Full wwPDB EM Validation Report ⓘ

Mar 31, 2025 – 05:09 PM JST

PDB ID	:	5WYK / pdb_00005wyk
EMDB ID	:	EMD-6696
Title	:	Cryo-EM structure of the 90S small subunit pre-ribosome (Mtr4-depleted, Enp1-TAP)
Authors	:	Ye, K.; Zhu, X.; Sun, Q.
Deposited on	:	2017-01-13
Resolution	:	4.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

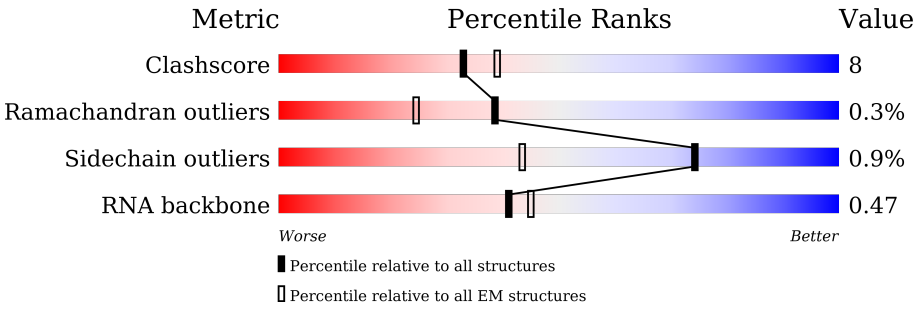
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance

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

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	3A	333	23% 19% 53%
2	3B	327	59% 14% 27%
2	3C	327	61% 12% 27%
3	3D	504	62% 12% 27%
4	3E	511	62% 12% 25%
5	3F	573	48% 16% 36%
6	3G	126	80% 17%
6	3H	126	88% 9%

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Mol	Chain	Length	Quality of chain
7	5A	700	34% 26% 5% 34%
8	AA	776	70% 27%
9	AB	643	54% 9% 37%
10	AC	713	56% 10% 34%
11	AD	575	16% 82%
12	AE	1769	19% 77%
13	AF	513	66% 7% 27%
14	AG	896	58% 10% 32%
15	B1	1183	36% 9% 55%
16	BA	923	61% 20% 18%
17	BB	943	58% 24% 17%
18	BC	817	74% 22%
19	BD	594	33% 21% 45%
20	BE	939	60% 19% 20%
21	CA	297	49% 16% 34%
22	CB	1237	67% 21% 11%
23	E1	252	72% 14% 14%
23	E2	252	66% 19% 14%
24	E4	707	38% 60%
25	K1	316	46% 9% 45%
26	MA	183	63% 9% 27%
27	MB	290	47% 16% 37%
28	MC	593	7% 92%
29	P1	274	53% 11% 37%
30	R1	367	72% 25%

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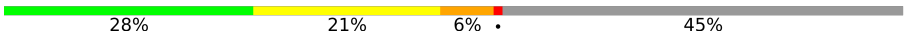
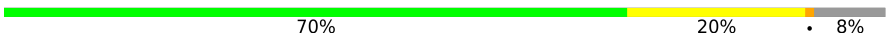
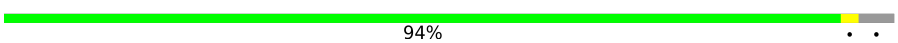
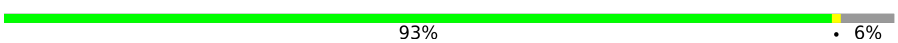
Mol	Chain	Length	Quality of chain
31	S1	489	
32	SA	1812	
33	SC	255	
34	SF	261	
35	SG	225	
36	SI	190	
37	SJ	200	
38	SK	197	
39	SM	156	
40	SO	151	
41	SP	137	
42	SR	143	
43	SX	130	
44	SY	145	
45	SZ	135	
46	Sc	82	
47	Sd	67	
48	Sf	63	
49	U1	554	
50	U2	250	
51	U4	189	
52	U5	274	
53	UA	1615	
54	UB	987	
55	UC	1033	

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 150760 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called U3 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3A	157	Total	C	N	O	P	0	0
			3327	1488	575	1107	157		

- Molecule 2 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3B	239	Total	C	N	O	S	0	0
			1866	1183	332	341	10		
2	3C	239	Total	C	N	O	S	0	0
			1866	1183	332	341	10		

- Molecule 3 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3D	370	Total	C	N	O	S	0	0
			2915	1843	503	560	9		

- Molecule 4 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3E	382	Total	C	N	O	S	0	0
			2935	1859	498	570	8		

- Molecule 5 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3F	365	Total	C	N	O	S	0	0
			2916	1871	506	529	10		

- Molecule 6 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3G	122	Total 924	C 589	N 159	O 172	S 4	0	0
6	3H	122	Total 924	C 589	N 159	O 172	S 4	0	0

- Molecule 7 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	5A	462	Total 9867	C 4406	N 1749	O 3250	P 462	0	0

- Molecule 8 is a protein called Utp4.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AA	569	Total 2845	C 1707	N 569	O 569	0	0

- Molecule 9 is a protein called Utp5.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	AB	403	Total 2015	C 1209	N 403	O 403	0	0

- Molecule 10 is a protein called Utp8.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	AC	472	Total 2360	C 1416	N 472	O 472	0	0

- Molecule 11 is a protein called Utp9.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	AD	101	Total 505	C 303	N 101	O 101	0	0

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AE	413	Total 3331	C 2156	N 547	O 616	S 12	0	0

- Molecule 13 is a protein called Utp15.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	AF	376	Total 1880	C 1128	N 376	O 376	0	0

- Molecule 14 is a protein called Utp17.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	AG	612	Total 3060	C 1836	N 612	O 612	0	0

- Molecule 15 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	B1	536	Total 4325	C 2801	N 758	O 746	S 20	0	0

- Molecule 16 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	BA	755	Total 6026	C 3862	N 1025	O 1123	S 16	0	0

- Molecule 17 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BB	778	Total 6138	C 3931	N 1019	O 1161	S 27	0	0

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	BC	783	Total 6117	C 3870	N 1033	O 1187	S 27	0	0

- Molecule 19 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	325	Total 2539	C 1606	N 458	O 466	S 9	0	0

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BE	753	Total	C	N	O	S	0	0
			5936	3769	1020	1126	21		

- Molecule 21 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CA	196	Total	C	N	O	S	0	0
			1582	1016	259	300	7		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CB	1098	Total	C	N	O	S	0	0
			8870	5763	1462	1621	24		

- Molecule 23 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E1	217	Total	C	N	O	S	0	0
			1689	1073	293	312	11		
23	E2	216	Total	C	N	O	S	0	0
			1695	1078	295	313	9		

- Molecule 24 is a protein called Enp2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	E4	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 25 is a protein called KRR1 small subunit processome component.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	K1	175	Total	C	N	O	S	0	0
			1410	903	252	245	10		

- Molecule 26 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	MA	133	Total	C	N	O	S	0	0
			1097	692	204	194	7		

- Molecule 27 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	MB	184	Total	C	N	O	S	0	0
			1465	926	273	260	6		

- Molecule 28 is a protein called Mpp10,U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	MC	46	Total	C	N	O	0	0
			307	193	52	62		

- Molecule 29 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P1	173	Total	C	N	O	S	0	0
			1368	876	245	243	4		

- Molecule 30 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	R1	355	Total	C	N	O	S	0	0
			2742	1756	466	509	11		

- Molecule 31 is a protein called Sof1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	S1	285	Total	C	N	O	0	0
			1425	855	285	285		

- Molecule 32 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	SA	1000	Total	C	N	O	P	0	0
			21307	9529	3794	6984	1000		

- Molecule 33 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	SC	214	Total	C	N	O	S	0	0
			1709	1084	310	311	4		

- Molecule 34 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	SF	237	Total	C	N	O	S	0	0
			1881	1205	345	328	3		

- Molecule 35 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	SG	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 36 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	SI	165	Total	C	N	O	0	0
			1322	856	227	239		

- Molecule 37 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	SJ	170	Total	C	N	O	S	0	0
			1350	839	268	241	2		

- Molecule 38 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	SK	175	Total	C	N	O	S	0	0
			1412	892	272	247	1		

- Molecule 39 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	SM	141	Total	C	N	O	S	0	0
			1143	733	216	191	3		

- Molecule 40 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	SO	134	Total	C	N	O	S	0	0
			1087	698	202	186	1		

- Molecule 41 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	SP	112	Total	C	N	O	S	0	0
			771	477	150	143	1		

- Molecule 42 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	SR	125	Total	C	N	O	0	0
			973	625	174	174		

- Molecule 43 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	SX	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 44 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	SY	103	Total	C	N	O	S	0	0
			785	501	144	138	2		

- Molecule 45 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	SZ	101	Total	C	N	O	0	0
			801	512	144	145		

- Molecule 46 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Sc	79	Total	C	N	O	S	0	0
			595	371	108	111	5		

- Molecule 47 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Sd	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 48 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Sf	30	Total 251	C 162	N 50	O 39	0	0

- Molecule 49 is a protein called Utp7.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	U1	285	Total 1425	C 855	N 285	O 285	0	0

- Molecule 50 is a protein called Utp11.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	U2	73	Total 365	C 219	N 73	O 73	0	0

- Molecule 51 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	U4	126	Total 990	C 633	N 179	O 168	S 10	0	0

- Molecule 52 is a protein called Ribosome biogenesis protein UTP30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	U5	248	Total 2009	C 1285	N 357	O 359	S 8	0	0

- Molecule 53 is a protein called Helical domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	UA	338	Total 1690	C 1014	N 338	O 338	0	0

- Molecule 54 is a protein called Helical domain protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	UB	555	Total 2775	C 1665	N 555	O 555	0	0

- Molecule 55 is a protein called Unassigned helices.

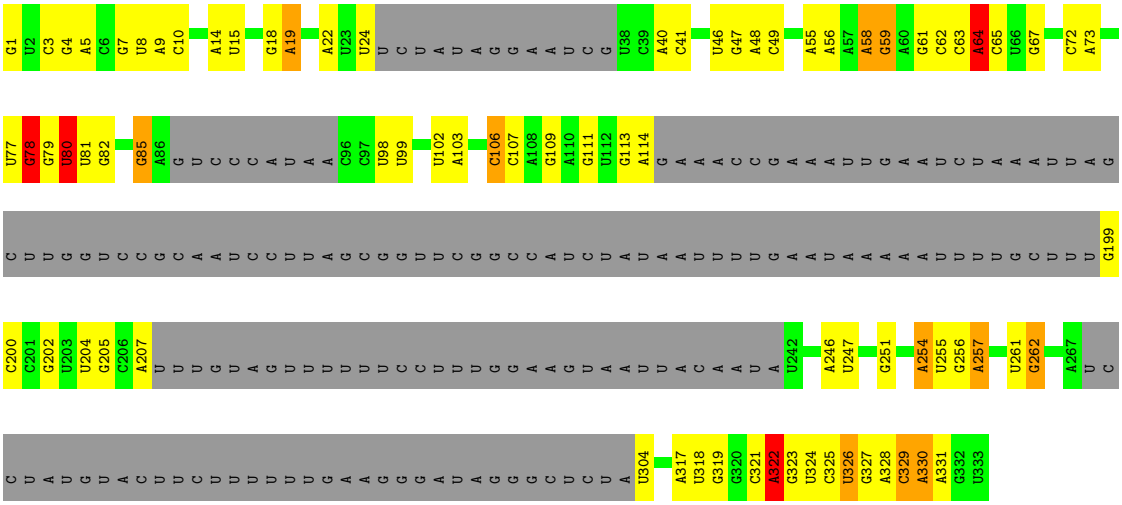
Mol	Chain	Residues	Atoms				AltConf	Trace
55	UC	660	Total 3300	C 1980	N 660	O 660	0	0

3 Residue-property plots (i)

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. 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. 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.

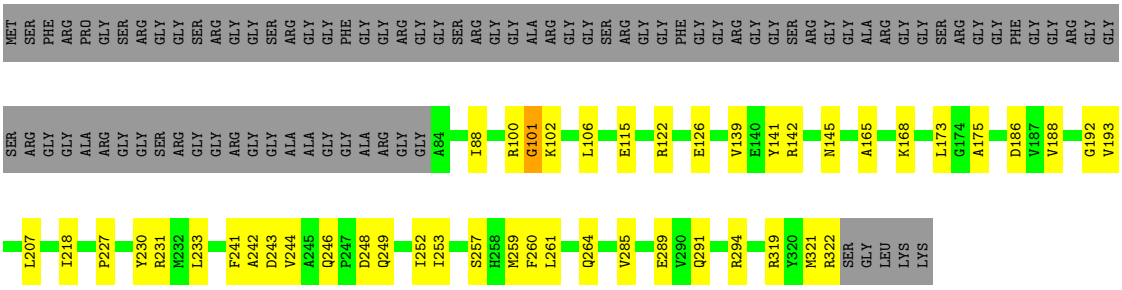
- Molecule 1: U3 RNA

Chain 3A:



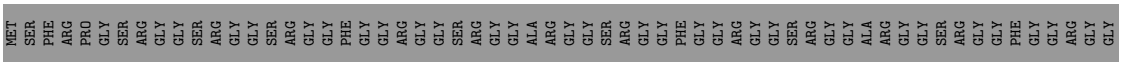
- Molecule 2: rRNA 2'-O-methyltransferase fibrillarin

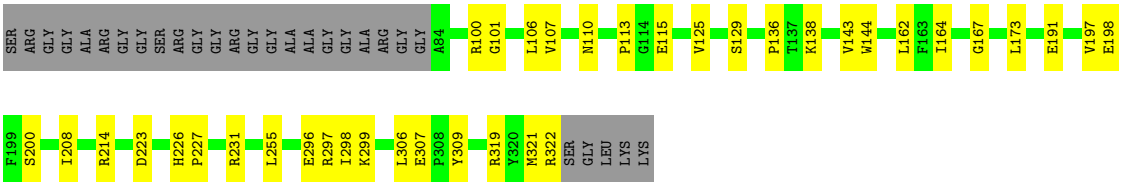
Chain 3B:



- Molecule 2: rRNA 2'-O-methyltransferase fibrillarin

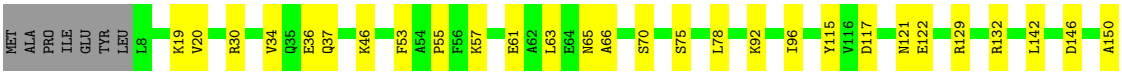
Chain 3C:

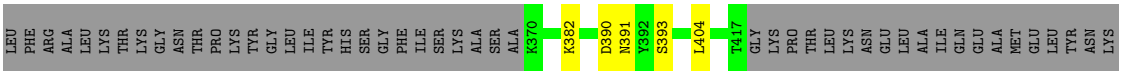




• Molecule 3: Nucleolar protein 56

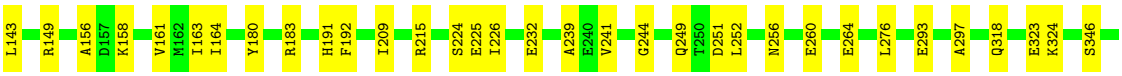
Chain 3D:





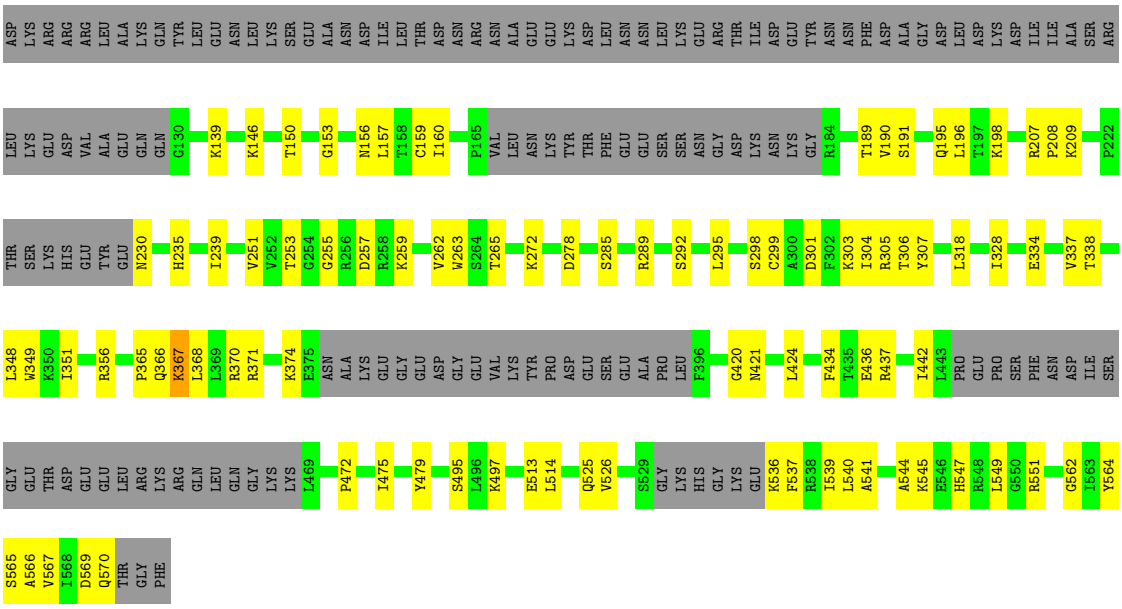
• Molecule 4: Nucleolar protein 58

Chain 3E:



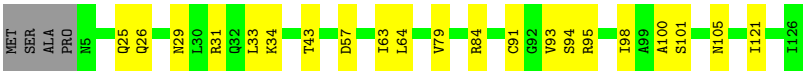
• Molecule 5: Ribosomal RNA-processing protein 9

Chain 3F:



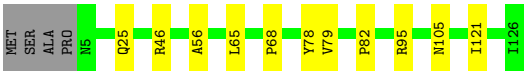
• Molecule 6: 13 kDa ribonucleoprotein-associated protein

Chain 3G:



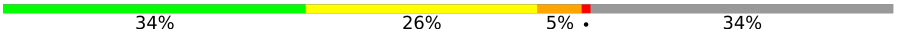
• Molecule 6: 13 kDa ribonucleoprotein-associated protein

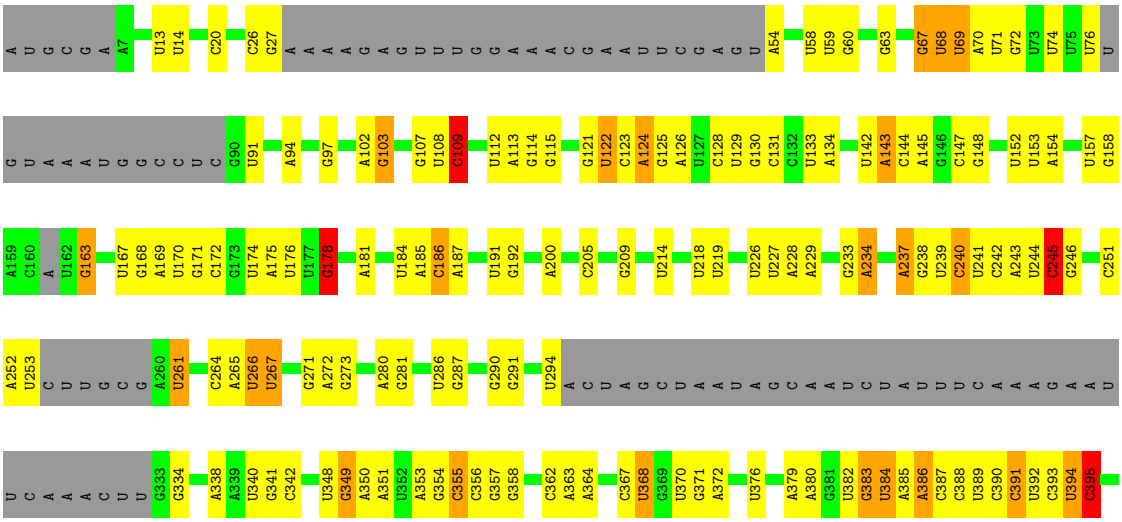
Chain 3H:

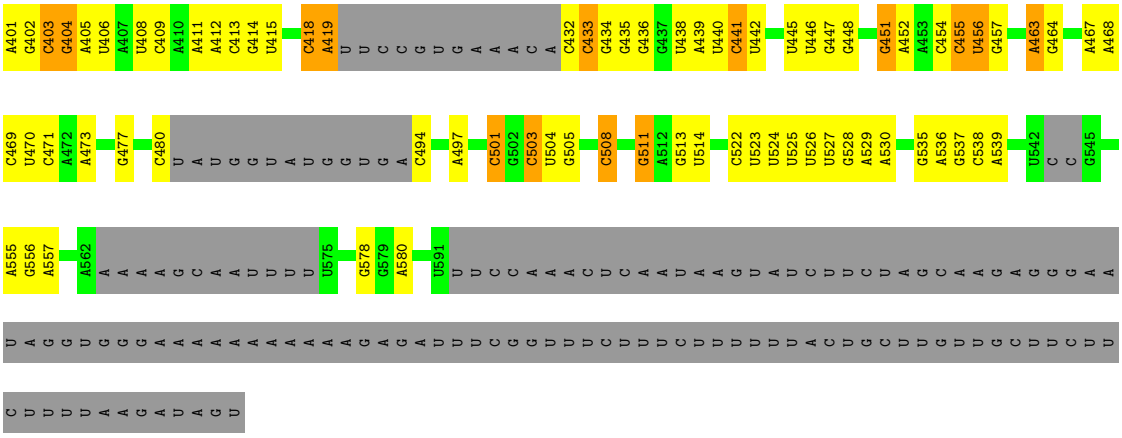


• Molecule 7: 5ETS RNA

Chain 5A:

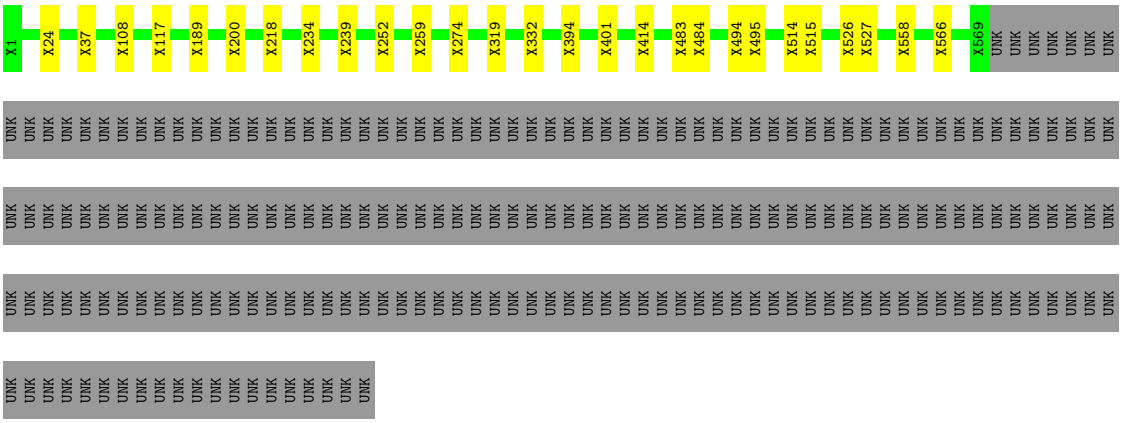






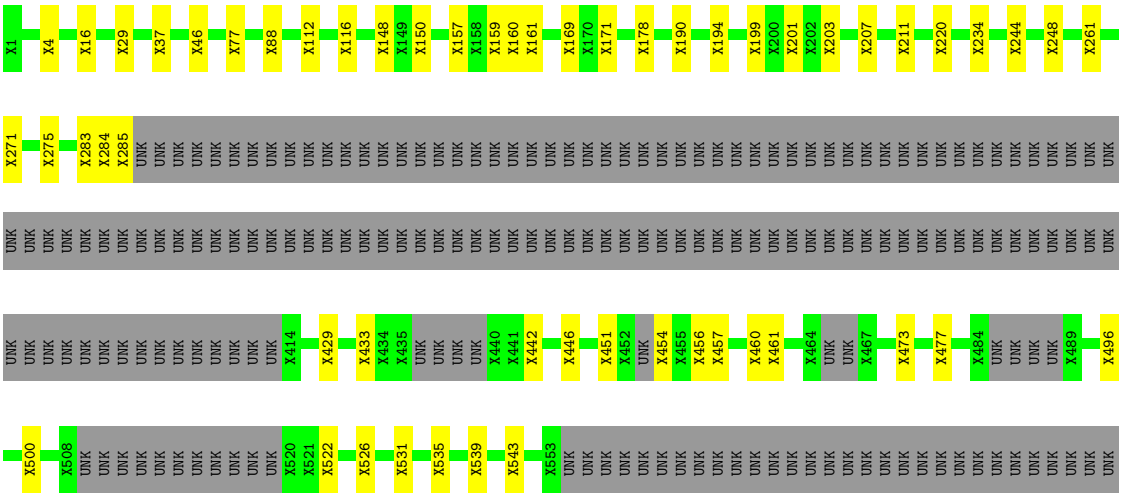
• Molecule 8: Utp4

Chain AA: 70% • 27%



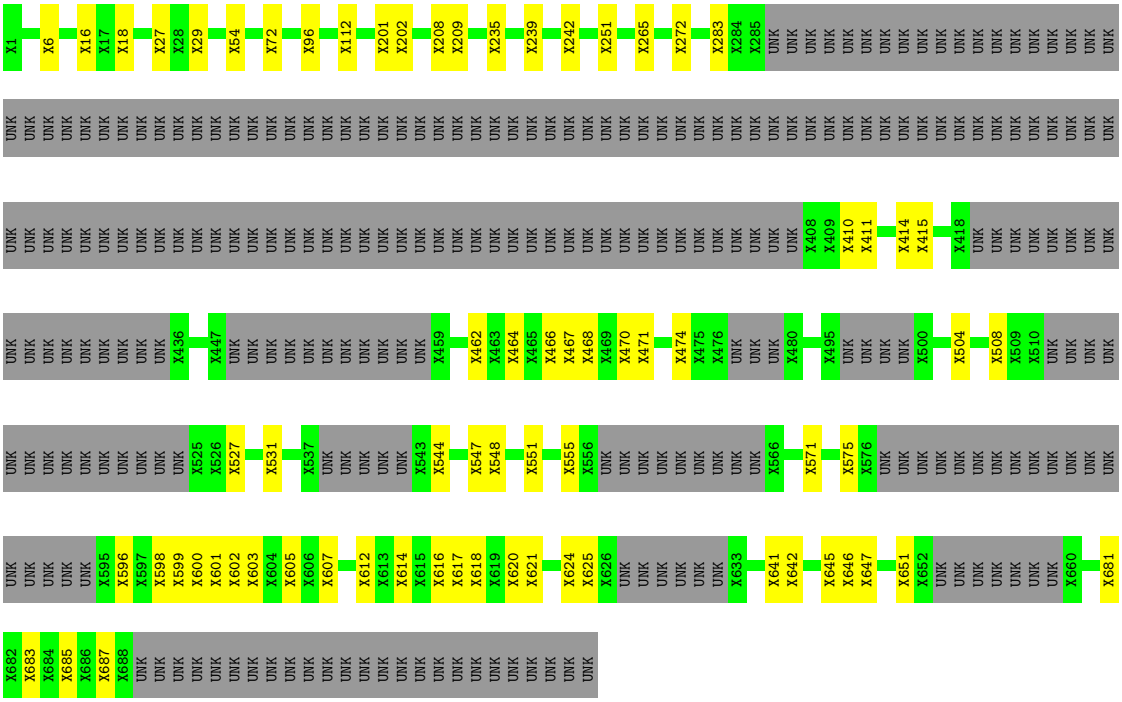
• Molecule 9: Utp5

Chain AB: 54% 9% 37%



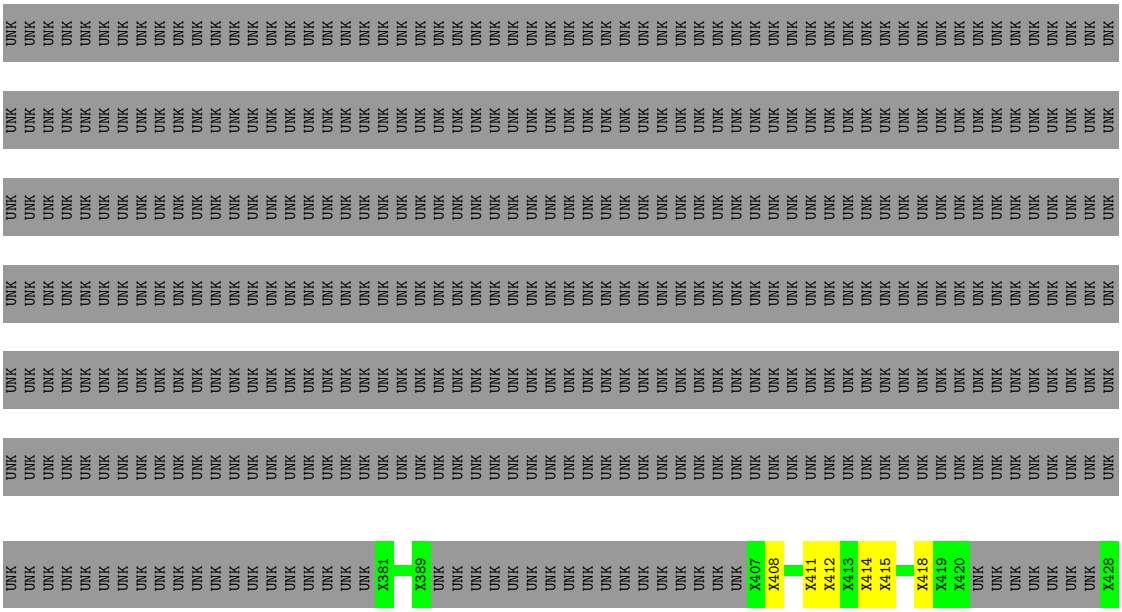
• Molecule 10: Utp8

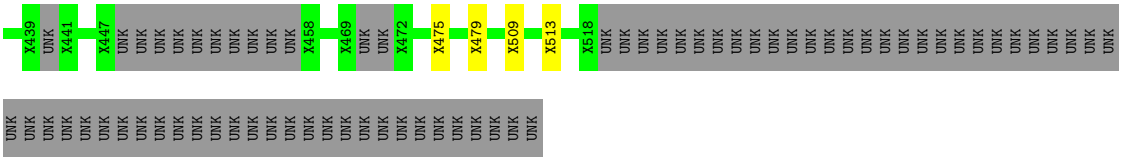
Chain AC:



• Molecule 11: Utp9

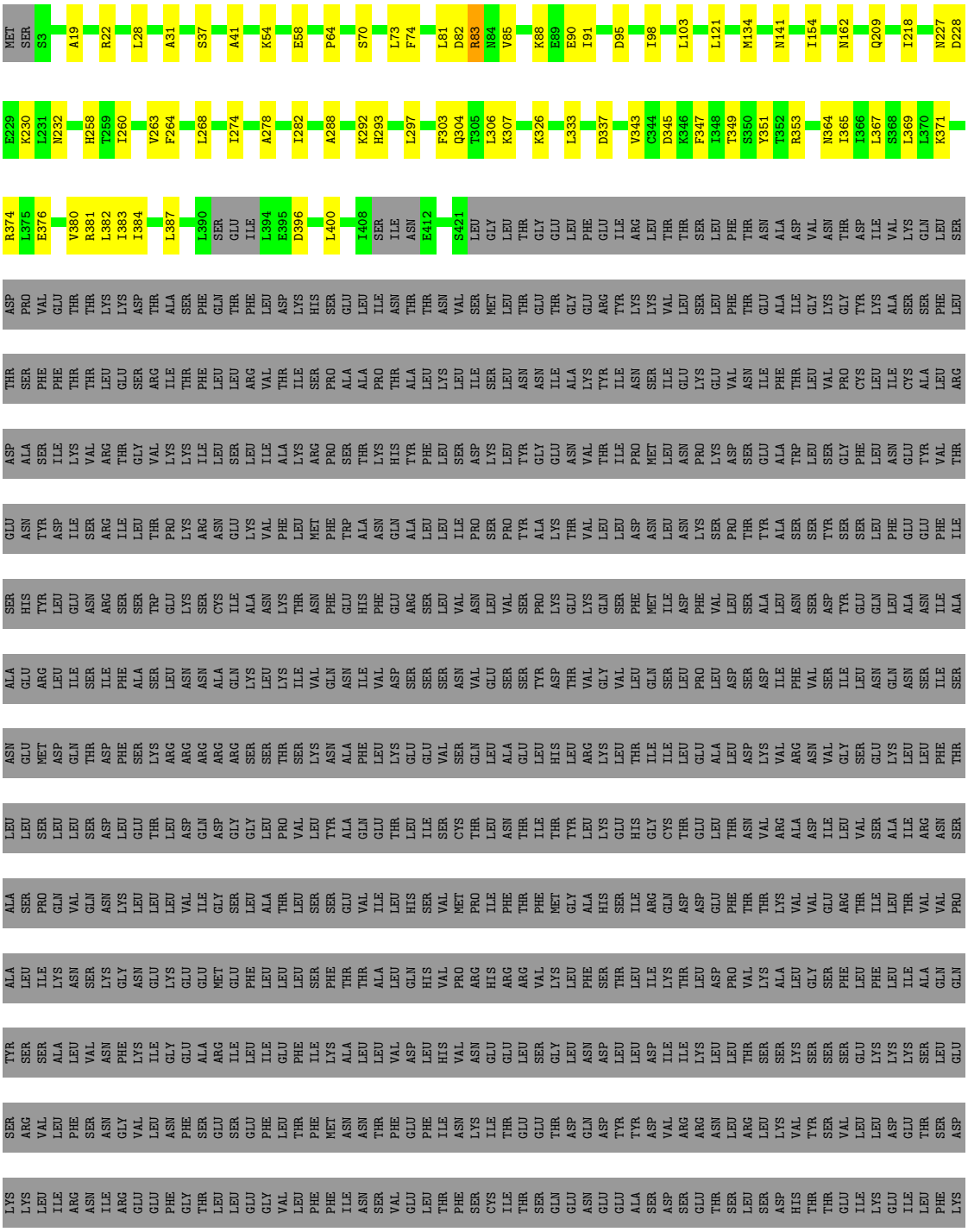
Chain AD:

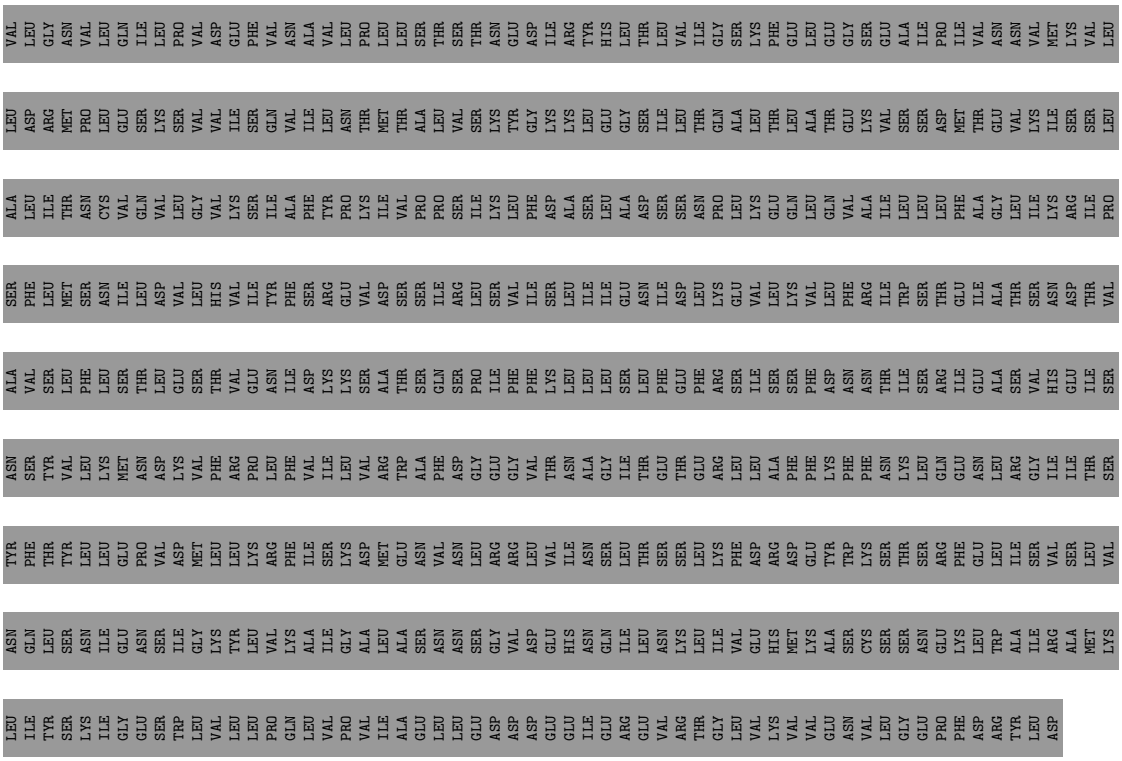




• Molecule 12: U3 small nucleolar RNA-associated protein 10

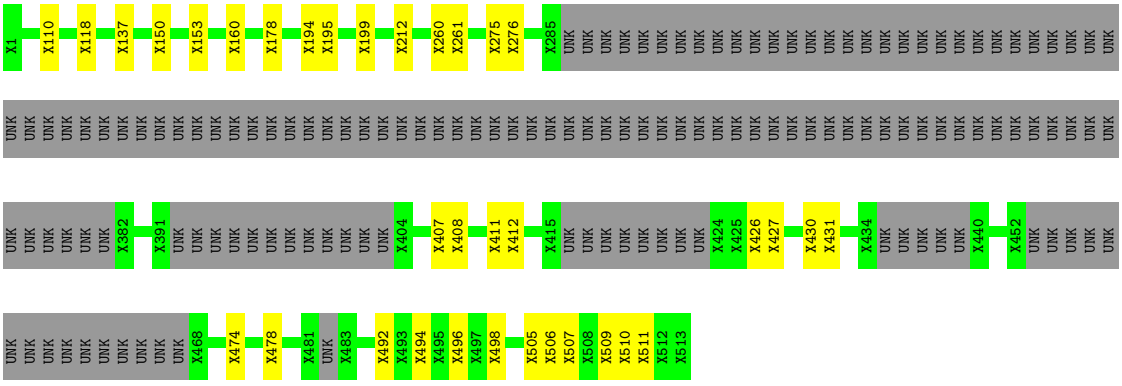
Chain AE:





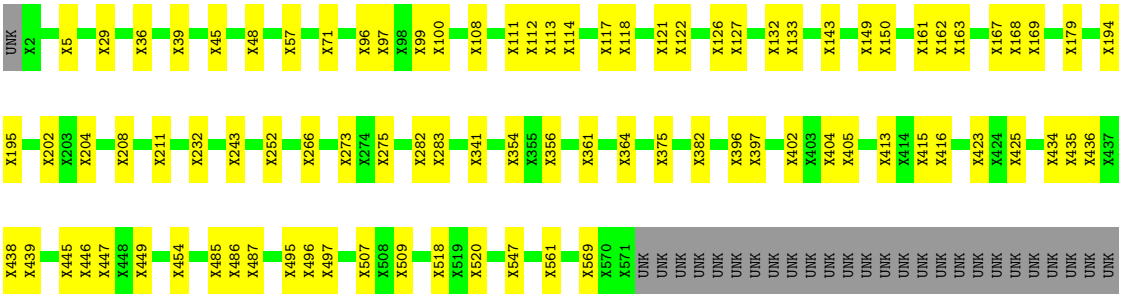
- Molecule 13: Utp15

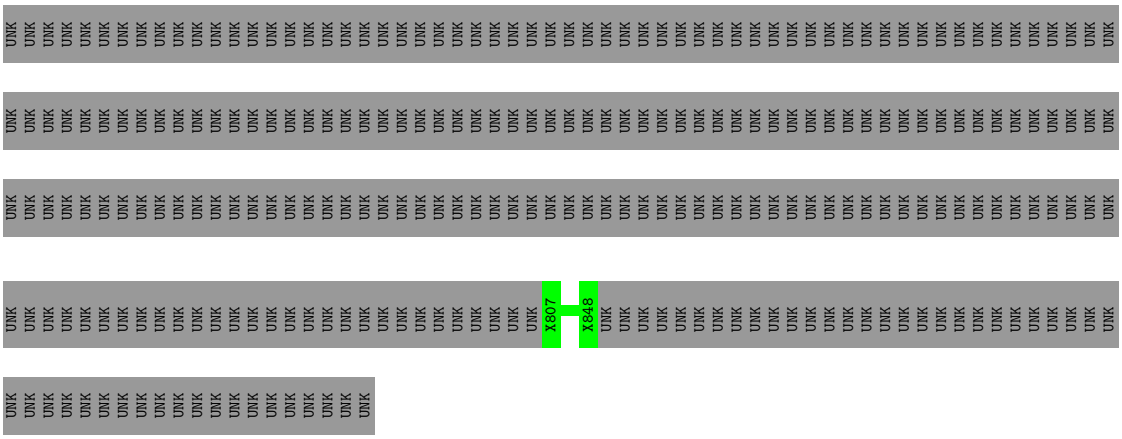
Chain AF:



- Molecule 14: Utp17

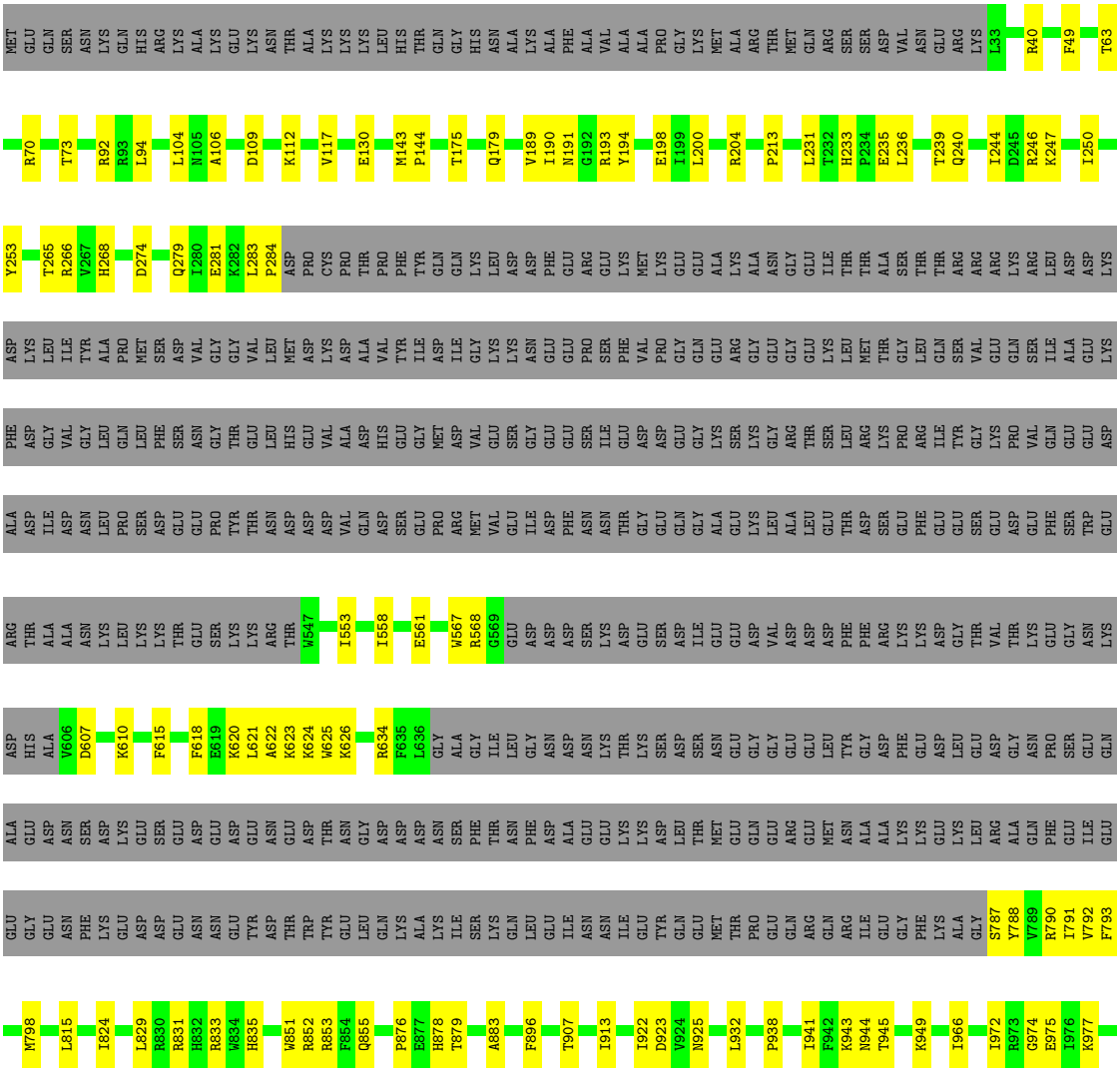
Chain AG:

