VAL:H	1.48	0.78
38:A:947:PRO:CD	38:A:948:PRO:CD	2.59	0.78
7:U:631:PRO:HG2	7:U:1044:LEU:CB	2.13	0.78
12:q:7:ASN:HA	12:q:13:LYS:HA	1.66	0.78
24:Y:103:GLY:O	24:Y:107:PRO:CG	2.31	0.78
38:A:1468:ASN:O	38:A:1470:TYR:N	2.15	0.78
48:u:417:PRO:CB	48:u:418:PRO:HD2	2.11	0.78
5:w:17:VAL:O	5:w:56:TYR:HA	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:224:LYS:O	47:4:497:ARG:O	2.01	0.78
22:r:376:PRO:HB3	38:A:388:LEU:CB	2.13	0.78
36:Z:147:U:H6	36:Z:147:U:C5'	1.96	0.78
2:E:189:TYR:CA	8:x:73:LEU:CB	2.61	0.78
9:6:28:A:H61	43:P:167:PHE:CB	1.94	0.78
38:A:407:ALA:HB1	38:A:408:PRO:HD3	1.66	0.78
9:6:28:A:H3'	9:6:28:A:N3	1.98	0.78
38:A:138:PRO:HD2	38:A:139:VAL:N	1.96	0.78
30:2:100:U:C1'	6:k:65:ASN:CB	2.62	0.78
38:A:409:ARG:N	38:A:410:PRO:HD3	1.98	0.78
22:r:93:ILE:O	31:G:276:GLU:HA	1.83	0.77
48:u:460:PRO:HG3	48:u:479:LEU:C	2.06	0.77
9:6:50:A:H4'	9:6:50:A:OP2	1.83	0.77
9:6:75:G:N3	9:6:75:G:H3'	2.00	0.77
26:M:52:ARG:O	26:M:56:LEU:CB	2.33	0.77
7:U:745:PRO:HB2	7:U:782:HIS:O	1.84	0.77
33:o:27:ILE:HA	33:o:67:MET:CB	2.14	0.77
38:A:1641:ARG:CB	38:A:1642:PRO:CD	2.62	0.77
38:A:1719:PHE:CB	38:A:1720:PRO:HD3	2.14	0.77
36:Z:142:U:O4	47:4:396:LEU:O	2.02	0.77
16:0:274:TYR:CA	48:u:437:PRO:HA	2.10	0.77
30:2:150:U:H3	30:2:181:G:H1	1.31	0.77
38:A:1738:PRO:CD	38:A:1739:ALA:H	1.97	0.77
9:6:8:C:H5''	9:6:8:C:C6	2.19	0.77
36:Z:70:G:N2	38:A:512:ASN:HA	1.99	0.77
38:A:1214:TRP:C	38:A:1228:CYS:CB	2.58	0.77
46:F:51:LEU:CA	48:u:1141:LEU:H	1.97	0.77
9:6:78:A:C8	30:2:19:G:O6	2.37	0.77
9:6:85:U:O2	30:2:14:C:N3	2.18	0.77
7:U:632:ASN:CB	7:U:668:ALA:CA	2.62	0.76
7:U:977:ALA:HB1	7:U:978:PRO:HD3	1.66	0.76
38:A:410:PRO:CD	38:A:411:PHE:H	1.98	0.76
31:G:298:PRO:HG2	31:G:340:ALA:CA	2.15	0.76
42:n:75:PRO:HG2	47:4:357:GLU:N	1.99	0.76
7:U:427:TYR:CB	7:U:637:ASP:CA	2.63	0.76
10:B:224:LYS:O	47:4:497:ARG:C	2.28	0.76
15:3:583:ARG:O	18:1:57:SER:CB	2.33	0.76
7:U:747:PHE:HA	7:U:781:PRO:HA	1.67	0.76
9:6:38:G:N2	36:Z:67:C:C2	2.54	0.76
38:A:947:PRO:HG2	38:A:948:PRO:CD	2.00	0.76
17:Q:19:GLU:N	17:Q:20:PRO:HD2	1.99	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:948:PRO:HD2	38:A:949:PRO:CG	2.15	0.76
38:A:1084:PRO:HD2	38:A:1085:ILE:N	1.91	0.76
44:5:44:A:H3'	44:5:45:C:H5''	1.66	0.76
26:M:517:THR:H	26:M:518:PRO:HD3	1.47	0.76
7:U:1102:PRO:CG	7:U:1116:GLU:O	2.34	0.76
9:6:66:C:H1'	38:A:651:TRP:CB	2.16	0.76
30:2:105:G:OP2	32:h:104:ASP:CB	2.33	0.76
38:A:1609:VAL:CB	38:A:2064:THR:C	2.58	0.76
2:E:695:GLY:N	25:7:178:ARG:CB	2.49	0.76
9:6:40:U:H2'	9:6:41:A:C8	2.20	0.76
2:E:113:ARG:CB	48:u:1278:ASP:CA	2.64	0.75
9:6:24:A:C2	9:6:26:U:C4	2.73	0.75
16:0:292:ILE:CB	48:u:433:ALA:HB3	2.15	0.75
38:A:725:PRO:HD2	38:A:726:TRP:H	1.51	0.75
9:6:48:A:N3	9:6:48:A:H2'	1.99	0.75
14:v:222:PRO:N	14:v:223:PRO:HD2	2.00	0.75
38:A:175:PRO:HD2	38:A:176:LEU:H	1.51	0.75
46:F:164:ARG:O	46:F:165:ARG:CB	2.34	0.75
9:6:23:U:C5'	17:Q:117:CYS:HA	2.16	0.75
38:A:617:ASN:HA	38:A:622:GLY:CA	2.14	0.75
46:F:174:GLU:N	46:F:175:PRO:HD2	2.01	0.75
38:A:731:LEU:CB	38:A:732:PRO:CD	2.65	0.75
38:A:1496:PRO:HD2	38:A:1497:THR:N	2.02	0.75
38:A:913:PRO:HD2	38:A:914:LEU:N	2.00	0.74
36:Z:63:G:O2'	36:Z:64:A:O4'	2.04	0.74
38:A:425:PRO:CD	38:A:426:LEU:H	1.99	0.74
7:U:977:ALA:HB1	7:U:978:PRO:HD2	1.67	0.74
9:6:23:U:H4'	17:Q:117:CYS:HA	1.68	0.74
9:6:33:G:N2	36:Z:72:A:N1	2.35	0.74
20:N:97:ASP:CB	36:Z:68:U:H4'	2.18	0.74
38:A:937:PRO:HB2	38:A:938:PRO:CD	2.17	0.74
31:G:382:PRO:CG	31:G:422:ASN:O	2.36	0.74
38:A:1120:PRO:CD	38:A:1121:ASN:H	1.99	0.74
48:u:434:THR:CB	48:u:435:PRO:HD3	2.17	0.74
48:u:460:PRO:CD	48:u:479:LEU:HA	2.17	0.74
2:E:114:ARG:CA	8:x:41:CYS:CB	2.65	0.74
9:6:66:C:P	38:A:541:GLY:HA2	2.28	0.74
33:o:28:PRO:N	33:o:63:ALA:HB1	2.01	0.74
38:A:564:TYR:O	38:A:569:VAL:CB	2.35	0.74
38:A:1538:TRP:C	38:A:1540:PRO:CD	2.60	0.74
7:U:532:PRO:O	7:U:631:PRO:O	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:23:HIS:CA	33:o:31:ASP:CA	2.60	0.74
38:A:202:PRO:HD2	38:A:203:VAL:N	2.01	0.74
38:A:1609:VAL:CB	38:A:2063:GLU:C	2.60	0.74
16:0:226:PHE:CA	18:1:49:GLU:CB	2.66	0.74
19:L:29:ASN:CB	30:2:24:A:H2	2.00	0.74
27:K:383:PHE:CB	44:5:39:C:HO2'	1.99	0.73
33:o:29:PHE:CB	33:o:54:PHE:HA	2.18	0.73
38:A:439:GLN:N	38:A:440:PRO:CD	2.51	0.73
24:Y:103:GLY:O	24:Y:107:PRO:HG3	1.88	0.73
22:r:196:LYS:CA	37:e:12:GLU:HA	2.19	0.73
48:u:311:ALA:O	48:u:314:PRO:CD	2.36	0.73
36:Z:158:C:H4'	36:Z:158:C:OP1	1.88	0.73
37:l:48:VAL:O	37:l:55:VAL:HA	1.88	0.73
2:E:325:ILE:O	2:E:375:SER:N	2.22	0.73
9:6:34:G:N3	9:6:34:G:H5''	2.03	0.73
9:6:31:U:H5''	9:6:31:U:H6	1.54	0.73
48:u:428:ALA:O	48:u:432:THR:N	2.22	0.73
7:U:527:ILE:C	7:U:1051:LYS:CB	2.60	0.73
9:6:5:U:H3'	9:6:7:G:H5''	1.71	0.73
38:A:734:PRO:HD2	38:A:735:ILE:N	2.00	0.72
38:A:1609:VAL:N	38:A:2065:GLN:HA	2.04	0.72
38:A:1609:VAL:H	38:A:2065:GLN:HA	1.54	0.72
9:6:36:A:N6	36:Z:68:U:N3	2.36	0.72
38:A:1382:SER:CA	38:A:1415:GLY:CA	2.55	0.72
44:5:92:U:H2'	32:a:62:HIS:CB	2.20	0.72
46:F:51:LEU:C	48:u:1140:GLU:HA	2.14	0.72
30:2:105:G:N1	42:n:20:LYS:CB	2.53	0.72
38:A:201:ALA:N	38:A:202:PRO:HD3	2.03	0.72
38:A:1723:LYS:N	38:A:1724:PRO:HD3	2.04	0.72
48:u:328:THR:N	48:u:329:PRO:HD2	2.03	0.72
21:S:485:ARG:HA	21:S:489:GLY:HA3	1.70	0.72
38:A:1084:PRO:CD	38:A:1085:ILE:H	1.96	0.72
38:A:1616:PRO:CD	38:A:1617:ARG:H	2.02	0.72
38:A:1641:ARG:CB	38:A:1642:PRO:HD3	2.20	0.72
38:A:347:LEU:CB	38:A:348:PRO:CD	2.67	0.72
44:5:92:U:C2'	32:a:62:HIS:CB	2.68	0.72
38:A:344:ASP:CB	38:A:345:PRO:CD	2.68	0.72
38:A:1313:PRO:HG2	38:A:1336:PRO:HD3	1.72	0.72
9:6:92:A:O3'	28:O:348:SER:CB	2.39	0.71
42:n:75:PRO:HG2	47:4:357:GLU:HA	1.71	0.71
14:v:129:ASP:N	14:v:130:PRO:HD2	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:596:TYR:N	44:5:45:C:P	2.43	0.71
2:E:274:ARG:HA	2:E:387:PHE:O	1.90	0.71
9:6:34:G:N3	9:6:34:G:H3'	2.05	0.71
38:A:175:PRO:HD2	38:A:176:LEU:N	2.06	0.71
38:A:270:ASN:CB	38:A:282:LEU:CB	2.67	0.71
44:5:37:G:H1	44:5:45:C:H42	1.39	0.71
44:5:39:C:OP1	44:5:39:C:H4'	1.88	0.71
9:6:24:A:OP1	17:Q:111:THR:HA	1.90	0.71
7:U:488:SER:CB	7:U:567:VAL:CB	2.69	0.71
9:6:33:G:C2	36:Z:72:A:N1	2.59	0.71
2:E:272:PRO:CB	2:E:385:PHE:O	2.36	0.71
38:A:372:PRO:HD2	38:A:373:ASP:N	2.06	0.71
48:u:324:GLY:O	48:u:327:PRO:CD	2.38	0.71
38:A:596:TYR:H	44:5:45:C:P	2.07	0.71
2:E:193:ASP:HA	8:x:78:PRO:CB	1.82	0.70
14:v:198:ARG:O	43:P:36:MET:N	2.19	0.70
38:A:646:PRO:CD	38:A:647:LEU:H	2.00	0.70
7:U:977:ALA:CB	7:U:978:PRO:CD	2.68	0.70
28:O:305:THR:C	28:O:307:PRO:HD3	2.15	0.70
30:2:101:U:H1'	37:l:66:SER:H	1.50	0.70
5:w:25:SER:C	5:w:27:PRO:CD	2.61	0.70
31:G:382:PRO:HB2	31:G:423:SER:CA	2.22	0.70
38:A:211:GLN:N	38:A:212:PRO:CD	2.53	0.70
48:u:311:ALA:C	48:u:314:PRO:CD	2.54	0.70
30:2:44:U:C4	36:Z:144:A:N1	2.59	0.70
38:A:1540:PRO:HD2	38:A:1541:THR:N	2.00	0.70
38:A:1608:THR:CB	38:A:2065:GLN:C	2.64	0.70
9:6:31:U:H4'	9:6:31:U:OP1	1.91	0.70
9:6:38:G:H8	9:6:38:G:P	2.14	0.70
38:A:1695:TYR:CB	38:A:1696:PRO:CD	2.69	0.70
2:E:195:ASP:H	8:x:78:PRO:HB2	1.56	0.70
31:G:187:LYS:N	31:G:188:PRO:CD	2.54	0.70
34:t:135:ASN:O	34:t:141:PHE:HA	1.91	0.70
7:U:632:ASN:CB	7:U:668:ALA:HA	2.22	0.70
30:2:19:G:N3	30:2:19:G:H2'	2.06	0.70
38:A:1530:PRO:CD	38:A:1531:ASN:H	2.00	0.70
48:u:324:GLY:C	48:u:327:PRO:HG2	2.16	0.70
38:A:947:PRO:CD	38:A:949:PRO:HD3	2.13	0.69
38:A:1313:PRO:HD2	38:A:1314:VAL:H	1.57	0.69
46:F:51:LEU:C	48:u:1141:LEU:H	2.00	0.69
38:A:1608:THR:CB	38:A:2066:THR:N	2.55	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:v:179:TYR:HA	39:8:115:ALA:HA	1.73	0.69
36:Z:59:G:OP1	38:A:1305:SER:CB	2.40	0.69
48:u:324:GLY:O	48:u:327:PRO:HD2	1.92	0.69
9:6:50:A:N3	9:6:50:A:H5'	2.06	0.69
12:q:44:LEU:HA	12:q:69:GLU:O	1.92	0.69
36:Z:143:G:C4	47:4:399:LEU:CB	2.75	0.69
38:A:464:PRO:CD	38:A:465:LYS:H	2.05	0.69
33:o:27:ILE:CB	33:o:28:PRO:CD	2.70	0.69
38:A:1183:PRO:HD2	38:A:1184:ASN:N	2.07	0.69
48:u:311:ALA:CA	48:u:314:PRO:HD2	2.23	0.69
7:U:494:PRO:HG2	7:U:587:VAL:HA	1.74	0.69
18:1:2:ASN:N	18:1:3:PRO:HD2	2.07	0.69
2:E:113:ARG:CB	48:u:1278:ASP:HA	2.23	0.69
9:6:37:C:H4'	9:6:38:G:OP2	1.91	0.69
48:u:431:LEU:CB	48:u:435:PRO:CG	2.71	0.69
28:O:337:MET:HA	28:O:341:PRO:HG3	1.73	0.69
38:A:1313:PRO:HD2	38:A:1314:VAL:N	2.08	0.69
8:x:72:MET:O	8:x:75:PRO:HD3	1.93	0.68
38:A:138:PRO:CD	38:A:139:VAL:H	2.04	0.68
38:A:167:PRO:HD2	38:A:167:PRO:O	1.93	0.68
38:A:273:ILE:H	38:A:277:PRO:CG	2.05	0.68
38:A:1724:PRO:CD	38:A:1725:LEU:N	2.51	0.68
7:U:1217:LEU:O	7:U:1337:PRO:HB2	1.94	0.68
9:6:33:G:H1	36:Z:72:A:N6	1.90	0.68
22:r:93:ILE:HA	31:G:275:LEU:O	1.94	0.68
33:o:23:HIS:CA	33:o:31:ASP:HA	2.23	0.68
38:A:63:PRO:HD2	38:A:64:GLU:H	1.58	0.68
48:u:326:THR:N	48:u:327:PRO:CD	2.55	0.68
48:u:431:LEU:CB	48:u:435:PRO:CD	2.70	0.68
9:6:50:A:N3	9:6:50:A:H3'	2.09	0.68
34:t:142:ARG:HA	34:t:149:PRO:HA	1.75	0.68
7:U:494:PRO:HG2	7:U:587:VAL:CA	2.24	0.68
15:3:583:ARG:N	18:1:57:SER:O	2.26	0.68
44:5:19:A:O2'	44:5:21:A:N1	2.26	0.68
26:M:213:ALA:HB1	26:M:216:SER:CB	2.24	0.68
38:A:466:ALA:HB3	44:5:20:G:H1	1.53	0.68
38:A:874:PRO:CD	38:A:875:HIS:H	2.03	0.68
38:A:410:PRO:CD	38:A:411:PHE:N	2.57	0.68
38:A:1065:PRO:CD	38:A:1066:GLN:H	2.05	0.68
7:U:630:ASP:CB	7:U:631:PRO:CD	2.72	0.68
7:U:1339:PRO:HD2	7:U:1339:PRO:O	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:1102:PRO:HG2	7:U:1116:GLU:O	1.94	0.68
30:2:19:G:OP2	30:2:19:G:O3'	2.12	0.68
48:u:417:PRO:HB2	48:u:418:PRO:HD2	1.67	0.67
8:x:71:LYS:O	8:x:75:PRO:CA	2.43	0.67
38:A:96:PRO:O	38:A:99:VAL:N	2.23	0.67
9:6:26:U:O2'	43:P:180:PRO:HG3	1.94	0.67
38:A:211:GLN:N	38:A:212:PRO:HD3	2.08	0.67
46:F:51:LEU:HA	48:u:1140:GLU:CA	2.25	0.67
2:E:349:VAL:N	2:E:357:TYR:O	2.25	0.67
38:A:1695:TYR:CB	38:A:1696:PRO:HD3	2.25	0.67
9:6:81:C:H6	9:6:81:C:O5'	1.77	0.67
38:A:63:PRO:HD2	38:A:64:GLU:N	2.10	0.67
38:A:464:PRO:CD	38:A:465:LYS:N	2.58	0.67
7:U:494:PRO:HG2	7:U:587:VAL:CB	2.23	0.67
38:A:371:LEU:CB	38:A:372:PRO:HD3	2.25	0.67
9:6:51:U:H6	9:6:51:U:OP2	1.78	0.67
26:M:50:LYS:CB	26:M:51:PRO:CD	2.72	0.67
36:Z:142:U:O4	47:4:396:LEU:CA	2.43	0.67
2:E:359:TYR:HA	2:E:397:LEU:HA	1.77	0.67
7:U:631:PRO:CG	7:U:1044:LEU:CB	2.73	0.67
17:Q:45:SER:O	17:Q:48:PRO:HD2	1.95	0.67
48:u:422:VAL:N	48:u:423:PRO:HD2	2.09	0.67
2:E:695:GLY:N	25:7:178:ARG:CA	2.58	0.67
31:G:374:SER:O	31:G:392:PRO:HD3	1.94	0.67
38:A:273:ILE:CB	38:A:277:PRO:CG	2.70	0.66
5:w:25:SER:CB	5:w:27:PRO:HD2	2.25	0.66
38:A:409:ARG:N	38:A:410:PRO:CD	2.57	0.66
30:2:136:G:C3'	32:h:87:SER:N	2.54	0.66
38:A:1697:SER:CB	38:A:1698:PRO:CD	2.74	0.66
7:U:1217:LEU:O	7:U:1338:PHE:N	2.20	0.66
38:A:425:PRO:CD	38:A:426:LEU:N	2.57	0.66
9:6:61:C:H3'	9:6:61:C:H6	1.60	0.66
30:2:39:U:H3	36:Z:149:A:H61	1.43	0.66
2:E:347:LEU:N	2:E:359:TYR:O	2.28	0.66
9:6:24:A:H2	9:6:26:U:H3	1.37	0.66
14:v:427:ASP:CB	38:A:1262:LYS:HA	2.26	0.66
38:A:1064:PRO:HD2	38:A:1064:PRO:O	1.95	0.66
33:o:29:PHE:CB	33:o:54:PHE:CA	2.74	0.66
30:2:101:U:C1'	37:l:66:SER:H	2.06	0.65
36:Z:160:G:H3'	36:Z:160:G:N3	2.11	0.65
38:A:646:PRO:CD	38:A:647:LEU:N	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:913:PRO:CD	38:A:914:LEU:H	2.09	0.65
38:A:1458:GLN:O	38:A:1462:GLY:N	2.29	0.65
2:E:326:ARG:HA	2:E:374:SER:HA	1.77	0.65
9:6:82:A:O2'	30:2:16:U:O4	2.14	0.65
10:B:53:PHE:CB	30:2:165:A:C2	2.77	0.65
26:M:347:SER:O	26:M:351:ARG:CB	2.44	0.65
38:A:947:PRO:HD2	38:A:948:PRO:N	2.10	0.65
31:G:298:PRO:CG	31:G:339:GLN:C	2.67	0.65
38:A:273:ILE:CB	38:A:274:PRO:CD	2.75	0.65
2:E:193:ASP:C	8:x:78:PRO:CG	2.41	0.65
7:U:481:ILE:O	7:U:592:VAL:N	2.30	0.65
15:3:582:TYR:CA	18:1:57:SER:O	2.45	0.65
30:2:103:U:OP1	35:m:75:GLU:HA	1.96	0.65
7:U:632:ASN:H	7:U:668:ALA:CB	2.09	0.65
31:G:339:GLN:CB	31:G:343:PRO:HD3	2.27	0.65
38:A:407:ALA:HB1	38:A:408:PRO:CD	2.26	0.65
48:u:1257:PRO:HG3	49:T:482:ALA:CB	2.22	0.65
5:w:15:VAL:O	5:w:58:PHE:HA	1.98	0.64
33:o:8:LEU:CB	33:o:28:PRO:CG	2.63	0.64
15:3:563:ARG:CB	15:3:564:PRO:CD	2.74	0.64
48:u:311:ALA:HA	48:u:314:PRO:CG	2.25	0.64
2:E:192:ALA:CB	8:x:74:GLN:CB	2.74	0.64
30:2:44:U:O4	36:Z:144:A:N1	2.29	0.64
38:A:386:PRO:HD2	38:A:386:PRO:O	1.95	0.64
38:A:1609:VAL:H	38:A:2065:GLN:CA	2.10	0.64
38:A:1738:PRO:CD	38:A:1739:ALA:N	2.58	0.64
9:6:92:A:O3'	28:O:348:SER:CA	2.44	0.64
30:2:32:U:O2	36:Z:158:C:C5	2.50	0.64
31:G:185:MET:O	31:G:188:PRO:HD3	1.97	0.64
38:A:1118:PRO:HD2	38:A:1118:PRO:O	1.98	0.64
24:Y:91:GLY:CA	48:u:607:ALA:HB1	2.16	0.64
30:2:17:U:H6	30:2:17:U:H5''	1.63	0.64
30:2:47:U:H1'	30:2:48:A:H8	1.61	0.64
30:2:103:U:C5	35:m:37:HIS:O	2.51	0.64
9:6:52:U:H4'	9:6:53:A:H5'	1.79	0.64
38:A:596:TYR:N	44:5:44:A:O3'	2.31	0.64
44:5:51:A:O2'	44:5:52:U:O5'	2.15	0.64
9:6:40:U:H2'	9:6:41:A:H8	1.61	0.64
14:v:133:GLN:C	31:G:385:TYR:N	2.56	0.64
38:A:435:CYS:CB	38:A:436:PRO:CD	2.76	0.64
38:A:466:ALA:HB1	44:5:20:G:O6	1.88	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:643:GLY:O	38:A:646:PRO:HD3	1.98	0.64
38:A:1312:PRO:HD2	38:A:1312:PRO:O	1.97	0.64
48:u:599:ASN:O	48:u:603:ALA:HB2	1.98	0.64
47:4:472:GLN:H	47:4:473:PRO:CD	2.05	0.64
9:6:38:G:H8	9:6:38:G:O5'	1.79	0.64
38:A:734:PRO:CD	38:A:735:ILE:H	2.09	0.64
38:A:948:PRO:N	38:A:949:PRO:HD3	2.13	0.64
2:E:695:GLY:N	25:7:178:ARG:HA	2.13	0.63
9:6:36:A:OP2	36:Z:69:A:N6	2.29	0.63
33:o:22:LEU:O	33:o:26:PHE:CB	2.47	0.63
38:A:463:PRO:HD2	38:A:463:PRO:O	1.98	0.63
38:A:625:PRO:HD2	38:A:625:PRO:O	1.98	0.63
38:A:1567:PRO:CD	38:A:1568:THR:N	2.56	0.63
38:A:1642:PRO:HD2	38:A:1642:PRO:O	1.97	0.63
2:E:346:PHE:HA	2:E:360:GLN:HA	1.79	0.63
2:E:347:LEU:O	2:E:359:TYR:N	2.32	0.63
9:6:79:C:H5''	30:2:18:U:H3	1.62	0.63
38:A:1084:PRO:CD	38:A:1085:ILE:N	2.58	0.63
7:U:485:ILE:CA	7:U:591:TYR:O	2.44	0.63
10:B:47:LYS:O	30:2:163:G:O2'	2.08	0.63
30:2:44:U:H3	36:Z:144:A:H2	1.37	0.63
14:v:281:ASN:CB	38:A:798:GLY:CA	2.76	0.63
48:u:847:ALA:O	48:u:851:SER:CB	2.46	0.63
7:U:632:ASN:CA	7:U:668:ALA:HB2	2.29	0.63
22:r:86:THR:C	31:G:239:LYS:O	2.41	0.63
9:6:25:C:H5'	9:6:26:U:H5''	1.81	0.63
30:2:100:U:O2	6:k:64:GLY:CA	2.46	0.63
44:5:33:U:H2'	44:5:34:U:H5''	1.80	0.63
48:u:812:PRO:HB2	48:u:813:PRO:HD3	1.81	0.63
7:U:1101:PRO:HB2	7:U:1102:PRO:HD2	1.81	0.63
9:6:33:G:OP2	9:6:33:G:H8	1.80	0.63
14:v:129:ASP:N	14:v:130:PRO:CD	2.60	0.63
24:Y:106:TRP:N	24:Y:107:PRO:HD2	2.14	0.63
38:A:1616:PRO:CD	38:A:1617:ARG:N	2.60	0.63
7:U:1338:PHE:CB	7:U:1339:PRO:CD	2.75	0.63
36:Z:167:U:H3'	36:Z:167:U:OP2	1.98	0.63
38:A:138:PRO:CD	38:A:139:VAL:N	2.62	0.63
38:A:725:PRO:HD2	38:A:726:TRP:N	2.10	0.63
38:A:1539:SER:N	38:A:1540:PRO:CD	2.61	0.63
44:5:60:G:O2'	44:5:61:A:O4'	2.16	0.63
48:u:431:LEU:CA	48:u:435:PRO:HD3	2.20	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:332:ALA:O	26:M:336:GLN:CB	2.47	0.62
30:2:47:U:H1'	30:2:48:A:C8	2.34	0.62
31:G:342:GLU:CB	31:G:343:PRO:HD3	2.29	0.62
31:G:386:THR:HA	31:G:399:LYS:HA	1.80	0.62
36:Z:163:C:H3'	36:Z:163:C:H6	1.64	0.62
38:A:948:PRO:CD	38:A:949:PRO:N	2.53	0.62
38:A:1540:PRO:CD	38:A:1541:THR:H	2.11	0.62
42:n:75:PRO:HG3	47:4:356:ARG:O	1.98	0.62
7:U:747:PHE:CA	7:U:780:GLU:O	2.46	0.62
38:A:335:PRO:HD2	38:A:335:PRO:O	1.99	0.62
38:A:907:PRO:HD2	38:A:907:PRO:O	1.99	0.62
36:Z:54:G:C6	44:5:44:A:N7	2.66	0.62
44:5:44:A:H3'	44:5:45:C:C5'	2.29	0.62
48:u:713:ALA:HA	48:u:716:ALA:HB3	1.80	0.62
14:v:196:VAL:O	43:P:33:TYR:CA	2.40	0.62
26:M:214:GLY:HA2	33:o:79:VAL:O	2.00	0.62
36:Z:142:U:O4	47:4:396:LEU:C	2.42	0.62
38:A:347:LEU:CB	38:A:348:PRO:HD3	2.30	0.62
38:A:1488:THR:C	38:A:1540:PRO:HG2	2.25	0.62
38:A:1698:PRO:CD	38:A:1699:THR:H	2.13	0.62
38:A:1723:LYS:N	38:A:1724:PRO:CD	2.62	0.62
7:U:171:SER:C	7:U:173:PRO:HD2	2.24	0.62
9:6:36:A:N7	36:Z:69:A:N3	2.46	0.62
9:6:78:A:C6	30:2:19:G:C6	2.88	0.62
16:0:255:PRO:HG2	16:0:276:HIS:HA	1.82	0.62
16:0:255:PRO:HG2	16:0:276:HIS:CA	2.29	0.62
2:E:1111:PRO:O	25:7:176:GLN:C	2.43	0.62
2:E:349:VAL:O	2:E:357:TYR:O	2.17	0.61
36:Z:54:G:N2	44:5:44:A:H8	1.97	0.61
38:A:321:ASN:O	38:A:324:PRO:HG3	2.00	0.61
2:E:194:ASN:N	8:x:78:PRO:CB	2.56	0.61
7:U:532:PRO:HG2	7:U:632:ASN:O	2.00	0.61
7:U:747:PHE:CA	7:U:781:PRO:HA	2.30	0.61
15:3:584:TRP:CB	18:1:54:CYS:HA	2.30	0.61
36:Z:70:G:HO2'	36:Z:71:C:P	2.23	0.61
38:A:1336:PRO:HG2	38:A:1339:ASP:CB	2.30	0.61
17:Q:47:TRP:N	17:Q:48:PRO:HD2	2.16	0.61
30:2:103:U:H5	35:m:37:HIS:O	1.83	0.61
36:Z:168:U:H6	36:Z:168:U:O5'	1.84	0.61
7:U:481:ILE:CB	7:U:592:VAL:O	2.48	0.61
38:A:1065:PRO:CD	38:A:1066:GLN:N	2.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:648:LEU:O	48:u:651:VAL:N	2.33	0.61
9:6:6:C:H4'	9:6:6:C:OP2	1.99	0.61
30:2:102:U:O3'	35:m:75:GLU:CB	2.49	0.61
38:A:826:PRO:HD2	38:A:826:PRO:O	2.00	0.61
26:M:519:GLN:O	26:M:523:ASN:CB	2.49	0.61
38:A:1120:PRO:CD	38:A:1121:ASN:N	2.61	0.61
9:6:36:A:C5	36:Z:69:A:C2	2.88	0.61
34:t:52:PRO:HA	34:t:62:ASP:HA	1.82	0.61
38:A:697:MET:CB	38:A:698:PRO:CD	2.79	0.61
9:6:45:A:H4'	9:6:46:G:H21	1.66	0.61
14:v:415:SER:HA	15:3:606:ALA:CB	2.31	0.61
33:o:202:ASP:HA	33:o:210:GLY:O	2.01	0.61
18:1:2:ASN:N	18:1:3:PRO:CD	2.64	0.60
26:M:214:GLY:N	33:o:79:VAL:O	2.34	0.60
2:E:407:ILE:CB	2:E:1122:LEU:N	2.63	0.60
21:S:455:ALA:CB	21:S:489:GLY:HA2	2.30	0.60
33:o:27:ILE:C	33:o:63:ALA:HB1	2.26	0.60
3:i:30:LYS:O	3:i:47:THR:HA	2.00	0.60
48:u:1067:LYS:HA	48:u:1107:GLN:CB	2.30	0.60
9:6:7:G:H5'	9:6:7:G:H8	1.66	0.60
38:A:1698:PRO:CD	38:A:1699:THR:N	2.60	0.60
47:4:445:HIS:CA	49:T:473:ASP:HA	2.32	0.60
2:E:92:TYR:HA	2:E:99:PHE:HA	1.84	0.60
7:U:491:ARG:HA	7:U:507:TRP:O	2.01	0.60
31:G:298:PRO:HG2	31:G:340:ALA:HB2	1.82	0.60
49:T:612:GLU:O	49:T:615:ILE:N	2.33	0.60
2:E:428:GLY:HA3	2:E:433:SER:HA	1.82	0.60
9:6:42:C:H5''	38:A:2055:ILE:CA	2.31	0.60
38:A:111:GLU:CB	38:A:210:HIS:CB	2.80	0.60
38:A:874:PRO:CD	38:A:875:HIS:N	2.63	0.60
10:B:41:VAL:HA	30:2:167:U:O4	2.02	0.60
15:3:568:GLY:N	15:3:569:PRO:HD3	2.16	0.60
9:6:38:G:P	9:6:38:G:C8	2.94	0.60
38:A:358:PRO:HD2	38:A:358:PRO:O	2.00	0.60
38:A:725:PRO:CD	38:A:726:TRP:H	2.13	0.60
38:A:1530:PRO:CD	38:A:1531:ASN:N	2.60	0.60
38:A:1468:ASN:C	38:A:1470:TYR:H	2.09	0.60
7:U:684:PRO:HG2	7:U:687:LEU:CB	2.31	0.59
38:A:133:PRO:HD2	38:A:133:PRO:O	2.01	0.59
15:3:563:ARG:CB	15:3:564:PRO:HD3	2.32	0.59
38:A:827:PHE:CB	38:A:828:PRO:HD3	2.31	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:5:39:C:H5''	44:5:39:C:H6	1.66	0.59
26:M:211:SER:O	33:o:68:ASN:CB	2.50	0.59
31:G:186:PRO:C	31:G:188:PRO:HD2	2.28	0.59
36:Z:157:C:H2'	36:Z:158:C:H5''	1.83	0.59
9:6:28:A:H5'	17:Q:41:ARG:CB	2.30	0.59
16:0:270:LEU:CB	16:0:271:PRO:HD3	2.32	0.59
38:A:177:ASP:O	38:A:181:ASN:CB	2.51	0.59
38:A:201:ALA:N	38:A:202:PRO:CD	2.64	0.59
38:A:1496:PRO:CD	38:A:1497:THR:H	2.13	0.59
44:5:59:G:O2'	44:5:60:G:H5'	2.03	0.59
2:E:94:PRO:C	2:E:96:LYS:H	2.10	0.59
38:A:913:PRO:CD	38:A:914:LEU:N	2.66	0.59
38:A:1068:PRO:HD2	38:A:1068:PRO:O	2.01	0.59
29:y:84:GLY:O	29:y:86:PRO:HD3	2.01	0.59
36:Z:143:G:C2	47:4:395:TRP:O	2.55	0.59
38:A:1198:PRO:HD2	38:A:1198:PRO:O	2.03	0.59
7:U:744:ILE:N	7:U:745:PRO:HD2	2.13	0.59
30:2:32:U:C2	36:Z:158:C:N4	2.62	0.59
30:2:56:A:H2'	30:2:57:A:C8	2.38	0.59
38:A:117:PRO:CG	38:A:131:GLU:CB	2.81	0.59
38:A:734:PRO:CD	38:A:735:ILE:N	2.66	0.59
38:A:824:PRO:HD2	38:A:824:PRO:O	2.03	0.59
14:v:227:ALA:HB1	14:v:228:PRO:HD2	1.84	0.58
21:S:448:TYR:HA	21:S:451:ALA:HB3	1.84	0.58
38:A:174:PRO:CB	38:A:175:PRO:HD3	2.28	0.58
38:A:168:PRO:CD	38:A:169:PHE:N	2.55	0.58
44:5:37:G:N2	44:5:45:C:C2	2.71	0.58
2:E:201:ALA:CB	8:x:74:GLN:CB	2.80	0.58
2:E:273:ARG:O	2:E:387:PHE:N	2.35	0.58
24:Y:104:GLU:C	24:Y:107:PRO:HD2	2.28	0.58
19:L:86:ALA:HB3	19:L:87:PRO:HD3	1.86	0.58
2:E:916:ASN:N	2:E:917:PRO:CD	2.67	0.58
38:A:1720:PRO:HD2	38:A:1720:PRO:O	2.04	0.58
48:u:311:ALA:CA	48:u:314:PRO:HG2	2.30	0.58
36:Z:143:G:N2	47:4:395:TRP:O	2.37	0.58
38:A:202:PRO:CD	38:A:203:VAL:N	2.67	0.58
16:0:272:VAL:O	48:u:438:LEU:CA	2.51	0.58
22:r:196:LYS:O	37:e:12:GLU:CA	2.48	0.58
38:A:1496:PRO:CD	38:A:1497:THR:N	2.66	0.58
38:A:1540:PRO:CD	38:A:1541:THR:N	2.66	0.58
26:M:723:MET:O	26:M:727:ARG:CB	2.52	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:943:LYS:CB	48:u:947:VAL:CB	2.82	0.58
2:E:404:LEU:CA	2:E:1124:GLY:HA3	2.32	0.58
26:M:668:CYS:O	26:M:672:ALA:HB2	2.04	0.58
38:A:70:ILE:C	38:A:72:ASP:H	2.11	0.58
9:6:61:C:C3'	9:6:61:C:C6	2.87	0.58
33:o:23:HIS:CB	33:o:31:ASP:CB	2.82	0.58
9:6:66:C:OP2	38:A:541:GLY:HA2	2.04	0.57
22:r:80:ILE:O	31:G:200:ILE:HA	2.04	0.57
30:2:56:A:O3'	49:T:481:THR:CB	2.51	0.57
36:Z:145:U:H6	36:Z:145:U:O5'	1.87	0.57
38:A:408:PRO:O	38:A:408:PRO:HD2	2.04	0.57
38:A:224:THR:CB	44:5:12:U:O5'	2.52	0.57
38:A:1319:PRO:HD2	38:A:1319:PRO:O	2.04	0.57
48:u:416:PRO:HB2	48:u:417:PRO:CD	2.34	0.57
2:E:114:ARG:HA	8:x:41:CYS:CB	2.33	0.57
31:G:187:LYS:N	31:G:188:PRO:HD3	2.18	0.57
38:A:725:PRO:CD	38:A:726:TRP:N	2.66	0.57
38:A:1545:ALA:O	38:A:1548:TYR:O	2.23	0.57
48:u:313:THR:N	48:u:314:PRO:CD	2.66	0.57
3:b:39:TYR:CB	44:5:93:U:C4	2.88	0.57
16:0:274:TYR:N	48:u:438:LEU:N	2.45	0.57
22:r:196:LYS:HA	37:e:12:GLU:HA	1.87	0.57
26:M:517:THR:N	26:M:518:PRO:HD2	2.18	0.57
38:A:526:PRO:HD2	38:A:526:PRO:O	2.02	0.57
26:M:48:ALA:HB1	26:M:49:PRO:HD3	1.82	0.57
36:Z:161:U:H4'	36:Z:161:U:OP1	2.05	0.57
14:v:429:ILE:HA	15:3:617:GLU:O	2.04	0.57
31:G:339:GLN:CB	31:G:343:PRO:CD	2.83	0.57
36:Z:167:U:C6	36:Z:167:U:H5'	2.39	0.57
48:u:324:GLY:CA	48:u:327:PRO:CD	2.82	0.57
2:E:347:LEU:O	2:E:359:TYR:O	2.23	0.57
30:2:181:G:H1'	37:l:52:ASP:HA	1.87	0.57
38:A:1308:PRO:HD2	38:A:1308:PRO:O	2.04	0.57
38:A:1313:PRO:CG	38:A:1336:PRO:HD3	2.34	0.57
46:F:115:PRO:HD2	46:F:177:GLU:N	2.19	0.57
26:M:479:ARG:O	26:M:483:SER:CB	2.53	0.57
43:P:278:GLN:O	43:P:281:GLU:CB	2.52	0.57
16:0:270:LEU:CB	16:0:271:PRO:CD	2.83	0.57
9:6:28:A:O3'	9:6:28:A:OP2	2.23	0.56
31:G:298:PRO:HG2	31:G:340:ALA:HA	1.87	0.56
5:w:25:SER:CA	5:w:27:PRO:HD2	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:100:U:C2	6:k:64:GLY:N	2.73	0.56
36:Z:54:G:H22	44:5:44:A:H8	1.51	0.56
38:A:797:ASP:C	38:A:799:PRO:HD3	2.29	0.56
48:u:460:PRO:HD3	48:u:479:LEU:HA	1.86	0.56
7:U:489:VAL:C	7:U:491:ARG:H	2.13	0.56
15:3:567:SER:CB	15:3:569:PRO:HD3	2.34	0.56
17:Q:47:TRP:N	17:Q:48:PRO:CD	2.68	0.56
30:2:71:C:C2	30:2:72:U:C5	2.94	0.56
38:A:200:ASP:O	38:A:202:PRO:CD	2.53	0.56
9:6:42:C:O5'	38:A:2055:ILE:CB	2.53	0.56
9:6:61:C:H3'	9:6:61:C:C6	2.39	0.56
26:M:480:VAL:O	26:M:484:LEU:CB	2.53	0.56
38:A:324:PRO:HD2	38:A:324:PRO:O	2.05	0.56
30:2:70:C:C2	30:2:71:C:C5	2.94	0.56
44:5:109:C:H2'	44:5:110:A:H8	1.70	0.56
30:2:72:U:H2'	30:2:73:C:H6	1.71	0.56
36:Z:147:U:C5'	36:Z:147:U:C6	2.85	0.56
38:A:117:PRO:HG3	38:A:131:GLU:CB	2.34	0.56
38:A:1313:PRO:HD3	38:A:1336:PRO:CG	2.21	0.56
48:u:326:THR:HA	48:u:329:PRO:HG2	1.86	0.56
9:6:93:G:OP1	28:O:347:HIS:O	2.24	0.56
36:Z:70:G:O2'	36:Z:71:C:O5'	2.08	0.56
30:2:83:A:H2'	30:2:84:C:H6	1.70	0.56
31:G:298:PRO:CG	31:G:340:ALA:CA	2.81	0.56
38:A:76:MET:C	38:A:78:ASN:H	2.14	0.56
38:A:949:PRO:CD	38:A:950:LEU:N	2.55	0.56
48:u:331:ALA:O	48:u:335:LYS:N	2.34	0.56
48:u:422:VAL:N	48:u:423:PRO:CD	2.69	0.56
21:S:484:ARG:O	21:S:489:GLY:CA	2.53	0.56
30:2:70:C:H2'	30:2:71:C:H6	1.71	0.56
44:5:108:G:O3'	42:g:50:ARG:HA	2.06	0.56
31:G:298:PRO:HG2	31:G:340:ALA:CB	2.35	0.55
38:A:1468:ASN:C	38:A:1470:TYR:N	2.62	0.55
9:6:31:U:H6	9:6:31:U:C5'	2.19	0.55
9:6:51:U:H2'	9:6:51:U:O2	2.07	0.55
26:M:163:GLU:O	26:M:167:ARG:CB	2.54	0.55
30:2:105:G:C2	42:n:20:LYS:CB	2.89	0.55
31:G:374:SER:O	31:G:392:PRO:CD	2.54	0.55
2:E:113:ARG:N	48:u:1278:ASP:CB	2.69	0.55
30:2:72:U:C2	30:2:73:C:C5	2.94	0.55
8:x:6:THR:O	8:x:8:HIS:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:r:356:PHE:H	38:A:377:GLU:CB	2.19	0.55
26:M:406:GLU:HA	26:M:410:GLN:HA	1.87	0.55
30:2:101:U:O5'	37:l:66:SER:CB	2.51	0.55
33:o:23:HIS:CB	33:o:31:ASP:HA	2.37	0.55
36:Z:142:U:O4	47:4:396:LEU:CB	2.55	0.55
38:A:617:ASN:C	38:A:622:GLY:HA3	2.29	0.55
44:5:9:G:H1'	44:5:10:U:H5	1.71	0.55
14:v:188:PHE:CB	43:P:154:THR:H	2.19	0.55
17:Q:19:GLU:H	17:Q:20:PRO:HD2	1.70	0.55
30:2:39:U:H3	36:Z:149:A:N6	2.03	0.55
33:o:27:ILE:O	33:o:63:ALA:HB1	2.06	0.55
7:U:744:ILE:N	7:U:745:PRO:HD3	2.11	0.55
14:v:429:ILE:O	15:3:617:GLU:HA	2.07	0.55
18:1:26:VAL:CB	48:u:861:ALA:CA	2.82	0.55
30:2:71:C:H2'	30:2:72:U:H6	1.70	0.55
44:5:109:C:H2'	44:5:110:A:C8	2.42	0.55
38:A:75:ASP:C	38:A:77:THR:H	2.14	0.55
11:z:49:ARG:CB	48:u:412:TYR:CB	2.85	0.55
38:A:175:PRO:CD	38:A:176:LEU:N	2.70	0.55
1:D:282:HIS:HA	1:D:304:SER:HA	1.88	0.54
22:r:633:GLY:H	22:r:636:TYR:CB	2.20	0.54
30:2:83:A:C4	30:2:84:C:C5	2.95	0.54
31:G:416:ILE:HA	31:G:431:ALA:HA	1.89	0.54
33:o:28:PRO:CB	33:o:63:ALA:CB	2.60	0.54
38:A:200:ASP:O	38:A:202:PRO:HD2	2.07	0.54
38:A:1703:ILE:HA	38:A:1714:ALA:HB2	1.89	0.54
7:U:489:VAL:CB	7:U:504:PHE:CA	2.85	0.54
7:U:581:ARG:CB	7:U:582:PRO:HD2	2.38	0.54
14:v:415:SER:HA	15:3:606:ALA:HB1	1.88	0.54
15:3:567:SER:O	15:3:569:PRO:HD2	2.05	0.54
28:O:305:THR:O	28:O:307:PRO:HD3	2.07	0.54
31:G:382:PRO:CB	31:G:423:SER:HA	2.29	0.54
44:5:108:G:H5''	42:g:49:ASN:C	2.33	0.54
38:A:372:PRO:CD	38:A:373:ASP:H	2.16	0.54
38:A:1214:TRP:CB	38:A:1228:CYS:C	2.80	0.54
2:E:3:LEU:HA	2:E:1131:PRO:HA	1.89	0.54
7:U:747:PHE:HA	7:U:781:PRO:CA	2.38	0.54
43:P:278:GLN:O	43:P:281:GLU:N	2.40	0.54
38:A:307:PRO:HD2	38:A:307:PRO:O	2.08	0.54
38:A:564:TYR:C	38:A:569:VAL:CB	2.81	0.54
38:A:1183:PRO:CD	38:A:1184:ASN:H	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:311:ALA:CA	48:u:314:PRO:CD	2.85	0.54
46:F:115:PRO:HD2	46:F:115:PRO:O	2.07	0.54
2:E:327:LEU:O	2:E:372:GLU:HA	2.08	0.54
7:U:745:PRO:CB	7:U:746:PRO:CD	2.82	0.54
9:6:23:U:H4'	17:Q:117:CYS:CA	2.36	0.54
22:r:354:ARG:O	38:A:377:GLU:O	2.26	0.54
36:Z:54:G:C2	44:5:44:A:C8	2.96	0.54
9:6:38:G:H2'	9:6:39:A:C8	2.43	0.54
14:v:254:TRP:CB	19:L:29:ASN:CB	2.86	0.54
48:u:421:TYR:N	48:u:423:PRO:HD2	2.23	0.54
2:E:1111:PRO:O	25:7:176:GLN:CB	2.53	0.53
38:A:464:PRO:CB	44:5:20:G:N1	2.49	0.53
44:5:36:C:H42	44:5:46:U:H3	1.56	0.53
30:2:151:C:H2'	30:2:152:G:H8	1.74	0.53
44:5:98:C:H2'	44:5:99:C:C6	2.44	0.53
47:4:445:HIS:CB	49:T:473:ASP:CA	2.85	0.53
7:U:426:LEU:O	7:U:636:GLN:CB	2.40	0.53
26:M:342:PRO:C	26:M:344:LEU:H	2.16	0.53
33:o:29:PHE:O	33:o:53:GLU:C	2.49	0.53
38:A:63:PRO:CD	38:A:64:GLU:N	2.72	0.53
48:u:325:GLU:C	48:u:327:PRO:HD2	2.33	0.53
48:u:599:ASN:O	48:u:603:ALA:CB	2.57	0.53
38:A:211:GLN:H	38:A:212:PRO:CD	2.13	0.53
7:U:172:LEU:N	7:U:173:PRO:HD2	2.24	0.53
38:A:202:PRO:CD	38:A:203:VAL:H	2.19	0.53
7:U:481:ILE:O	7:U:485:ILE:CB	2.57	0.53
14:v:207:MET:HA	38:A:91:ALA:CB	2.38	0.53
16:0:255:PRO:CG	16:0:276:HIS:HA	2.39	0.53
38:A:946:GLU:CB	38:A:947:PRO:HD3	2.38	0.53
42:n:78:THR:CB	47:4:354:GLU:N	2.72	0.53
44:5:9:G:O5'	44:5:9:G:H8	1.91	0.53
14:v:207:MET:CB	38:A:91:ALA:HB2	2.27	0.53
48:u:1010:THR:O	48:u:1012:PRO:HD3	2.08	0.53
48:u:1257:PRO:HB3	49:T:481:THR:C	2.34	0.53
15:3:567:SER:CB	15:3:569:PRO:CD	2.87	0.53
9:6:23:U:H4'	17:Q:117:CYS:CB	2.39	0.53
2:E:404:LEU:C	2:E:1124:GLY:HA3	2.33	0.53
7:U:1340:THR:C	7:U:1342:ARG:H	2.16	0.53
26:M:231:ASN:O	26:M:233:ASP:N	2.41	0.52
31:G:396:LYS:HA	31:G:408:ASN:HA	1.91	0.52
38:A:946:GLU:CB	38:A:947:PRO:CD	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6:28:A:H3'	9:6:28:A:OP2	2.10	0.52
11:z:95:ASN:HA	48:u:128:ILE:H	1.74	0.52
38:A:947:PRO:CB	38:A:948:PRO:HD3	2.34	0.52
38:A:947:PRO:HG3	38:A:1455:TRP:O	2.10	0.52
17:Q:46:LEU:C	17:Q:48:PRO:HD2	2.35	0.52
36:Z:76:A:N6	43:P:198:ILE:N	2.57	0.52
38:A:1214:TRP:CA	38:A:1228:CYS:CB	2.85	0.52
38:A:1412:TRP:HA	38:A:1419:ILE:CB	2.39	0.52
30:2:55:U:H1'	30:2:58:U:H5	1.74	0.52
30:2:101:U:H1'	37:l:65:GLY:C	2.33	0.52
38:A:1313:PRO:CG	38:A:1336:PRO:HG3	2.39	0.52
2:E:637:PRO:HA	2:E:669:LEU:HA	1.92	0.52
