



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:57 AM BST

PDB ID : 6ORD
Title : Crystal structure of tRNA^{Ala}(GGC) U32-A38 bound to cognate 70S A site
Authors : Nguyen, H.A.; Sunita, S.; Dunham, C.M.
Deposited on : 2019-04-30
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

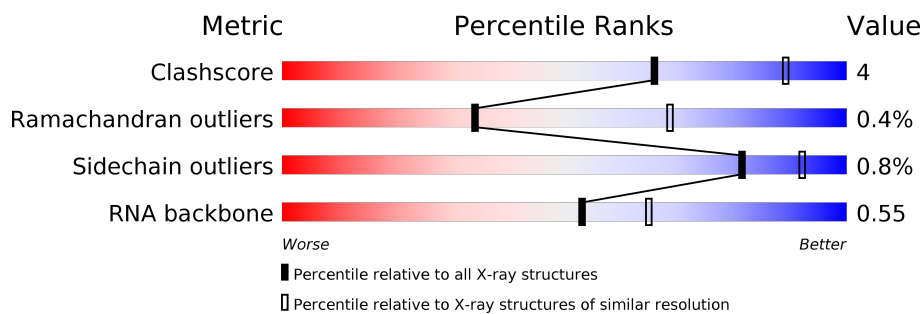
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)















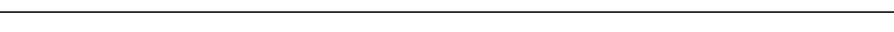

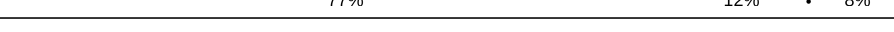

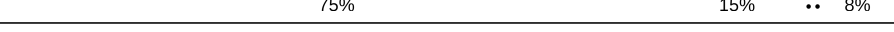



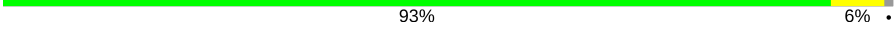


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	QA	1522	69% 25% . .
1	XA	1522	69% 25% . .
2	QB	256	71% 18% . 10%
2	XB	256	74% 16% 10%
3	QC	239	74% 11% . 14%
3	XC	239	75% 10% 14%
4	QD	209	80% 18% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	XD	209	 84% 16%
5	QE	162	 76% 15% 9%
5	XE	162	 78% 14% 9%
6	QF	101	 87% 12% .
6	XF	101	 77% 20% ..
7	QG	156	 81% 17% ..
7	XG	156	 91% 8% .
8	QH	138	 80% 19% .
8	XH	138	 84% 15% .
9	QI	128	 74% 23% ..
9	XI	128	 73% 26% .
10	QJ	105	 78% 14% 8%
10	XJ	105	 74% 17% 9%
11	QK	129	 74% 14% 12%
11	XK	129	 76% 12% 12%
12	QL	132	 77% 12% . 8%
12	XL	132	 75% 16% .. 8%
13	QM	126	 75% 15% .. 8%
13	XM	126	 67% 22% . 10%
14	QN	61	 85% 13% .
14	XN	61	 84% 15% .
15	QO	89	 93% 6% .
15	XO	89	 92% 7% .
16	QP	88	 78% 13% . 7%
16	XP	88	 72% 18% .. 7%


























Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	QQ	105	
17	XQ	105	
18	QR	88	
18	XR	88	
19	QS	93	
19	XS	93	
20	QT	106	
20	XT	106	
21	QU	27	
21	XU	27	
22	QV	77	
22	XV	77	
23	QX	19	
23	XX	19	
24	QY	76	
24	XY	76	
25	R0	85	
25	Y0	85	
26	R1	98	
26	Y1	98	
27	R2	72	
27	Y2	72	
28	R3	60	
28	Y3	60	
29	R4	71	





















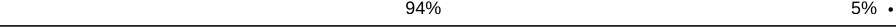




Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	Y4	71	
30	R5	60	
30	Y5	60	
31	R6	54	
31	Y6	54	
32	R7	49	
32	Y7	49	
33	R8	65	
33	Y8	65	
34	R9	37	
34	Y9	37	
35	RA	2915	
35	YA	2915	
36	RB	122	
36	YB	122	
37	RD	276	
37	YD	276	
38	RE	206	
38	YE	206	
39	RF	210	
39	YF	210	
40	RG	182	
40	YG	182	
41	RH	180	
41	YH	180	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
42	RI	148	 94% 5% .
42	YI	148	 93% 6% .
43	RN	140	 84% 15% .
43	YN	140	 91% 9%
44	RO	122	 80% 20% .
44	YO	122	 79% 21%
45	RP	150	 81% 18% .
45	YP	150	 79% 20% .
46	RQ	141	 82% 18%
46	YQ	141	 87% 13%
47	RR	118	 92% 8%
47	YR	118	 89% 11%
48	RS	112	 84% 13% ..
48	YS	112	 88% 9% ..
49	RT	146	 73% 16% . 10%
49	YT	146	 75% 14% . 10%
50	RU	118	 85% 12% ...
50	YU	118	 88% 8% ...
51	RV	101	 79% 18% .
51	YV	101	 94% 5% .
52	RW	113	 88% 11% .
52	YW	113	 88% 12% .
53	RX	96	 85% 14% .
53	YX	96	 91% 8% .
54	RY	110	 86% 11% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	YY	110	<div><div></div><div>79%</div><div>17%</div><div></div><div></div></div>
55	RZ	206	<div><div></div><div>74%</div><div>12%</div><div>14%</div><div></div></div>
55	YZ	206	<div><div></div><div>74%</div><div>11%</div><div></div><div>14%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 293819 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	QA	1500	Total	C	N	O	P	0	0	0
			32246	14358	5975	10413	1500			
1	XA	1504	Total	C	N	O	P	0	0	0
			32331	14396	5990	10441	1504			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	QB	231	Total	C	N	O	S	0	0	0
			1842	1175	330	332	5			
2	XB	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	QC	206	Total	C	N	O	S	0	0	0
			1558	979	305	273	1			
3	XC	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	QD	208	Total	C	N	O	S	0	0	0
			1665	1043	329	286	7			
4	XD	208	Total	C	N	O	S	0	0	0
			1668	1047	330	284	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	QE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			
5	XE	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	QF	100	Total	C	N	O	S	0	0	0
			814	516	144	151	3			
6	XF	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	QG	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			
7	XG	155	Total	C	N	O	S	0	0	0
			1229	766	241	216	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	QH	137	Total	C	N	O	S	0	0	0
			1098	694	210	192	2			
8	XH	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	QI	127	Total	C	N	O		0	0	0
			986	625	193	168				
9	XI	126	Total	C	N	O		0	0	0
			966	613	186	167				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	QJ	97	Total	C	N	O		0	0	0
			719	446	142	131				

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	XJ	96	Total	C	N	O			
			710	442	137	131	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	QK	114	Total	C	N	O	S		
			834	520	156	155	3	0	0
11	XK	114	Total	C	N	O	S		
			833	519	156	155	3	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	QL	122	Total	C	N	O	S		
			932	586	185	159	2	0	0
12	XL	122	Total	C	N	O	S		
			932	586	185	159	2	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	QM	116	Total	C	N	O	S		
			914	564	189	159	2	0	0
13	XM	114	Total	C	N	O	S		
			895	550	186	157	2	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	QN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0
14	XN	60	Total	C	N	O	S		
			492	312	104	72	4	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	QO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0
15	XO	88	Total	C	N	O	S		
			728	456	144	126	2	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	QP	82	Total	C	N	O	S	0	0	0
			681	433	134	113	1			
16	XP	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	QQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
17	XQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	QR	68	Total	C	N	O	0	0	0
			555	355	108	92			
18	XR	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	QS	83	Total	C	N	O	S	0	0	0
			648	415	120	111	2			
19	XS	83	Total	C	N	O	S	0	0	0
			645	410	118	115	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	QT	96	Total	C	N	O	S	0	0	0
			732	449	157	124	2			
20	XT	98	Total	C	N	O	S	0	0	0
			733	451	154	126	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	QU	23	Total	C	N	O	0	0	0
			199	122	48	29			
21	XU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called P-site tRNA^{fMet}.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	QV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	XV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	QX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			
23	XX	18	Total	C	N	O	P	0	0	0
			394	176	80	120	18			

- Molecule 24 is a RNA chain called A-site tRNA^{Ala}(GGC) U32-A38.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	QY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			
24	XY	76	Total	C	N	O	P	0	0	0
			1625	724	293	532	76			

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	R0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			
25	Y0	77	Total	C	N	O	S	0	0	0
			608	375	129	103	1			

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	R1	97	Total	C	N	O	S	0	0	0
			754	475	148	130	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Y1	97	Total	C	N	O	S	0	0	0
			759	478	149	131	1			

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	R2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			
27	Y2	70	Total	C	N	O	S	0	0	0
			592	368	119	103	2			

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	R3	59	Total	C	N	O		0	0	0
			469	298	90	81				
28	Y3	59	Total	C	N	O		0	0	0
			464	296	90	78				

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	R4	69	Total	C	N	O	S	0	0	0
			546	346	96	99	5			
29	Y4	69	Total	C	N	O	S	0	0	0
			536	342	98	91	5			

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	R5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
30	Y5	59	Total	C	N	O	S	0	0	0
			455	285	89	76	5			

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	R6	53	Total	C	N	O	S	0	0	0
			453	281	91	77	4			
31	Y6	53	Total	C	N	O	S	0	0	0
			449	279	91	75	4			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	R7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
32	Y7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	R8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			
33	Y8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	R9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
34	Y9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 35 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	RA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			
35	YA	2867	Total	C	N	O	P	0	0	0
			61758	27491	11552	19850	2865			

- Molecule 36 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	RB	120	Total	C	N	O	P	0	0	0
			2572	1145	476	832	119			
36	YB	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 37 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	RD	275	Total	C	N	O	S	0	0	0
			2131	1346	422	360	3			
37	YD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 38 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	RE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			
38	YE	204	Total	C	N	O	S	0	0	0
			1559	985	298	270	6			

- Molecule 39 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	RF	202	Total	C	N	O	S	0	0	0
			1583	1009	297	275	2			
39	YF	202	Total	C	N	O	S	0	0	0
			1579	1007	296	274	2			

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	RG	181	Total	C	N	O	S	0	0	0
			1426	916	253	253	4			
40	YG	181	Total	C	N	O	S	0	0	0
			1424	912	259	249	4			

- Molecule 41 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	RH	174	Total	C	N	O	S	0	0	0
			1330	845	248	236	1			
41	YH	173	Total	C	N	O	S	0	0	0
			1324	842	247	234	1			

- Molecule 42 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	RI	147	Total	C	N	O	S	0	0	0
			1094	699	191	203	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	YI	146	Total	C	N	O	S	0	0	0
			1076	687	186	202	1			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	RN	140	Total	C	N	O	S	0	0	0
			1121	722	208	187	4			
43	YN	140	Total	C	N	O	S	0	0	0
			1117	719	207	187	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	RO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
44	YO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	RP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			
45	YP	149	Total	C	N	O	S	0	0	0
			1135	706	230	196	3			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	RQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
46	YQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	RR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
47	YR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	RS	110	Total	C	N	O	0	0	0
			877	553	175	149			
48	YS	110	Total	C	N	O	0	0	0
			870	549	173	148			

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	RT	131	Total	C	N	O	S	0	0	0
			1091	680	225	185	1			
49	YT	131	Total	C	N	O	S	0	0	0
			1083	675	224	183	1			

- Molecule 50 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	RU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
50	YU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	RV	101	Total	C	N	O	S	0	0	0
			775	498	141	135	1			
51	YV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	RW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			
52	YW	112	Total	C	N	O	S	0	0	0
			886	557	174	153	2			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	RX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			
53	YX	95	Total	C	N	O	S	0	0	0
			750	488	135	126	1			

- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	RY	107	Total	C	N	O	S	0	0	0
			810	520	153	131	6			
54	YY	107	Total	C	N	O	S	0	0	0
			810	519	153	132	6			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	RZ	178	Total	C	N	O	S	0	0	0
			1406	898	253	253	2			
55	YZ	177	Total	C	N	O	S	0	0	0
			1381	885	246	248	2			

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	QA	221	Total	Mg	0	0
			221	221		
56	YV	1	Total	Mg	0	0
			1	1		
56	RP	3	Total	Mg	0	0
			3	3		
56	R7	3	Total	Mg	0	0
			3	3		
56	YA	707	Total	Mg	0	0
			707	707		
56	Y5	1	Total	Mg	0	0
			1	1		
56	YR	2	Total	Mg	0	0
			2	2		
56	RT	4	Total	Mg	0	0
			4	4		
56	QD	4	Total	Mg	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	RN	2	Total 2	Mg 2	0	0
56	XE	2	Total 2	Mg 2	0	0
56	RG	4	Total 4	Mg 4	0	0
56	QI	1	Total 1	Mg 1	0	0
56	YD	7	Total 7	Mg 7	0	0
56	QV	5	Total 5	Mg 5	0	0
56	YE	5	Total 5	Mg 5	0	0
56	Y8	1	Total 1	Mg 1	0	0
56	YO	1	Total 1	Mg 1	0	0
56	XA	193	Total 193	Mg 193	0	0
56	Y1	2	Total 2	Mg 2	0	0
56	RQ	4	Total 4	Mg 4	0	0
56	R0	3	Total 3	Mg 3	0	0
56	XT	1	Total 1	Mg 1	0	0
56	QL	3	Total 3	Mg 3	0	0
56	RU	2	Total 2	Mg 2	0	0
56	QG	2	Total 2	Mg 2	0	0
56	RO	1	Total 1	Mg 1	0	0
56	XJ	1	Total 1	Mg 1	0	0
56	Y7	2	Total 2	Mg 2	0	0
56	QH	2	Total 2	Mg 2	0	0

Continued on next page...

Continued from previous page...

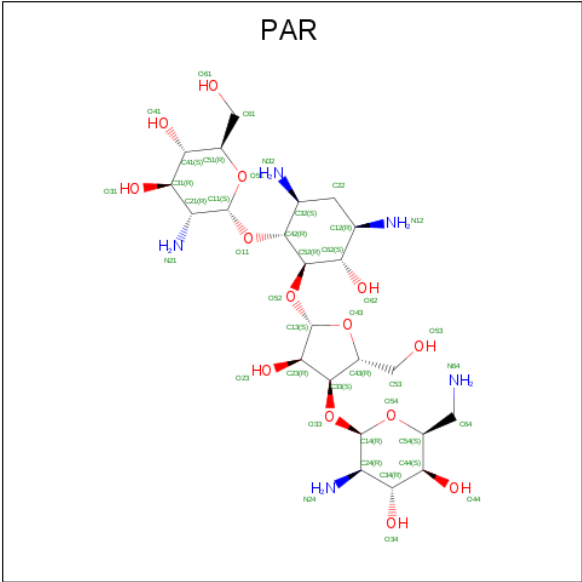
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	YG	3	Total 3	Mg 3	0	0
56	XY	1	Total 1	Mg 1	0	0
56	YQ	2	Total 2	Mg 2	0	0
56	YN	1	Total 1	Mg 1	0	0
56	XF	2	Total 2	Mg 2	0	0
56	RR	2	Total 2	Mg 2	0	0
56	RD	8	Total 8	Mg 8	0	0
56	R1	1	Total 1	Mg 1	0	0
56	QO	2	Total 2	Mg 2	0	0
56	YT	3	Total 3	Mg 3	0	0
56	RV	3	Total 3	Mg 3	0	0
56	QF	2	Total 2	Mg 2	0	0
56	RH	2	Total 2	Mg 2	0	0
56	R5	2	Total 2	Mg 2	0	0
56	Y0	1	Total 1	Mg 1	0	0
56	RA	709	Total 709	Mg 709	0	0
56	QK	1	Total 1	Mg 1	0	0
56	YF	3	Total 3	Mg 3	0	0
56	YP	2	Total 2	Mg 2	0	0
56	RZ	1	Total 1	Mg 1	0	0
56	QB	1	Total 1	Mg 1	0	0

Continued on next page...

Continued from previous page...

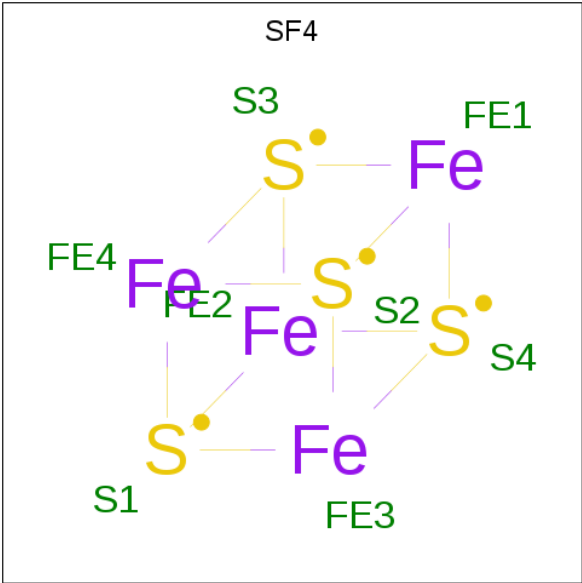
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	R9	1	Total 1	Mg 1	0	0
56	RE	4	Total 4	Mg 4	0	0
56	XL	2	Total 2	Mg 2	0	0
56	YB	20	Total 20	Mg 20	0	0
56	QT	1	Total 1	Mg 1	0	0
56	Y6	1	Total 1	Mg 1	0	0
56	QN	1	Total 1	Mg 1	0	0
56	YW	2	Total 2	Mg 2	0	0
56	RW	1	Total 1	Mg 1	0	0
56	R6	1	Total 1	Mg 1	0	0
56	XV	3	Total 3	Mg 3	0	0
56	QP	1	Total 1	Mg 1	0	0
56	RB	17	Total 17	Mg 17	0	0
56	YI	1	Total 1	Mg 1	0	0
56	QE	4	Total 4	Mg 4	0	0
56	XR	1	Total 1	Mg 1	0	0
56	RF	4	Total 4	Mg 4	0	0
56	R3	3	Total 3	Mg 3	0	0
56	Y3	1	Total 1	Mg 1	0	0

- Molecule 57 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
57	QA	1	Total	C	N	O	0	0
			42	23	5	14		
57	XA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
58	QD	1	Total	Fe	S	0	0
			8	4	4		
58	XD	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

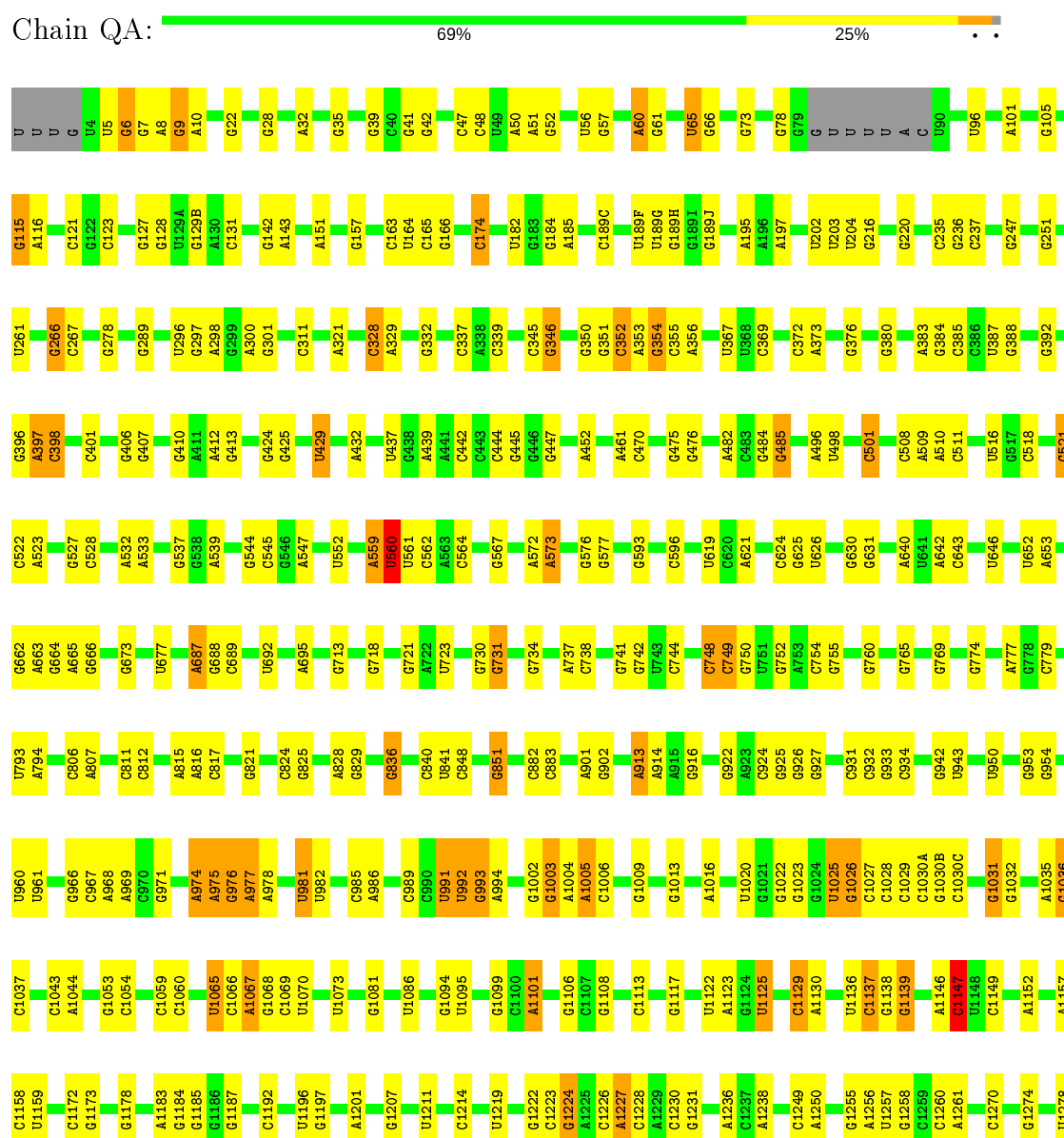
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	Y9	1	Total	Zn	0	0
			1	1		
59	Y6	1	Total	Zn	0	0
			1	1		
59	QN	1	Total	Zn	0	0
			1	1		
59	XN	1	Total	Zn	0	0
			1	1		
59	R9	1	Total	Zn	0	0
			1	1		
59	Y4	1	Total	Zn	0	0
			1	1		
59	R6	1	Total	Zn	0	0
			1	1		
59	Y5	1	Total	Zn	0	0
			1	1		
59	R5	1	Total	Zn	0	0
			1	1		
59	R4	1	Total	Zn	0	0
			1	1		
59	RY	1	Total	Zn	0	0
			1	1		
59	YY	1	Total	Zn	0	0
			1	1		

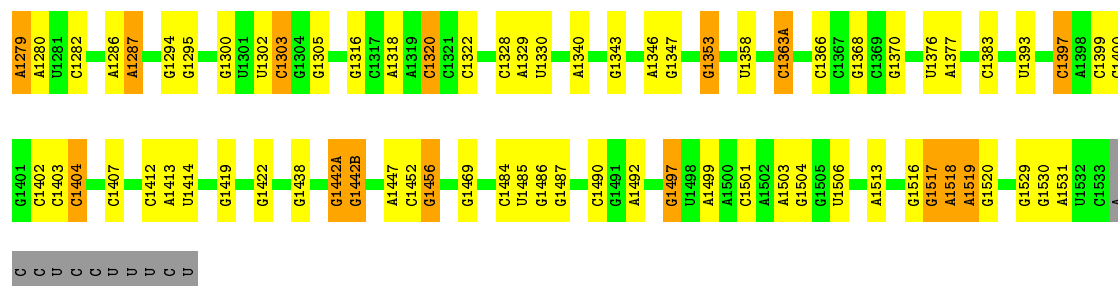
3 Residue-property plots [i](#)

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.

Note EDS failed to run properly.

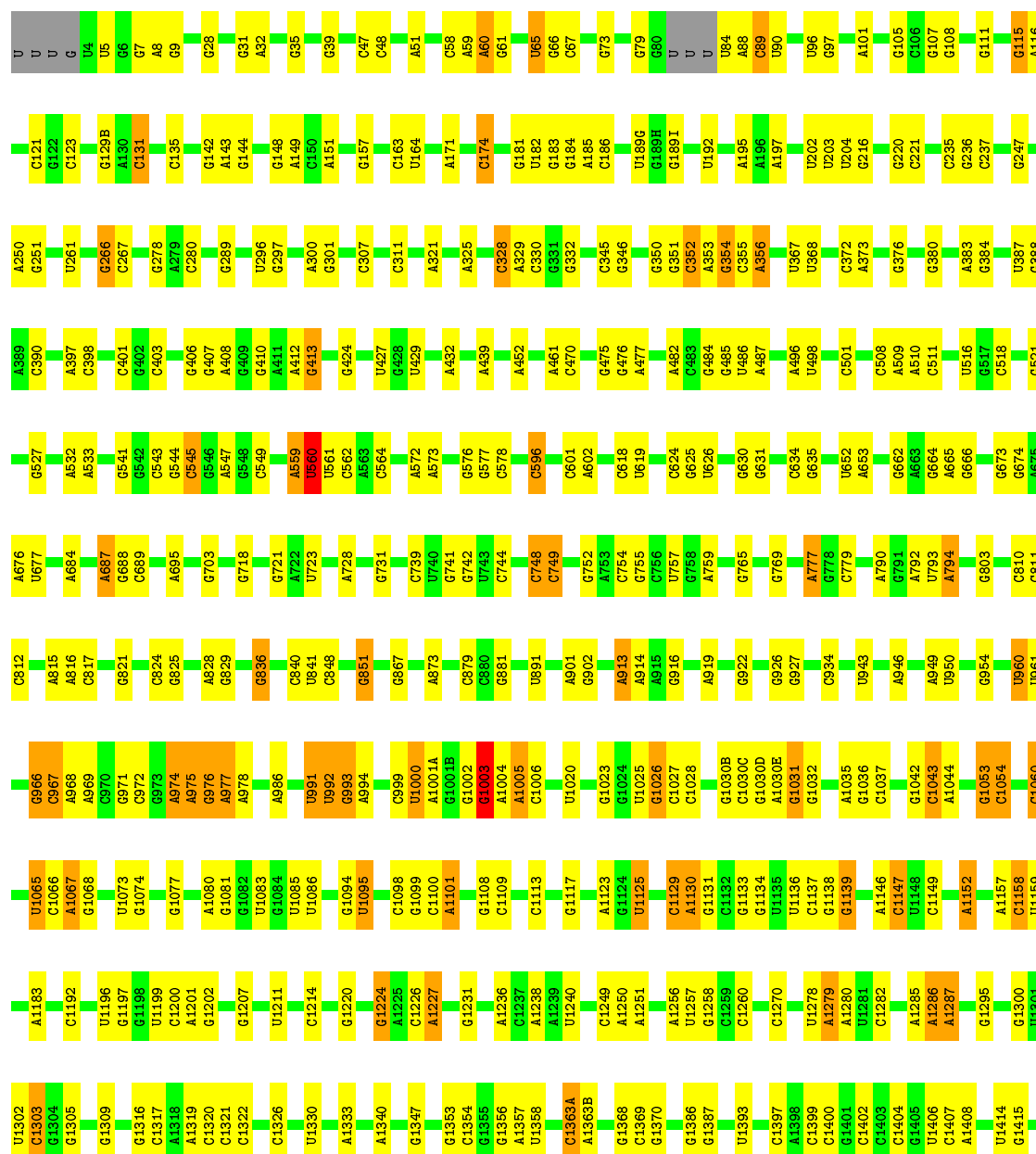
• Molecule 1: 16S rRNA

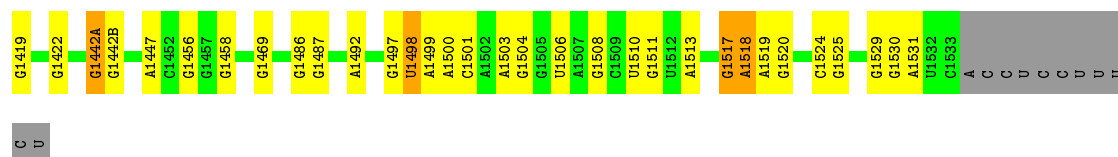




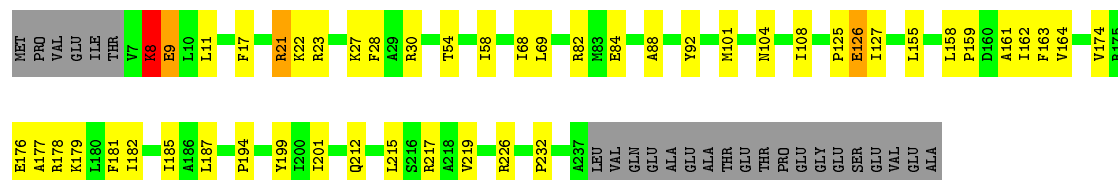
• Molecule 1: 16S rRNA

Chain XA:  69% 25% . .