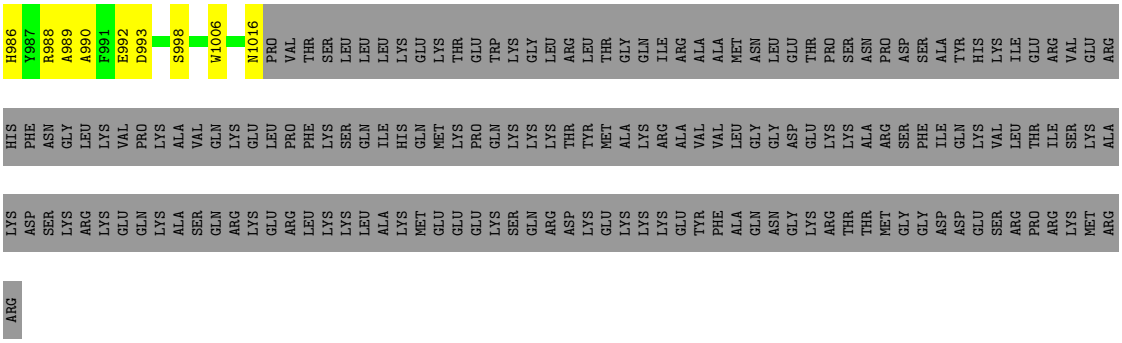




• Molecule 15: Ribosome biogenesis protein BMS1

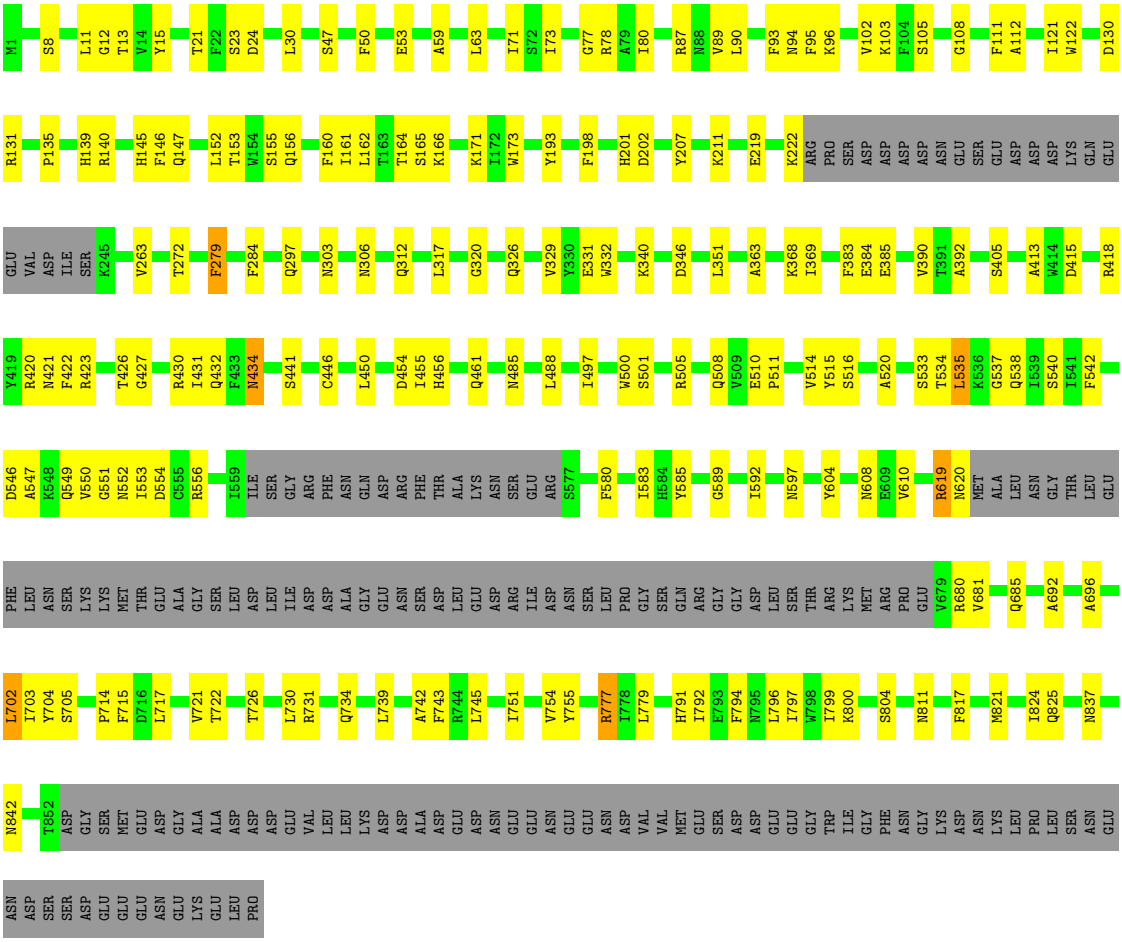
Chain B1:





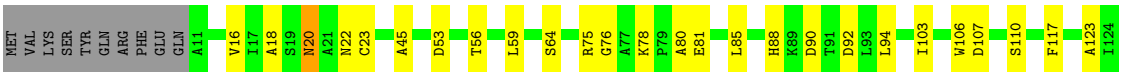
• Molecule 16: Periodic tryptophan protein 2

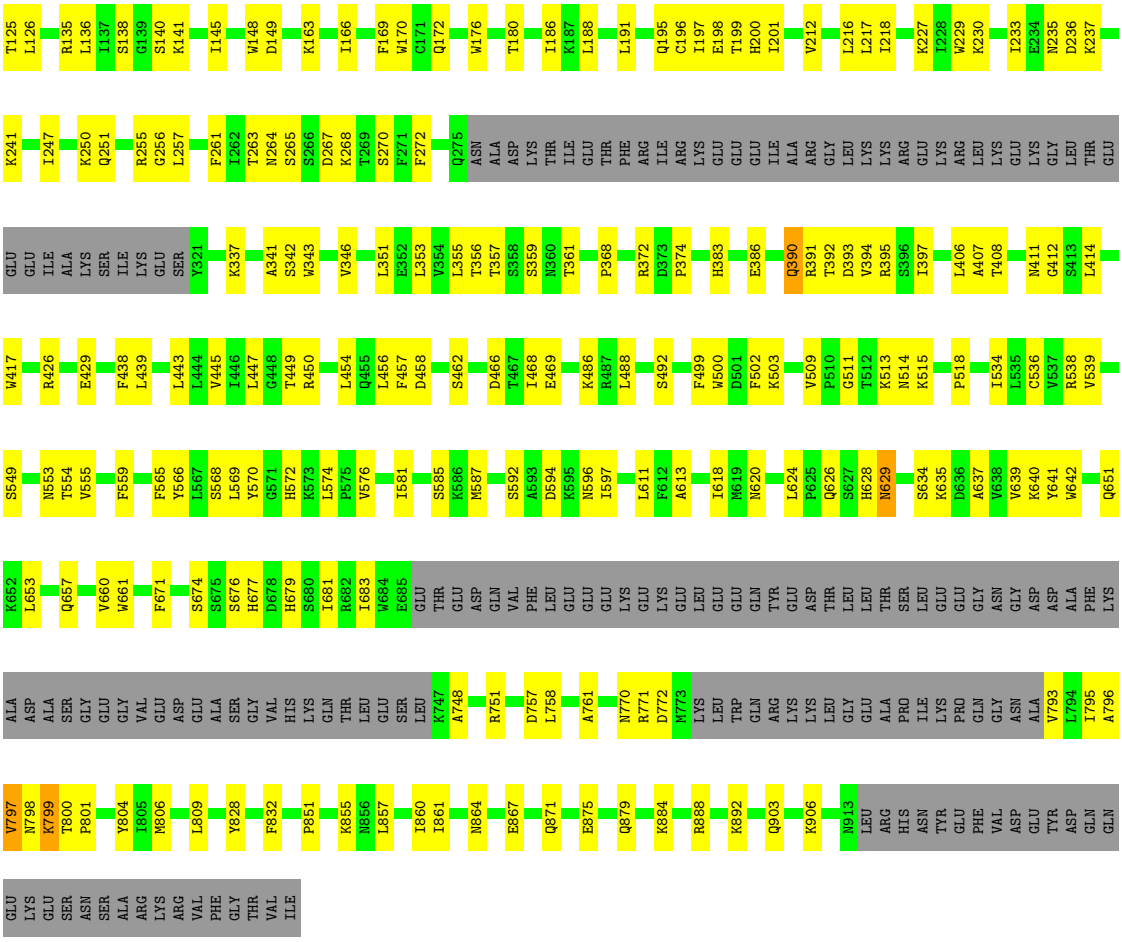
Chain BA:



• Molecule 17: U3 small nucleolar RNA-associated protein 12

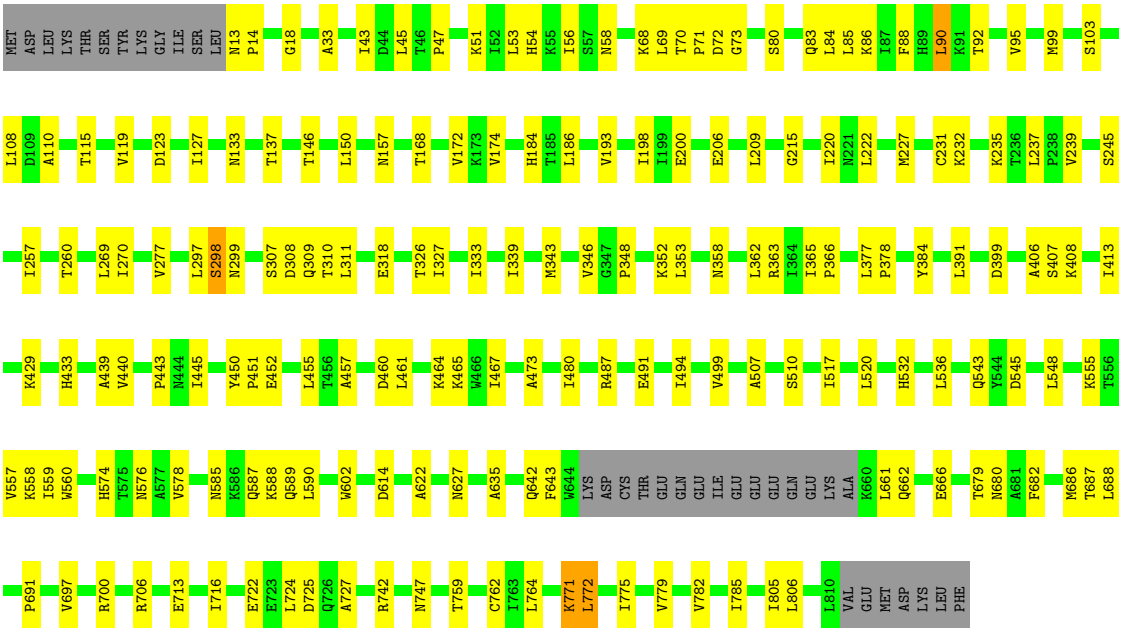
Chain BB:





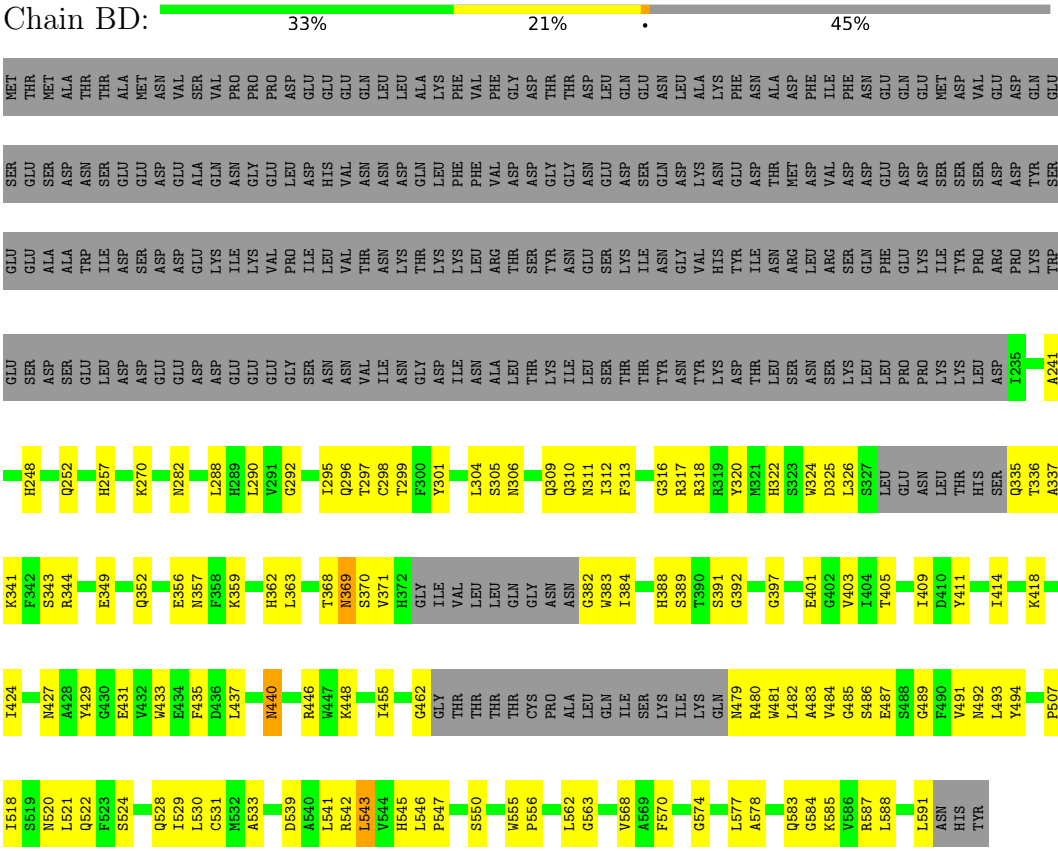
• Molecule 18: U3 small nucleolar RNA-associated protein 13

Chain BC:



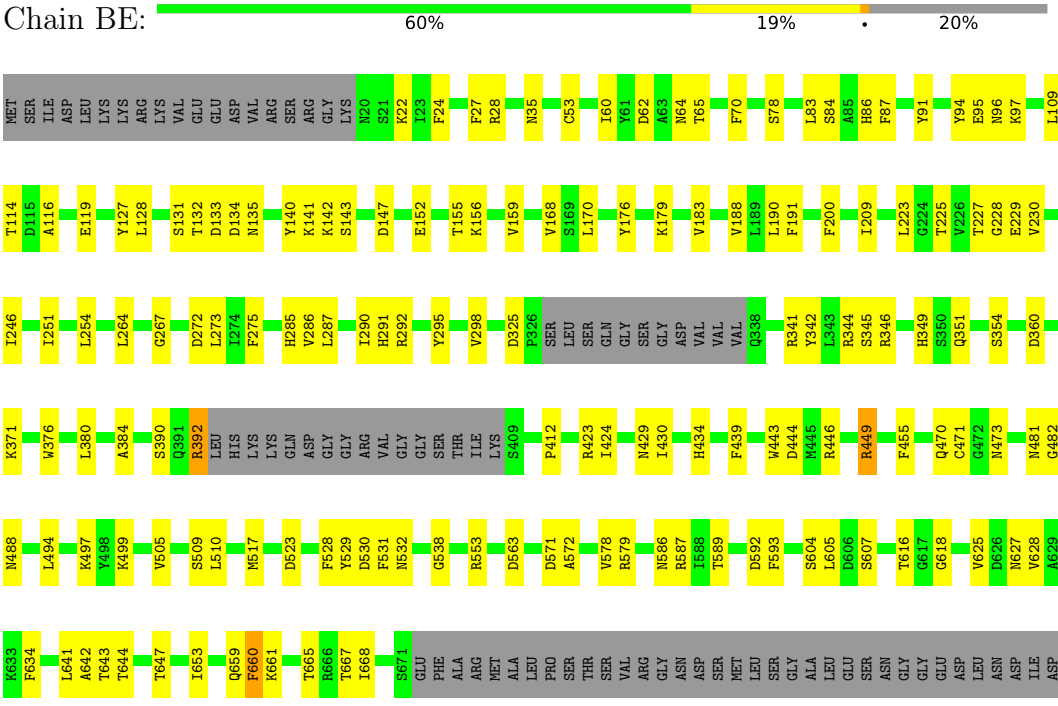
• Molecule 19: U3 small nucleolar RNA-associated protein 18

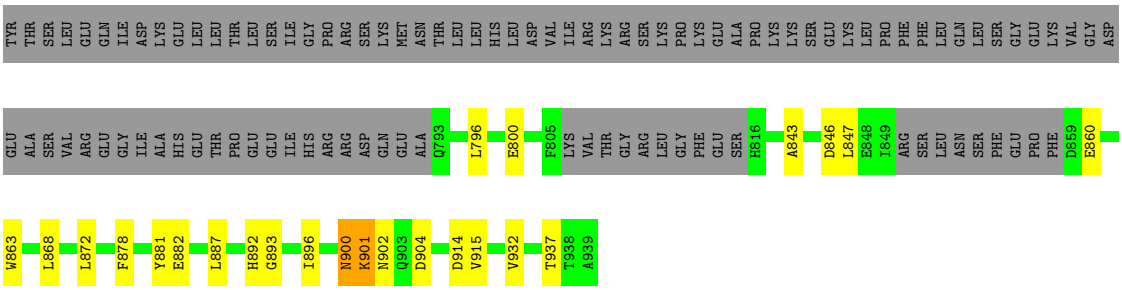
Chain BD:



• Molecule 20: U3 small nucleolar RNA-associated protein 21

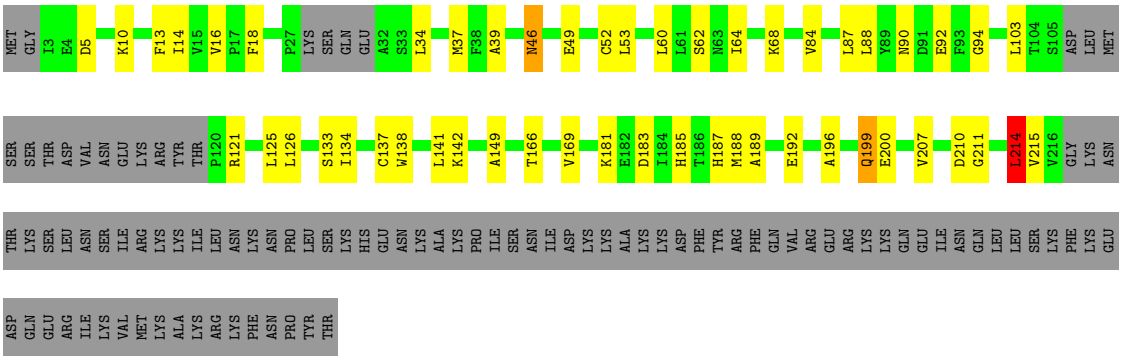
Chain BE:





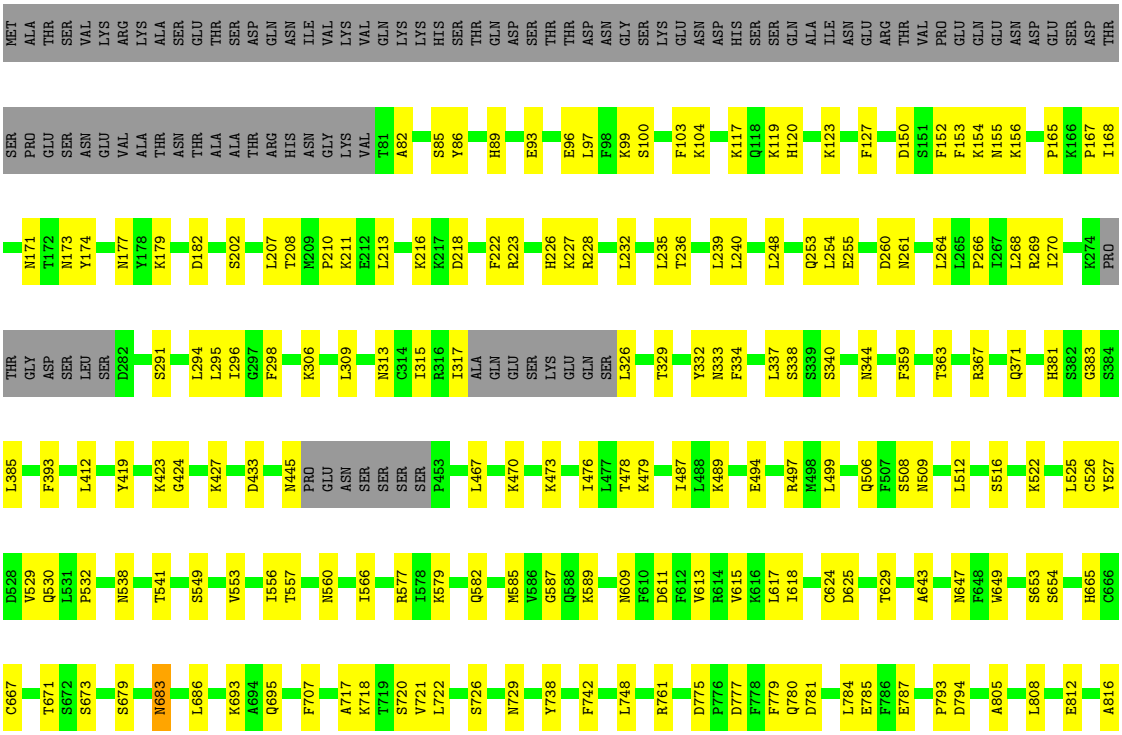
• Molecule 21: Ribosomal RNA-processing protein 7

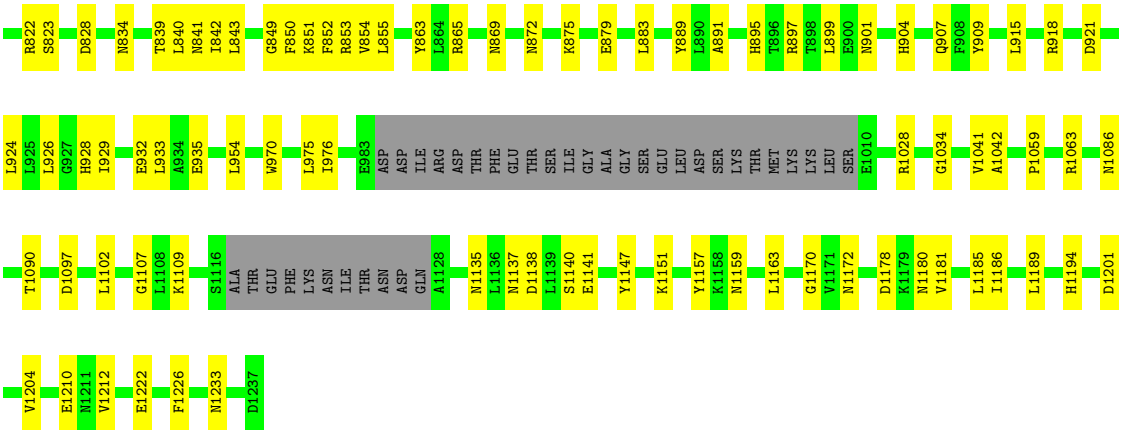
Chain CA:



• Molecule 22: U3 small nucleolar RNA-associated protein 22

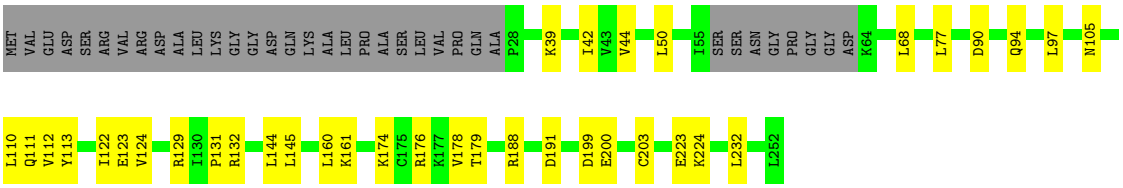
Chain CB:





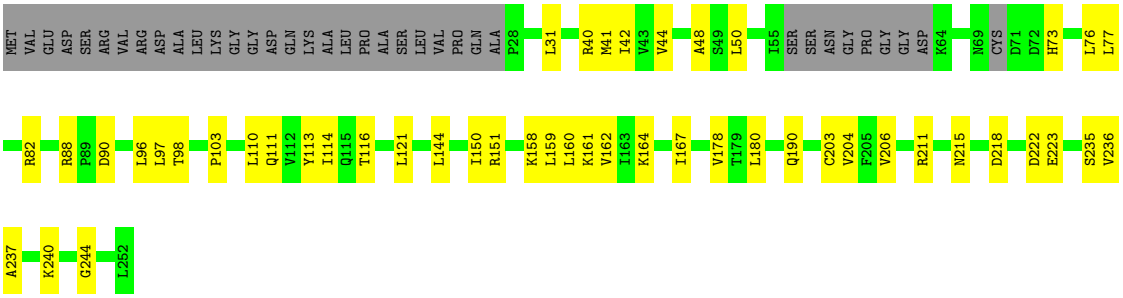
• Molecule 23: Ribosomal RNA small subunit methyltransferase NEP1

Chain E1:



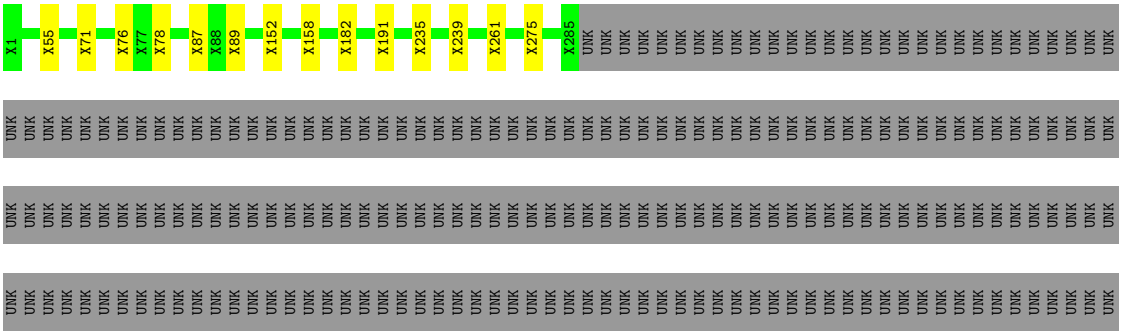
• Molecule 23: Ribosomal RNA small subunit methyltransferase NEP1

Chain E2:



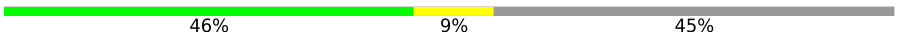
• Molecule 24: Enp2

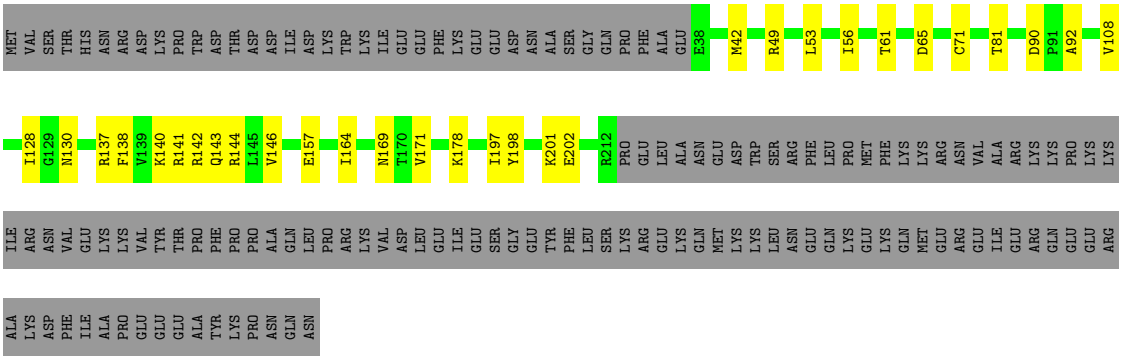
Chain E4:



• Molecule 25: KRR1 small subunit processome component

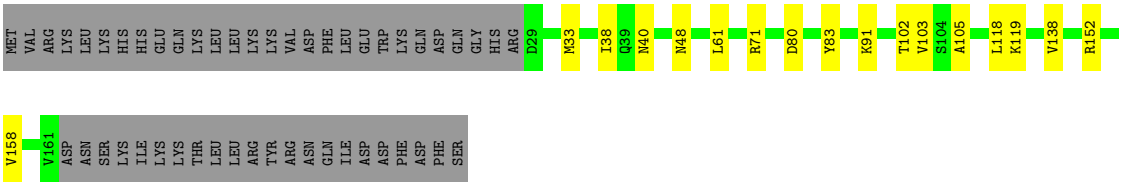
Chain K1:





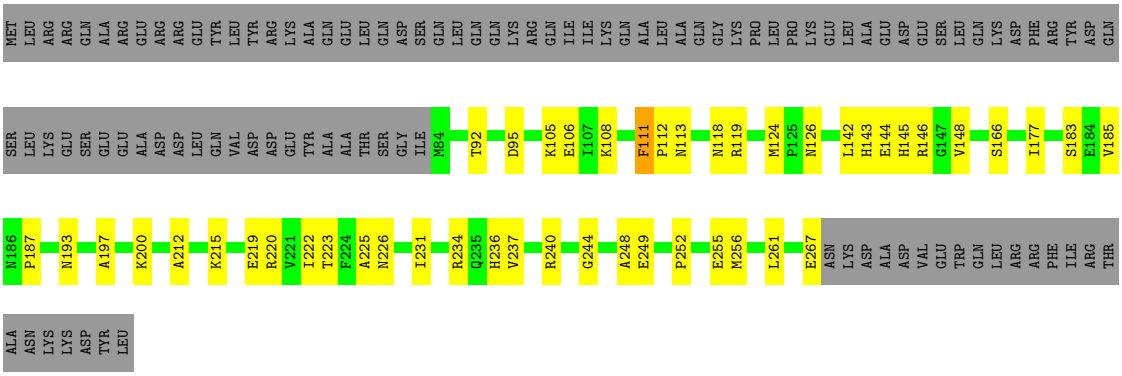
• Molecule 26: U3 small nucleolar ribonucleoprotein protein IMP3

Chain MA:



• Molecule 27: U3 small nucleolar ribonucleoprotein protein IMP4

Chain MB:

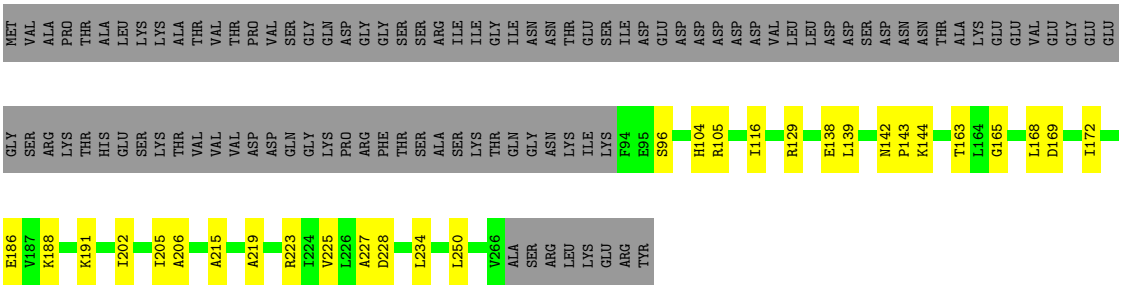


• Molecule 28: Mpp10,U3 small nucleolar RNA-associated protein MPP10

Chain MC:

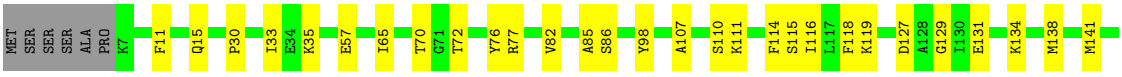
• Molecule 29: Pre-rRNA-processing protein PNO1

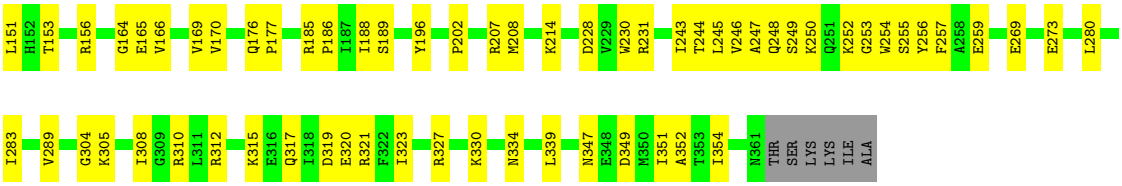
Chain P1:



• Molecule 30: RNA 3'-terminal phosphate cyclase-like protein

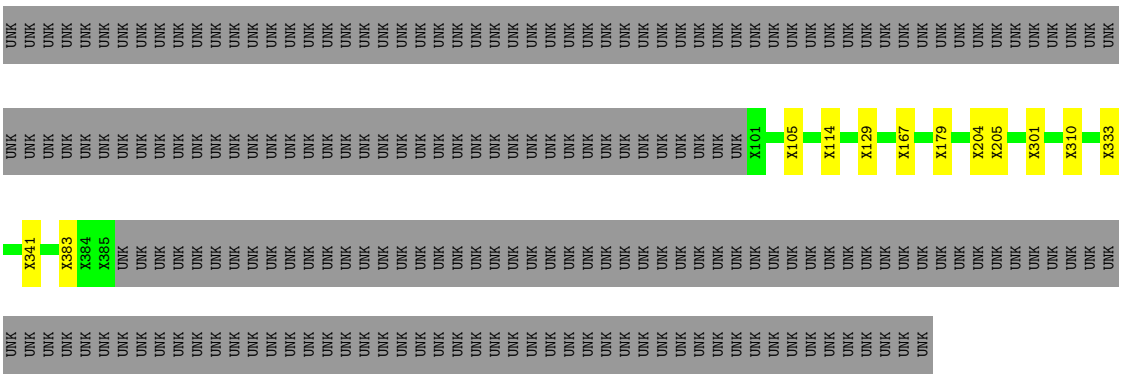
Chain R1:





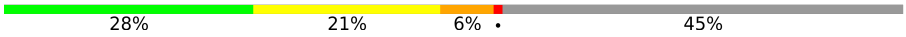
• Molecule 31: Sof1

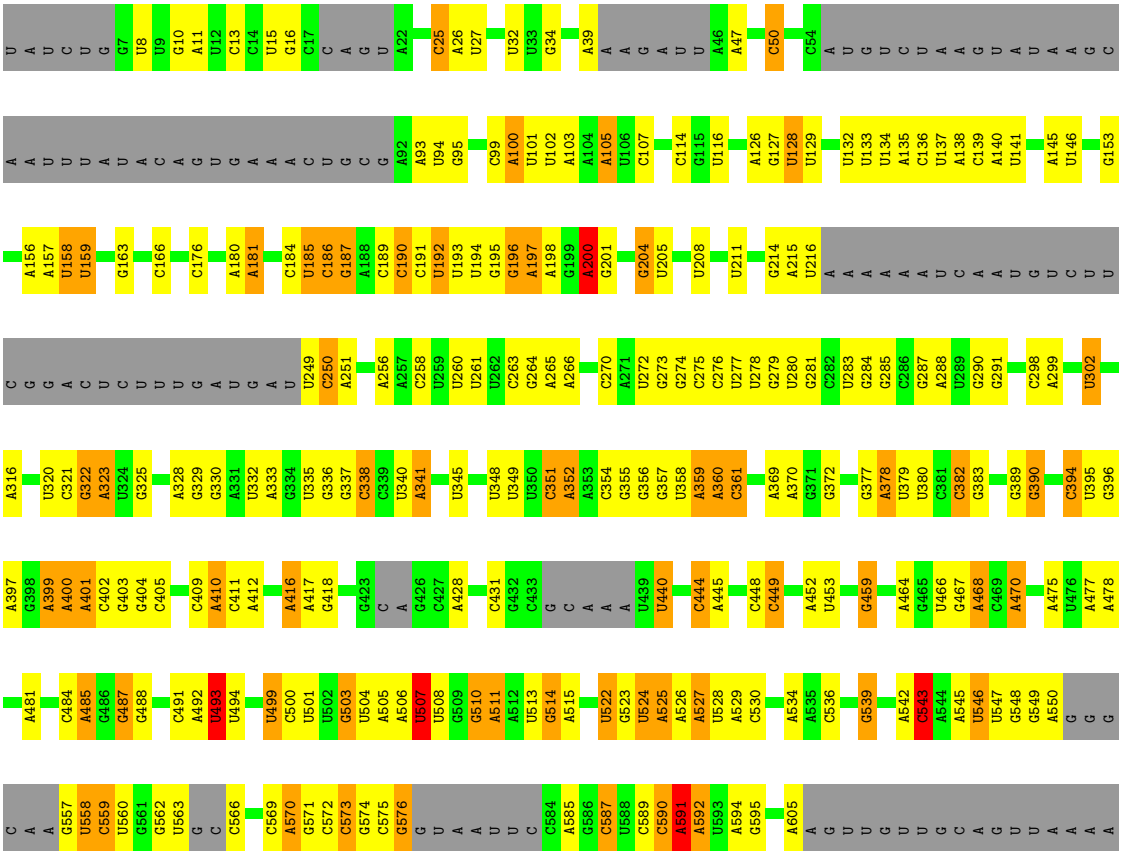
Chain S1:

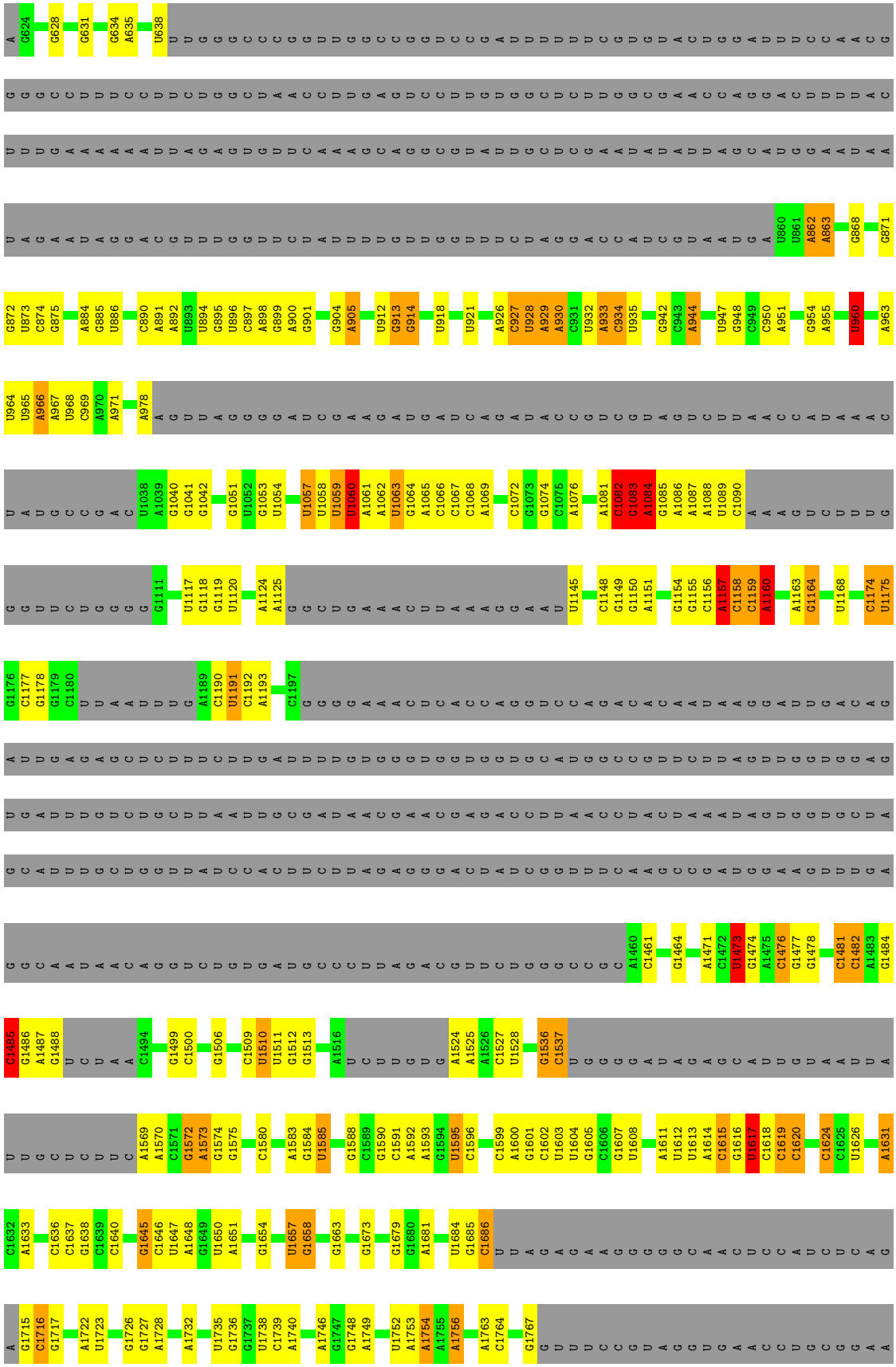


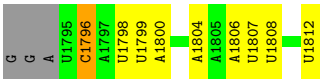
• Molecule 32: 18S ribosomal RNA

Chain SA:



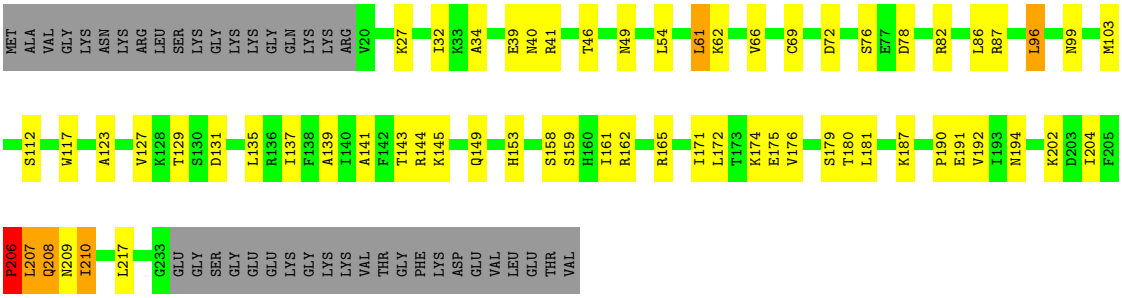






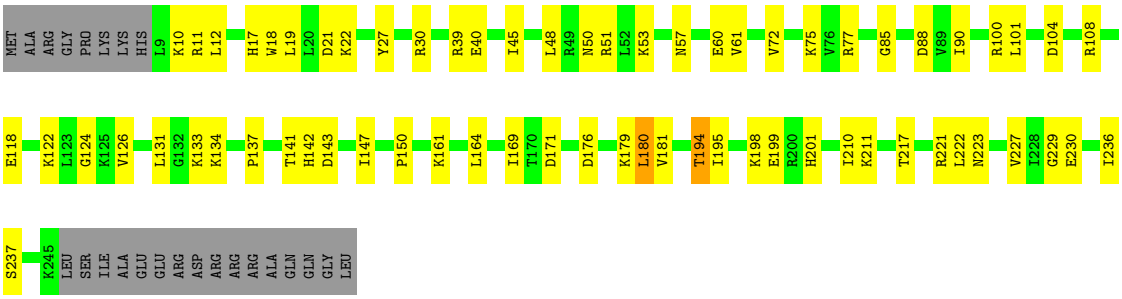
• Molecule 33: 40S ribosomal protein S1-A