24:Y:106:TRP:N	24:Y:107:PRO:CD	2.72	0.52
38:A:947:PRO:CG	38:A:1455:TRP:O	2.58	0.52
38:A:1183:PRO:CD	38:A:1184:ASN:N	2.71	0.52
2:E:345:GLY:O	2:E:360:GLN:CB	2.57	0.52
7:U:789:PRO:O	7:U:978:PRO:CD	2.58	0.52
30:2:100:U:O2	6:k:64:GLY:C	2.52	0.52
38:A:117:PRO:HD2	38:A:117:PRO:O	2.09	0.52
38:A:372:PRO:CD	38:A:373:ASP:N	2.72	0.52
38:A:1545:ALA:O	38:A:1548:TYR:C	2.53	0.52
37:e:32:LEU:HA	37:e:43:MET:HA	1.91	0.52
9:6:50:A:N3	9:6:50:A:C3'	2.73	0.52
9:6:52:U:O3'	9:6:52:U:O5'	2.28	0.52
9:6:28:A:H5''	17:Q:41:ARG:HA	0.57	0.52
9:6:28:A:N3	9:6:28:A:C2'	2.73	0.52
22:r:353:THR:O	38:A:381:PRO:HA	2.10	0.52
30:2:56:A:O2'	49:T:481:THR:CB	2.58	0.52
30:2:56:A:N6	49:T:505:CYS:HA	2.25	0.52
30:2:120:A:N1	30:2:137:U:O4	2.43	0.52
33:o:23:HIS:HA	33:o:31:ASP:N	2.24	0.52
38:A:829:PRO:HD2	38:A:829:PRO:O	2.10	0.52
7:U:484:ASP:CB	7:U:563:PHE:CB	2.88	0.52
38:A:1330:MET:CA	38:A:1367:ASN:CB	2.88	0.52
44:5:29:A:H2'	44:5:30:A:C8	2.45	0.52
9:6:50:A:N3	9:6:50:A:C5'	2.73	0.51
9:6:61:C:H2'	9:6:62:C:C6	2.44	0.51
48:u:325:GLU:N	48:u:327:PRO:HD2	2.23	0.51
9:6:34:G:N3	9:6:34:G:C3'	2.72	0.51
33:o:30:GLY:HA3	33:o:52:VAL:CB	2.39	0.51
2:E:347:LEU:O	2:E:358:LEU:C	2.53	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:A:167:PRO:O	38:A:167:PRO:CD	2.57	0.51
38:A:938:PRO:HD2	38:A:939:TRP:N	2.25	0.51
44:5:29:A:H2'	44:5:30:A:H8	1.74	0.51
9:6:66:C:OP1	38:A:541:GLY:HA2	2.10	0.51
22:r:594:PRO:HA	22:r:653:ILE:HA	1.91	0.51
38:A:947:PRO:CD	38:A:948:PRO:N	2.72	0.51
38:A:1597:PHE:C	38:A:1599:GLN:H	2.18	0.51
7:U:485:ILE:CB	7:U:591:TYR:O	2.59	0.51
9:6:43:A:O2'	9:6:44:G:H5'	2.11	0.51
9:6:78:A:H5''	9:6:78:A:H8	1.76	0.51
44:5:49:A:H2'	44:5:50:G:H8	1.76	0.51
2:E:336:ALA:HA	2:E:351:SER:HA	1.91	0.51
4:W:81:GLU:HA	4:W:108:PRO:HB3	1.92	0.51
9:6:38:G:O6	36:Z:67:C:N4	2.44	0.51
11:z:95:ASN:CB	48:u:128:ILE:N	2.72	0.51
14:v:281:ASN:CB	38:A:798:GLY:N	2.74	0.51
29:y:4:HIS:HA	36:Z:156:U:H4'	1.92	0.51
38:A:63:PRO:CD	38:A:64:GLU:H	2.23	0.51
5:w:16:TYR:HA	5:w:57:GLY:O	2.10	0.51
7:U:119:PHE:N	7:U:120:PRO:HD2	2.26	0.51
9:6:34:G:N3	9:6:34:G:C5'	2.73	0.51
17:Q:45:SER:O	17:Q:48:PRO:CD	2.58	0.51
46:F:174:GLU:N	46:F:175:PRO:CD	2.73	0.51
48:u:328:THR:N	48:u:329:PRO:CD	2.72	0.51
9:6:48:A:N3	9:6:48:A:C2'	2.73	0.51
44:5:28:A:H2'	44:5:29:A:C8	2.45	0.51
14:v:188:PHE:HA	43:P:154:THR:HA	1.93	0.51
15:3:582:TYR:CB	18:1:58:GLN:HA	2.40	0.51
36:Z:70:G:H22	38:A:512:ASN:HA	1.76	0.51
48:u:1213:ASN:CB	49:T:589:ASP:O	2.59	0.51
5:w:34:LEU:HA	5:w:37:GLY:O	2.11	0.50
7:U:1101:PRO:CB	7:U:1102:PRO:HD2	2.38	0.50
36:Z:147:U:H5''	36:Z:147:U:C6	2.29	0.50
38:A:425:PRO:HG3	44:5:26:A:O5'	2.11	0.50
3:b:25:TRP:O	44:5:116:A:H2	1.90	0.50
9:6:66:C:OP1	38:A:542:ASN:N	2.44	0.50
14:v:427:ASP:O	38:A:1261:ASN:CB	2.58	0.50
36:Z:70:G:H22	38:A:512:ASN:CB	2.23	0.50
38:A:435:CYS:CB	38:A:436:PRO:HD3	2.41	0.50
38:A:797:ASP:CB	38:A:799:PRO:HG3	2.41	0.50
48:u:669:GLN:O	48:u:672:ALA:N	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:PRO:HG2	1:D:337:PRO:HA	1.94	0.50
2:E:349:VAL:CA	2:E:357:TYR:O	2.59	0.50
7:U:1339:PRO:O	7:U:1339:PRO:CD	2.60	0.50
9:6:75:G:N3	9:6:75:G:C3'	2.72	0.50
44:5:48:A:O2'	44:5:49:A:H5'	2.11	0.50
7:U:485:ILE:CB	7:U:591:TYR:C	2.84	0.50
7:U:824:PRO:HB2	7:U:825:PRO:HD2	1.93	0.50
30:2:51:A:N6	30:2:63:G:O6	2.43	0.50
38:A:634:TRP:O	38:A:638:LEU:CB	2.60	0.50
38:A:1661:TRP:N	38:A:1699:THR:O	2.45	0.50
26:M:328:GLU:O	26:M:332:ALA:CB	2.60	0.50
9:6:8:C:H6	9:6:8:C:C5'	2.15	0.50
38:A:175:PRO:CD	38:A:176:LEU:H	2.19	0.50
40:j:32:GLN:N	40:j:88:GLN:O	2.44	0.50
44:5:16:U:H2'	44:5:17:U:C6	2.46	0.50
38:A:1691:ASN:O	38:A:1693:SER:N	2.45	0.50
38:A:2068:SER:C	38:A:2070:LYS:H	2.19	0.50
42:n:78:THR:CB	47:4:353:GLY:O	2.60	0.50
5:w:14:THR:CA	5:w:59:VAL:O	2.27	0.50
17:Q:19:GLU:N	17:Q:20:PRO:CD	2.74	0.50
20:N:105:GLN:O	20:N:110:MET:N	2.33	0.50
36:Z:163:C:H3'	36:Z:163:C:C6	2.46	0.50
38:A:1475:ILE:O	38:A:1480:GLY:N	2.44	0.50
7:U:527:ILE:CB	7:U:1051:LYS:CB	2.90	0.50
29:y:93:SER:C	30:2:34:U:O2'	2.52	0.50
24:Y:49:LYS:N	24:Y:50:PRO:HD2	2.27	0.49
30:2:23:A:H8	30:2:23:A:H3'	1.77	0.49
38:A:174:PRO:CB	38:A:175:PRO:CD	2.78	0.49
38:A:1643:SER:N	38:A:1716:GLY:O	2.42	0.49
44:5:9:G:H2'	44:5:9:G:P	2.52	0.49
44:5:99:C:H2'	44:5:100:U:C6	2.47	0.49
49:T:611:ASP:O	49:T:614:ARG:CB	2.60	0.49
2:E:113:ARG:CA	48:u:1278:ASP:HA	2.42	0.49
2:E:1111:PRO:O	25:7:176:GLN:O	2.30	0.49
9:6:38:G:C2	36:Z:67:C:C2	2.99	0.49
9:6:41:A:H2'	9:6:42:C:C6	2.47	0.49
26:M:214:GLY:CA	33:o:79:VAL:C	2.85	0.49
36:Z:147:U:C6	36:Z:147:U:C4'	2.94	0.49
2:E:1012:VAL:HA	2:E:1023:ILE:HA	1.94	0.49
30:2:100:U:H1'	6:k:65:ASN:CA	2.42	0.49
38:A:2068:SER:C	38:A:2070:LYS:N	2.70	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6:62:C:OP2	9:6:62:C:H6	1.95	0.49
22:r:376:PRO:CB	38:A:388:LEU:CB	2.86	0.49
27:K:386:SER:O	44:5:46:U:O2'	2.23	0.49
38:A:1336:PRO:HD2	38:A:1336:PRO:O	2.12	0.49
44:5:28:A:H2'	44:5:29:A:H8	1.78	0.49
44:5:97:G:H2'	44:5:98:C:H6	1.77	0.49
42:g:70:LEU:H	32:a:99:MET:HA	1.78	0.49
26:M:615:VAL:O	26:M:619:ALA:CB	2.61	0.49
30:2:46:U:O2'	30:2:47:U:OP2	2.25	0.49
38:A:117:PRO:HG2	38:A:131:GLU:N	2.27	0.49
38:A:1064:PRO:O	38:A:1064:PRO:CD	2.59	0.49
38:A:1313:PRO:CD	38:A:1314:VAL:N	2.73	0.49
38:A:1342:TRP:O	38:A:1353:PHE:N	2.39	0.49
38:A:2125:ALA:HA	38:A:2179:HIS:HA	1.93	0.49
44:5:12:U:H3	44:5:65:G:H1	1.59	0.49
44:5:49:A:H2'	44:5:50:G:C8	2.48	0.49
22:r:93:ILE:C	31:G:275:LEU:O	2.53	0.49
31:G:186:PRO:C	31:G:188:PRO:CD	2.85	0.49
37:l:23:ASN:N	37:l:67:LYS:O	2.46	0.49
48:u:323:ILE:O	48:u:327:PRO:HD2	1.96	0.49
2:E:404:LEU:CB	2:E:1124:GLY:C	2.79	0.49
27:K:386:SER:O	44:5:46:U:H1'	2.13	0.49
30:2:37:U:H2'	30:2:38:A:H8	1.78	0.49
36:Z:54:G:N2	44:5:44:A:C8	2.77	0.49
38:A:724:ILE:CB	38:A:725:PRO:CD	2.91	0.49
48:u:1132:LEU:O	48:u:1135:GLU:N	2.45	0.49
7:U:630:ASP:CB	7:U:631:PRO:HD2	2.43	0.49
9:6:61:C:H6	9:6:61:C:C3'	2.22	0.49
36:Z:165:U:H6	36:Z:165:U:OP1	1.96	0.49
41:I:129:LYS:HA	41:I:143:HIS:HA	1.94	0.49
5:w:72:LYS:CB	33:o:217:LYS:CB	2.91	0.49
26:M:211:SER:C	26:M:213:ALA:H	2.21	0.49
38:A:239:TYR:HA	38:A:242:ALA:HB3	1.95	0.49
44:5:39:C:H2'	44:5:40:U:H2'	1.95	0.49
7:U:1074:ILE:N	7:U:1075:PRO:HD2	2.27	0.48
31:G:437:HIS:HA	31:G:449:ARG:HA	1.95	0.48
36:Z:163:C:C6	36:Z:163:C:C3'	2.96	0.48
38:A:386:PRO:CD	38:A:386:PRO:O	2.60	0.48
49:T:652:GLY:N	49:T:655:SER:O	2.46	0.48
7:U:486:GLU:CB	7:U:589:LEU:CB	2.91	0.48
29:y:21:ARG:HA	29:y:68:ASP:HA	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Z:167:U:O2	36:Z:167:U:H2'	2.12	0.48
38:A:729:PRO:HD2	38:A:729:PRO:O	2.13	0.48
44:5:13:C:H2'	44:5:14:U:C6	2.48	0.48
31:G:185:MET:N	31:G:186:PRO:HD2	2.28	0.48
38:A:942:PRO:HD2	38:A:943:ALA:N	2.29	0.48
38:A:1458:GLN:O	38:A:1462:GLY:CA	2.61	0.48
44:5:97:G:H2'	44:5:98:C:C6	2.48	0.48
48:u:323:ILE:C	48:u:327:PRO:CD	2.72	0.48
9:6:53:A:O5'	9:6:53:A:H8	1.95	0.48
17:Q:45:SER:C	17:Q:48:PRO:HD2	2.38	0.48
18:1:70:ASP:H	18:1:75:LYS:HA	1.77	0.48
26:M:456:LEU:O	26:M:460:THR:CB	2.62	0.48
48:u:1110:VAL:O	48:u:1113:THR:CB	2.61	0.48
2:E:113:ARG:HA	48:u:1278:ASP:HA	1.95	0.48
2:E:916:ASN:H	2:E:917:PRO:HD2	1.75	0.48
42:n:75:PRO:CG	47:4:357:GLU:HA	2.40	0.48
44:5:24:G:N3	44:5:26:A:N6	2.61	0.48
38:A:280:GLU:CB	38:A:281:PRO:HD2	2.44	0.48
38:A:1451:ASN:CB	38:A:1452:PRO:CD	2.91	0.48
44:5:54:U:H2'	44:5:55:C:O4'	2.13	0.48
17:Q:109:ARG:O	38:A:480:LYS:CB	2.62	0.48
30:2:120:A:N1	30:2:137:U:C4	2.82	0.48
2:E:201:ALA:HB1	8:x:74:GLN:CB	2.43	0.48
48:u:535:ILE:O	48:u:538:LEU:N	2.47	0.48
9:6:60:C:H3'	9:6:60:C:O2	2.13	0.48
18:1:31:GLU:CB	48:u:821:HIS:H	2.26	0.48
19:L:86:ALA:HB3	19:L:87:PRO:CD	2.44	0.48
30:2:37:U:H2'	30:2:38:A:C8	2.49	0.48
33:o:41:TYR:HA	33:o:154:GLY:HA3	1.95	0.48
48:u:434:THR:CB	48:u:435:PRO:CD	2.92	0.48
9:6:22:A:H5''	17:Q:116:ASN:C	2.38	0.48
26:M:177:PRO:CG	33:o:65:ASP:CB	2.87	0.48
40:j:63:GLU:O	40:j:71:ARG:HA	2.14	0.48
7:U:489:VAL:C	7:U:491:ARG:N	2.72	0.47
38:A:597:LYS:N	44:5:45:C:OP1	2.42	0.47
48:u:326:THR:HA	48:u:329:PRO:CG	2.44	0.47
38:A:371:LEU:CB	38:A:372:PRO:CD	2.92	0.47
47:4:409:GLU:HA	47:4:413:ASN:HA	1.96	0.47
30:2:72:U:H2'	30:2:73:C:C6	2.50	0.47
30:2:83:A:H2'	30:2:84:C:C6	2.49	0.47
31:G:298:PRO:HG3	31:G:340:ALA:H	1.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:G:298:PRO:CG	31:G:340:ALA:HB2	2.43	0.47
36:Z:160:G:N3	36:Z:160:G:C3'	2.76	0.47
8:x:74:GLN:N	8:x:75:PRO:HD3	2.29	0.47
9:6:12:G:H2'	9:6:13:G:O4'	2.15	0.47
12:q:3:GLU:O	12:q:65:GLY:N	2.45	0.47
38:A:1642:PRO:CD	38:A:1642:PRO:O	2.61	0.47
44:5:98:C:H2'	44:5:99:C:H6	1.79	0.47
7:U:171:SER:CB	7:U:173:PRO:HD2	2.45	0.47
15:3:582:TYR:CB	18:1:58:GLN:CA	2.92	0.47
22:r:946:ASP:C	22:r:948:SER:H	2.22	0.47
30:2:100:U:H1'	6:k:65:ASN:N	2.30	0.47
38:A:180:ASP:HA	38:A:183:LEU:HA	1.96	0.47
38:A:1640:SER:HA	38:A:1652:MET:HA	1.97	0.47
2:E:207:THR:HA	2:E:227:PRO:HA	1.96	0.47
9:6:23:U:O2	17:Q:134:CYS:HA	2.14	0.47
9:6:24:A:N3	9:6:26:U:C2	2.83	0.47
36:Z:147:U:H6	36:Z:147:U:C4'	2.28	0.47
1:D:154:VAL:HA	1:D:171:SER:HA	1.97	0.47
2:E:62:ILE:HA	2:E:82:SER:HA	1.97	0.47
7:U:526:ASN:CB	7:U:1048:ASP:CB	2.92	0.47
14:v:132:LEU:O	31:G:384:HIS:CB	2.60	0.47
14:v:188:PHE:CB	43:P:154:THR:N	2.78	0.47
22:r:93:ILE:CA	31:G:275:LEU:O	2.61	0.47
27:K:386:SER:CB	44:5:46:U:O4'	2.63	0.47
30:2:68:G:N3	30:2:68:G:H2'	2.30	0.47
36:Z:143:G:H1'	47:4:399:LEU:CB	2.45	0.47
38:A:233:PRO:HD2	38:A:234:MET:N	2.30	0.47
42:n:78:THR:CB	47:4:354:GLU:HA	2.45	0.47
44:5:91:U:O4	42:g:37:ASN:CB	2.63	0.47
9:6:38:G:C2	36:Z:67:C:O2	2.65	0.47
30:2:57:A:H2'	30:2:58:U:O4'	2.14	0.47
36:Z:147:U:C6	36:Z:147:U:C3'	2.97	0.47
38:A:334:THR:CB	38:A:335:PRO:HD3	2.44	0.47
40:c:62:GLU:HA	40:c:73:GLN:HA	1.97	0.47
2:E:347:LEU:C	2:E:359:TYR:O	2.58	0.47
2:E:796:ASN:HA	2:E:871:PRO:HD3	1.97	0.47
7:U:1157:LEU:CB	7:U:1158:PRO:HD2	2.45	0.47
31:G:196:LEU:HA	31:G:489:TYR:HA	1.97	0.47
38:A:765:ALA:O	38:A:767:VAL:N	2.47	0.47
48:u:501:LEU:O	48:u:504:ILE:N	2.48	0.47
30:2:124:G:H2'	30:2:125:G:C8	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:m:69:LEU:O	37:l:73:LEU:N	2.40	0.47
38:A:425:PRO:HG3	44:5:26:A:P	2.54	0.46
46:F:50:HIS:HA	48:u:1139:PRO:CB	2.45	0.46
9:6:31:U:C6	9:6:31:U:C5'	2.92	0.46
9:6:37:C:H2'	9:6:37:C:O2	2.15	0.46
36:Z:165:U:O5'	36:Z:165:U:C6	2.69	0.46
38:A:1313:PRO:CD	38:A:1314:VAL:H	2.27	0.46
48:u:728:LEU:O	48:u:731:LEU:N	2.48	0.46
14:v:221:GLY:CA	14:v:223:PRO:HD2	2.42	0.46
40:j:44:GLU:O	40:j:61:ALA:HA	2.15	0.46
44:5:32:C:H2'	44:5:33:U:H6	1.81	0.46
44:5:33:U:C2'	44:5:34:U:H5''	2.45	0.46
38:A:625:PRO:O	38:A:625:PRO:CD	2.63	0.46
38:A:643:GLY:HA3	44:5:28:A:O2'	2.15	0.46
44:5:15:C:O2'	44:5:16:U:O5'	2.32	0.46
2:E:43:PRO:HA	2:E:50:VAL:HA	1.97	0.46
7:U:531:TRP:CB	7:U:632:ASN:HA	2.45	0.46
9:6:36:A:C5	36:Z:69:A:N1	2.83	0.46
14:v:179:TYR:CA	39:8:115:ALA:HA	2.43	0.46
14:v:427:ASP:CB	38:A:1265:THR:CB	2.94	0.46
22:r:139:HIS:HA	50:r:1500:GTP:O3B	2.16	0.46
30:2:23:A:H3'	30:2:23:A:C8	2.50	0.46
38:A:1489:LEU:CB	38:A:1540:PRO:HG3	2.45	0.46
46:F:114:ARG:HA	46:F:177:GLU:CB	2.46	0.46
48:u:862:GLU:O	48:u:865:ARG:N	2.48	0.46
2:E:349:VAL:C	2:E:357:TYR:O	2.59	0.46
30:2:60:U:H2'	30:2:61:C:H6	1.81	0.46
40:j:36:TYR:N	40:j:83:ASN:O	2.45	0.46
44:5:110:A:H2'	44:5:111:A:C8	2.50	0.46
7:U:264:LEU:N	7:U:265:PRO:HD2	2.30	0.46
9:6:23:U:C4'	17:Q:117:CYS:CA	2.87	0.46
38:A:463:PRO:O	38:A:463:PRO:CD	2.63	0.46
8:x:74:GLN:N	8:x:75:PRO:CD	2.78	0.46
21:S:455:ALA:HB2	21:S:489:GLY:HA2	1.98	0.46
38:A:348:PRO:HD2	38:A:348:PRO:O	2.15	0.46
38:A:1118:PRO:O	38:A:1118:PRO:CD	2.63	0.46
7:U:1358:MET:N	7:U:1359:PRO:HD2	2.30	0.46
10:B:182:LEU:O	10:B:184:PRO:HD3	2.15	0.46
30:2:45:C:N3	47:4:395:TRP:CA	2.74	0.46
33:o:22:LEU:O	33:o:26:PHE:N	2.49	0.46
46:F:42:LYS:O	46:F:44:PRO:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:84:ALA:HB1	30:2:165:A:H61	1.81	0.46
20:N:82:CYS:O	20:N:86:ASP:N	2.49	0.46
22:r:675:PHE:O	22:r:955:ASP:CB	2.65	0.46
30:2:101:U:O4	6:k:38:MET:CB	2.64	0.46
38:A:1312:PRO:O	38:A:1312:PRO:CD	2.62	0.46
7:U:977:ALA:CB	7:U:978:PRO:HD2	2.41	0.45
30:2:47:U:H4'	30:2:48:A:OP1	2.15	0.45
2:E:37:ILE:HA	2:E:57:GLU:HA	1.98	0.45
11:z:46:ARG:N	11:z:63:VAL:O	2.50	0.45
26:M:211:SER:C	26:M:213:ALA:N	2.73	0.45
9:6:38:G:C2	36:Z:67:C:N3	2.84	0.45
11:z:96:ARG:CA	48:u:537:PRO:HG3	2.46	0.45
12:q:33:ALA:O	27:K:347:PHE:CB	2.64	0.45
30:2:84:C:H2'	30:2:85:A:H8	1.82	0.45
36:Z:162:C:C6	48:u:586:ASP:HA	2.52	0.45
36:Z:165:U:OP1	36:Z:165:U:C6	2.69	0.45
38:A:173:GLU:CB	38:A:174:PRO:CD	2.94	0.45
38:A:458:ALA:C	38:A:460:LYS:H	2.24	0.45
38:A:458:ALA:C	38:A:460:LYS:N	2.75	0.45
44:5:26:A:O2'	44:5:27:U:H2'	2.16	0.45
13:s:1047:PRO:HB3	38:A:2074:ARG:CA	2.45	0.45
30:2:81:G:H2'	30:2:82:G:H8	1.81	0.45
33:o:218:LYS:HA	33:o:244:ASN:O	2.16	0.45
38:A:826:PRO:O	38:A:826:PRO:CD	2.65	0.45
38:A:1477:ALA:C	38:A:1479:GLY:H	2.25	0.45
38:A:2231:THR:O	38:A:2235:TYR:N	2.45	0.45
9:6:26:U:O2'	43:P:180:PRO:CG	2.64	0.45
9:6:52:U:C4'	9:6:53:A:H5'	2.45	0.45
26:M:51:PRO:O	26:M:55:GLN:N	2.48	0.45
38:A:828:PRO:HD2	38:A:828:PRO:O	2.17	0.45
38:A:947:PRO:CB	38:A:948:PRO:CD	2.95	0.45
38:A:1068:PRO:O	38:A:1068:PRO:CD	2.65	0.45
43:P:280:ALA:O	43:P:283:ALA:HB3	2.16	0.45
2:E:348:PHE:HA	2:E:358:LEU:HA	1.97	0.45
2:E:785:PRO:HA	2:E:801:GLU:HA	1.98	0.45
9:6:5:U:H5'	9:6:6:C:OP2	2.17	0.45
30:2:17:U:H6	30:2:17:U:C5'	2.28	0.45
30:2:70:C:H2'	30:2:71:C:C6	2.49	0.45
30:2:71:C:H2'	30:2:72:U:C6	2.50	0.45
30:2:120:A:C6	30:2:137:U:O4	2.70	0.45
36:Z:147:U:C5	36:Z:147:U:OP2	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:I:29:ILE:HA	41:I:67:PRO:HG3	1.98	0.45
47:4:445:HIS:CB	49:T:473:ASP:N	2.79	0.45
2:E:970:TYR:HA	2:E:979:ARG:HA	1.99	0.45
9:6:27:A:OP1	9:6:27:A:H4'	2.16	0.45
9:6:47:A:C4	9:6:47:A:O5'	2.69	0.45
9:6:53:A:O5'	9:6:53:A:C8	2.69	0.45
31:G:467:ALA:HB3	31:G:480:ALA:HB3	1.98	0.45
36:Z:162:C:H5	48:u:586:ASP:N	2.15	0.45
41:I:11:SER:HA	41:I:17:PRO:HG3	1.99	0.45
44:5:13:C:H2'	44:5:14:U:H6	1.82	0.45
44:5:107:G:H3'	44:5:108:G:H8	1.82	0.45
48:u:1125:PRO:O	48:u:1128:VAL:N	2.49	0.45
48:u:1257:PRO:HA	49:T:482:ALA:HA	1.98	0.45
2:E:113:ARG:CA	48:u:1278:ASP:CB	2.95	0.45
9:6:38:G:OP2	9:6:38:G:C8	2.69	0.45
9:6:62:C:C6	9:6:62:C:OP2	2.70	0.45
16:0:226:PHE:HA	18:1:49:GLU:N	2.08	0.45
25:7:101:HIS:CB	48:u:1051:SER:CB	2.95	0.45
30:2:80:A:H2'	30:2:81:G:H8	1.81	0.45
36:Z:168:U:OP2	36:Z:168:U:C6	2.70	0.45
38:A:697:MET:CB	38:A:698:PRO:HD2	2.46	0.45
38:A:827:PHE:CB	38:A:828:PRO:CD	2.94	0.45
36:Z:142:U:O4	47:4:396:LEU:HA	2.17	0.45
9:6:9:U:H2'	9:6:10:U:C6	2.52	0.45
9:6:39:A:H2'	9:6:40:U:C6	2.52	0.45
9:6:93:G:P	28:O:351:ASN:CB	3.04	0.45
22:r:196:LYS:HA	37:e:12:GLU:CA	2.46	0.45
30:2:82:G:H2'	30:2:83:A:H8	1.82	0.45
7:U:481:ILE:O	7:U:592:VAL:CA	2.65	0.44
10:B:224:LYS:C	47:4:497:ARG:O	2.59	0.44
22:r:831:TYR:HA	22:r:876:PRO:HA	1.99	0.44
36:Z:166:U:H4'	36:Z:167:U:C5	2.52	0.44
38:A:121:HIS:HA	38:A:482:PHE:HA	1.99	0.44
44:5:74:U:H2'	44:5:75:G:C8	2.52	0.44
48:u:810:ILE:O	48:u:813:PRO:HD2	2.17	0.44
2:E:12:THR:CB	2:E:404:LEU:H	2.30	0.44
5:w:67:ALA:HA	5:w:70:ALA:HB3	2.00	0.44
13:s:1045:PRO:HB3	38:A:2313:HIS:O	2.17	0.44
14:v:420:SER:O	38:A:1458:GLN:CB	2.65	0.44
36:Z:146:G:C8	36:Z:146:G:O5'	2.70	0.44
38:A:335:PRO:O	38:A:335:PRO:CD	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:345:PHE:HA	7:U:346:PRO:HD2	1.86	0.44
9:6:22:A:C5'	17:Q:116:ASN:O	2.58	0.44
30:2:60:U:H2'	30:2:61:C:C6	2.52	0.44
30:2:166:G:N2	30:2:166:G:OP2	2.50	0.44
36:Z:145:U:C5	36:Z:145:U:OP2	2.70	0.44
38:A:1720:PRO:CD	38:A:1720:PRO:O	2.65	0.44
48:u:326:THR:CA	48:u:329:PRO:HG2	2.47	0.44
48:u:416:PRO:HB2	48:u:417:PRO:HD2	1.98	0.44
48:u:762:ALA:O	48:u:766:THR:CB	2.65	0.44
13:s:957:VAL:O	13:s:961:ALA:N	2.46	0.44
30:2:33:G:C2	36:Z:157:C:O2	2.71	0.44
38:A:907:PRO:O	38:A:907:PRO:CD	2.64	0.44
38:A:1489:LEU:N	38:A:1540:PRO:HG3	2.32	0.44
44:5:37:G:H3'	44:5:37:G:C8	2.53	0.44
2:E:1045:ALA:HA	2:E:1055:VAL:HA	1.99	0.44
9:6:28:A:N3	9:6:28:A:C3'	2.73	0.44
9:6:46:G:C2	9:6:46:G:OP2	2.70	0.44
11:z:98:PHE:O	11:z:100:LYS:N	2.50	0.44
17:Q:19:GLU:CB	17:Q:20:PRO:HD3	2.47	0.44
22:r:79:THR:HA	31:G:199:VAL:CB	2.48	0.44
44:5:12:U:O2'	44:5:13:C:H5'	2.17	0.44
49:T:611:ASP:O	49:T:614:ARG:N	2.50	0.44
30:2:44:U:N3	36:Z:144:A:H2	2.02	0.44
14:v:179:TYR:CB	39:8:115:ALA:HA	2.48	0.44
14:v:207:MET:HA	38:A:91:ALA:HB1	1.99	0.44
30:2:17:U:C6	30:2:17:U:OP2	2.70	0.44
30:2:19:G:OP2	30:2:19:G:H4'	2.18	0.44
30:2:79:G:H2'	30:2:80:A:H8	1.81	0.44
44:5:54:U:H2'	44:5:55:C:C6	2.52	0.44
9:6:93:G:H5''	28:O:347:HIS:C	2.43	0.44
30:2:34:U:C4	30:2:35:A:N7	2.85	0.44
40:j:57:VAL:HA	40:j:77:ILE:O	2.18	0.44
2:E:642:ILE:HA	2:E:665:LEU:HA	2.00	0.44
9:6:61:C:H4'	9:6:61:C:OP1	2.18	0.44
30:2:100:U:H3	6:k:64:GLY:H	1.65	0.44
38:A:727:LYS:O	38:A:729:PRO:HD3	2.18	0.44
44:5:17:U:O4	44:5:60:G:O6	2.36	0.44
9:6:28:A:N3	9:6:28:A:H2'	2.33	0.43
33:o:49:PHE:O	33:o:50:ALA:HB2	2.18	0.43
48:u:1110:VAL:O	48:u:1113:THR:N	2.51	0.43
15:3:593:PHE:CB	18:1:95:ASP:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:u:427:PRO:O	48:u:431:LEU:N	2.45	0.43
2:E:89:ILE:O	2:E:102:ILE:N	2.47	0.43
3:b:23:LEU:HA	3:b:69:VAL:HA	2.00	0.43
7:U:1340:THR:C	7:U:1342:ARG:N	2.75	0.43
19:L:29:ASN:CB	30:2:24:A:C2	2.91	0.43
30:2:144:C:H2'	30:2:145:A:H2'	2.00	0.43
32:h:30:SER:O	32:h:34:GLN:N	2.45	0.43
36:Z:160:G:N3	36:Z:160:G:C2'	2.81	0.43
38:A:1661:TRP:CB	38:A:1696:PRO:HG3	2.48	0.43
2:E:94:PRO:C	2:E:96:LYS:N	2.76	0.43
9:6:26:U:H3'	9:6:27:A:H5''	2.00	0.43
11:z:16:GLU:CB	48:u:542:PRO:CB	2.96	0.43
25:7:337:PRO:HB2	25:7:341:LYS:CB	2.48	0.43
38:A:358:PRO:O	38:A:358:PRO:CD	2.65	0.43
22:r:685:ILE:HA	22:r:794:ALA:HA	2.00	0.43
36:Z:145:U:H6	36:Z:145:U:P	2.41	0.43
38:A:133:PRO:O	38:A:133:PRO:CD	2.66	0.43
45:p:105:LYS:CB	46:F:117:TYR:HA	2.48	0.43
48:u:426:THR:CB	48:u:427:PRO:HD3	2.49	0.43
17:Q:19:GLU:CB	17:Q:20:PRO:CD	2.96	0.43
30:2:33:G:N3	36:Z:157:C:O2	2.51	0.43
8:x:30:GLU:N	8:x:79:PRO:HG3	2.29	0.43
26:M:683:ARG:O	26:M:687:ILE:CB	2.67	0.43
30:2:100:U:O3'	6:k:65:ASN:CB	2.66	0.43
33:o:27:ILE:CA	33:o:67:MET:CB	2.90	0.43
36:Z:54:G:C2	44:5:44:A:H8	2.35	0.43
38:A:1330:MET:HA	38:A:1367:ASN:CB	2.49	0.43
1:D:249:TYR:HA	1:D:263:ASP:HA	2.00	0.43
9:6:34:G:H2'	9:6:35:A:C4	2.54	0.43
9:6:36:A:N9	36:Z:69:A:N1	2.66	0.43
9:6:42:C:H2'	9:6:43:A:C8	2.53	0.43
14:v:207:MET:CA	38:A:91:ALA:HB1	2.39	0.43
30:2:56:A:OP1	48:u:1258:ALA:HA	2.19	0.43
36:Z:167:U:OP2	36:Z:167:U:C6	2.71	0.43
38:A:385:GLU:CB	38:A:386:PRO:HD2	2.45	0.43
38:A:2216:CYS:HA	38:A:2225:LEU:HA	2.01	0.43
46:F:51:LEU:HA	48:u:1140:GLU:HA	2.01	0.43
2:E:255:TYR:HA	2:E:270:PRO:HA	2.00	0.43
2:E:931:VAL:N	2:E:936:LYS:O	2.50	0.43
9:6:47:A:OP1	9:6:47:A:C8	2.71	0.43
22:r:176:GLU:O	38:A:330:THR:CB	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:6:22:A:N1	39:8:130:ARG:HA	2.34	0.42
11:z:114:LYS:HA	11:z:119:ILE:O	2.19	0.42
30:2:151:C:H2'	30:2:152:G:C8	2.53	0.42
46:F:141:ILE:CB	46:F:175:PRO:HG3	2.48	0.42
42:g:29:ILE:HA	42:g:40:LEU:HA	2.01	0.42
48:u:722:GLU:O	48:u:725:ASP:CB	2.67	0.42
13:s:912:ASN:HA	13:s:978:ASN:HA	2.01	0.42
13:s:1433:ASP:O	13:s:1437:ARG:CB	2.67	0.42
26:M:214:GLY:HA2	33:o:79:VAL:C	2.44	0.42
31:G:185:MET:N	31:G:186:PRO:CD	2.81	0.42
38:A:1615:HIS:CB	38:A:1616:PRO:CD	2.97	0.42
44:5:49:A:O2'	44:5:50:G:H5'	2.19	0.42
44:5:63:A:O2'	44:5:64:G:H5'	2.19	0.42
48:u:436:THR:CB	48:u:437:PRO:HD3	2.49	0.42
2:E:915:LEU:CB	2:E:917:PRO:HD2	2.49	0.42
7:U:748:ARG:O	7:U:779:VAL:HA	2.19	0.42
30:2:41:U:O3'	46:F:75:GLY:HA3	2.19	0.42
36:Z:74:G:O2'	36:Z:75:U:OP1	2.29	0.42
38:A:2273:VAL:O	38:A:2297:GLN:N	2.50	0.42
48:u:707:LEU:O	48:u:710:ALA:HB3	2.20	0.42
2:E:201:ALA:HB2	8:x:74:GLN:CB	2.49	0.42
21:S:492:VAL:O	21:S:496:ILE:CB	2.67	0.42
38:A:1722:SER:C	38:A:1724:PRO:CD	2.92	0.42
44:5:73:C:H2'	44:5:74:U:H6	1.83	0.42
46:F:141:ILE:HA	46:F:175:PRO:HB3	2.00	0.42
49:T:614:ARG:O	49:T:618:GLY:N	2.51	0.42
2:E:888:ALA:HA	2:E:909:VAL:HA	2.01	0.42
2:E:1052:ASN:HA	2:E:1096:HIS:HA	2.01	0.42
5:w:66:ASP:HA	49:T:643:PRO:HG2	2.01	0.42
38:A:408:PRO:O	38:A:408:PRO:CD	2.68	0.42
38:A:765:ALA:C	38:A:767:VAL:N	2.77	0.42
44:5:9:G:H1'	44:5:10:U:C5	2.54	0.42
44:5:41:U:O2'	44:5:42:U:H5'	2.19	0.42
48:u:311:ALA:CA	48:u:314:PRO:CG	2.94	0.42
2:E:440:HIS:HA	2:E:774:PHE:HA	2.01	0.42
26:M:560:TYR:O	26:M:564:PHE:CB	2.67	0.42
30:2:69:U:H2'	30:2:70:C:H6	1.84	0.42
38:A:938:PRO:HD2	38:A:939:TRP:H	1.85	0.42
45:p:103:GLU:CB	46:F:115:PRO:CG	2.94	0.42
46:F:51:LEU:C	48:u:1141:LEU:N	2.67	0.42
48:u:323:ILE:O	48:u:327:PRO:CG	2.57	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:264:ASP:O	26:M:268:ARG:CB	2.67	0.42
38:A:173:GLU:CB	38:A:174:PRO:HD3	2.49	0.42
44:5:55:C:H2'	44:5:56:C:C6	2.54	0.42
2:E:193:ASP:C	8:x:78:PRO:HB2	2.17	0.42
2:E:456:PRO:HA	2:E:478:PHE:HA	2.02	0.42
25:7:275:ALA:HB1	25:7:348:GLY:C	2.44	0.42
26:M:668:CYS:O	26:M:672:ALA:CB	2.68	0.42
30:2:19:G:N3	30:2:19:G:C2'	2.81	0.42
30:2:56:A:H61	49:T:505:CYS:HA	1.82	0.42
38:A:829:PRO:HG2	38:A:832:TYR:CB	2.49	0.42
38:A:2126:GLY:N	38:A:2178:ILE:O	2.52	0.42
42:n:14:THR:HA	42:n:28:THR:HA	2.02	0.42
46:F:51:LEU:CA	48:u:1140:GLU:HA	2.49	0.42
49:T:630:PRO:HA	49:T:631:PRO:HD3	1.77	0.42
2:E:436:ARG:HA	2:E:778:ALA:HA	2.02	0.42
38:A:324:PRO:O	38:A:324:PRO:CD	2.68	0.42
33:o:10:VAL:O	33:o:49:PHE:CB	2.68	0.41
35:m:26:ILE:O	35:m:47:GLU:HA	2.20	0.41
44:5:24:G:H1'	44:5:26:A:N7	2.35	0.41
9:6:7:G:H5'	9:6:7:G:C8	2.52	0.41
24:Y:49:LYS:N	24:Y:50:PRO:CD	2.83	0.41
38:A:1198:PRO:O	38:A:1198:PRO:CD	2.67	0.41
38:A:1661:TRP:CB	38:A:1696:PRO:CG	2.98	0.41
44:5:10:U:H2'	44:5:11:U:H6	1.84	0.41
44:5:12:U:H2'	44:5:13:C:H6	1.85	0.41
48:u:417:PRO:CG	48:u:418:PRO:CD	2.76	0.41
48:u:699:GLN:O	48:u:700:LYS:C	2.63	0.41
9:6:36:A:H8	36:Z:69:A:H2	1.47	0.41
31:G:249:VAL:HA	31:G:265:GLY:HA3	2.01	0.41
36:Z:146:G:H2'	36:Z:147:U:C4	2.55	0.41
38:A:824:PRO:O	38:A:824:PRO:CD	2.67	0.41
2:E:347:LEU:H	2:E:360:GLN:HA	1.85	0.41
7:U:1317:THR:N	7:U:1318:PRO:HD2	2.36	0.41
9:6:38:G:N1	36:Z:67:C:C2	2.87	0.41
13:s:2032:GLY:H	13:s:2096:ALA:HB3	1.85	0.41
26:M:543:ARG:O	26:M:547:LEU:CB	2.69	0.41
42:g:16:THR:HA	42:g:26:HIS:HA	2.02	0.41
9:6:37:C:C5	36:Z:62:A:OP2	2.73	0.41
38:A:1134:TRP:O	38:A:1136:ARG:N	2.53	0.41
44:5:75:G:H2'	44:5:76:A:C8	2.55	0.41
45:p:104:GLY:HA3	46:F:139:PRO:CG	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:209:THR:HA	2:E:225:SER:HA	2.02	0.41
2:E:743:SER:O	2:E:755:VAL:N	2.52	0.41
36:Z:70:G:H22	38:A:512:ASN:CA	2.34	0.41
38:A:70:ILE:C	38:A:72:ASP:N	2.75	0.41
38:A:937:PRO:HB2	38:A:938:PRO:HD2	2.00	0.41
42:n:78:THR:N	47:4:353:GLY:HA3	2.35	0.41
2:E:805:ASN:CB	8:x:58:ASN:CB	2.98	0.41
7:U:370:GLY:N	7:U:371:PRO:HD2	2.35	0.41
9:6:39:A:H2'	9:6:40:U:O4'	2.21	0.41
22:r:358:LYS:CB	38:A:370:PRO:HA	2.51	0.41
26:M:452:ALA:O	26:M:456:LEU:CB	2.68	0.41
48:u:1120:ALA:HB1	48:u:1125:PRO:HB3	2.01	0.41
1:D:163:GLY:HA3	1:D:164:PRO:HD3	1.90	0.41
38:A:938:PRO:CD	38:A:939:TRP:N	2.84	0.41
9:6:27:A:OP1	9:6:27:A:C4'	2.69	0.41
9:6:56:A:N6	30:2:20:G:C6	2.89	0.41
31:G:455:GLN:CB	31:G:456:PRO:HD2	2.51	0.41
38:A:1615:HIS:CB	38:A:1616:PRO:HD3	2.51	0.41
44:5:5:U:H2'	44:5:6:C:C6	2.56	0.41
35:f:16:ARG:HA	35:f:30:THR:HA	2.02	0.41
5:w:67:ALA:O	5:w:70:ALA:HB3	2.21	0.41
7:U:1102:PRO:CD	7:U:1116:GLU:O	2.68	0.41
11:z:16:GLU:CB	48:u:542:PRO:HB3	2.51	0.41
30:2:103:U:P	35:m:75:GLU:CB	3.09	0.41
44:5:99:C:H2'	44:5:100:U:H6	1.86	0.41
7:U:494:PRO:HB2	7:U:569:PRO:HB3	2.03	0.40
21:S:490:LEU:O	21:S:494:GLN:CB	2.68	0.40
30:2:44:U:C2	36:Z:144:A:H2	2.39	0.40
38:A:1319:PRO:O	38:A:1319:PRO:CD	2.68	0.40
48:u:1029:GLU:O	48:u:1033:GLU:N	2.30	0.40
9:6:8:C:C6	9:6:8:C:C5'	2.97	0.40
26:M:326:ASP:C	26:M:328:GLU:H	2.28	0.40
26:M:597:LEU:O	26:M:601:GLN:CB	2.69	0.40
30:2:152:G:H2'	30:2:153:A:H8	1.87	0.40
33:o:37:ILE:HA	33:o:38:PRO:HD3	1.94	0.40
36:Z:143:G:H22	47:4:395:TRP:CB	2.34	0.40
36:Z:160:G:H21	36:Z:161:U:H5''	1.86	0.40
38:A:942:PRO:CD	38:A:943:ALA:N	2.85	0.40
45:p:103:GLU:C	46:F:139:PRO:HG2	2.46	0.40
48:u:943:LYS:CB	48:u:947:VAL:H	2.33	0.40
9:6:40:U:O4	9:6:41:A:N6	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:v:217:LYS:O	14:v:219:PRO:HD3	2.22	0.40
26:M:328:GLU:O	26:M:332:ALA:HB2	2.22	0.40
30:2:180:G:N2	37:l:53:GLY:HA3	2.36	0.40
34:t:142:ARG:O	34:t:150:PHE:CB	2.70	0.40
48:u:324:GLY:CA	48:u:327:PRO:HG2	2.43	0.40
5:w:17:VAL:CA	5:w:85:ARG:O	2.45	0.40
7:U:746:PRO:HD2	7:U:782:HIS:H	1.86	0.40
9:6:42:C:H2'	9:6:43:A:O4'	2.21	0.40
9:6:42:C:C2	9:6:43:A:C8	3.09	0.40
15:3:567:SER:CA	15:3:569:PRO:HD2	2.48	0.40
2:E:720:TRP:HA	2:E:733:PRO:HA	2.03	0.40
9:6:30:A:O4'	43:P:166:SER:CB	2.70	0.40
9:6:36:A:H2'	9:6:36:A:P	2.61	0.40
11:z:96:ARG:HA	48:u:537:PRO:HG3	2.03	0.40
22:r:179:VAL:HA	50:r:1500:GTP:O2G	2.22	0.40
44:5:9:G:O5'	44:5:9:G:C8	2.72	0.40
44:5:58:U:H2'	44:5:59:G:H8	1.85	0.40
45:p:105:LYS:CB	46:F:117:TYR:CA	2.99	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	D	300/357 (84%)	292 (97%)	8 (3%)	0	100	100
2	E	1165/1217 (96%)	1126 (97%)	27 (2%)	12 (1%)	12	49
3	b	71/86 (83%)	71 (100%)	0	0	100	100
3	i	70/86 (81%)	69 (99%)	1 (1%)	0	100	100
4	W	160/255 (63%)	147 (92%)	13 (8%)	0	100	100
5	w	76/424 (18%)	68 (90%)	7 (9%)	1 (1%)	9	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	d	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
6	k	71/76 (93%)	69 (97%)	2 (3%)	0	100	100
7	U	1319/1485 (89%)	1273 (96%)	36 (3%)	10 (1%)	16	54
8	x	77/86 (90%)	66 (86%)	10 (13%)	1 (1%)	9	42
10	B	165/225 (73%)	158 (96%)	4 (2%)	3 (2%)	6	34
11	z	106/125 (85%)	90 (85%)	16 (15%)	0	100	100
12	q	71/73 (97%)	64 (90%)	7 (10%)	0	100	100
13	s	1720/2136 (80%)	1691 (98%)	29 (2%)	0	100	100
14	v	198/536 (37%)	181 (91%)	17 (9%)	0	100	100
15	3	53/619 (9%)	48 (91%)	5 (9%)	0	100	100
16	0	148/396 (37%)	145 (98%)	3 (2%)	0	100	100
17	Q	136/144 (94%)	127 (93%)	8 (6%)	1 (1%)	18	56
18	1	120/322 (37%)	111 (92%)	6 (5%)	3 (2%)	4	26
19	L	112/802 (14%)	108 (96%)	4 (4%)	0	100	100
20	N	54/199 (27%)	47 (87%)	7 (13%)	0	100	100
21	S	353/563 (63%)	344 (98%)	8 (2%)	1 (0%)	36	72
22	r	893/972 (92%)	813 (91%)	76 (8%)	4 (0%)	30	67
23	R	42/229 (18%)	38 (90%)	4 (10%)	0	100	100
24	Y	93/904 (10%)	92 (99%)	1 (1%)	0	100	100
25	7	230/393 (58%)	225 (98%)	4 (2%)	1 (0%)	30	67
26	M	704/855 (82%)	597 (85%)	96 (14%)	11 (2%)	7	38
27	K	121/439 (28%)	96 (79%)	25 (21%)	0	100	100
28	O	246/848 (29%)	234 (95%)	12 (5%)	0	100	100
29	y	98/110 (89%)	93 (95%)	3 (3%)	2 (2%)	6	31
31	G	318/514 (62%)	292 (92%)	21 (7%)	5 (2%)	7	38
32	a	74/118 (63%)	73 (99%)	1 (1%)	0	100	100
32	h	91/118 (77%)	86 (94%)	5 (6%)	0	100	100
33	o	221/301 (73%)	196 (89%)	19 (9%)	6 (3%)	4	25
34	t	247/520 (48%)	234 (95%)	12 (5%)	1 (0%)	30	67
35	f	60/240 (25%)	60 (100%)	0	0	100	100
35	m	80/240 (33%)	74 (92%)	6 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	e	76/126 (60%)	76 (100%)	0	0	100	100
37	l	81/126 (64%)	76 (94%)	5 (6%)	0	100	100
38	A	2153/2335 (92%)	1791 (83%)	296 (14%)	66 (3%)	3	22
39	8	16/579 (3%)	15 (94%)	1 (6%)	0	100	100
40	c	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
40	j	79/92 (86%)	77 (98%)	2 (2%)	0	100	100
41	I	174/312 (56%)	166 (95%)	8 (5%)	0	100	100
42	g	89/119 (75%)	88 (99%)	1 (1%)	0	100	100
42	n	78/119 (66%)	75 (96%)	3 (4%)	0	100	100
43	P	231/420 (55%)	191 (83%)	39 (17%)	1 (0%)	30	67
45	p	120/793 (15%)	115 (96%)	3 (2%)	2 (2%)	7	36
46	F	159/464 (34%)	145 (91%)	10 (6%)	4 (2%)	4	26
47	4	415/501 (83%)	370 (89%)	36 (9%)	9 (2%)	5	29
48	u	931/1304 (71%)	822 (88%)	103 (11%)	6 (1%)	21	59
49	T	175/895 (20%)	159 (91%)	15 (9%)	1 (1%)	21	59
All	All	14983/25366 (59%)	13804 (92%)	1028 (7%)	151 (1%)	15	49