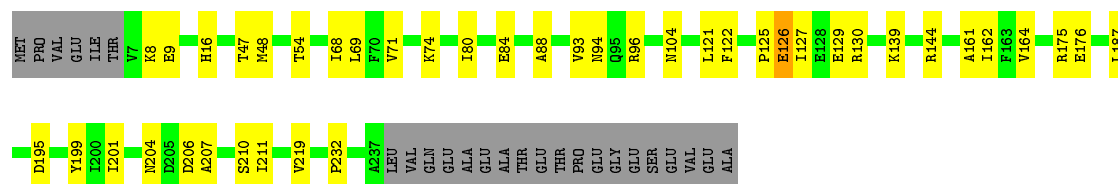
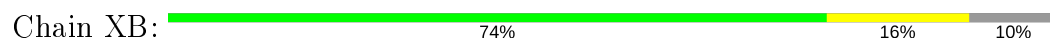




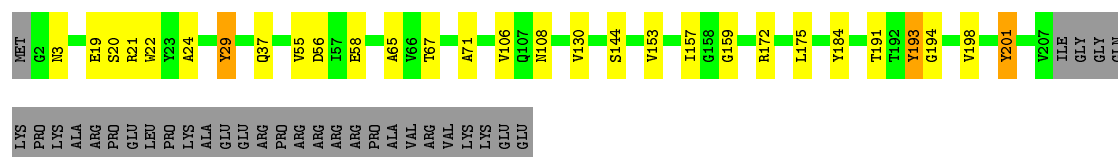
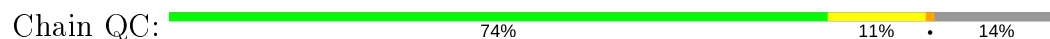
- Molecule 2: 30S ribosomal protein S2



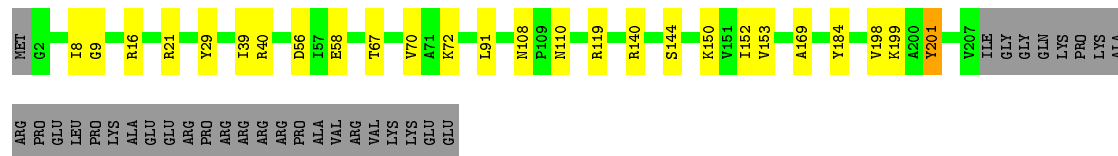
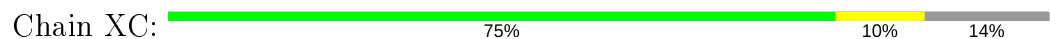
- Molecule 2: 30S ribosomal protein S2



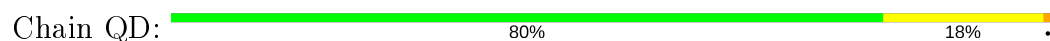
- Molecule 3: 30S ribosomal protein S3



- Molecule 3: 30S ribosomal protein S3



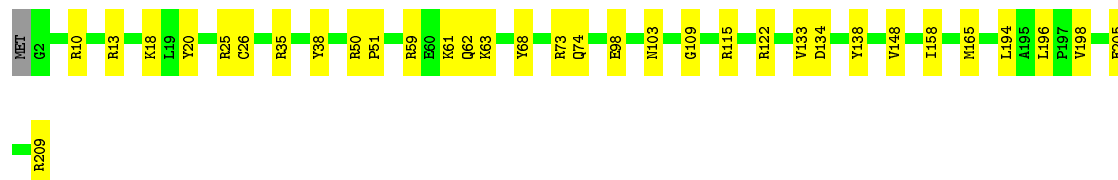
- Molecule 4: 30S ribosomal protein S4





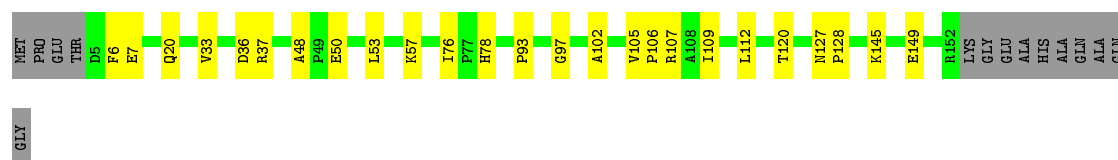
- Molecule 4: 30S ribosomal protein S4

Chain XD: 84% 16%



- Molecule 5: 30S ribosomal protein S5

Chain QE: 76% 15% 9%



- Molecule 5: 30S ribosomal protein S5

Chain XE: 78% 14% 9%



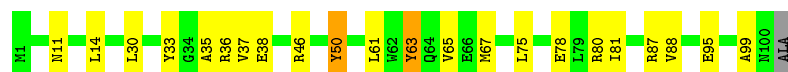
- Molecule 6: 30S ribosomal protein S6

Chain QF: 87% 12%




- Molecule 6: 30S ribosomal protein S6

Chain XF: 77% 20%



- Molecule 7: 30S ribosomal protein S7

Chain QG:  81% 17% ..




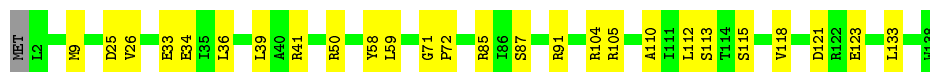
- Molecule 7: 30S ribosomal protein S7

Chain XG:  91% 8% .




- Molecule 8: 30S ribosomal protein S8

Chain QH:  80% 19% .



- Molecule 8: 30S ribosomal protein S8

Chain XH:  84% 15% .



- Molecule 9: 30S ribosomal protein S9

Chain QI:  74% 23% ..




- Molecule 9: 30S ribosomal protein S9

Chain XI:  73% 26% .



- Molecule 10: 30S ribosomal protein S10

Chain QJ:  78% 14% 8%



- Molecule 10: 30S ribosomal protein S10

Chain XJ: 74% 17% 9%



- Molecule 11: 30S ribosomal protein S11

Chain QK: 74% 14% 12%



- Molecule 11: 30S ribosomal protein S11

Chain XK: 76% 12% 12%



- Molecule 12: 30S ribosomal protein S12

Chain QL: 77% 12% 8%



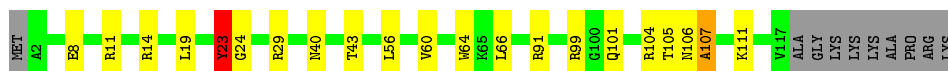
- Molecule 12: 30S ribosomal protein S12

Chain XL: 75% 16% 8%



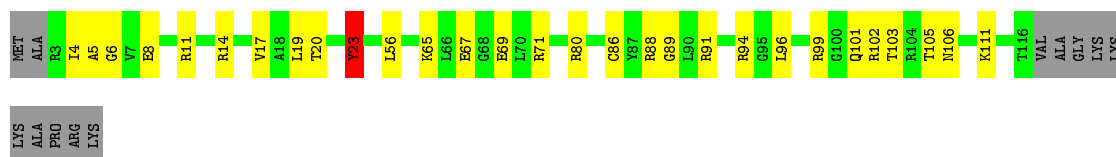
- Molecule 13: 30S ribosomal protein S13

Chain QM: 75% 15% 8%



- Molecule 13: 30S ribosomal protein S13

Chain XM: 67% 22% 10%



- Molecule 14: 30S ribosomal protein S14 type Z

Chain QN: 85% 13% .



- Molecule 14: 30S ribosomal protein S14 type Z

Chain XN: 84% 15% .



- Molecule 15: 30S ribosomal protein S15

Chain QO: 93% 6% .



- Molecule 15: 30S ribosomal protein S15

Chain XO: 92% 7% .



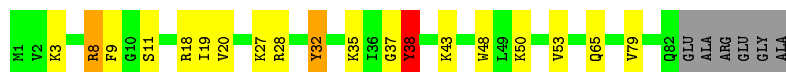
- Molecule 16: 30S ribosomal protein S16

Chain QP: 78% 13% 7% .




- Molecule 16: 30S ribosomal protein S16

Chain XP: 72% 18% 7% .




- Molecule 17: 30S ribosomal protein S17

Chain QQ:  81% 13% 6%



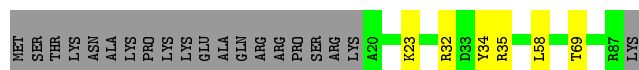
- Molecule 17: 30S ribosomal protein S17

Chain XQ:  78% 16% 6%



- Molecule 18: 30S ribosomal protein S18

Chain QR:  70% 7% 23%




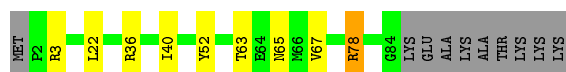
- Molecule 18: 30S ribosomal protein S18

Chain XR:  64% 14% 23%



- Molecule 19: 30S ribosomal protein S19

Chain QS:  80% 9% 11%




- Molecule 19: 30S ribosomal protein S19

Chain XS:  76% 13% 11%




- Molecule 20: 30S ribosomal protein S20

Chain QT:  79% 11% 9%




- Molecule 20: 30S ribosomal protein S20

Chain XT:  86% 7% 8%




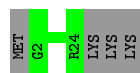
- Molecule 21: 30S ribosomal protein Thx

Chain QU:  81% 15%



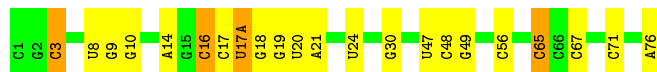
- Molecule 21: 30S ribosomal protein Thx

Chain XU:  85% 15%




- Molecule 22: P-site tRNA^{fMet}

Chain QV:  71% 23% 5%



- Molecule 22: P-site tRNA^{fMet}

Chain XV:  77% 18% 5%



- Molecule 23: mRNA

Chain QX:  53% 37% 5% 5%



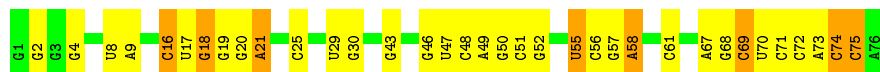
- Molecule 23: mRNA

Chain XX:  42% 47% 5% 5%



- Molecule 24: A-site tRNA^{Ala}(GGC) U32-A38

Chain QY:  54% 36% 11%




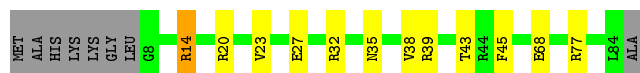
- Molecule 24: A-site tRNAAla(GGC) U32-A38

Chain XY:  47% 43% 9%



- Molecule 25: 50S ribosomal protein L27

Chain R0:  76% 13% 9%



- Molecule 25: 50S ribosomal protein L27

Chain Y0:  71% 19% 9%



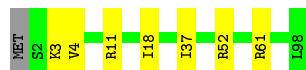
- Molecule 26: 50S ribosomal protein L28

Chain R1:  86% 13% 9%




- Molecule 26: 50S ribosomal protein L28

Chain Y1:  92% 7% 9%




- Molecule 27: 50S ribosomal protein L29

Chain R2:  79% 18% 9%



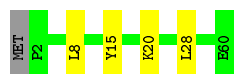
- Molecule 27: 50S ribosomal protein L29

Chain Y2:  85% 13%




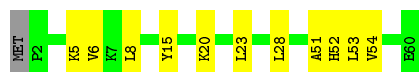
- Molecule 28: 50S ribosomal protein L30

Chain R3:  92% 7%




- Molecule 28: 50S ribosomal protein L30

Chain Y3:  80% 18%



- Molecule 29: 50S ribosomal protein L31

Chain R4:  77% 20%




- Molecule 29: 50S ribosomal protein L31

Chain Y4:  68% 24%




- Molecule 30: 50S ribosomal protein L32

Chain R5:  85% 13%



- Molecule 30: 50S ribosomal protein L32

Chain Y5:  85% 13%




- Molecule 31: 50S ribosomal protein L33

Chain R6:  89% 9%




- Molecule 31: 50S ribosomal protein L33

Chain Y6:  85% 13%




- Molecule 32: 50S ribosomal protein L34

Chain R7:  86% 12%



- Molecule 32: 50S ribosomal protein L34

Chain Y7:  84% 14%




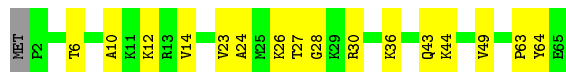
- Molecule 33: 50S ribosomal protein L35

Chain R8:  72% 26%




- Molecule 33: 50S ribosomal protein L35

Chain Y8:  74% 25%



- Molecule 34: 50S ribosomal protein L36

Chain R9:  78% 22%



- Molecule 34: 50S ribosomal protein L36

Chain Y9:

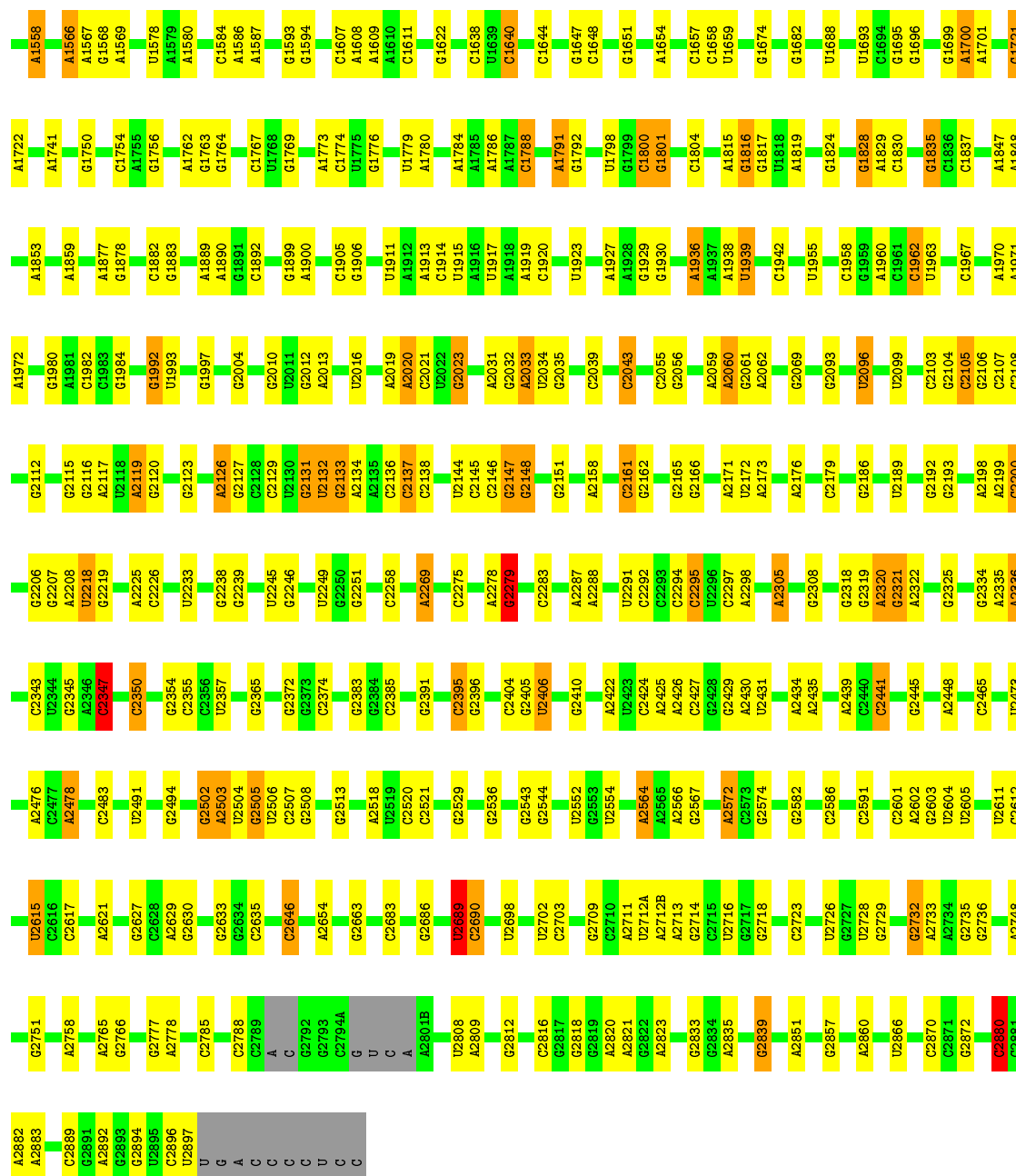


- Molecule 35: 23S rRNA

Chain RA:

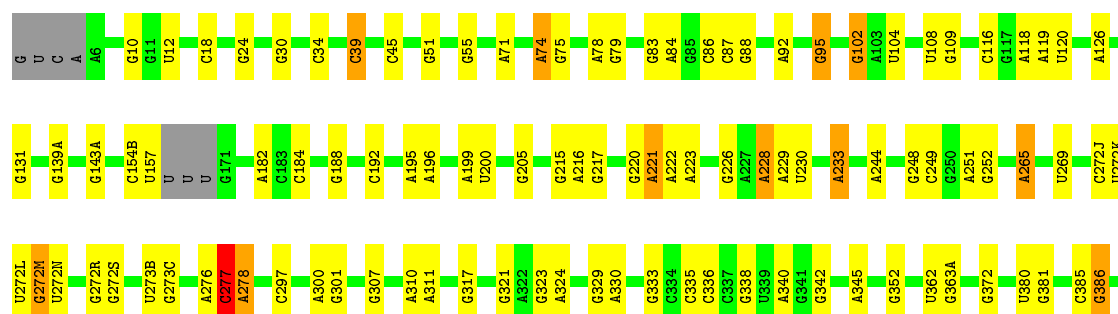


U1420	A1253	U1108	C1041	A918	C	G573	A457	C318	U200
G1421	A1254	C1109	G1042	G919	A	C574	G458	C319	G
G1422	U1255	G1110	G1043	U922	C	A575	U459	A320	U
G1423	G1256	A1111	G1044	G905	C	U576	A460	G321	C
G1424	C1257	G1112	A1045	G932	C	A577	C461	A322	A
A1427	U1113	U1114	A1046	U907	C	A578	G462	G323	G6
C1428	G1047	G1047	G1047	A941	C	G579	G463	A324	G10
G1429	G1048	A1048	A1048	A941	C	C580	C	A216	G15
C1437	C1124	C1124	G1051	G944	C	C581	A466	G329	G18
A1445A	A1128	A1128	C1052	A945	C	G582	A467	A330	C13
A1272	A1129	A1129	C1053	G946	C	G583	G468	A331	A222
U1273	U1130	U1130	A1054	A953	C	A586	G469	G338	A223
G1450A	C1135	C1135	G1055	G954	C	U587	C	U339	C39
U1288	G1136	G1136	A057	G956	C	G830	G470	A340	C34
G1455	U1300	U1300	G1058	A957	C	G831	A479	G342	C45
U1300	A1301	A1301	C1059	G958	C	G601	A480	G342	C51
A1460	G1461	G1461	U1060	A959	C	G602	G481	A345	A71
G1309	G1153	G1153	U	U947	C	A603	G491	G352	G242
G1311	G1154	G1154	G1062	C961	C	G604	C605	U362	G248
G1312	A1155	A1155	C1063	G954	C	U606	G500	G363A	C249
C1467	U1312	U1312	C1064	G955	C	G607	A503	C365	G83
A1471	G1162	G1162	G1065	C975A	C	A508	U504	G372	A265
C1314	C1314	C1314	G975B	C957	C	G608	A505	G386	U269
G1333	G1171	G1171	U858	C976	C	A609	C	A390	G117
C1333	G	G	G859	G969	C	G613	G	G392	A118
U1341	A	A	U860	U860	C	U614A	G508	C409	A119
U1352	U	U	A861	A861	C	G614C	C509	A411	U120
A1353	G	G	C986	G973	C	A614D	G521	A412	U126
C1493	C1178	C1178	U1072	G983	C	G615	G522	C420	A157
A1494	A1074	A1074	A1073	G987	C	G620	A526	A428	U
U1497	U1188	U1188	C1075	G993	C	C624	G527	A435	U
G1500	A1189	A1189	C1076	C994	C	C730	A528	G442	A
A1365	G1195	G1195	U1077	C995	C	A734	A529	A443	A181
A1366	U1078	U1078	C988	A996	C	G734	C	C444	A182
A1367	C1206	C1206	C989	A1000	C	A631	C	G307	G188
G1368	G1206	G1206	U082	A1000	C	A631	C	U273B	A195
G1369	A1210	A1210	U1083	C1005	C	G832	C531	G273C	A196
C1370	U1211	U1211	A1084	C1006	C	C993	A532	A276	U
C1376	A1220	A1220	C085	U1085	C	C894	C533	C277	U
A1379	G1223	G1223	G1087	A1008	C	U895	C535	A278	U
G1514	C1224	C1224	A1088	A1009	C	A764	C	C297	U
G1515	G1225	G1225	C997	C997	C	G765	G545	C297	U
C1516	U1012	U1012	C998	C998	C	C766	C	C297	U
G1517	C1013	C1013	U012	U012	C	C645	C	C297	U
G1533	G1091	G1091	C1013	C1013	C	A646	A	C297	U
U	C1092	C1092	A1021	A1021	C	G647	A	C297	U
A	G1093	G1093	U907	U907	C	G647	A	C297	U
C1536	U1023	U1023	G775	G775	C	A652C	G549	C298	A181
A1542	G1232	G1232	U1023	U1023	C	G652D	U55A	A299	A