Chain SC:



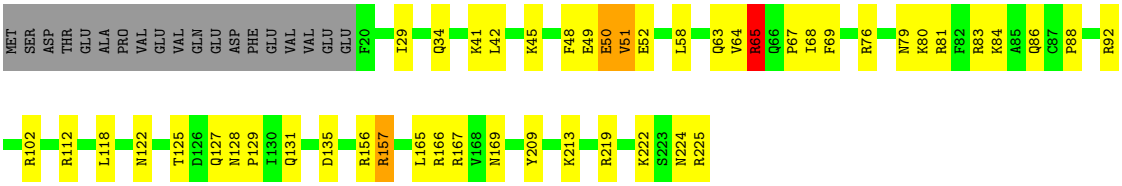
• Molecule 34: 40S ribosomal protein S4-A

Chain SF:



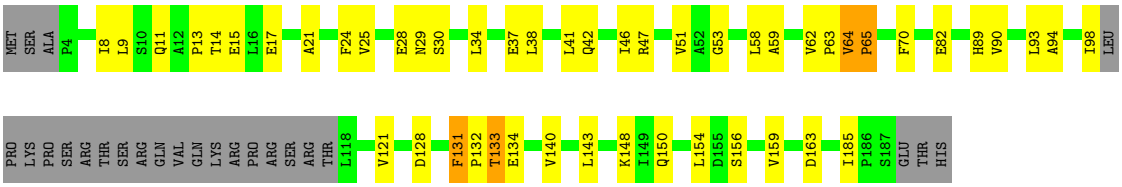
• Molecule 35: 40S ribosomal protein S5

Chain SG:



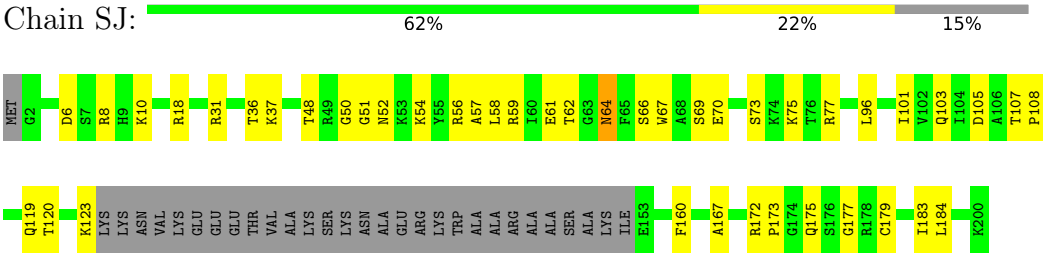
• Molecule 36: 40S ribosomal protein S7-A

Chain SI:



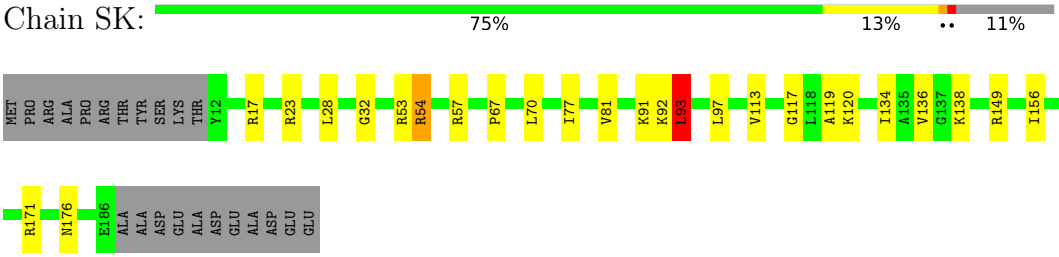
• Molecule 37: 40S ribosomal protein S8-A

Chain SJ:



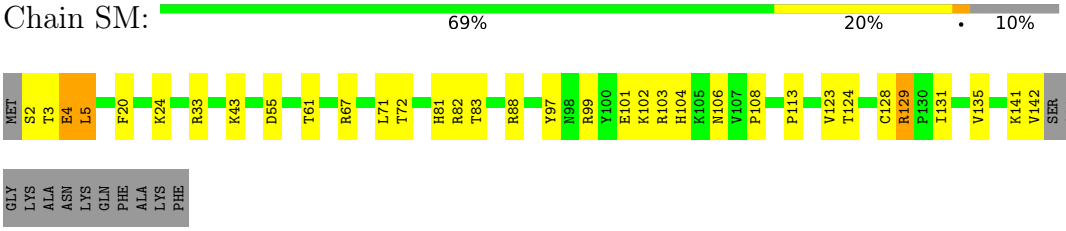
• Molecule 38: 40S ribosomal protein S9-A

Chain SK:



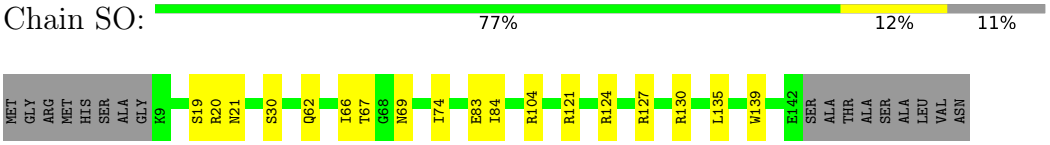
• Molecule 39: 40S ribosomal protein S11-A

Chain SM:



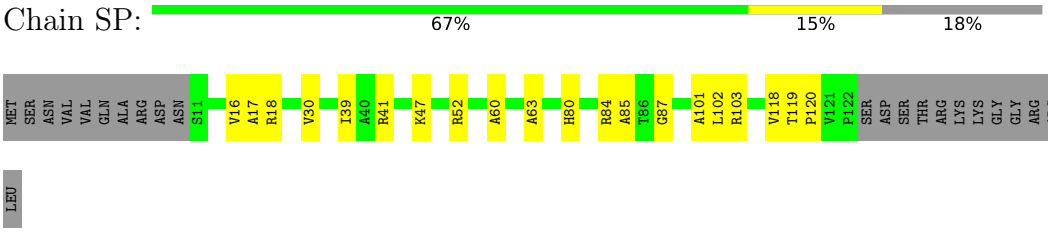
• Molecule 40: 40S ribosomal protein S13

Chain SO:



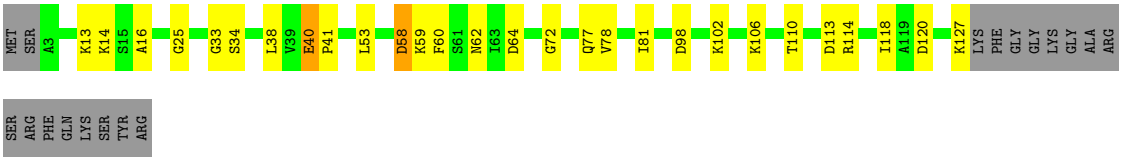
• Molecule 41: 40S ribosomal protein S14-A

Chain SP:



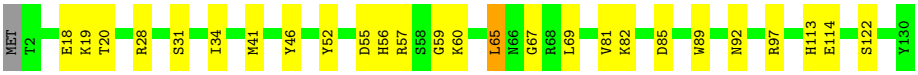
• Molecule 42: 40S ribosomal protein S16-A

Chain SR:



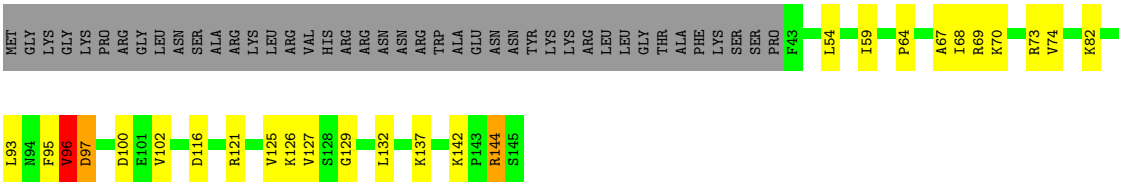
• Molecule 43: 40S ribosomal protein S22-A

Chain SX:



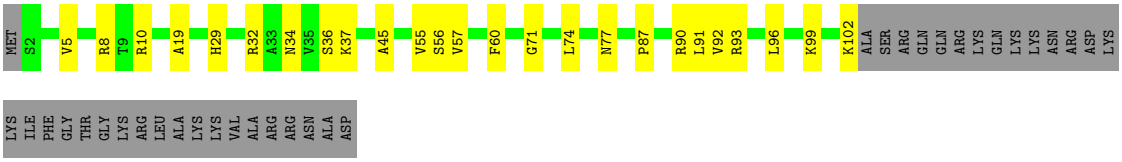
• Molecule 44: 40S ribosomal protein S23-A

Chain SY:



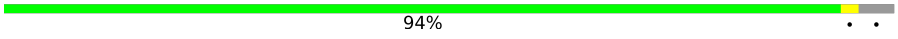
• Molecule 45: 40S ribosomal protein S24-A

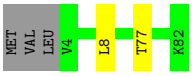
Chain SZ:



• Molecule 46: 40S ribosomal protein S27-A

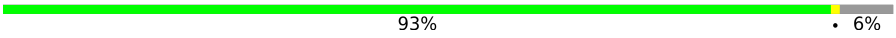
Chain Sc:

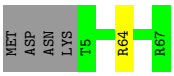




• Molecule 47: 40S ribosomal protein S28-A

Chain Sd:



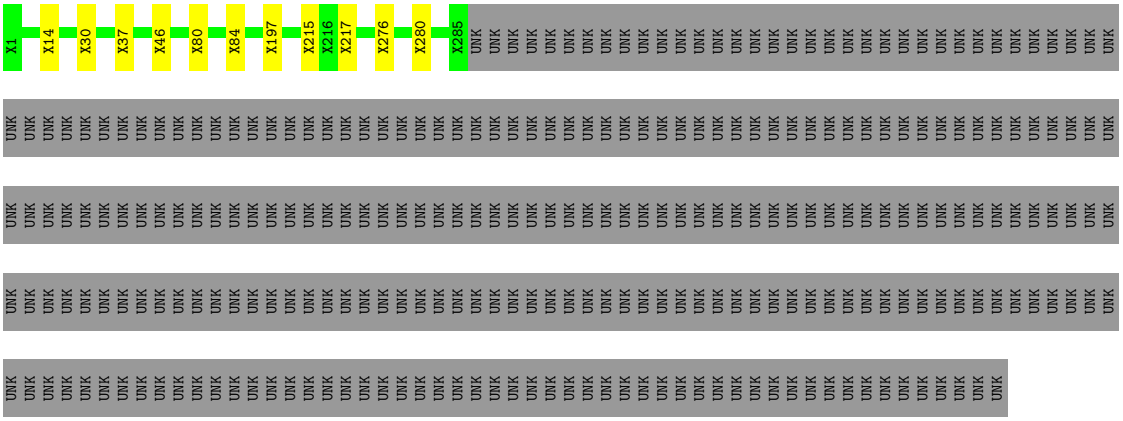


• Molecule 48: 40S ribosomal protein S30-A

Chain Sf:

• Molecule 49: Utp7

Chain U1:

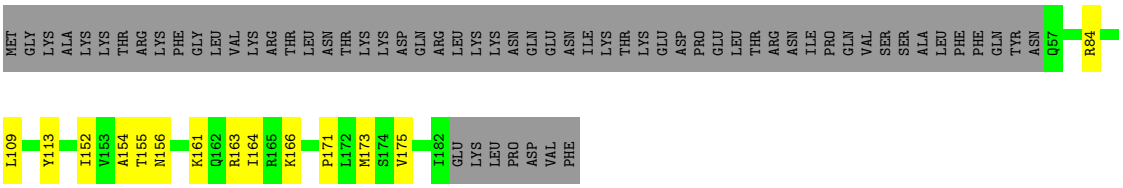


• Molecule 50: Utp11

Chain U2:

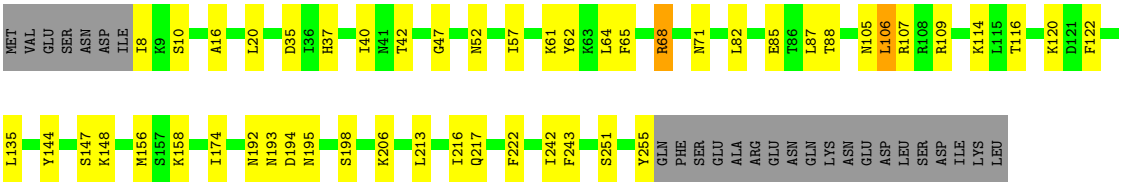
• Molecule 51: rRNA-processing protein FCF1

Chain U4:



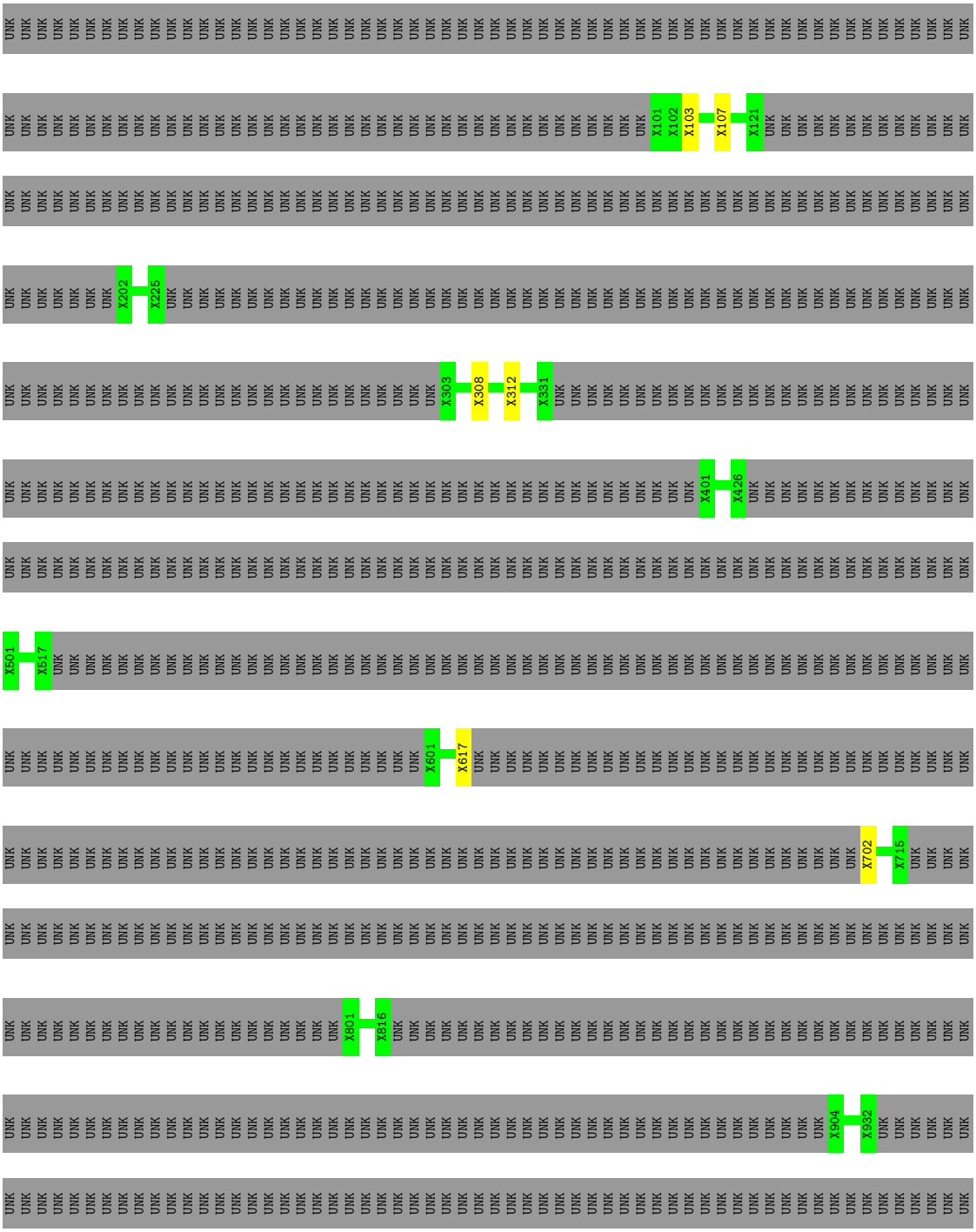
• Molecule 52: Ribosome biogenesis protein UTP30

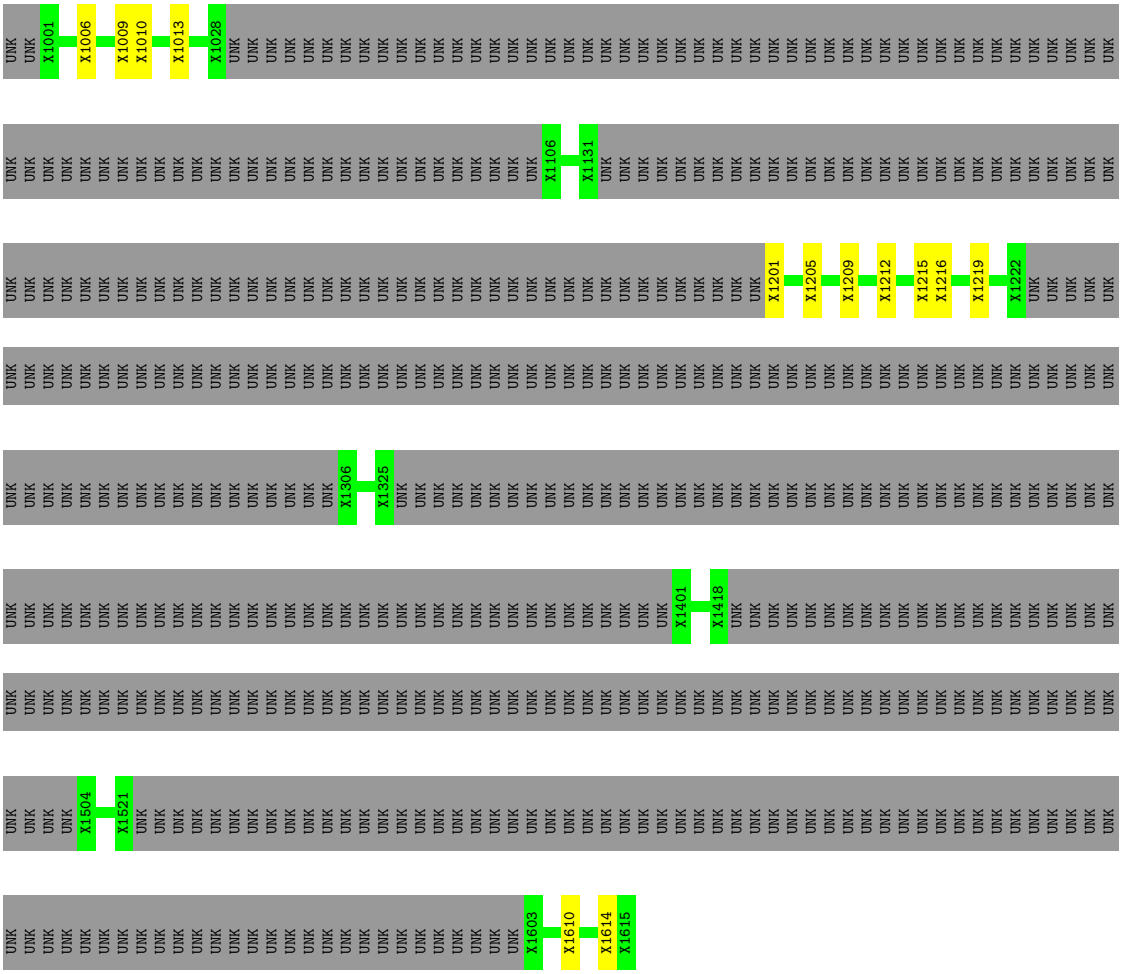
Chain U5:



• Molecule 53: Helical domain protein

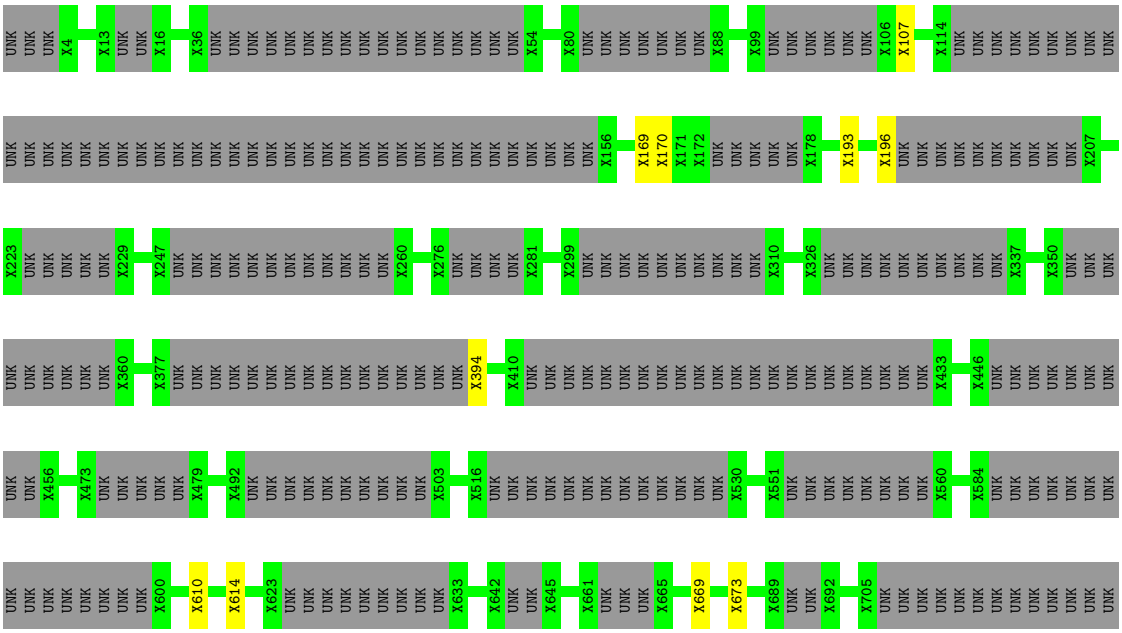
Chain UA: 20% 79%

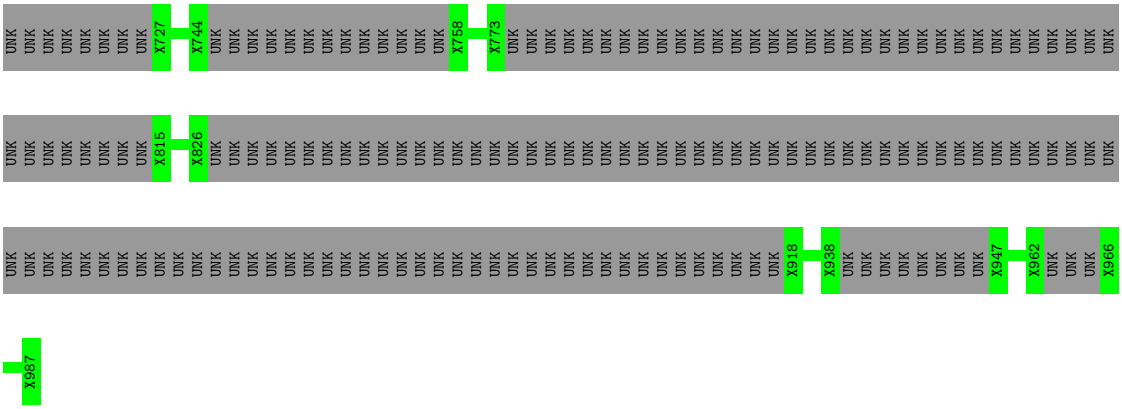




• Molecule 54: Helical domain protein

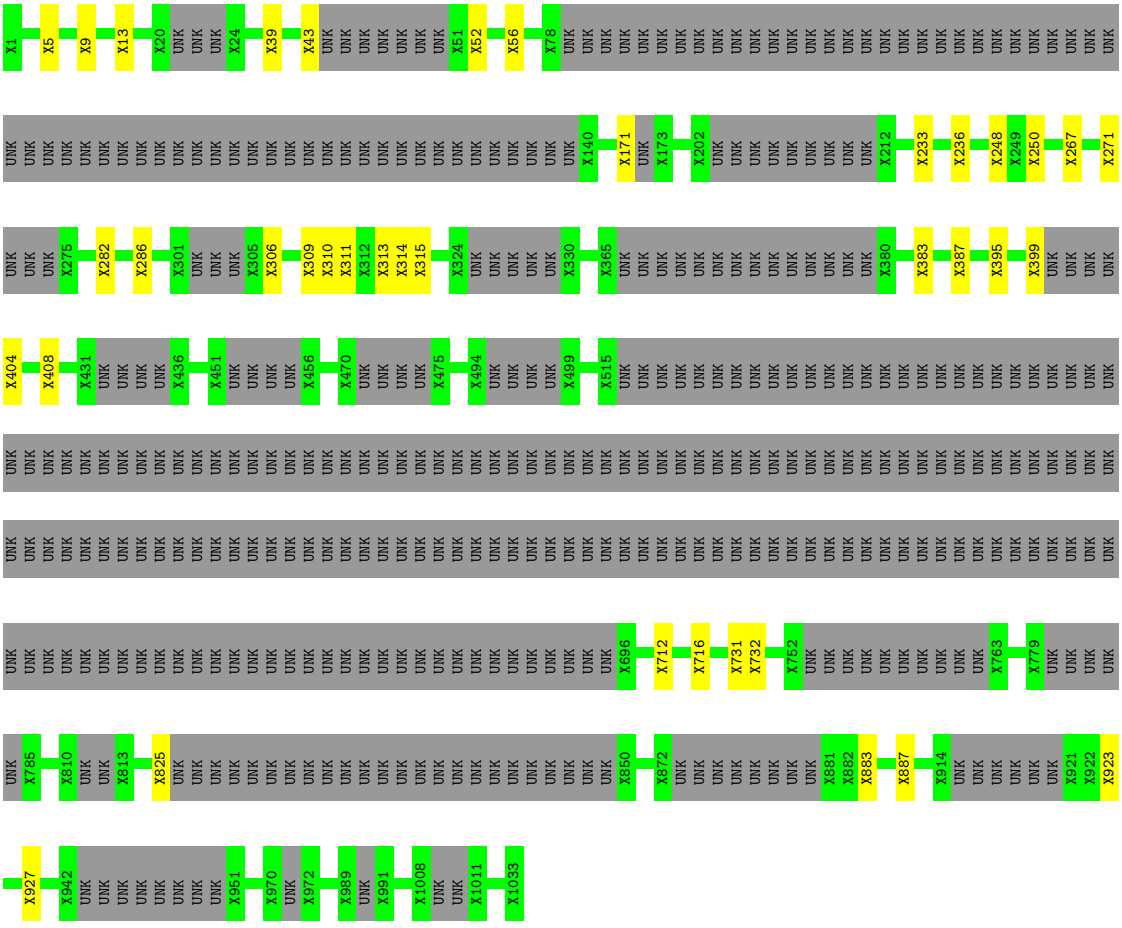
Chain UB:





• Molecule 55: Unassigned helices

Chain UC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73543	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	79545	Depositor
Image detector	OTHER	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	3A	0.53	0/3710	1.13	14/5763 (0.2%)
2	3B	0.41	0/1903	0.61	1/2572 (0.0%)
2	3C	0.30	0/1903	0.56	1/2572 (0.0%)
3	3D	0.35	0/2960	0.58	0/3987
4	3E	0.31	0/2970	0.52	0/4004
5	3F	0.33	0/2975	0.58	0/4008
6	3G	0.32	0/936	0.55	0/1273
6	3H	0.34	0/936	0.59	0/1273
7	5A	0.51	0/11029	1.19	66/17170 (0.4%)
12	AE	0.35	0/3386	0.56	0/4577
15	B1	0.36	0/4431	0.62	1/5988 (0.0%)
16	BA	0.42	0/6164	0.66	5/8349 (0.1%)
17	BB	0.31	0/6264	0.62	1/8473 (0.0%)
18	BC	0.31	0/6226	0.63	3/8442 (0.0%)
19	BD	0.37	0/2597	0.65	0/3520
20	BE	0.39	0/6056	0.62	1/8189 (0.0%)
21	CA	0.34	0/1621	0.55	2/2196 (0.1%)
22	CB	0.29	0/9081	0.49	0/12283
23	E1	0.28	0/1716	0.49	0/2319
23	E2	0.30	0/1721	0.50	0/2323
25	K1	0.35	0/1432	0.56	0/1926
26	MA	0.42	0/1117	0.64	0/1509
27	MB	0.36	0/1496	0.65	2/2025 (0.1%)
28	MC	0.38	0/209	0.67	1/282 (0.4%)
29	P1	0.30	0/1394	0.56	0/1881
30	R1	0.31	0/2793	0.52	0/3774
32	SA	0.47	5/23814 (0.0%)	1.22	200/37055 (0.5%)
33	SC	0.34	0/1735	0.77	2/2335 (0.1%)
34	SF	0.30	0/1920	0.63	1/2589 (0.0%)
35	SG	0.44	0/1629	0.68	0/2202
36	SI	0.32	0/1343	0.62	1/1808 (0.1%)
37	SJ	0.29	0/1373	0.62	0/1834
38	SK	0.34	0/1434	0.66	1/1920 (0.1%)
39	SM	0.30	0/1169	0.57	0/1576

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
40	SO	0.30	0/1109	0.53	0/1495
41	SP	0.30	0/781	0.56	0/1062
42	SR	0.39	0/990	0.71	1/1335 (0.1%)
43	SX	0.33	0/1038	0.62	1/1395 (0.1%)
44	SY	0.34	0/796	0.71	0/1062
45	SZ	0.30	0/814	0.54	0/1093
46	Sc	0.33	0/605	0.62	0/817
47	Sd	0.34	0/499	0.65	0/670
48	Sf	0.34	0/255	0.63	0/339
51	U4	0.39	0/1007	0.59	0/1357
52	U5	0.32	0/2043	0.59	1/2747 (0.0%)
All	All	0.39	5/131380 (0.0%)	0.84	306/185369 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	3B	0	1
3	3D	0	2
5	3F	0	1
12	AE	0	1
15	B1	0	3
16	BA	0	5
17	BB	0	7
18	BC	0	6
19	BD	0	1
20	BE	0	5
21	CA	0	1
29	P1	0	1
32	SA	0	1
33	SC	0	4
34	SF	0	1
35	SG	0	8
36	SI	0	4
37	SJ	0	1
38	SK	0	2
39	SM	0	1
42	SR	0	1
44	SY	0	2
45	SZ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
46	Sc	0	2
52	U5	0	1
55	UC	0	2
All	All	0	65

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	SA	493	U	C2-N3	-14.24	1.27	1.37
32	SA	487	G	C5-C4	8.67	1.44	1.38
32	SA	487	G	C5-C6	5.81	1.48	1.42
32	SA	1160	A	N9-C4	-5.30	1.34	1.37
32	SA	487	G	C8-N7	-5.17	1.27	1.30

All (306) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	487	G	C5-C6-O6	30.25	146.75	128.60
32	SA	487	G	N1-C6-O6	-28.75	102.65	119.90
32	SA	487	G	C4-C5-N7	-26.03	100.39	110.80
32	SA	493	U	C5-C4-O4	24.09	140.36	125.90
32	SA	493	U	N3-C4-O4	-21.06	104.66	119.40
32	SA	487	G	C6-C5-N7	19.95	142.37	130.40
32	SA	487	G	C5-N7-C8	19.04	113.82	104.30
32	SA	493	U	C2-N3-C4	15.12	136.07	127.00
32	SA	493	U	N1-C2-N3	-14.20	106.38	114.90
32	SA	487	G	C6-N1-C2	11.14	131.78	125.10
32	SA	1485	C	N1-C2-O2	11.11	125.57	118.90
32	SA	487	G	N3-C4-N9	-10.99	119.40	126.00
32	SA	559	C	C2-N1-C1'	10.49	130.34	118.80
32	SA	487	G	N9-C4-C5	10.27	109.51	105.40
32	SA	487	G	C5-C6-N1	-10.14	106.43	111.50
7	5A	456	U	C5-C6-N1	10.00	127.70	122.70
7	5A	522	C	N3-C2-O2	-9.74	115.08	121.90
32	SA	493	U	C4-C5-C6	-9.59	113.94	119.70
32	SA	559	C	N1-C2-O2	9.37	124.52	118.90
32	SA	558	U	N3-C2-O2	-9.24	115.73	122.20
32	SA	1485	C	N3-C2-O2	-9.12	115.51	121.90
7	5A	356	C	N3-C2-O2	-9.11	115.52	121.90
32	SA	1082	C	C2-N1-C1'	9.01	128.71	118.80
38	SK	93	LEU	CA-CB-CG	9.00	136.00	115.30
32	SA	1596	C	C2-N1-C1'	8.90	128.59	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	1082	C	N1-C2-O2	8.52	124.01	118.90
32	SA	1624	C	N1-C2-O2	8.50	124.00	118.90
32	SA	1596	C	N1-C2-O2	8.26	123.86	118.90
7	5A	108	U	C2-N1-C1'	8.11	127.44	117.70
7	5A	433	C	N1-C2-O2	8.11	123.77	118.90
32	SA	1057	U	N1-C2-O2	8.02	128.41	122.80
32	SA	1057	U	C2-N1-C1'	8.01	127.31	117.70
7	5A	432	C	N1-C2-O2	7.89	123.64	118.90
32	SA	1537	C	N1-C2-O2	7.84	123.61	118.90
32	SA	1060	U	N1-C2-O2	7.84	128.29	122.80
7	5A	356	C	C6-N1-C2	-7.77	117.19	120.30
32	SA	1057	U	N3-C2-O2	-7.74	116.79	122.20
32	SA	107	C	N1-C2-O2	7.68	123.51	118.90
32	SA	50	C	C2-N1-C1'	7.66	127.23	118.80
7	5A	356	C	N1-C2-O2	7.62	123.47	118.90
32	SA	1063	U	N3-C2-O2	-7.55	116.91	122.20
7	5A	522	C	N1-C2-O2	7.51	123.41	118.90
32	SA	184	C	N1-C2-O2	7.48	123.39	118.90
7	5A	441	C	C6-N1-C2	-7.42	117.33	120.30
32	SA	1536	G	C4-N9-C1'	7.41	136.13	126.50
7	5A	391	C	C5-C6-N1	7.39	124.70	121.00
32	SA	559	C	C6-N1-C1'	-7.38	111.94	120.80
32	SA	1537	C	C6-N1-C2	-7.33	117.37	120.30
32	SA	1537	C	N3-C2-O2	-7.32	116.78	121.90
32	SA	440	U	N3-C2-O2	-7.32	117.08	122.20
32	SA	1063	U	N1-C2-O2	7.30	127.91	122.80
32	SA	1536	G	N3-C4-C5	-7.29	124.96	128.60
32	SA	574	G	N3-C4-N9	7.26	130.35	126.00
32	SA	965	U	N1-C2-O2	7.19	127.83	122.80
7	5A	432	C	C2-N1-C1'	7.18	126.70	118.80
32	SA	440	U	N1-C2-O2	7.12	127.79	122.80
1	3A	304	U	C2-N1-C1'	7.11	126.24	117.70
32	SA	1596	C	N3-C2-O2	-7.11	116.92	121.90
32	SA	1624	C	N3-C2-O2	-7.08	116.94	121.90
32	SA	499	U	N3-C2-O2	-7.06	117.26	122.20
32	SA	1063	U	C2-N1-C1'	6.97	126.07	117.70
32	SA	185	U	C2-N1-C1'	6.97	126.06	117.70
32	SA	1060	U	N3-C2-O2	-6.93	117.35	122.20
32	SA	1060	U	C2-N1-C1'	6.92	126.00	117.70
7	5A	456	U	C5-C4-O4	-6.88	121.77	125.90
32	SA	1082	C	C6-N1-C1'	-6.84	112.59	120.80
32	SA	1159	C	C2-N1-C1'	6.84	126.32	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	5A	108	U	N1-C2-O2	6.84	127.59	122.80
7	5A	433	C	C2-N1-C1'	6.82	126.30	118.80
21	CA	214	LEU	CA-CB-CG	6.79	130.93	115.30
1	3A	304	U	N1-C2-O2	6.78	127.55	122.80
32	SA	965	U	C2-N1-C1'	6.75	125.80	117.70
7	5A	391	C	C6-N1-C2	-6.74	117.60	120.30
32	SA	1072	C	C2-N1-C1'	6.73	126.20	118.80
32	SA	1536	G	N3-C4-N9	6.71	130.02	126.00
1	3A	10	C	C6-N1-C2	-6.66	117.64	120.30
36	SI	143	LEU	CA-CB-CG	6.63	130.55	115.30
32	SA	185	U	N1-C2-O2	6.61	127.43	122.80
18	BC	133	ASN	C-N-CA	6.58	136.12	122.30
27	MB	111	PHE	C-N-CD	-6.58	106.13	120.60
32	SA	934	C	N1-C2-O2	6.55	122.83	118.90
7	5A	522	C	C6-N1-C2	-6.54	117.69	120.30
1	3A	304	U	N3-C2-O2	-6.48	117.66	122.20
32	SA	25	C	P-O3'-C3'	6.48	127.47	119.70
32	SA	1159	C	N1-C2-O2	6.48	122.78	118.90
32	SA	965	U	N3-C2-O2	-6.46	117.68	122.20
32	SA	559	C	C6-N1-C2	-6.45	117.72	120.30
32	SA	449	C	C5-C6-N1	6.43	124.22	121.00
32	SA	913	G	C4-N9-C1'	6.43	134.86	126.50
7	5A	441	C	C2-N1-C1'	6.41	125.85	118.80
32	SA	559	C	C5-C6-N1	6.36	124.18	121.00
7	5A	433	C	N3-C2-O2	-6.33	117.47	121.90
7	5A	508	C	C2-N1-C1'	6.31	125.74	118.80
32	SA	591	A	C6-N1-C2	-6.27	114.84	118.60
7	5A	386	A	C2-N3-C4	6.27	113.74	110.60
32	SA	136	C	C2-N1-C1'	6.27	125.70	118.80
32	SA	507	U	C2-N1-C1'	6.25	125.20	117.70
32	SA	558	U	N1-C2-N3	6.25	118.65	114.90
32	SA	107	C	N3-C2-O2	-6.24	117.54	121.90
32	SA	285	G	C4-N9-C1'	6.23	134.60	126.50
7	5A	456	U	N3-C4-O4	6.22	123.75	119.40
32	SA	1158	C	C5-C6-N1	6.22	124.11	121.00
32	SA	192	U	P-O3'-C3'	6.21	127.15	119.70
32	SA	1624	C	C2-N1-C1'	6.21	125.63	118.80
32	SA	574	G	C6-C5-N7	-6.19	126.68	130.40
32	SA	638	U	C2-N1-C1'	6.17	125.10	117.70
32	SA	1536	G	C2-N3-C4	6.16	114.98	111.90
7	5A	245	C	P-O3'-C3'	6.14	127.07	119.70
32	SA	559	C	N3-C2-O2	-6.13	117.61	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	1485	C	C2-N1-C1'	6.12	125.54	118.80
32	SA	1083	G	OP1-P-O3'	6.12	118.66	105.20
32	SA	1596	C	C6-N1-C2	-6.11	117.86	120.30
21	CA	214	LEU	CB-CG-CD2	6.11	121.38	111.00
7	5A	128	C	N1-C2-O2	6.10	122.56	118.90
32	SA	1573	A	P-O3'-C3'	6.09	127.01	119.70
32	SA	440	U	C2-N1-C1'	6.09	125.01	117.70
32	SA	1596	C	C6-N1-C1'	-6.09	113.49	120.80
32	SA	934	C	C2-N1-C1'	6.08	125.48	118.80
16	BA	546	ASP	CB-CG-OD1	6.07	123.76	118.30
32	SA	250	C	C6-N1-C2	-6.07	117.87	120.30
32	SA	1536	G	C8-N9-C1'	-6.06	119.13	127.00
7	5A	109	C	C2-N1-C1'	6.05	125.45	118.80
7	5A	355	C	N1-C2-O2	6.04	122.53	118.90
32	SA	1063	U	C5-C6-N1	6.04	125.72	122.70
2	3C	306	LEU	C-N-CA	6.02	136.74	121.70
32	SA	1072	C	N1-C2-O2	6.02	122.51	118.90
32	SA	1658	G	C4-N9-C1'	6.01	134.31	126.50
33	SC	61	LEU	CA-CB-CG	6.00	129.11	115.30
32	SA	499	U	N1-C2-O2	6.00	127.00	122.80
32	SA	507	U	N1-C2-O2	5.99	127.00	122.80
7	5A	108	U	N3-C2-O2	-5.99	118.01	122.20
7	5A	432	C	N3-C2-O2	-5.98	117.71	121.90
7	5A	172	C	C5-C6-N1	5.98	123.99	121.00
32	SA	453	U	N1-C2-O2	5.97	126.98	122.80
32	SA	50	C	N1-C2-O2	5.96	122.48	118.90
32	SA	453	U	N3-C2-O2	-5.95	118.03	122.20
32	SA	1620	C	N1-C2-O2	5.95	122.47	118.90
32	SA	1585	U	C5-C6-N1	5.94	125.67	122.70
32	SA	159	U	C5-C6-N1	5.92	125.66	122.70
7	5A	508	C	N1-C2-O2	5.92	122.45	118.90
32	SA	1640	C	N1-C2-O2	5.91	122.45	118.90
32	SA	431	C	C5-C6-N1	5.90	123.95	121.00
32	SA	1067	C	C6-N1-C2	-5.89	117.94	120.30
32	SA	394	C	N1-C2-O2	5.89	122.43	118.90
7	5A	240	C	N1-C2-O2	5.88	122.43	118.90
18	BC	545	ASP	CB-CG-OD1	5.88	123.59	118.30
32	SA	1063	U	C6-N1-C2	-5.86	117.48	121.00
32	SA	285	G	N3-C4-N9	5.83	129.50	126.00
32	SA	1573	A	OP2-P-O3'	5.83	118.02	105.20
43	SX	65	LEU	CA-CB-CG	5.81	128.66	115.30
32	SA	185	U	N3-C2-O2	-5.81	118.13	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	1072	C	C6-N1-C2	-5.79	117.98	120.30
32	SA	159	U	N1-C2-O2	5.78	126.84	122.80
32	SA	50	C	C6-N1-C1'	-5.78	113.87	120.80
32	SA	260	U	C2-N1-C1'	5.78	124.63	117.70
32	SA	260	U	N1-C2-O2	5.77	126.84	122.80
32	SA	487	G	C4-N9-C1'	5.76	133.99	126.50
32	SA	1658	G	N3-C4-N9	5.76	129.46	126.00
7	5A	186	C	C5-C6-N1	5.74	123.87	121.00
32	SA	136	C	N1-C2-O2	5.74	122.34	118.90
7	5A	251	C	C6-N1-C2	-5.73	118.01	120.30
32	SA	260	U	N3-C2-O2	-5.73	118.19	122.20
1	3A	49	C	C6-N1-C2	-5.73	118.01	120.30
32	SA	1066	C	N3-C2-O2	-5.73	117.89	121.90
1	3A	326	U	N1-C2-O2	5.71	126.80	122.80
7	5A	355	C	C6-N1-C2	-5.69	118.02	120.30
32	SA	1082	C	O4'-C1'-N1	5.68	112.75	108.20
32	SA	1619	C	N3-C2-O2	-5.67	117.93	121.90
32	SA	159	U	C2-N1-C1'	5.66	124.49	117.70
32	SA	159	U	N3-C2-O2	-5.66	118.24	122.20
16	BA	535	LEU	CA-CB-CG	5.65	128.30	115.30
32	SA	249	U	C2-N1-C1'	5.65	124.48	117.70
32	SA	400	A	O4'-C1'-N9	-5.64	103.69	108.20
7	5A	342	C	N1-C2-O2	5.64	122.28	118.90
16	BA	11	LEU	CA-CB-CG	5.64	128.27	115.30
32	SA	960	U	N3-C2-O2	-5.64	118.25	122.20
32	SA	1527	C	N1-C2-O2	5.63	122.28	118.90
7	5A	413	C	N3-C2-O2	-5.63	117.96	121.90
1	3A	326	U	C2-N1-C1'	5.63	124.45	117.70
7	5A	108	U	C6-N1-C1'	-5.63	113.32	121.20
7	5A	267	U	C2-N1-C1'	5.63	124.45	117.70
7	5A	342	C	N3-C2-O2	-5.62	117.96	121.90
32	SA	453	U	C2-N1-C1'	5.62	124.44	117.70
32	SA	913	G	N3-C4-N9	5.62	129.37	126.00
32	SA	1510	U	N3-C2-O2	-5.61	118.27	122.20
7	5A	442	U	C2-N1-C1'	5.61	124.43	117.70
32	SA	1084	A	O5'-P-OP1	-5.61	100.65	105.70
7	5A	294	U	N3-C2-O2	-5.58	118.29	122.20
7	5A	178	G	C4-N9-C1'	5.58	133.75	126.50
32	SA	1615	C	N3-C2-O2	-5.57	118.00	121.90
32	SA	913	G	N3-C4-C5	-5.55	125.83	128.60
1	3A	80	U	N1-C2-O2	5.54	126.68	122.80
32	SA	1481	C	OP1-P-O3'	5.54	117.39	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	263	C	N3-C2-O2	-5.53	118.03	121.90
32	SA	1619	C	N1-C2-O2	5.53	122.22	118.90
7	5A	214	U	N3-C2-O2	-5.53	118.33	122.20
32	SA	249	U	N1-C2-O2	5.53	126.67	122.80
32	SA	560	U	N1-C2-O2	5.50	126.65	122.80
32	SA	913	G	C8-N9-C1'	-5.50	119.86	127.00
7	5A	178	G	N3-C4-N9	5.48	129.29	126.00
7	5A	172	C	N1-C2-O2	5.47	122.18	118.90
32	SA	1191	U	C2-N1-C1'	5.47	124.27	117.70
32	SA	960	U	N1-C2-O2	5.47	126.63	122.80
32	SA	1607	G	N1-C6-O6	-5.47	116.62	119.90
32	SA	184	C	N3-C2-O2	-5.47	118.07	121.90
32	SA	1510	U	N1-C2-O2	5.46	126.62	122.80
7	5A	355	C	N3-C2-O2	-5.46	118.08	121.90
32	SA	200	A	O4'-C1'-N9	5.45	112.56	108.20
32	SA	1723	U	N3-C2-O2	-5.43	118.40	122.20
32	SA	285	G	C8-N9-C1'	-5.42	119.96	127.00
32	SA	1157	A	P-O3'-C3'	5.40	126.18	119.70
1	3A	80	U	N3-C2-O2	-5.39	118.42	122.20
7	5A	383	G	O5'-P-OP2	-5.39	100.84	105.70
27	MB	111	PHE	C-N-CA	5.39	144.66	122.00
32	SA	543	C	C2-N1-C1'	5.39	124.73	118.80
32	SA	574	G	C4-N9-C1'	5.39	133.51	126.50
16	BA	721	VAL	C-N-CA	-5.39	108.22	121.70
32	SA	574	G	C8-N9-C1'	-5.38	120.00	127.00
32	SA	184	C	C2-N1-C1'	5.38	124.72	118.80
32	SA	1658	G	C8-N9-C1'	-5.37	120.02	127.00
7	5A	480	C	C2-N1-C1'	5.36	124.69	118.80
32	SA	590	C	N1-C2-O2	5.36	122.11	118.90
32	SA	449	C	C6-N1-C2	-5.35	118.16	120.30
32	SA	1057	U	C6-N1-C1'	-5.35	113.72	121.20
1	3A	107	C	C6-N1-C2	-5.34	118.16	120.30
32	SA	1082	C	C5-C6-N1	5.34	123.67	121.00
32	SA	302	U	N3-C2-O2	-5.33	118.47	122.20
2	3B	101	GLY	N-CA-C	5.33	126.43	113.10
7	5A	388	C	C2-N1-C1'	5.33	124.66	118.80
17	BB	353	LEU	CA-CB-CG	5.33	127.56	115.30
32	SA	1082	C	N3-C2-O2	-5.31	118.19	121.90
32	SA	587	C	N1-C2-O2	5.31	122.08	118.90
32	SA	1617	U	C2-N1-C1'	5.31	124.07	117.70
7	5A	280	A	C4-C5-C6	-5.30	114.35	117.00
7	5A	415	U	C5-C6-N1	5.30	125.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	1585	U	N1-C2-O2	5.30	126.51	122.80
32	SA	50	C	C5-C6-N1	5.29	123.65	121.00
32	SA	1624	C	C6-N1-C2	-5.29	118.18	120.30
32	SA	1473	U	N3-C2-O2	-5.29	118.50	122.20
32	SA	1481	C	P-O3'-C3'	5.29	126.04	119.70
32	SA	302	U	N1-C2-O2	5.28	126.50	122.80
32	SA	158	U	OP1-P-O3'	5.28	116.81	105.20
20	BE	494	LEU	CA-CB-CG	5.27	127.42	115.30
32	SA	250	C	C5-C6-N1	5.26	123.63	121.00
34	SF	222	LEU	CA-CB-CG	5.26	127.41	115.30
32	SA	159	U	C6-N1-C2	-5.25	117.85	121.00
32	SA	390	G	N3-C4-N9	5.24	129.14	126.00
32	SA	1168	U	N3-C2-O2	-5.24	118.53	122.20
42	SR	41	PRO	N-CA-C	5.24	125.71	112.10
7	5A	432	C	C6-N1-C1'	-5.23	114.52	120.80
32	SA	405	C	N1-C2-O2	5.23	122.04	118.90
52	U5	106	LEU	CA-CB-CG	5.23	127.34	115.30
32	SA	574	G	C5-C6-O6	-5.23	125.46	128.60
16	BA	702	LEU	CA-CB-CG	5.22	127.30	115.30
7	5A	186	C	C6-N1-C2	-5.21	118.22	120.30
7	5A	455	C	O4'-C1'-N1	5.21	112.37	108.20
1	3A	326	U	N3-C2-O2	-5.20	118.56	122.20
32	SA	1615	C	N1-C2-O2	5.20	122.02	118.90
32	SA	1159	C	N3-C2-O2	-5.19	118.27	121.90
32	SA	934	C	N3-C2-O2	-5.19	118.27	121.90
32	SA	1636	C	N1-C2-O2	5.18	122.01	118.90
32	SA	1175	U	C5-C6-N1	5.17	125.29	122.70
1	3A	64	A	N7-C8-N9	5.17	116.39	113.80
32	SA	1658	G	N3-C4-C5	-5.17	126.02	128.60
7	5A	172	C	C2-N3-C4	5.17	122.48	119.90
1	3A	78	G	P-O3'-C3'	5.16	125.90	119.70
32	SA	1657	U	N1-C2-O2	5.16	126.42	122.80
32	SA	1723	U	N1-C2-O2	5.16	126.41	122.80
7	5A	267	U	N1-C2-O2	5.15	126.41	122.80
32	SA	394	C	N3-C2-O2	-5.15	118.30	121.90
32	SA	1612	U	N1-C2-O2	5.15	126.41	122.80
28	MC	430	LEU	CA-CB-CG	5.14	127.13	115.30
32	SA	638	U	N1-C2-O2	5.14	126.40	122.80
32	SA	591	A	P-O3'-C3'	5.13	125.86	119.70
7	5A	20	C	C5-C6-N1	5.12	123.56	121.00
32	SA	1614	A	O4'-C1'-N9	5.12	112.30	108.20
32	SA	1060	U	P-O3'-C3'	5.12	125.84	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	SA	186	C	C5-C6-N1	5.11	123.56	121.00
7	5A	395	C	C2-N1-C1'	5.11	124.42	118.80
32	SA	927	C	N3-C2-O2	-5.10	118.33	121.90
7	5A	109	C	N1-C2-O2	5.10	121.96	118.90
32	SA	158	U	P-O3'-C3'	5.10	125.82	119.70
32	SA	285	G	N3-C4-C5	-5.09	126.05	128.60
1	3A	322	A	O5'-P-OP1	-5.09	101.12	105.70
32	SA	1067	C	C5-C6-N1	5.08	123.54	121.00
32	SA	1527	C	C2-N1-C1'	5.07	124.38	118.80
32	SA	1072	C	C5-C6-N1	5.07	123.53	121.00
32	SA	287	G	O4'-C1'-N9	5.07	112.25	108.20
32	SA	527	A	C4-N9-C1'	5.07	135.42	126.30
32	SA	591	A	C5-C6-N1	5.07	120.23	117.70
7	5A	251	C	C5-C6-N1	5.05	123.53	121.00
32	SA	1488	G	C8-N9-C4	-5.05	104.38	106.40
32	SA	1617	U	N1-C2-O2	5.05	126.33	122.80
7	5A	501	C	N1-C2-O2	5.04	121.92	118.90
15	B1	104	LEU	CA-CB-CG	5.04	126.89	115.30
32	SA	574	G	N3-C4-C5	-5.04	126.08	128.60
18	BC	18	GLY	C-N-CA	5.03	134.28	121.70
7	5A	409	C	C6-N1-C2	-5.03	118.29	120.30
7	5A	205	C	C6-N1-C2	-5.03	118.29	120.30
32	SA	1051	G	C4-N9-C1'	-5.03	119.97	126.50
7	5A	441	C	N1-C2-O2	5.02	121.91	118.90
7	5A	418	C	C5-C6-N1	5.02	123.51	121.00
32	SA	13	C	C6-N1-C2	-5.01	118.30	120.30
32	SA	1640	C	N3-C2-O2	-5.01	118.39	121.90
33	SC	96	LEU	CA-CB-CG	5.01	126.82	115.30
7	5A	205	C	C2-N1-C1'	5.00	124.30	118.80