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	405	SER
2	E	914	ILE
7	U	744	ILE
7	U	980	PRO
7	U	1338	PHE
8	x	7	ILE
10	B	175	PRO
18	1	72	LYS
26	M	48	ALA
26	M	50	LYS
26	M	720	ILE
31	G	343	PRO
31	G	371	HIS
38	A	233	PRO
38	A	250	VAL
38	A	381	PRO
38	A	462	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A	463	PRO
38	A	697	MET
38	A	766	THR
38	A	942	PRO
38	A	947	PRO
38	A	948	PRO
38	A	1417	PRO
38	A	1469	ASN
38	A	1698	PRO
45	p	192	ASN
46	F	165	ARG
47	4	78	PRO
47	4	463	LYS
47	4	473	PRO
48	u	417	PRO
48	u	718	PRO
48	u	942	ASN
2	E	95	SER
2	E	361	ILE
2	E	385	PHE
2	E	392	LEU
2	E	397	LEU
2	E	402	ASP
2	E	406	PRO
7	U	982	PHE
10	B	176	GLY
17	Q	11	PRO
22	r	947	VAL
22	r	948	SER
29	y	4	HIS
31	G	382	PRO
33	o	28	PRO
38	A	77	THR
38	A	113	ILE
38	A	283	VAL
38	A	393	LEU
38	A	435	CYS
38	A	436	PRO
38	A	701	ILE
38	A	704	ASN
38	A	857	ASN
38	A	946	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A	1015	VAL
38	A	1367	ASN
38	A	1415	GLY
43	P	278	GLN
47	4	227	PRO
47	4	292	SER
48	u	720	GLY
49	T	604	LYS
7	U	490	SER
18	1	73	THR
26	M	206	ASP
26	M	207	GLU
26	M	385	VAL
29	y	3	LYS
31	G	383	ARG
33	o	27	ILE
34	t	143	ASP
38	A	285	ASP
38	A	323	LEU
38	A	395	THR
38	A	623	LYS
38	A	729	PRO
38	A	1467	LEU
38	A	1692	MET
38	A	2058	THR
45	p	218	ILE
47	4	308	LYS
47	4	482	SER
2	E	386	PHE
2	E	773	VAL
7	U	977	ALA
25	7	104	HIS
26	M	357	VAL
26	M	585	ASP
31	G	344	GLN
33	o	48	GLY
33	o	203	PHE
38	A	208	TYR
38	A	472	LEU
38	A	532	THR
38	A	622	GLY
38	A	763	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A	1348	VAL
38	A	1369	TYR
38	A	1414	ARG
38	A	1416	ILE
38	A	1691	ASN
38	A	2068	SER
48	u	456	VAL
2	E	96	LYS
7	U	745	PRO
22	r	941	LYS
26	M	337	LEU
33	o	208	GLY
38	A	364	SER
38	A	370	PRO
38	A	433	GLU
38	A	439	GLN
38	A	706	ALA
38	A	1120	PRO
38	A	2066	THR
46	F	115	PRO
46	F	208	LEU
47	4	99	PRO
7	U	493	LYS
10	B	213	THR
18	1	74	GLY
26	M	212	LYS
33	o	25	ALA
38	A	1600	GLU
38	A	1696	PRO
7	U	630	ASP
7	U	631	PRO
38	A	137	GLU
38	A	731	LEU
38	A	913	PRO
47	4	472	GLN
22	r	955	ASP
38	A	384	VAL
38	A	1496	PRO
46	F	188	ILE
5	w	27	PRO
26	M	517	THR
38	A	569	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	A	1084	PRO
38	A	1697	SER
21	S	376	ILE
38	A	191	ILE
38	A	1016	VAL
38	A	409	ARG
38	A	1956	PRO
48	u	932	ILE