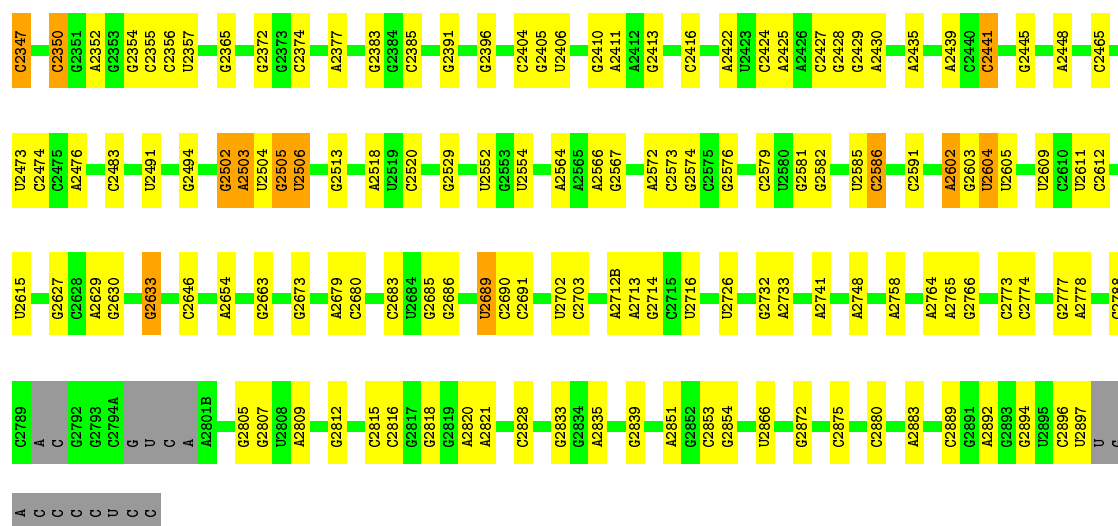


- Molecule 35: 23S rRNA

Chain YA:  71% 23% 6%



A2225	U2118	G1816	A1669	G1533	U1394	A1220	C1082	A1009	G692	G775	G649	G549	G396
A2119	A2119	G1824	G1674	U	A1395	G1223	C1082	U1012	C893	G776	A652C	U557	U405
G2120	G2120	G1827	G1674	A	G1400	A1226	A1095	C1013	U895	A782	G652D	U557	G411
G2121	G2121	G1828	G1674	C1536	G1401	A1226	U1097	G1022	A896	A783	G652E	C560	A412
G2122	G2122	A1829	G1682	G1537	U1415	G1236	A1098	U1023	C997	A784	G	G563	C413
A2126	A2126	C1830	U1693	U1540	G1416	G1243	G1099	G1024	G906	G786	G	C564	C414
G2127	G2127	G1835	G1694	U1541	G1417	G1243	C1102	U1025	U907	C787	C	C565	A415
C2128	C2128	G1835	G1695	A1542	G1418	G1243	C1103	U1026	G906	U787	C	C573	C420
C2129	C2129	G1835	G1696	C1543	G1419	G1250	A1103	U1026	U907	U788	C	C574	C420
U2130	U2130	A1847	G1697	C1543	U1420	G1250	U1104	U1033	A910	A789	C	A575	A428
G2131	G2131	A1848	A1698	C1546	G1421	A1253	U1105	G1034	A910	A789	A	A575	A428
U2132	U2132	A1853	G1699	C1547	G1422	A1253	G1106	U1035	C915	G792	C	A575	A428
G2133	G2133	A1853	A1700	A1558	G1423	G1256	G1107	U1035	G916	A793	C	A575	A428
A2134	A2134	A1853	A1701	A1558	G1424	G1256	U1108	C1038	A917	G794	C	A575	A428
A2135	A2135	A1853	A1701	A1558	G1425	G1266	C1109	C1038	A918	C795	C	A575	A428
C2136	C2136	A1853	A1701	A1558	G1426	G1266	G1110	C1041	A919	C795	C	A575	A428
C2137	C2137	A1853	A1701	A1558	G1427	G1266	A1111	C1041	A919	C795	C	A575	A428
C2138	C2138	A1853	A1701	A1558	G1428	G1266	A1112	C1041	A919	C795	C	A575	A428
C2139	C2139	A1853	A1701	A1558	G1429	G1266	U1113	A1045	G932	A802	C	A575	A428
C2140	C2140	A1853	A1701	A1558	G1430	G1266	U1114	A1046	G932	A802	C	A575	A428
C2141	C2141	A1853	A1701	A1558	G1431	G1266	U1115	A1047	G932	A802	C	A575	A428
C2142	C2142	A1853	A1701	A1558	G1432	G1266	U1116	A1048	G932	A802	C	A575	A428
C2143	C2143	A1853	A1701	A1558	G1433	G1266	U1117	A1049	G932	A802	C	A575	A428
C2144	C2144	A1853	A1701	A1558	G1434	G1266	U1118	A1050	G932	A802	C	A575	A428
C2145	C2145	A1853	A1701	A1558	G1435	G1266	U1119	A1051	G932	A802	C	A575	A428
C2146	C2146	A1853	A1701	A1558	G1436	G1266	U1120	A1052	G932	A802	C	A575	A428
C2147	C2147	A1853	A1701	A1558	G1437	G1266	U1121	A1053	G932	A802	C	A575	A428
C2148	C2148	A1853	A1701	A1558	G1438	G1266	U1122	A1054	G932	A802	C	A575	A428
C2149	C2149	A1853	A1701	A1558	G1439	G1266	U1123	A1055	G932	A802	C	A575	A428
C2150	C2150	A1853	A1701	A1558	G1440	G1266	U1124	A1056	G932	A802	C	A575	A428
C2151	C2151	A1853	A1701	A1558	G1441	G1266	U1125	A1057	G932	A802	C	A575	A428
C2152	C2152	A1853	A1701	A1558	G1442	G1266	U1126	A1058	G932	A802	C	A575	A428
C2153	C2153	A1853	A1701	A1558	G1443	G1266	U1127	A1059	G932	A802	C	A575	A428
C2154	C2154	A1853	A1701	A1558	G1444	G1266	U1128	A1060	G932	A802	C	A575	A428
C2155	C2155	A1853	A1701	A1558	G1445	G1266	U1129	A1061	G932	A802	C	A575	A428
C2156	C2156	A1853	A1701	A1558	G1446	G1266	U1130	A1062	G932	A802	C	A575	A428
C2157	C2157	A1853	A1701	A1558	G1447	G1266	U1131	A1063	G932	A802	C	A575	A428
C2158	C2158	A1853	A1701	A1558	G1448	G1266	U1132	A1064	G932	A802	C	A575	A428
C2159	C2159	A1853	A1701	A1558	G1449	G1266	U1133	A1065	G932	A802	C	A575	A428
C2160	C2160	A1853	A1701	A1558	G1450	G1266	U1134	A1066	G932	A802	C	A575	A428
C2161	C2161	A1853	A1701	A1558	G1451	G1266	U1135	A1067	G932	A802	C	A575	A428
C2162	C2162	A1853	A1701	A1558	G1452	G1266	U1136	A1068	G932	A802	C	A575	A428
C2163	C2163	A1853	A1701	A1558	G1453	G1266	U1137	A1069	G932	A802	C	A575	A428
C2164	C2164	A1853	A1701	A1558	G1454	G1266	U1138	A1070	G932	A802	C	A575	A428
C2165	C2165	A1853	A1701	A1558	G1455	G1266	U1139	A1071	G932	A802	C	A575	A428
C2166	C2166	A1853	A1701	A1558	G1456	G1266	U1140	A1072	G932	A802	C	A575	A428
C2167	C2167	A1853	A1701	A1558	G1457	G1266	U1141	A1073	G932	A802	C	A575	A428
C2168	C2168	A1853	A1701	A1558	G1458	G1266	U1142	A1074	G932	A802	C	A575	A428
C2169	C2169	A1853	A1701	A1558	G1459	G1266	U1143	A1075	G932	A802	C	A575	A428
C2170	C2170	A1853	A1701	A1558	G1460	G1266	U1144	A1076	G932	A802	C	A575	A428
C2171	C2171	A1853	A1701	A1558	G1461	G1266	U1145	A1077	G932	A802	C	A575	A428
C2172	C2172	A1853	A1701	A1558	G1462	G1266	U1146	A1078	G932	A802	C	A575	A428
C2173	C2173	A1853	A1701	A1558	G1463	G1266	U1147	A1079	G932	A802	C	A575	A428
C2174	C2174	A1853	A1701	A1558	G1464	G1266	U1148	A1080	G932	A802	C	A575	A428
C2175	C2175	A1853	A1701	A1558	G1465	G1266	U1149	A1081	G932	A802	C	A575	A428
C2176	C2176	A1853	A1701	A1558	G1466	G1266	U1150	A1082	G932	A802	C	A575	A428
C2177	C2177	A1853	A1701	A1558	G1467	G1266	U1151	A1083	G932	A802	C	A575	A428
C2178	C2178	A1853	A1701	A1558	G1468	G1266	U1152	A1084	G932	A802	C	A575	A428
C2179	C2179	A1853	A1701	A1558	G1469	G1266	U1153	A1085	G932	A802	C	A575	A428
C2180	C2180	A1853	A1701	A1558	G1470	G1266	U1154	A1086	G932	A802	C	A575	A428
C2181	C2181	A1853	A1701	A1558	G1471	G1266	U1155	A1087	G932	A802	C	A575	A428
C2182	C2182	A1853	A1701	A1558	G1472	G1266	U1156	A1088	G932	A802	C	A575	A428
C2183	C2183	A1853	A1701	A1558	G1473	G1266	U1157	A1089	G932	A802	C	A575	A428
C2184	C2184	A1853	A1701	A1558	G1474	G1266	U1158	A1090	G932	A802	C	A575	A428
C2185	C2185	A1853	A1701	A1558	G1475	G1266	U1159	A1091	G932	A802	C	A575	A428
C2186	C2186	A1853	A1701	A1558	G1476	G1266	U1160	A1092	G932	A802	C	A575	A428
C2187	C2187	A1853	A1701	A1558	G1477	G1266	U1161	A1093	G932	A802	C	A575	A428
C2188	C2188	A1853	A1701	A1558	G1478	G1266	U1162	A1094	G932	A802	C	A575	A428
C2189	C2189	A1853	A1701	A1558	G1479	G1266	U1163	A1095	G932	A802	C	A575	A428
C2190	C2190	A1853	A1701	A1558	G1480	G1266	U1164	A1096	G932	A802	C	A575	A428
C2191	C2191	A1853	A1701	A1558	G1481	G1266	U1165	A1097	G932	A802	C	A575	A428
C2192	C2192	A1853	A1701	A1558	G1482	G1266	U1166	A1098	G932	A802	C	A575	A428
C2193	C2193	A1853	A1701	A1558	G1483	G1266	U1167	A1099	G932	A802	C	A575	A428
C2194	C2194	A1853	A1701	A1558	G1484	G1266	U1168	A1100	G932	A802	C	A575	A428
C2195	C2195	A1853	A1701	A1558	G1485	G1266	U1169	A1101	G932	A802	C	A575	A428
C2196	C2196	A1853	A1701	A1558	G1486	G1266	U1170	A1102	G932	A802	C	A575	A428
C2197	C2197	A1853	A1701	A1558	G1487	G1266	U1171	A1103	G932	A802	C	A575	A428
C2198	C2198	A1853	A1701	A1558	G1488	G1266	U1172	A1104	G932	A802	C	A575	A428
C2199	C2199	A1853	A1701	A1558	G1489	G1266	U1173	A1105	G932	A802	C	A575	A428
C2200	C2200	A1853	A1701	A1558	G1490	G1266	U1174	A1106	G932	A802	C	A575	A428
C2201	C2201	A1853	A1701	A1558	G1491	G1266	U1175	A1107	G932	A802	C	A575	A428
C2202	C2202	A1853	A1701	A1558	G1492	G1266	U1176	A1108	G932	A802	C	A575	A428
C2203	C2203	A1853	A1701	A1558	G1493	G1266	U1177	A1109	G932	A802	C	A575	A428
C2204	C2204	A1853	A1701	A1558	G1494	G1266	U1178	A1110	G932	A802	C	A575	A428
C2205	C2205	A1853	A1701	A1558	G1495	G1266	U1179	A1111	G932	A802	C	A575	A428
C2206	C2206	A1853	A1701	A1558	G1496	G1266	U1180	A1112	G932	A802	C	A575	A428
C2207	C2207	A1853	A1701	A1558	G1497	G1266	U1181	A1113	G932	A802	C	A575	A428
C2208	C2208	A1853	A1701	A1558	G1498	G1266	U1182	A1114	G932	A802	C	A575	A428
C2209	C2209	A1853	A1701	A1558	G1499	G1266	U1183	A1115	G932	A802	C	A575	A428
C2210	C2210	A1853	A1701	A1558	G1500	G1266	U1184	A1116	G932	A802	C	A575	A428
C2211	C2211	A1853	A1701	A1558	G1501	G1266	U1185	A1117	G932	A802	C	A575	A428
C2212	C2212	A1853	A1701	A1558	G1502	G1266	U1186	A1118	G932	A802	C	A575	A428
C2213	C2213	A1853	A1701	A1558	G1503	G1266	U1187	A1119	G932	A802	C	A575	A428
C2214	C2214	A1853	A1701	A1558	G1504	G1266	U1188	A1120	G932	A802	C	A575	A428
C2215	C2215	A1853	A1701	A1558	G1505	G1266	U1189	A1121	G932	A802	C	A575	A428
C2216	C2216	A1853	A1701	A1558	G1506	G1266	U1190	A1122	G932	A802	C	A575	A428
C2217	C2217	A1853	A1701	A1558	G1507	G1266	U1191	A1123	G932	A802	C	A575	A428
C2218	C2218	A1853	A1701	A1558	G1508	G1266	U1192	A1124	G932	A802	C	A575	A428
C2219	C2219	A1853	A1701	A1558	G1509	G1266	U1193	A11					



- Molecule 36: 5S rRNA

Chain RB: 86% 10%



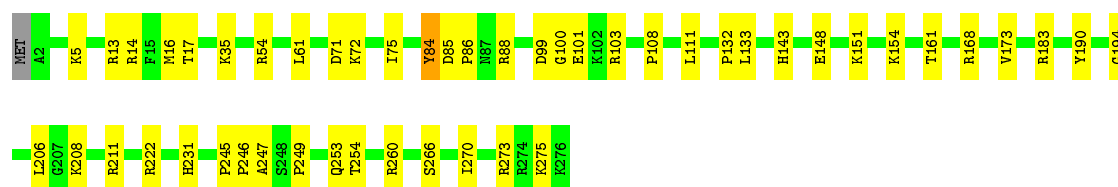
- Molecule 36: 5S rRNA

Chain YB: 81% 16%



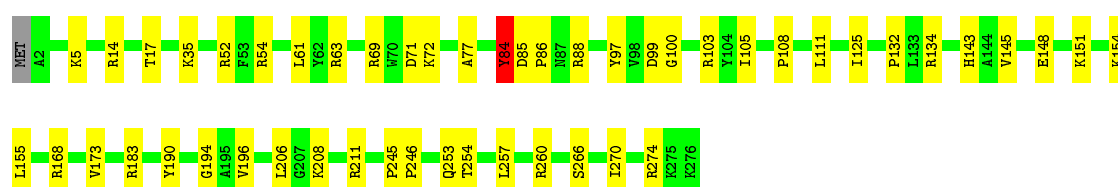
- Molecule 37: 50S ribosomal protein L2

Chain RD: 82% 17%




- Molecule 37: 50S ribosomal protein L2

Chain YD: 82% 18%




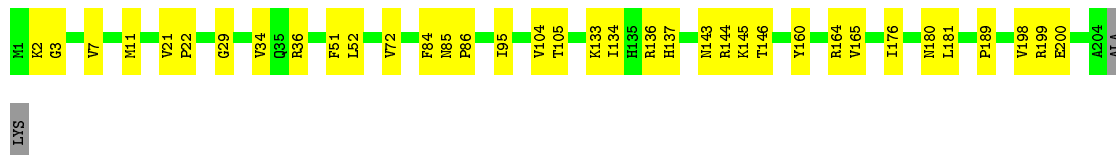
- Molecule 38: 50S ribosomal protein L3

Chain RE:  86% 13% .




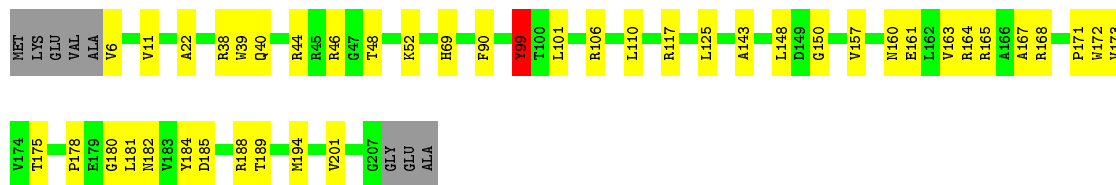
- Molecule 38: 50S ribosomal protein L3

Chain YE:  82% 17% .




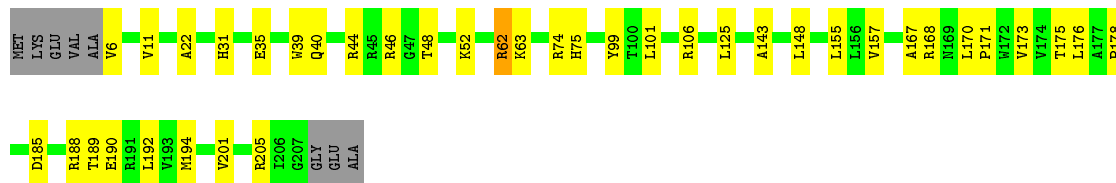
- Molecule 39: 50S ribosomal protein L4

Chain RF:  76% 20% .




- Molecule 39: 50S ribosomal protein L4

Chain YF:  78% 18% .




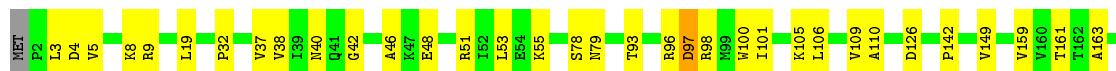
- Molecule 40: 50S ribosomal protein L5

Chain RG:  87% 12% ..



- Molecule 40: 50S ribosomal protein L5

Chain YG:  80% 19% ..





- Molecule 41: 50S ribosomal protein L6

Chain RH: 86% 10% ..



- Molecule 41: 50S ribosomal protein L6

Chain YH: 84% 12% ..



- Molecule 42: 50S ribosomal protein L9

Chain RI: 94% 5% .



- Molecule 42: 50S ribosomal protein L9

Chain YI: 93% 6% .



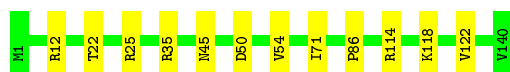
- Molecule 43: 50S ribosomal protein L13

Chain RN: 84% 15% .



- Molecule 43: 50S ribosomal protein L13

Chain YN: 91% 9%

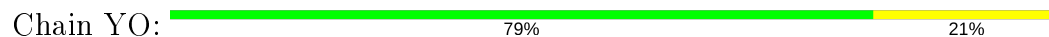


- Molecule 44: 50S ribosomal protein L14

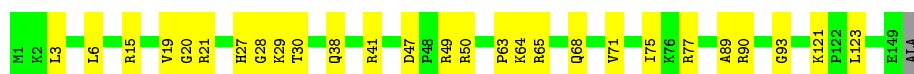
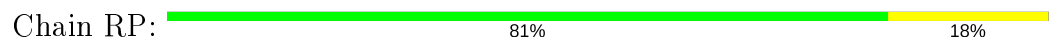
Chain RO: 80% 20% .



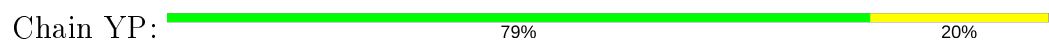
- Molecule 44: 50S ribosomal protein L14



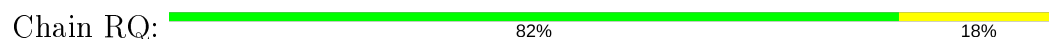
- Molecule 45: 50S ribosomal protein L15



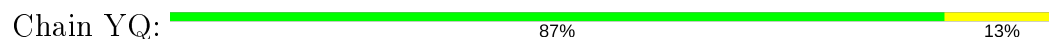
- Molecule 45: 50S ribosomal protein L15



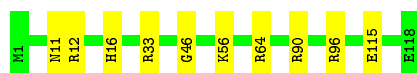
- Molecule 46: 50S ribosomal protein L16



- Molecule 46: 50S ribosomal protein L16



- Molecule 47: 50S ribosomal protein L17



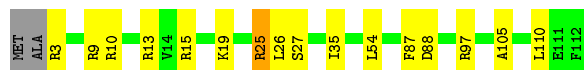
- Molecule 47: 50S ribosomal protein L17





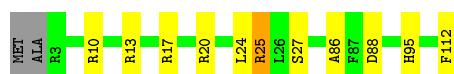
- Molecule 48: 50S ribosomal protein L18

Chain RS: 84% 13% ..



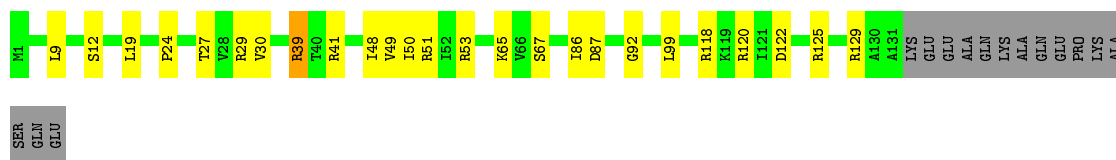
- Molecule 48: 50S ribosomal protein L18

Chain YS: 88% 9% ..



- Molecule 49: 50S ribosomal protein L19

Chain RT: 73% 16% • 10%



- Molecule 49: 50S ribosomal protein L19

Chain YT: 75% 14% • 10%



- Molecule 50: 50S ribosomal protein L20

Chain RU: 85% 12% ...




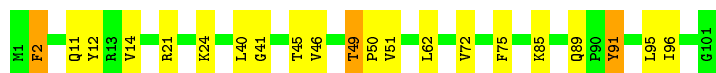
- Molecule 50: 50S ribosomal protein L20

Chain YU: 88% 8% ...



- Molecule 51: 50S ribosomal protein L21

Chain RV:  79% 18% .



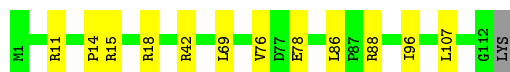
- Molecule 51: 50S ribosomal protein L21

Chain YV:  94% 5% .



- Molecule 52: 50S ribosomal protein L22

Chain RW:  88% 11% .




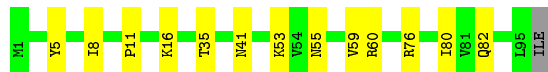
- Molecule 52: 50S ribosomal protein L22

Chain YW:  88% 12% .



- Molecule 53: 50S ribosomal protein L23

Chain RX:  85% 14% .



- Molecule 53: 50S ribosomal protein L23

Chain YX:  91% 8% .



- Molecule 54: 50S ribosomal protein L24

Chain RY:  86% 11% .



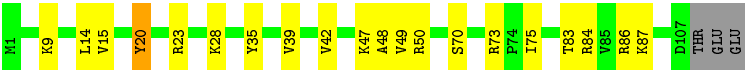
- Molecule 54: 50S ribosomal protein L24

Chain YY:

79%

17%

••



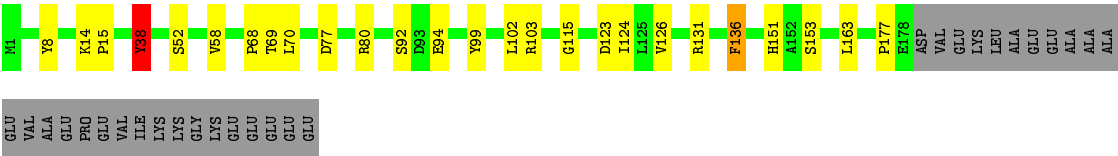
• Molecule 55: 50S ribosomal protein L25

Chain RZ:

74%

12%

14%



• Molecule 55: 50S ribosomal protein L25

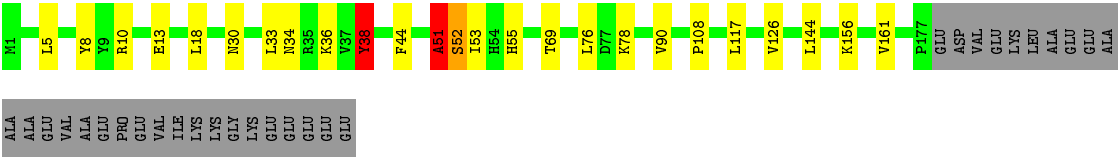
Chain YZ:

74%

11%

14%

•



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.38Å 445.83Å 616.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.10	Depositor
% Data completeness (in resolution range)	95.2 (50.00-3.10)	Depositor
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.231 , 0.268	Depositor
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.273	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	293819	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, OMC, PAR, M2G, OMG, 5MC, MA6, G7M, SF4, 0TD, MG, 2MA, 2MG, OMU, UR3, 4OC, ZN, PSU

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	QA	0.71	0/35795	0.97	64/55864 (0.1%)
1	XA	0.76	3/35890 (0.0%)	0.99	84/56012 (0.1%)
2	QB	0.45	0/1876	0.78	3/2533 (0.1%)
2	XB	0.44	0/1860	0.75	2/2518 (0.1%)
3	QC	0.42	0/1582	0.65	2/2137 (0.1%)
3	XC	0.49	0/1566	0.70	2/2119 (0.1%)
4	QD	0.54	0/1695	0.71	1/2274 (0.0%)
4	XD	0.48	0/1698	0.66	1/2277 (0.0%)
5	QE	0.40	0/1149	0.63	0/1548
5	XE	0.42	0/1149	0.63	0/1548
6	QF	0.53	0/827	0.69	2/1120 (0.2%)
6	XF	0.54	0/829	0.67	1/1123 (0.1%)
7	QG	0.44	0/1254	0.61	0/1683
7	XG	0.49	0/1248	0.63	0/1676
8	QH	0.45	0/1118	0.66	0/1506
8	XH	0.45	0/1108	0.64	0/1494
9	QI	0.42	1/1005 (0.1%)	0.70	1/1351 (0.1%)
9	XI	0.41	0/985	0.67	0/1329
10	QJ	0.42	0/732	0.72	0/993
10	XJ	0.45	0/723	0.65	0/984
11	QK	0.42	0/849	0.60	0/1150
11	XK	0.41	0/848	0.60	1/1149 (0.1%)
12	QL	0.55	0/937	0.81	3/1260 (0.2%)
12	XL	0.58	1/937 (0.1%)	0.84	3/1260 (0.2%)
13	QM	0.44	0/924	0.76	2/1242 (0.2%)
13	XM	0.47	0/905	0.76	1/1217 (0.1%)
14	QN	0.44	0/501	0.66	0/664
14	XN	0.46	0/501	0.66	0/664
15	QO	0.45	0/739	0.64	0/985
15	XO	0.43	0/739	0.62	0/985
16	QP	0.48	0/697	0.77	2/939 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	XP	0.49	0/693	0.76	1/935 (0.1%)
17	QQ	0.48	0/836	0.62	0/1117
17	XQ	0.47	0/836	0.66	1/1117 (0.1%)
18	QR	0.42	0/560	0.59	0/746
18	XR	0.48	0/560	0.60	0/746
19	QS	0.44	0/663	0.67	0/895
19	XS	0.41	0/660	0.68	0/893
20	QT	0.37	0/734	0.60	0/969
20	XT	0.37	0/736	0.56	0/976
21	QU	0.38	0/203	0.58	0/266
21	XU	0.39	0/203	0.59	0/266
22	QV	0.64	0/1832	1.00	6/2855 (0.2%)
22	XV	0.70	0/1832	1.01	6/2855 (0.2%)
23	QX	0.59	0/443	1.07	3/690 (0.4%)
23	XX	0.61	0/443	1.12	2/690 (0.3%)
24	QY	0.56	0/1816	1.07	8/2830 (0.3%)
24	XY	0.58	0/1816	1.08	11/2830 (0.4%)
25	R0	0.49	0/616	0.72	0/821
25	Y0	0.52	0/616	0.74	0/821
26	R1	0.47	0/761	0.61	0/1013
26	Y1	0.51	0/766	0.61	0/1018
27	R2	0.45	0/590	0.57	0/781
27	Y2	0.48	0/594	0.65	0/785
28	R3	0.45	0/474	0.64	0/635
28	Y3	0.51	0/469	0.63	0/630
29	R4	0.54	0/559	0.85	1/754 (0.1%)
29	Y4	0.54	0/549	0.94	5/741 (0.7%)
30	R5	0.59	1/473 (0.2%)	0.68	0/639
30	Y5	0.54	0/469	0.64	0/635
31	R6	0.55	0/460	0.67	0/613
31	Y6	0.57	0/456	0.65	0/608
32	R7	0.50	0/426	0.69	0/561
32	Y7	0.52	0/426	0.69	0/561
33	R8	0.47	0/525	0.58	0/691
33	Y8	0.50	0/525	0.59	0/691
34	R9	0.54	0/310	0.66	0/407
34	Y9	0.58	0/310	0.66	0/407
35	RA	0.83	0/68903	1.02	168/107552 (0.2%)
35	YA	0.92	0/68903	1.03	186/107552 (0.2%)
36	RB	0.71	0/2876	1.03	13/4486 (0.3%)
36	YB	0.84	0/2878	1.05	11/4490 (0.2%)
37	RD	0.54	0/2181	0.71	1/2940 (0.0%)
37	YD	0.57	0/2186	0.70	1/2944 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	RE	0.48	0/1592	0.67	0/2149
38	YE	0.53	0/1592	0.68	0/2149
39	RF	0.54	0/1618	0.68	1/2191 (0.0%)
39	YF	0.54	0/1614	0.66	0/2186
40	RG	0.47	0/1451	0.67	1/1961 (0.1%)
40	YG	0.47	0/1449	0.67	0/1957
41	RH	0.45	0/1356	0.65	1/1834 (0.1%)
41	YH	0.53	0/1350	0.61	0/1826
42	RI	0.43	0/1109	0.68	0/1512
42	YI	0.48	0/1091	0.63	1/1490 (0.1%)
43	RN	0.49	1/1148 (0.1%)	0.58	0/1547
43	YN	0.51	0/1144	0.61	0/1543
44	RO	0.51	0/943	0.66	0/1269
44	YO	0.55	0/943	0.65	0/1269
45	RP	0.47	0/1152	0.70	0/1533
45	YP	0.53	0/1152	0.70	0/1533
46	RQ	0.45	0/1143	0.65	0/1527
46	YQ	0.49	0/1143	0.66	1/1527 (0.1%)
47	RR	0.45	0/982	0.65	0/1312
47	YR	0.47	0/982	0.65	0/1312
48	RS	0.45	0/887	0.66	0/1180
48	YS	0.48	0/880	0.61	0/1172
49	RT	0.47	0/1105	0.65	0/1477
49	YT	0.48	0/1097	0.66	0/1468
50	RU	0.49	0/977	0.69	2/1301 (0.2%)
50	YU	0.54	0/977	0.71	3/1301 (0.2%)
51	RV	0.55	0/786	0.78	3/1053 (0.3%)
51	YV	0.54	0/782	0.69	0/1049
52	RW	0.47	0/897	0.59	0/1205
52	YW	0.51	0/897	0.59	0/1205
53	RX	0.49	0/764	0.63	0/1025
53	YX	0.49	0/764	0.64	0/1025
54	RY	0.46	0/823	0.66	0/1099
54	YY	0.53	0/823	0.67	0/1100
55	RZ	0.45	0/1438	0.76	1/1955 (0.1%)
55	YZ	0.50	0/1413	0.77	2/1924 (0.1%)
All	All	0.74	7/316097 (0.0%)	0.94	615/473222 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1042	G	C5-C4	9.41	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	1042	G	C6-N1	6.72	1.44	1.39
30	R5	59	GLU	CD-OE1	5.69	1.31	1.25
1	XA	1042	G	N9-C4	-5.68	1.33	1.38
9	QI	121	ARG	C-N	-5.32	1.21	1.34
43	RN	77	GLY	C-N	-5.16	1.22	1.34
12	XL	47	LYS	C-N	5.11	1.44	1.34