There are no chirality outliers.

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	3B	102	LYS	Peptide
3	3D	393	SER	Peptide
3	3D	46	LYS	Peptide
5	3F	437	ARG	Peptide
12	AE	64	PRO	Peptide
15	B1	190	ILE	Peptide
15	B1	233	HIS	Peptide
15	B1	73	THR	Peptide

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Mol	Chain	Res	Type	Group
16	BA	12	GLY	Peptide
16	BA	415	ASP	Peptide
16	BA	515	TYR	Peptide
16	BA	608	ASN	Peptide
16	BA	702	LEU	Peptide
17	BB	169	PHE	Peptide
17	BB	235	ASN	Peptide
17	BB	390	GLN	Peptide
17	BB	795	ILE	Peptide
17	BB	796	ALA	Peptide
17	BB	797	VAL	Peptide
17	BB	864	ASN	Peptide
18	BC	200	GLU	Peptide
18	BC	326	THR	Peptide
18	BC	365	ILE	Peptide
18	BC	771	LYS	Peptide
18	BC	772	LEU	Peptide
18	BC	90	LEU	Peptide
19	BD	304	LEU	Peptide
20	BE	660	PHE	Peptide
20	BE	665	THR	Peptide
20	BE	667	THR	Peptide
20	BE	900	ASN	Peptide
20	BE	94	TYR	Peptide
21	CA	199	GLN	Peptide
29	P1	227	ALA	Peptide
32	SA	493	U	Sidechain
33	SC	179	SER	Peptide
33	SC	206	PRO	Peptide
33	SC	208	GLN	Peptide
33	SC	54	LEU	Peptide
34	SF	194	THR	Peptide
35	SG	125	THR	Peptide
35	SG	127	GLN	Peptide
35	SG	128	ASN	Peptide
35	SG	48	PHE	Peptide
35	SG	49	GLU	Peptide
35	SG	50	GLU	Peptide
35	SG	64	VAL	Peptide
35	SG	65	ARG	Peptide
36	SI	131	PHE	Peptide
36	SI	156	SER	Peptide

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Mol	Chain	Res	Type	Group
36	SI	64	VAL	Peptide
36	SI	65	PRO	Peptide
37	SJ	103	GLN	Peptide
38	SK	117	GLY	Peptide
38	SK	163	PRO	Peptide
39	SM	4	GLU	Peptide
42	SR	40	GLU	Peptide
44	SY	137	LYS	Peptide
44	SY	96	VAL	Peptide
45	SZ	36	SER	Peptide
46	Sc	77	THR	Peptide
46	Sc	8	LEU	Peptide
52	U5	62	TYR	Peptide
55	UC	233	UNK	Peptide,Mainchain

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	3A	3327	0	1687	51	0
2	3B	1866	0	1904	25	0
2	3C	1866	0	1904	20	0
3	3D	2915	0	2930	36	0
4	3E	2935	0	3033	44	0
5	3F	2916	0	2947	59	0
6	3G	924	0	975	14	0
6	3H	924	0	975	9	0
7	5A	9867	0	4954	86	0
8	AA	2845	0	688	14	0
9	AB	2015	0	470	28	0
10	AC	2360	0	542	38	0
11	AD	505	0	116	5	0
12	AE	3331	0	3466	48	0
13	AF	1880	0	442	18	0
14	AG	3060	0	735	50	0
15	B1	4325	0	4434	78	0
16	BA	6026	0	5940	115	0
17	BB	6138	0	6163	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	BC	6117	0	6141	102	0
19	BD	2539	0	2520	82	0
20	BE	5936	0	5882	119	0
21	CA	1582	0	1528	40	0
22	CB	8870	0	8975	168	0
23	E1	1689	0	1738	22	0
23	E2	1695	0	1757	38	0
24	E4	1425	0	329	8	0
25	K1	1410	0	1503	22	0
26	MA	1097	0	1130	10	0
27	MB	1465	0	1486	35	0
28	MC	307	0	231	4	0
29	P1	1368	0	1436	17	0
30	R1	2742	0	2829	59	0
31	S1	1425	0	335	7	0
32	SA	21307	0	10756	251	0
33	SC	1709	0	1784	36	0
34	SF	1881	0	1958	48	0
35	SG	1609	0	1675	41	0
36	SI	1322	0	1394	28	0
37	SJ	1350	0	1374	31	0
38	SK	1412	0	1486	12	0
39	SM	1143	0	1210	26	0
40	SO	1087	0	1152	13	0
41	SP	771	0	751	14	0
42	SR	973	0	1029	21	0
43	SX	1021	0	1060	16	0
44	SY	785	0	840	20	0
45	SZ	801	0	828	17	0
46	Sc	595	0	613	0	0
47	Sd	497	0	535	0	0
48	Sf	251	0	277	0	0
49	U1	1425	0	351	6	0
50	U2	365	0	75	3	0
51	U4	990	0	1054	8	0
52	U5	2009	0	2130	31	0
53	UA	1690	0	373	10	0
54	UB	2775	0	625	6	0
55	UC	3300	0	731	21	0
All	All	150760	0	116186	2077	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 8.