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	D	10/300 (3%)	10 (100%)	0	100	100
2	E	60/1051 (6%)	60 (100%)	0	100	100
3	b	4/74 (5%)	4 (100%)	0	100	100
3	i	4/74 (5%)	4 (100%)	0	100	100
4	W	6/218 (3%)	6 (100%)	0	100	100
5	w	4/336 (1%)	4 (100%)	0	100	100
6	d	3/66 (4%)	3 (100%)	0	100	100
6	k	3/66 (4%)	3 (100%)	0	100	100
7	U	71/1336 (5%)	70 (99%)	1 (1%)	59	72
8	x	3/77 (4%)	3 (100%)	0	100	100
10	B	8/195 (4%)	8 (100%)	0	100	100
11	z	5/109 (5%)	5 (100%)	0	100	100
13	s	79/1908 (4%)	79 (100%)	0	100	100
14	v	15/459 (3%)	15 (100%)	0	100	100
15	3	6/545 (1%)	6 (100%)	0	100	100
16	0	10/349 (3%)	10 (100%)	0	100	100
17	Q	6/130 (5%)	6 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	1	3/291 (1%)	3 (100%)	0	100	100
19	L	3/709 (0%)	3 (100%)	0	100	100
21	S	8/510 (2%)	8 (100%)	0	100	100
22	r	55/866 (6%)	55 (100%)	0	100	100
24	Y	4/831 (0%)	4 (100%)	0	100	100
25	7	6/354 (2%)	6 (100%)	0	100	100
26	M	24/749 (3%)	24 (100%)	0	100	100
27	K	2/395 (0%)	2 (100%)	0	100	100
28	O	3/751 (0%)	3 (100%)	0	100	100
29	y	4/95 (4%)	4 (100%)	0	100	100
31	G	13/441 (3%)	13 (100%)	0	100	100
32	a	3/110 (3%)	3 (100%)	0	100	100
32	h	5/110 (4%)	5 (100%)	0	100	100
33	o	8/252 (3%)	8 (100%)	0	100	100
34	t	14/456 (3%)	14 (100%)	0	100	100
35	f	2/177 (1%)	2 (100%)	0	100	100
35	m	4/177 (2%)	4 (100%)	0	100	100
37	e	3/101 (3%)	3 (100%)	0	100	100
37	l	3/101 (3%)	3 (100%)	0	100	100
38	A	123/2108 (6%)	123 (100%)	0	100	100
39	8	1/502 (0%)	1 (100%)	0	100	100
40	c	1/84 (1%)	1 (100%)	0	100	100
40	j	1/84 (1%)	1 (100%)	0	100	100
41	I	6/293 (2%)	6 (100%)	0	100	100
42	g	4/101 (4%)	4 (100%)	0	100	100
42	n	3/101 (3%)	3 (100%)	0	100	100
43	P	12/361 (3%)	12 (100%)	0	100	100
45	p	7/709 (1%)	7 (100%)	0	100	100
46	F	8/382 (2%)	8 (100%)	0	100	100
47	4	12/446 (3%)	11 (92%)	1 (8%)	10	30
48	u	49/1104 (4%)	48 (98%)	1 (2%)	48	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	T	19/776 (2%)	19 (100%)	0	100	100
All	All	710/21820 (3%)	707 (100%)	3 (0%)	81	84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	U	980	PRO
47	4	78	PRO
48	u	718	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	2	161/188 (85%)	40 (24%)	3 (1%)
36	Z	55/324 (16%)	26 (47%)	5 (9%)
44	5	113/116 (97%)	39 (34%)	3 (2%)
9	6	88/106 (83%)	40 (45%)	13 (14%)
All	All	417/734 (56%)	145 (34%)	24 (5%)