All (615) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	999	C	N1-C2-O2	15.66	128.30	118.90
1	XA	999	C	C5-C6-N1	13.88	127.94	121.00
1	XA	1042	G	C6-N1-C2	12.73	132.74	125.10
2	QB	232	PRO	C-N-CA	12.22	152.25	121.70
1	XA	1042	G	C5-C6-N1	-12.10	105.45	111.50
55	RZ	38	TYR	CA-CB-CG	11.11	134.50	113.40
50	YU	52	ARG	CG-CD-NE	10.62	134.11	111.80
1	XA	999	C	C2-N3-C4	10.51	125.15	119.90
36	RB	73	A	C5-C6-N6	-10.31	115.45	123.70
13	QM	23	TYR	CA-CB-CG	9.99	132.37	113.40
50	RU	52	ARG	CG-CD-NE	9.93	132.66	111.80
35	YA	2506	U	N1-C2-O2	9.88	129.72	122.80
35	RA	847	U	C2-N1-C1'	9.79	129.45	117.70
35	YA	1064	C	C6-N1-C2	-9.65	116.44	120.30
1	XA	999	C	N3-C2-O2	-9.57	115.20	121.90
16	QP	38	TYR	CA-CB-CG	9.53	131.50	113.40
35	RA	1313	U	C2-N1-C1'	9.42	129.00	117.70
37	YD	84	TYR	CA-CB-CG	9.41	131.27	113.40
55	YZ	38	TYR	CA-CB-CG	9.34	131.15	113.40
35	YA	2506	U	C2-N1-C1'	9.32	128.89	117.70
35	YA	847	U	C2-N1-C1'	9.32	128.88	117.70
35	YA	2506	U	N3-C2-O2	-9.21	115.76	122.20
35	YA	1064	C	C5-C6-N1	9.07	125.54	121.00
1	QA	266	G	P-O3'-C3'	9.04	130.54	119.70
1	QA	1158	C	C2-N1-C1'	8.97	128.67	118.80
35	YA	1313	U	C2-N1-C1'	8.95	128.44	117.70
35	RA	847	U	N1-C2-O2	8.83	128.98	122.80
35	YA	2689	U	N3-C2-O2	-8.83	116.02	122.20
1	XA	1003	G	C4-N9-C1'	8.83	137.97	126.50
35	RA	856	C	C6-N1-C2	-8.74	116.80	120.30
37	RD	84	TYR	CA-CB-CG	8.72	129.96	113.40
1	QA	1003	G	C4-N9-C1'	8.68	137.78	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	RB	73	A	N9-C4-C5	-8.67	102.33	105.80
35	RA	2506	U	C2-N1-C1'	8.66	128.10	117.70
35	RA	2506	U	N1-C2-O2	8.66	128.86	122.80
1	XA	266	G	P-O3'-C3'	8.65	130.08	119.70
36	YB	73	A	C5-C6-N6	-8.62	116.81	123.70
35	YA	847	U	N1-C2-O2	8.47	128.73	122.80
35	RA	847	U	N3-C2-O2	-8.43	116.30	122.20
1	QA	1003	G	N3-C4-C5	-8.43	124.39	128.60
13	XM	23	TYR	CA-CB-CG	8.40	129.36	113.40
1	XA	1042	G	N3-C2-N2	8.39	125.78	119.90
35	YA	1065	U	N3-C2-O2	-8.39	116.33	122.20
36	RB	73	A	C5-C6-N1	8.37	121.89	117.70
1	QA	1158	C	N1-C2-O2	8.37	123.92	118.90
1	XA	1042	G	N1-C2-N3	-8.28	118.93	123.90
35	YA	2689	U	N1-C2-O2	8.26	128.58	122.80
35	YA	847	U	N3-C2-O2	-8.24	116.44	122.20
35	RA	2137	C	N3-C2-O2	-8.16	116.19	121.90
16	XP	38	TYR	CA-CB-CG	8.14	128.87	113.40
24	XY	55	U	C2-N1-C1'	8.07	127.39	117.70
39	RF	99	TYR	CA-CB-CG	8.06	128.71	113.40
1	XA	1003	G	C8-N9-C4	-8.05	103.18	106.40
35	YA	856	C	C6-N1-C2	-8.02	117.09	120.30
35	YA	614(A)	U	C2-N1-C1'	8.00	127.30	117.70
35	RA	1064	C	C6-N1-C2	-7.98	117.11	120.30
35	RA	614(A)	U	N1-C2-O2	7.95	128.36	122.80
24	QY	55	U	C2-N1-C1'	7.94	127.22	117.70
35	RA	1313	U	N1-C2-O2	7.92	128.34	122.80
35	RA	2506	U	N3-C2-O2	-7.89	116.68	122.20
35	RA	614(A)	U	N3-C2-O2	-7.88	116.69	122.20
1	XA	1003	G	N3-C4-C5	-7.85	124.67	128.60
35	RA	1313	U	N3-C2-O2	-7.84	116.71	122.20
35	RA	2689	U	N3-C2-O2	-7.84	116.71	122.20
35	RA	614(A)	U	C2-N1-C1'	7.81	127.07	117.70
35	YA	2321	G	C4-N9-C1'	7.77	136.60	126.50
35	RA	1052	C	N1-C2-O2	7.75	123.55	118.90
51	RV	49	THR	N-CA-C	-7.75	90.09	111.00
35	YA	1065	U	N1-C2-O2	7.66	128.16	122.80
35	YA	1052	C	C6-N1-C2	-7.63	117.25	120.30
35	YA	1052	C	C5-C6-N1	7.59	124.80	121.00
35	YA	1314	C	C6-N1-C2	-7.53	117.29	120.30
24	XY	55	U	N3-C2-O2	-7.52	116.94	122.20
35	RA	2321	G	C4-N9-C1'	7.51	136.26	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1158	C	C2-N1-C1'	7.51	127.06	118.80
35	RA	1065	U	C5-C6-N1	7.50	126.45	122.70
1	XA	1003	G	N7-C8-N9	7.46	116.83	113.10
35	YA	1065	U	P-O3'-C3'	7.46	128.65	119.70
35	RA	1064	C	C5-C6-N1	7.45	124.72	121.00
24	QY	55	U	N3-C2-O2	-7.39	117.03	122.20
35	YA	1313	U	N3-C2-O2	-7.39	117.03	122.20
1	XA	999	C	C4-C5-C6	-7.38	113.71	117.40
35	YA	2591	C	C6-N1-C2	-7.36	117.36	120.30
1	QA	1158	C	N3-C2-O2	-7.29	116.80	121.90
1	XA	1442(A)	G	C4-N9-C1'	7.25	135.93	126.50
35	RA	1065	U	P-O3'-C3'	7.25	128.40	119.70
35	YA	1065	U	C5-C6-N1	7.25	126.32	122.70
35	RA	1065	U	N1-C2-O2	7.22	127.85	122.80
35	RA	2137	C	C4-C5-C6	7.22	121.01	117.40
35	RA	1899	G	C4-N9-C1'	7.21	135.88	126.50
35	RA	269	U	N1-C2-O2	7.21	127.85	122.80
35	YA	1313	U	N1-C2-O2	7.20	127.84	122.80
35	YA	1065	U	C6-N1-C2	-7.20	116.68	121.00
9	QI	36	TYR	CA-CB-CG	7.17	127.03	113.40
35	RA	1065	U	N3-C2-O2	-7.16	117.19	122.20
35	RA	2889	C	N1-C2-O2	7.15	123.19	118.90
2	XB	232	PRO	C-N-CA	7.14	139.54	121.70
35	YA	1314	C	C5-C6-N1	7.12	124.56	121.00
1	QA	1003	G	C8-N9-C4	-7.12	103.55	106.40
1	QA	1067	A	P-O3'-C3'	7.11	128.23	119.70
35	YA	2473	U	C2-N1-C1'	7.07	126.19	117.70
1	XA	1067	A	P-O3'-C3'	7.07	128.19	119.70
36	RB	73	A	C4-C5-N7	7.03	114.22	110.70
35	YA	2473	U	N1-C2-O2	7.03	127.72	122.80
1	QA	754	C	C2-N1-C1'	7.01	126.51	118.80
1	QA	1158	C	C6-N1-C2	-6.99	117.50	120.30
36	YB	30	C	N1-C2-O2	6.98	123.09	118.90
50	YU	52	ARG	CD-NE-CZ	6.96	133.34	123.60
35	YA	2506	U	C5-C6-N1	6.95	126.18	122.70
35	YA	1314	C	N1-C2-O2	6.95	123.07	118.90
1	XA	1442(A)	G	N3-C4-C5	-6.94	125.13	128.60
35	YA	1052	C	C2-N1-C1'	6.91	126.40	118.80
35	YA	1052	C	N1-C2-O2	6.85	123.01	118.90
35	RA	269	U	N3-C2-O2	-6.85	117.40	122.20
35	YA	753	C	C6-N1-C2	-6.85	117.56	120.30
1	QA	1065	U	P-O3'-C3'	6.81	127.87	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	991	U	P-O3'-C3'	6.80	127.86	119.70
35	RA	2473	U	C2-N1-C1'	6.79	125.85	117.70
1	XA	1065	U	P-O3'-C3'	6.79	127.85	119.70
1	XA	999	C	C6-N1-C2	-6.76	117.59	120.30
1	QA	687	A	P-O3'-C3'	6.76	127.81	119.70
22	XV	65	C	N1-C2-O2	6.74	122.95	118.90
24	XY	55	U	C6-N1-C2	-6.74	116.95	121.00
36	YB	73	A	C5-C6-N1	6.74	121.07	117.70
35	YA	1899	G	C4-N9-C1'	6.74	135.26	126.50
36	YB	73	A	N9-C4-C5	-6.73	103.11	105.80
35	YA	2465	C	N1-C2-O2	6.73	122.94	118.90
36	RB	73	A	N1-C6-N6	6.72	122.63	118.60
35	RA	1065	U	C6-N1-C2	-6.72	116.97	121.00
2	XB	129	GLU	C-N-CA	6.71	138.47	121.70
3	XC	29	TYR	CA-CB-CG	6.71	126.14	113.40
51	RV	12	TYR	CA-CB-CG	6.68	126.10	113.40
12	QL	87	GLY	N-CA-C	6.67	129.76	113.10
35	YA	614(A)	U	N1-C2-O2	6.65	127.45	122.80
1	QA	748	C	P-O3'-C3'	6.65	127.68	119.70
1	QA	266	G	OP2-P-O3'	6.63	119.80	105.20
35	RA	2179	C	N1-C2-O2	6.63	122.88	118.90
36	RB	30	C	C6-N1-C2	-6.63	117.65	120.30
36	RB	30	C	N1-C2-O2	6.63	122.88	118.90
1	XA	748	C	P-O3'-C3'	6.62	127.64	119.70
35	YA	2321	G	C8-N9-C1'	-6.60	118.42	127.00
35	RA	847	U	C6-N1-C1'	-6.59	111.97	121.20
35	RA	2279	G	C5-N7-C8	6.58	107.59	104.30
35	YA	614(A)	U	N3-C2-O2	-6.58	117.60	122.20
35	YA	2889	C	C6-N1-C2	-6.57	117.67	120.30
1	QA	1003	G	N3-C4-N9	6.57	129.94	126.00
35	YA	1882	C	N1-C2-O2	6.53	122.82	118.90
1	XA	266	G	OP2-P-O3'	6.52	119.55	105.20
1	XA	545	C	N3-C2-O2	-6.52	117.33	121.90
35	RA	753	C	C6-N1-C2	-6.52	117.69	120.30
1	XA	1442(A)	G	N3-C4-N9	6.49	129.90	126.00
1	XA	687	A	P-O3'-C3'	6.49	127.49	119.70
35	YA	1788	C	C6-N1-C2	-6.49	117.70	120.30
35	RA	2689	U	N1-C2-O2	6.48	127.34	122.80
1	XA	960	U	N1-C2-O2	6.48	127.34	122.80
35	RA	2137	C	N1-C2-O2	6.48	122.79	118.90
1	XA	991	U	P-O3'-C3'	6.47	127.47	119.70
1	XA	913	A	P-O3'-C3'	6.46	127.45	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	QY	55	U	N1-C2-O2	6.45	127.32	122.80
35	RA	2889	C	N3-C2-O2	-6.45	117.39	121.90
1	XA	60	A	P-O3'-C3'	6.45	127.44	119.70
1	QA	1003	G	C8-N9-C1'	-6.44	118.62	127.00
35	YA	2126	A	P-O3'-C3'	6.44	127.43	119.70
35	YA	2473	U	N3-C2-O2	-6.44	117.69	122.20
35	RA	1314	C	N1-C2-O2	6.44	122.76	118.90
35	RA	1314	C	C2-N1-C1'	6.44	125.88	118.80
35	YA	512	G	O4'-C1'-N9	6.43	113.34	108.20
35	RA	277	C	P-O3'-C3'	6.43	127.42	119.70
35	YA	1314	C	C2-N1-C1'	6.43	125.87	118.80
50	RU	52	ARG	CD-NE-CZ	6.42	132.59	123.60
35	YA	618	C	N1-C2-O2	6.42	122.75	118.90
12	XL	119	LYS	N-CA-C	-6.42	93.66	111.00
35	YA	12	U	N3-C2-O2	-6.42	117.71	122.20
35	YA	944	G	C4-N9-C1'	6.42	134.84	126.50
35	RA	2126	A	P-O3'-C3'	6.42	127.40	119.70
35	RA	1905	C	N1-C2-O2	6.41	122.75	118.90
24	QY	70	U	OP1-P-O3'	6.40	119.28	105.20
12	QL	119	LYS	N-CA-C	-6.40	93.73	111.00
1	XA	1003	G	N3-C4-N9	6.39	129.83	126.00
1	QA	60	A	P-O3'-C3'	6.38	127.36	119.70
35	RA	461	C	C6-N1-C2	-6.37	117.75	120.30
24	XY	55	U	N1-C2-O2	6.37	127.26	122.80
35	RA	1493	C	N1-C2-O2	6.37	122.72	118.90
35	RA	1314	C	C6-N1-C2	-6.37	117.75	120.30
35	RA	2039	C	C6-N1-C2	-6.36	117.76	120.30
29	Y4	58	ARG	N-CA-CB	6.35	122.03	110.60
35	RA	1005	C	C6-N1-C2	-6.33	117.77	120.30
35	RA	1892	C	C6-N1-C2	-6.33	117.77	120.30
1	XA	1003	G	C8-N9-C1'	-6.32	118.79	127.00
35	RA	2179	C	C2-N1-C1'	6.31	125.74	118.80
3	QC	29	TYR	CA-CB-CG	6.30	125.37	113.40
35	YA	272(M)	G	P-O3'-C3'	6.30	127.26	119.70
35	YA	783	A	C2-N3-C4	6.30	113.75	110.60
1	XA	754	C	C2-N1-C1'	6.29	125.72	118.80
1	QA	1442(A)	G	P-O3'-C3'	6.28	127.24	119.70
35	RA	1135	C	N1-C2-O2	6.28	122.67	118.90
1	QA	65	U	P-O3'-C3'	6.28	127.23	119.70
35	RA	1313	U	C6-N1-C1'	-6.27	112.42	121.20
1	XA	1109	C	C6-N1-C2	-6.27	117.79	120.30
1	QA	913	A	P-O3'-C3'	6.25	127.21	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	XX	18	G	OP2-P-O3'	6.25	118.95	105.20
1	XA	1158	C	N1-C2-O2	6.25	122.65	118.90
35	RA	530	G	C4-N9-C1'	6.24	134.62	126.50
35	RA	1052	C	N3-C2-O2	-6.23	117.54	121.90
35	RA	2279	G	C4-C5-N7	-6.23	108.31	110.80
1	XA	1060	C	N1-C2-O2	6.23	122.64	118.90
1	QA	115	G	P-O3'-C3'	6.22	127.17	119.70
36	RB	73	A	C8-N9-C4	6.22	108.29	105.80
35	YA	2320	A	C2-N3-C4	6.22	113.71	110.60
35	RA	1005	C	N1-C2-O2	6.21	122.62	118.90
35	RA	272(M)	G	P-O3'-C3'	6.20	127.14	119.70
35	YA	1057	A	P-O3'-C3'	6.18	127.12	119.70
23	QX	18	G	P-O3'-C3'	6.17	127.11	119.70
1	XA	960	U	C2-N1-C1'	6.17	125.10	117.70
1	XA	1303	C	N3-C2-O2	-6.16	117.59	121.90
35	YA	1497	U	C2-N1-C1'	6.16	125.09	117.70
1	QA	337	C	C6-N1-C2	-6.16	117.84	120.30
35	YA	1879	C	C6-N1-C2	-6.16	117.84	120.30
1	QA	501	C	C6-N1-C2	-6.15	117.84	120.30
35	YA	2889	C	N1-C2-O2	6.14	122.58	118.90
35	RA	272(M)	G	OP1-P-O3'	6.13	118.68	105.20
12	XL	87	GLY	N-CA-C	6.13	128.42	113.10
1	QA	1003	G	N7-C8-N9	6.13	116.16	113.10
35	RA	1052	C	C2-N1-C1'	6.13	125.54	118.80
35	RA	753	C	C5-C6-N1	6.12	124.06	121.00
35	YA	2889	C	N3-C2-O2	-6.12	117.62	121.90
6	QF	63	TYR	CA-CB-CG	6.12	125.03	113.40
1	XA	115	G	P-O3'-C3'	6.12	127.04	119.70
35	RA	2321	G	C8-N9-C1'	-6.12	119.05	127.00
35	YA	269	U	N1-C2-O2	6.11	127.08	122.80
35	YA	1905	C	N1-C2-O2	6.11	122.57	118.90
35	YA	2095	C	C6-N1-C2	-6.10	117.86	120.30
24	XY	55	U	C5-C6-N1	6.10	125.75	122.70
3	XC	201	TYR	CA-CB-CG	6.10	124.99	113.40
35	YA	1992	G	OP2-P-O3'	6.09	118.61	105.20
35	RA	885	C	C6-N1-C2	-6.09	117.86	120.30
35	RA	1497	U	C2-N1-C1'	6.09	125.01	117.70
35	YA	2321	G	N3-C4-C5	-6.09	125.56	128.60
35	RA	1314	C	C5-C6-N1	6.08	124.04	121.00
1	QA	1043	C	N1-C2-O2	6.08	122.55	118.90
35	YA	12	U	N1-C2-O2	6.08	127.06	122.80
1	QA	992	U	P-O3'-C3'	6.07	126.99	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	2506	U	C5-C6-N1	6.07	125.73	122.70
1	XA	1442(A)	G	P-O3'-C3'	6.07	126.99	119.70
35	RA	1376	C	N1-C2-O2	6.05	122.53	118.90
35	YA	752	A	P-O3'-C3'	6.05	126.97	119.70
35	RA	1899	G	N3-C4-C5	-6.03	125.58	128.60
22	QV	71	C	C6-N1-C2	-6.03	117.89	120.30
35	RA	2617	C	N1-C2-O2	6.02	122.51	118.90
35	YA	893	C	N1-C2-O2	6.02	122.51	118.90
35	YA	1065	U	C2-N1-C1'	6.02	124.92	117.70
35	YA	1992	G	P-O3'-C3'	6.02	126.92	119.70
35	YA	272(M)	G	OP1-P-O3'	6.02	118.44	105.20
1	XA	1279	A	C2-N3-C4	6.01	113.61	110.60
35	YA	624	C	C6-N1-C2	-6.01	117.90	120.30
35	RA	2880	C	N3-C2-O2	-6.00	117.70	121.90
1	XA	972	C	C6-N1-C2	-6.00	117.90	120.30
35	YA	12	U	C2-N1-C1'	6.00	124.90	117.70
35	RA	893	C	N1-C2-O2	6.00	122.50	118.90
1	QA	354	G	C4-N9-C1'	5.99	134.29	126.50
1	XA	545	C	N1-C2-O2	5.99	122.50	118.90
23	XX	18	G	P-O3'-C3'	5.99	126.89	119.70
35	RA	1057	A	P-O3'-C3'	5.99	126.89	119.70
1	XA	65	U	P-O3'-C3'	5.99	126.89	119.70
35	YA	269	U	C2-N1-C1'	5.98	124.87	117.70
35	RA	269	U	C2-N1-C1'	5.97	124.86	117.70
35	YA	753	C	C5-C6-N1	5.96	123.98	121.00
35	YA	795	C	C6-N1-C2	-5.95	117.92	120.30
1	XA	992	U	P-O3'-C3'	5.95	126.84	119.70
1	XA	999	C	N3-C4-C5	-5.95	119.52	121.90
1	XA	960	U	N3-C2-O2	-5.94	118.04	122.20
35	RA	752	A	P-O3'-C3'	5.94	126.83	119.70
35	RA	976	C	N1-C2-O2	5.94	122.46	118.90
35	RA	774	A	C2-N3-C4	5.93	113.57	110.60
35	RA	1899	G	C8-N9-C1'	-5.93	119.29	127.00
35	RA	1062	G	N3-C4-N9	5.92	129.56	126.00
1	XA	560	U	P-O3'-C3'	5.92	126.81	119.70
35	RA	1992	G	P-O3'-C3'	5.90	126.78	119.70
1	XA	1158	C	N3-C2-O2	-5.90	117.77	121.90
35	YA	277	C	N1-C2-O2	5.90	122.44	118.90
4	QD	138	TYR	CA-CB-CG	5.90	124.61	113.40
1	QA	1442(A)	G	C4-N9-C1'	5.90	134.17	126.50
24	XY	70	U	OP1-P-O3'	5.89	118.16	105.20
35	RA	2880	C	N1-C2-O2	5.88	122.43	118.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1899	G	N3-C4-C5	-5.88	125.66	128.60
35	RA	856	C	N3-C2-O2	-5.88	117.79	121.90
35	YA	825	C	C6-N1-C2	-5.88	117.95	120.30
35	YA	1082	U	C5-C6-N1	5.88	125.64	122.70
1	XA	810	C	N1-C2-O2	5.87	122.42	118.90
35	YA	510	C	N1-C2-O2	5.87	122.42	118.90
1	XA	749	C	C6-N1-C2	-5.87	117.95	120.30
35	YA	530	G	C4-N9-C1'	5.87	134.13	126.50
35	YA	1497	U	N3-C2-O2	-5.87	118.09	122.20
36	YB	73	A	N1-C6-N6	5.87	122.12	118.60
35	RA	645	C	N1-C2-O2	5.86	122.41	118.90
1	QA	643	C	C6-N1-C2	-5.85	117.96	120.30
1	QA	442	C	N1-C2-O2	5.85	122.41	118.90
35	YA	560	C	C6-N1-C2	-5.85	117.96	120.30
35	YA	601	C	C6-N1-C2	-5.84	117.96	120.30
1	XA	1442(A)	G	C8-N9-C1'	-5.84	119.41	127.00
36	YB	30	C	N3-C2-O2	-5.84	117.81	121.90
22	QV	67	C	N1-C2-O2	5.84	122.40	118.90
1	QA	1158	C	C6-N1-C1'	-5.83	113.81	120.80
35	RA	2395	C	C6-N1-C2	-5.82	117.97	120.30
35	YA	277	C	P-O3'-C3'	5.81	126.68	119.70
35	YA	847	U	C5-C6-N1	5.81	125.60	122.70
35	RA	783	A	C2-N3-C4	5.80	113.50	110.60
35	YA	1644	C	C6-N1-C2	-5.80	117.98	120.30
35	YA	1064	C	N3-C4-N4	5.80	122.06	118.00
1	QA	1043	C	C2-N1-C1'	5.79	125.17	118.80
24	QY	55	U	C6-N1-C2	-5.79	117.53	121.00
36	YB	73	A	C4-C5-N7	5.78	113.59	110.70
1	XA	810	C	N3-C2-O2	-5.78	117.86	121.90
29	Y4	43	TYR	CA-CB-CG	5.78	124.38	113.40
35	RA	601	C	C6-N1-C2	-5.77	117.99	120.30
40	RG	48	GLU	C-N-CA	5.77	136.13	121.70
35	YA	2465	C	C2-N1-C1'	5.77	125.15	118.80
35	RA	2689	U	P-O3'-C3'	5.77	126.62	119.70
1	XA	1303	C	N1-C2-O2	5.77	122.36	118.90
35	YA	758	C	C6-N1-C2	-5.77	117.99	120.30
35	YA	1135	C	N1-C2-O2	5.76	122.36	118.90
36	RB	30	C	C5-C6-N1	5.75	123.87	121.00
35	YA	2689	U	C2-N1-C1'	5.75	124.60	117.70
35	YA	2880	C	C6-N1-C2	-5.74	118.00	120.30
35	YA	2342	C	C6-N1-C2	-5.74	118.00	120.30
35	RA	1005	C	N3-C2-O2	-5.73	117.89	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1992	G	OP2-P-O3'	5.73	117.81	105.20
35	RA	1493	C	N3-C2-O2	-5.73	117.89	121.90
6	XF	63	TYR	CA-CB-CG	5.73	124.28	113.40
35	RA	1065	U	C2-N1-C1'	5.72	124.57	117.70
35	YA	2321	G	N3-C4-N9	5.72	129.43	126.00
35	YA	1102	C	C6-N1-C2	-5.72	118.01	120.30
3	QC	201	TYR	CA-CB-CG	5.71	124.25	113.40
35	RA	2138	C	C5-C6-N1	5.71	123.86	121.00
35	YA	635	C	N1-C2-O2	5.70	122.32	118.90
35	YA	269	U	N3-C2-O2	-5.70	118.21	122.20
35	RA	1899	G	N3-C4-N9	5.70	129.42	126.00
35	RA	2179	C	N3-C2-O2	-5.69	117.92	121.90
35	YA	39	C	C6-N1-C2	-5.69	118.03	120.30
24	QY	16	C	C6-N1-C2	-5.68	118.03	120.30
35	RA	2179	C	C6-N1-C2	-5.68	118.03	120.30
12	XL	48	PRO	N-CA-C	5.68	126.87	112.10
35	YA	2689	U	P-O3'-C3'	5.68	126.51	119.70
1	QA	1059	C	C6-N1-C2	-5.67	118.03	120.30
35	YA	991	C	C6-N1-C2	-5.67	118.03	120.30
35	RA	635	C	C6-N1-C2	-5.66	118.04	120.30
35	YA	2356	C	C6-N1-C2	-5.66	118.04	120.30
35	RA	2294	C	N1-C2-O2	5.65	122.29	118.90
35	RA	2870	C	C6-N1-C2	-5.65	118.04	120.30
1	QA	1442(A)	G	N3-C4-C5	-5.64	125.78	128.60
35	RA	1776	G	C4-N9-C1'	5.64	133.83	126.50
35	RA	2473	U	N3-C2-O2	-5.64	118.25	122.20
35	YA	560	C	N3-C2-O2	-5.64	117.95	121.90
35	YA	1644	C	N1-C2-O2	5.63	122.28	118.90
35	YA	564	C	C6-N1-C2	-5.63	118.05	120.30
35	YA	2506	U	C6-N1-C1'	-5.63	113.31	121.20