All (2077) 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)
7:5A:408:U:H3	7:5A:448:G:H1	1.03	1.01
32:SA:126:A:H62	32:SA:291:G:N2	1.61	0.99
32:SA:126:A:N6	32:SA:291:G:H21	1.61	0.98
34:SF:75:LYS:NZ	34:SF:77:ARG:HH12	1.62	0.98
7:5A:513:G:H1	7:5A:523:U:H3	1.03	0.97
20:BE:796:LEU:O	20:BE:800:GLU:HB2	1.66	0.96
16:BA:538:GLN:HA	16:BA:552:ASN:O	1.63	0.96
20:BE:273:LEU:O	20:BE:286:VAL:HA	1.66	0.95
17:BB:828:TYR:O	17:BB:832:PHE:HB2	1.68	0.94
7:5A:511:G:H1	7:5A:525:U:H3	1.16	0.94
5:3F:146:LYS:O	5:3F:566:ALA:HA	1.67	0.93
16:BA:317:LEU:HB2	16:BA:332:TRP:O	1.71	0.90
1:3A:251:G:N7	5:3F:545:LYS:NZ	2.19	0.90
5:3F:497:LYS:NZ	5:3F:513:GLU:OE2	2.06	0.89
19:BD:311:ASN:HA	19:BD:324:TRP:O	1.72	0.88
22:CB:679:SER:O	22:CB:683:ASN:HB2	1.73	0.87
32:SA:126:A:H62	32:SA:291:G:H21	0.89	0.87
34:SF:75:LYS:HZ2	34:SF:77:ARG:HH12	1.20	0.87
20:BE:227:THR:OG1	20:BE:245:LYS:NZ	2.08	0.87
15:B1:143:MET:O	44:SY:144:ARG:NH1	2.07	0.87
20:BE:325:ASP:OD2	20:BE:341:ARG:NE	2.07	0.86
32:SA:1608:U:OP2	42:SR:14:LYS:NZ	2.08	0.86
5:3F:301:ASP:O	5:3F:303:LYS:NZ	2.10	0.85
35:SG:52:GLU:HA	35:SG:65:ARG:HH12	1.41	0.84
30:R1:131:GLU:OE2	30:R1:156:ARG:NH2	2.10	0.84
19:BD:431:GLU:OE2	20:BE:587:ARG:NH1	2.11	0.84
37:SJ:110:ARG:NH1	37:SJ:160:PHE:O	2.10	0.84
32:SA:1175:U:H3	32:SA:1464:G:H1	0.84	0.83
22:CB:707:PHE:O	22:CB:918:ARG:NH1	2.11	0.83
25:K1:138:PHE:O	25:K1:142:ARG:HB2	1.77	0.83
23:E2:164:LYS:NZ	32:SA:1575:G:OP1	2.10	0.83
20:BE:127:TYR:OH	20:BE:141:LYS:NZ	2.11	0.83
1:3A:5:A:H2	32:SA:1119:G:H1	1.25	0.83
5:3F:421:ASN:HA	5:3F:436:GLU:O	1.79	0.83
16:BA:21:THR:O	16:BA:30:LEU:HB2	1.78	0.83
15:B1:634:ARG:NH1	30:R1:186:PRO:O	2.12	0.82
21:CA:68:LYS:NZ	21:CA:84:VAL:O	2.12	0.82
27:MB:215:LYS:NZ	32:SA:1624:C:O3'	2.12	0.82
32:SA:868:G:OP1	40:SO:121:ARG:NH1	2.13	0.82
8:AA:515:UNK:O	8:AA:526:UNK:HA	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BE:272:ASP:HA	20:BE:287:LEU:O	1.79	0.82
32:SA:322:G:O2'	37:SJ:10:LYS:NZ	2.11	0.82
22:CB:100:SER:O	22:CB:104:LYS:HB2	1.79	0.81
22:CB:794:ASP:OD2	22:CB:865:ARG:NH1	2.13	0.81
6:3G:57:ASP:O	6:3G:84:ARG:NH1	2.14	0.81
17:BB:554:THR:HA	17:BB:569:LEU:O	1.80	0.81
30:R1:85:ALA:HA	30:R1:115:SER:O	1.81	0.81
20:BE:439:PHE:HA	20:BE:455:PHE:O	1.81	0.81
30:R1:114:PHE:O	30:R1:169:VAL:HA	1.81	0.81
22:CB:152:PHE:O	22:CB:156:LYS:NZ	2.14	0.81
15:B1:283:LEU:O	15:B1:788:TYR:HB3	1.79	0.80
32:SA:523:G:N2	32:SA:529:A:OP2	2.14	0.80
32:SA:1085:G:N2	32:SA:1088:A:OP2	2.15	0.80
18:BC:548:LEU:O	18:BC:559:ILE:HA	1.82	0.80
22:CB:840:LEU:O	22:CB:851:LYS:HA	1.81	0.80
23:E2:151:ARG:NH2	32:SA:1572:G:OP2	2.14	0.80
22:CB:470:LYS:O	22:CB:473:LYS:NZ	2.15	0.79
27:MB:236:HIS:HA	27:MB:248:ALA:O	1.81	0.79
20:BE:528:PHE:HB2	20:BE:538:GLY:O	1.82	0.79
32:SA:333:A:OP2	37:SJ:31:ARG:NH2	2.14	0.79
14:AG:341:UNK:HA	14:AG:356:UNK:O	1.83	0.79
9:AB:150:UNK:HA	9:AB:159:UNK:O	1.82	0.79
30:R1:196:TYR:HA	30:R1:228:ASP:O	1.83	0.79
32:SA:522:U:OP1	45:SZ:37:LYS:NZ	2.16	0.79
37:SJ:70:GLU:OE1	39:SM:24:LYS:NZ	2.16	0.79
32:SA:349:U:OP2	39:SM:106:ASN:ND2	2.16	0.78
3:3D:323:THR:HG22	3:3D:327:LYS:HZ2	1.48	0.78
22:CB:643:ALA:O	22:CB:647:ASN:HB2	1.84	0.78
22:CB:1147:TYR:O	22:CB:1151:LYS:HB2	1.84	0.78
45:SZ:29:HIS:HB3	45:SZ:32:ARG:HH11	1.48	0.78
16:BA:739:LEU:O	16:BA:743:PHE:HB2	1.84	0.78
32:SA:1645:G:H1	32:SA:1756:A:N6	1.82	0.77
15:B1:279:GLN:O	15:B1:792:VAL:HB	1.84	0.77
35:SG:76:ARG:NH1	42:SR:120:ASP:OD1	2.18	0.77
30:R1:310:ARG:HA	30:R1:352:ALA:O	1.85	0.77
17:BB:555:VAL:O	17:BB:568:SER:HA	1.84	0.76
43:SX:113:HIS:NE2	43:SX:114:GLU:OE2	2.18	0.76
27:MB:197:ALA:O	27:MB:200:LYS:NZ	2.17	0.76
19:BD:382:GLY:N	19:BD:405:THR:HG1	1.84	0.76
27:MB:225:ALA:O	27:MB:231:ILE:HA	1.85	0.76
23:E1:178:VAL:HA	23:E1:223:GLU:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:SY:96:VAL:O	44:SY:142:LYS:NZ	2.19	0.76
1:3A:246:A:OP2	5:3F:207:ARG:NH2	2.19	0.75
15:B1:247:LYS:HA	15:B1:793:PHE:O	1.85	0.75
19:BD:522:GLN:HB3	19:BD:531:CYS:HB3	1.68	0.75
23:E2:88:ARG:NH1	32:SA:1191:U:OP1	2.19	0.75
18:BC:662:GLN:O	18:BC:666:GLU:HB2	1.87	0.75
20:BE:142:LYS:NZ	20:BE:147:ASP:O	2.20	0.74
8:AA:483:UNK:O	8:AA:495:UNK:HA	1.86	0.74
17:BB:126:LEU:O	17:BB:138:SER:HA	1.86	0.74
22:CB:150:ASP:O	22:CB:154:LYS:HB2	1.87	0.74
35:SG:156:ARG:HH12	35:SG:224:ASN:HB3	1.52	0.74
5:3F:367:LYS:O	5:3F:370:ARG:HB2	1.88	0.74
17:BB:406:LEU:HB2	17:BB:417:TRP:HB2	1.70	0.74
25:K1:157:GLU:OE2	25:K1:164:ILE:N	2.21	0.73
21:CA:134:ILE:O	21:CA:138:TRP:HB2	1.88	0.73
25:K1:61:THR:O	25:K1:65:ASP:HB2	1.89	0.73
8:AA:514:UNK:HA	8:AA:527:UNK:O	1.88	0.73
20:BE:64:ASN:O	20:BE:344:ARG:NH1	2.21	0.73
21:CA:88:LEU:HB2	21:CA:125:LEU:O	1.88	0.73
15:B1:876:PRO:HG2	15:B1:879:THR:H	1.53	0.73
20:BE:230:VAL:O	20:BE:243:THR:HA	1.88	0.73
32:SA:176:C:N4	32:SA:266:A:OP2	2.21	0.73
1:3A:80:U:OP2	6:3H:95:ARG:NH1	2.16	0.73
14:AG:486:UNK:HA	14:AG:496:UNK:O	1.89	0.72
19:BD:325:ASP:H	19:BD:337:ALA:HA	1.53	0.72
32:SA:1663:G:H1	32:SA:1738:U:H3	0.80	0.72
3:3D:291:TYR:OH	4:3E:251:ASP:OD1	2.02	0.72
32:SA:1084:A:H61	32:SA:1089:U:H3	1.35	0.72
17:BB:801:PRO:O	17:BB:804:TYR:HB3	1.89	0.72
37:SJ:105:ASP:OD2	37:SJ:107:THR:OG1	2.06	0.72
39:SM:72:THR:O	39:SM:88:ARG:NH1	2.22	0.71
15:B1:922:ILE:O	30:R1:111:LYS:NZ	2.22	0.71
15:B1:49:PHE:HB3	15:B1:94:LEU:HG	1.73	0.71
33:SC:27:LYS:NZ	33:SC:49:ASN:OD1	2.22	0.71
22:CB:823:SER:HA	22:CB:841:ASN:O	1.90	0.71
7:5A:69:U:OP2	7:5A:71:U:O2'	2.08	0.70
32:SA:896:U:O2'	41:SP:41:ARG:NH1	2.24	0.70
44:SY:95:PHE:O	44:SY:142:LYS:NZ	2.24	0.70
35:SG:222:LYS:HG3	35:SG:225:ARG:HH12	1.56	0.70
20:BE:360:ASP:OD2	20:BE:364:HIS:N	2.22	0.70
34:SF:50:ASN:O	34:SF:53:LYS:NZ	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:AE:365:ILE:O	12:AE:369:LEU:HB3	1.91	0.70
5:3F:540:LEU:HA	5:3F:564:TYR:O	1.93	0.69
17:BB:875:GLU:O	17:BB:879:GLN:HB2	1.92	0.69
39:SM:97:TYR:HB3	39:SM:99:ARG:HH11	1.55	0.69
1:3A:80:U:O2	6:3H:95:ARG:NH1	2.24	0.69
32:SA:1085:G:N2	32:SA:1088:A:N7	2.39	0.69
16:BA:516:SER:HB3	16:BA:535:LEU:H	1.58	0.69
23:E2:31:LEU:HD22	23:E2:40:ARG:HH21	1.58	0.69
32:SA:15:U:O2'	51:U4:163:ARG:NH2	2.25	0.69
33:SC:158:SER:O	33:SC:162:ARG:NH1	2.25	0.69
20:BE:97:LYS:NZ	20:BE:111:GLU:OE1	2.26	0.69
23:E1:179:THR:HB	23:E1:224:LYS:HG2	1.74	0.69
32:SA:966:A:OP2	40:SO:124:ARG:NH2	2.26	0.69
17:BB:261:PHE:O	17:BB:272:PHE:HA	1.93	0.68
22:CB:99:LYS:O	22:CB:103:PHE:HB3	1.92	0.68
27:MB:124:MET:HG2	27:MB:126:ASN:H	1.58	0.68
2:3C:319:ARG:HD2	2:3C:322:ARG:HD3	1.75	0.68
22:CB:654:SER:O	22:CB:665:HIS:HA	1.92	0.68
25:K1:137:ARG:HG3	25:K1:140:LYS:HD2	1.75	0.68
7:5A:122:U:O2'	7:5A:125:G:OP2	2.09	0.68
27:MB:119:ARG:NH1	27:MB:124:MET:SD	2.67	0.68
35:SG:209:TYR:OH	35:SG:213:LYS:NZ	2.24	0.68
17:BB:391:ARG:HG3	17:BB:392:THR:HG23	1.75	0.68
20:BE:142:LYS:HD3	20:BE:147:ASP:HB2	1.76	0.68
20:BE:275:PHE:HB2	20:BE:285:HIS:HB3	1.76	0.68
17:BB:488:LEU:HB2	17:BB:500:TRP:HB2	1.74	0.68
19:BD:252:GLN:HE22	19:BD:295:ILE:HG23	1.58	0.68
2:3C:299:LYS:HD2	2:3C:322:ARG:HB3	1.74	0.67
12:AE:367:LEU:O	12:AE:371:LYS:HB2	1.93	0.67
32:SA:1645:G:N1	32:SA:1756:A:N6	2.43	0.67
1:3A:3:C:H2'	1:3A:4:G:H8	1.59	0.67
6:3G:34:LYS:HB2	6:3G:101:SER:HB3	1.75	0.67
14:AG:423:UNK:HA	14:AG:438:UNK:O	1.94	0.67
33:SC:175:GLU:OE2	33:SC:187:LYS:NZ	2.19	0.67
7:5A:209:G:N2	7:5A:209:G:OP2	2.27	0.67
16:BA:533:SER:HB3	16:BA:580:PHE:HB2	1.74	0.67
23:E2:158:LYS:HE2	23:E2:161:LYS:NZ	2.09	0.67
32:SA:205:U:OP1	34:SF:134:LYS:NZ	2.28	0.67
29:P1:188:LYS:HA	29:P1:191:LYS:HZ3	1.60	0.67
32:SA:950:C:O2'	40:SO:104:ARG:NH1	2.27	0.67
32:SA:1484:G:H22	32:SA:1591:C:H1'	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:577:ARG:NH1	22:CB:624:CYS:O	2.27	0.66
20:BE:481:ASN:O	20:BE:499:LYS:NZ	2.28	0.66
5:3F:299:CYS:SG	5:3F:305:ARG:NH1	2.68	0.66
8:AA:484:UNK:HA	8:AA:494:UNK:O	1.94	0.66
3:3D:187:ASP:OD2	4:3E:180:TYR:OH	2.07	0.66
26:MA:33:MET:HA	26:MA:38:ILE:HD12	1.77	0.66
16:BA:547:ALA:O	16:BA:549:GLN:NE2	2.28	0.66
17:BB:748:ALA:HA	17:BB:751:ARG:HE	1.60	0.66
27:MB:231:ILE:O	27:MB:255:GLU:HA	1.96	0.66
32:SA:396:G:N1	32:SA:399:A:OP2	2.29	0.66
34:SF:75:LYS:HZ2	34:SF:77:ARG:NH1	1.92	0.66
15:B1:49:PHE:HB2	15:B1:92:ARG:HH11	1.59	0.65
16:BA:508:GLN:O	42:SR:127:LYS:NZ	2.29	0.65
35:SG:29:ILE:HB	35:SG:34:GLN:HE21	1.61	0.65
15:B1:988:ARG:HH12	27:MB:146:ARG:NH1	1.95	0.65
16:BA:488:LEU:HB3	16:BA:500:TRP:HB2	1.78	0.65
19:BD:421:THR:HA	19:BD:435:PHE:O	1.95	0.65
22:CB:921:ASP:OD2	22:CB:1172:ASN:ND2	2.27	0.65
31:S1:114:UNK:HA	31:S1:129:UNK:O	1.95	0.65
4:3E:323:GLU:OE1	4:3E:324:LYS:NZ	2.30	0.65
15:B1:988:ARG:HH12	27:MB:146:ARG:HH11	1.44	0.65
16:BA:103:LYS:O	16:BA:112:ALA:HB3	1.96	0.65
22:CB:207:LEU:HB2	22:CB:295:LEU:O	1.96	0.65
22:CB:897:ARG:O	22:CB:901:ASN:HB2	1.97	0.65
1:3A:64:A:H5'	20:BE:392:ARG:NH1	2.12	0.65
33:SC:171:ILE:HA	33:SC:174:LYS:HZ2	1.61	0.65
1:3A:5:A:N1	32:SA:1119:G:O6	2.30	0.65
25:K1:49:ARG:NH2	25:K1:108:VAL:O	2.29	0.65
35:SG:222:LYS:HG3	35:SG:225:ARG:NH1	2.11	0.65
12:AE:260:ILE:O	12:AE:264:PHE:HB2	1.97	0.64
18:BC:47:PRO:HD2	18:BC:51:LYS:H	1.61	0.64
27:MB:105:LYS:HD2	27:MB:177:ILE:HB	1.79	0.64
16:BA:89:VAL:HG12	16:BA:90:LEU:HG	1.79	0.64
20:BE:632:VAL:HG12	20:BE:643:THR:HG22	1.79	0.64
41:SP:47:LYS:HZ2	41:SP:63:ALA:HA	1.63	0.64
12:AE:54:LYS:O	12:AE:58:GLU:HB3	1.97	0.64
17:BB:799:LYS:HD2	17:BB:800:THR:HG23	1.78	0.64
21:CA:18:PHE:O	21:CA:34:LEU:HA	1.96	0.64
30:R1:347:ASN:ND2	30:R1:349:ASP:OD2	2.30	0.64
34:SF:39:ARG:NH1	34:SF:40:GLU:OE2	2.31	0.64
16:BA:620:ASN:OD1	16:BA:680:ARG:NH2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:349:GLU:O	19:BD:352:GLN:NE2	2.31	0.64
27:MB:240:ARG:HA	27:MB:244:GLY:O	1.96	0.64
3:3D:96:ILE:O	3:3D:117:ASP:HB3	1.98	0.64
22:CB:879:GLU:O	22:CB:883:LEU:HB2	1.98	0.64
32:SA:1685:G:N2	32:SA:1716:C:N3	2.46	0.64
27:MB:261:LEU:O	32:SA:571:G:N2	2.30	0.63
3:3D:157:ALA:O	3:3D:161:ALA:HB2	1.97	0.63
5:3F:551:ARG:HH11	6:3G:94:SER:HA	1.61	0.63
23:E2:178:VAL:HG12	23:E2:223:GLU:HB3	1.81	0.63
7:5A:234:A:N6	7:5A:237:A:N1	2.45	0.63
23:E2:31:LEU:HD13	23:E2:40:ARG:HE	1.64	0.63
17:BB:136:LEU:HB3	17:BB:148:TRP:HB2	1.80	0.63
18:BC:33:ALA:H	18:BC:69:LEU:HD21	1.64	0.63
45:SZ:37:LYS:HE3	45:SZ:93:ARG:HD3	1.79	0.63
32:SA:523:G:H1'	32:SA:530:C:H42	1.63	0.63
3:3D:323:THR:HG22	3:3D:327:LYS:NZ	2.14	0.63
14:AG:485:UNK:O	14:AG:497:UNK:HA	1.99	0.63
17:BB:597:ILE:O	17:BB:611:LEU:HB2	1.99	0.63
5:3F:371:ARG:HH21	5:3F:374:LYS:NZ	1.97	0.63
34:SF:133:LYS:HG3	34:SF:134:LYS:HG3	1.80	0.63
10:AC:272:UNK:O	10:AC:283:UNK:HA	1.99	0.62
17:BB:499:PHE:HB2	17:BB:518:PRO:HG2	1.81	0.62
20:BE:292:ARG:HH22	20:BE:351:GLN:HG3	1.64	0.62
32:SA:348:U:H5"	39:SM:106:ASN:HB2	1.79	0.62
52:U5:47:GLY:HA2	52:U5:52:ASN:HD22	1.64	0.62
7:5A:26:C:N4	7:5A:54:A:OP2	2.32	0.62
26:MA:61:LEU:HD13	28:MC:437:ILE:HG21	1.80	0.62
40:SO:20:ARG:HH21	43:SX:56:HIS:HB3	1.63	0.62
2:3C:125:VAL:O	2:3C:138:LYS:HA	2.00	0.62
19:BD:482:LEU:HB2	19:BD:494:TYR:O	2.00	0.62
22:CB:268:LEU:HD23	22:CB:294:LEU:HD12	1.82	0.62
23:E1:176:ARG:NH1	23:E1:200:GLU:OE2	2.33	0.62
27:MB:193:ASN:HB3	27:MB:226:ASN:HB2	1.81	0.62
33:SC:32:ILE:HD11	33:SC:46:THR:HG23	1.82	0.62
25:K1:178:LYS:NZ	32:SA:904:G:H5"	2.15	0.62
4:3E:191:HIS:O	4:3E:215:ARG:NH2	2.33	0.61
22:CB:1107:GLY:HA2	22:CB:1178:ASP:HB3	1.82	0.61
19:BD:344:ARG:HH21	19:BD:392:GLY:HA3	1.65	0.61
19:BD:429:TYR:HB3	19:BD:431:GLU:HG2	1.81	0.61
20:BE:179:LYS:HA	20:BE:191:PHE:O	1.99	0.61
35:SG:131:GLN:NE2	35:SG:135:ASP:OD2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BE:390:SER:HB3	20:BE:449:ARG:HA	1.82	0.61
23:E1:50:LEU:HB3	23:E1:145:LEU:HD11	1.83	0.61
25:K1:130:ASN:ND2	32:SA:930:A:OP1	2.30	0.61
32:SA:513:U:H3'	38:SK:171:ARG:HH22	1.64	0.61
4:3E:371:LEU:O	4:3E:375:ALA:HB2	2.01	0.61
20:BE:291:HIS:HD2	20:BE:298:VAL:HG22	1.65	0.61
20:BE:847:LEU:HD12	20:BE:887:LEU:HD11	1.82	0.61
15:B1:634:ARG:NH1	30:R1:185:ARG:HG2	2.15	0.61
16:BA:554:ASP:O	16:BA:556:ARG:NH1	2.33	0.61
17:BB:230:LYS:HD3	17:BB:237:LYS:HB3	1.83	0.61
19:BD:570:PHE:HB3	19:BD:574:GLY:HA2	1.83	0.61
23:E2:73:HIS:HD2	23:E2:76:LEU:HD22	1.65	0.61
30:R1:129:GLY:N	30:R1:259:GLU:OE2	2.34	0.61
17:BB:45:ALA:HB2	17:BB:85:LEU:HB2	1.83	0.61
21:CA:62:SER:O	21:CA:90:ASN:ND2	2.34	0.61
22:CB:317:ILE:HG12	22:CB:549:SER:HB3	1.82	0.61
23:E2:150:ILE:O	23:E2:159:LEU:HB2	2.00	0.61
15:B1:268:HIS:ND1	15:B1:274:ASP:OD1	2.32	0.61
16:BA:147:GLN:HG3	16:BA:166:LYS:HB3	1.82	0.61
18:BC:548:LEU:HB3	18:BC:560:TRP:HB2	1.82	0.61
33:SC:117:TRP:HE3	33:SC:153:HIS:HB3	1.65	0.61
34:SF:18:TRP:O	34:SF:51:ARG:NH1	2.34	0.61
32:SA:562:G:H1	44:SY:64:PRO:HB2	1.66	0.61
19:BD:545:HIS:HB3	19:BD:550:SER:HB2	1.83	0.61
35:SG:42:LEU:HD21	35:SG:45:LYS:NZ	2.15	0.61
38:SK:17:ARG:O	38:SK:23:ARG:NH2	2.34	0.61
19:BD:484:VAL:O	19:BD:491:VAL:HA	2.01	0.60
3:3D:30:ARG:NH2	31:S1:204:UNK:O	2.33	0.60
52:U5:243:PHE:HB3	52:U5:251:SER:HB2	1.83	0.60
12:AE:353:ARG:HH12	12:AE:382:LEU:HB2	1.64	0.60
41:SP:30:VAL:HG13	41:SP:39:ILE:HG23	1.83	0.60
16:BA:842:ASN:ND2	20:BE:882:GLU:OE1	2.34	0.60
35:SG:51:VAL:HG21	35:SG:131:GLN:HB2	1.82	0.60
4:3E:95:ALA:O	4:3E:99:ASN:HB2	2.01	0.60
14:AG:402:UNK:HA	14:AG:416:UNK:O	2.01	0.60
18:BC:588:LYS:HG2	18:BC:589:GLN:HE21	1.64	0.60
25:K1:42:MET:SD	33:SC:112:SER:OG	2.59	0.60
18:BC:353:LEU:HD12	18:BC:366:PRO:HG2	1.82	0.60
30:R1:11:PHE:HB2	30:R1:33:ILE:HG12	1.84	0.60
41:SP:85:ALA:H	41:SP:119:THR:HG22	1.66	0.60
44:SY:102:VAL:HG12	44:SY:127:VAL:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3D:180:LEU:HD13	4:3E:183:ARG:HG2	1.83	0.60
17:BB:757:ASP:O	17:BB:761:ALA:HB2	2.01	0.60
25:K1:198:TYR:O	25:K1:202:GLU:HB2	2.01	0.60
32:SA:1585:U:H3	32:SA:1611:A:H2	1.48	0.60
5:3F:198:LYS:NZ	5:3F:265:THR:O	2.34	0.60
17:BB:884:LYS:HZ3	18:BC:806:LEU:HB3	1.67	0.60
34:SF:45:ILE:HG13	34:SF:61:VAL:HG21	1.84	0.60
38:SK:54:ARG:HG3	38:SK:57:ARG:HH21	1.66	0.60
7:5A:494:C:OP1	7:5A:497:A:N6	2.35	0.60
12:AE:304:GLN:NE2	12:AE:343:VAL:O	2.32	0.59
18:BC:68:LYS:HG3	18:BC:110:ALA:HA	1.83	0.59
22:CB:891:ALA:O	22:CB:895:HIS:HB2	2.01	0.59
32:SA:929:A:H4'	32:SA:930:A:OP2	1.99	0.59
43:SX:28:ARG:HD3	43:SX:60:LYS:HE2	1.84	0.59
52:U5:116:THR:O	52:U5:120:LYS:NZ	2.32	0.59
4:3E:225:GLU:HG3	4:3E:226:ILE:HG13	1.82	0.59
17:BB:454:LEU:O	17:BB:468:ILE:HB	2.02	0.59
27:MB:112:PRO:HD2	27:MB:212:ALA:HB1	1.84	0.59
30:R1:289:VAL:O	30:R1:317:GLN:NE2	2.35	0.59
35:SG:156:ARG:NH1	35:SG:157:ARG:O	2.35	0.59
41:SP:87:GLY:HA3	41:SP:120:PRO:HG2	1.83	0.59
7:5A:438:U:H2'	7:5A:439:A:H8	1.68	0.59
12:AE:383:ILE:O	12:AE:387:LEU:HB2	2.03	0.59
19:BD:485:GLY:HA3	19:BD:521:LEU:HD21	1.83	0.59
21:CA:103:LEU:O	22:CB:869:ASN:ND2	2.35	0.59
22:CB:228:ARG:NH1	22:CB:266:PRO:O	2.34	0.59
20:BE:135:ASN:HB3	20:BE:159:VAL:HB	1.83	0.59
19:BD:401:GLU:HB3	20:BE:628:VAL:HG21	1.85	0.59
19:BD:462:GLY:HA2	19:BD:480:ARG:H	1.67	0.59
20:BE:28:ARG:NH2	20:BE:380:LEU:O	2.35	0.59
37:SJ:120:THR:HB	37:SJ:123:LYS:NZ	2.18	0.59
1:3A:5:A:C2	32:SA:1119:G:N1	2.62	0.59
5:3F:150:THR:O	5:3F:562:GLY:HA3	2.02	0.59
25:K1:141:ARG:HG2	25:K1:144:ARG:NH1	2.17	0.59
12:AE:274:ILE:O	12:AE:278:ALA:HB2	2.03	0.59
15:B1:253:TYR:HA	15:B1:787:SER:O	2.03	0.59
16:BA:351:LEU:HB3	16:BA:685:GLN:HE22	1.66	0.59
19:BD:427:ASN:HB3	19:BD:455:ILE:HD12	1.84	0.59
35:SG:80:LYS:NZ	35:SG:83:ARG:NH1	2.50	0.59
14:AG:179:UNK:HA	14:AG:195:UNK:HA	1.83	0.59
19:BD:242:ASN:ND2	19:BD:282:ASN:OD1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:292:GLY:O	19:BD:318:ARG:NH1	2.36	0.59
19:BD:483:ALA:HA	19:BD:492:ASN:O	2.02	0.59
19:BD:491:VAL:HG13	19:BD:511:LEU:HB2	1.85	0.59
25:K1:71:CYS:HA	25:K1:81:THR:O	2.02	0.59
32:SA:481:A:H2	32:SA:507:U:H3	1.49	0.59
3:3D:36:GLU:OE1	3:3D:37:GLN:NE2	2.36	0.59
7:5A:357:G:O6	7:5A:368:U:C2	2.55	0.59
14:AG:266:UNK:HA	14:AG:273:UNK:HA	1.85	0.59
32:SA:163:G:OP2	32:SA:163:G:N2	2.28	0.59
32:SA:1485:C:H3'	32:SA:1486:G:H21	1.68	0.59
29:P1:96:SER:HA	29:P1:139:LEU:O	2.02	0.58
36:SI:62:VAL:HG12	36:SI:64:VAL:H	1.67	0.58
52:U5:64:LEU:HB3	52:U5:68:ARG:HD2	1.85	0.58
22:CB:975:LEU:HD23	22:CB:1041:VAL:HG22	1.86	0.58
25:K1:197:ILE:HG12	25:K1:201:LYS:HE3	1.84	0.58
37:SJ:57:ALA:HB2	37:SJ:177:GLY:HA2	1.83	0.58
45:SZ:29:HIS:HB3	45:SZ:32:ARG:NH1	2.18	0.58
14:AG:446:UNK:O	14:AG:454:UNK:N	2.36	0.58
16:BA:24:ASP:O	16:BA:312:GLN:NE2	2.36	0.58
22:CB:738:TYR:O	22:CB:742:PHE:HB3	2.04	0.58
32:SA:1648:A:H61	32:SA:1752:U:H3	1.52	0.58
44:SY:125:VAL:HG12	44:SY:126:LYS:HG3	1.84	0.58
5:3F:536:LYS:NZ	5:3F:569:ASP:OD1	2.31	0.58
22:CB:96:GLU:O	22:CB:100:SER:HB2	2.03	0.58
18:BC:543:GLN:HB2	18:BC:587:GLN:HE21	1.67	0.58
22:CB:529:VAL:HB	22:CB:613:VAL:O	2.02	0.58
22:CB:1138:ASP:O	22:CB:1141:GLU:HB2	2.03	0.58
28:MC:58:UNK:O	28:MC:62:UNK:CB	2.52	0.58
14:AG:161:UNK:O	14:AG:169:UNK:N	2.36	0.58
17:BB:903:GLN:HE22	17:BB:906:LYS:HD2	1.68	0.58
34:SF:180:LEU:HA	34:SF:194:THR:HG22	1.85	0.58
36:SI:30:SER:HB2	36:SI:34:LEU:HB2	1.85	0.58
44:SY:97:ASP:HB2	44:SY:100:ASP:OD2	2.04	0.58
5:3F:139:LYS:HB3	5:3F:570:GLN:HG2	1.86	0.58
17:BB:75:ARG:HD2	17:BB:78:LYS:HG2	1.85	0.58
20:BE:630:THR:N	20:BE:644:THR:O	2.37	0.58
22:CB:494:GLU:OE1	22:CB:497:ARG:NH2	2.37	0.58
2:3C:208:ILE:HD12	4:3E:156:ALA:HA	1.86	0.58
16:BA:553:ILE:HG23	16:BA:556:ARG:HH12	1.68	0.58
30:R1:330:LYS:O	30:R1:334:ASN:ND2	2.37	0.58
32:SA:960:U:H5"	40:SO:62:GLN:HE22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:SP:47:LYS:NZ	41:SP:63:ALA:HA	2.18	0.58
15:B1:966:ILE:N	15:B1:974:GLY:O	2.35	0.58
25:K1:92:ALA:HB2	41:SP:102:LEU:HD22	1.85	0.58
32:SA:918:U:O3'	41:SP:18:ARG:NH1	2.37	0.58
1:3A:80:U:H3	6:3H:95:ARG:HH22	1.52	0.58
5:3F:348:LEU:O	5:3F:356:ARG:HA	2.04	0.58
14:AG:423:UNK:HA	14:AG:439:UNK:HA	1.86	0.58
18:BC:722:GLU:O	18:BC:725:ASP:HB2	2.04	0.58
7:5A:357:G:O6	7:5A:368:U:O2	2.22	0.57
15:B1:621:LEU:O	15:B1:625:TRP:HB2	2.04	0.57
18:BC:339:ILE:HD11	18:BC:358:ASN:HB2	1.86	0.57
20:BE:190:LEU:HB3	20:BE:200:PHE:HB3	1.85	0.57
27:MB:92:THR:HG22	27:MB:142:LEU:HB2	1.85	0.57
3:3D:55:PRO:HB2	3:3D:57:LYS:HG3	1.85	0.57
22:CB:333:ASN:O	22:CB:337:LEU:HB3	2.03	0.57
22:CB:412:LEU:HD21	22:CB:424:GLY:HA3	1.85	0.57
22:CB:557:THR:H	22:CB:560:ASN:HD22	1.53	0.57
32:SA:389:G:H3'	32:SA:390:G:H21	1.69	0.57
52:U5:40:ILE:HG22	52:U5:242:ILE:HG12	1.86	0.57
5:3F:251:VAL:O	5:3F:263:TRP:HB2	2.04	0.57
12:AE:73:LEU:HD21	12:AE:121:LEU:HD11	1.85	0.57
15:B1:281:GLU:HB2	15:B1:790:ARG:O	2.05	0.57
22:CB:179:LYS:HB2	22:CB:210:PRO:HG2	1.86	0.57
16:BA:585:TYR:HA	16:BA:592:ILE:HG22	1.87	0.57
22:CB:383:GLY:HA3	22:CB:585:MET:HG2	1.86	0.57
22:CB:1059:PRO:O	22:CB:1063:ARG:HB2	2.04	0.57
1:3A:63:C:H2'	1:3A:64:A:H8	1.70	0.57
54:UB:170:UNK:HA	54:UB:196:UNK:HA	1.86	0.57
16:BA:817:PHE:O	16:BA:821:MET:CB	2.53	0.57
19:BD:433:TRP:HE1	19:BD:435:PHE:HB2	1.69	0.57
22:CB:235:LEU:O	22:CB:239:LEU:CB	2.52	0.57
25:K1:143:GLN:HA	25:K1:146:VAL:HG12	1.87	0.57
15:B1:944:ASN:ND2	32:SA:572:C:OP1	2.37	0.57
18:BC:13:ASN:N	18:BC:643:PHE:O	2.38	0.57
18:BC:231:CYS:SG	18:BC:232:LYS:N	2.78	0.57
18:BC:559:ILE:HD11	18:BC:590:LEU:HD22	1.85	0.57
18:BC:771:LYS:HB3	18:BC:775:ILE:HD12	1.87	0.57
20:BE:632:VAL:HA	20:BE:642:ALA:O	2.03	0.57
23:E2:158:LYS:HE2	23:E2:161:LYS:HZ2	1.69	0.57
37:SJ:61:GLU:HG3	37:SJ:62:THR:HG23	1.87	0.57
16:BA:202:ASP:OD1	16:BA:202:ASP:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:BE:843:ALA:HB1	20:BE:846:ASP:HB3	1.86	0.57
42:SR:102:LYS:NZ	42:SR:106:LYS:NZ	2.53	0.57
7:5A:414:G:H1	7:5A:440:U:H3	1.52	0.57
16:BA:166:LYS:NZ	16:BA:193:TYR:OH	2.33	0.57
17:BB:264:ASN:HD21	17:BB:341:ALA:HB3	1.69	0.57
36:SI:51:VAL:HG23	36:SI:53:GLY:H	1.70	0.57
44:SY:96:VAL:HA	44:SY:142:LYS:HZ1	1.70	0.57
1:3A:322:A:N6	55:UC:825:UNK:O	2.38	0.56
18:BC:805:ILE:HD12	20:BE:932:VAL:HG23	1.86	0.56
37:SJ:120:THR:HB	37:SJ:123:LYS:HZ2	1.70	0.56
16:BA:392:ALA:HB3	16:BA:405:SER:HB3	1.86	0.56
3:3D:92:LYS:HD3	3:3D:115:TYR:HA	1.87	0.56
14:AG:405:UNK:O	14:AG:413:UNK:N	2.38	0.56
17:BB:393:ASP:HA	17:BB:679:HIS:HB3	1.87	0.56
17:BB:536:CYS:H	17:BB:549:SER:HB2	1.71	0.56
19:BD:325:ASP:HB2	19:BD:337:ALA:H	1.71	0.56
29:P1:105:ARG:NH1	32:SA:1798:U:O2'	2.37	0.56
30:R1:312:ARG:HH21	30:R1:347:ASN:HD21	1.51	0.56
32:SA:1118:G:H2'	32:SA:1119:G:H8	1.70	0.56
15:B1:40:ARG:HH22	15:B1:213:PRO:HB3	1.70	0.56
4:3E:18:SER:HB2	4:3E:83:LYS:HZ3	1.69	0.56
15:B1:974:GLY:CA	15:B1:990:ALA:O	2.53	0.56
16:BA:284:PHE:O	16:BA:297:GLN:HA	2.05	0.56
19:BD:320:TYR:HB3	19:BD:343:SER:HB2	1.88	0.56
19:BD:446:ARG:HH11	20:BE:586:ASN:HB2	1.71	0.56
22:CB:334:PHE:O	22:CB:338:SER:HB3	2.05	0.56
29:P1:186:GLU:HG2	29:P1:188:LYS:H	1.69	0.56
41:SP:60:ALA:HB1	41:SP:101:ALA:HB2	1.88	0.56
7:5A:556:G:H2'	7:5A:557:A:H8	1.70	0.56
16:BA:431:ILE:HG23	16:BA:432:GLN:HG3	1.88	0.56
22:CB:85:SER:O	22:CB:89:HIS:HB2	2.06	0.56
23:E2:236:VAL:HG12	23:E2:240:LYS:NZ	2.21	0.56
37:SJ:172:ARG:HE	37:SJ:175:GLN:HG3	1.70	0.56
18:BC:362:LEU:HB2	18:BC:384:TYR:HB2	1.88	0.56
20:BE:354:SER:O	20:BE:631:ASN:ND2	2.39	0.56
22:CB:334:PHE:O	22:CB:338:SER:CB	2.54	0.56
23:E1:112:VAL:O	23:E1:124:VAL:HB	2.05	0.56
30:R1:249:SER:O	30:R1:253:GLY:HA2	2.06	0.56
32:SA:566:C:O2'	32:SA:576:G:N2	2.39	0.56
2:3B:142:ARG:NH2	2:3B:186:ASP:OD2	2.39	0.56
7:5A:178:G:O6	7:5A:219:U:O2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BA:556:ARG:CZ	20:BE:423:ARG:HH12	2.19	0.56
18:BC:84:LEU:HD22	18:BC:86:LYS:HD2	1.88	0.56
20:BE:132:THR:OG1	20:BE:134:ASP:OD1	2.11	0.56
22:CB:165:PRO:HD2	22:CB:222:PHE:HE2	1.70	0.56
23:E2:31:LEU:HB3	23:E2:111:GLN:HE21	1.70	0.56
37:SJ:54:LYS:HD2	37:SJ:56:ARG:HH12	1.71	0.56
14:AG:361:UNK:HA	14:AG:375:UNK:O	2.06	0.56
20:BE:176:TYR:HB3	20:BE:179:LYS:HB2	1.87	0.56
20:BE:346:ARG:NH2	20:BE:384:ALA:O	2.39	0.56
22:CB:93:GLU:O	22:CB:97:LEU:HB2	2.06	0.56
22:CB:828:ASP:OD2	22:CB:853:ARG:NH2	2.38	0.56
27:MB:185:VAL:HA	27:MB:215:LYS:HG3	1.87	0.56
30:R1:214:LYS:HD3	30:R1:273:GLU:OE2	2.06	0.56
1:3A:7:G:O6	32:SA:1117:U:O4	2.24	0.55
1:3A:106:C:O2	1:3A:262:G:N2	2.39	0.55
9:AB:199:UNK:O	9:AB:211:UNK:HA	2.07	0.55
15:B1:945:THR:OG1	32:SA:1595:U:OP1	2.23	0.55
16:BA:751:ILE:O	16:BA:755:TYR:HB3	2.05	0.55
32:SA:591:A:H2'	32:SA:592:A:C8	2.41	0.55
1:3A:1:G:C6	32:SA:1124:A:N1	2.74	0.55
2:3B:230:TYR:HB2	2:3B:233:LEU:HB2	1.88	0.55
15:B1:200:LEU:O	15:B1:204:ARG:HB2	2.06	0.55
16:BA:413:ALA:HB3	16:BA:422:PHE:HB2	1.87	0.55
17:BB:456:LEU:HB3	17:BB:466:ASP:O	2.06	0.55
18:BC:713:GLU:HB3	18:BC:762:CYS:HB2	1.89	0.55
22:CB:99:LYS:O	22:CB:103:PHE:CB	2.53	0.55
23:E2:164:LYS:HZ1	32:SA:1575:G:P	2.29	0.55
32:SA:1615:C:H2'	35:SG:81:ARG:HD2	1.89	0.55
36:SI:25:VAL:O	36:SI:29:ASN:ND2	2.39	0.55
39:SM:33:ARG:HH11	39:SM:61:THR:HG21	1.71	0.55
6:3G:34:LYS:HG3	6:3G:43:THR:HG21	1.87	0.55
17:BB:554:THR:HG22	17:BB:570:TYR:HB2	1.88	0.55
18:BC:43:ILE:HB	18:BC:56:ILE:O	2.07	0.55
22:CB:526:CYS:HA	22:CB:615:VAL:O	2.06	0.55
35:SG:69:PHE:HZ	42:SR:53:LEU:HD11	1.72	0.55
4:3E:293:GLU:O	4:3E:297:ALA:HB2	2.06	0.55
16:BA:430:ARG:HE	16:BA:431:ILE:H	1.53	0.55
20:BE:119:GLU:OE2	20:BE:133:ASP:HB3	2.06	0.55
34:SF:181:VAL:HG22	34:SF:194:THR:H	1.72	0.55
38:SK:136:VAL:HG22	38:SK:156:ILE:HG12	1.87	0.55
2:3B:227:PRO:HB2	2:3B:260:PHE:HE2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:315:ILE:HB	22:CB:553:VAL:HG13	1.88	0.55
22:CB:1097:ASP:OD2	22:CB:1186:ILE:N	2.26	0.55
23:E2:121:LEU:HD11	23:E2:167:ILE:HD13	1.88	0.55
23:E2:222:ASP:OD2	35:SG:219:ARG:NH1	2.31	0.55
24:E4:55:UNK:HA	24:E4:71:UNK:HA	1.89	0.55
2:3B:115:GLU:O	2:3B:122:ARG:NH1	2.40	0.55
14:AG:435:UNK:O	14:AG:447:UNK:CB	2.55	0.55
17:BB:218:ILE:HA	17:BB:227:LYS:O	2.07	0.55
33:SC:171:ILE:HA	33:SC:174:LYS:NZ	2.21	0.55
5:3F:328:ILE:HA	5:3F:337:VAL:O	2.07	0.55
19:BD:301:TYR:HB2	19:BD:313:PHE:H	1.71	0.55
20:BE:128:LEU:HB3	20:BE:140:TYR:HB2	1.89	0.55
20:BE:578:VAL:O	20:BE:579:ARG:NE	2.39	0.55
21:CA:183:ASP:O	21:CA:187:HIS:HB2	2.07	0.55
23:E1:129:ARG:NH1	32:SA:1192:C:H5”	2.20	0.55
25:K1:169:ASN:ND2	32:SA:933:A:OP2	2.40	0.55
29:P1:215:ALA:O	29:P1:219:ALA:HB2	2.07	0.55
32:SA:1588:G:H1	32:SA:1608:U:H3	1.53	0.55
2:3C:227:PRO:HG3	2:3C:255:LEU:HB3	1.89	0.55
18:BC:298:SER:OG	18:BC:299:ASN:N	2.38	0.55
22:CB:1222:GLU:O	22:CB:1226:PHE:HB2	2.06	0.55
52:U5:47:GLY:H	52:U5:193:ASN:HA	1.70	0.55
18:BC:172:VAL:HB	18:BC:186:LEU:HB2	1.89	0.55
32:SA:99:C:O2’	32:SA:101:U:O4	2.24	0.55
9:AB:190:UNK:O	9:AB:201:UNK:HA	2.07	0.55
20:BE:370:SER:OG	20:BE:371:LYS:N	2.39	0.55
20:BE:872:LEU:HD22	20:BE:915:VAL:HB	1.89	0.55
32:SA:190:C:N4	32:SA:196:G:O6	2.41	0.55
33:SC:143:THR:O	33:SC:208:GLN:NE2	2.40	0.55
5:3F:539:ILE:O	5:3F:565:SER:HA	2.07	0.54
7:5A:394:U:N3	7:5A:463:A:N1	2.55	0.54
16:BA:739:LEU:O	16:BA:743:PHE:CB	2.54	0.54
17:BB:188:LEU:HD12	17:BB:198:GLU:HB3	1.89	0.54
17:BB:613:ALA:O	17:BB:640:LYS:NZ	2.40	0.54
23:E2:96:LEU:HD21	23:E2:114:ILE:HD11	1.90	0.54
30:R1:207:ARG:NE	30:R1:269:GLU:OE2	2.37	0.54
30:R1:228:ASP:OD2	30:R1:230:TRP:NE1	2.40	0.54
30:R1:339:LEU:HA	30:R1:351:ILE:O	2.07	0.54
33:SC:144:ARG:HB3	33:SC:208:GLN:HB3	1.89	0.54
52:U5:35:ASP:OD2	52:U5:37:HIS:NE2	2.41	0.54
52:U5:71:ASN:HB2	52:U5:122:PHE:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:1:G:C6	32:SA:1124:A:C2	2.95	0.54
3:3D:157:ALA:O	3:3D:161:ALA:CB	2.55	0.54
5:3F:160:ILE:O	5:3F:525:GLN:NE2	2.40	0.54
32:SA:394:C:O2	32:SA:401:A:N6	2.39	0.54
32:SA:1663:G:O6	32:SA:1738:U:O4	2.24	0.54
38:SK:77:ILE:HD11	38:SK:93:LEU:HB3	1.90	0.54
4:3E:76:LEU:HA	4:3E:84:LYS:HZ3	1.72	0.54
19:BD:524:SER:OG	19:BD:528:GLN:N	2.37	0.54
39:SM:124:THR:HB	39:SM:141:LYS:HB3	1.89	0.54
2:3B:264:GLN:NE2	2:3B:321:MET:O	2.41	0.54
17:BB:176:TRP:H	17:BB:191:LEU:HB2	1.73	0.54
17:BB:359:SER:O	17:BB:391:ARG:NH2	2.40	0.54
22:CB:268:LEU:HB3	22:CB:294:LEU:HB2	1.89	0.54
52:U5:156:MET:HG3	52:U5:158:LYS:H	1.73	0.54
2:3C:173:LEU:HD23	2:3C:197:VAL:HG21	1.89	0.54
9:AB:261:UNK:N	9:AB:275:UNK:O	2.40	0.54
14:AG:122:UNK:N	14:AG:126:UNK:O	2.41	0.54
29:P1:228:ASP:OD1	32:SA:1796:C:N4	2.39	0.54
32:SA:631:G:H1	32:SA:968:U:H3	1.54	0.54
7:5A:124:A:OP1	54:UB:107:UNK:N	2.40	0.54
15:B1:972:ILE:HG21	15:B1:993:ASP:HB2	1.90	0.54
18:BC:193:VAL:HG23	18:BC:215:GLY:H	1.71	0.54
19:BD:522:GLN:O	19:BD:530:LEU:HA	2.07	0.54
20:BE:97:LYS:HD3	20:BE:109:LEU:HD21	1.89	0.54
22:CB:487:ILE:HD12	22:CB:582:GLN:HE21	1.71	0.54
32:SA:1650:U:H2'	32:SA:1651:A:H8	1.72	0.54
2:3C:231:ARG:NH1	4:3E:7:GLU:O	2.40	0.54
13:AF:137:UNK:HA	13:AF:153:UNK:HA	1.89	0.54
16:BA:201:HIS:HB2	16:BA:272:THR:HG21	1.90	0.54
17:BB:771:ARG:NH1	17:BB:772:ASP:OD1	2.40	0.54
32:SA:550:A:H2'	32:SA:557:G:H2'	1.90	0.54
34:SF:100:ARG:HG2	34:SF:236:ILE:HD11	1.90	0.54
36:SI:140:VAL:HB	43:SX:52:TYR:HB3	1.90	0.54
1:3A:5:A:H2	32:SA:1119:G:N1	2.02	0.54
16:BA:825:GLN:NE2	20:BE:937:THR:OG1	2.33	0.54
19:BD:270:LYS:HA	19:BD:295:ILE:HG22	1.88	0.54
22:CB:840:LEU:HB3	22:CB:852:PHE:HB2	1.89	0.54
32:SA:1604:U:H2'	32:SA:1605:G:H8	1.73	0.54
40:SO:83:GLU:HG2	40:SO:84:ILE:HG12	1.90	0.54
2:3B:261:LEU:O	3:3D:129:ARG:NH2	2.41	0.54
3:3D:34:VAL:HG23	3:3D:36:GLU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3E:125:PRO:HB3	4:3E:132:SER:HA	1.89	0.54
16:BA:351:LEU:HD13	16:BA:696:ALA:HB2	1.90	0.54
16:BA:797:ILE:HD12	16:BA:800:LYS:HD3	1.90	0.54
17:BB:555:VAL:HG22	17:BB:569:LEU:HB2	1.89	0.54
20:BE:273:LEU:HD23	20:BE:287:LEU:HD12	1.88	0.54
20:BE:627:ASN:ND2	20:BE:647:THR:OG1	2.41	0.54
30:R1:247:ALA:O	30:R1:255:SER:HA	2.08	0.54
44:SY:74:VAL:N	44:SY:82:LYS:HZ2	2.06	0.54
5:3F:262:VAL:HB	5:3F:272:LYS:HB3	1.90	0.53
14:AG:97:UNK:HA	14:AG:113:UNK:HA	1.90	0.53
15:B1:938:PRO:HB2	15:B1:941:ILE:HD11	1.89	0.53
19:BD:409:ILE:HG12	19:BD:427:ASN:HD21	1.73	0.53
20:BE:116:ALA:HB1	20:BE:133:ASP:OD1	2.08	0.53
21:CA:16:VAL:HB	21:CA:37:MET:O	2.09	0.53
22:CB:313:ASN:HD22	22:CB:326:LEU:HB3	1.71	0.53
32:SA:16:G:OP1	51:U4:166:LYS:NZ	2.32	0.53
32:SA:354:C:H2'	32:SA:355:G:H8	1.74	0.53
38:SK:28:LEU:O	38:SK:32:GLY:N	2.41	0.53
13:AF:150:UNK:HA	13:AF:160:UNK:HA	1.90	0.53
49:U1:197:UNK:O	49:U1:215:UNK:N	2.41	0.53
5:3F:368:LEU:O	5:3F:371:ARG:HB2	2.07	0.53
16:BA:817:PHE:O	16:BA:821:MET:HB2	2.08	0.53
17:BB:426:ARG:HG2	17:BB:462:SER:HA	1.90	0.53
20:BE:251:ILE:HA	20:BE:267:GLY:O	2.09	0.53
32:SA:1068:C:H2'	32:SA:1069:A:H8	1.73	0.53
42:SR:110:THR:HA	42:SR:113:ASP:HB2	1.89	0.53
2:3B:319:ARG:HG3	2:3B:322:ARG:HD2	1.90	0.53
9:AB:178:UNK:HA	9:AB:194:UNK:HA	1.89	0.53
16:BA:87:ARG:HD3	16:BA:89:VAL:HG22	1.89	0.53
16:BA:198:PHE:O	16:BA:207:TYR:HB3	2.09	0.53
18:BC:45:LEU:HD12	18:BC:54:HIS:HB3	1.90	0.53
21:CA:181:LYS:HZ3	22:CB:808:LEU:HD13	1.73	0.53
32:SA:330:G:OP2	37:SJ:172:ARG:NH1	2.41	0.53
32:SA:1163:A:N3	32:SA:1613:U:O2'	2.41	0.53
52:U5:8:ILE:N	52:U5:255:TYR:O	2.40	0.53
4:3E:45:ALA:HB1	4:3E:83:LYS:HZ3	1.74	0.53
22:CB:793:PRO:HA	32:SA:1059:U:H5"	1.90	0.53
26:MA:83:TYR:HE1	26:MA:91:LYS:HA	1.73	0.53
26:MA:138:VAL:HG22	26:MA:158:VAL:HG22	1.90	0.53
32:SA:1175:U:O4	32:SA:1464:G:O6	2.27	0.53
40:SO:124:ARG:HG2	40:SO:127:ARG:HH21	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SX:18:GLU:HG3	43:SX:69:LEU:HD12	1.90	0.53
44:SY:68:ILE:HB	44:SY:70:LYS:NZ	2.23	0.53
5:3F:424:LEU:HB3	5:3F:434:PHE:HB3	1.90	0.53
7:5A:242:C:H2'	7:5A:243:A:H8	1.72	0.53
18:BC:759:THR:O	18:BC:762:CYS:HB3	2.08	0.53
9:AB:4:UNK:HA	9:AB:283:UNK:O	2.08	0.53
12:AE:141:ASN:ND2	12:AE:209:GLN:OE1	2.41	0.53
14:AG:112:UNK:HA	14:AG:118:UNK:HA	1.90	0.53
17:BB:251:GLN:NE2	17:BB:342:SER:O	2.36	0.53
19:BD:541:LEU:O	19:BD:542:ARG:NH1	2.37	0.53
22:CB:100:SER:O	22:CB:104:LYS:CB	2.54	0.53
22:CB:532:PRO:HG2	22:CB:693:LYS:HE2	1.91	0.53
27:MB:223:THR:HB	27:MB:234:ARG:HB2	1.90	0.53
34:SF:11:ARG:NH1	34:SF:21:ASP:O	2.35	0.53
34:SF:39:ARG:HG3	34:SF:40:GLU:HG3	1.89	0.53
13:AF:474:UNK:O	13:AF:478:UNK:CB	2.57	0.53
17:BB:123:ALA:HB3	17:BB:141:LYS:HE2	1.90	0.53
21:CA:134:ILE:O	21:CA:138:TRP:CB	2.56	0.53
23:E1:144:LEU:HD22	23:E1:160:LEU:HD13	1.91	0.53
23:E2:44:VAL:HA	23:E2:113:TYR:O	2.08	0.53
35:SG:63:GLN:NE2	35:SG:86:GLN:OE1	2.40	0.53
20:BE:143:SER:HB3	20:BE:152:GLU:OE2	2.09	0.53
32:SA:514:G:H8	32:SA:514:G:OP2	1.92	0.53
1:3A:72:C:H2'	1:3A:73:A:H8	1.74	0.53
7:5A:557:A:H61	7:5A:580:A:H61	1.55	0.53
12:AE:333:LEU:HD11	12:AE:369:LEU:HD12	1.91	0.53
12:AE:381:ARG:HA	12:AE:384:ILE:HD12	1.90	0.53
16:BA:320:GLY:HA2	16:BA:329:VAL:HG22	1.91	0.53
16:BA:514:VAL:HG13	42:SR:118:ILE:HB	1.90	0.53
16:BA:799:ILE:HD11	16:BA:824:ILE:HD12	1.91	0.53
19:BD:528:GLN:HA	19:BD:546:LEU:HB2	1.91	0.53
20:BE:342:TYR:HH	20:BE:345:SER:HG	1.56	0.53
23:E1:131:PRO:HA	32:SA:1192:C:H1'	1.90	0.53
39:SM:129:ARG:HE	39:SM:131:ILE:HD13	1.74	0.53
9:AB:271:UNK:HA	9:AB:284:UNK:O	2.09	0.52
11:AD:509:UNK:O	11:AD:513:UNK:CB	2.57	0.52
12:AE:37:SER:O	12:AE:41:ALA:HB2	2.08	0.52
18:BC:353:LEU:HB3	18:BC:366:PRO:HD2	1.91	0.52
18:BC:391:LEU:HD23	18:BC:407:SER:HB2	1.91	0.52
5:3F:334:GLU:HG2	5:3F:351:ILE:HB	1.90	0.52
7:5A:419:A:N1	7:5A:436:G:N2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AC:603:UNK:O	10:AC:607:UNK:CB	2.57	0.52
15:B1:876:PRO:HB2	15:B1:878:HIS:H	1.72	0.52
18:BC:747:ASN:HD22	18:BC:785:ILE:HD12	1.73	0.52
22:CB:467:LEU:HB3	22:CB:476:ILE:HB	1.90	0.52
22:CB:629:THR:HB	22:CB:667:CYS:HB2	1.90	0.52
32:SA:1615:C:OP1	35:SG:81:ARG:NH2	2.42	0.52
33:SC:129:THR:OG1	33:SC:131:ASP:O	2.20	0.52
5:3F:235:HIS:NE2	5:3F:253:THR:OG1	2.37	0.52
12:AE:371:LYS:O	12:AE:374:ARG:NH2	2.41	0.52
19:BD:568:VAL:HA	19:BD:578:ALA:O	2.10	0.52
21:CA:207:VAL:HG21	32:SA:1060:U:H1'	1.91	0.52
15:B1:815:LEU:HD21	15:B1:852:ARG:HD2	1.91	0.52
16:BA:105:SER:OG	16:BA:108:GLY:N	2.42	0.52
18:BC:222:LEU:HD12	18:BC:235:LYS:HB2	1.91	0.52
22:CB:748:LEU:HB3	22:CB:787:GLU:HG2	1.92	0.52
27:MB:187:PRO:HB3	27:MB:220:ARG:HG3	1.90	0.52
30:R1:119:LYS:HG2	30:R1:165:GLU:HG2	1.92	0.52
30:R1:246:VAL:HA	30:R1:256:TYR:O	2.09	0.52
34:SF:75:LYS:HZ1	34:SF:77:ARG:HH12	1.51	0.52
5:3F:442:ILE:HA	5:3F:472:PRO:HA	1.91	0.52
12:AE:333:LEU:O	12:AE:337:ASP:CB	2.58	0.52
17:BB:263:THR:O	17:BB:270:SER:HA	2.10	0.52
22:CB:173:ASN:ND2	32:SA:1686:C:OP1	2.42	0.52
32:SA:382:C:H2'	32:SA:383:G:H8	1.75	0.52
39:SM:55:ASP:OD2	39:SM:113:PRO:HD2	2.10	0.52
1:3A:254:A:OP2	6:3G:95:ARG:NH1	2.42	0.52
3:3D:30:ARG:NH2	31:S1:205:UNK:O	2.43	0.52
5:3F:285:SER:N	5:3F:298:SER:OG	2.43	0.52
5:3F:497:LYS:HG2	5:3F:513:GLU:HG2	1.91	0.52
7:5A:446:U:H2'	7:5A:447:G:H8	1.74	0.52
9:AB:244:UNK:N	9:AB:248:UNK:O	2.42	0.52
11:AD:408:UNK:O	11:AD:412:UNK:CB	2.58	0.52
12:AE:288:ALA:HB1	12:AE:292:LYS:HG2	1.90	0.52
12:AE:293:HIS:O	12:AE:297:LEU:CB	2.58	0.52
15:B1:620:LYS:O	15:B1:624:LYS:CB	2.57	0.52
21:CA:181:LYS:NZ	22:CB:808:LEU:HB3	2.24	0.52
22:CB:235:LEU:O	22:CB:239:LEU:HB3	2.09	0.52
22:CB:381:HIS:NE2	22:CB:478:THR:O	2.35	0.52
29:P1:105:ARG:HH21	29:P1:163:THR:HA	1.74	0.52
52:U5:85:GLU:HB3	52:U5:174:ILE:HD11	1.91	0.52
1:3A:41:C:H42	7:5A:477:G:H1	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3D:156:HIS:O	3:3D:160:ARG:HB3	2.10	0.52
8:AA:259:UNK:HA	8:AA:274:UNK:O	2.10	0.52
12:AE:365:ILE:O	12:AE:369:LEU:CB	2.57	0.52
16:BA:730:LEU:HD22	16:BA:734:GLN:HB2	1.92	0.52
17:BB:337:LYS:HD3	17:BB:355:LEU:HD21	1.91	0.52
18:BC:309:GLN:O	18:BC:363:ARG:NH1	2.43	0.52
18:BC:465:LYS:HE3	18:BC:520:LEU:HD11	1.89	0.52
19:BD:529:ILE:HD12	19:BD:545:HIS:HA	1.91	0.52
35:SG:79:ASN:HB2	35:SG:83:ARG:HH22	1.75	0.52
14:AG:96:UNK:O	14:AG:114:UNK:N	2.42	0.52
21:CA:214:LEU:HD23	21:CA:215:VAL:HG23	1.92	0.52
28:MC:54:UNK:O	28:MC:58:UNK:CB	2.58	0.52
36:SI:9:LEU:HD22	36:SI:17:GLU:HB3	1.92	0.52
36:SI:47:ARG:HB2	36:SI:59:ALA:HB3	1.91	0.52
37:SJ:67:TRP:NE1	37:SJ:69:SER:OG	2.42	0.52
52:U5:213:LEU:HA	52:U5:216:ILE:HD12	1.92	0.52
1:3A:4:G:H1	32:SA:1120:U:H3	1.57	0.52
1:3A:80:U:OP2	6:3H:95:ARG:HD2	2.09	0.52
1:3A:330:A:H2'	1:3A:331:A:H8	1.75	0.52
15:B1:244:ILE:O	15:B1:246:ARG:NH2	2.43	0.52
16:BA:742:ALA:HA	16:BA:745:LEU:HD12	1.92	0.52
20:BE:587:ARG:HB3	20:BE:605:LEU:HD13	1.90	0.52
32:SA:1528:U:H5"	35:SG:112:ARG:HH22	1.74	0.52
38:SK:67:PRO:HA	38:SK:70:LEU:HB2	1.91	0.52
39:SM:108:PRO:HB2	39:SM:135:VAL:HG22	1.92	0.52
40:SO:19:SER:OG	40:SO:21:ASN:OD1	2.27	0.52
5:3F:365:PRO:O	5:3F:368:LEU:HB2	2.10	0.52
8:AA:218:UNK:HA	8:AA:234:UNK:HA	1.92	0.52
17:BB:426:ARG:NH1	17:BB:458:ASP:O	2.43	0.52
18:BC:346:VAL:HB	18:BC:352:LYS:HB3	1.92	0.52
20:BE:860:GLU:HA	20:BE:863:TRP:HE3	1.75	0.52
21:CA:13:PHE:HA	21:CA:39:ALA:O	2.09	0.52
32:SA:900:A:H3'	32:SA:901:G:H21	1.75	0.52
32:SA:1511:U:H2'	32:SA:1512:G:H8	1.75	0.52
39:SM:71:LEU:HB3	39:SM:88:ARG:NH1	2.24	0.52
2:3B:248:ASP:OD1	2:3B:248:ASP:N	2.42	0.51
16:BA:430:ARG:HE	16:BA:432:GLN:H	1.58	0.51
21:CA:210:ASP:O	21:CA:214:LEU:HB3	2.10	0.51
23:E1:44:VAL:HG22	23:E1:113:TYR:HB2	1.92	0.51
32:SA:1638:G:H22	32:SA:1763:A:H2	1.57	0.51
32:SA:1739:C:H2'	32:SA:1740:A:H8	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:U5:109:ARG:HA	52:U5:114:LYS:HE3	1.91	0.51
3:3D:146:ASP:HB2	4:3E:241:VAL:HG11	1.91	0.51
4:3E:346:SER:O	4:3E:350:GLN:HB2	2.09	0.51
12:AE:347:PHE:O	12:AE:351:TYR:HB2	2.10	0.51
16:BA:193:TYR:HB3	16:BA:211:LYS:HD3	1.92	0.51
17:BB:553:ASN:HB3	17:BB:572:HIS:HB2	1.92	0.51
19:BD:288:LEU:HD22	19:BD:324:TRP:CD1	2.45	0.51
31:S1:167:UNK:CB	31:S1:179:UNK:O	2.59	0.51
32:SA:325:G:O2'	39:SM:81:HIS:O	2.27	0.51
35:SG:58:LEU:HD11	35:SG:167:ARG:HH12	1.74	0.51
14:AG:113:UNK:N	14:AG:117:UNK:O	2.43	0.51
16:BA:537:GLY:HA3	16:BA:554:ASP:HA	1.92	0.51
17:BB:250:LYS:H	17:BB:265:SER:HA	1.76	0.51
18:BC:614:ASP:OD1	18:BC:614:ASP:N	2.40	0.51
20:BE:62:ASP:OD2	20:BE:65:THR:OG1	2.11	0.51
23:E1:188:ARG:HD3	23:E1:191:ASP:OD2	2.10	0.51
45:SZ:92:VAL:HG21	45:SZ:99:LYS:HE2	1.91	0.51
55:UC:311:UNK:O	55:UC:315:UNK:N	2.44	0.51
5:3F:159:CYS:SG	5:3F:160:ILE:N	2.83	0.51
7:5A:174:U:H2'	7:5A:175:A:C8	2.45	0.51
15:B1:553:ILE:HG23	30:R1:323:ILE:HG23	1.93	0.51
16:BA:441:SER:OG	16:BA:485:ASN:ND2	2.43	0.51
20:BE:488:ASN:HD21	42:SR:98:ASP:HB3	1.74	0.51
22:CB:587:GLY:HA3	22:CB:611:ASP:OD2	2.10	0.51
23:E2:44:VAL:HG22	23:E2:113:TYR:HB2	1.93	0.51
12:AE:227:ASN:HD22	12:AE:230:LYS:HD2	1.76	0.51
16:BA:59:ALA:HA	16:BA:73:ILE:O	2.10	0.51
17:BB:637:ALA:HA	17:BB:660:VAL:HG12	1.92	0.51
21:CA:52:CYS:HA	21:CA:126:LEU:O	2.09	0.51
22:CB:228:ARG:HH21	22:CB:296:ILE:H	1.58	0.51
35:SG:63:GLN:HB3	35:SG:88:PRO:HA	1.91	0.51
55:UC:309:UNK:O	55:UC:313:UNK:N	2.43	0.51
4:3E:209:ILE:O	4:3E:256:ASN:ND2	2.44	0.51
10:AC:504:UNK:O	10:AC:508:UNK:CB	2.59	0.51
16:BA:619:ARG:NH1	16:BA:620:ASN:O	2.44	0.51
18:BC:119:VAL:HG21	18:BC:127:ILE:HG13	1.93	0.51
20:BE:229:GLU:HA	20:BE:244:ILE:O	2.11	0.51
22:CB:433:ASP:HB2	22:CB:489:LYS:NZ	2.25	0.51
32:SA:361:C:H3'	32:SA:378:A:OP2	2.11	0.51
32:SA:1510:U:OP1	52:U5:144:TYR:OH	2.29	0.51
34:SF:85:GLY:N	34:SF:88:ASP:OD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:SX:31:SER:H	43:SX:34:ILE:HD12	1.74	0.51
2:3B:188:VAL:HG22	2:3B:192:GLY:HA3	1.93	0.51
7:5A:513:G:N2	7:5A:523:U:O2	2.33	0.51
10:AC:6:UNK:O	10:AC:283:UNK:N	2.43	0.51
13:AF:407:UNK:O	13:AF:411:UNK:CB	2.58	0.51
15:B1:824:ILE:HD12	15:B1:925:ASN:H	1.76	0.51
22:CB:508:SER:HA	22:CB:512:LEU:HB2	1.92	0.51
23:E1:122:ILE:HA	23:E1:161:LYS:O	2.10	0.51
32:SA:1160:A:H1'	32:SA:1620:C:H42	1.75	0.51
53:UA:617:UNK:O	53:UA:702:UNK:N	2.38	0.51
53:UA:1212:UNK:O	53:UA:1216:UNK:N	2.44	0.51
4:3E:163:ILE:HG23	4:3E:276:LEU:HD11	1.93	0.51
7:5A:511:G:O6	7:5A:525:U:O4	2.28	0.51
12:AE:81:LEU:HD11	12:AE:85:VAL:HG22	1.93	0.51
17:BB:196:CYS:SG	17:BB:199:THR:OG1	2.68	0.51
23:E1:68:LEU:HD13	23:E1:77:LEU:HD21	1.92	0.51
32:SA:1145:U:H3	32:SA:1633:A:H2'	1.76	0.51
35:SG:41:LYS:NZ	35:SG:67:PRO:HG2	2.25	0.51
13:AF:408:UNK:O	13:AF:412:UNK:CB	2.59	0.51
14:AG:382:UNK:HA	14:AG:397:UNK:O	2.11	0.51
16:BA:146:PHE:HE1	49:U1:217:UNK:HA	1.76	0.51
32:SA:485:A:N3	32:SA:503:G:N2	2.53	0.51
53:UA:1006:UNK:O	53:UA:1010:UNK:N	2.44	0.51
2:3B:249:GLN:HA	2:3B:252:ILE:HD12	1.93	0.51
8:AA:319:UNK:CB	8:AA:332:UNK:O	2.59	0.51
9:AB:148:UNK:HA	9:AB:161:UNK:O	2.11	0.51
14:AG:143:UNK:HA	14:AG:150:UNK:HA	1.93	0.51
19:BD:369:ASN:O	19:BD:384:ILE:HA	2.11	0.51
22:CB:822:ARG:O	22:CB:842:ILE:HA	2.10	0.51
22:CB:904:HIS:O	22:CB:907:GLN:NE2	2.44	0.51
22:CB:924:LEU:HD21	22:CB:1181:VAL:HG13	1.92	0.51
32:SA:1727:G:H2'	32:SA:1728:A:H8	1.76	0.51
37:SJ:37:LYS:HB2	37:SJ:59:ARG:HG2	1.93	0.51
37:SJ:105:ASP:OD2	37:SJ:108:PRO:HD3	2.10	0.51
49:U1:37:UNK:N	49:U1:46:UNK:O	2.44	0.51
5:3F:295:LEU:O	5:3F:306:THR:HA	2.11	0.50
10:AC:18:UNK:N	10:AC:27:UNK:O	2.44	0.50
10:AC:242:UNK:CB	10:AC:251:UNK:O	2.59	0.50
15:B1:607:ASP:O	30:R1:321:ARG:NH1	2.43	0.50
17:BB:757:ASP:O	17:BB:761:ALA:CB	2.58	0.50
20:BE:868:LEU:HB3	20:BE:881:TYR:HE1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:1063:ARG:HH21	22:CB:1185:LEU:HD11	1.76	0.50
32:SA:103:A:H4'	32:SA:105:A:H61	1.76	0.50
32:SA:1647:U:H2'	32:SA:1648:A:H8	1.76	0.50
44:SY:59:ILE:O	44:SY:69:ARG:N	2.43	0.50
2:3C:162:LEU:HG	2:3C:164:ILE:H	1.76	0.50
9:AB:77:UNK:HA	9:AB:88:UNK:HA	1.93	0.50
12:AE:260:ILE:O	12:AE:264:PHE:CB	2.59	0.50
14:AG:100:UNK:HA	14:AG:111:UNK:HA	1.92	0.50
19:BD:296:GLN:H	19:BD:316:GLY:HA2	1.75	0.50
22:CB:506:GLN:OE1	22:CB:509:ASN:ND2	2.44	0.50
36:SI:62:VAL:HB	36:SI:94:ALA:HA	1.93	0.50
5:3F:371:ARG:HH21	5:3F:374:LYS:HZ3	1.58	0.50
7:5A:67:G:H5'	7:5A:68:U:OP2	2.10	0.50
11:AD:475:UNK:O	11:AD:479:UNK:CB	2.60	0.50
15:B1:70:ARG:NH2	15:B1:193:ARG:O	2.44	0.50
16:BA:23:SER:HA	16:BA:63:LEU:HD21	1.94	0.50
16:BA:430:ARG:HH21	16:BA:431:ILE:HG22	1.75	0.50
18:BC:348:PRO:HB3	18:BC:399:ASP:HA	1.92	0.50
22:CB:85:SER:O	22:CB:89:HIS:CB	2.59	0.50
30:R1:107:ALA:HB1	30:R1:170:VAL:HG11	1.93	0.50
35:SG:80:LYS:HZ3	35:SG:83:ARG:NH1	2.09	0.50
35:SG:156:ARG:NH1	35:SG:157:ARG:HD2	2.27	0.50
3:3D:75:SER:HB2	3:3D:78:LEU:HD23	1.93	0.50
4:3E:149:ARG:HE	4:3E:156:ALA:HB2	1.76	0.50
7:5A:408:U:O4	7:5A:448:G:O6	2.29	0.50
9:AB:157:UNK:HA	9:AB:171:UNK:O	2.11	0.50
17:BB:492:SER:H	17:BB:534:ILE:HD11	1.77	0.50
18:BC:680:ASN:N	18:BC:680:ASN:OD1	2.44	0.50
22:CB:915:LEU:HD22	22:CB:954:LEU:HD21	1.93	0.50
22:CB:928:HIS:NE2	22:CB:1163:LEU:O	2.43	0.50
34:SF:72:VAL:N	34:SF:75:LYS:O	2.41	0.50
34:SF:118:GLU:OE2	34:SF:237:SER:N	2.30	0.50
18:BC:257:ILE:HB	18:BC:269:LEU:HD22	1.94	0.50
18:BC:687:THR:HG23	18:BC:688:LEU:HG	1.93	0.50
20:BE:444:ASP:OD1	20:BE:446:ARG:N	2.36	0.50
33:SC:145:LYS:HB3	33:SC:149:GLN:HG3	1.93	0.50
43:SX:55:ASP:OD1	43:SX:59:GLY:N	2.43	0.50
12:AE:367:LEU:HA	12:AE:400:LEU:HD11	1.92	0.50
18:BC:72:ASP:OD1	18:BC:72:ASP:N	2.45	0.50
19:BD:414:ILE:HB	19:BD:479:ASN:HD21	1.76	0.50
20:BE:254:LEU:HD22	20:BE:264:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:SF:126:VAL:HA	34:SF:141:THR:HA	1.94	0.50
49:U1:14:UNK:HA	49:U1:30:UNK:HA	1.93	0.50
52:U5:16:ALA:O	52:U5:20:LEU:N	2.45	0.50
7:5A:446:U:H2'	7:5A:447:G:C8	2.47	0.50
9:AB:203:UNK:N	9:AB:207:UNK:O	2.45	0.50
15:B1:923:ASP:OD1	15:B1:923:ASP:N	2.44	0.50
16:BA:538:GLN:HE21	16:BA:551:GLY:HA3	1.77	0.50
17:BB:624:LEU:N	17:BB:629:ASN:O	2.40	0.50
20:BE:168:VAL:HB	20:BE:183:VAL:HG23	1.94	0.50
44:SY:67:ALA:HB3	44:SY:69:ARG:HH22	1.76	0.50
3:3D:19:LYS:HE3	3:3D:142:LEU:HD13	1.92	0.50
5:3F:190:VAL:HA	5:3F:195:GLN:O	2.12	0.50
7:5A:107:G:OP2	7:5A:109:C:H5'	2.12	0.50
19:BD:362:HIS:H	19:BD:418:LYS:HD3	1.77	0.50
21:CA:169:VAL:HB	22:CB:1140:SER:HB2	1.93	0.50
32:SA:340:U:H2'	32:SA:341:A:C8	2.47	0.50
34:SF:12:LEU:HD21	34:SF:22:LYS:HG2	1.94	0.50
34:SF:57:ASN:HB2	34:SF:60:GLU:HG3	1.93	0.50
2:3C:107:VAL:HG12	2:3C:143:VAL:HA	1.94	0.50
16:BA:303:ASN:HD22	16:BA:326:GLN:HG3	1.75	0.50
17:BB:227:LYS:HG3	17:BB:241:LYS:HG2	1.93	0.50
18:BC:318:GLU:HB3	18:BC:327:ILE:HG22	1.93	0.50
19:BD:241:ALA:HB2	19:BD:587:ARG:HG2	1.93	0.50
27:MB:105:LYS:HD3	32:SA:1580:C:H5"	1.94	0.50
32:SA:329:G:H2'	32:SA:330:G:H8	1.77	0.50
33:SC:190:PRO:HG2	33:SC:192:VAL:HG23	1.93	0.50
2:3C:129:SER:H	2:3C:136:PRO:HG3	1.76	0.49
2:3C:297:ARG:HE	2:3C:321:MET:HG2	1.77	0.49
5:3F:230:ASN:HB2	5:3F:259:LYS:HD3	1.94	0.49
19:BD:520:ASN:HD22	19:BD:533:ALA:HB3	1.77	0.49
22:CB:970:TRP:O	22:CB:1028:ARG:NH2	2.45	0.49
32:SA:359:A:OP2	32:SA:360:A:N6	2.45	0.49
34:SF:17:HIS:HA	34:SF:108:ARG:HG2	1.94	0.49
34:SF:48:LEU:HD21	34:SF:61:VAL:HG22	1.94	0.49
12:AE:349:THR:HG23	12:AE:383:ILE:HD11	1.94	0.49
18:BC:123:ASP:OD1	18:BC:146:THR:OG1	2.29	0.49
32:SA:1041:G:H2'	32:SA:1042:G:H8	1.77	0.49
34:SF:137:PRO:HG2	34:SF:150:PRO:HD2	1.94	0.49
39:SM:101:GLU:OE2	39:SM:103:ARG:NE	2.44	0.49
7:5A:503:C:H1'	7:5A:535:G:H1	1.77	0.49
10:AC:96:UNK:HA	10:AC:112:UNK:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:AC:621:UNK:O	10:AC:625:UNK:CB	2.60	0.49
16:BA:71:ILE:HD11	16:BA:102:VAL:HG11	1.94	0.49
17:BB:397:ILE:HG22	17:BB:408:THR:HG22	1.94	0.49
22:CB:207:LEU:O	22:CB:296:ILE:HA	2.11	0.49
24:E4:261:UNK:N	24:E4:275:UNK:O	2.45	0.49
26:MA:102:THR:OG1	26:MA:103:VAL:N	2.45	0.49
32:SA:1164:G:OP1	35:SG:166:ARG:NH2	2.45	0.49
42:SR:62:ASN:OD1	42:SR:62:ASN:N	2.44	0.49
55:UC:404:UNK:O	55:UC:408:UNK:N	2.44	0.49
5:3F:156:ASN:HA	5:3F:544:ALA:HB1	1.94	0.49
17:BB:407:ALA:HB1	17:BB:414:LEU:HD11	1.95	0.49
20:BE:84:SER:O	20:BE:91:TYR:HB2	2.12	0.49
20:BE:273:LEU:HB3	20:BE:287:LEU:HB2	1.93	0.49
20:BE:523:ASP:OD1	20:BE:523:ASP:N	2.43	0.49
22:CB:855:LEU:HD13	22:CB:889:TYR:HD2	1.76	0.49
22:CB:970:TRP:HZ3	22:CB:1034:GLY:HA3	1.78	0.49
22:CB:1109:LYS:NZ	22:CB:1170:GLY:O	2.28	0.49
23:E1:42:ILE:O	23:E1:203:CYS:HA	2.11	0.49
30:R1:98:TYR:HB2	30:R1:127:ASP:OD2	2.13	0.49
15:B1:558:ILE:O	30:R1:327:ARG:NH2	2.41	0.49
22:CB:96:GLU:O	22:CB:100:SER:CB	2.60	0.49
29:P1:215:ALA:O	29:P1:219:ALA:CB	2.60	0.49
35:SG:41:LYS:HZ3	35:SG:67:PRO:HB2	1.77	0.49
36:SI:159:VAL:HG23	36:SI:163:ASP:OD2	2.12	0.49
51:U4:161:LYS:HA	51:U4:164:ILE:HD12	1.92	0.49
53:UA:1215:UNK:O	53:UA:1219:UNK:N	2.45	0.49
3:3D:66:ALA:O	3:3D:70:SER:OG	2.27	0.49
4:3E:260:GLU:O	4:3E:264:GLU:HB2	2.12	0.49
10:AC:681:UNK:O	10:AC:685:UNK:CB	2.60	0.49
14:AG:487:UNK:O	14:AG:495:UNK:N	2.45	0.49
17:BB:212:VAL:HB	17:BB:217:LEU:HD23	1.94	0.49
17:BB:828:TYR:O	17:BB:832:PHE:CB	2.51	0.49
17:BB:861:ILE:HG12	18:BC:806:LEU:HG	1.94	0.49
19:BD:310:GLN:HA	19:BD:326:LEU:HB2	1.94	0.49
21:CA:14:ILE:HG21	21:CA:141:LEU:HB3	1.94	0.49
23:E2:42:ILE:O	23:E2:203:CYS:HA	2.11	0.49
37:SJ:10:LYS:O	37:SJ:18:ARG:NH2	2.46	0.49
55:UC:248:UNK:O	55:UC:250:UNK:N	2.46	0.49
1:3A:5:A:N1	32:SA:1119:G:C6	2.81	0.49
9:AB:539:UNK:O	9:AB:543:UNK:CB	2.60	0.49
15:B1:246:ARG:NH2	15:B1:798:MET:SD	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BB:351:LEU:HA	17:BB:372:ARG:HG2	1.95	0.49
22:CB:976:ILE:HA	22:CB:1042:ALA:O	2.13	0.49
5:3F:304:ILE:HB	5:3F:318:LEU:HB2	1.95	0.49
6:3G:63:ILE:HG13	6:3G:64:LEU:HG	1.95	0.49
7:5A:125:G:H2'	7:5A:126:A:C8	2.47	0.49
7:5A:286:U:H2'	7:5A:287:G:H8	1.77	0.49
10:AC:462:UNK:O	10:AC:466:UNK:CB	2.61	0.49
15:B1:117:VAL:HG23	15:B1:144:PRO:HG2	1.95	0.49
16:BA:219:GLU:O	16:BA:222:LYS:NZ	2.45	0.49
23:E2:178:VAL:HA	23:E2:223:GLU:O	2.13	0.49
32:SA:273:G:H2'	32:SA:274:G:H8	1.77	0.49
36:SI:46:ILE:HD11	36:SI:58:LEU:HB3	1.93	0.49
36:SI:58:LEU:HD12	36:SI:90:VAL:HG22	1.93	0.49
38:SK:81:VAL:HG21	38:SK:91:LYS:HE2	1.95	0.49
10:AC:265:UNK:HA	10:AC:272:UNK:HA	1.94	0.49
32:SA:200:A:H2'	32:SA:201:G:H8	1.78	0.49
32:SA:251:A:O2'	34:SF:131:LEU:O	2.31	0.49
32:SA:954:G:H2'	32:SA:955:A:C8	2.48	0.49
45:SZ:5:VAL:HG22	45:SZ:32:ARG:HH22	1.78	0.49
12:AE:293:HIS:O	12:AE:297:LEU:HB2	2.13	0.49
17:BB:565:PHE:HD2	30:R1:207:ARG:NH1	2.11	0.49
19:BD:313:PHE:HE2	19:BD:389:SER:HB2	1.77	0.49
22:CB:423:LYS:O	22:CB:427:LYS:HB2	2.13	0.49
22:CB:721:VAL:HG13	22:CB:722:LEU:HG	1.93	0.49
22:CB:1159:ASN:HD22	22:CB:1201:ASP:HB3	1.77	0.49
22:CB:1189:LEU:O	22:CB:1194:HIS:NE2	2.44	0.49
32:SA:1482:C:H4'	42:SR:77:GLN:HE22	1.78	0.49
4:3E:355:ASN:ND2	4:3E:401:LEU:O	2.46	0.48
5:3F:549:LEU:HB2	5:3F:551:ARG:HG2	1.95	0.48
10:AC:16:UNK:O	10:AC:29:UNK:N	2.46	0.48
15:B1:975:GLU:O	15:B1:990:ALA:HB3	2.13	0.48
17:BB:247:ILE:HG22	17:BB:267:ASP:HB2	1.95	0.48
19:BD:296:GLN:HG3	19:BD:317:ARG:HB3	1.94	0.48
20:BE:78:SER:OG	20:BE:95:GLU:OE2	2.29	0.48
20:BE:893:GLY:HA2	20:BE:896:ILE:HD12	1.94	0.48
45:SZ:5:VAL:HG13	45:SZ:32:ARG:HH12	1.77	0.48
1:3A:40:A:OP1	12:AE:22:ARG:NH1	2.46	0.48
9:AB:473:UNK:O	9:AB:477:UNK:CB	2.60	0.48
16:BA:751:ILE:HA	16:BA:754:VAL:HG12	1.95	0.48
17:BB:641:TYR:HD2	17:BB:651:GLN:HB2	1.78	0.48
18:BC:467:ILE:H	18:BC:480:ILE:HG21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:539:ASP:H	19:BD:563:GLY:H	1.61	0.48
24:E4:78:UNK:CB	24:E4:87:UNK:O	2.61	0.48
2:3C:198:GLU:HG3	2:3C:200:SER:H	1.78	0.48
9:AB:160:UNK:CB	9:AB:169:UNK:O	2.61	0.48
10:AC:614:UNK:O	10:AC:618:UNK:CB	2.61	0.48
10:AC:647:UNK:O	10:AC:651:UNK:CB	2.62	0.48
12:AE:85:VAL:HG21	12:AE:90:GLU:HG2	1.95	0.48
12:AE:367:LEU:O	12:AE:371:LYS:CB	2.61	0.48
17:BB:135:ARG:NH1	17:BB:149:ASP:OD1	2.46	0.48
17:BB:861:ILE:HG21	18:BC:806:LEU:HD11	1.94	0.48
19:BD:424:ILE:HB	19:BD:433:TRP:HB3	1.94	0.48
22:CB:538:ASN:OD1	22:CB:541:THR:OG1	2.31	0.48
26:MA:38:ILE:HG22	26:MA:40:ASN:H	1.78	0.48
30:R1:188:ILE:HA	30:R1:249:SER:HB2	1.95	0.48
33:SC:87:ARG:O	33:SC:99:ASN:N	2.43	0.48
35:SG:118:LEU:HD22	35:SG:129:PRO:HB2	1.95	0.48
37:SJ:54:LYS:CD	37:SJ:56:ARG:HH12	2.26	0.48
12:AE:88:LYS:HA	12:AE:91:ILE:HD12	1.95	0.48
15:B1:284:PRO:HA	15:B1:787:SER:HB3	1.95	0.48
17:BB:676:SER:OG	17:BB:677:HIS:N	2.44	0.48
30:R1:208:MET:HB3	30:R1:243:ILE:HD12	1.94	0.48
32:SA:905:A:H4'	41:SP:52:ARG:HD3	1.95	0.48
36:SI:133:THR:OG1	36:SI:134:GLU:N	2.41	0.48
7:5A:341:G:H1	7:5A:384:U:H3	1.61	0.48
14:AG:232:UNK:O	14:AG:243:UNK:HA	2.14	0.48
17:BB:486:LYS:HA	17:BB:502:PHE:HB3	1.96	0.48
18:BC:71:PRO:HD2	18:BC:115:THR:HG22	1.96	0.48
20:BE:127:TYR:HA	20:BE:140:TYR:O	2.13	0.48
20:BE:430:ILE:HB	20:BE:443:TRP:HB2	1.94	0.48
20:BE:592:ASP:OD1	20:BE:593:PHE:N	2.46	0.48
30:R1:280:LEU:HD23	30:R1:283:ILE:HD12	1.96	0.48
32:SA:99:C:O2	32:SA:100:A:N6	2.44	0.48
32:SA:1592:A:H2'	32:SA:1593:A:H8	1.78	0.48
51:U4:109:LEU:HB3	51:U4:113:TYR:HD2	1.78	0.48
7:5A:408:U:O2	7:5A:448:G:N2	2.34	0.48
10:AC:620:UNK:O	10:AC:624:UNK:CB	2.62	0.48
17:BB:94:LEU:HB3	17:BB:106:TRP:O	2.14	0.48
17:BB:394:VAL:HG23	17:BB:679:HIS:HB2	1.95	0.48
17:BB:509:VAL:HG13	17:BB:515:LYS:HE2	1.96	0.48
18:BC:47:PRO:HD3	18:BC:53:LEU:HG	1.96	0.48
23:E2:164:LYS:HZ2	32:SA:1575:G:H5"	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SA:325:G:H4'	39:SM:83:THR:HG21	1.95	0.48
32:SA:377:G:H5"	32:SA:378:A:H3'	1.95	0.48
32:SA:1482:C:O2'	42:SR:72:GLY:O	2.29	0.48
55:UC:39:UNK:O	55:UC:43:UNK:N	2.47	0.48
14:AG:404:UNK:HA	14:AG:415:UNK:HA	1.94	0.48
17:BB:88:HIS:CD2	17:BB:90:ASP:H	2.31	0.48
19:BD:555:TRP:HZ3	19:BD:591:LEU:HD22	1.79	0.48
23:E2:178:VAL:HG23	23:E2:204:VAL:HG23	1.96	0.48
32:SA:1509:C:O2'	52:U5:192:ASN:ND2	2.46	0.48
35:SG:52:GLU:HA	35:SG:65:ARG:NH1	2.21	0.48
40:SO:30:SER:OG	40:SO:66:ILE:O	2.31	0.48
45:SZ:8:ARG:NH1	45:SZ:10:ARG:NH1	2.61	0.48
1:3A:18:G:H2'	1:3A:19:A:H8	1.77	0.48
1:3A:46:U:H2'	1:3A:47:G:H8	1.79	0.48
15:B1:175:THR:O	15:B1:179:GLN:NE2	2.46	0.48
16:BA:597:ASN:ND2	16:BA:681:VAL:O	2.46	0.48
18:BC:83:GLN:NE2	18:BC:103:SER:O	2.46	0.48
22:CB:235:LEU:O	22:CB:239:LEU:HB2	2.13	0.48
22:CB:624:CYS:SG	22:CB:625:ASP:N	2.87	0.48
22:CB:1086:ASN:O	22:CB:1090:THR:OG1	2.26	0.48
32:SA:897:C:O2'	32:SA:914:G:N2	2.46	0.48
2:3B:88:ILE:HD13	2:3B:141:TYR:HD2	1.79	0.48
7:5A:241:U:OP2	7:5A:266:U:N3	2.47	0.48
14:AG:354:UNK:HA	14:AG:364:UNK:HA	1.94	0.48
15:B1:231:LEU:HB2	15:B1:247:LYS:O	2.13	0.48
16:BA:434:ASN:HB2	16:BA:450:LEU:HB2	1.94	0.48
16:BA:791:HIS:HB3	16:BA:794:PHE:HB3	1.96	0.48
18:BC:220:ILE:HD11	18:BC:260:THR:HG21	1.96	0.48
18:BC:507:ALA:HB2	18:BC:517:ILE:HG12	1.96	0.48
19:BD:290:LEU:HD22	19:BD:339:ILE:HD11	1.96	0.48
20:BE:530:ASP:OD1	20:BE:532:ASN:N	2.40	0.48
33:SC:66:VAL:HB	33:SC:86:LEU:HB2	1.96	0.48
42:SR:58:ASP:O	42:SR:60:PHE:N	2.47	0.48
52:U5:116:THR:HG22	52:U5:120:LYS:HZ3	1.78	0.48
7:5A:406:U:O2	7:5A:451:G:N2	2.47	0.48
12:AE:307:LYS:NZ	12:AE:376:GLU:OE2	2.47	0.48
16:BA:111:PHE:O	16:BA:121:ILE:HA	2.13	0.48