All (145) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	6	5	U
9	6	6	C
9	6	7	G
9	6	8	C
9	6	10	U
9	6	12	G
9	6	25	C
9	6	26	U
9	6	27	A
9	6	28	A
9	6	29	A
9	6	31	U
9	6	32	U
9	6	33	G
9	6	34	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	6	36	A
9	6	37	C
9	6	38	G
9	6	44	G
9	6	45	A
9	6	46	G
9	6	47	A
9	6	48	A
9	6	49	G
9	6	50	A
9	6	51	U
9	6	52	U
9	6	53	A
9	6	54	G
9	6	61	C
9	6	62	C
9	6	69	A
9	6	73	A
9	6	75	G
9	6	79	C
9	6	80	G
9	6	81	C
9	6	83	A
9	6	84	A
9	6	85	U
30	2	15	U
30	2	18	U
30	2	19	G
30	2	20	G
30	2	23	A
30	2	24	A
30	2	25	G
30	2	27	U
30	2	29	A
30	2	30	A
30	2	31	G
30	2	32	U
30	2	44	U
30	2	45	C
30	2	46	U
30	2	47	U
30	2	48	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	2	65	U
30	2	68	G
30	2	101	U
30	2	102	U
30	2	103	U
30	2	111	G
30	2	116	A
30	2	117	U
30	2	121	A
30	2	122	U
30	2	123	A
30	2	124	G
30	2	128	C
30	2	129	U
30	2	130	U
30	2	131	G
30	2	136	G
30	2	138	C
30	2	146	C
30	2	147	G
30	2	157	G
30	2	164	C
30	2	177	A
36	Z	51	U
36	Z	52	C
36	Z	53	C
36	Z	54	G
36	Z	55	A
36	Z	60	U
36	Z	61	A
36	Z	62	A
36	Z	63	G
36	Z	71	C
36	Z	72	A
36	Z	75	U
36	Z	78	A
36	Z	146	G
36	Z	147	U
36	Z	149	A
36	Z	151	A
36	Z	155	A
36	Z	158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	Z	159	U
36	Z	160	G
36	Z	161	U
36	Z	162	C
36	Z	163	C
36	Z	167	U
36	Z	168	U
44	5	8	G
44	5	9	G
44	5	10	U
44	5	11	U
44	5	16	U
44	5	17	U
44	5	19	A
44	5	20	G
44	5	21	A
44	5	22	U
44	5	26	A
44	5	27	U
44	5	34	U
44	5	38	C
44	5	39	C
44	5	40	U
44	5	41	U
44	5	44	A
44	5	45	C
44	5	48	A
44	5	52	U
44	5	53	U
44	5	61	A
44	5	62	G
44	5	68	C
44	5	69	A
44	5	72	U
44	5	79	C
44	5	80	U
44	5	81	U
44	5	82	A
44	5	83	A
44	5	88	A
44	5	90	U
44	5	92	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	5	93	U
44	5	95	G
44	5	96	A
44	5	109	C