35	YA	847	U	C6-N1-C1'	-5.63	113.32	121.20
1	QA	560	U	P-O3'-C3'	5.63	126.45	119.70
35	YA	2506	U	C6-N1-C2	-5.63	117.62	121.00
35	RA	1788	C	C6-N1-C2	-5.62	118.05	120.30
1	QA	397	A	C2-N3-C4	5.62	113.41	110.60
35	RA	2473	U	N1-C2-O2	5.62	126.74	122.80
24	XY	36	C	C5-C6-N1	5.62	123.81	121.00
35	YA	1210	A	P-O3'-C3'	5.62	126.45	119.70
35	YA	1493	C	N1-C2-O2	5.61	122.27	118.90
35	RA	915	C	C6-N1-C2	-5.61	118.06	120.30
35	RA	1804	C	C6-N1-C2	-5.61	118.06	120.30
35	YA	385	C	C2-N1-C1'	5.60	124.96	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1437	C	N1-C2-O2	5.58	122.25	118.90
35	RA	277	C	OP2-P-O3'	5.58	117.48	105.20
35	RA	1654	A	N1-C6-N6	-5.58	115.25	118.60
22	XV	65	C	C2-N1-C1'	5.58	124.94	118.80
23	QX	18	G	OP2-P-O3'	5.58	117.48	105.20
35	RA	837	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	154(B)	C	N1-C2-O2	5.58	122.25	118.90
35	YA	18	C	C6-N1-C2	-5.58	118.07	120.30
35	YA	277	C	C2-N1-C1'	5.58	124.93	118.80
22	QV	71	C	N1-C2-O2	5.57	122.24	118.90
35	YA	2474	C	N1-C2-O2	5.57	122.24	118.90
35	RA	1005	C	C2-N1-C1'	5.56	124.92	118.80
1	XA	354	G	C4-N9-C1'	5.56	133.72	126.50
35	RA	2506	U	C6-N1-C1'	-5.54	113.44	121.20
35	YA	817	C	C6-N1-C2	-5.54	118.08	120.30
1	XA	754	C	N1-C2-O2	5.54	122.22	118.90
24	XY	36	C	C6-N1-C2	-5.54	118.08	120.30
35	YA	1531	C	C6-N1-C2	-5.54	118.08	120.30
35	YA	1882	C	C2-N1-C1'	5.54	124.89	118.80
36	YB	30	C	C6-N1-C2	-5.54	118.08	120.30
35	RA	1257	C	C6-N1-C2	-5.52	118.09	120.30
35	YA	1882	C	N3-C2-O2	-5.52	118.04	121.90
1	QA	1060	C	C6-N1-C2	-5.51	118.09	120.30
1	QA	1125	U	C2-N1-C1'	5.51	124.31	117.70
12	QL	48	PRO	C-N-CA	5.51	135.46	121.70
22	XV	65	C	C6-N1-C2	-5.50	118.10	120.30
35	YA	1640	C	C6-N1-C2	-5.49	118.10	120.30
35	YA	1493	C	N3-C2-O2	-5.49	118.06	121.90
1	XA	596	C	N1-C2-O2	5.49	122.19	118.90
35	RA	2808	U	N1-C2-O2	5.48	126.64	122.80
1	QA	989	C	N1-C2-O2	5.48	122.19	118.90
35	YA	2889	C	C2-N1-C1'	5.48	124.83	118.80
35	RA	2347	C	N1-C2-O2	5.47	122.19	118.90
35	YA	2465	C	C5-C6-N1	5.47	123.74	121.00
35	RA	195	A	P-O3'-C3'	5.46	126.25	119.70
1	XA	1158	C	C6-N1-C2	-5.46	118.11	120.30
1	XA	1060	C	N3-C2-O2	-5.46	118.08	121.90
1	QA	354	G	C8-N9-C1'	-5.45	119.91	127.00
35	RA	277	C	C2-N1-C1'	5.45	124.80	118.80
35	YA	838	C	N1-C2-O2	5.45	122.17	118.90
35	YA	976	C	C6-N1-C2	-5.45	118.12	120.30
35	YA	1314	C	N3-C2-O2	-5.45	118.08	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	1147	C	N1-C2-O2	5.45	122.17	118.90
1	XA	1326	C	N1-C2-O2	5.44	122.16	118.90
1	XA	58	C	N1-C2-O2	5.44	122.16	118.90
1	QA	1442(A)	G	N3-C4-N9	5.43	129.26	126.00
35	RA	1210	A	P-O3'-C3'	5.43	126.22	119.70
35	YA	1313	U	C6-N1-C1'	-5.43	113.59	121.20
35	RA	560	C	N3-C2-O2	-5.43	118.10	121.90
35	RA	1658	C	C5-C6-N1	5.43	123.72	121.00
35	RA	2591	C	C6-N1-C2	-5.43	118.13	120.30
35	YA	2774	C	N1-C2-O2	5.43	122.16	118.90
35	YA	2465	C	C6-N1-C2	-5.42	118.13	120.30
35	YA	752	A	OP2-P-O3'	5.42	117.12	105.20
35	RA	1767	C	C6-N1-C2	-5.42	118.13	120.30
1	QA	1026	G	C4-N9-C1'	5.41	133.54	126.50
22	XV	65	C	N3-C2-O2	-5.41	118.11	121.90
35	YA	1150	C	C6-N1-C2	-5.41	118.13	120.30
35	RA	601	C	N3-C2-O2	-5.41	118.11	121.90
11	XK	116	HIS	C-N-CA	5.41	135.21	121.70
35	YA	1899	G	C8-N9-C1'	-5.41	119.97	127.00
35	YA	1827	C	C6-N1-C2	-5.40	118.14	120.30
35	YA	2473	U	C5-C6-N1	5.40	125.40	122.70
36	YB	70	C	C6-N1-C2	-5.40	118.14	120.30
1	XA	810	C	C6-N1-C2	-5.40	118.14	120.30
29	Y4	67	TYR	CA-CB-CG	5.40	123.65	113.40
35	YA	1073	A	P-O3'-C3'	5.39	126.17	119.70
35	RA	2723	C	C6-N1-C2	-5.39	118.14	120.30
1	XA	1109	C	N3-C2-O2	-5.39	118.13	121.90
24	QY	70	U	P-O3'-C3'	5.39	126.17	119.70
35	RA	1314	C	N3-C2-O2	-5.39	118.13	121.90
35	RA	766	C	C6-N1-C2	-5.39	118.14	120.30
35	RA	1092	C	C5-C6-N1	5.38	123.69	121.00
2	QB	126	GLU	C-N-CA	5.38	135.15	121.70
36	YB	71	C	N1-C2-O2	5.38	122.13	118.90
22	QV	3	C	N1-C2-O2	5.38	122.13	118.90
35	RA	2320	A	C2-N3-C4	5.38	113.29	110.60
35	RA	1658	C	C6-N1-C2	-5.37	118.15	120.30
1	XA	174	C	N1-C2-O2	5.37	122.12	118.90
35	RA	2465	C	N1-C2-O2	5.37	122.12	118.90
1	XA	972	C	N3-C2-O2	-5.37	118.14	121.90
35	YA	614(A)	U	C6-N1-C1'	-5.37	113.69	121.20
35	YA	2039	C	C6-N1-C2	-5.36	118.15	120.30
35	YA	333	G	C4-N9-C1'	5.36	133.47	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1905	C	N3-C2-O2	-5.35	118.15	121.90
1	XA	330	C	N1-C2-O2	5.35	122.11	118.90
36	RB	30	C	N3-C2-O2	-5.35	118.15	121.90
35	YA	1062	G	N3-C4-N9	5.35	129.21	126.00
35	YA	560	C	N1-C2-O2	5.35	122.11	118.90
35	YA	1899	G	N3-C4-N9	5.35	129.21	126.00
35	RA	944	G	C4-N9-C1'	5.35	133.45	126.50
1	QA	1030(A)	C	N1-C2-O2	5.34	122.11	118.90
24	XY	70	U	P-O3'-C3'	5.34	126.11	119.70
35	RA	1837	C	N1-C2-O2	5.34	122.10	118.90
35	YA	847	U	C6-N1-C2	-5.33	117.80	121.00
35	RA	2200	C	C6-N1-C2	-5.33	118.17	120.30
35	YA	1038	C	N1-C2-O2	5.33	122.10	118.90
35	YA	1644	C	N3-C2-O2	-5.33	118.17	121.90
17	XQ	42	TYR	CA-CB-CG	5.32	123.51	113.40
35	YA	893	C	C2-N1-C1'	5.32	124.65	118.80
35	RA	1067	A	OP2-P-O3'	5.31	116.88	105.20
35	RA	2889	C	C2-N1-C1'	5.30	124.64	118.80
41	RH	163	TYR	CA-CB-CG	5.30	123.48	113.40
35	YA	1979	C	N1-C2-O2	5.30	122.08	118.90
1	QA	1303	C	N1-C2-O2	5.30	122.08	118.90
35	RA	1082	U	C5-C6-N1	5.30	125.35	122.70
1	XA	1125	U	C2-N1-C1'	5.30	124.06	117.70
1	QA	385	C	C6-N1-C2	-5.30	118.18	120.30
1	XA	131	C	N1-C2-O2	5.30	122.08	118.90
1	QA	442	C	C6-N1-C2	-5.29	118.18	120.30
35	YA	1669	A	C2-N3-C4	5.29	113.25	110.60
2	QB	8	LYS	C-N-CA	5.29	134.93	121.70
1	QA	1158	C	C5-C6-N1	5.29	123.64	121.00
35	RA	1073	A	P-O3'-C3'	5.29	126.05	119.70
35	YA	992	C	N1-C2-O2	5.28	122.07	118.90
35	YA	1005	C	N1-C2-O2	5.28	122.07	118.90
1	QA	1026	G	N3-C4-N9	5.28	129.16	126.00
35	YA	1578	U	N3-C2-O2	-5.27	118.51	122.20
35	YA	634	C	C6-N1-C2	-5.27	118.19	120.30
35	RA	198	C	N1-C2-O2	5.26	122.06	118.90
35	YA	2179	C	C2-N1-C1'	5.26	124.59	118.80
16	QP	32	TYR	CA-CB-CG	5.25	123.39	113.40
46	YQ	60	ARG	NE-CZ-NH2	-5.25	117.67	120.30
35	RA	461	C	C5-C6-N1	5.25	123.63	121.00
35	RA	912	C	N1-C2-O2	5.25	122.05	118.90
1	XA	354	G	C8-N9-C1'	-5.25	120.18	127.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	601	C	N3-C2-O2	-5.24	118.23	121.90
23	QX	23	A	C2-N3-C4	5.24	113.22	110.60
35	RA	2689	U	OP2-P-O3'	5.24	116.72	105.20
35	YA	2095	C	N3-C2-O2	-5.24	118.23	121.90
35	RA	686	G	N3-C2-N2	5.23	123.56	119.90
35	YA	1052	C	N3-C2-O2	-5.23	118.24	121.90
1	QA	1003	G	C2-N3-C4	5.23	114.52	111.90
1	QA	931	C	C6-N1-C2	-5.23	118.21	120.30
1	XA	221	C	C6-N1-C2	-5.23	118.21	120.30
1	QA	643	C	C5-C6-N1	5.22	123.61	121.00
35	RA	1882	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	645	C	N1-C2-O2	5.22	122.03	118.90
35	YA	1882	C	C6-N1-C2	-5.22	118.21	120.30
35	YA	1656	C	C6-N1-C2	-5.21	118.22	120.30
1	XA	739	C	C6-N1-C2	-5.21	118.22	120.30
35	RA	2297	C	N1-C2-O2	5.21	122.03	118.90
35	YA	2591	C	C5-C6-N1	5.21	123.60	121.00
1	QA	1383	C	N1-C2-O2	5.21	122.02	118.90
35	RA	2889	C	C6-N1-C2	-5.21	118.22	120.30
35	YA	1064	C	C5-C4-N4	-5.20	116.56	120.20
1	XA	754	C	N3-C2-O2	-5.20	118.26	121.90
36	RB	57	A	C4-C5-N7	5.19	113.30	110.70
35	RA	530	G	C8-N9-C1'	-5.19	120.25	127.00
36	YB	84	C	C6-N1-C2	-5.19	118.22	120.30
1	QA	1113	C	C6-N1-C2	-5.19	118.22	120.30
35	RA	614(A)	U	C6-N1-C1'	-5.19	113.94	121.20
35	YA	755	C	C6-N1-C2	-5.19	118.22	120.30
35	YA	1788	C	C5-C6-N1	5.19	123.59	121.00
35	RA	2295	C	C6-N1-C2	-5.18	118.23	120.30
35	YA	1640	C	C5-C6-N1	5.18	123.59	121.00
36	RB	8	U	C5-C6-N1	5.18	125.29	122.70
6	QF	15	ASP	CB-CG-OD1	5.17	122.95	118.30
35	YA	565	C	N1-C2-O2	5.17	122.00	118.90
35	YA	944	G	C8-N9-C1'	-5.16	120.29	127.00
35	RA	1882	C	N1-C2-O2	5.16	122.00	118.90
1	XA	810	C	C2-N1-C1'	5.16	124.47	118.80
35	RA	1640	C	C5-C6-N1	5.15	123.58	121.00
35	YA	672	C	C6-N1-C2	-5.15	118.24	120.30
1	QA	174	C	N1-C2-O2	5.14	121.99	118.90
35	RA	1102	C	N1-C2-O2	5.14	121.98	118.90
35	RA	1644	C	N1-C2-O2	5.14	121.98	118.90
24	XY	25	C	N3-C2-O2	-5.14	118.30	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y4	25	TYR	CA-CB-CG	5.14	123.16	113.40
35	YA	1313	U	C5-C6-N1	5.14	125.27	122.70
35	RA	1437	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	1467	C	N1-C2-O2	5.13	121.98	118.90
35	RA	624	C	C6-N1-C2	-5.13	118.25	120.30
35	RA	856	C	C5-C6-N1	5.13	123.56	121.00
22	QV	71	C	C5-C6-N1	5.13	123.56	121.00
35	RA	2766	G	C4-N9-C1'	5.12	133.16	126.50
1	XA	1042	G	N9-C4-C5	-5.12	103.35	105.40
29	R4	52	THR	N-CA-C	-5.12	97.17	111.00
35	RA	1333	C	C6-N1-C2	-5.12	118.25	120.30
1	XA	135	C	C6-N1-C2	-5.12	118.25	120.30
35	YA	2465	C	N3-C2-O2	-5.11	118.32	121.90
36	RB	70	C	C6-N1-C2	-5.11	118.26	120.30
24	QY	25	C	N1-C2-O2	5.11	121.96	118.90
35	YA	195	A	P-O3'-C3'	5.10	125.82	119.70
1	QA	369	C	N1-C2-O2	5.10	121.96	118.90
22	QV	65	C	N1-C2-O2	5.10	121.96	118.90
35	RA	976	C	N3-C2-O2	-5.10	118.33	121.90
35	RA	893	C	C2-N1-C1'	5.10	124.41	118.80
1	QA	1397	C	N1-C2-O2	5.09	121.96	118.90
13	QM	107	ALA	N-CA-CB	5.09	117.23	110.10
35	YA	1313	U	C6-N1-C2	-5.09	117.94	121.00
1	QA	1303	C	N3-C2-O2	-5.09	118.34	121.90
35	RA	1497	U	N3-C2-O2	-5.09	118.64	122.20
35	RA	1333	C	N1-C2-O2	5.09	121.95	118.90
42	YI	126	TYR	CA-CB-CG	5.09	123.06	113.40
35	YA	1765	C	C6-N1-C2	-5.08	118.27	120.30
35	RA	1370	C	N1-C2-O2	5.08	121.95	118.90
1	XA	1054	C	N1-C2-O2	5.08	121.95	118.90
35	YA	2320	A	N3-C4-N9	5.08	131.46	127.40
1	XA	999	C	N1-C2-N3	-5.07	115.65	119.20
1	XA	1000	U	C4-C5-C6	5.07	122.74	119.70
35	YA	1578	U	N1-C2-O2	5.07	126.35	122.80
35	RA	1333	C	N3-C2-O2	-5.07	118.35	121.90
1	XA	972	C	N1-C2-O2	5.06	121.94	118.90
35	RA	1021	A	C2-N3-C4	5.06	113.13	110.60
55	YZ	51	ALA	C-N-CA	5.06	134.36	121.70
1	XA	307	C	N1-C2-O2	5.06	121.93	118.90
50	YU	52	ARG	CB-CG-CD	5.06	124.75	111.60
1	QA	1026	G	N3-C4-C5	-5.05	126.07	128.60
35	RA	1064	C	C5-C4-N4	-5.05	116.66	120.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	485	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	1359	A	C2-N3-C4	5.05	113.13	110.60
1	XA	354	G	N3-C4-N9	5.05	129.03	126.00
35	YA	815	C	C6-N1-C2	-5.05	118.28	120.30
35	YA	1372	U	N1-C2-O2	5.05	126.33	122.80
22	XV	65	C	C5-C6-N1	5.05	123.52	121.00
35	YA	154(B)	C	N3-C2-O2	-5.05	118.37	121.90
35	YA	1064	C	C2-N1-C1'	5.05	124.35	118.80
35	RA	856	C	N1-C2-O2	5.04	121.93	118.90
4	XD	38	TYR	CA-CB-CG	5.04	122.99	113.40
35	YA	614(A)	U	O4'-C1'-N1	5.04	112.24	108.20
35	YA	645	C	C2-N1-C1'	5.04	124.35	118.80
35	RA	1038	C	C6-N1-C2	-5.04	118.28	120.30
35	RA	2880	C	C6-N1-C2	-5.04	118.28	120.30
51	RV	2	PHE	N-CA-CB	5.04	119.67	110.60
35	YA	2095	C	N1-C2-O2	5.04	121.92	118.90
1	QA	266	G	N3-C4-C5	-5.04	126.08	128.60
35	YA	665	C	N1-C2-O2	5.03	121.92	118.90
35	YA	1067	A	OP2-P-O3'	5.03	116.27	105.20
1	QA	1279	A	C2-N3-C4	5.03	113.11	110.60
1	XA	186	C	C6-N1-C2	-5.03	118.29	120.30
35	RA	313	C	C6-N1-C2	-5.03	118.29	120.30
1	XA	1003	G	C2-N3-C4	5.03	114.41	111.90
35	YA	1979	C	C6-N1-C2	-5.02	118.29	120.30
1	QA	882	C	N1-C2-O2	5.02	121.91	118.90
35	YA	783	A	N3-C4-N9	5.02	131.41	127.40
24	XY	16	C	C6-N1-C2	-5.02	118.29	120.30
35	YA	2416	C	C5-C6-N1	5.02	123.51	121.00
35	RA	915	C	N3-C2-O2	-5.01	118.39	121.90
35	RA	1135	C	N3-C2-O2	-5.01	118.39	121.90
29	Y4	57	GLU	C-N-CA	5.01	134.23	121.70
22	XV	67	C	N1-C2-O2	5.01	121.91	118.90
1	XA	1113	C	C6-N1-C2	-5.01	118.30	120.30
35	YA	2828	C	C6-N1-C2	-5.01	118.30	120.30
1	QA	1376	U	N3-C2-O2	-5.00	118.70	122.20
35	RA	1835	G	N3-C4-N9	5.00	129.00	126.00
1	XA	1026	G	C4-N9-C1'	5.00	133.00	126.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	QA	32246	0	16295	169	0
1	XA	32331	0	16337	177	0
2	QB	1842	0	1861	26	0
2	XB	1825	0	1828	22	0
3	QC	1558	0	1557	29	0
3	XC	1542	0	1517	16	0
4	QD	1665	0	1691	33	0
4	XD	1668	0	1707	26	0
5	QE	1133	0	1191	16	0
5	XE	1133	0	1191	14	0
6	QF	814	0	808	7	0
6	XF	816	0	808	19	0
7	QG	1235	0	1249	17	0
7	XG	1229	0	1238	8	0
8	QH	1098	0	1143	18	0
8	XH	1088	0	1126	13	0
9	QI	986	0	990	24	0
9	XI	966	0	953	24	0
10	QJ	719	0	672	10	0
10	XJ	710	0	661	13	0
11	QK	834	0	838	12	0
11	XK	833	0	836	11	0
12	QL	932	0	981	17	0
12	XL	932	0	981	11	0
13	QM	914	0	954	14	0
13	XM	895	0	920	22	0
14	QN	492	0	529	10	0
14	XN	492	0	529	10	0
15	QO	728	0	760	2	0
15	XO	728	0	760	3	0
16	QP	681	0	697	20	0
16	XP	677	0	686	22	0
17	QQ	823	0	891	10	0
17	XQ	823	0	891	10	0
18	QR	555	0	618	4	0
18	XR	555	0	618	11	0
19	QS	648	0	658	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	XS	645	0	635	15	0
20	QT	732	0	809	8	0
20	XT	733	0	795	8	0
21	QU	199	0	208	1	0
21	XU	199	0	208	0	0
22	QV	1640	0	837	5	0
22	XV	1640	0	837	5	0
23	QX	394	0	197	1	0
23	XX	394	0	197	1	0
24	QY	1625	0	822	5	0
24	XY	1625	0	822	5	0
25	R0	608	0	622	8	0
25	Y0	608	0	622	12	0
26	R1	754	0	823	10	0
26	Y1	759	0	837	5	0
27	R2	588	0	643	8	0
27	Y2	592	0	654	6	0
28	R3	469	0	518	2	0
28	Y3	464	0	514	8	0
29	R4	546	0	522	9	0
29	Y4	536	0	514	12	0
30	R5	459	0	476	8	0
30	Y5	455	0	465	6	0
31	R6	453	0	473	3	0
31	Y6	449	0	469	4	0
32	R7	418	0	466	5	0
32	Y7	418	0	466	4	0
33	R8	517	0	582	14	0
33	Y8	517	0	582	13	0
34	R9	307	0	335	5	0
34	Y9	307	0	335	7	0
35	RA	61758	0	31137	265	0
35	YA	61758	0	31138	256	0
36	RB	2572	0	1304	3	0
36	YB	2573	0	1306	6	0
37	RD	2131	0	2205	41	0
37	YD	2136	0	2217	43	0
38	RE	1559	0	1618	20	0
38	YE	1559	0	1618	33	0
39	RF	1583	0	1624	43	0
39	YF	1579	0	1618	27	0
40	RG	1426	0	1445	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	YG	1424	0	1441	22	0
41	RH	1330	0	1407	16	0
41	YH	1324	0	1402	14	0
42	RI	1094	0	1127	4	0
42	YI	1076	0	1094	4	0
43	RN	1121	0	1195	16	0
43	YN	1117	0	1184	8	0
44	RO	933	0	996	15	0
44	YO	933	0	996	18	0
45	RP	1135	0	1212	22	0
45	YP	1135	0	1212	24	0
46	RQ	1122	0	1179	19	0
46	YQ	1122	0	1179	14	0
47	RR	968	0	1033	8	0
47	YR	968	0	1033	10	0
48	RS	877	0	938	10	0
48	YS	870	0	923	8	0
49	RT	1091	0	1151	16	0
49	YT	1083	0	1136	15	0
50	RU	959	0	1019	15	0
50	YU	959	0	1019	11	0
51	RV	775	0	841	14	0
51	YV	771	0	830	8	0
52	RW	886	0	940	8	0
52	YW	886	0	940	9	0
53	RX	750	0	814	11	0
53	YX	750	0	814	6	0
54	RY	810	0	892	7	0
54	YY	810	0	887	14	0
55	RZ	1406	0	1418	17	0
55	YZ	1381	0	1386	15	0
56	QA	221	0	0	0	0
56	QB	1	0	0	0	0
56	QD	4	0	0	0	0
56	QE	4	0	0	0	0
56	QF	2	0	0	0	0
56	QG	2	0	0	0	0
56	QH	2	0	0	0	0
56	QI	1	0	0	0	0
56	QK	1	0	0	0	0
56	QL	3	0	0	0	0
56	QN	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	QO	2	0	0	0	0
56	QP	1	0	0	0	0
56	QT	1	0	0	0	0
56	QV	5	0	0	0	0
56	R0	3	0	0	0	0
56	R1	1	0	0	0	0
56	R3	3	0	0	0	0
56	R5	2	0	0	0	0
56	R6	1	0	0	0	0
56	R7	3	0	0	0	0
56	R9	1	0	0	0	0
56	RA	709	0	0	0	0
56	RB	17	0	0	0	0
56	RD	8	0	0	0	0
56	RE	4	0	0	0	0
56	RF	4	0	0	0	0
56	RG	4	0	0	0	0
56	RH	2	0	0	0	0
56	RN	2	0	0	0	0
56	RO	1	0	0	0	0
56	RP	3	0	0	0	0
56	RQ	4	0	0	0	0
56	RR	2	0	0	0	0
56	RT	4	0	0	0	0
56	RU	2	0	0	0	0
56	RV	3	0	0	0	0
56	RW	1	0	0	0	0
56	RZ	1	0	0	0	0
56	XA	193	0	0	0	0
56	XE	2	0	0	0	0
56	XF	2	0	0	0	0
56	XJ	1	0	0	0	0
56	XL	2	0	0	0	0
56	XR	1	0	0	0	0
56	XT	1	0	0	0	0
56	XV	3	0	0	0	0
56	XY	1	0	0	0	0
56	Y0	1	0	0	0	0
56	Y1	2	0	0	0	0
56	Y3	1	0	0	0	0
56	Y5	1	0	0	0	0
56	Y6	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	Y7	2	0	0	0	0
56	Y8	1	0	0	0	0
56	YA	707	0	0	0	0
56	YB	20	0	0	0	0
56	YD	7	0	0	0	0
56	YE	5	0	0	0	0
56	YF	3	0	0	0	0
56	YG	3	0	0	0	0
56	YI	1	0	0	0	0
56	YN	1	0	0	0	0
56	YO	1	0	0	0	0
56	YP	2	0	0	0	0
56	YQ	2	0	0	0	0
56	YR	2	0	0	0	0
56	YT	3	0	0	0	0
56	YV	1	0	0	0	0
56	YW	2	0	0	0	0
57	QA	42	0	45	1	0
57	XA	42	0	45	1	0
58	QD	8	0	0	0	0
58	XD	8	0	0	1	0
59	QN	1	0	0	0	0
59	R4	1	0	0	0	0
59	R5	1	0	0	0	0
59	R6	1	0	0	0	0
59	R9	1	0	0	0	0
59	RY	1	0	0	0	0
59	XN	1	0	0	0	0
59	Y4	1	0	0	0	0
59	Y5	1	0	0	0	0
59	Y6	1	0	0	0	0
59	Y9	1	0	0	0	0
59	YY	1	0	0	0	0
All	All	293819	0	196213	1738	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 4.