16:BA:423:ARG:NH2	16:BA:461:GLN:O	2.47	0.48
18:BC:445:ILE:HD12	18:BC:451:PRO:HG3	1.96	0.48
18:BC:460:ASP:OD2	18:BC:464:LYS:NZ	2.44	0.48
22:CB:173:ASN:OD1	22:CB:223:ARG:NH2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:1135:ASN:HD21	22:CB:1137:ASN:HD22	1.62	0.48
32:SA:1650:U:H2'	32:SA:1651:A:C8	2.49	0.48
36:SI:148:LYS:NZ	36:SI:150:GLN:HG3	2.28	0.48
14:AG:396:UNK:CB	14:AG:404:UNK:O	2.61	0.47
18:BC:146:THR:HG22	18:BC:168:THR:HB	1.96	0.47
18:BC:206:GLU:HA	18:BC:209:LEU:HB2	1.96	0.47
21:CA:183:ASP:O	21:CA:187:HIS:CB	2.62	0.47
39:SM:33:ARG:NH1	39:SM:61:THR:HG21	2.29	0.47
53:UA:1610:UNK:O	53:UA:1614:UNK:N	2.47	0.47
6:3G:25:GLN:OE1	6:3G:29:ASN:ND2	2.43	0.47
16:BA:501:SER:OG	16:BA:508:GLN:NE2	2.48	0.47
17:BB:94:LEU:HD12	17:BB:106:TRP:HB2	1.96	0.47
17:BB:629:ASN:ND2	17:BB:642:TRP:O	2.47	0.47
18:BC:222:LEU:HB2	18:BC:235:LYS:H	1.79	0.47
18:BC:237:LEU:HB3	18:BC:239:VAL:HG22	1.96	0.47
21:CA:87:LEU:HD21	21:CA:90:ASN:HD22	1.79	0.47
32:SA:128:U:OP1	32:SA:264:G:O2'	2.29	0.47
34:SF:10:LYS:HA	34:SF:27:TYR:HA	1.95	0.47
34:SF:104:ASP:N	34:SF:108:ARG:O	2.46	0.47
36:SI:154:LEU:HB2	36:SI:185:ILE:HG13	1.96	0.47
37:SJ:101:ILE:HD12	37:SJ:184:LEU:HD21	1.96	0.47
55:UC:395:UNK:O	55:UC:399:UNK:N	2.47	0.47
1:3A:85:G:N7	4:3E:361:ARG:NH1	2.61	0.47
2:3B:291:GLN:OE1	2:3B:294:ARG:NH2	2.47	0.47
2:3C:223:ASP:OD2	2:3C:226:HIS:ND1	2.36	0.47
9:AB:442:UNK:O	9:AB:446:UNK:CB	2.62	0.47
10:AC:617:UNK:O	10:AC:621:UNK:CB	2.63	0.47
13:AF:492:UNK:O	13:AF:496:UNK:CB	2.61	0.47
17:BB:268:LYS:HA	17:BB:337:LYS:HE2	1.96	0.47
17:BB:851:PRO:O	17:BB:855:LYS:HB2	2.15	0.47
21:CA:10:LYS:HB2	22:CB:1210:GLU:HG2	1.95	0.47
27:MB:222:ILE:HA	27:MB:234:ARG:O	2.14	0.47
32:SA:628:G:H21	32:SA:971:A:H62	1.62	0.47
32:SA:947:U:H2'	32:SA:948:G:H8	1.77	0.47
32:SA:1118:G:H2'	32:SA:1119:G:C8	2.48	0.47
32:SA:1645:G:N2	32:SA:1756:A:N1	2.62	0.47
34:SF:19:LEU:HD21	34:SF:108:ARG:HH21	1.80	0.47
3:3D:194:ARG:NH2	3:3D:197:GLU:OE1	2.48	0.47
4:3E:161:VAL:HA	4:3E:164:ILE:HD12	1.96	0.47
5:3F:189:THR:O	5:3F:196:LEU:HA	2.14	0.47
5:3F:547:HIS:HB3	5:3F:551:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5A:271:G:H2'	7:5A:272:A:H8	1.78	0.47
7:5A:455:C:H2'	7:5A:456:U:C6	2.49	0.47
12:AE:333:LEU:O	12:AE:337:ASP:HB2	2.14	0.47
13:AF:199:UNK:O	13:AF:212:UNK:CB	2.63	0.47
14:AG:29:UNK:O	14:AG:36:UNK:HA	2.14	0.47
14:AG:36:UNK:O	14:AG:48:UNK:HA	2.14	0.47
16:BA:604:TYR:HE1	16:BA:610:VAL:HG22	1.78	0.47
18:BC:724:LEU:HD22	18:BC:727:ALA:HB3	1.95	0.47
21:CA:185:HIS:O	21:CA:189:ALA:CB	2.62	0.47
22:CB:419:TYR:HE1	22:CB:499:LEU:HD22	1.78	0.47
25:K1:178:LYS:HZ3	32:SA:904:G:H5"	1.79	0.47
27:MB:111:PHE:HA	27:MB:113:ASN:H	1.79	0.47
32:SA:1511:U:H2'	32:SA:1512:G:C8	2.49	0.47
38:SK:163:PRO:HA	38:SK:165:GLY:H	1.80	0.47
49:U1:276:UNK:N	49:U1:280:UNK:O	2.48	0.47
4:3E:158:LYS:HG3	4:3E:380:ARG:HH22	1.79	0.47
4:3E:224:SER:HA	4:3E:232:GLU:OE2	2.14	0.47
8:AA:401:UNK:O	8:AA:414:UNK:CB	2.63	0.47
11:AD:411:UNK:O	11:AD:415:UNK:CB	2.63	0.47
17:BB:180:THR:HG22	17:BB:186:ILE:HG23	1.96	0.47
18:BC:443:PRO:HB2	18:BC:450:TYR:HB3	1.96	0.47
20:BE:35:ASN:ND2	20:BE:53:CYS:SG	2.83	0.47
22:CB:232:LEU:O	22:CB:236:THR:OG1	2.22	0.47
22:CB:367:ARG:O	22:CB:371:GLN:HB2	2.14	0.47
30:R1:118:PHE:O	30:R1:165:GLU:HA	2.14	0.47
1:3A:82:G:N3	1:3A:327:G:N2	2.62	0.47
7:5A:133:U:H2'	7:5A:134:A:C8	2.50	0.47
10:AC:571:UNK:O	10:AC:575:UNK:CB	2.63	0.47
18:BC:310:THR:HB	18:BC:363:ARG:HH12	1.79	0.47
20:BE:429:ASN:N	20:BE:429:ASN:OD1	2.47	0.47
21:CA:185:HIS:O	21:CA:189:ALA:HB2	2.13	0.47
22:CB:218:ASP:OD2	22:CB:227:LYS:NZ	2.47	0.47
29:P1:202:ILE:O	29:P1:206:ALA:HB3	2.15	0.47
32:SA:1512:G:H2'	32:SA:1513:G:C8	2.48	0.47
42:SR:13:LYS:HG3	42:SR:14:LYS:H	1.79	0.47
44:SY:127:VAL:HG13	44:SY:132:LEU:HD21	1.96	0.47
4:3E:45:ALA:HB1	4:3E:83:LYS:NZ	2.29	0.47
5:3F:157:LEU:HA	5:3F:191:SER:HA	1.96	0.47
5:3F:367:LYS:HA	5:3F:370:ARG:HD3	1.97	0.47
5:3F:537:PHE:O	5:3F:567:VAL:HA	2.13	0.47
6:3G:26:GLN:HA	6:3G:29:ASN:HD22	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:AB:220:UNK:CB	9:AB:234:UNK:O	2.63	0.47
14:AG:5:UNK:CB	14:AG:569:UNK:O	2.63	0.47
14:AG:39:UNK:HA	14:AG:45:UNK:HA	1.96	0.47
14:AG:204:UNK:N	14:AG:208:UNK:O	2.48	0.47
14:AG:507:UNK:N	14:AG:520:UNK:O	2.45	0.47
15:B1:974:GLY:HA2	15:B1:990:ALA:O	2.14	0.47
16:BA:385:GLU:OE1	16:BA:421:ASN:ND2	2.48	0.47
16:BA:717:LEU:HG	16:BA:745:LEU:HD23	1.95	0.47
18:BC:406:ALA:HB2	18:BC:440:VAL:HB	1.96	0.47
19:BD:359:LYS:O	19:BD:368:THR:OG1	2.28	0.47
20:BE:60:ILE:HB	20:BE:70:PHE:HB2	1.95	0.47
20:BE:183:VAL:HG12	20:BE:188:VAL:HG22	1.96	0.47
22:CB:240:LEU:HD13	22:CB:254:LEU:HD22	1.96	0.47
22:CB:530:GLN:HB2	22:CB:695:GLN:HB2	1.97	0.47
23:E2:90:ASP:N	23:E2:90:ASP:OD1	2.47	0.47
24:E4:235:UNK:CB	24:E4:239:UNK:O	2.63	0.47
25:K1:141:ARG:HG2	25:K1:144:ARG:HH11	1.79	0.47
30:R1:319:ASP:OD2	30:R1:321:ARG:HD3	2.15	0.47
32:SA:1064:G:H2'	32:SA:1065:A:H8	1.79	0.47
33:SC:135:LEU:HB3	33:SC:217:LEU:HG	1.96	0.47
34:SF:180:LEU:N	34:SF:229:GLY:O	2.44	0.47
34:SF:199:GLU:OE1	34:SF:201:HIS:NE2	2.44	0.47
34:SF:211:LYS:HB3	34:SF:217:THR:HG22	1.96	0.47
37:SJ:48:THR:OG1	37:SJ:51:GLY:O	2.32	0.47
7:5A:504:U:H2'	7:5A:505:G:H8	1.79	0.47
14:AG:163:UNK:N	14:AG:167:UNK:O	2.46	0.47
16:BA:77:GLY:O	16:BA:95:PHE:N	2.42	0.47
16:BA:111:PHE:HB3	16:BA:122:TRP:HB2	1.97	0.47
17:BB:80:ALA:HB2	17:BB:657:GLN:HG3	1.97	0.47
17:BB:195:GLN:HE22	17:BB:197:ILE:HB	1.79	0.47
17:BB:447:LEU:O	17:BB:454:LEU:HA	2.15	0.47
18:BC:85:LEU:O	18:BC:99:MET:HB3	2.14	0.47
19:BD:577:LEU:O	19:BD:588:LEU:HA	2.14	0.47
21:CA:60:LEU:HA	21:CA:92:GLU:OE2	2.13	0.47
21:CA:62:SER:HB2	21:CA:90:ASN:HD21	1.80	0.47
22:CB:117:LYS:HE3	22:CB:120:HIS:HE1	1.79	0.47
32:SA:1064:G:O2'	33:SC:204:ILE:O	2.32	0.47
33:SC:76:SER:OG	33:SC:78:ASP:OD1	2.32	0.47
34:SF:75:LYS:NZ	34:SF:77:ARG:NH1	2.46	0.47
37:SJ:64:ASN:HA	37:SJ:75:LYS:HA	1.97	0.47
55:UC:306:UNK:O	55:UC:310:UNK:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:82:G:N2	1:3A:327:G:O2'	2.44	0.47
3:3D:156:HIS:O	3:3D:160:ARG:CB	2.63	0.47
7:5A:357:G:H2'	7:5A:358:G:H8	1.80	0.47
14:AG:179:UNK:HA	14:AG:194:UNK:O	2.15	0.47
14:AG:509:UNK:O	14:AG:518:UNK:N	2.47	0.47
16:BA:751:ILE:O	16:BA:755:TYR:CB	2.63	0.47
18:BC:622:ALA:H	18:BC:635:ALA:HB3	1.80	0.47
23:E1:105:ASN:HB2	23:E1:110:LEU:HD23	1.97	0.47
23:E1:113:TYR:HE1	23:E1:123:GLU:HG3	1.80	0.47
23:E1:232:LEU:HD21	23:E2:103:PRO:HG3	1.96	0.47
30:R1:176:GLN:HG3	30:R1:305:LYS:HB3	1.96	0.47
32:SA:1679:G:H1'	32:SA:1722:A:H61	1.80	0.47
39:SM:4:GLU:HB3	39:SM:5:LEU:HB2	1.97	0.47
52:U5:10:SER:OG	52:U5:217:GLN:NE2	2.38	0.47
52:U5:61:LYS:HB3	52:U5:64:LEU:HD21	1.96	0.47
10:AC:410:UNK:O	10:AC:414:UNK:CB	2.63	0.47
15:B1:998:SER:OG	55:UC:171:UNK:O	2.33	0.47
17:BB:426:ARG:HD2	17:BB:457:PHE:HB3	1.97	0.47
20:BE:287:LEU:HD13	20:BE:290:ILE:HD13	1.97	0.47
20:BE:287:LEU:HD22	20:BE:290:ILE:HG21	1.97	0.47
22:CB:841:ASN:HA	22:CB:850:PHE:O	2.15	0.47
32:SA:445:A:C4	32:SA:525:A:H4'	2.50	0.47
32:SA:899:G:H2'	32:SA:900:A:H8	1.79	0.47
33:SC:137:ILE:HD11	33:SC:172:LEU:HD13	1.97	0.47
33:SC:191:GLU:OE1	33:SC:194:ASN:ND2	2.48	0.47
34:SF:181:VAL:HA	34:SF:227:VAL:HA	1.96	0.47
36:SI:14:THR:OG1	36:SI:15:GLU:N	2.47	0.47
52:U5:57:ILE:HG13	52:U5:222:PHE:HD1	1.80	0.47
10:AC:612:UNK:O	10:AC:616:UNK:CB	2.63	0.46
14:AG:149:UNK:HA	14:AG:162:UNK:O	2.15	0.46
35:SG:80:LYS:HZ2	35:SG:83:ARG:HH12	1.64	0.46
36:SI:94:ALA:HB3	36:SI:128:ASP:OD2	2.15	0.46
51:U4:152:ILE:HG23	51:U4:171:PRO:HB2	1.97	0.46
55:UC:5:UNK:O	55:UC:9:UNK:N	2.49	0.46
2:3B:285:VAL:O	2:3B:289:GLU:HB2	2.15	0.46
10:AC:551:UNK:O	10:AC:555:UNK:CB	2.63	0.46
15:B1:618:PHE:O	15:B1:622:ALA:CB	2.62	0.46
20:BE:22:LYS:HB3	20:BE:661:LYS:HE2	1.96	0.46
20:BE:97:LYS:HZ1	20:BE:111:GLU:CD	2.17	0.46
20:BE:517:MET:HB3	20:BE:529:TYR:HB2	1.96	0.46
22:CB:566:ILE:HG23	22:CB:686:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R1:249:SER:O	30:R1:253:GLY:CA	2.62	0.46
44:SY:74:VAL:CA	44:SY:82:LYS:HZ2	2.28	0.46
51:U4:155:THR:OG1	51:U4:156:ASN:N	2.49	0.46
7:5A:350:A:H2'	7:5A:351:A:C8	2.51	0.46
8:AA:394:UNK:O	8:AA:401:UNK:HA	2.16	0.46
16:BA:692:ALA:HB2	16:BA:705:SER:H	1.79	0.46
17:BB:64:SER:O	17:BB:76:GLY:N	2.45	0.46
17:BB:200:HIS:CD2	17:BB:236:ASP:HB3	2.50	0.46
21:CA:211:GLY:HA2	21:CA:214:LEU:HD22	1.98	0.46
27:MB:106:GLU:HG2	27:MB:252:PRO:HG2	1.97	0.46
29:P1:143:PRO:HA	29:P1:144:LYS:HA	1.66	0.46
32:SA:513:U:H2'	32:SA:514:G:C8	2.50	0.46
32:SA:1715:G:H8	32:SA:1715:G:OP2	1.98	0.46
35:SG:42:LEU:HD21	35:SG:45:LYS:HZ3	1.79	0.46
6:3G:64:LEU:HD21	6:3G:98:ILE:HD13	1.97	0.46
9:AB:457:UNK:O	9:AB:461:UNK:CB	2.63	0.46
18:BC:555:LYS:HE2	18:BC:576:ASN:HA	1.98	0.46
21:CA:133:SER:O	21:CA:137:CYS:HB3	2.14	0.46
22:CB:909:TYR:OH	22:CB:935:GLU:O	2.32	0.46
23:E1:39:LYS:HB2	23:E1:199:ASP:HA	1.97	0.46
36:SI:14:THR:OG1	36:SI:15:GLU:OE1	2.33	0.46
45:SZ:91:LEU:O	45:SZ:96:LEU:N	2.47	0.46
55:UC:52:UNK:O	55:UC:56:UNK:N	2.49	0.46
7:5A:71:U:H2'	7:5A:72:G:C8	2.51	0.46
10:AC:544:UNK:O	10:AC:548:UNK:CB	2.64	0.46
13:AF:261:UNK:N	13:AF:275:UNK:O	2.48	0.46
14:AG:547:UNK:N	14:AG:561:UNK:O	2.48	0.46
15:B1:49:PHE:HB2	15:B1:92:ARG:NH1	2.29	0.46
15:B1:620:LYS:O	15:B1:624:LYS:HB3	2.16	0.46
16:BA:15:TYR:HE1	16:BA:346:ASP:HA	1.80	0.46
17:BB:125:THR:H	17:BB:140:SER:HA	1.80	0.46
17:BB:343:TRP:N	17:BB:356:THR:OG1	2.48	0.46
20:BE:872:LEU:HG	20:BE:878:PHE:HE1	1.79	0.46
32:SA:351:C:H2'	39:SM:102:LYS:H	1.80	0.46
34:SF:147:ILE:HG21	34:SF:169:ILE:HG13	1.97	0.46
35:SG:92:ARG:NH2	35:SG:169:ASN:OD1	2.49	0.46
1:3A:64:A:H5'	20:BE:392:ARG:HH12	1.78	0.46
12:AE:258:HIS:HE1	12:AE:282:ILE:HG23	1.80	0.46
16:BA:363:ALA:HB1	16:BA:390:VAL:HB	1.96	0.46
19:BD:422:ILE:HD11	19:BD:437:LEU:HD13	1.97	0.46
23:E2:98:THR:OG1	23:E2:235:SER:OG	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K1:128:ILE:HG21	25:K1:171:VAL:HG23	1.97	0.46
32:SA:10:G:H2'	32:SA:11:A:H8	1.81	0.46
32:SA:128:U:O2	32:SA:181:A:N6	2.45	0.46
32:SA:1663:G:N2	32:SA:1738:U:O2	2.37	0.46
36:SI:24:PHE:O	36:SI:28:GLU:N	2.45	0.46
10:AC:641:UNK:O	10:AC:645:UNK:CB	2.64	0.46
18:BC:407:SER:OG	18:BC:408:LYS:N	2.49	0.46
18:BC:706:ARG:NE	18:BC:716:ILE:O	2.46	0.46
19:BD:489:GLY:HA2	19:BD:518:ILE:HD12	1.97	0.46
22:CB:1102:LEU:HB2	22:CB:1180:ASN:HB3	1.98	0.46
23:E2:77:LEU:O	23:E2:82:ARG:N	2.40	0.46
30:R1:177:PRO:HD2	30:R1:304:GLY:HA2	1.97	0.46
32:SA:396:G:H22	32:SA:399:A:H5'	1.81	0.46
55:UC:923:UNK:O	55:UC:927:UNK:N	2.49	0.46
12:AE:364:ASN:ND2	12:AE:396:ASP:OD2	2.49	0.46
32:SA:1537:C:H1'	32:SA:1569:A:OP2	2.16	0.46
33:SC:61:LEU:HD12	33:SC:62:LYS:H	1.81	0.46
44:SY:70:LYS:HG2	44:SY:93:LEU:HD22	1.98	0.46
44:SY:116:ASP:OD1	44:SY:116:ASP:N	2.48	0.46
55:UC:282:UNK:O	55:UC:286:UNK:N	2.49	0.46
5:3F:366:GLN:HG3	5:3F:370:ARG:NH1	2.31	0.46
13:AF:427:UNK:O	13:AF:431:UNK:CB	2.64	0.46
15:B1:250:ILE:HG22	15:B1:791:ILE:HB	1.97	0.46
16:BA:112:ALA:HB1	16:BA:152:LEU:HD21	1.98	0.46
19:BD:556:PRO:HB2	19:BD:562:LEU:HD11	1.98	0.46
22:CB:761:ARG:HD2	22:CB:899:LEU:HD22	1.97	0.46
26:MA:102:THR:HG23	26:MA:105:ALA:H	1.80	0.46
37:SJ:66:SER:HA	37:SJ:73:SER:HA	1.98	0.46
1:3A:202:G:H1	1:3A:247:U:H3	1.64	0.46
2:3B:244:VAL:HG12	2:3B:246:GLN:HG2	1.97	0.46
5:3F:420:GLY:HA2	5:3F:475:ILE:HD11	1.97	0.46
7:5A:438:U:H2'	7:5A:439:A:C8	2.48	0.46
15:B1:567:TRP:HZ2	30:R1:315:LYS:HZ2	1.62	0.46
17:BB:357:THR:OG1	17:BB:361:THR:O	2.28	0.46
17:BB:449:THR:OG1	17:BB:450:ARG:N	2.49	0.46
27:MB:95:ASP:OD1	27:MB:95:ASP:N	2.40	0.46
28:MC:57:UNK:O	28:MC:61:UNK:CB	2.64	0.46
30:R1:248:GLN:HE22	30:R1:250:LYS:HA	1.80	0.46
33:SC:69:CYS:HB3	33:SC:72:ASP:OD2	2.16	0.46
41:SP:16:VAL:HG12	41:SP:18:ARG:HG3	1.98	0.46
42:SR:34:SER:HB3	42:SR:38:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:AD:414:UNK:O	11:AD:418:UNK:CB	2.64	0.45
12:AE:218:ILE:HG23	12:AE:263:VAL:HG11	1.99	0.45
15:B1:561:GLU:HB3	30:R1:320:GLU:OE2	2.16	0.45
16:BA:497:ILE:HG21	16:BA:542:PHE:HZ	1.80	0.45
16:BA:692:ALA:HB1	16:BA:704:TYR:H	1.81	0.45
18:BC:307:SER:OG	18:BC:308:ASP:N	2.47	0.45
18:BC:443:PRO:HA	18:BC:499:VAL:HG21	1.98	0.45
30:R1:82:VAL:O	30:R1:110:SER:OG	2.35	0.45
34:SF:75:LYS:HZ2	34:SF:75:LYS:HB3	1.80	0.45
34:SF:221:ARG:HH11	34:SF:223:ASN:HB2	1.81	0.45
53:UA:1205:UNK:O	53:UA:1209:UNK:N	2.49	0.45
1:3A:204:U:H2'	1:3A:205:G:C8	2.52	0.45
2:3B:193:VAL:HG13	2:3B:218:ILE:HD13	1.97	0.45
4:3E:76:LEU:HD11	4:3E:98:ILE:HG12	1.98	0.45
6:3H:56:ALA:HB3	6:3H:82:PRO:HA	1.97	0.45
7:5A:379:A:H2'	7:5A:380:A:C8	2.52	0.45
13:AF:505:UNK:O	13:AF:509:UNK:CB	2.65	0.45
14:AG:202:UNK:CB	14:AG:211:UNK:O	2.64	0.45
14:AG:275:UNK:O	14:AG:282:UNK:HA	2.16	0.45
17:BB:661:TRP:HE1	17:BB:677:HIS:HB2	1.81	0.45
19:BD:241:ALA:HB3	19:BD:585:LYS:HE2	1.97	0.45
31:S1:301:UNK:CB	31:S1:310:UNK:O	2.64	0.45
32:SA:335:U:O2'	39:SM:129:ARG:NH1	2.49	0.45
32:SA:1602:C:H2'	32:SA:1603:U:C6	2.52	0.45
13:AF:110:UNK:CB	13:AF:118:UNK:O	2.65	0.45
20:BE:485:THR:HG22	20:BE:497:LYS:HG3	1.99	0.45
22:CB:625:ASP:OD2	22:CB:722:LEU:HB2	2.16	0.45
27:MB:113:ASN:OD1	27:MB:113:ASN:N	2.50	0.45
32:SA:510:G:H8	32:SA:510:G:OP2	1.99	0.45
34:SF:179:LYS:HE3	34:SF:230:GLU:OE2	2.15	0.45
43:SX:18:GLU:OE2	43:SX:65:LEU:HD12	2.17	0.45
2:3B:259:MET:SD	3:3D:132:ARG:NH1	2.90	0.45
3:3D:280:SER:OG	4:3E:264:GLU:OE2	2.29	0.45
4:3E:76:LEU:HA	4:3E:84:LYS:NZ	2.31	0.45
4:3E:293:GLU:O	4:3E:297:ALA:CB	2.64	0.45
7:5A:191:U:H2'	7:5A:192:G:C8	2.51	0.45
7:5A:536:A:H2'	7:5A:537:G:C8	2.52	0.45
14:AG:132:UNK:HA	14:AG:133:UNK:HA	1.74	0.45
16:BA:369:ILE:HG13	16:BA:383:PHE:HB2	1.97	0.45
19:BD:388:HIS:HD2	19:BD:391:SER:H	1.62	0.45
22:CB:168:ILE:HD12	22:CB:171:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:E4:152:UNK:HA	24:E4:158:UNK:HA	1.99	0.45
29:P1:205:ILE:HA	29:P1:250:LEU:HD13	1.98	0.45
32:SA:356:G:H2'	32:SA:357:G:C8	2.52	0.45
32:SA:1157:A:H3'	32:SA:1160:A:H62	1.81	0.45
35:SG:42:LEU:HD21	35:SG:45:LYS:HZ1	1.81	0.45
42:SR:102:LYS:HZ2	42:SR:106:LYS:NZ	2.12	0.45
1:3A:67:G:H1	7:5A:286:U:H3	1.63	0.45
6:3G:33:LEU:HD11	6:3G:100:ALA:HB1	1.98	0.45
7:5A:513:G:O6	7:5A:523:U:O4	2.34	0.45
13:AF:494:UNK:O	13:AF:498:UNK:CB	2.65	0.45
14:AG:243:UNK:CB	14:AG:252:UNK:O	2.65	0.45
15:B1:235:GLU:OE2	15:B1:240:GLN:NE2	2.45	0.45
19:BD:363:LEU:HB2	19:BD:418:LYS:HZ1	1.81	0.45
30:R1:245:LEU:O	30:R1:257:PHE:HA	2.17	0.45
39:SM:128:CYS:SG	39:SM:129:ARG:N	2.90	0.45
7:5A:290:G:H2'	7:5A:291:G:H8	1.81	0.45
10:AC:596:UNK:O	10:AC:600:UNK:CB	2.65	0.45
14:AG:108:UNK:HA	14:AG:122:UNK:HA	1.98	0.45
16:BA:368:LYS:HG2	16:BA:384:GLU:HG2	1.98	0.45
17:BB:576:VAL:HA	17:BB:592:SER:HA	1.98	0.45
20:BE:482:GLY:HA2	20:BE:505:VAL:HG23	1.98	0.45
21:CA:94:GLY:CA	21:CA:121:ARG:HH12	2.30	0.45
25:K1:90:ASP:OD1	41:SP:103:ARG:NH2	2.50	0.45
32:SA:352:A:OP2	32:SA:352:A:H8	1.99	0.45
32:SA:394:C:H2'	32:SA:395:U:H6	1.82	0.45
32:SA:1499:G:N2	52:U5:194:ASP:OD2	2.49	0.45
33:SC:39:GLU:HG3	33:SC:40:ASN:H	1.81	0.45
1:3A:59:G:C8	1:3A:61:G:H5'	2.51	0.45
1:3A:330:A:H2'	1:3A:331:A:C8	2.51	0.45
4:3E:376:LEU:HD13	6:3H:65:LEU:HB2	1.99	0.45
9:AB:37:UNK:CB	9:AB:46:UNK:O	2.65	0.45
9:AB:451:UNK:O	9:AB:454:UNK:N	2.49	0.45
10:AC:235:UNK:CB	10:AC:239:UNK:O	2.65	0.45
18:BC:270:ILE:HA	18:BC:277:VAL:HA	1.98	0.45
22:CB:1059:PRO:O	22:CB:1063:ARG:CB	2.64	0.45
23:E2:180:LEU:HD13	23:E2:237:ALA:HB1	1.98	0.45
32:SA:863:A:OP1	43:SX:57:ARG:NH2	2.40	0.45
33:SC:144:ARG:NH2	33:SC:207:LEU:O	2.40	0.45
33:SC:202:LYS:HG2	33:SC:206:PRO:HA	1.99	0.45
37:SJ:48:THR:OG1	37:SJ:52:ASN:O	2.29	0.45
39:SM:97:TYR:HB3	39:SM:99:ARG:NH1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:UC:310:UNK:O	55:UC:314:UNK:N	2.50	0.45
17:BB:163:LYS:O	32:SA:1764:C:O2'	2.33	0.45
18:BC:80:SER:O	18:BC:84:LEU:HB2	2.17	0.45
22:CB:82:ALA:O	22:CB:86:TYR:HB2	2.17	0.45
22:CB:673:SER:N	22:CB:717:ALA:O	2.45	0.45
22:CB:784:LEU:O	22:CB:854:VAL:HA	2.17	0.45
38:SK:113:VAL:HG12	38:SK:119:ALA:HB2	1.99	0.45
1:3A:47:G:H2'	1:3A:48:A:H8	1.82	0.45
5:3F:479:TYR:HE2	5:3F:526:VAL:HB	1.82	0.45
7:5A:394:U:O4	7:5A:463:A:N6	2.49	0.45
9:AB:16:UNK:O	9:AB:29:UNK:N	2.49	0.45
9:AB:112:UNK:CB	9:AB:116:UNK:O	2.65	0.45
16:BA:47:SER:HB3	16:BA:50:PHE:CE2	2.52	0.45
16:BA:446:CYS:HA	16:BA:456:HIS:O	2.16	0.45
19:BD:305:SER:OG	19:BD:306:ASN:N	2.50	0.45
22:CB:153:PHE:HA	22:CB:156:LYS:HZ3	1.80	0.45
22:CB:359:PHE:O	22:CB:363:THR:OG1	2.27	0.45
32:SA:323:A:H61	32:SA:345:U:H3	1.65	0.45
32:SA:356:G:H2'	32:SA:357:G:H8	1.82	0.45
32:SA:444:C:N4	32:SA:459:G:OP2	2.48	0.45
32:SA:1739:C:H2'	32:SA:1740:A:C8	2.51	0.45
40:SO:67:THR:HG21	40:SO:74:ILE:HD11	1.97	0.45
1:3A:326:U:OP1	6:3H:46:ARG:NH1	2.48	0.45
2:3C:106:LEU:O	2:3C:144:TRP:HB3	2.17	0.45
3:3D:63:LEU:HD22	3:3D:157:ALA:HB1	1.99	0.45
5:3F:160:ILE:HG23	5:3F:525:GLN:HG2	1.98	0.45
5:3F:541:ALA:HB3	5:3F:564:TYR:HB3	1.98	0.45
7:5A:228:A:H2'	7:5A:229:A:C8	2.52	0.45
7:5A:445:U:H2'	7:5A:446:U:C6	2.52	0.45
9:AB:429:UNK:O	9:AB:433:UNK:CB	2.64	0.45
10:AC:601:UNK:O	10:AC:605:UNK:CB	2.65	0.45
18:BC:90:LEU:O	18:BC:92:THR:N	2.50	0.45
18:BC:174:VAL:HB	18:BC:184:HIS:O	2.17	0.45
18:BC:494:ILE:HA	18:BC:510:SER:HA	1.99	0.45
21:CA:5:ASP:HA	21:CA:149:ALA:HB2	1.99	0.45
21:CA:199:GLN:HB3	21:CA:200:GLU:H	1.54	0.45
22:CB:433:ASP:HB2	22:CB:489:LYS:HZ1	1.82	0.45
32:SA:187:G:H22	32:SA:197:A:H2'	1.81	0.45
32:SA:524:U:C4	45:SZ:93:ARG:NH1	2.85	0.45
32:SA:546:U:H2'	32:SA:547:U:C6	2.51	0.45
40:SO:67:THR:HG22	40:SO:69:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:264:GLN:HE22	2:3B:322:ARG:HA	1.82	0.44
3:3D:121:ASN:HA	3:3D:122:GLU:HA	1.81	0.44
5:3F:239:ILE:HA	5:3F:255:GLY:HA3	1.99	0.44
7:5A:191:U:H2'	7:5A:192:G:H8	1.82	0.44
14:AG:436:UNK:HA	14:AG:445:UNK:O	2.18	0.44
15:B1:949:LYS:HG2	15:B1:986:HIS:HE1	1.82	0.44
17:BB:439:LEU:HD23	17:BB:443:LEU:HB2	1.98	0.44
18:BC:557:VAL:HG22	18:BC:578:VAL:HG11	1.99	0.44
19:BD:383:TRP:HZ3	19:BD:397:GLY:HA3	1.81	0.44
19:BD:481:TRP:HE1	19:BD:547:PRO:HB3	1.82	0.44
22:CB:127:PHE:HE1	22:CB:248:LEU:HD13	1.82	0.44
32:SA:1054:U:H3	32:SA:1065:A:H61	1.65	0.44
33:SC:202:LYS:NZ	33:SC:206:PRO:HB3	2.31	0.44
36:SI:98:ILE:HG12	36:SI:121:VAL:HG11	1.99	0.44
52:U5:106:LEU:HD11	52:U5:135:LEU:HD21	1.99	0.44
5:3F:338:THR:OG1	5:3F:349:TRP:NE1	2.44	0.44
8:AA:189:UNK:O	8:AA:200:UNK:HA	2.17	0.44
10:AC:547:UNK:O	10:AC:551:UNK:CB	2.65	0.44
18:BC:14:PRO:HB3	18:BC:642:GLN:HG2	1.99	0.44
19:BD:257:HIS:HE2	19:BD:309:GLN:HG2	1.81	0.44
19:BD:326:LEU:HA	19:BD:335:GLN:HA	1.99	0.44
20:BE:97:LYS:HB3	20:BE:109:LEU:HD11	2.00	0.44
20:BE:847:LEU:O	20:BE:892:HIS:NE2	2.37	0.44
22:CB:649:TRP:HB2	22:CB:653:SER:HB2	1.99	0.44
22:CB:738:TYR:O	22:CB:742:PHE:CB	2.64	0.44
30:R1:86:SER:O	30:R1:116:ILE:HA	2.18	0.44
30:R1:138:MET:HA	30:R1:141:MET:HG2	1.99	0.44
32:SA:329:G:H2'	32:SA:330:G:C8	2.51	0.44
32:SA:1059:U:H6	32:SA:1060:U:H3	1.65	0.44
32:SA:1084:A:OP1	43:SX:19:LYS:NZ	2.43	0.44
32:SA:1156:C:H2'	32:SA:1157:A:C8	2.52	0.44
34:SF:124:GLY:HA2	34:SF:142:HIS:CE1	2.51	0.44
43:SX:81:VAL:O	43:SX:122:SER:OG	2.35	0.44
52:U5:147:SER:HA	52:U5:148:LYS:HA	1.61	0.44
55:UC:267:UNK:O	55:UC:271:UNK:N	2.50	0.44
55:UC:731:UNK:HA	55:UC:732:UNK:HA	1.81	0.44
5:3F:150:THR:HG21	5:3F:208:PRO:HD2	2.00	0.44
9:AB:496:UNK:O	9:AB:500:UNK:CB	2.65	0.44
10:AC:54:UNK:O	10:AC:72:UNK:N	2.50	0.44
12:AE:19:ALA:HB2	12:AE:28:LEU:HD12	1.99	0.44
15:B1:236:LEU:O	15:B1:239:THR:OG1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B1:977:LYS:H	15:B1:989:ALA:HA	1.82	0.44
17:BB:857:LEU:HA	17:BB:860:ILE:HG22	2.00	0.44
18:BC:352:LYS:HG3	18:BC:377:LEU:HD11	1.99	0.44
18:BC:455:LEU:HD13	18:BC:465:LYS:HD3	1.98	0.44
18:BC:691:PRO:HG3	18:BC:742:ARG:HE	1.81	0.44
20:BE:796:LEU:O	20:BE:800:GLU:CB	2.53	0.44
22:CB:579:LYS:HB2	22:CB:618:ILE:HG22	1.99	0.44
23:E2:215:ASN:HB2	23:E2:218:ASP:OD2	2.17	0.44
32:SA:273:G:H2'	32:SA:274:G:C8	2.52	0.44
2:3C:110:ASN:HD21	2:3C:113:PRO:HA	1.82	0.44
15:B1:607:ASP:OD2	30:R1:15:GLN:HA	2.18	0.44
17:BB:412:GLY:HA2	17:BB:429:GLU:HB2	2.00	0.44
22:CB:777:ASP:O	22:CB:780:GLN:NE2	2.50	0.44
24:E4:182:UNK:O	24:E4:191:UNK:N	2.50	0.44
41:SP:84:ARG:HB2	41:SP:118:VAL:HG23	1.99	0.44
52:U5:37:HIS:ND1	52:U5:198:SER:OG	2.51	0.44
2:3B:100:ARG:HA	2:3B:101:GLY:HA2	1.66	0.44
5:3F:551:ARG:NH1	6:3G:94:SER:HA	2.32	0.44
7:5A:348:U:H3	7:5A:376:U:H3	1.66	0.44
12:AE:70:SER:HA	12:AE:74:PHE:HB2	1.99	0.44
14:AG:121:UNK:HA	14:AG:127:UNK:HA	1.99	0.44
15:B1:829:LEU:HD11	15:B1:896:PHE:HE2	1.83	0.44
16:BA:161:ILE:HB	16:BA:173:TRP:HB2	1.99	0.44
22:CB:921:ASP:HB2	22:CB:926:LEU:HD22	1.98	0.44
32:SA:1726:G:H2'	32:SA:1727:G:H8	1.82	0.44
33:SC:161:ILE:HG22	33:SC:165:ARG:NH1	2.32	0.44
36:SI:82:GLU:OE2	36:SI:89:HIS:HA	2.18	0.44
37:SJ:62:THR:HG22	37:SJ:77:ARG:HA	2.00	0.44
1:3A:329:C:H2'	1:3A:330:A:C8	2.53	0.44
7:5A:163:G:H8	7:5A:163:G:OP2	2.00	0.44
7:5A:349:G:H2'	7:5A:350:A:C8	2.53	0.44
12:AE:228:ASP:HB3	12:AE:268:LEU:HD11	1.99	0.44
16:BA:121:ILE:HD11	16:BA:140:ARG:HB2	1.98	0.44
17:BB:16:VAL:HG13	17:BB:18:ALA:H	1.82	0.44
17:BB:386:GLU:HB3	17:BB:390:GLN:HE22	1.83	0.44
20:BE:589:THR:HG23	20:BE:604:SER:HA	1.98	0.44
20:BE:616:THR:HG23	20:BE:618:GLY:H	1.83	0.44
22:CB:671:THR:OG1	22:CB:718:LYS:O	2.36	0.44
22:CB:1147:TYR:O	22:CB:1151:LYS:CB	2.59	0.44
23:E2:41:MET:O	23:E2:110:LEU:HA	2.18	0.44
32:SA:1083:G:H22	32:SA:1090:C:H42	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:SJ:6:ASP:OD1	37:SJ:6:ASP:N	2.50	0.44
52:U5:87:LEU:HA	52:U5:88:THR:HA	1.59	0.44
7:5A:538:C:H2'	7:5A:539:A:H8	1.82	0.44
14:AG:275:UNK:CB	14:AG:283:UNK:O	2.65	0.44
15:B1:283:LEU:HB3	15:B1:788:TYR:HD2	1.82	0.44
16:BA:121:ILE:HD12	16:BA:139:HIS:HB3	1.98	0.44
16:BA:145:HIS:CE1	16:BA:171:LYS:HD2	2.52	0.44
19:BD:248:HIS:HB3	19:BD:583:GLN:HA	2.00	0.44
20:BE:131:SER:HB3	20:BE:170:LEU:HD11	2.00	0.44
20:BE:225:THR:OG1	20:BE:227:THR:O	2.32	0.44
21:CA:188:MET:O	21:CA:192:GLU:HB2	2.17	0.44
22:CB:834:ASN:ND2	22:CB:863:TYR:OH	2.51	0.44
30:R1:30:PRO:HB3	30:R1:77:ARG:HG2	2.00	0.44
32:SA:1727:G:H2'	32:SA:1728:A:C8	2.52	0.44
51:U4:154:ALA:HA	51:U4:173:MET:HB2	2.00	0.44
4:3E:18:SER:HB2	4:3E:83:LYS:NZ	2.33	0.44
7:5A:242:C:H2'	7:5A:243:A:C8	2.51	0.44
12:AE:95:ASP:HA	12:AE:98:ILE:HD12	2.00	0.44
16:BA:263:VAL:HG22	16:BA:279:PHE:HE1	1.83	0.44
17:BB:88:HIS:HB3	17:BB:92:ASP:H	1.82	0.44
17:BB:201:ILE:HD12	18:BC:661:LEU:HD22	1.99	0.44
20:BE:668:ILE:H	20:BE:668:ILE:HG13	1.59	0.44
20:BE:904:ASP:N	20:BE:904:ASP:OD1	2.49	0.44
24:E4:76:UNK:O	24:E4:89:UNK:CB	2.65	0.44
32:SA:397:A:H5"	37:SJ:50:GLY:HA2	1.99	0.44
32:SA:491:C:H2'	32:SA:492:A:C8	2.53	0.44
32:SA:511:A:OP2	38:SK:176:ASN:ND2	2.51	0.44
2:3C:167:GLY:HA2	2:3C:191:GLU:HB2	2.00	0.44
7:5A:97:G:O2'	7:5A:154:A:N3	2.50	0.44
12:AE:82:ASP:HB3	12:AE:83:ARG:HD3	2.00	0.44
19:BD:369:ASN:HD22	19:BD:370:SER:H	1.65	0.44
19:BD:435:PHE:HZ	19:BD:440:ASN:HA	1.83	0.44
22:CB:173:ASN:HD22	32:SA:1686:C:H5"	1.83	0.44
22:CB:516:SER:HA	22:CB:522:LYS:HD2	2.00	0.44
32:SA:204:G:O6	32:SA:264:G:N2	2.43	0.44
42:SR:102:LYS:HZ2	42:SR:106:LYS:CE	2.31	0.44
45:SZ:56:SER:HB3	45:SZ:74:LEU:HB2	1.99	0.44
49:U1:80:UNK:N	49:U1:84:UNK:O	2.51	0.44
50:U2:27:UNK:O	50:U2:31:UNK:N	2.51	0.44
2:3B:106:LEU:HD12	2:3B:106:LEU:HA	1.82	0.43
3:3D:20:VAL:O	3:3D:53:PHE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3D:221:LEU:HD13	3:3D:275:ALA:HB3	2.00	0.43
3:3D:296:MET:HG2	3:3D:309:GLU:HA	2.00	0.43
4:3E:76:LEU:HD13	4:3E:101:LEU:HD22	1.98	0.43
5:3F:289:ARG:HB3	5:3F:292:SER:HB3	1.99	0.43
15:B1:281:GLU:HB2	15:B1:790:ARG:HB2	1.99	0.43
15:B1:943:LYS:HD2	32:SA:573:C:OP2	2.18	0.43
16:BA:53:GLU:HB2	16:BA:80:ILE:HD12	2.00	0.43
16:BA:505:ARG:HD3	32:SA:1617:U:OP2	2.18	0.43
16:BA:520:ALA:HB1	16:BA:583:ILE:HG22	1.99	0.43
17:BB:503:LYS:H	17:BB:511:GLY:HA3	1.83	0.43
18:BC:413:ILE:HD11	18:BC:429:LYS:HE2	2.00	0.43
19:BD:411:TYR:HB2	19:BD:424:ILE:HA	2.00	0.43
19:BD:486:SER:OG	19:BD:487:GLU:N	2.51	0.43
21:CA:192:GLU:O	21:CA:196:ALA:HB2	2.18	0.43
22:CB:775:ASP:OD2	22:CB:777:ASP:HB2	2.18	0.43
23:E1:111:GLN:NE2	23:E1:113:TYR:OH	2.51	0.43
23:E2:211:ARG:HH12	32:SA:1190:C:H3'	1.82	0.43
24:E4:182:UNK:N	24:E4:191:UNK:O	2.51	0.43
25:K1:178:LYS:HZ1	32:SA:904:G:H5"	1.81	0.43
32:SA:409:C:H2'	32:SA:410:A:H8	1.81	0.43
1:3A:1:G:N1	32:SA:1124:A:C2	2.86	0.43
10:AC:470:UNK:O	10:AC:474:UNK:CB	2.66	0.43
13:AF:260:UNK:HA	13:AF:276:UNK:HA	1.99	0.43
13:AF:507:UNK:O	13:AF:511:UNK:CB	2.66	0.43
18:BC:88:PHE:HE1	18:BC:95:VAL:HG22	1.83	0.43
18:BC:585:ASN:HD22	18:BC:627:ASN:HA	1.83	0.43
19:BD:297:THR:HG21	19:BD:356:GLU:HA	2.00	0.43
19:BD:298:CYS:SG	19:BD:299:THR:N	2.91	0.43
20:BE:571:ASP:OD1	20:BE:572:ALA:N	2.50	0.43
20:BE:914:ASP:OD1	20:BE:914:ASP:N	2.48	0.43
21:CA:46:ASN:HB3	21:CA:49:GLU:HB2	2.00	0.43
22:CB:174:TYR:HB3	22:CB:223:ARG:NH1	2.32	0.43
32:SA:340:U:H2'	32:SA:341:A:H8	1.83	0.43
32:SA:1041:G:H2'	32:SA:1042:G:C8	2.53	0.43
42:SR:16:ALA:HB2	42:SR:72:GLY:HA3	2.00	0.43
42:SR:78:VAL:HA	42:SR:81:ILE:HG12	2.00	0.43
44:SY:73:ARG:HH21	44:SY:82:LYS:HG2	1.82	0.43
45:SZ:19:ALA:HB1	45:SZ:77:ASN:HD22	1.82	0.43
1:3A:58:A:H2'	1:3A:59:G:C8	2.53	0.43
10:AC:202:UNK:HA	10:AC:208:UNK:HA	2.00	0.43
15:B1:236:LEU:HB3	15:B1:239:THR:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:BB:626:GLN:HG3	17:BB:628:HIS:HD2	1.81	0.43
17:BB:671:PHE:HB2	17:BB:683:ILE:HG23	2.00	0.43
19:BD:313:PHE:HA	19:BD:322:HIS:O	2.18	0.43
19:BD:522:GLN:H	19:BD:530:LEU:HD22	1.83	0.43
32:SA:352:A:H5"	39:SM:104:HIS:HE1	1.83	0.43
32:SA:510:G:O6	32:SA:539:G:N1	2.44	0.43
32:SA:862:A:O2'	32:SA:963:A:N1	2.42	0.43
32:SA:928:U:H5"	32:SA:944:A:H3'	2.00	0.43
45:SZ:57:VAL:HG22	45:SZ:60:PHE:HE2	1.82	0.43
4:3E:68:VAL:HG13	4:3E:72:LEU:HD22	2.00	0.43
4:3E:76:LEU:HD23	4:3E:84:LYS:NZ	2.33	0.43
7:5A:529:A:H2'	7:5A:530:A:C8	2.53	0.43
10:AC:599:UNK:O	10:AC:603:UNK:CB	2.66	0.43
12:AE:81:LEU:HD11	12:AE:85:VAL:H	1.83	0.43
15:B1:106:ALA:HA	15:B1:109:ASP:HB2	1.99	0.43
15:B1:194:TYR:CE2	15:B1:198:GLU:HB2	2.53	0.43
15:B1:932:LEU:H	15:B1:1006:TRP:HB2	1.83	0.43
17:BB:103:ILE:HB	17:BB:117:PHE:HB2	1.99	0.43
20:BE:155:THR:OG1	20:BE:156:LYS:N	2.51	0.43
20:BE:607:SER:OG	20:BE:625:VAL:O	2.34	0.43
22:CB:182:ASP:HB2	22:CB:208:THR:HB	1.99	0.43
31:S1:333:UNK:CB	31:S1:341:UNK:O	2.67	0.43
36:SI:21:ALA:HA	36:SI:24:PHE:HD2	1.83	0.43
52:U5:42:THR:H	52:U5:195:ASN:HB3	1.84	0.43
7:5A:114:G:H2'	7:5A:115:G:C8	2.54	0.43
8:AA:108:UNK:HA	8:AA:117:UNK:O	2.18	0.43
10:AC:683:UNK:O	10:AC:687:UNK:CB	2.67	0.43
17:BB:233:ILE:HG13	17:BB:237:LYS:HD3	2.00	0.43
17:BB:581:ILE:HD11	17:BB:585:SER:HA	2.00	0.43
32:SA:571:G:H5"	32:SA:572:C:OP2	2.19	0.43
33:SC:141:ALA:HA	33:SC:210:ILE:HG12	2.01	0.43
35:SG:156:ARG:HH11	35:SG:157:ARG:HD2	1.82	0.43
37:SJ:173:PRO:HG3	37:SJ:179:CYS:HA	2.00	0.43
53:UA:1009:UNK:O	53:UA:1013:UNK:N	2.50	0.43
13:AF:195:UNK:O	54:UB:394:UNK:N	2.49	0.43
14:AG:57:UNK:CB	14:AG:71:UNK:O	2.65	0.43
16:BA:800:LYS:O	16:BA:804:SER:HB3	2.19	0.43
17:BB:107:ASP:OD2	17:BB:110:SER:N	2.46	0.43
21:CA:181:LYS:HZ3	22:CB:808:LEU:HB3	1.82	0.43
32:SA:298:C:O3'	34:SF:30:ARG:NH2	2.52	0.43
32:SA:947:U:H2'	32:SA:948:G:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:SG:68:ILE:HD13	42:SR:114:ARG:NH1	2.33	0.43
3:3D:230:ASN:HD22	3:3D:252:ILE:HD13	1.84	0.43
4:3E:56:ALA:HB1	4:3E:143:LEU:HD22	1.98	0.43
6:3H:79:VAL:HG23	6:3H:121:ILE:HG23	2.00	0.43
7:5A:252:A:N6	7:5A:261:U:O4	2.52	0.43
14:AG:99:UNK:O	14:AG:112:UNK:N	2.51	0.43
19:BD:482:LEU:HD23	19:BD:482:LEU:HA	1.88	0.43
19:BD:539:ASP:HA	19:BD:562:LEU:HB2	2.00	0.43
22:CB:264:LEU:HD21	22:CB:556:ILE:HG21	1.99	0.43
22:CB:334:PHE:O	22:CB:338:SER:OG	2.35	0.43
22:CB:527:TYR:HB2	22:CB:615:VAL:HB	2.01	0.43
32:SA:10:G:H2'	32:SA:11:A:C8	2.53	0.43
32:SA:448:C:H2'	32:SA:449:C:C6	2.54	0.43
41:SP:17:ALA:N	41:SP:80:HIS:O	2.46	0.43
52:U5:65:PHE:HD1	52:U5:206:LYS:HE2	1.83	0.43
53:UA:103:UNK:O	53:UA:107:UNK:N	2.52	0.43
2:3C:296:GLU:HG3	2:3C:298:ILE:HG12	2.00	0.43
2:3C:307:GLU:O	2:3C:309:TYR:N	2.49	0.43
9:AB:456:UNK:O	9:AB:460:UNK:CB	2.67	0.43
16:BA:553:ILE:HG13	16:BA:554:ASP:H	1.84	0.43
18:BC:682:PHE:O	18:BC:686:MET:HB2	2.19	0.43
22:CB:260:ASP:OD2	22:CB:479:LYS:NZ	2.52	0.43
22:CB:589:LYS:O	22:CB:609:ASN:ND2	2.41	0.43
22:CB:726:SER:HA	22:CB:729:ASN:HD22	1.83	0.43
23:E2:180:LEU:HD12	23:E2:206:VAL:HG22	2.00	0.43
34:SF:88:ASP:HB2	34:SF:101:LEU:HD12	2.00	0.43
45:SZ:60:PHE:H	45:SZ:71:GLY:HA2	1.84	0.43
50:U2:67:UNK:O	50:U2:71:UNK:N	2.51	0.43
1:3A:8:U:H2'	1:3A:9:A:C8	2.53	0.43
7:5A:411:A:H2'	7:5A:412:A:H8	1.84	0.43
16:BA:331:GLU:HB2	16:BA:340:LYS:H	1.84	0.43
17:BB:341:ALA:HA	17:BB:357:THR:HA	2.01	0.43
22:CB:781:ASP:OD1	22:CB:853:ARG:NE	2.42	0.43
23:E2:158:LYS:HE2	23:E2:161:LYS:HZ3	1.80	0.43
30:R1:202:PRO:HD3	30:R1:231:ARG:HH22	1.83	0.43
35:SG:84:LYS:HG2	35:SG:92:ARG:HH12	1.83	0.43
37:SJ:6:ASP:OD2	37:SJ:8:ARG:HB2	2.19	0.43
37:SJ:36:THR:HG23	37:SJ:96:LEU:HB2	2.00	0.43
4:3E:215:ARG:NH1	4:3E:244:GLY:O	2.52	0.43
10:AC:527:UNK:O	10:AC:531:UNK:CB	2.67	0.43
16:BA:8:SER:HB2	16:BA:703:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BD:301:TYR:HB3	19:BD:312:ILE:HA	2.00	0.43
20:BE:901:LYS:HB3	20:BE:902:ASN:H	1.61	0.43
30:R1:65:ILE:HG12	30:R1:76:TYR:HD1	1.82	0.43
31:S1:105:UNK:CB	31:S1:383:UNK:O	2.67	0.43
32:SA:570:A:HO2'	32:SA:571:G:H8	1.65	0.43
32:SA:1524:A:H2'	32:SA:1525:A:C8	2.54	0.43
32:SA:1637:C:H42	32:SA:1764:C:H42	1.67	0.43
33:SC:34:ALA:HB3	33:SC:41:ARG:HA	2.01	0.43
52:U5:61:LYS:HE2	52:U5:64:LEU:HD21	2.00	0.43
2:3B:173:LEU:HB2	2:3B:242:ALA:HA	1.99	0.42
2:3B:241:PHE:CE2	2:3B:243:ASP:HB2	2.54	0.42
3:3D:214:TYR:HE1	3:3D:279:ALA:HA	1.84	0.42
7:5A:504:U:H2'	7:5A:505:G:C8	2.54	0.42
10:AC:642:UNK:O	10:AC:646:UNK:CB	2.67	0.42
15:B1:972:ILE:HD13	15:B1:993:ASP:HB2	2.01	0.42
16:BA:743:PHE:HZ	16:BA:777:ARG:HB3	1.84	0.42
17:BB:634:SER:OG	17:BB:635:LYS:N	2.51	0.42
18:BC:257:ILE:HG12	18:BC:299:ASN:HD22	1.84	0.42
20:BE:592:ASP:OD2	20:BE:634:PHE:N	2.45	0.42
23:E1:90:ASP:OD1	23:E1:90:ASP:N	2.52	0.42
23:E1:97:LEU:HD22	23:E1:132:ARG:HH21	1.84	0.42
23:E2:48:ALA:HB3	23:E2:116:THR:HA	2.01	0.42
32:SA:396:G:H1	32:SA:399:A:H5'	1.84	0.42
39:SM:123:VAL:HG23	39:SM:142:VAL:HA	2.01	0.42
44:SY:121:ARG:HH11	50:U2:10:UNK:CB	2.32	0.42
4:3E:379:ASP:OD2	4:3E:386:ILE:HD11	2.19	0.42
5:3F:551:ARG:NH1	6:3G:93:VAL:O	2.52	0.42
6:3G:79:VAL:HG23	6:3G:121:ILE:HG23	1.99	0.42
7:5A:71:U:H2'	7:5A:72:G:H8	1.84	0.42
7:5A:147:C:H2'	7:5A:148:G:H8	1.84	0.42
12:AE:288:ALA:HB3	12:AE:326:LYS:HB3	2.00	0.42
15:B1:974:GLY:HA3	15:B1:990:ALA:O	2.19	0.42
22:CB:839:THR:HB	22:CB:851:LYS:HB2	2.01	0.42
27:MB:166:SER:O	27:MB:256:MET:HA	2.19	0.42
32:SA:156:A:H1'	32:SA:416:A:C8	2.54	0.42
32:SA:874:C:H2'	32:SA:875:G:C8	2.54	0.42
32:SA:912:U:H5'	32:SA:914:G:H5'	2.01	0.42
32:SA:1753:A:H2'	32:SA:1754:A:H2'	2.00	0.42
33:SC:82:ARG:HH11	33:SC:103:MET:CE	2.32	0.42
39:SM:2:SER:HB2	39:SM:82:ARG:HA	2.00	0.42
1:3A:64:A:H5"	1:3A:65:C:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5A:467:A:H2'	7:5A:468:A:H8	1.84	0.42
16:BA:619:ARG:NH1	16:BA:619:ARG:O	2.52	0.42
18:BC:532:HIS:CE1	18:BC:558:LYS:HD2	2.53	0.42
18:BC:697:VAL:HG12	18:BC:700:ARG:HH21	1.83	0.42
20:BE:292:ARG:HB2	20:BE:295:TYR:HB2	2.01	0.42
21:CA:138:TRP:CD1	21:CA:142:LYS:HE3	2.53	0.42
22:CB:228:ARG:NH2	22:CB:296:ILE:H	2.17	0.42
22:CB:253:GLN:O	22:CB:270:ILE:HA	2.19	0.42
22:CB:742:PHE:CE2	33:SC:190:PRO:HG3	2.54	0.42
23:E2:144:LEU:HD22	23:E2:160:LEU:HD13	2.01	0.42
26:MA:80:ASP:HA	26:MA:83:TYR:HD2	1.84	0.42
32:SA:208:U:N3	32:SA:258:C:O2	2.52	0.42
32:SA:1476:C:H2'	32:SA:1477:G:H8	1.84	0.42
37:SJ:113:PHE:HE2	37:SJ:119:GLN:HB3	1.84	0.42
43:SX:97:ARG:HG3	51:U4:84:ARG:HH12	1.85	0.42
7:5A:184:U:H2'	7:5A:185:A:C8	2.55	0.42
15:B1:63:THR:HG22	15:B1:193:ARG:HE	1.85	0.42
15:B1:992:GLU:HB2	32:SA:570:A:C5	2.55	0.42
16:BA:714:PRO:HB2	16:BA:715:PHE:CD2	2.55	0.42
17:BB:674:SER:H	17:BB:681:ILE:HG23	1.84	0.42
18:BC:311:LEU:HD12	18:BC:333:ILE:HD11	2.00	0.42
21:CA:68:LYS:HG2	21:CA:84:VAL:HB	2.01	0.42
22:CB:153:PHE:HA	22:CB:156:LYS:NZ	2.34	0.42
22:CB:385:LEU:HD13	22:CB:582:GLN:HG3	2.01	0.42
30:R1:189:SER:H	30:R1:249:SER:HA	1.85	0.42
32:SA:1148:C:H1'	32:SA:1631:A:H61	1.84	0.42
36:SI:63:PRO:HB2	36:SI:65:PRO:HD2	2.01	0.42
40:SO:84:ILE:HG22	40:SO:135:LEU:HD21	2.01	0.42
7:5A:133:U:H2'	7:5A:134:A:H8	1.83	0.42
7:5A:271:G:H2'	7:5A:272:A:C8	2.54	0.42
16:BA:585:TYR:HE1	16:BA:589:GLY:HA2	1.85	0.42
17:BB:59:LEU:HB2	17:BB:383:HIS:HB3	2.01	0.42
18:BC:439:ALA:HB3	18:BC:457:ALA:HB3	2.01	0.42
22:CB:643:ALA:O	22:CB:647:ASN:CB	2.61	0.42
23:E2:121:LEU:O	23:E2:162:VAL:HA	2.20	0.42
30:R1:57:GLU:HG3	30:R1:65:ILE:HD12	2.00	0.42
30:R1:244:THR:HG23	30:R1:259:GLU:HB3	2.02	0.42
32:SA:1673:G:H1	32:SA:1728:A:H61	1.67	0.42
33:SC:159:SER:HA	33:SC:162:ARG:HH11	1.84	0.42
36:SI:131:PHE:CD2	36:SI:132:PRO:HD3	2.54	0.42
53:UA:1201:UNK:O	53:UA:1205:UNK:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:5A:447:G:H2'	7:5A:448:G:H8	1.85	0.42
17:BB:438:PHE:HA	17:BB:445:VAL:HG23	2.00	0.42
17:BB:576:VAL:HG12	17:BB:592:SER:HB2	2.02	0.42
20:BE:424:ILE:HG23	20:BE:446:ARG:NH1	2.35	0.42
27:MB:108:LYS:HD3	27:MB:177:ILE:HD11	2.01	0.42
30:R1:153:THR:HA	30:R1:166:VAL:HG12	2.01	0.42
43:SX:82:LYS:HB3	43:SX:85:ASP:OD2	2.20	0.42
7:5A:395:C:OP1	26:MA:119:LYS:NZ	2.49	0.42
7:5A:451:G:H2'	7:5A:451:G:OP2	2.19	0.42
8:AA:24:UNK:HA	8:AA:37:UNK:O	2.19	0.42
10:AC:411:UNK:O	10:AC:415:UNK:CB	2.67	0.42
12:AE:345:ASP:OD1	12:AE:345:ASP:N	2.51	0.42
13:AF:426:UNK:O	13:AF:430:UNK:CB	2.68	0.42
15:B1:620:LYS:O	15:B1:624:LYS:HB2	2.20	0.42
15:B1:623:LYS:HA	15:B1:626:LYS:HE2	2.01	0.42
16:BA:164:THR:OG1	16:BA:165:SER:N	2.52	0.42
19:BD:341:LYS:O	19:BD:344:ARG:NH1	2.52	0.42
19:BD:493:LEU:H	19:BD:507:PRO:HB3	1.83	0.42
22:CB:298:PHE:HB2	22:CB:340:SER:HA	2.02	0.42
27:MB:144:GLU:O	32:SA:1603:U:O2'	2.29	0.42
32:SA:514:G:H22	32:SA:543:C:H5	1.68	0.42
34:SF:176:ASP:HB2	34:SF:179:LYS:HD2	2.02	0.42
35:SG:165:LEU:O	35:SG:169:ASN:ND2	2.53	0.42
39:SM:2:SER:N	39:SM:82:ARG:HG2	2.35	0.42
1:3A:3:C:H2'	1:3A:4:G:C8	2.48	0.42
1:3A:46:U:H2'	1:3A:47:G:C8	2.55	0.42
3:3D:61:GLU:O	3:3D:65:ASN:ND2	2.53	0.42
3:3D:150:ALA:O	3:3D:154:LEU:CB	2.68	0.42
4:3E:249:GLN:HA	4:3E:252:LEU:HD12	2.01	0.42
8:AA:239:UNK:CB	8:AA:252:UNK:O	2.68	0.42
10:AC:467:UNK:O	10:AC:471:UNK:CB	2.68	0.42
18:BC:108:LEU:HB3	18:BC:150:LEU:HD22	2.02	0.42
18:BC:679:THR:HA	18:BC:724:LEU:HD23	2.01	0.42
19:BD:448:LYS:HE3	20:BE:563:ASP:OD2	2.20	0.42
20:BE:470:GLN:HA	20:BE:553:ARG:HH12	1.84	0.42
22:CB:167:PRO:HD3	22:CB:226:HIS:CE1	2.54	0.42
22:CB:363:THR:HA	22:CB:393:PHE:HE2	1.85	0.42
22:CB:779:PHE:HA	22:CB:849:GLY:O	2.20	0.42
22:CB:822:ARG:HB2	22:CB:843:LEU:HB2	2.01	0.42
27:MB:143:HIS:HB2	32:SA:1604:U:H5"	2.01	0.42
32:SA:926:A:H2'	32:SA:927:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:UB:669:UNK:O	54:UB:673:UNK:N	2.52	0.42
5:3F:495:SER:HA	5:3F:514:LEU:O	2.19	0.42
7:5A:103:G:C8	7:5A:143:A:H1'	2.54	0.42
12:AE:162:ASN:N	12:AE:162:ASN:OD1	2.52	0.42
15:B1:189:VAL:HG13	15:B1:193:ARG:HA	2.01	0.42
17:BB:145:ILE:HB	17:BB:166:ILE:HD13	2.01	0.42
17:BB:236:ASP:OD1	17:BB:236:ASP:N	2.53	0.42
17:BB:639:VAL:HB	17:BB:653:LEU:HB2	2.02	0.42
17:BB:641:TYR:HB2	17:BB:651:GLN:O	2.20	0.42
17:BB:867:GLU:O	17:BB:871:GLN:NE2	2.47	0.42
17:BB:888:ARG:O	17:BB:892:LYS:HB2	2.20	0.42
20:BE:27:PHE:HB3	20:BE:653:ILE:O	2.19	0.42
20:BE:53:CYS:HB2	20:BE:83:LEU:HD11	2.02	0.42
22:CB:761:ARG:NH1	22:CB:932:GLU:OE2	2.53	0.42
22:CB:1204:VAL:HB	22:CB:1212:VAL:HB	2.02	0.42
27:MB:185:VAL:HG11	27:MB:219:GLU:HB3	2.02	0.42
32:SA:336:G:H2'	32:SA:338:C:H5	1.85	0.42
32:SA:468:A:H8	32:SA:470:A:OP2	2.03	0.42
32:SA:1174:C:H2'	32:SA:1175:U:C6	2.54	0.42
32:SA:1619:C:H2'	32:SA:1620:C:H6	1.85	0.42
35:SG:58:LEU:HD11	35:SG:167:ARG:NH1	2.34	0.42
37:SJ:167:ALA:HA	37:SJ:183:ILE:HA	2.01	0.42
53:UA:308:UNK:O	53:UA:312:UNK:N	2.53	0.42
1:3A:63:C:O2'	20:BE:392:ARG:NH2	2.53	0.42
5:3F:289:ARG:NH1	5:3F:334:GLU:HB2	2.34	0.42
14:AG:162:UNK:HA	14:AG:168:UNK:HA	2.01	0.42
20:BE:86:HIS:CD2	20:BE:87:PHE:H	2.38	0.42
22:CB:202:SER:HA	22:CB:291:SER:HB2	2.01	0.42
27:MB:267:GLU:OE2	55:UC:13:UNK:N	2.53	0.42
29:P1:129:ARG:HB2	29:P1:138:GLU:HG2	2.02	0.42
30:R1:134:LYS:NZ	30:R1:151:LEU:O	2.44	0.42
32:SA:351:C:H2'	39:SM:101:GLU:HB2	2.02	0.42
32:SA:1124:A:H2'	32:SA:1125:A:C8	2.55	0.42
32:SA:1806:A:H8	32:SA:1806:A:OP2	2.03	0.42
33:SC:123:ALA:HB3	33:SC:139:ALA:HB3	2.02	0.42
36:SI:37:GLU:OE2	36:SI:38:LEU:HD22	2.20	0.42
2:3C:100:ARG:HA	2:3C:101:GLY:HA2	1.83	0.41
3:3D:303:LEU:HG	3:3D:390:ASP:OD2	2.20	0.41
6:3G:91:CYS:HB2	6:3G:93:VAL:HB	2.01	0.41
9:AB:522:UNK:O	9:AB:526:UNK:CB	2.67	0.41
9:AB:531:UNK:O	9:AB:535:UNK:CB	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:AF:506:UNK:O	13:AF:510:UNK:CB	2.68	0.41
15:B1:855:GLN:H	15:B1:1016:ASN:HD22	1.68	0.41
18:BC:574:HIS:CE1	18:BC:602:TRP:HE1	2.38	0.41
19:BD:403:VAL:HG21	20:BE:589:THR:HG21	2.02	0.41
22:CB:150:ASP:O	22:CB:154:LYS:CB	2.64	0.41
22:CB:344:ASN:HD21	22:CB:445:ASN:HD21	1.68	0.41
22:CB:1178:ASP:OD1	22:CB:1178:ASP:N	2.53	0.41
32:SA:187:G:O2'	32:SA:198:A:N6	2.53	0.41
32:SA:214:G:N2	32:SA:250:C:OP2	2.52	0.41
32:SA:524:U:H2'	45:SZ:93:ARG:HH22	1.85	0.41
32:SA:1807:U:H2'	32:SA:1808:U:H6	1.85	0.41
1:3A:77:U:H2'	1:3A:78:G:C8	2.55	0.41
2:3B:165:ALA:HB3	2:3B:168:LYS:HE2	2.02	0.41
4:3E:121:LYS:HA	4:3E:124:LEU:HB2	2.00	0.41
7:5A:244:U:H2'	7:5A:245:C:C6	2.55	0.41
16:BA:779:LEU:HD23	16:BA:779:LEU:HA	1.91	0.41
17:BB:53:ASP:OD2	17:BB:56:THR:N	2.54	0.41
17:BB:256:GLY:H	17:BB:346:VAL:HG21	1.84	0.41
20:BE:179:LYS:HB3	20:BE:190:LEU:HD11	2.02	0.41
20:BE:228:GLY:O	20:BE:246:ILE:N	2.46	0.41
20:BE:659:GLN:HB2	20:BE:660:PHE:HD1	1.85	0.41
22:CB:177:ASN:HB3	22:CB:213:LEU:HD22	2.02	0.41
22:CB:255:GLU:OE2	22:CB:269:ARG:HD2	2.20	0.41
23:E2:190:GLN:HE21	23:E2:244:GLY:HA2	1.85	0.41
30:R1:35:LYS:N	30:R1:72:THR:O	2.53	0.41
32:SA:1057:U:H6	32:SA:1062:A:H61	1.67	0.41
32:SA:1512:G:H2'	32:SA:1513:G:H8	1.85	0.41
35:SG:80:LYS:HB2	35:SG:83:ARG:NH1	2.35	0.41
36:SI:8:ILE:HA	36:SI:42:GLN:HG3	2.02	0.41
45:SZ:87:PRO:HD2	45:SZ:90:ARG:HD2	2.01	0.41
1:3A:102:U:H2'	1:3A:103:A:C8	2.55	0.41
2:3C:115:GLU:OE1	2:3C:214:ARG:NH2	2.53	0.41
5:3F:295:LEU:HB3	5:3F:307:TYR:HB2	2.03	0.41
7:5A:186:C:H2'	7:5A:187:A:C8	2.55	0.41
16:BA:155:SER:HB3	16:BA:160:PHE:HB3	2.02	0.41
17:BB:368:PRO:HA	17:BB:374:PRO:HA	2.01	0.41
19:BD:352:GLN:HG3	19:BD:371:VAL:HG22	2.01	0.41
21:CA:196:ALA:HA	21:CA:199:GLN:HG3	2.01	0.41
29:P1:165:GLY:HA3	29:P1:225:VAL:HG11	2.02	0.41
30:R1:207:ARG:HB3	30:R1:269:GLU:OE2	2.19	0.41
32:SA:966:A:H2'	32:SA:967:A:H8	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:SA:1081:A:H1'	32:SA:1082:C:N3	2.36	0.41
32:SA:1177:C:H2'	32:SA:1178:G:H8	1.86	0.41
32:SA:1748:G:H2'	32:SA:1749:A:C8	2.56	0.41
4:3E:192:PHE:HE1	4:3E:239:ALA:HA	1.85	0.41
6:3H:68:PRO:HB3	6:3H:78:TYR:CZ	2.56	0.41
8:AA:558:UNK:CB	8:AA:566:UNK:O	2.69	0.41
12:AE:380:VAL:HA	12:AE:383:ILE:HD12	2.03	0.41
15:B1:829:LEU:HD13	15:B1:883:ALA:HB3	2.02	0.41
16:BA:317:LEU:O	16:BA:331:GLU:HA	2.21	0.41
17:BB:20:ASN:HD21	17:BB:23:CYS:H	1.68	0.41
17:BB:618:ILE:H	17:BB:618:ILE:HG13	1.73	0.41
17:BB:758:LEU:HD11	17:BB:793:VAL:HG11	2.02	0.41
17:BB:806:MET:O	17:BB:809:LEU:HB2	2.20	0.41
18:BC:343:MET:HB2	18:BC:353:LEU:HD21	2.02	0.41
22:CB:525:LEU:HB2	22:CB:617:LEU:HB2	2.02	0.41
29:P1:104:HIS:CD2	32:SA:1799:U:H1'	2.55	0.41
34:SF:181:VAL:HG21	34:SF:210:ILE:HD12	2.01	0.41
35:SG:80:LYS:NZ	35:SG:83:ARG:HH12	2.15	0.41
52:U5:106:LEU:HB3	52:U5:107:ARG:HD2	2.02	0.41
4:3E:44:ILE:HG23	4:3E:127:LEU:HD22	2.01	0.41
15:B1:130:GLU:HB3	15:B1:907:THR:HB	2.03	0.41
16:BA:817:PHE:O	16:BA:821:MET:HB3	2.20	0.41
25:K1:138:PHE:O	25:K1:142:ARG:CB	2.60	0.41
27:MB:118:ASN:OD1	27:MB:119:ARG:N	2.52	0.41
27:MB:183:SER:HA	27:MB:220:ARG:NH1	2.36	0.41
29:P1:169:ASP:HA	29:P1:172:ILE:HD12	2.02	0.41
30:R1:308:ILE:HA	30:R1:354:ILE:O	2.20	0.41
32:SA:894:U:H2'	32:SA:895:G:H8	1.85	0.41
32:SA:966:A:H2'	32:SA:967:A:C8	2.56	0.41
34:SF:122:LYS:NZ	34:SF:143:ASP:OD2	2.38	0.41
44:SY:54:LEU:HD12	44:SY:82:LYS:NZ	2.36	0.41
52:U5:82:LEU:HA	52:U5:174:ILE:HD13	2.02	0.41
55:UC:712:UNK:O	55:UC:716:UNK:N	2.53	0.41
1:3A:18:G:H2'	1:3A:19:A:C8	2.55	0.41
7:5A:112:U:H2'	7:5A:113:A:H8	1.86	0.41
12:AE:31:ALA:HA	12:AE:154:ILE:HD11	2.01	0.41
15:B1:634:ARG:HA	15:B1:634:ARG:HD2	1.90	0.41
20:BE:349:HIS:CE1	20:BE:376:TRP:HD1	2.38	0.41
22:CB:785:GLU:OE2	22:CB:855:LEU:HD23	2.20	0.41
22:CB:929:ILE:HG23	22:CB:933:LEU:HD23	2.02	0.41
27:MB:237:VAL:HB	27:MB:248:ALA:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:UB:169:UNK:HA	54:UB:193:UNK:HA	2.03	0.41
55:UC:883:UNK:O	55:UC:887:UNK:N	2.54	0.41
5:3F:235:HIS:ND1	5:3F:257:ASP:OD2	2.48	0.41
7:5A:168:G:H1	7:5A:228:A:N6	2.19	0.41
7:5A:357:G:C6	7:5A:368:U:O2	2.74	0.41
9:AB:271:UNK:HA	9:AB:285:UNK:HA	2.01	0.41
10:AC:201:UNK:O	10:AC:209:UNK:N	2.54	0.41
15:B1:112:LYS:HE3	15:B1:851:TRP:HA	2.03	0.41
18:BC:461:LEU:HD13	18:BC:491:GLU:HA	2.03	0.41
18:BC:779:VAL:HA	18:BC:782:VAL:HG22	2.03	0.41
20:BE:96:ASN:ND2	20:BE:114:THR:O	2.35	0.41
22:CB:119:LYS:O	22:CB:123:LYS:HB2	2.21	0.41
29:P1:223:ARG:HB2	29:P1:234:LEU:HB2	2.01	0.41
32:SA:478:A:H2	32:SA:510:G:H22	1.67	0.41
32:SA:549:G:H2'	32:SA:550:A:H8	1.84	0.41
34:SF:161:LYS:HB3	34:SF:171:ASP:HB3	2.01	0.41
34:SF:181:VAL:HG12	34:SF:227:VAL:HG12	2.03	0.41
36:SI:59:ALA:HB1	36:SI:93:LEU:HD12	2.02	0.41
37:SJ:36:THR:HA	37:SJ:58:LEU:HD22	2.03	0.41
54:UB:610:UNK:O	54:UB:614:UNK:N	2.54	0.41
2:3B:253:ILE:O	2:3B:257:SER:CB	2.69	0.41
10:AC:464:UNK:O	10:AC:468:UNK:CB	2.69	0.41
12:AE:303:PHE:HA	12:AE:306:LEU:HB3	2.02	0.41
16:BA:454:ASP:OD1	16:BA:455:ILE:N	2.52	0.41
16:BA:792:ILE:O	16:BA:796:LEU:HB2	2.21	0.41
19:BD:245:HIS:HD2	19:BD:584:GLY:HA2	1.85	0.41
20:BE:471:CYS:SG	20:BE:473:ASN:ND2	2.94	0.41
21:CA:166:THR:HA	21:CA:169:VAL:HG22	2.03	0.41
23:E1:174:LYS:HB3	23:E1:200:GLU:HA	2.01	0.41
32:SA:156:A:H2'	32:SA:157:A:H8	1.86	0.41
32:SA:589:C:H2'	32:SA:590:C:H6	1.86	0.41
32:SA:929:A:H2'	32:SA:929:A:N3	2.36	0.41
44:SY:126:LYS:HE2	44:SY:129:GLY:HA2	2.01	0.41
52:U5:47:GLY:HA2	52:U5:52:ASN:ND2	2.33	0.41
2:3B:126:GLU:HG3	2:3B:139:VAL:H	1.86	0.41
3:3D:198:TRP:NE1	3:3D:271:VAL:HG21	2.36	0.41
7:5A:403:C:OP2	7:5A:404:G:O2'	2.37	0.41
10:AC:598:UNK:O	10:AC:602:UNK:CB	2.69	0.41
12:AE:258:HIS:CE1	12:AE:282:ILE:HD12	2.55	0.41
14:AG:425:UNK:O	14:AG:438:UNK:N	2.54	0.41
16:BA:93:PHE:HZ	16:BA:96:LYS:HD3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:BA:534:THR:OG1	16:BA:538:GLN:O	2.29	0.41
16:BA:540:SER:HA	16:BA:550:VAL:O	2.20	0.41
16:BA:800:LYS:O	16:BA:804:SER:CB	2.69	0.41
17:BB:255:ARG:HG2	17:BB:257:LEU:H	1.86	0.41
17:BB:469:GLU:HB2	17:BB:513:LYS:HE3	2.02	0.41
17:BB:538:ARG:NH1	17:BB:539:VAL:O	2.54	0.41
18:BC:70:THR:HG23	18:BC:73:GLY:H	1.85	0.41
18:BC:174:VAL:HB	18:BC:184:HIS:H	1.85	0.41
20:BE:530:ASP:OD1	20:BE:531:PHE:N	2.53	0.41
22:CB:812:GLU:O	22:CB:816:ALA:HB2	2.20	0.41
25:K1:53:LEU:HD23	25:K1:56:ILE:HD11	2.03	0.41
27:MB:236:HIS:HE1	27:MB:249:GLU:HG2	1.85	0.41
29:P1:116:ILE:HD11	29:P1:168:LEU:HD13	2.01	0.41
30:R1:252:LYS:HD2	30:R1:254:TRP:HE1	1.86	0.41
32:SA:328:A:H2'	32:SA:329:G:C8	2.56	0.41
32:SA:493:U:O2'	55:UC:236:UNK:O	2.30	0.41
32:SA:1473:U:C4	35:SG:102:ARG:HD2	2.56	0.41
32:SA:1654:G:H21	32:SA:1746:A:H62	1.69	0.41
38:SK:53:ARG:NH1	38:SK:97:LEU:O	2.49	0.41
43:SX:41:MET:HB3	43:SX:46:TYR:HB2	2.01	0.41
45:SZ:45:ALA:HB2	45:SZ:55:VAL:HG21	2.02	0.41
55:UC:383:UNK:O	55:UC:387:UNK:N	2.54	0.41
4:3E:50:PHE:HD1	4:3E:50:PHE:HA	1.75	0.41
7:5A:115:G:N2	7:5A:131:C:O2	2.43	0.41
16:BA:153:THR:OG1	16:BA:162:LEU:O	2.33	0.41
17:BB:216:LEU:HA	17:BB:229:TRP:O	2.21	0.41
17:BB:634:SER:HG	17:BB:635:LYS:H	1.69	0.41
18:BC:198:ILE:HD13	18:BC:245:SER:HA	2.03	0.41
21:CA:53:LEU:HB2	21:CA:126:LEU:HB3	2.03	0.41
22:CB:671:THR:HG21	22:CB:720:SER:HB2	2.02	0.41
32:SA:103:A:H4'	32:SA:105:A:N6	2.36	0.41
32:SA:871:G:H2'	32:SA:872:G:C8	2.55	0.41
32:SA:884:A:H2'	32:SA:885:G:C8	2.56	0.41
33:SC:127:VAL:HG13	33:SC:176:VAL:HG11	2.02	0.41
34:SF:122:LYS:HG2	34:SF:164:LEU:HD21	2.02	0.41
7:5A:403:C:H3'	7:5A:404:G:H4'	2.03	0.40
15:B1:615:PHE:HB3	15:B1:621:LEU:HD11	2.02	0.40
17:BB:559:PHE:HB3	17:BB:566:TYR:CZ	2.57	0.40
17:BB:574:LEU:HD23	17:BB:594:ASP:HB3	2.03	0.40
18:BC:377:LEU:HA	18:BC:378:PRO:HD3	1.88	0.40
20:BE:24:PHE:CZ	20:BE:641:LEU:HD22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:CB:872:ASN:HA	22:CB:875:LYS:HE2	2.03	0.40
32:SA:1082:C:C2	43:SX:20:THR:HG22	2.56	0.40
32:SA:1177:C:H2'	32:SA:1178:G:C8	2.57	0.40
33:SC:207:LEU:HD22	33:SC:210:ILE:HD11	2.03	0.40
36:SI:41:LEU:HB3	36:SI:70:PHE:HE1	1.86	0.40
1:3A:199:G:C2	5:3F:153:GLY:HA2	2.56	0.40
3:3D:382:LYS:HB3	3:3D:404:LEU:HD11	2.03	0.40
5:3F:278:ASP:OD2	5:3F:301:ASP:OD2	2.39	0.40
12:AE:103:LEU:HD23	12:AE:103:LEU:HA	1.83	0.40
15:B1:175:THR:HG22	15:B1:179:GLN:HE22	1.85	0.40
15:B1:835:HIS:ND1	15:B1:913:ILE:O	2.54	0.40
16:BA:90:LEU:HD22	16:BA:135:PRO:HG3	2.03	0.40
16:BA:556:ARG:CZ	20:BE:423:ARG:NH1	2.84	0.40
16:BA:722:THR:O	16:BA:726:THR:OG1	2.33	0.40
16:BA:731:ARG:HH21	16:BA:754:VAL:HB	1.86	0.40
16:BA:743:PHE:CZ	16:BA:777:ARG:HB3	2.56	0.40
17:BB:170:TRP:NE1	17:BB:172:GLN:HA	2.37	0.40
18:BC:433:HIS:CE1	18:BC:464:LYS:HD2	2.56	0.40
19:BD:325:ASP:O	19:BD:336:THR:N	2.52	0.40
20:BE:412:PRO:O	20:BE:434:HIS:ND1	2.54	0.40
20:BE:509:SER:OG	20:BE:510:LEU:N	2.54	0.40
22:CB:805:ALA:HA	22:CB:808:LEU:HD12	2.02	0.40
22:CB:1157:TYR:OH	22:CB:1222:GLU:OE1	2.39	0.40
27:MB:145:HIS:CE1	27:MB:148:VAL:H	2.39	0.40
30:R1:70:THR:HG23	30:R1:72:THR:H	1.86	0.40
30:R1:119:LYS:HA	30:R1:164:GLY:O	2.22	0.40
32:SA:914:G:H8	32:SA:914:G:OP2	2.04	0.40
33:SC:87:ARG:N	33:SC:99:ASN:O	2.53	0.40
35:SG:76:ARG:O	35:SG:83:ARG:NH2	2.44	0.40
43:SX:89:TRP:HA	43:SX:92:ASN:HD22	1.85	0.40
7:5A:334:G:O6	7:5A:390:C:N4	2.55	0.40
14:AG:434:UNK:HA	14:AG:449:UNK:N	2.36	0.40
16:BA:510:GLU:HA	16:BA:511:PRO:HD3	1.85	0.40
17:BB:393:ASP:HB2	17:BB:395:ARG:HH12	1.86	0.40
18:BC:682:PHE:CD2	18:BC:724:LEU:HD21	2.56	0.40
19:BD:531:CYS:HA	19:BD:543:LEU:HA	2.02	0.40
23:E2:50:LEU:HD12	23:E2:116:THR:HG22	2.04	0.40
26:MA:83:TYR:HD1	26:MA:152:ARG:HH12	1.69	0.40
34:SF:72:VAL:HG22	34:SF:90:ILE:HG12	2.03	0.40
36:SI:11:GLN:HG3	36:SI:13:PRO:HD2	2.02	0.40
40:SO:130:ARG:HD3	40:SO:139:TRP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:175:ALA:HB1	2:3B:207:LEU:HD11	2.02	0.40
13:AF:178:UNK:HA	13:AF:194:UNK:HA	2.04	0.40
15:B1:265:THR:OG1	15:B1:266:ARG:N	2.54	0.40
15:B1:610:LYS:O	30:R1:321:ARG:NH2	2.51	0.40
16:BA:156:GLN:HE21	16:BA:201:HIS:CE1	2.38	0.40
17:BB:500:TRP:HB3	17:BB:514:ASN:HB3	2.03	0.40
18:BC:532:HIS:CD2	18:BC:536:LEU:HD11	2.57	0.40
18:BC:764:LEU:H	18:BC:764:LEU:HG	1.60	0.40
20:BE:209:ILE:HG21	20:BE:223:LEU:HD22	2.04	0.40
22:CB:306:LYS:HA	22:CB:309:LEU:HG	2.03	0.40
22:CB:329:THR:HB	22:CB:332:TYR:HB3	2.04	0.40
32:SA:103:A:OP2	32:SA:358:U:OP2	2.39	0.40
32:SA:211:U:H5"	39:SM:20:PHE:CG	2.56	0.40
32:SA:448:C:H2'	32:SA:449:C:H6	1.86	0.40
32:SA:890:C:H2'	32:SA:891:A:H8	1.87	0.40
42:SR:25:GLY:HA3	42:SR:64:ASP:OD2	2.22	0.40
42:SR:58:ASP:N	42:SR:58:ASP:OD1	2.54	0.40
1:3A:113:G:H1'	1:3A:257:A:H61	1.86	0.40
7:5A:264:C:H2'	7:5A:265:A:C8	2.56	0.40
7:5A:556:G:H2'	7:5A:557:A:C8	2.53	0.40
16:BA:426:THR:OG1	16:BA:427:GLY:N	2.55	0.40
18:BC:452:GLU:HB3	18:BC:473:ALA:HB3	2.04	0.40
21:CA:64:ILE:HG13	21:CA:68:LYS:HE2	2.04	0.40
23:E1:94:GLN:HE22	23:E2:97:LEU:HB3	1.86	0.40
32:SA:891:A:H2'	32:SA:892:A:H8	1.85	0.40
32:SA:1476:C:H2'	32:SA:1477:G:C8	2.57	0.40
32:SA:1735:U:H2'	32:SA:1736:G:C8	2.57	0.40
34:SF:124:GLY:HA2	34:SF:142:HIS:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	3B	237/327 (72%)	222 (94%)	15 (6%)	0	100	100
2	3C	237/327 (72%)	218 (92%)	19 (8%)	0	100	100
3	3D	366/504 (73%)	339 (93%)	27 (7%)	0	100	100
4	3E	378/511 (74%)	352 (93%)	26 (7%)	0	100	100
5	3F	353/573 (62%)	332 (94%)	21 (6%)	0	100	100
6	3G	120/126 (95%)	114 (95%)	6 (5%)	0	100	100
6	3H	120/126 (95%)	115 (96%)	5 (4%)	0	100	100
12	AE	407/1769 (23%)	380 (93%)	27 (7%)	0	100	100
15	B1	528/1183 (45%)	477 (90%)	50 (10%)	1 (0%)	44	78
16	BA	747/923 (81%)	657 (88%)	89 (12%)	1 (0%)	48	83
17	BB	770/943 (82%)	681 (88%)	86 (11%)	3 (0%)	30	68
18	BC	779/817 (95%)	682 (88%)	93 (12%)	4 (0%)	25	64
19	BD	317/594 (53%)	265 (84%)	52 (16%)	0	100	100
20	BE	741/939 (79%)	683 (92%)	57 (8%)	1 (0%)	48	83
21	CA	190/297 (64%)	182 (96%)	8 (4%)	0	100	100
22	CB	1086/1237 (88%)	1050 (97%)	36 (3%)	0	100	100
23	E1	213/252 (84%)	209 (98%)	4 (2%)	0	100	100
23	E2	210/252 (83%)	200 (95%)	10 (5%)	0	100	100
25	K1	173/316 (55%)	163 (94%)	10 (6%)	0	100	100
26	MA	131/183 (72%)	126 (96%)	5 (4%)	0	100	100
27	MB	182/290 (63%)	164 (90%)	18 (10%)	0	100	100
28	MC	24/593 (4%)	24 (100%)	0	0	100	100
29	P1	171/274 (62%)	163 (95%)	8 (5%)	0	100	100
30	R1	353/367 (96%)	339 (96%)	14 (4%)	0	100	100
33	SC	212/255 (83%)	169 (80%)	37 (18%)	6 (3%)	4	24
34	SF	235/261 (90%)	212 (90%)	22 (9%)	1 (0%)	30	68
35	SG	204/225 (91%)	178 (87%)	24 (12%)	2 (1%)	13	49
36	SI	161/190 (85%)	141 (88%)	19 (12%)	1 (1%)	22	60
37	SJ	166/200 (83%)	144 (87%)	22 (13%)	0	100	100
38	SK	173/197 (88%)	150 (87%)	22 (13%)	1 (1%)	22	60
39	SM	139/156 (89%)	129 (93%)	8 (6%)	2 (1%)	9	40
40	SO	132/151 (87%)	128 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
41	SP	110/137 (80%)	97 (88%)	13 (12%)	0	100 100
42	SR	123/143 (86%)	107 (87%)	12 (10%)	4 (3%)	3 21
43	SX	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	16 54
44	SY	101/145 (70%)	78 (77%)	21 (21%)	2 (2%)	6 32
45	SZ	99/135 (73%)	91 (92%)	8 (8%)	0	100 100
46	Sc	77/82 (94%)	70 (91%)	7 (9%)	0	100 100
47	Sd	61/67 (91%)	51 (84%)	10 (16%)	0	100 100
48	Sf	28/63 (44%)	27 (96%)	1 (4%)	0	100 100
51	U4	124/189 (66%)	111 (90%)	12 (10%)	1 (1%)	16 54
52	U5	246/274 (90%)	222 (90%)	24 (10%)	0	100 100
All	All	11351/16723 (68%)	10354 (91%)	966 (8%)	31 (0%)	38 72