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	6	5	U
9	6	7	G
9	6	28	A
9	6	31	U
9	6	33	G
9	6	37	C
9	6	46	G
9	6	47	A
9	6	48	A
9	6	49	G
9	6	52	U
9	6	79	C
9	6	83	A
30	2	23	A
30	2	46	U
30	2	47	U
36	Z	70	G
36	Z	74	G
36	Z	160	G
36	Z	161	U
36	Z	167	U
44	5	26	A
44	5	40	U
44	5	78	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 1 is 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
50	GTP	r	1500	51	33,34,34	1.19	4 (12%)	50,54,54	1.98	9 (18%)
52	IHP	A	3001	-	36,36,36	1.58	6 (16%)	60,60,60	0.93	2 (3%)

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
50	GTP	r	1500	51	-	8/22/38/38	0/3/3/3
52	IHP	A	3001	-	-	3/30/54/54	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	A	3001	IHP	P2-O12	3.76	1.66	1.59
52	A	3001	IHP	P3-O13	3.43	1.65	1.59
52	A	3001	IHP	P1-O11	3.36	1.65	1.59
50	r	1500	GTP	C6-N1	-3.35	1.32	1.38
52	A	3001	IHP	P5-O15	3.25	1.65	1.59
52	A	3001	IHP	P6-O16	3.24	1.65	1.59
52	A	3001	IHP	P4-O14	3.24	1.65	1.59
50	r	1500	GTP	C5-N7	-2.73	1.33	1.39
50	r	1500	GTP	C4-N9	-2.33	1.32	1.38
50	r	1500	GTP	C5-C4	2.19	1.44	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	r	1500	GTP	C5-C4-N3	-6.56	117.95	128.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	r	1500	GTP	N9-C4-N3	5.77	137.49	125.95
50	r	1500	GTP	C2-N3-C4	5.50	121.78	112.30
50	r	1500	GTP	O6-C6-C5	-3.85	116.36	126.53
52	A	3001	IHP	O12-C2-C1	3.26	115.69	108.76
50	r	1500	GTP	C5-C6-N1	3.17	121.33	113.25
50	r	1500	GTP	C2-N1-C6	-3.04	119.59	125.11
50	r	1500	GTP	C6-C5-N7	2.63	135.08	130.29
50	r	1500	GTP	O2G-PG-O3B	2.46	112.88	104.64
52	A	3001	IHP	P3-O13-C3	-2.14	117.73	123.43
50	r	1500	GTP	C8-N9-C4	2.06	109.89	106.03