All (1738) 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)
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CE1	1.78	1.17
16:QP:20:VAL:HG21	16:QP:32:TYR:HD2	1.09	1.13
55:RZ:8:TYR:HB2	55:RZ:38:TYR:CD1	1.90	1.07
35:RA:660:G:H5'	39:RF:99:TYR:CE2	1.94	1.03
16:QP:20:VAL:HG21	16:QP:32:TYR:CD2	1.94	1.02
4:QD:38:TYR:HE2	4:QD:45:GLN:HG2	1.26	1.00
16:XP:20:VAL:HG21	16:XP:32:TYR:CD2	1.96	0.99
3:QC:159:GLY:N	3:QC:193:TYR:HE2	1.60	0.99
35:RA:660:G:C5'	39:RF:99:TYR:CE2	2.47	0.97
35:RA:660:G:C5'	39:RF:99:TYR:HE2	1.78	0.95
35:YA:2604:U:H6	35:YA:2604:U:H5''	1.31	0.94
16:XP:20:VAL:HG21	16:XP:32:TYR:HD2	1.30	0.94
16:QP:38:TYR:CD1	16:QP:50:LYS:HB3	2.04	0.91
55:RZ:8:TYR:CB	55:RZ:38:TYR:CE1	2.56	0.87
35:YA:1567:A:C5	37:YD:84:TYR:HE2	1.92	0.87
35:RA:528:A:H2	43:RN:114:ARG:NH2	1.72	0.86
16:QP:38:TYR:CE1	16:QP:50:LYS:HB3	2.12	0.85
3:QC:159:GLY:HA2	3:QC:193:TYR:CE2	2.11	0.85
1:XA:765:G:H1	1:XA:812:C:HO2'	1.20	0.85
38:YE:84:PHE:CD2	38:YE:86:PRO:HD3	2.11	0.84
19:XS:41:VAL:CG2	19:XS:43:GLU:OE1	2.25	0.84
35:RA:528:A:H2	43:RN:114:ARG:HH21	1.21	0.83
35:YA:1567:A:C5	37:YD:84:TYR:CE2	2.68	0.82
19:XS:41:VAL:HB	19:XS:43:GLU:OE1	1.80	0.82
3:QC:159:GLY:CA	3:QC:193:TYR:HE2	1.92	0.81
35:RA:660:G:H4'	39:RF:99:TYR:HE2	1.45	0.80
35:RA:660:G:H5'	39:RF:99:TYR:CD2	2.17	0.79
19:XS:41:VAL:HG23	19:XS:43:GLU:OE1	1.80	0.79
3:QC:159:GLY:HA2	3:QC:193:TYR:CD2	2.18	0.79
35:YA:1567:A:N7	37:YD:84:TYR:HE2	1.80	0.79
1:QA:1422:G:H5''	44:RO:48:PRO:HB3	1.65	0.79
4:QD:98:GLU:OE1	4:QD:189:PRO:CG	2.30	0.78
39:RF:39:TRP:HA	39:RF:99:TYR:HE1	1.48	0.78
1:XA:1330:U:H4'	13:XM:23:TYR:CD1	2.17	0.78
4:QD:38:TYR:CE2	4:QD:45:GLN:HG2	2.15	0.78
1:QA:1330:U:H4'	13:QM:23:TYR:CD1	2.18	0.77
50:RU:49:HIS:HA	50:RU:52:ARG:HB3	1.66	0.77
4:QD:98:GLU:OE2	4:QD:194:LEU:HD23	1.83	0.77
55:RZ:8:TYR:CB	55:RZ:38:TYR:HE1	1.97	0.77
1:QA:626:U:H4'	16:QP:38:TYR:CE2	2.20	0.76
16:QP:38:TYR:CE1	16:QP:50:LYS:CB	2.69	0.76
29:Y4:11:PRO:HG3	29:Y4:25:TYR:CE2	2.21	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2604:U:H5''	35:YA:2604:U:C6	2.19	0.75
3:QC:159:GLY:H	3:QC:193:TYR:HE2	1.33	0.75
1:QA:626:U:H4'	16:QP:38:TYR:HE2	1.51	0.74
19:XS:43:GLU:OE1	19:XS:43:GLU:N	2.20	0.74
3:QC:159:GLY:CA	3:QC:193:TYR:CE2	2.69	0.74
19:XS:41:VAL:CB	19:XS:43:GLU:OE1	2.35	0.74
35:RA:660:G:C4'	39:RF:99:TYR:HE2	2.00	0.74
50:YU:49:HIS:HA	50:YU:52:ARG:HB3	1.70	0.74
1:XA:1043:C:H4'	1:XA:1043:C:OP1	1.87	0.74
1:QA:1086:U:H3	1:QA:1099:G:H22	1.36	0.73
3:QC:184:TYR:HE1	3:QC:201:TYR:HE1	1.36	0.73
1:XA:626:U:H4'	16:XP:38:TYR:CE2	2.24	0.73
1:XA:1393:U:HO2'	1:XA:1501:C:HO2'	1.37	0.72
1:XA:501:C:OP1	12:XL:117:ARG:NH2	2.22	0.72
4:QD:98:GLU:OE1	4:QD:189:PRO:HG3	1.90	0.72
38:YE:84:PHE:CE2	38:YE:86:PRO:HD3	2.24	0.72
41:RH:154:PRO:HB3	41:RH:163:TYR:CE1	2.24	0.72
1:XA:1422:G:H5''	44:YO:48:PRO:HB3	1.71	0.71
4:QD:68:TYR:HE2	4:QD:103:ASN:ND2	1.88	0.71
48:YS:25:ARG:NH1	48:YS:88:ASP:OD2	2.22	0.71
3:QC:184:TYR:CE1	3:QC:201:TYR:CE1	2.79	0.71
6:XF:50:TYR:HE1	18:XR:77:GLY:HA2	1.55	0.70
1:XA:1249:C:O2'	9:XI:73:GLN:NE2	2.24	0.70
35:YA:1041:C:H42	35:YA:1114:G:H1	1.39	0.70
3:QC:159:GLY:N	3:QC:193:TYR:CE2	2.53	0.70
10:QJ:10:GLY:HA3	10:QJ:16:LEU:HD21	1.72	0.70
16:QP:38:TYR:HE1	16:QP:50:LYS:HB2	1.55	0.70
24:QY:4:G:H1	24:QY:69:C:H42	1.37	0.70
35:RA:2131:G:H5''	35:RA:2132:U:H5'	1.74	0.70
1:XA:664:G:H22	1:XA:741:G:H1	1.38	0.69
1:QA:236:G:H5''	17:QQ:42:TYR:OH	1.92	0.69
1:QA:559:A:H4'	1:QA:560:U:H3'	1.72	0.69
2:QB:185:ILE:HG22	2:QB:199:TYR:HB2	1.74	0.69
16:QP:5:ARG:HH12	16:QP:28:ARG:HA	1.56	0.69
35:RA:528:A:C2	43:RN:114:ARG:NH2	2.60	0.69
35:RA:660:G:C5'	39:RF:99:TYR:CD2	2.76	0.69
1:QA:544:G:OP1	4:QD:59:ARG:NH2	2.25	0.69
1:XA:544:G:OP1	4:XD:59:ARG:NH2	2.26	0.69
35:RA:881:G:H1	35:RA:895:U:H3	1.39	0.69
33:Y8:30:ARG:HH21	45:YP:63:PRO:HB2	1.57	0.69
35:YA:1056:G:H21	35:YA:1103:A:H62	1.39	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:122:PHE:HE2	2:XB:139:LYS:HD3	1.58	0.68
1:QA:429:U:OP1	4:QD:13:ARG:NH1	2.27	0.68
16:QP:38:TYR:HE1	16:QP:50:LYS:CB	2.07	0.68
1:XA:1130:A:O2'	9:XI:3:GLN:NE2	2.26	0.68
27:R2:66:GLU:HA	27:R2:69:ARG:HD3	1.76	0.67
44:RO:35:VAL:HG11	44:RO:103:ALA:HB3	1.76	0.67
35:RA:83:G:H1	35:RA:102:G:HO2'	1.41	0.67
35:RA:1153:C:OP1	50:RU:92:ARG:NH2	2.25	0.67
51:YV:21:ARG:NE	51:YV:91:TYR:HE2	1.93	0.67
1:QA:1295:G:O2'	13:QM:14:ARG:NH1	2.27	0.67
2:QB:8:LYS:O	2:QB:217:ARG:NH2	2.28	0.67
4:QD:98:GLU:OE1	4:QD:189:PRO:HG2	1.94	0.67
1:XA:559:A:H4'	1:XA:560:U:H3'	1.77	0.67
34:R9:27:CYS:SG	34:R9:28:GLU:N	2.68	0.66
5:XE:102:ALA:HB1	5:XE:106:PRO:HG2	1.77	0.66
25:Y0:39:ARG:HH21	35:YA:2355:C:H1'	1.61	0.66
3:QC:184:TYR:HE1	3:QC:201:TYR:CE1	2.13	0.66
52:RW:14:PRO:HG2	52:RW:78:GLU:HG2	1.76	0.66
35:RA:958:U:OP2	46:RQ:14:ARG:NH1	2.29	0.66
16:QP:38:TYR:HD1	16:QP:50:LYS:HB3	1.60	0.66
40:RG:47:LYS:NZ	40:RG:80:PHE:O	2.25	0.66
35:YA:881:G:H1	35:YA:895:U:H3	1.43	0.66
35:RA:1041:C:H42	35:RA:1114:G:H1	1.44	0.66
20:XT:100:ILE:HG22	20:XT:101:GLY:H	1.59	0.66
9:QI:86:VAL:HG21	9:QI:93:ARG:HE	1.59	0.66
29:R4:16:CYS:SG	29:R4:17:GLY:N	2.69	0.66
55:YZ:51:ALA:HB1	55:YZ:55:HIS:HB2	1.78	0.66
8:XH:114:THR:HG23	8:XH:116:LYS:H	1.61	0.66
10:XJ:57:LYS:HE2	10:XJ:60:ARG:HH22	1.60	0.66
55:YZ:10:ARG:HE	55:YZ:36:LYS:HB3	1.61	0.65
1:XA:8:A:N6	4:XD:205:GLU:O	2.29	0.65
35:YA:2131:G:H5''	35:YA:2132:U:H5'	1.77	0.65
39:RF:157:VAL:HB	39:RF:194:MET:HG2	1.78	0.65
35:YA:2506:U:C2	35:YA:2585:U:O4	2.49	0.65
35:YA:2298:A:H62	35:YA:2318:G:H8	1.44	0.65
1:QA:501:C:OP1	12:QL:117:ARG:NH2	2.29	0.65
1:QA:545:C:OP1	4:QD:61:LYS:NZ	2.29	0.65
4:XD:98:GLU:HA	4:XD:103:ASN:HD22	1.62	0.65
12:XL:47:LYS:O	12:XL:49:ASN:N	2.30	0.65
35:YA:483:A:H5''	54:YY:50:ARG:HE	1.61	0.65
38:YE:84:PHE:HE2	38:YE:86:PRO:HG3	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:187:LEU:HA	2:QB:201:ILE:HB	1.77	0.65
1:XA:1123:A:H4'	10:XJ:36:GLY:HA3	1.78	0.65
6:XF:81:ILE:HD11	37:YD:125:ILE:HB	1.79	0.65
51:RV:21:ARG:HH11	51:RV:91:TYR:HE2	1.45	0.65
29:Y4:14:ILE:HB	29:Y4:22:ILE:HB	1.79	0.65
35:YA:2010:G:H5''	52:YW:42:ARG:HB2	1.79	0.65
39:RF:143:ALA:HB1	39:RF:148:LEU:HB2	1.78	0.64
13:XM:6:GLY:HA3	13:XM:67:GLU:HG3	1.78	0.64
35:YA:1153:C:OP1	50:YU:92:ARG:NH2	2.29	0.64
4:QD:4:TYR:O	4:QD:6:GLY:N	2.31	0.64
37:RD:85:ASP:OD2	37:RD:88:ARG:NH1	2.29	0.64
38:RE:2:LYS:HB2	38:RE:95:ILE:HD12	1.78	0.64
17:QQ:26:GLN:HG2	17:QQ:37:LYS:HG2	1.78	0.64
35:RA:2010:G:H5''	52:RW:42:ARG:HB2	1.79	0.64
6:XF:87:ARG:NH1	18:XR:75:ILE:O	2.31	0.64
1:XA:1101:A:N7	2:XB:175:ARG:NH2	2.46	0.64
55:RZ:115:GLY:HA2	55:RZ:177:PRO:HD3	1.79	0.64
38:YE:84:PHE:HE2	38:YE:86:PRO:CG	2.10	0.64
1:QA:664:G:H22	1:QA:741:G:H1	1.45	0.63
33:R8:6:THR:HG22	33:R8:63:PRO:HD2	1.81	0.63
35:YA:39:C:O2	39:YF:46:ARG:NH2	2.28	0.63
9:QI:121:ARG:NH1	9:QI:122:ALA:O	2.30	0.63
4:QD:18:LYS:NZ	4:QD:31:CYS:SG	2.72	0.63
1:XA:626:U:H4'	16:XP:38:TYR:HE2	1.61	0.63
34:Y9:27:CYS:SG	34:Y9:28:GLU:N	2.71	0.63
5:QE:102:ALA:HB1	5:QE:106:PRO:HG2	1.79	0.63
35:RA:1791:A:H5'	37:RD:206:LEU:HD12	1.81	0.63
3:QC:108:ASN:ND2	3:QC:144:SER:OG	2.32	0.63
22:QV:9:G:O2'	22:QV:10:G:N7	2.32	0.63
29:Y4:16:CYS:SG	29:Y4:17:GLY:N	2.72	0.63
35:YA:1824:G:N3	37:YD:254:THR:OG1	2.32	0.63
35:YA:2604:U:H6	35:YA:2604:U:C5'	2.10	0.63
35:RA:2851:A:O2'	47:RR:64:ARG:NH2	2.32	0.62
35:YA:1470:G:N2	35:YA:1520:G:OP2	2.31	0.62
35:YA:2032:G:N2	38:YE:146:THR:OG1	2.32	0.62
33:R8:30:ARG:HH21	45:RP:63:PRO:HB2	1.63	0.62
4:QD:68:TYR:CE2	4:QD:103:ASN:ND2	2.67	0.62
12:QL:71:PRO:O	12:QL:102:ARG:NH1	2.33	0.62
35:RA:1607:C:N4	35:RA:1622:G:OP2	2.30	0.62
49:RT:125:ARG:O	49:RT:129:ARG:NH1	2.32	0.62
35:RA:993:G:N3	51:RV:89:GLN:NE2	2.46	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:YS:25:ARG:HD3	48:YS:27:SER:HB2	1.81	0.62
33:R8:28:GLY:O	33:R8:36:LYS:NZ	2.31	0.62
43:RN:12:ARG:NH1	43:RN:50:ASP:OD2	2.32	0.62
35:YA:1721:G:H8	35:YA:1741:A:H62	1.46	0.62
17:QQ:66:SER:O	17:QQ:70:ARG:NH1	2.33	0.62
26:R1:51:VAL:HG11	26:R1:74:VAL:HG21	1.81	0.62
29:R4:34:GLU:OE1	29:R4:35:VAL:HG23	2.00	0.62
38:RE:36:ARG:NH1	38:RE:85:ASN:OD1	2.33	0.62
3:XC:56:ASP:HB2	3:XC:67:THR:HB	1.82	0.62
37:YD:108:PRO:HD2	37:YD:111:LEU:HD22	1.80	0.62
54:YY:9:LYS:NZ	54:YY:28:LYS:O	2.30	0.62
2:QB:54:THR:HG22	2:QB:199:TYR:HB3	1.81	0.62
1:QA:539:A:OP2	12:QL:115:LYS:NZ	2.33	0.62
35:RA:1195:G:OP2	45:RP:15:ARG:NH1	2.32	0.62
35:YA:993:G:OP1	50:YU:50:ARG:NH2	2.31	0.62
39:YF:157:VAL:HB	39:YF:194:MET:HG2	1.81	0.62
35:RA:1695:G:N7	37:RD:14:ARG:NH2	2.48	0.62
41:YH:86:GLU:OE2	41:YH:130:ARG:NH1	2.33	0.62
17:XQ:26:GLN:HG2	17:XQ:37:LYS:HG2	1.82	0.61
37:RD:108:PRO:HD2	37:RD:111:LEU:HD22	1.82	0.61
40:YG:48:GLU:O	40:YG:51:ARG:NH1	2.33	0.61
1:QA:352:C:O2	1:QA:355:C:N4	2.32	0.61
1:QA:626:U:H5''	16:QP:38:TYR:HD2	1.64	0.61
3:XC:184:TYR:HE1	3:XC:201:TYR:HE1	1.48	0.61
1:QA:1497:G:H1'	1:QA:1518:MA6:H2	1.82	0.61
3:QC:56:ASP:HB2	3:QC:67:THR:HB	1.83	0.61
1:QA:1328:C:O2'	13:QM:29:ARG:NH2	2.34	0.61
1:QA:1137:C:O2	1:QA:1138:G:N2	2.34	0.61
51:RV:40:LEU:HB2	51:RV:46:VAL:HG22	1.82	0.61
35:YA:83:G:H1	35:YA:102:G:HO2'	1.45	0.61
35:RA:807:U:O2'	35:RA:2060:A:N1	2.33	0.61
17:XQ:66:SER:O	17:XQ:70:ARG:NH1	2.34	0.61
24:XY:18:G:N2	24:XY:58:A:OP1	2.33	0.61
35:YA:2413:G:H21	45:YP:70:GLN:HE22	1.48	0.61
45:YP:93:GLY:H	45:YP:123:LEU:HD22	1.66	0.61
38:YE:84:PHE:CE2	38:YE:86:PRO:CD	2.84	0.61
43:YN:22:THR:HB	43:YN:25:ARG:HB2	1.83	0.61
35:RA:660:G:H5''	39:RF:99:TYR:CE2	2.35	0.60
44:RO:23:ARG:NH2	44:RO:28:SER:O	2.34	0.60
35:YA:1567:A:N7	37:YD:84:TYR:CE2	2.67	0.60
44:YO:35:VAL:HG11	44:YO:103:ALA:HB3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:958:U:OP2	46:YQ:14:ARG:NH1	2.34	0.60
1:QA:737:A:H1'	6:QF:73:ASN:HD21	1.66	0.60
25:Y0:20:ARG:HH12	35:YA:2357:U:H5'	1.66	0.60
1:QA:8:A:N6	4:QD:205:GLU:O	2.32	0.60
9:QI:17:VAL:HG21	9:QI:81:ILE:HG22	1.84	0.60
26:Y1:52:ARG:NH1	35:YA:2218:U:O2	2.35	0.60
7:QG:150:ALA:HB1	11:QK:57:THR:HG21	1.83	0.60
1:XA:974:A:OP2	14:YN:41:ARG:NH1	2.34	0.60
8:QH:110:ALA:HB3	8:QH:121:ASP:HB3	1.82	0.60
35:RA:613:G:N2	35:RA:614(D):A:O2'	2.35	0.60
35:YA:2292:C:OP1	48:YS:17:ARG:NH2	2.34	0.60
2:QB:69:LEU:HB3	2:QB:162:ILE:HG22	1.82	0.60
24:QY:74:C:H42	35:RA:2508:G:H5'	1.65	0.60
55:RZ:99:TYR:HB3	55:RZ:123:ASP:HB2	1.82	0.60
38:YE:105:THR:OG1	38:YE:199:ARG:NH2	2.34	0.60
35:RA:1824:G:N3	37:RD:254:THR:OG1	2.35	0.60
3:QC:58:GLU:HB2	3:QC:65:ALA:HB3	1.84	0.60
40:RG:64:THR:HB	40:RG:94:LEU:HD21	1.83	0.60
49:RT:92:GLY:O	49:RT:120:ARG:NH2	2.34	0.60
16:XP:38:TYR:HE1	16:XP:50:LYS:CB	2.13	0.60
1:XA:954:G:H21	1:XA:1227:A:H62	1.48	0.60
30:Y5:29:THR:HG21	35:YA:2815:C:H5'	1.83	0.60
37:YD:85:ASP:OD2	37:YD:88:ARG:NH1	2.32	0.60
35:YA:674:G:H1'	39:YF:74:ARG:HD3	1.83	0.60
35:YA:336:C:O2'	54:YY:35:TYR:OH	2.20	0.60
35:YA:301:G:OP2	54:YY:84:ARG:NH2	2.34	0.60
35:RA:987:G:O2'	35:RA:1000:A:N3	2.34	0.59
3:XC:110:ASN:OD1	3:XC:140:ARG:NH1	2.35	0.59
50:YU:97:ASP:OD1	50:YU:101:ARG:NH1	2.34	0.59
37:YD:143:HIS:ND1	37:YD:194:GLY:O	2.33	0.59
38:YE:29:GLY:HA2	38:YE:180:ASN:HB3	1.83	0.59
1:XA:978:A:H61	1:XA:1316:G:H1'	1.66	0.59
1:XA:1406:U:O2	1:XA:1517:G:N2	2.35	0.59
1:XA:427:U:OP1	4:XD:13:ARG:NH1	2.35	0.59
1:QA:425:G:O3'	4:QD:45:GLN:NE2	2.35	0.59
4:QD:20:TYR:CD2	4:QD:26:CYS:HB3	2.37	0.59
35:YA:2602:A:H2'	35:YA:2602:A:N3	2.18	0.59
3:QC:21:ARG:NH2	3:QC:58:GLU:OE2	2.36	0.59
1:QA:974:A:OP2	14:QN:41:ARG:NH1	2.35	0.59
35:RA:2096:U:H3	35:RA:2193:G:H1	1.50	0.59
16:XP:8:ARG:HB3	16:XP:28:ARG:HH12	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1330:U:H4'	13:QM:23:TYR:CE1	2.37	0.59
35:RA:1815:A:OP2	37:RD:54:ARG:NH2	2.36	0.59
2:XB:68:ILE:HG12	2:XB:161:ALA:HB3	1.84	0.59
8:XH:10:LEU:HD22	8:XH:83:ILE:HD11	1.84	0.59
55:YZ:8:TYR:HB2	55:YZ:38:TYR:CE1	2.38	0.59
35:RA:181:A:H1'	35:RA:435:C:H5'	1.85	0.59
1:XA:1500:A:H5''	1:XA:1508:G:H5''	1.84	0.59
1:XA:508:C:OP1	4:XD:209:ARG:NH2	2.35	0.59
10:XJ:17:ASP:OD1	10:XJ:70:ARG:NH1	2.35	0.59
1:QA:1013:G:N2	1:QA:1016:A:OP2	2.36	0.59
33:R8:14:VAL:HG12	33:R8:24:ALA:HB2	1.85	0.59
37:YD:260:ARG:NH2	37:YD:266:SER:OG	2.36	0.59
40:YG:19:LEU:HD23	40:YG:32:PRO:HD2	1.85	0.59
54:YY:15:VAL:HG21	54:YY:42:VAL:HG11	1.84	0.59
1:QA:933:G:O6	7:QG:3:ARG:NH2	2.36	0.58
48:RS:105:ALA:HB1	48:RS:110:LEU:HD12	1.85	0.58
5:XE:33:VAL:HG21	5:XE:109:ILE:HA	1.85	0.58
35:RA:1791:A:H4'	37:RD:206:LEU:HB2	1.85	0.58
35:YA:987:G:O2'	35:YA:1000:A:N3	2.35	0.58
55:YZ:8:TYR:HB2	55:YZ:38:TYR:CD1	2.38	0.58
28:R3:15:TYR:O	28:R3:20:LYS:NZ	2.37	0.58
39:RF:101:LEU:O	39:RF:106:ARG:NH1	2.35	0.58
41:RH:159:GLU:HG3	41:RH:171:LEU:HD11	1.85	0.58
24:XY:4:G:H1	24:XY:69:C:H42	1.50	0.58
35:YA:1058:G:N2	35:YA:1080:C:O2	2.35	0.58
35:YA:2096:U:H3	35:YA:2193:G:H1	1.50	0.58
45:YP:29:LYS:HD3	45:YP:30:THR:HG23	1.85	0.58
20:QT:51:GLU:HA	20:QT:54:LYS:HE2	1.84	0.58
33:R8:30:ARG:NH2	45:RP:64:LYS:O	2.36	0.58
25:R0:14:ARG:NH1	35:RA:2279:G:O6	2.36	0.58
35:YA:2604:U:C5'	35:YA:2604:U:C6	2.85	0.58
16:XP:18:ARG:NH1	16:XP:32:TYR:OH	2.36	0.58
35:RA:2298:A:H62	35:RA:2318:G:H8	1.51	0.58
35:YA:526:A:O2'	35:YA:2043:C:O2	2.21	0.58
33:Y8:43:GLN:NE2	35:YA:2365:G:O6	2.30	0.58
35:YA:1155:A:OP1	50:YU:55:ARG:HG2	2.04	0.58
24:XY:75:C:O2'	35:YA:2573:C:N4	2.37	0.58
35:YA:631:A:OP1	45:YP:65:ARG:NH1	2.36	0.58
34:R9:36:GLN:NE2	35:RA:1124:C:O2	2.36	0.58
35:RA:956:G:H2'	35:RA:957:A:H2'	1.86	0.58
17:QQ:9:VAL:HG22	17:QQ:56:VAL:HG22	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1286:A:H2'	1:XA:1287:A:H4'	1.85	0.58
24:XY:20:G:N2	24:XY:21:A:O2'	2.37	0.58
35:YA:2574:G:N3	38:YE:143:ASN:ND2	2.52	0.58
1:QA:779:C:O2'	11:QK:120:ARG:NH1	2.37	0.58
35:RA:2646:C:OP2	35:RA:2732:G:O2'	2.22	0.58
1:QA:528:C:N4	12:QL:49:ASN:OD1	2.34	0.57
35:RA:340:A:O2'	39:RF:168:ARG:NH2	2.37	0.57
35:RA:39:C:O2	39:RF:46:ARG:NH2	2.33	0.57
35:RA:1800:C:OP2	37:RD:183:ARG:NH2	2.37	0.57
27:Y2:16:LEU:O	27:Y2:67:LYS:NZ	2.36	0.57
35:YA:2483:C:N3	46:YQ:124:LYS:NZ	2.42	0.57
35:YA:1791:A:H5'	37:YD:206:LEU:HD12	1.86	0.57
1:XA:1086:U:H3	1:XA:1099:G:H22	1.52	0.57
35:RA:1791:A:N6	35:RA:1828:G:O2'	2.34	0.57
35:RA:2627:G:N2	35:RA:2777:G:OP2	2.36	0.57
3:XC:40:ARG:HH12	14:XN:52:GLN:HG2	1.69	0.57
35:RA:994:C:OP1	50:RU:53:ARG:NH2	2.37	0.57
12:XL:70:ILE:HG13	12:XL:100:ILE:HD12	1.86	0.57
35:YA:693:C:O2'	35:YA:1353:A:N3	2.34	0.57
39:YF:190:GLU:HA	45:YP:2:LYS:HE3	1.86	0.57
1:QA:977:A:N6	1:QA:1224:G:OP1	2.29	0.57
28:R3:8:LEU:HB2	28:R3:28:LEU:HD13	1.86	0.57
35:RA:1162:G:H4'	51:RV:24:LYS:HB3	1.87	0.57
35:RA:500:G:N1	35:RA:503:A:OP2	2.37	0.57
35:RA:631:A:OP1	45:RP:65:ARG:NH1	2.37	0.57
4:XD:18:LYS:HD2	58:XD:301:SF4:S2	2.44	0.57
25:R0:20:ARG:HH12	35:RA:2357:U:H5'	1.69	0.57
37:RD:143:HIS:ND1	37:RD:194:GLY:O	2.34	0.57
44:RO:104:ARG:NH2	44:RO:121:VAL:O	2.38	0.57