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	BE	901	LYS
33	SC	206	PRO
33	SC	207	LEU
33	SC	209	ASN
34	SF	195	ILE
35	SG	50	GLU
35	SG	51	VAL
42	SR	59	LYS
18	BC	298	SER
44	SY	97	ASP
16	BA	130	ASP
18	BC	137	THR
18	BC	297	LEU
18	BC	772	LEU
33	SC	181	LEU
39	SM	5	LEU
42	SR	58	ASP
17	BB	797	VAL
36	SI	133	THR
15	B1	191	ASN
17	BB	798	ASN
33	SC	180	THR
39	SM	3	THR

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Mol	Chain	Res	Type
17	BB	81	GLU
33	SC	210	ILE
38	SK	134	ILE
42	SR	33	GLY
44	SY	96	VAL
51	U4	175	VAL
42	SR	40	GLU
43	SX	67	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	3B	202/240 (84%)	200 (99%)	2 (1%)	73 81
2	3C	202/240 (84%)	202 (100%)	0	100 100
3	3D	317/435 (73%)	315 (99%)	2 (1%)	84 88
4	3E	314/433 (72%)	312 (99%)	2 (1%)	84 88
5	3F	317/503 (63%)	315 (99%)	2 (1%)	84 88
6	3G	101/104 (97%)	99 (98%)	2 (2%)	50 68
6	3H	101/104 (97%)	99 (98%)	2 (2%)	50 68
12	AE	381/1633 (23%)	378 (99%)	3 (1%)	79 84
15	B1	471/1039 (45%)	467 (99%)	4 (1%)	79 84
16	BA	663/812 (82%)	650 (98%)	13 (2%)	50 68
17	BB	687/832 (83%)	678 (99%)	9 (1%)	65 77
18	BC	687/719 (96%)	683 (99%)	4 (1%)	84 88
19	BD	281/529 (53%)	277 (99%)	4 (1%)	62 75
20	BE	657/819 (80%)	654 (100%)	3 (0%)	86 89
21	CA	178/274 (65%)	176 (99%)	2 (1%)	70 80
22	CB	1000/1125 (89%)	994 (99%)	6 (1%)	84 88
23	E1	191/222 (86%)	191 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	E2	193/222 (87%)	193 (100%)	0	100	100
25	K1	158/289 (55%)	158 (100%)	0	100	100
26	MA	123/172 (72%)	120 (98%)	3 (2%)	44	63
27	MB	164/258 (64%)	164 (100%)	0	100	100
28	MC	24/148 (16%)	24 (100%)	0	100	100
29	P1	151/238 (63%)	150 (99%)	1 (1%)	81	87
30	R1	302/312 (97%)	302 (100%)	0	100	100
33	SC	191/224 (85%)	190 (100%)	1 (0%)	86	89
34	SF	203/222 (91%)	201 (99%)	2 (1%)	73	81
35	SG	173/191 (91%)	170 (98%)	3 (2%)	56	72
36	SI	146/170 (86%)	146 (100%)	0	100	100
37	SJ	138/161 (86%)	137 (99%)	1 (1%)	81	87
38	SK	149/166 (90%)	143 (96%)	6 (4%)	27	48
39	SM	128/137 (93%)	125 (98%)	3 (2%)	45	64
40	SO	117/128 (91%)	117 (100%)	0	100	100
41	SP	69/105 (66%)	69 (100%)	0	100	100
42	SR	105/119 (88%)	105 (100%)	0	100	100
43	SX	110/111 (99%)	110 (100%)	0	100	100
44	SY	85/120 (71%)	84 (99%)	1 (1%)	67	79
45	SZ	85/113 (75%)	83 (98%)	2 (2%)	44	63
46	Sc	68/71 (96%)	68 (100%)	0	100	100
47	Sd	56/60 (93%)	55 (98%)	1 (2%)	54	71
48	Sf	27/54 (50%)	26 (96%)	1 (4%)	29	51
51	U4	110/169 (65%)	110 (100%)	0	100	100
52	U5	231/256 (90%)	229 (99%)	2 (1%)	75	83
All	All	10056/14279 (70%)	9969 (99%)	87 (1%)	74	83