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	r	1500	GTP	C5'-O5'-PA-O3A
50	r	1500	GTP	C5'-O5'-PA-O1A
50	r	1500	GTP	C5'-O5'-PA-O2A
50	r	1500	GTP	O4'-C4'-C5'-O5'
52	A	3001	IHP	C1-C2-O12-P2
50	r	1500	GTP	C3'-C4'-C5'-O5'
52	A	3001	IHP	C4-O14-P4-O24
52	A	3001	IHP	C3-C2-O12-P2
50	r	1500	GTP	PB-O3B-PG-O3G
50	r	1500	GTP	PG-O3B-PB-O1B
50	r	1500	GTP	PG-O3B-PB-O2B

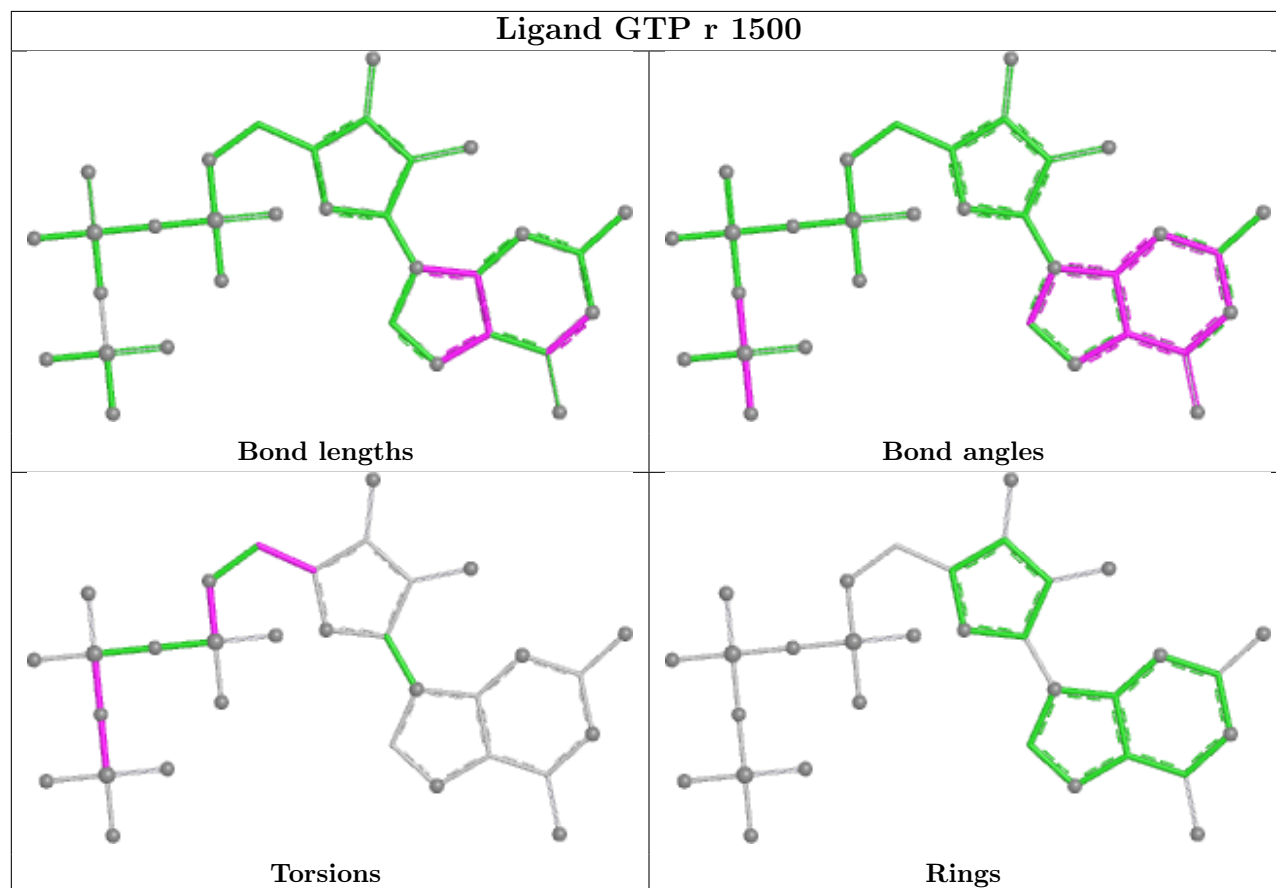
There are no ring outliers.

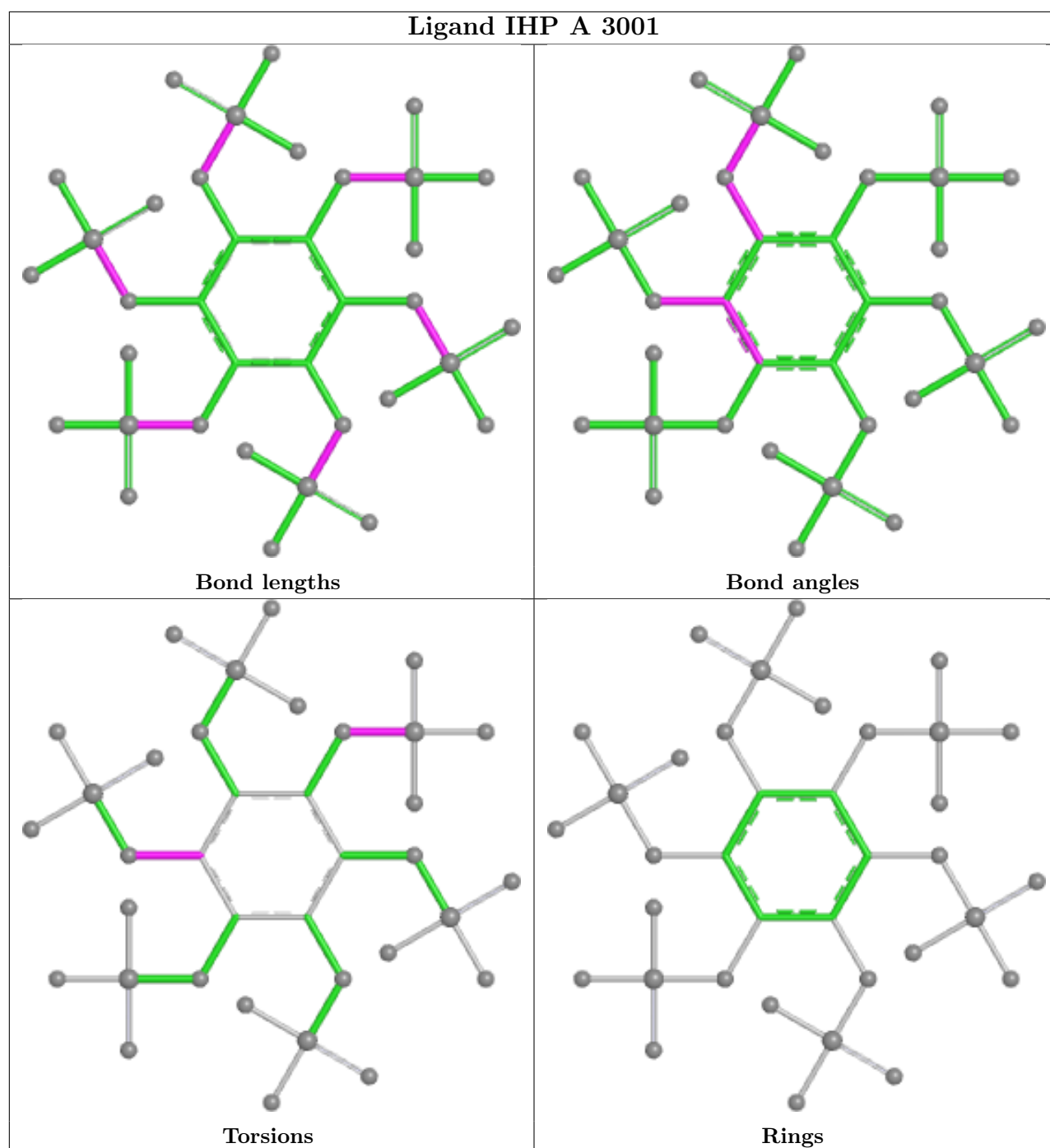
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	r	1500	GTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

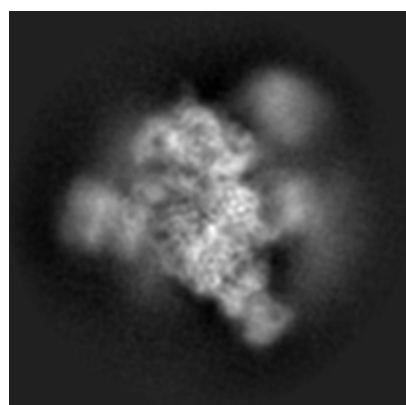
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11697. These allow visual inspection of the internal detail of the map and identification of artifacts.

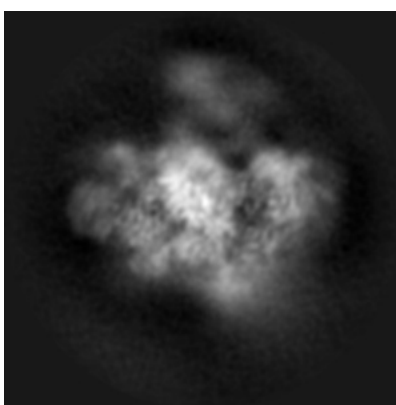
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

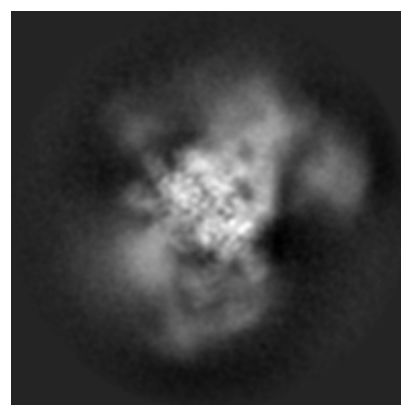
6.1.1 Primary map



X



Y

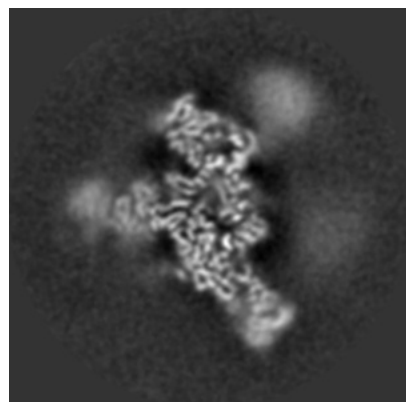


Z

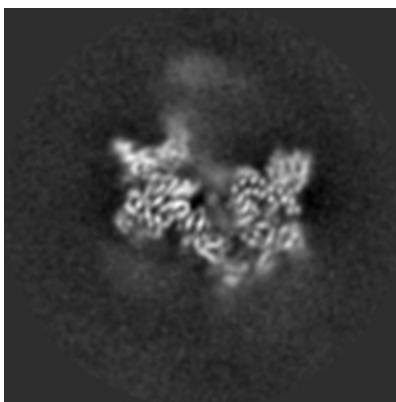
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

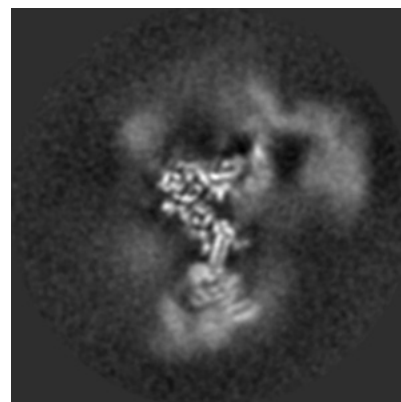
6.2.1 Primary map



X Index: 192



Y Index: 192

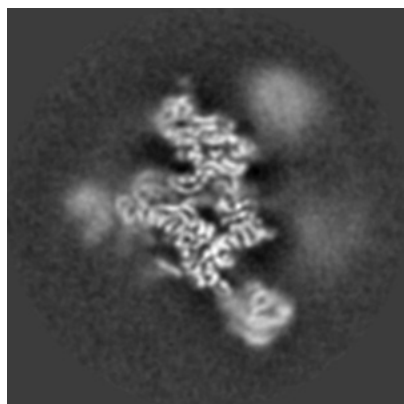


Z Index: 192

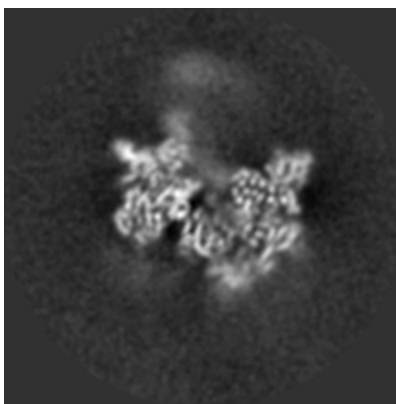
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

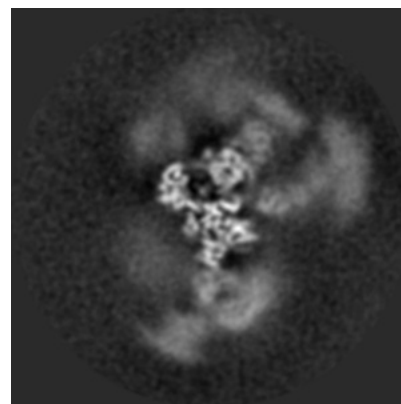
6.3.1 Primary map



X Index: 198



Y Index: 195

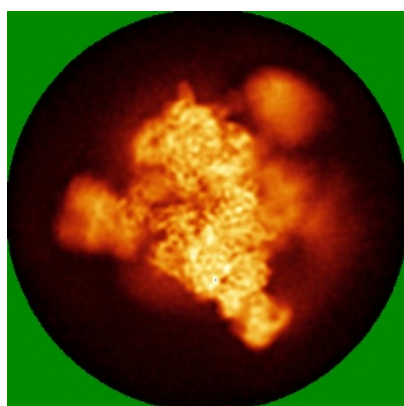


Z Index: 175

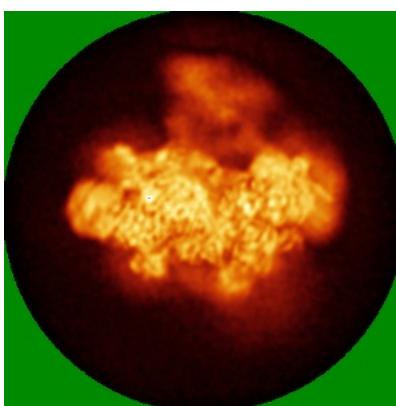
The images above show the largest variance slices of the map in three orthogonal directions.

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

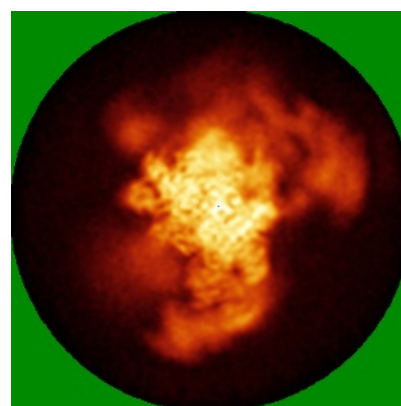
6.4.1 Primary map



X



Y



Z

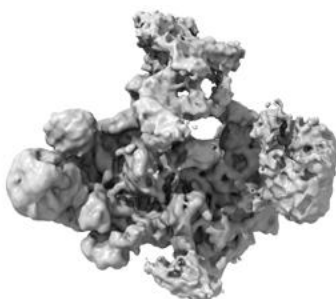
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

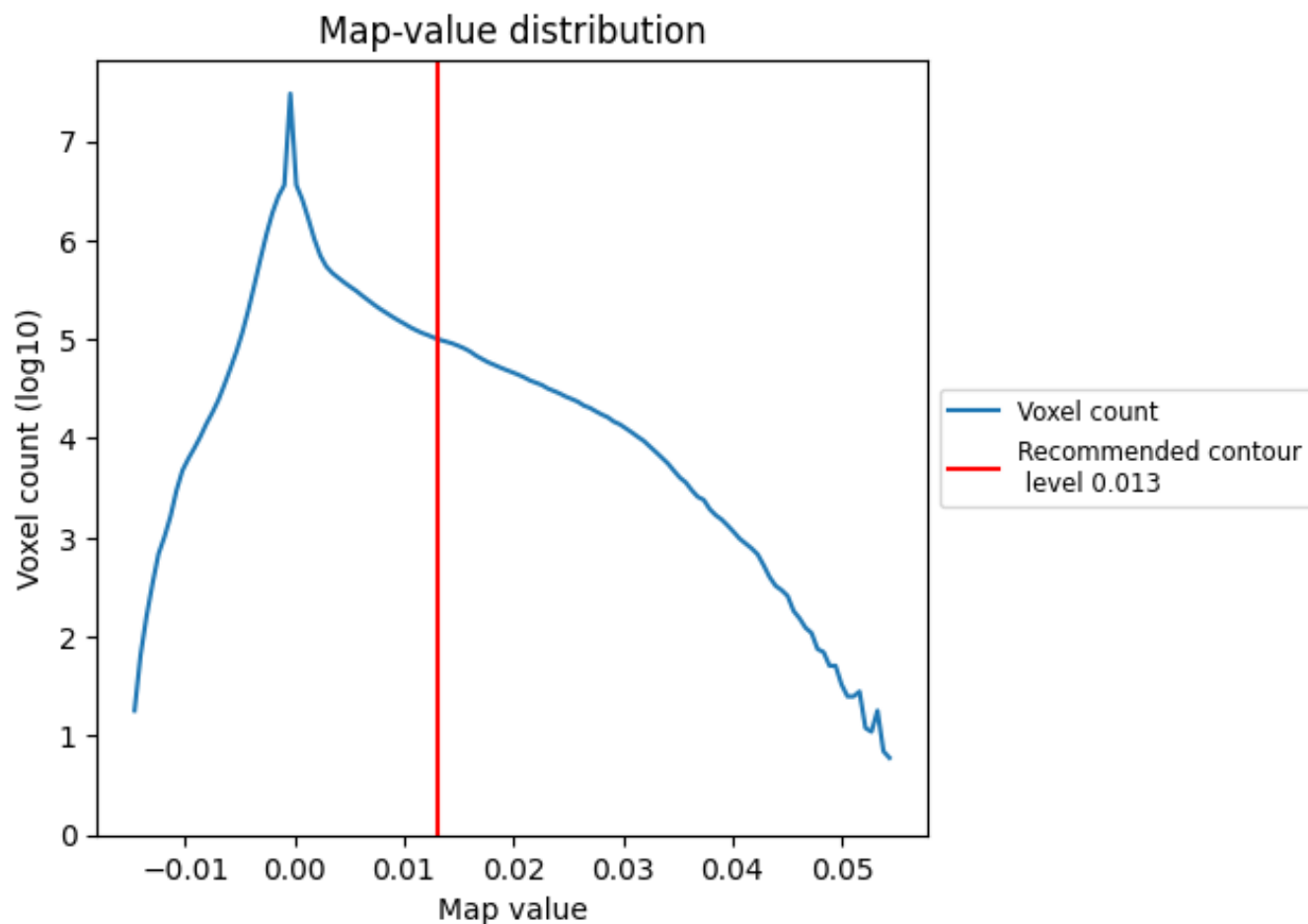
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