35:RA:143(A):G:H4'	53:RX:35:THR:HG21	1.87	0.57
35:YA:859:G:O2'	35:YA:916:G:O6	2.22	0.57
13:QM:99:ARG:HB2	13:QM:101:GLN:HE22	1.69	0.57
35:RA:615:G:OP1	39:RF:40:GLN:NE2	2.38	0.57
41:RH:154:PRO:HG3	41:RH:163:TYR:CD1	2.40	0.57
28:Y3:15:TYR:O	28:Y3:20:LYS:NZ	2.37	0.57
31:Y6:35:GLU:OE2	31:Y6:50:ARG:NH1	2.38	0.57
1:XA:1295:G:O2'	13:XM:14:ARG:NH1	2.38	0.57
35:RA:1009:A:OP2	43:RN:37:LYS:NZ	2.35	0.57
35:YA:1791:A:N6	35:YA:1828:G:O2'	2.38	0.57
39:RF:11:VAL:HG22	39:RF:125:LEU:HB2	1.86	0.56
45:RP:93:GLY:H	45:RP:123:LEU:HD22	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:8:GLU:OE2	13:XM:11:ARG:NH2	2.38	0.56
10:QJ:49:VAL:HG23	14:QN:41:ARG:HB2	1.86	0.56
26:R1:52:ARG:NH1	35:RA:2218:U:O2	2.38	0.56
35:RA:2839:G:H5'	47:RR:46:GLY:HA2	1.87	0.56
33:Y8:28:GLY:O	33:Y8:36:LYS:NZ	2.36	0.56
47:YR:103:ARG:NH1	47:YR:108:GLY:O	2.38	0.56
35:YA:1651:G:N7	47:YR:11:ASN:ND2	2.52	0.56
1:XA:545:C:OP1	4:XD:61:LYS:NZ	2.38	0.56
1:XA:626:U:H5''	16:XP:38:TYR:HD2	1.69	0.56
19:XS:63:THR:HG23	19:XS:65:ASN:H	1.70	0.56
1:QA:1318:A:OP1	19:QS:3:ARG:NH2	2.37	0.56
54:RY:47:LYS:NZ	54:RY:48:ALA:O	2.39	0.56
35:YA:1695:G:N7	37:YD:14:ARG:NH2	2.54	0.56
26:R1:3:LYS:NZ	35:RA:1366:A:OP1	2.38	0.56
49:RT:122:ASP:OD1	49:RT:125:ARG:NH2	2.35	0.56
1:XA:1003:G:H1	1:XA:1035:A:H61	1.52	0.56
29:Y4:43:TYR:OH	40:YG:179:PRO:HG3	2.05	0.56
40:RG:137:GLU:HG3	40:RG:140:ILE:HG12	1.88	0.56
5:QE:7:GLU:OE1	5:QE:37:ARG:NE	2.35	0.56
34:Y9:22:ARG:HH12	35:YA:2741:A:H5''	1.71	0.56
35:YA:1466:G:HO2'	35:YA:1546:C:HO2'	1.50	0.56
25:Y0:51:VAL:O	48:YS:20:ARG:NH2	2.39	0.56
1:QA:1226:C:O2'	13:QM:111:LYS:NZ	2.34	0.56
35:RA:297:C:OP1	54:RY:87:LYS:NZ	2.38	0.56
50:RU:97:ASP:OD1	50:RU:101:ARG:NH1	2.38	0.56
55:RZ:126:VAL:HG12	55:RZ:163:LEU:HA	1.86	0.56
8:XH:9:MET:HG3	8:XH:26:VAL:HG11	1.87	0.56
1:QA:619:U:N3	4:QD:134:ASP:OD1	2.38	0.56
19:XS:50:ALA:HB1	19:XS:57:HIS:HB3	1.88	0.56
1:XA:1321:C:O2'	19:XS:78:ARG:NH1	2.39	0.56
38:YE:84:PHE:CE2	38:YE:86:PRO:CG	2.88	0.56
1:QA:7:G:O2'	5:QE:120:THR:O	2.23	0.56
12:QL:117:ARG:HB2	12:QL:122:THR:HB	1.86	0.56
38:RE:105:THR:OG1	38:RE:199:ARG:NH2	2.38	0.56
1:QA:345:C:OP2	49:RT:39:ARG:NH2	2.39	0.56
1:XA:1226:C:O2'	13:XM:111:LYS:NZ	2.37	0.56
4:QD:157:LEU:O	4:QD:161:ASN:ND2	2.38	0.56
35:RA:1466:G:HO2'	35:RA:1546:C:HO2'	1.54	0.56
2:XB:187:LEU:HA	2:XB:201:ILE:HB	1.87	0.56
1:XA:562:C:H1'	12:XL:15:ARG:HB3	1.88	0.56
29:Y4:53:GLU:HG3	29:Y4:56:VAL:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:2144:U:O2	35:YA:2148:G:N1	2.34	0.56
35:YA:615:G:OP1	39:YF:40:GLN:NE2	2.39	0.56
30:R5:19:ARG:NH2	35:RA:1264:G:OP1	2.38	0.55
1:XA:352:C:O2	1:XA:355:C:N4	2.39	0.55
2:XB:195:ASP:O	8:XH:68:ARG:NH2	2.39	0.55
20:XT:50:GLU:HB2	20:XT:99:LEU:HD22	1.88	0.55
50:YU:83:LEU:HD13	50:YU:88:ILE:HB	1.89	0.55
35:RA:1250:G:OP2	45:RP:21:ARG:NH1	2.39	0.55
35:RA:1266:G:O5'	52:RW:15:ARG:NH2	2.39	0.55
1:XA:662:G:O2'	1:XA:836:G:OP1	2.25	0.55
3:XC:184:TYR:CE1	3:XC:201:TYR:CE1	2.94	0.55
12:XL:71:PRO:O	12:XL:102:ARG:NH1	2.39	0.55
13:XM:19:LEU:HD11	13:XM:56:LEU:HD21	1.87	0.55
37:YD:72:LYS:NZ	37:YD:99:ASP:OD2	2.40	0.55
35:RA:1638:C:O2	35:RA:2698:U:O2'	2.24	0.55
35:RA:2635:C:O2'	38:RE:48:GLN:NE2	2.38	0.55
51:RV:21:ARG:HD3	51:RV:91:TYR:HE2	1.72	0.55
1:XA:1152:A:OP1	10:XJ:70:ARG:NH2	2.39	0.55
41:YH:124:GLU:HB2	41:YH:132:ARG:HB3	1.89	0.55
1:QA:1249:C:O2'	9:QI:73:GLN:NE2	2.39	0.55
1:QA:297:G:N2	1:QA:300:A:OP2	2.40	0.55
8:QH:9:MET:HG3	8:QH:26:VAL:HG11	1.87	0.55
35:RA:1066:U:O2'	35:RA:1068:G:OP2	2.21	0.55
35:RA:1721:G:H8	35:RA:1741:A:H62	1.53	0.55
38:RE:7:VAL:HG13	38:RE:51:PHE:HE2	1.72	0.55
49:RT:29:ARG:HB3	49:RT:87:ASP:HB2	1.88	0.55
39:YF:143:ALA:HB1	39:YF:148:LEU:HB2	1.87	0.55
44:YO:104:ARG:NH2	44:YO:121:VAL:O	2.38	0.55
24:QY:20:G:N2	24:QY:21:A:O2'	2.38	0.55
27:R2:16:LEU:HB3	27:R2:20:GLU:HG3	1.89	0.55
35:RA:526:A:O2'	35:RA:2043:C:O2	2.23	0.55
41:RH:86:GLU:OE2	41:RH:132:ARG:NH2	2.37	0.55
49:RT:65:LYS:HE3	49:RT:67:SER:HB2	1.89	0.55
3:XC:70:VAL:HG12	3:XC:72:LYS:H	1.72	0.55
11:XK:34:ASP:OD1	11:XK:38:ASN:N	2.40	0.55
32:Y7:24:THR:HG23	32:Y7:27:GLY:H	1.71	0.55
1:QA:1320:C:O2	19:QS:36:ARG:NH2	2.35	0.55
1:QA:922:G:H4'	5:QE:20:GLN:HA	1.88	0.55
35:RA:1246:A:OP1	39:RF:38:ARG:NH2	2.37	0.55
1:QA:1178:G:OP1	9:QI:93:ARG:NH1	2.40	0.55
1:QA:978:A:O2'	1:QA:1322:C:N3	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:QI:11:LYS:HA	9:QI:108:VAL:HG12	1.88	0.55
35:RA:919:G:N2	35:RA:2269:A:OP2	2.40	0.55
33:R8:43:GLN:NE2	35:RA:2365:G:O6	2.38	0.55
35:RA:604:G:OP2	45:RP:90:ARG:NH1	2.40	0.55
35:RA:993:G:OP1	50:RU:50:ARG:NH2	2.39	0.55
1:XA:1414:U:H3	1:XA:1486:G:H1	1.54	0.55
3:XC:184:TYR:HE1	3:XC:201:TYR:CE1	2.25	0.55
35:YA:918:A:N3	36:YB:80:U:O2'	2.40	0.55
37:YD:168:ARG:HG2	37:YD:173:VAL:HG12	1.89	0.55
1:QA:573:A:N3	1:QA:883:C:O2'	2.36	0.55
6:QF:41:GLU:OE1	18:QR:35:ARG:NH1	2.37	0.55
35:RA:2683:C:OP1	49:RT:53:ARG:NH2	2.34	0.55
35:RA:458:G:O2'	35:RA:469:G:O6	2.24	0.55
39:RF:40:GLN:HE22	39:RF:182:ASN:HB2	1.72	0.55
55:RZ:8:TYR:HB3	55:RZ:38:TYR:HE1	1.71	0.55
1:XA:79:G:H1	1:XA:90:U:H3	1.55	0.55
8:QH:41:ARG:NH2	8:QH:123:GLU:OE1	2.40	0.54
35:YA:2291:U:O2'	35:YA:2374:C:O2	2.24	0.54
35:YA:604:G:OP2	45:YP:90:ARG:NH1	2.39	0.54
38:YE:84:PHE:CE2	38:YE:86:PRO:HB3	2.42	0.54
9:QI:10:ARG:HG3	9:QI:11:LYS:H	1.72	0.54
35:RA:237:C:O2	35:RA:609:A:O2'	2.25	0.54
25:Y0:30:VAL:HG22	25:Y0:66:VAL:HG22	1.89	0.54
35:YA:451:C:OP1	39:YF:52:LYS:NZ	2.39	0.54
4:QD:20:TYR:HD2	4:QD:26:CYS:HB3	1.72	0.54
9:QI:49:PRO:HD2	9:QI:81:ILE:HD11	1.89	0.54
35:RA:861:A:N3	36:RB:79:C:O2'	2.40	0.54
35:YA:807:U:O2'	35:YA:2060:A:N1	2.41	0.54
35:YA:2788:C:O2'	35:YA:2809:A:N3	2.35	0.54
35:YA:613:G:N2	35:YA:614(D):A:O2'	2.40	0.54
44:YO:23:ARG:NH2	44:YO:28:SER:O	2.40	0.54
1:QA:261:U:OP2	20:QT:79:ARG:NH2	2.40	0.54
35:RA:600:G:N2	35:RA:605:C:O3'	2.40	0.54
35:RA:907:U:O2'	46:RQ:101:ARG:NH2	2.38	0.54
1:XA:67:C:O2'	1:XA:171:A:N3	2.35	0.54
6:XF:36:ARG:NH2	6:XF:38:GLU:OE2	2.41	0.54
1:QA:1003:G:H1	1:QA:1035:A:H61	1.56	0.54
1:QA:1484:C:HO2'	35:RA:1960:A:HO2'	1.48	0.54
35:RA:660:G:H4'	39:RF:99:TYR:CE2	2.34	0.54
46:RQ:32:TYR:CE1	46:RQ:133:ARG:HG3	2.42	0.54
1:XA:676:A:H1'	11:XK:115:PRO:HB3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Y7:34:ARG:HG3	32:Y7:39:ARG:HG3	1.90	0.54
38:YE:36:ARG:NH1	38:YE:85:ASN:OD1	2.41	0.54
1:QA:692:U:OP2	11:QK:26:ASN:ND2	2.37	0.54
7:QG:94:ARG:NH1	7:QG:98:SER:OG	2.41	0.54
35:RA:2115:G:N1	35:RA:2119:A:OP2	2.36	0.54
45:RP:29:LYS:HD3	45:RP:30:THR:HG23	1.89	0.54
1:XA:1101:A:N6	2:XB:176:GLU:OE2	2.40	0.54
1:XA:1060:C:OP1	14:XN:45:ARG:NH2	2.41	0.54
36:RB:117:G:H4'	48:RS:54:LEU:HD22	1.89	0.54
2:XB:74:LYS:NZ	2:XB:206:ASP:OD1	2.37	0.54
35:YA:1652:A:N6	47:YR:11:ASN:OD1	2.34	0.54
54:YY:47:LYS:NZ	54:YY:48:ALA:O	2.41	0.54
35:YA:2683:C:OP1	49:YT:53:ARG:NH2	2.36	0.54
46:YQ:137:TYR:HB3	55:YZ:76:LEU:HD11	1.90	0.54
37:RD:5:LYS:HG2	37:RD:17:THR:HG22	1.90	0.54
55:RZ:92:SER:OG	55:RZ:94:GLU:OE1	2.25	0.54
35:YA:307:G:N1	35:YA:310:A:OP2	2.39	0.54
1:XA:626:U:C5'	16:XP:38:TYR:HD2	2.21	0.54
40:YG:46:ALA:HB2	40:YG:53:LEU:HD12	1.90	0.54
2:QB:28:PHE:HD1	2:QB:194:PRO:HG3	1.73	0.53
35:RA:2012:G:OP1	52:RW:11:ARG:NH2	2.41	0.53
29:Y4:31:ILE:HG21	40:YG:142:PRO:HB2	1.89	0.53
46:YQ:32:TYR:CE1	46:YQ:133:ARG:HG3	2.43	0.53
5:QE:33:VAL:HG21	5:QE:109:ILE:HA	1.89	0.53
7:QG:15:ASP:OD1	7:QG:19:GLY:N	2.42	0.53
38:RE:176:ILE:HB	38:RE:181:LEU:HB2	1.90	0.53
44:RO:9:GLU:OE2	44:RO:18:LYS:NZ	2.39	0.53
2:XB:47:THR:OG1	2:XB:48:MET:N	2.39	0.53
34:Y9:16:VAL:HG22	34:Y9:25:VAL:HG22	1.90	0.53
35:YA:1754:C:N3	35:YA:2716:U:O2'	2.33	0.53
46:YQ:30:GLY:N	46:YQ:105:GLU:OE2	2.41	0.53
1:QA:1368:G:OP1	9:QI:111:ARG:NH2	2.41	0.53
35:RA:2245:U:H5''	35:RA:2246:G:H5'	1.91	0.53
1:XA:977:A:N6	1:XA:1224:G:OP1	2.35	0.53
3:XC:152:ILE:HD11	3:XC:199:LYS:HD2	1.89	0.53
4:XD:59:ARG:HH21	4:XD:62:GLN:HG3	1.71	0.53
20:XT:50:GLU:HG3	20:XT:100:ILE:HD11	1.90	0.53
25:Y0:77:ARG:NH2	35:YA:857:C:OP2	2.40	0.53
35:YA:1607:C:N4	35:YA:1622:G:OP2	2.34	0.53
45:YP:89:ALA:O	45:YP:121:LYS:NZ	2.38	0.53
35:YA:1066:U:O2'	35:YA:1068:G:OP2	2.21	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1398:C:OP1	53:RX:53:LYS:NZ	2.40	0.53
35:RA:2258:C:O2'	35:RA:2427:C:OP2	2.26	0.53
35:RA:2502:G:H5''	35:RA:2503:2MA:H5''	1.91	0.53
35:YA:2115:G:N1	35:YA:2119:A:OP2	2.41	0.53
39:YF:185:ASP:OD1	39:YF:188:ARG:NH1	2.41	0.53
4:QD:168:ARG:HH22	37:YD:134:ARG:HH21	1.57	0.53
35:RA:1788:C:OP1	37:RD:222:ARG:NH2	2.41	0.53
1:XA:578:C:O2'	1:XA:728:A:N3	2.38	0.53
1:XA:811:C:O2'	1:XA:901:A:N1	2.42	0.53
35:YA:300:A:OP1	54:YY:86:ARG:NH2	2.42	0.53
38:YE:2:LYS:HB2	38:YE:95:ILE:HD12	1.91	0.53
35:RA:1801:G:OP2	37:RD:154:LYS:NZ	2.42	0.53
39:RF:46:ARG:HG3	39:RF:48:THR:HG23	1.91	0.53
6:XF:99:ALA:HB2	18:XR:31:LEU:HD11	1.91	0.53
34:Y9:36:GLN:NE2	35:YA:1124:C:O2	2.42	0.53
52:YW:22:ASP:OD1	52:YW:25:ARG:NH1	2.38	0.53
1:QA:437:U:O2'	4:QD:123:HIS:ND1	2.39	0.53
16:QP:53:VAL:HG13	16:QP:79:VAL:HG12	1.90	0.53
35:RA:2572:A:OP1	35:RA:2574:G:O2'	2.25	0.53
1:XA:976:G:OP2	1:XA:1358:U:O2'	2.27	0.53
13:XM:99:ARG:HB2	13:XM:101:GLN:HE22	1.73	0.53
1:QA:662:G:O2'	1:QA:836:G:OP1	2.27	0.53
18:QR:32:ARG:HA	18:QR:69:THR:HG21	1.91	0.53
39:RF:117:ARG:NH2	39:RF:189:THR:O	2.42	0.53
4:XD:109:GLY:HA3	4:XD:165:MET:HG3	1.90	0.53
9:XI:7:THR:OG1	9:XI:83:ARG:NH1	2.39	0.53
42:YI:23:PRO:HB3	42:YI:27:ARG:HE	1.73	0.53
35:YA:2851:A:O2'	47:YR:64:ARG:NH2	2.41	0.53
24:QY:18:G:N2	24:QY:58:A:OP1	2.41	0.53
40:RG:32:PRO:HB2	40:RG:172:LEU:HD22	1.90	0.53
50:RU:89:GLU:O	51:RV:11:GLN:NE2	2.35	0.53
6:XF:33:TYR:HB2	6:XF:75:LEU:HD12	1.91	0.53
35:YA:600:G:N2	35:YA:605:C:O3'	2.42	0.53
39:YF:63:LYS:NZ	39:YF:75:HIS:O	2.38	0.53
8:QH:36:LEU:HD23	8:QH:39:LEU:HD12	1.91	0.52
31:R6:23:THR:OG1	31:R6:24:GLU:N	2.41	0.52
16:XP:20:VAL:HG23	16:XP:35:LYS:HA	1.91	0.52
35:YA:2404:C:O3'	45:YP:77:ARG:NH2	2.40	0.52
4:QD:98:GLU:HA	4:QD:103:ASN:HD22	1.75	0.52
7:QG:76:ARG:HD3	7:QG:89:MET:HG3	1.92	0.52
35:RA:1817:G:OP1	37:RD:88:ARG:NH2	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:574:C:N4	35:RA:2034:U:OP1	2.41	0.52
55:RZ:69:THR:OG1	55:RZ:70:LEU:N	2.42	0.52
1:XA:824:C:H2'	1:XA:825:G:H8	1.73	0.52
3:XC:39:ILE:HG23	3:XC:91:LEU:HD11	1.89	0.52
40:YG:161:THR:HG22	40:YG:163:ALA:H	1.74	0.52
35:RA:1693:U:O2'	37:RD:14:ARG:NH2	2.42	0.52
26:Y1:11:ARG:NH2	35:YA:1365:A:O2'	2.42	0.52
42:YI:92:VAL:HG23	42:YI:120:ILE:HB	1.91	0.52
1:QA:677:U:H3	1:QA:713:G:H22	1.58	0.52
46:RQ:31:ASP:N	46:RQ:106:VAL:O	2.42	0.52
30:Y5:16:ARG:NH1	30:Y5:17:ASP:OD1	2.43	0.52
1:QA:738:C:OP1	6:QF:4:TYR:OH	2.24	0.52
9:QI:48:GLU:HG3	9:QI:51:ARG:HH11	1.75	0.52
32:R7:39:ARG:NH2	35:RA:468:G:N7	2.51	0.52
47:RR:56:LYS:NZ	47:RR:90:ARG:O	2.43	0.52
54:RY:14:LEU:HB2	54:RY:75:ILE:HD11	1.92	0.52
1:XA:1030(D):G:H2'	1:XA:1030(E):A:H8	1.73	0.52
1:XA:486:U:H2'	1:XA:487:A:H8	1.74	0.52
35:YA:2033:A:O2'	35:YA:2035:G:OP2	2.24	0.52
44:YO:98:VAL:HG21	44:YO:114:ILE:HG23	1.92	0.52
2:QB:88:ALA:HB2	2:QB:219:VAL:HG13	1.92	0.52
5:QE:105:VAL:HG21	5:QE:128:PRO:HB3	1.90	0.52
35:RA:859:G:O2'	35:RA:916:G:O6	2.25	0.52
44:RO:98:VAL:HG21	44:RO:114:ILE:HG23	1.91	0.52
1:XA:413:G:N7	4:XD:35:ARG:NH1	2.57	0.52
9:XI:121:ARG:NH1	9:XI:122:ALA:O	2.43	0.52
19:XS:32:LYS:HA	19:XS:50:ALA:HB3	1.92	0.52
35:YA:805:G:N2	35:YA:829:A:OP1	2.40	0.52
40:YG:55:LYS:HZ1	40:YG:149:VAL:HA	1.75	0.52
1:QA:1003:G:N2	1:QA:1025:U:O4	2.42	0.52
1:QA:1286:A:H2'	1:QA:1287:A:H4'	1.91	0.52
1:QA:1438:G:OP2	20:QT:34:LYS:NZ	2.37	0.52
1:QA:157:G:H1	1:QA:164:U:H3	1.57	0.52
3:QC:20:SER:OG	3:QC:22:TRP:NE1	2.43	0.52
1:XA:950:U:H3	1:XA:1231:G:H1	1.58	0.52
35:YA:86:C:H4'	35:YA:104:U:H1'	1.92	0.52
38:YE:2:LYS:HG2	38:YE:200:GLU:HB2	1.92	0.52
44:YO:87:ILE:HD12	44:YO:91:LEU:HA	1.91	0.52
1:QA:954:G:H21	1:QA:1227:A:H62	1.57	0.52
52:YW:69:LEU:HB3	52:YW:107:LEU:HD23	1.90	0.52
35:RA:200:U:O2	35:RA:386:G:N2	2.43	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:RZ:103:ARG:HE	55:RZ:136:PHE:HD2	1.58	0.52
2:XB:88:ALA:HB2	2:XB:219:VAL:HG13	1.92	0.52
33:Y8:6:THR:HG22	33:Y8:63:PRO:HD2	1.92	0.52
35:YA:2313:C:O4'	40:YG:40:ASN:ND2	2.43	0.52
35:YA:641:C:O2'	35:YA:2350:C:OP1	2.23	0.52
35:YA:906:G:OP1	46:YQ:26:TYR:OH	2.22	0.52
35:YA:2602:A:C2'	35:YA:2602:A:N3	2.73	0.52
32:Y7:37:LYS:NZ	35:YA:468:G:OP2	2.42	0.52
35:YA:24:G:O2'	52:YW:78:GLU:O	2.26	0.52
1:QA:235:C:H2'	1:QA:236:G:H8	1.74	0.51
1:QA:742:G:OP2	15:QO:35:ARG:NH2	2.42	0.51
8:QH:36:LEU:HD12	8:QH:59:LEU:HD23	1.92	0.51
35:RA:1819:A:H5''	37:RD:161:THR:HG21	1.92	0.51
1:XA:35:G:N3	12:XL:118:SER:OG	2.42	0.51
35:YA:221:A:N1	35:YA:265:A:O2'	2.41	0.51
35:YA:2627:G:N2	35:YA:2777:G:OP2	2.42	0.51
53:YX:34:ALA:O	53:YX:77:LYS:NZ	2.42	0.51
1:QA:475:G:H2'	1:QA:476:G:H8	1.75	0.51
7:QG:26:PHE:HD1	7:QG:101:LEU:HD22	1.75	0.51
1:XA:1147:C:O2	9:XI:16:ARG:NH1	2.43	0.51
1:XA:1386:G:H2'	1:XA:1387:G:H8	1.75	0.51
1:XA:410:G:H21	1:XA:432:A:H62	1.59	0.51
1:XA:922:G:H4'	5:XE:20:GLN:HA	1.92	0.51
6:XF:37:VAL:HA	6:XF:65:VAL:HG12	1.91	0.51
30:Y5:29:THR:OG1	30:Y5:29:THR:O	2.26	0.51
39:YF:101:LEU:O	39:YF:106:ARG:NH1	2.42	0.51
1:QA:950:U:H3	1:QA:1231:G:H1	1.56	0.51
35:RA:577:G:O2'	35:RA:1254:A:OP1	2.27	0.51
35:RA:2133:G:O2'	35:RA:2158:A:N1	2.43	0.51
26:R1:76:ARG:O	35:RA:272(Q):G:O2'	2.28	0.51
43:RN:49:GLY:O	43:RN:119:ARG:NH1	2.43	0.51
35:YA:2306:C:N4	40:YG:42:GLY:O	2.43	0.51
47:YR:38:VAL:HG22	47:YR:112:ALA:HB2	1.91	0.51
51:YV:21:ARG:CD	51:YV:91:TYR:HE2	2.24	0.51
54:RY:83:THR:OG1	54:RY:84:ARG:N	2.44	0.51
1:XA:1077:G:N2	1:XA:1080:A:OP2	2.35	0.51
1:XA:390:C:O3'	16:XP:28:ARG:NH2	2.42	0.51
1:QA:339:C:OP2	44:RO:97:ARG:NH2	2.44	0.51
1:XA:73:G:H1	1:XA:96:U:H3	1.57	0.51
3:XC:153:VAL:HG22	3:XC:198:VAL:HG22	1.90	0.51
29:Y4:68:ARG:NH2	29:Y4:69:LYS:O	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:YD:148:GLU:HB3	37:YD:151:LYS:HD2	1.93	0.51
40:YG:4:ASP:OD2	40:YG:9:ARG:NH2	2.43	0.51
8:XH:81:HIS:N	8:XH:138:TRP:O	2.44	0.51
33:Y8:26:LYS:HD3	33:Y8:44:LYS:HA	1.93	0.51
34:Y9:25:VAL:HB	34:Y9:34:GLN:HB2	1.93	0.51
35:YA:1791:A:H4'	37:YD:206:LEU:HB2	1.92	0.51
43:YN:54:VAL:HB	43:YN:122:VAL:HG22	1.91	0.51
35:RA:2115:G:O2'	35:RA:2166:G:N2	2.43	0.51
49:RT:19:LEU:HD13	49:RT:86:ILE:HD12	1.92	0.51
9:XI:28:VAL:HG12	9:XI:63:ILE:HB	1.93	0.51
1:XA:401:C:OP2	4:XD:73:ARG:NH2	2.43	0.51
1:XA:403:C:OP2	4:XD:74:GLN:NE2	2.44	0.51
1:XA:993:G:O2'	1:XA:994:A:N7	2.43	0.51
1:XA:1525:G:OP1	11:XK:120:ARG:NH2	2.44	0.51
13:XM:65:LYS:HB2	13:XM:69:GLU:HB3	1.93	0.51
35:YA:116:C:O2'	35:YA:126:A:N3	2.37	0.51
5:QE:102:ALA:HB3	5:QE:107:ARG:HB2	1.93	0.51
16:QP:19:ILE:HB	16:QP:37:GLY:HA3	1.92	0.51
35:RA:2144:U:HO2'	35:RA:2147:G:H1	1.57	0.51