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3B	145	ASN
2	3B	231	ARG
3	3D	285	ARG

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Mol	Chain	Res	Type
3	3D	391	ASN
4	3E	50	PHE
4	3E	318	GLN
5	3F	209	LYS
5	3F	367	LYS
6	3G	31	ARG
6	3G	105	ASN
6	3H	25	GLN
6	3H	105	ASN
12	AE	83	ARG
12	AE	134	MET
12	AE	232	ASN
15	B1	568	ARG
15	B1	831	ARG
15	B1	833	ARG
15	B1	853	ARG
16	BA	13	THR
16	BA	78	ARG
16	BA	94	ASN
16	BA	131	ARG
16	BA	279	PHE
16	BA	306	ASN
16	BA	418	ARG
16	BA	420	ARG
16	BA	434	ASN
16	BA	619	ARG
16	BA	777	ARG
16	BA	811	ASN
16	BA	837	ASN
17	BB	20	ASN
17	BB	22	ASN
17	BB	411	ASN
17	BB	587	MET
17	BB	596	ASN
17	BB	620	ASN
17	BB	629	ASN
17	BB	770	ASN
17	BB	799	LYS
18	BC	58	ASN
18	BC	157	ASN
18	BC	227	MET
18	BC	487	ARG

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Mol	Chain	Res	Type
19	BD	357	ASN
19	BD	369	ASN
19	BD	440	ASN
19	BD	543	LEU
20	BE	392	ARG
20	BE	449	ARG
20	BE	900	ASN
21	CA	46	ASN
21	CA	214	LEU
22	CB	155	ASN
22	CB	211	LYS
22	CB	216	LYS
22	CB	261	ASN
22	CB	683	ASN
22	CB	1233	ASN
26	MA	48	ASN
26	MA	71	ARG
26	MA	118	LEU
29	P1	142	ASN
33	SC	96	LEU
34	SF	180	LEU
34	SF	198	LYS
35	SG	65	ARG
35	SG	122	ASN
35	SG	157	ARG
37	SJ	64	ASN
38	SK	54	ARG
38	SK	92	LYS
38	SK	93	LEU
38	SK	120	LYS
38	SK	138	LYS
38	SK	149	ARG
39	SM	43	LYS
39	SM	67	ARG
39	SM	129	ARG
44	SY	144	ARG
45	SZ	34	ASN
45	SZ	102	LYS
47	Sd	64	ARG
48	Sf	39	LEU
52	U5	68	ARG
52	U5	105	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (127) such sidechains are listed below:

Mol	Chain	Res	Type
2	3B	91	HIS
2	3B	145	ASN
2	3B	183	HIS
2	3B	264	GLN
3	3D	37	GLN
3	3D	151	GLN
3	3D	156	HIS
3	3D	170	ASN
3	3D	230	ASN
4	3E	355	ASN
6	3G	105	ASN
6	3H	105	ASN
12	AE	227	ASN
12	AE	232	ASN
12	AE	258	HIS
12	AE	364	ASN
15	B1	91	HIS
15	B1	179	GLN
15	B1	233	HIS
15	B1	893	ASN
15	B1	909	ASN
15	B1	986	HIS
16	BA	92	HIS
16	BA	94	ASN
16	BA	156	GLN
16	BA	302	GLN
16	BA	303	ASN
16	BA	306	ASN
16	BA	344	HIS
16	BA	456	HIS
16	BA	485	ASN
16	BA	538	GLN
16	BA	597	ASN
16	BA	811	ASN
16	BA	813	HIS
16	BA	825	GLN
16	BA	837	ASN
17	BB	20	ASN
17	BB	22	ASN
17	BB	88	HIS
17	BB	195	GLN

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Mol	Chain	Res	Type
17	BB	200	HIS
17	BB	360	ASN
17	BB	390	GLN
17	BB	403	ASN
17	BB	411	ASN
17	BB	620	ASN
17	BB	628	HIS
17	BB	629	ASN
17	BB	770	ASN
17	BB	903	GLN
18	BC	28	ASN
18	BC	54	HIS
18	BC	58	ASN
18	BC	157	ASN
18	BC	189	HIS
18	BC	532	HIS
18	BC	585	ASN
18	BC	587	GLN
18	BC	589	GLN
18	BC	747	ASN
18	BC	757	GLN
19	BD	242	ASN
19	BD	245	HIS
19	BD	276	HIS
19	BD	282	ASN
19	BD	357	ASN
19	BD	369	ASN
19	BD	440	ASN
19	BD	520	ASN
20	BE	86	HIS
20	BE	473	ASN
20	BE	627	ASN
20	BE	900	ASN
21	CA	46	ASN
21	CA	90	ASN
22	CB	120	HIS
22	CB	155	ASN
22	CB	261	ASN
22	CB	333	ASN
22	CB	378	ASN
22	CB	436	HIS
22	CB	445	ASN

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Mol	Chain	Res	Type
22	CB	560	ASN
22	CB	582	GLN
22	CB	683	ASN
22	CB	729	ASN
22	CB	834	ASN
22	CB	869	ASN
22	CB	1137	ASN
22	CB	1154	ASN
22	CB	1159	ASN
22	CB	1233	ASN
23	E1	111	GLN
23	E2	73	HIS
23	E2	111	GLN
23	E2	170	HIS
25	K1	167	GLN
26	MA	48	ASN
29	P1	142	ASN
30	R1	334	ASN
30	R1	347	ASN
33	SC	149	GLN
33	SC	208	GLN
34	SF	98	ASN
34	SF	142	HIS
35	SG	34	GLN
35	SG	100	ASN
35	SG	200	ASN
36	SI	29	ASN
36	SI	89	HIS
37	SJ	64	ASN
38	SK	139	GLN
38	SK	176	ASN
42	SR	77	GLN
43	SX	15	ASN
43	SX	24	GLN
43	SX	44	HIS
43	SX	92	ASN
44	SY	79	ASN
45	SZ	77	ASN
51	U4	148	HIS
51	U4	156	ASN
52	U5	52	ASN
52	U5	105	ASN

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Mol	Chain	Res	Type
52	U5	192	ASN
52	U5	217	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	3A	151/333 (45%)	40 (26%)	1 (0%)
32	SA	978/1812 (53%)	257 (26%)	18 (1%)
7	5A	452/700 (64%)	114 (25%)	5 (1%)
All	All	1581/2845 (55%)	411 (25%)	24 (1%)

All (411) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	3A	14	A
1	3A	15	U
1	3A	19	A
1	3A	22	A
1	3A	24	U
1	3A	55	A
1	3A	56	A
1	3A	58	A
1	3A	59	G
1	3A	62	C
1	3A	64	A
1	3A	79	G
1	3A	80	U
1	3A	81	U
1	3A	85	G
1	3A	98	U
1	3A	99	U
1	3A	106	C
1	3A	109	G
1	3A	111	G
1	3A	114	A
1	3A	200	C
1	3A	207	A
1	3A	254	A
1	3A	255	U
1	3A	256	G
1	3A	257	A

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Mol	Chain	Res	Type
1	3A	261	U
1	3A	262	G
1	3A	317	A
1	3A	318	U
1	3A	319	G
1	3A	321	C
1	3A	322	A
1	3A	323	G
1	3A	324	U
1	3A	325	C
1	3A	328	A
1	3A	329	C
1	3A	330	A
7	5A	13	U
7	5A	14	U
7	5A	27	G
7	5A	58	U
7	5A	59	U
7	5A	60	G
7	5A	63	G
7	5A	67	G
7	5A	68	U
7	5A	69	U
7	5A	70	A
7	5A	74	U
7	5A	76	U
7	5A	91	U
7	5A	94	A
7	5A	102	A
7	5A	103	G
7	5A	109	C
7	5A	121	G
7	5A	122	U
7	5A	123	C
7	5A	124	A
7	5A	129	U
7	5A	130	G
7	5A	142	U
7	5A	143	A
7	5A	144	C
7	5A	145	A
7	5A	152	U

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Mol	Chain	Res	Type
7	5A	153	U
7	5A	157	U
7	5A	158	G
7	5A	163	G
7	5A	167	U
7	5A	169	A
7	5A	170	U
7	5A	171	G
7	5A	176	U
7	5A	178	G
7	5A	181	A
7	5A	200	A
7	5A	218	U
7	5A	226	U
7	5A	227	U
7	5A	233	G
7	5A	234	A
7	5A	237	A
7	5A	238	G
7	5A	239	U
7	5A	240	C
7	5A	246	G
7	5A	253	U
7	5A	261	U
7	5A	266	U
7	5A	267	U
7	5A	273	G
7	5A	281	G
7	5A	338	A
7	5A	340	U
7	5A	349	G
7	5A	353	A
7	5A	354	G
7	5A	355	C
7	5A	362	C
7	5A	363	A
7	5A	364	A
7	5A	367	C
7	5A	368	U
7	5A	370	U
7	5A	371	G
7	5A	372	A

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Mol	Chain	Res	Type
7	5A	382	U
7	5A	383	G
7	5A	384	U
7	5A	385	A
7	5A	386	A
7	5A	387	C
7	5A	389	U
7	5A	391	C
7	5A	392	U
7	5A	393	C
7	5A	394	U
7	5A	395	C
7	5A	401	A
7	5A	402	G
7	5A	403	C
7	5A	404	G
7	5A	405	A
7	5A	418	C
7	5A	419	A
7	5A	433	C
7	5A	434	G
7	5A	435	G
7	5A	441	C
7	5A	451	G
7	5A	452	A
7	5A	454	C
7	5A	457	G
7	5A	463	A
7	5A	464	G
7	5A	469	C
7	5A	470	U
7	5A	471	C
7	5A	473	A
7	5A	501	C
7	5A	503	C
7	5A	508	C
7	5A	511	G
7	5A	514	U
7	5A	524	U
7	5A	527	U
7	5A	528	G
7	5A	555	A

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Mol	Chain	Res	Type
7	5A	578	G
32	SA	8	U
32	SA	25	C
32	SA	26	A
32	SA	27	U
32	SA	32	U
32	SA	34	G
32	SA	39	A
32	SA	47	A
32	SA	50	C
32	SA	93	A
32	SA	94	U
32	SA	95	G
32	SA	100	A
32	SA	102	U
32	SA	105	A
32	SA	114	C
32	SA	116	U
32	SA	127	G
32	SA	128	U
32	SA	129	U
32	SA	132	U
32	SA	133	U
32	SA	134	U
32	SA	135	A
32	SA	137	U
32	SA	138	A
32	SA	139	C
32	SA	140	A
32	SA	141	U
32	SA	145	A
32	SA	146	U
32	SA	153	G
32	SA	159	U
32	SA	166	C
32	SA	180	A
32	SA	181	A
32	SA	185	U
32	SA	186	C
32	SA	187	G
32	SA	189	C
32	SA	190	C

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Mol	Chain	Res	Type
32	SA	191	C
32	SA	192	U
32	SA	193	U
32	SA	194	U
32	SA	195	G
32	SA	196	G
32	SA	197	A
32	SA	200	A
32	SA	204	G
32	SA	215	A
32	SA	216	U
32	SA	256	A
32	SA	261	U
32	SA	265	A
32	SA	270	C
32	SA	272	U
32	SA	275	C
32	SA	276	C
32	SA	277	U
32	SA	278	U
32	SA	279	G
32	SA	280	U
32	SA	281	G
32	SA	283	U
32	SA	284	G
32	SA	288	A
32	SA	290	G
32	SA	299	A
32	SA	302	U
32	SA	316	A
32	SA	320	U
32	SA	321	C
32	SA	322	G
32	SA	323	A
32	SA	332	U
32	SA	337	G
32	SA	338	C
32	SA	341	A
32	SA	351	C
32	SA	352	A
32	SA	359	A
32	SA	360	A

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Mol	Chain	Res	Type
32	SA	361	C
32	SA	369	A
32	SA	370	A
32	SA	372	G
32	SA	378	A
32	SA	379	U
32	SA	380	U
32	SA	382	C
32	SA	399	A
32	SA	400	A
32	SA	401	A
32	SA	402	C
32	SA	403	G
32	SA	404	G
32	SA	410	A
32	SA	411	C
32	SA	412	A
32	SA	416	A
32	SA	417	A
32	SA	418	G
32	SA	428	A
32	SA	440	U
32	SA	444	C
32	SA	452	A
32	SA	459	G
32	SA	464	A
32	SA	466	U
32	SA	468	A
32	SA	470	A
32	SA	475	A
32	SA	477	A
32	SA	484	C
32	SA	485	A
32	SA	487	G
32	SA	488	G
32	SA	493	U
32	SA	494	U
32	SA	499	U
32	SA	500	C
32	SA	501	U
32	SA	503	G
32	SA	504	U

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Mol	Chain	Res	Type
32	SA	505	A
32	SA	506	A
32	SA	507	U
32	SA	508	U
32	SA	510	G
32	SA	511	A
32	SA	514	G
32	SA	515	A
32	SA	522	U
32	SA	524	U
32	SA	525	A
32	SA	526	A
32	SA	527	A
32	SA	528	U
32	SA	534	A
32	SA	536	C
32	SA	539	G
32	SA	542	A
32	SA	543	C
32	SA	545	A
32	SA	546	U
32	SA	548	G
32	SA	558	U
32	SA	559	C
32	SA	563	U
32	SA	569	C
32	SA	570	A
32	SA	573	C
32	SA	575	C
32	SA	576	G
32	SA	585	A
32	SA	587	C
32	SA	592	A
32	SA	594	A
32	SA	595	G
32	SA	605	A
32	SA	634	G
32	SA	635	A
32	SA	862	A
32	SA	863	A
32	SA	873	U
32	SA	886	U

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Mol	Chain	Res	Type
32	SA	898	A
32	SA	905	A
32	SA	913	G
32	SA	914	G
32	SA	921	U
32	SA	928	U
32	SA	929	A
32	SA	930	A
32	SA	932	U
32	SA	933	A
32	SA	934	C
32	SA	935	U
32	SA	942	G
32	SA	944	A
32	SA	951	A
32	SA	960	U
32	SA	964	U
32	SA	966	A
32	SA	969	C
32	SA	978	A
32	SA	1040	G
32	SA	1053	G
32	SA	1058	U
32	SA	1059	U
32	SA	1060	U
32	SA	1061	A
32	SA	1063	U
32	SA	1074	G
32	SA	1076	A
32	SA	1082	C
32	SA	1084	A
32	SA	1086	A
32	SA	1087	A
32	SA	1149	G
32	SA	1150	G
32	SA	1151	A
32	SA	1154	G
32	SA	1155	G
32	SA	1157	A
32	SA	1158	C
32	SA	1159	C
32	SA	1160	A

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Mol	Chain	Res	Type
32	SA	1164	G
32	SA	1174	C
32	SA	1193	A
32	SA	1461	C
32	SA	1471	A
32	SA	1473	U
32	SA	1474	G
32	SA	1476	C
32	SA	1478	G
32	SA	1482	C
32	SA	1485	C
32	SA	1487	A
32	SA	1500	C
32	SA	1506	G
32	SA	1536	G
32	SA	1570	A
32	SA	1572	G
32	SA	1573	A
32	SA	1574	G
32	SA	1583	A
32	SA	1584	G
32	SA	1590	G
32	SA	1595	U
32	SA	1599	C
32	SA	1600	A
32	SA	1601	G
32	SA	1616	G
32	SA	1617	U
32	SA	1618	C
32	SA	1626	U
32	SA	1631	A
32	SA	1645	G
32	SA	1646	C
32	SA	1657	U
32	SA	1658	G
32	SA	1681	A
32	SA	1684	U
32	SA	1686	C
32	SA	1716	C
32	SA	1717	G
32	SA	1732	A
32	SA	1754	A

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Mol	Chain	Res	Type
32	SA	1756	A
32	SA	1767	G
32	SA	1796	C
32	SA	1800	A
32	SA	1804	A
32	SA	1812	U

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	3A	78	G
7	5A	245	C
7	5A	382	U
7	5A	385	A
7	5A	526	U
7	5A	527	U
32	SA	25	C
32	SA	139	C
32	SA	158	U
32	SA	192	U
32	SA	278	U
32	SA	351	C
32	SA	369	A
32	SA	417	A
32	SA	467	G
32	SA	487	G
32	SA	503	G
32	SA	591	A
32	SA	913	G
32	SA	929	A
32	SA	1083	G
32	SA	1157	A
32	SA	1481	C
32	SA	1573	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

This section contains visualisations of the EMDB entry EMD-6696. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

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

9 Map-model fit

This section was not generated.