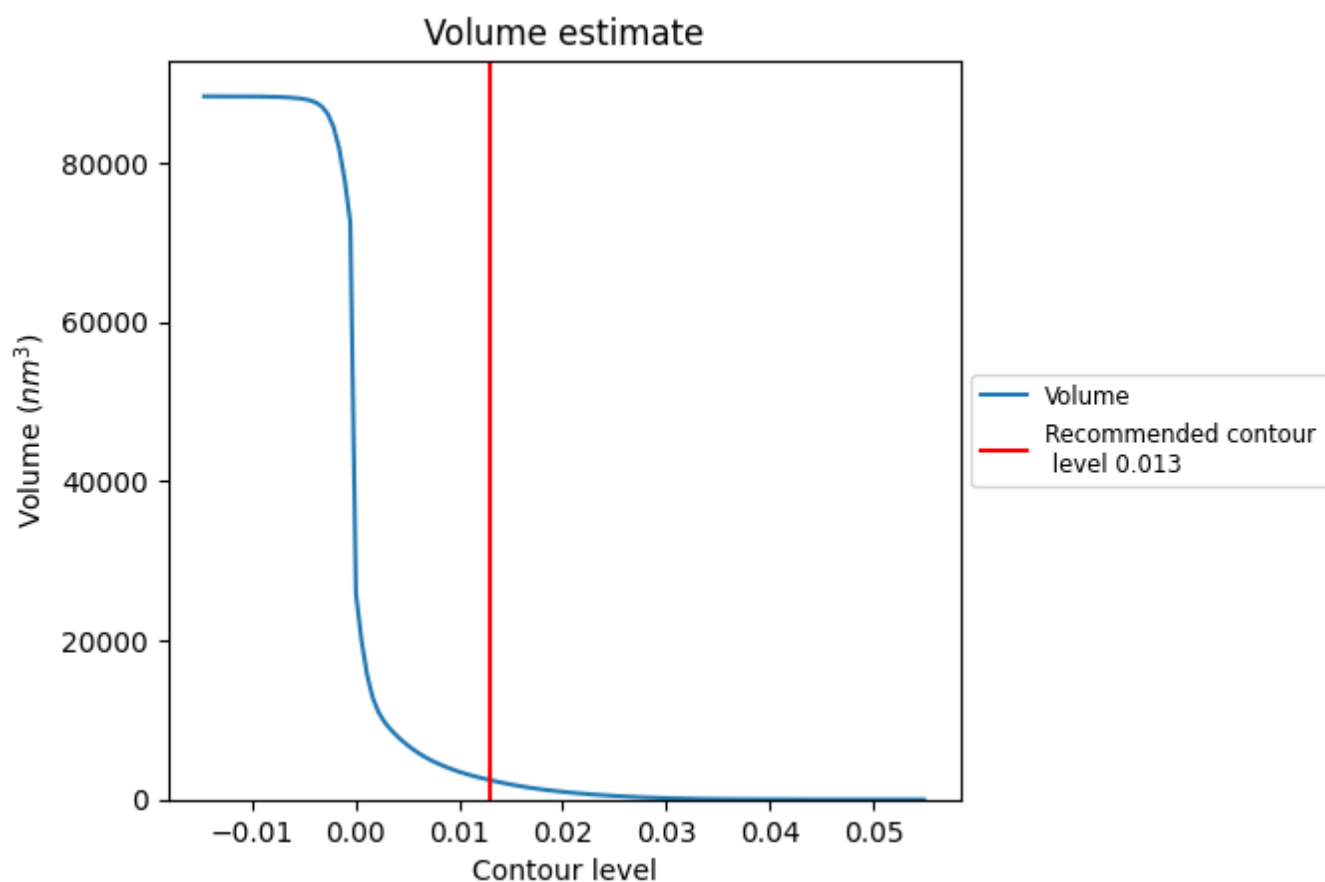
This section contains the results of statistical analysis of the map.

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.

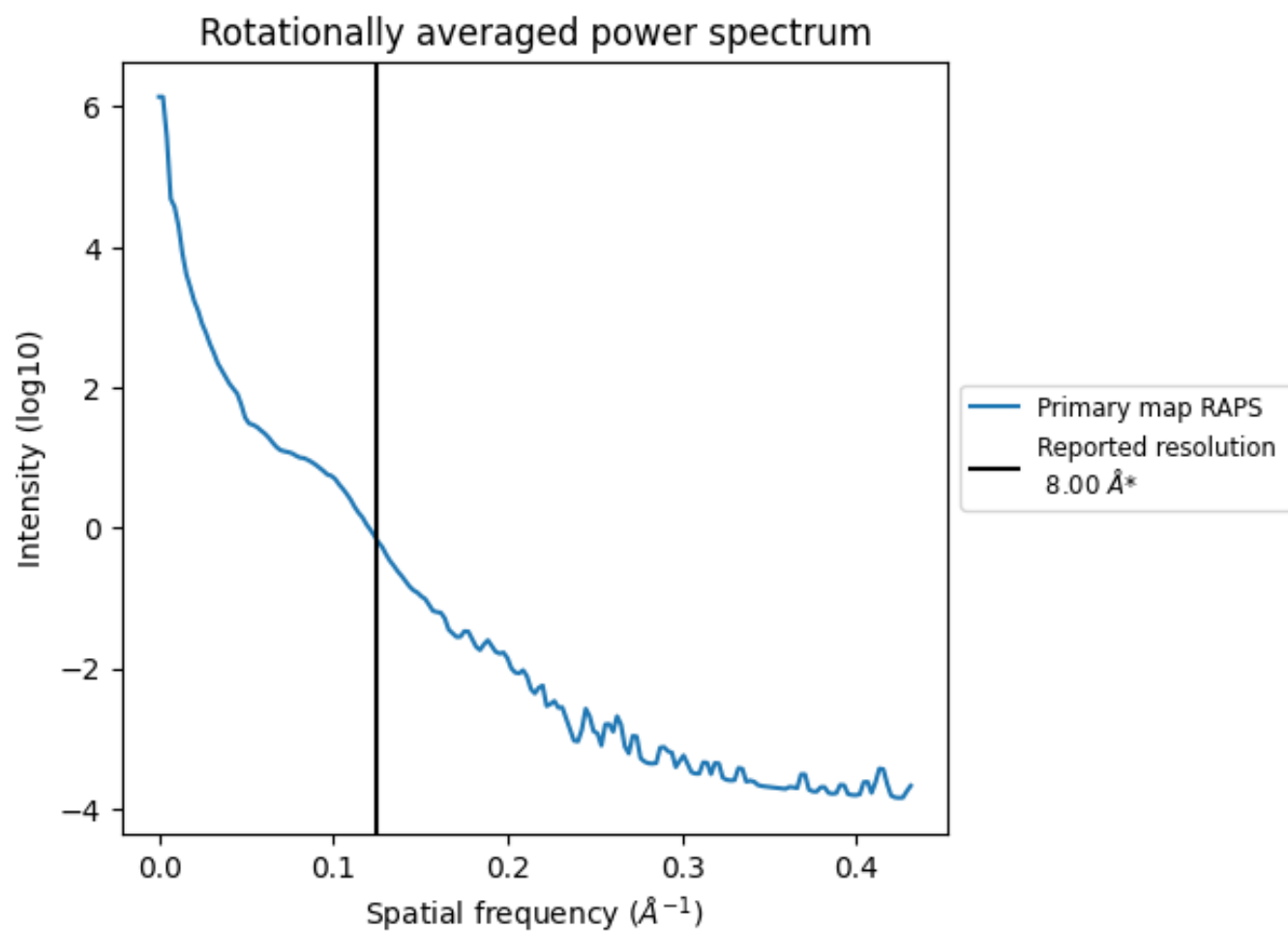
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2441 nm³; this corresponds to an approximate mass of 2205 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 0.125 Å⁻¹

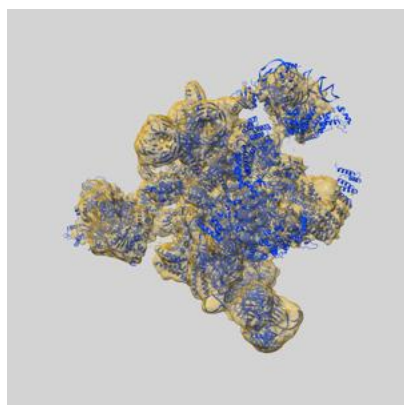
8 Fourier-Shell correlation ⓘ

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

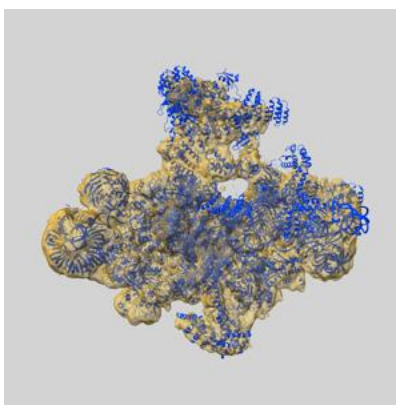
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11697 and PDB model 7ABI. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

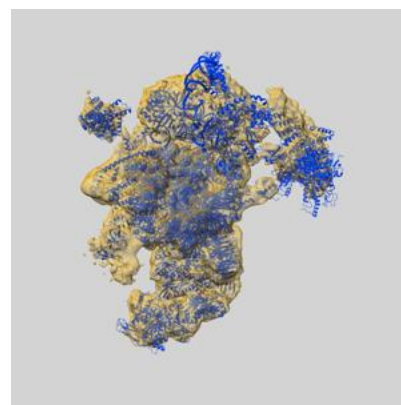
9.1 Map-model overlay [i](#)



X



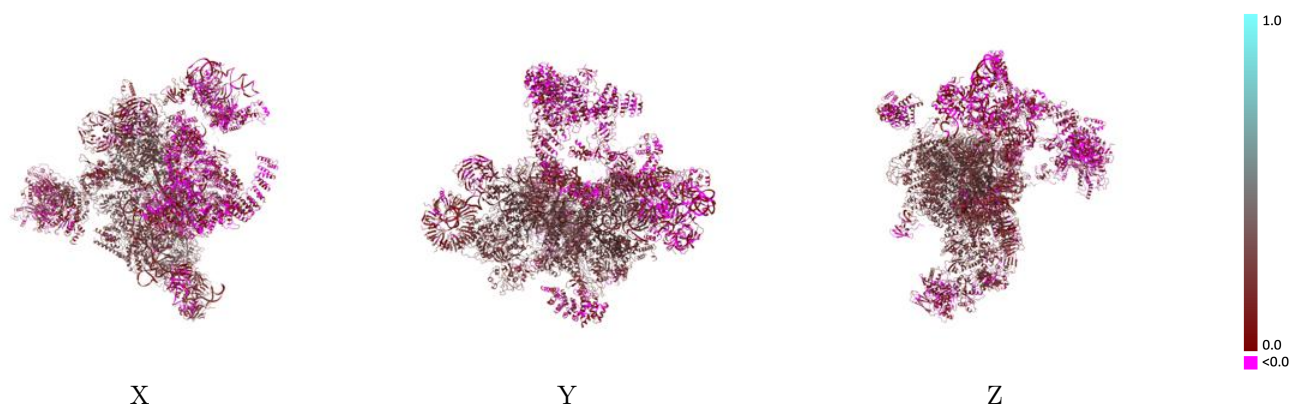
Y



Z

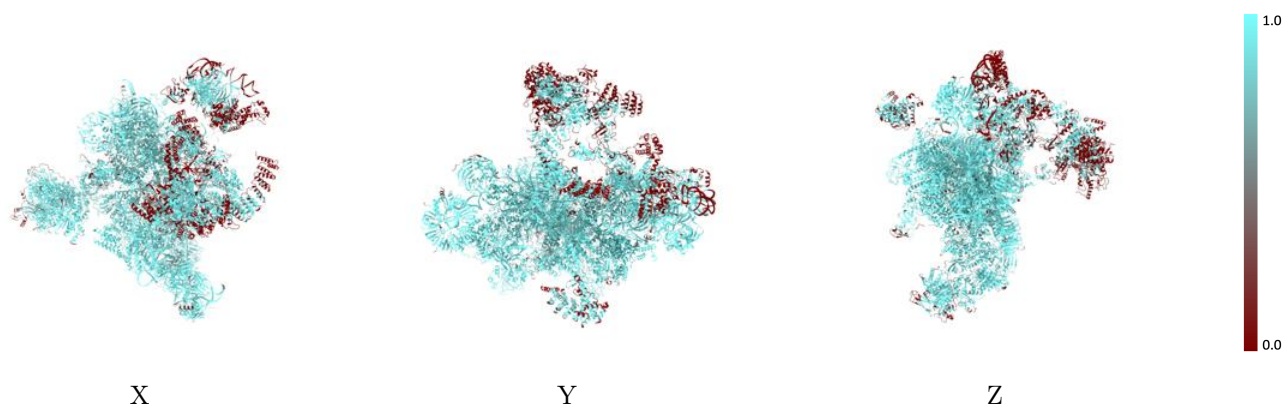
The images above show the 3D surface view of the map at the recommended contour level 0.013 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



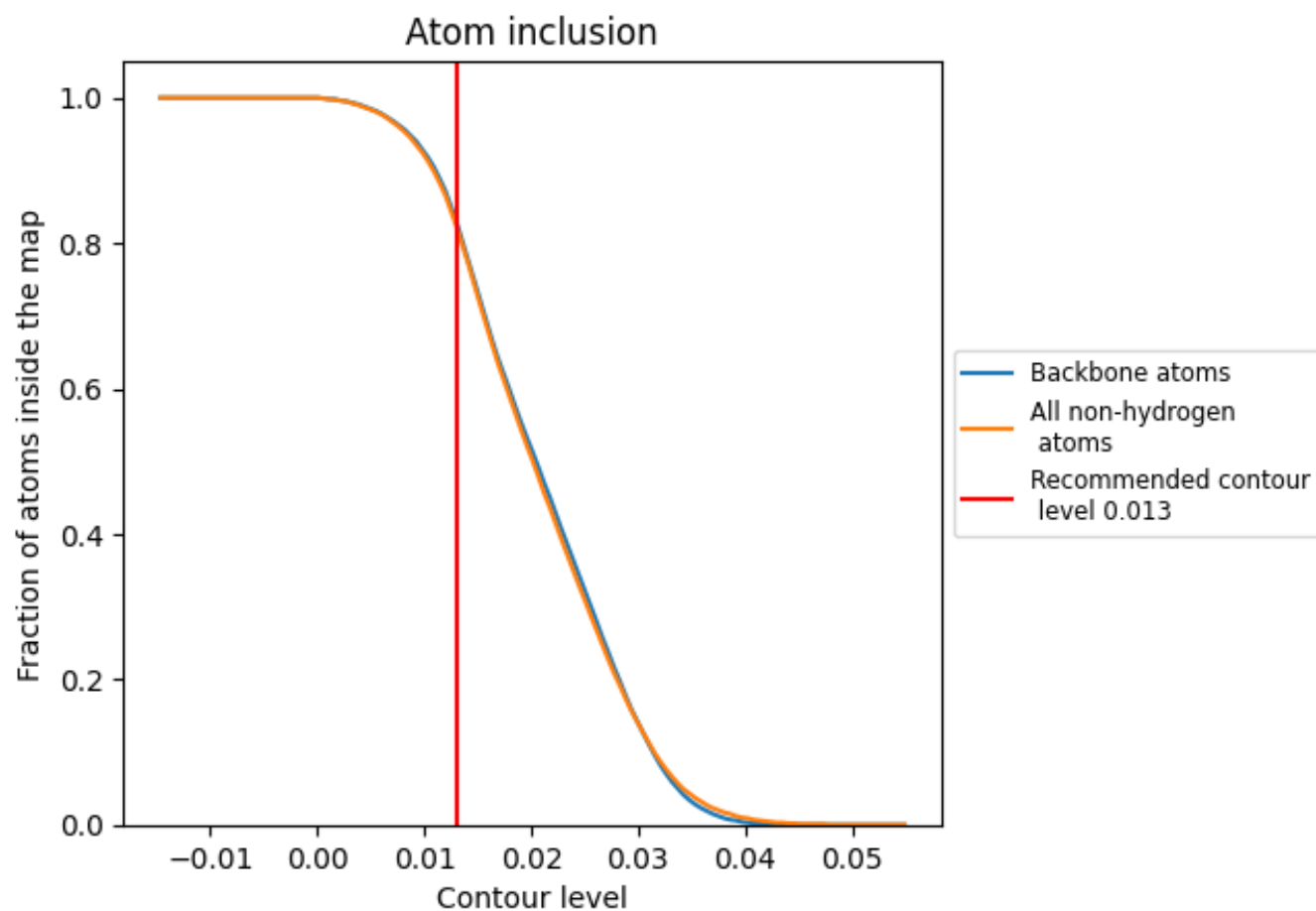
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.013).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 82% 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 (0.013) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8250	 0.1520
0	 0.9750	 0.1750
1	 0.9920	 0.2300
2	 0.6790	 0.0990
3	 0.9080	 0.2390
4	 0.4120	 0.0810
5	 0.9790	 0.1700
6	 0.9180	 0.1750
7	 0.7710	 0.1220
8	 0.9570	 0.1530
A	 0.9550	 0.2510
B	 0.4540	 0.0970
D	 0.9000	 0.0580
E	 0.9590	 0.1460
F	 0.7330	 0.1450
G	 0.9810	 0.2200
I	 0.9940	 0.2500
K	 0.9790	 0.2720
L	 0.9760	 0.2470
M	 0.4830	 0.0430
N	 0.9640	 0.2250
O	 0.8720	 0.1650
P	 0.9040	 0.1410
Q	 0.9910	 0.2330
R	 0.7170	 0.2070
S	 0.6130	 0.0610
T	 0.9440	 0.2090
U	 0.4180	 0.0250
W	 0.7450	 0.0360
Y	 0.9960	 0.2410
Z	 0.9780	 0.2070
a	 0.9820	 0.1340
b	 0.9420	 0.1000
c	 0.9460	 0.1440
d	 0.9740	 0.1730



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 1.0000	 0.2160
f	 0.9970	 0.1840
g	 0.8930	 0.1490
h	 0.8170	 0.0190
i	 0.9690	 0.0310
j	 0.9750	 0.0390
k	 0.9640	 0.0070
l	 0.8550	 0.0330
m	 0.9300	 0.0350
n	 0.5420	 -0.0150
o	 0.5370	 0.0480
p	 0.3950	 0.0320
q	 0.9860	 0.2730
r	 0.9890	 0.2430
s	 0.8770	 0.1020
t	 0.5620	 0.1020
u	 0.9800	 0.2790
v	 0.8920	 0.2330
w	 0.8800	 0.1230
x	 1.0000	 0.2590
y	 0.9960	 0.2310
z	 0.9850	 0.2420