35:RA:453:C:O2	35:RA:457:A:O2'	2.28	0.51
7:XG:113:GLU:HB2	7:XG:119:ARG:HG2	1.92	0.51
16:XP:8:ARG:NH2	16:XP:11:SER:O	2.44	0.51
35:YA:1266:G:O5'	52:YW:15:ARG:NH2	2.44	0.51
40:YG:37:VAL:HG22	40:YG:159:VAL:HG12	1.93	0.51
46:YQ:22:LYS:O	55:YZ:78:LYS:NZ	2.44	0.51
47:RR:33:ARG:NH2	47:RR:115:GLU:OE1	2.42	0.51
55:RZ:77:ASP:OD2	55:RZ:80:ARG:NH1	2.40	0.51
1:XA:376:G:H1	1:XA:387:U:H3	1.59	0.51
9:XI:53:VAL:HG23	9:XI:55:ALA:H	1.76	0.51
1:QA:642:A:N3	8:QH:113:SER:OG	2.44	0.50
1:QA:1123:A:H4'	10:QJ:36:GLY:HA3	1.93	0.50
29:R4:5:ILE:HD12	40:RG:67:LYS:HE2	1.92	0.50
39:RF:185:ASP:OD1	39:RF:188:ARG:NH1	2.42	0.50
25:Y0:27:GLU:HG3	25:Y0:68:GLU:HA	1.94	0.50
39:YF:62:ARG:HD2	39:YF:63:LYS:O	2.10	0.50
46:YQ:30:GLY:HA2	46:YQ:107:ALA:HB2	1.94	0.50
1:QA:765:G:N1	1:QA:812:C:O2'	2.38	0.50
1:QA:1101:A:N6	2:QB:176:GLU:OE2	2.44	0.50
35:RA:1056:G:H21	35:RA:1103:A:H62	1.59	0.50
5:XE:48:ALA:HB2	5:XE:57:LYS:HD3	1.93	0.50
35:YA:2302:G:N2	40:YG:126:ASP:OD1	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:175:LEU:HD21	3:QC:201:TYR:HE2	1.76	0.50
5:QE:33:VAL:HG13	5:QE:112:LEU:HD22	1.92	0.50
6:QF:11:ASN:HB3	6:QF:14:LEU:HG	1.93	0.50
37:RD:148:GLU:HB3	37:RD:151:LYS:HD2	1.93	0.50
41:RH:7:LEU:O	41:RH:69:ARG:NE	2.43	0.50
43:RN:22:THR:HB	43:RN:25:ARG:HB2	1.93	0.50
52:RW:86:LEU:HD22	52:RW:96:ILE:HD11	1.93	0.50
22:XV:33:U:N3	22:XV:36:U:OP2	2.31	0.50
33:Y8:14:VAL:HG12	33:Y8:24:ALA:HB2	1.93	0.50
35:YA:1426:G:O2'	35:YA:1572:A:N6	2.45	0.50
48:YS:10:ARG:HG3	48:YS:13:ARG:HH21	1.76	0.50
1:QA:1393:U:HO2'	1:QA:1501:C:HO2'	1.53	0.50
35:RA:2291:U:O2'	35:RA:2374:C:O2	2.28	0.50
46:RQ:30:GLY:HA2	46:RQ:107:ALA:HB2	1.92	0.50
26:Y1:4:VAL:HG12	26:Y1:11:ARG:HG2	1.94	0.50
35:RA:1779:U:OP2	35:RA:1784:A:N6	2.34	0.50
35:RA:2199:A:N1	35:RA:2226:C:N4	2.57	0.50
30:Y5:41:PRO:O	30:Y5:44:THR:OG1	2.30	0.50
35:YA:955:C:OP1	46:YQ:87:LYS:NZ	2.40	0.50
39:YF:46:ARG:HB3	39:YF:48:THR:HG23	1.94	0.50
10:QJ:53:PRO:O	14:QN:41:ARG:NH2	2.44	0.50
1:QA:626:U:H5''	16:QP:38:TYR:CD2	2.45	0.50
26:R1:50:ARG:HG2	26:R1:59:THR:HG22	1.93	0.50
35:RA:2816:C:O2	35:RA:2883:A:O2'	2.29	0.50
1:XA:978:A:OP2	1:XA:1363(A):C:N4	2.43	0.50
39:YF:168:ARG:HG2	39:YF:175:THR:HG21	1.93	0.50
2:QB:88:ALA:O	2:QB:226:ARG:NH2	2.45	0.50
11:QK:32:ILE:HG13	11:QK:72:ALA:HB2	1.94	0.50
33:R8:12:LYS:NZ	35:RA:249:C:O2	2.40	0.50
2:XB:121:LEU:HD23	2:XB:127:ILE:HD12	1.94	0.50
2:XB:84:GLU:HB3	2:XB:219:VAL:HG21	1.92	0.50
39:YF:155:LEU:HD23	39:YF:192:LEU:HD13	1.93	0.50
35:YA:1223:G:O6	51:YV:69:LYS:NZ	2.44	0.50
1:QA:1149:C:OP2	9:QI:9:ARG:NH2	2.45	0.50
35:RA:221:A:N1	35:RA:265:A:O2'	2.44	0.50
43:RN:15:LEU:HB2	43:RN:135:PRO:HB2	1.93	0.50
1:XA:1330:U:H4'	13:XM:23:TYR:CE1	2.46	0.50
1:XA:618:C:H5'	1:XA:619:U:H5''	1.94	0.50
26:Y1:3:LYS:HB2	26:Y1:61:ARG:HH11	1.77	0.50
29:Y4:1:MET:SD	40:YG:98:ARG:NH1	2.85	0.50
35:RA:693:C:O2'	35:RA:1353:A:N3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:1005:A:O3'	1:XA:1037:C:O2'	2.30	0.50
35:YA:1801:G:OP2	37:YD:154:LYS:NZ	2.44	0.50
35:YA:996:A:OP2	50:YU:93:LYS:NZ	2.39	0.50
1:QA:975:A:H4'	1:QA:976:G:H5''	1.93	0.49
18:QR:23:LYS:HD2	18:QR:58:LEU:HD23	1.94	0.49
35:RA:299:A:N3	35:RA:319:C:O2'	2.45	0.49
6:XF:11:ASN:HB3	6:XF:14:LEU:HG	1.94	0.49
35:YA:601:C:O2'	35:YA:605:C:OP1	2.28	0.49
1:QA:278:G:OP2	17:QQ:92:ARG:NH2	2.40	0.49
1:QA:993:G:O2'	1:QA:994:A:N7	2.44	0.49
35:RA:2882:A:H5'	47:RR:96:ARG:HG3	1.93	0.49
1:XA:757:U:O2'	1:XA:879:C:O2	2.30	0.49
8:XH:41:ARG:NH2	8:XH:123:GLU:OE2	2.45	0.49
35:YA:458:G:O2'	35:YA:469:G:O6	2.24	0.49
54:YY:20:TYR:HB3	54:YY:23:ARG:HG3	1.94	0.49
1:QA:769:G:H4'	1:QA:1513:A:H4'	1.93	0.49
1:QA:953:G:N7	13:QM:104:ARG:NH2	2.53	0.49
35:RA:1853:A:N3	35:RA:2233:U:O2'	2.41	0.49
44:RO:19:ILE:HG22	44:RO:43:VAL:HA	1.93	0.49
35:YA:1098:A:H3'	35:YA:1099:G:H8	1.77	0.49
35:YA:2875:C:OP1	49:YT:3:ARG:NH1	2.45	0.49
38:YE:7:VAL:HG23	38:YE:51:PHE:HE2	1.77	0.49
52:YW:86:LEU:HD22	52:YW:96:ILE:HD11	1.95	0.49
54:YY:14:LEU:HB2	54:YY:75:ILE:HD11	1.92	0.49
1:QA:410:G:H21	1:QA:432:A:H62	1.59	0.49
13:QM:24:GLY:O	13:QM:29:ARG:NH1	2.46	0.49
35:RA:392:C:H5''	35:RA:409:C:H5''	1.93	0.49
35:YA:2680:C:H5'	38:YE:189:PRO:HA	1.95	0.49
39:YF:11:VAL:HG22	39:YF:125:LEU:HB2	1.93	0.49
1:QA:1069:C:O2'	1:QA:1192:C:O2	2.27	0.49
35:RA:831:G:O2'	45:RP:38:GLN:OE1	2.27	0.49
1:XA:1129:C:OP1	9:XI:16:ARG:NH1	2.46	0.49
10:XJ:11:PHE:HE1	10:XJ:67:THR:HG22	1.77	0.49
35:YA:1047:G:H21	35:YA:1111:A:H62	1.59	0.49
1:QA:1255:G:OP2	10:QJ:45:ARG:NH2	2.45	0.49
35:RA:1309:G:HO2'	35:RA:1611:C:HO2'	1.56	0.49
18:XR:32:ARG:HA	18:XR:69:THR:HG21	1.94	0.49
39:YF:6:VAL:N	39:YF:22:ALA:O	2.45	0.49
35:YA:1277:G:O2'	47:YR:24:GLN:OE1	2.23	0.49
53:YX:59:VAL:HB	53:YX:76:ARG:HG3	1.95	0.49
1:QA:407:G:H5''	4:QD:115:ARG:HG2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:QD:88:VAL:HA	5:QE:97:GLY:HA3	1.94	0.49
35:RA:1490:A:O2'	37:RD:99:ASP:OD1	2.30	0.49
1:XA:1098:C:OP2	2:XB:144:ARG:NH1	2.46	0.49
35:YA:994:C:OP1	50:YU:53:ARG:NH2	2.45	0.49
2:XB:122:PHE:CE2	2:XB:139:LYS:HD3	2.43	0.49
2:XB:69:LEU:HB3	2:XB:162:ILE:HG22	1.95	0.49
31:Y6:21:TYR:OH	35:YA:2347:C:O2'	2.30	0.49
1:QA:1219:U:OP1	14:QN:19:ARG:NH2	2.46	0.49
8:QH:91:ARG:NE	17:QQ:32:TYR:O	2.45	0.49
9:QI:118:LYS:HB2	9:QI:121:ARG:HB3	1.93	0.49
29:R4:31:ILE:HG21	40:RG:142:PRO:HB2	1.95	0.49
33:Y8:26:LYS:HD3	33:Y8:44:LYS:HG2	1.94	0.49
57:QA:1821:PAR:O44	57:QA:1821:PAR:N64	2.44	0.49
25:R0:32:ARG:H	25:R0:35:ASN:ND2	2.09	0.49
35:RA:1022:G:N2	35:RA:1023:U:O4	2.41	0.49
39:RF:165:ARG:HG3	39:RF:168:ARG:HH12	1.78	0.49
51:RV:72:VAL:HG13	51:RV:85:LYS:HB3	1.94	0.49
1:XA:792:A:O2'	1:XA:794:A:N7	2.40	0.49
2:XB:16:HIS:HB2	2:XB:204:ASN:HB3	1.94	0.49
13:XM:102:ARG:NH2	13:XM:105:THR:OG1	2.43	0.49
13:XM:23:TYR:HE2	13:XM:71:ARG:HG2	1.78	0.49
41:YH:159:GLU:HG2	41:YH:169:VAL:HG11	1.94	0.49
1:QA:380:G:N2	1:QA:383:A:OP2	2.39	0.48
1:QA:401:C:O2'	1:QA:621:A:N3	2.42	0.48
39:RF:167:ALA:HB1	39:RF:173:VAL:HG11	1.95	0.48
45:RP:89:ALA:O	45:RP:121:LYS:NZ	2.36	0.48
8:XH:34:GLU:OE1	8:XH:37:ARG:NH2	2.46	0.48
12:XL:113:ARG:HH21	12:XL:116:SER:HG	1.61	0.48
6:XF:50:TYR:CE1	18:XR:77:GLY:HA2	2.43	0.48
39:YF:62:ARG:HD2	39:YF:63:LYS:C	2.33	0.48
44:YO:16:ALA:HA	44:YO:46:ALA:HA	1.94	0.48
1:QA:811:C:O2'	1:QA:901:A:N1	2.46	0.48
34:R9:25:VAL:HB	34:R9:34:GLN:HB2	1.94	0.48
33:R8:27:THR:HG22	45:RP:63:PRO:HD3	1.94	0.48
1:XA:1458:G:OP1	20:XT:35:THR:OG1	2.31	0.48
1:QA:978:A:H61	1:QA:1316:G:H1'	1.78	0.48
1:QA:663:A:H61	1:QA:742:G:H1	1.59	0.48
3:QC:191:THR:OG1	3:QC:194:GLY:O	2.27	0.48
13:QM:8:GLU:OE2	13:QM:11:ARG:NH1	2.46	0.48
35:RA:271:A:N3	35:RA:365:C:O2'	2.43	0.48
45:RP:19:VAL:HG12	45:RP:27:HIS:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:126:GLU:O	2:XB:130:ARG:NH1	2.46	0.48
14:YN:24:CYS:HB3	14:YN:29:ARG:H	1.78	0.48
3:XC:9:GLY:HA3	14:YN:49:HIS:HA	1.95	0.48
39:YF:167:ALA:HA	39:YF:170:LEU:HD23	1.95	0.48
2:QB:27:LYS:O	2:QB:30:ARG:NH1	2.46	0.48
6:QF:37:VAL:HA	6:QF:65:VAL:HG12	1.95	0.48
35:RA:1043:C:HO2'	35:RA:1048:A:HO2'	1.61	0.48
3:XC:152:ILE:HG12	3:XC:199:LYS:HB2	1.94	0.48
35:YA:1022:G:N2	35:YA:1023:U:O4	2.40	0.48
35:YA:1657:C:OP1	38:YE:136:ARG:N	2.46	0.48
37:RD:168:ARG:HG2	37:RD:173:VAL:HG12	1.95	0.48
52:RW:18:ARG:NH1	52:RW:76:VAL:O	2.46	0.48
1:QA:978:A:OP2	1:QA:1363(A):C:N4	2.42	0.48
29:R4:18:CYS:SG	29:R4:20:ASN:ND2	2.87	0.48
35:RA:1082:U:O4	35:RA:1086:A:N6	2.47	0.48
35:RA:2033:A:O2'	35:RA:2035:G:OP2	2.25	0.48
42:RI:4:ILE:HG12	42:RI:18:VAL:HG22	1.95	0.48
51:RV:21:ARG:HD3	51:RV:91:TYR:CE2	2.48	0.48
28:Y3:8:LEU:HD13	28:Y3:23:LEU:HD11	1.95	0.48
7:QG:57:GLU:HG3	7:QG:60:LYS:H	1.79	0.48
39:RF:164:ARG:HG3	39:RF:175:THR:HB	1.96	0.48
41:RH:3:ARG:HE	41:RH:4:ILE:H	1.62	0.48
1:XA:1309:G:N7	13:XM:99:ARG:NH2	2.61	0.48
10:XJ:9:ARG:HG2	10:XJ:69:ASN:HD22	1.79	0.48
35:YA:139(A):G:H21	53:YX:41:ASN:HD21	1.61	0.48
35:YA:919:G:N2	35:YA:2269:A:OP2	2.46	0.48
1:QA:1414:U:H3	1:QA:1486:G:H1	1.61	0.48
35:RA:220:G:O2'	35:RA:233:A:N3	2.40	0.48
44:RO:16:ALA:HA	44:RO:46:ALA:HA	1.95	0.48
51:RV:41:GLY:HA2	51:RV:45:THR:HA	1.95	0.48
35:YA:1682:G:OP1	35:YA:1699:G:N1	2.46	0.48
35:YA:223:A:O2'	35:YA:420:C:O2	2.29	0.48
44:YO:1:MET:HG3	44:YO:67:LYS:HG2	1.95	0.48
54:YY:39:VAL:HB	54:YY:42:VAL:HB	1.96	0.48
33:R8:26:LYS:HD3	33:R8:44:LYS:HG2	1.95	0.48
35:RA:307:G:N1	35:RA:310:A:OP2	2.47	0.48
37:RD:71:ASP:HB2	37:RD:103:ARG:HH12	1.79	0.48
1:XA:1085:U:H5''	1:XA:1086:U:H5	1.79	0.48
1:XA:280:C:OP1	17:XQ:91:ARG:NH1	2.43	0.48
6:XF:80:ARG:NH1	6:XF:88:VAL:O	2.47	0.48
35:YA:1568:G:H5''	37:YD:61:LEU:HG	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:861:A:N3	36:YB:79:C:O2'	2.45	0.48
39:YF:167:ALA:HB1	39:YF:173:VAL:HG11	1.96	0.48
35:RA:579:G:O2'	35:RA:2019:A:OP1	2.30	0.48
38:RE:134:ILE:HA	38:RE:137:HIS:HD2	1.77	0.48
35:RA:2751:G:H4'	41:RH:4:ILE:HD11	1.96	0.48
1:XA:380:G:N2	1:XA:383:A:OP2	2.35	0.48
17:XQ:28:PRO:HA	17:XQ:35:VAL:HA	1.96	0.48
41:YH:154:PRO:HB3	41:YH:163:TYR:CZ	2.48	0.48
49:YT:34:VAL:O	49:YT:41:ARG:N	2.43	0.48
55:YZ:69:THR:HG22	55:YZ:90:VAL:HA	1.95	0.48
16:QP:20:VAL:HG23	16:QP:35:LYS:HA	1.95	0.47
35:RA:1155:A:P	50:RU:55:ARG:HG2	2.54	0.47
3:XC:8:ILE:HG23	3:XC:16:ARG:HE	1.78	0.47
1:XA:718:G:O6	18:XR:74:ARG:NH1	2.47	0.47
27:Y2:22:GLU:OE2	27:Y2:68:ARG:NH2	2.47	0.47
35:YA:2572:A:OP1	35:YA:2574:G:O2'	2.30	0.47
1:QA:1261:A:H62	1:QA:1274:G:H21	1.62	0.47
9:QI:46:ALA:HB2	9:QI:74:ILE:HG23	1.95	0.47
27:R2:22:GLU:OE2	27:R2:68:ARG:NH2	2.46	0.47
35:RA:1657:C:OP1	38:RE:136:ARG:N	2.47	0.47
35:RA:918:A:N3	36:RB:80:U:O2'	2.46	0.47
35:RA:2574:G:N3	38:RE:143:ASN:ND2	2.61	0.47
45:RP:47:ASP:OD2	45:RP:49:ARG:NH2	2.43	0.47
35:YA:535:C:O3'	50:YU:53:ARG:NH1	2.47	0.47
37:YD:5:LYS:HG2	37:YD:17:THR:HG22	1.96	0.47
44:YO:80:ASP:OD2	49:YT:64:ARG:NH2	2.47	0.47
49:YT:73:GLU:OE2	49:YT:103:ARG:NH2	2.46	0.47
1:QA:1172:C:H2'	1:QA:1173:G:H8	1.79	0.47
1:QA:1422:G:O3'	44:RO:49:ARG:NH1	2.46	0.47
1:QA:376:G:H1	1:QA:387:U:H3	1.62	0.47
35:RA:1859:A:N6	35:RA:1883:G:O2'	2.46	0.47
25:Y0:33:ALA:N	25:Y0:64:ASP:OD1	2.45	0.47
35:YA:1798:U:OP2	37:YD:274:ARG:NH2	2.42	0.47
35:YA:1490:A:O2'	37:YD:99:ASP:OD1	2.29	0.47
35:YA:1250:G:OP2	45:YP:21:ARG:NH1	2.47	0.47
35:RA:1155:A:OP1	50:RU:55:ARG:HG2	2.14	0.47
32:R7:37:LYS:NZ	35:RA:468:G:OP2	2.47	0.47
37:RD:183:ARG:HG3	37:RD:270:ILE:HG12	1.96	0.47
44:RO:1:MET:HG3	44:RO:67:LYS:HG2	1.95	0.47
5:XE:94:ALA:HB1	5:XE:98:THR:HG21	1.97	0.47
25:Y0:32:ARG:H	25:Y0:35:ASN:ND2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:YE:144:ARG:HB3	38:YE:145:LYS:H	1.51	0.47
29:R4:37:SER:HB2	40:RG:108:ASN:HA	1.95	0.47
35:RA:660:G:H5''	39:RF:99:TYR:CD2	2.47	0.47
48:RS:27:SER:HA	48:RS:88:ASP:HB3	1.96	0.47
4:XD:68:TYR:OH	4:XD:98:GLU:OE2	2.21	0.47
10:XJ:50:ILE:HB	14:XN:41:ARG:HE	1.79	0.47
35:YA:2853:C:H2'	35:YA:2854:G:H8	1.79	0.47
38:YE:104:VAL:HG22	38:YE:198:VAL:HG22	1.97	0.47
40:YG:106:LEU:HA	40:YG:110:ALA:HB3	1.96	0.47
1:QA:1442(B):G:C8	49:RT:118:ARG:HG2	2.50	0.47
22:QV:16:C:H4'	22:QV:17(A):U:H5''	1.95	0.47
35:RA:2144:U:O2	35:RA:2148:G:N1	2.43	0.47
46:RQ:39:PRO:HB3	46:RQ:99:PRO:HD3	1.96	0.47
53:RX:59:VAL:HB	53:RX:76:ARG:HG3	1.96	0.47
9:XI:19:LEU:HB3	9:XI:59:PHE:HD2	1.79	0.47
27:Y2:48:HIS:ND1	35:YA:95:G:O2'	2.37	0.47
1:QA:123:C:OP1	1:QA:311:C:O2'	2.27	0.47
1:QA:593:G:H1	1:QA:646:U:H3	1.63	0.47
7:QG:51:GLN:NE2	7:QG:56:GLN:O	2.47	0.47
8:QH:85:ARG:NE	8:QH:87:SER:O	2.30	0.47
3:XC:58:GLU:HB3	10:XJ:92:THR:HG21	1.95	0.47
1:QA:562:C:H1'	12:QL:15:ARG:HB3	1.96	0.47
7:QG:28:ASN:OD1	7:QG:36:LYS:NZ	2.48	0.47
20:QT:50:GLU:HG3	20:QT:100:ILE:HD11	1.95	0.47
25:R0:27:GLU:HG3	25:R0:68:GLU:HA	1.96	0.47
34:R9:16:VAL:HG22	34:R9:25:VAL:HG22	1.96	0.47
1:XA:235:C:H2'	1:XA:236:G:H8	1.79	0.47
1:XA:261:U:OP2	20:XT:79:ARG:NH2	2.48	0.47
2:XB:71:VAL:HA	2:XB:93:VAL:HG22	1.97	0.47
26:Y1:18:ILE:HG12	26:Y1:37:ILE:HG12	1.97	0.47
35:YA:463:G:N2	35:YA:466:A:OP2	2.39	0.47
44:YO:19:ILE:HG22	44:YO:43:VAL:HA	1.97	0.47
49:YT:24:PRO:HA	49:YT:49:VAL:HG13	1.97	0.47
1:QA:1005:A:O2'	1:QA:1036:G:N2	2.47	0.47
1:QA:1358:U:H5''	14:QN:34:TYR:HA	1.95	0.47
35:RA:1074:G:C2	35:RA:1075:C:H1'	2.50	0.47
46:RQ:26:TYR:O	46:RQ:67:ARG:NH1	2.43	0.47
16:XP:38:TYR:CE1	16:XP:50:LYS:CB	2.97	0.47
27:Y2:55:ARG:HH12	35:YA:74:A:H5'	1.80	0.47
22:QV:56:C:O2	40:RG:78:SER:OG	2.32	0.47
33:R8:26:LYS:HD3	33:R8:44:LYS:HA	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:R9:1:MET:SD	34:R9:35:ARG:HB2	2.55	0.47
25:R0:43:THR:HG22	35:RA:2336:A:H61	1.79	0.47
1:XA:949:A:N7	13:XM:106:ASN:ND2	2.63	0.47
13:XM:94:ARG:HB3	13:XM:96:LEU:HD13	1.96	0.47
16:XP:8:ARG:NH1	16:XP:9:PHE:O	2.48	0.47
35:YA:530:G:N1	35:YA:2023:G:OP1	2.37	0.47
35:YA:184:C:O2'	35:YA:217:G:N3	2.42	0.47
38:YE:134:ILE:HA	38:YE:137:HIS:HD2	1.80	0.47
1:QA:73:G:H1	1:QA:96:U:H3	1.63	0.47
35:RA:321:G:O2'	35:RA:340:A:N3	2.46	0.47
35:RA:854:G:H2'	35:RA:855:G:H8	1.80	0.47
18:XR:23:LYS:HD2	18:XR:58:LEU:HD23	1.97	0.47
1:XA:1220:G:N2	19:XS:54:GLY:O	2.46	0.47
35:YA:745:G:O6	35:YA:746:A:N6	2.48	0.47
51:YV:21:ARG:NE	51:YV:91:TYR:CE2	2.79	0.47
52:YW:35:ILE:O	52:YW:39:THR:OG1	2.29	0.47
1:QA:689:C:OP1	11:QK:27:ASN:ND2	2.44	0.46
4:QD:166:LYS:HD2	4:QD:178:VAL:HG11	1.97	0.46
19:QS:40:ILE:HG22	19:QS:67:VAL:HG13	1.97	0.46
24:QY:75:C:O2	35:RA:2507:C:O2'	2.29	0.46
1:XA:975:A:H4'	1:XA:976:G:H5''	1.96	0.46
35:YA:2405:G:O2'	35:YA:2411:A:N6	2.45	0.46
35:YA:2680:C:O2'	38:YE:11:MET:SD	2.72	0.46
37:YD:71:ASP:HB2	37:YD:103:ARG:HH12	1.80	0.46
45:YP:88:LEU:HD11	45:YP:114:ILE:HD12	1.98	0.46
1:QA:932:C:H5''	7:QG:4:ARG:HE	1.80	0.46
3:QC:184:TYR:HD1	3:QC:201:TYR:CD1	2.34	0.46
20:QT:43:LEU:HD13	20:QT:51:GLU:HB3	1.97	0.46
30:R5:12:SER:HB3	35:RA:2020:A:H5'	1.98	0.46
1:XA:1330:U:H5'	13:XM:23:TYR:HD1	1.80	0.46
1:XA:634:C:H2'	1:XA:635:G:H8	1.80	0.46
6:XF:46:ARG:HH21	18:XR:78:LEU:HD22	1.80	0.46
10:XJ:6:ILE:HB	10:XJ:72:VAL:HG13	1.97	0.46
12:XL:57:LYS:HE3	12:XL:65:GLU:HG2	1.96	0.46
16:QP:32:TYR:CE2	16:QP:35:LYS:HB2	2.51	0.46
45:RP:20:GLY:HA2	45:RP:28:GLY:HA2	1.98	0.46
49:RT:27:THR:HG22	49:RT:48:ILE:HG12	1.96	0.46
12:XL:5:PRO:HD2	12:XL:15:ARG:HH22	1.80	0.46
35:YA:2816:C:O2	35:YA:2883:A:O2'	2.29	0.46
35:YA:793:A:OP2	35:YA:2071:A:O2'	2.33	0.46
39:YF:157:VAL:HG22	39:YF:176:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:345:C:OP2	49:YT:39:ARG:NH2	2.47	0.46
3:QC:71:ALA:HA	3:QC:106:VAL:HG22	1.96	0.46
35:RA:1288:U:O2'	35:RA:1647:G:N2	2.47	0.46
35:RA:2483:C:N3	46:RQ:124:LYS:NZ	2.55	0.46
46:RQ:13:GLN:O	46:RQ:72:LYS:NZ	2.33	0.46
1:XA:1414:U:H2'	1:XA:1415:G:H8	1.80	0.46
1:XA:619:U:N3	4:XD:134:ASP:OD1	2.38	0.46
35:YA:2503:2MA:O2'	35:YA:2505:G:OP2	2.25	0.46
38:YE:84:PHE:CZ	38:YE:86:PRO:HB3	2.51	0.46
1:QA:35:G:N3	12:QL:118:SER:OG	2.48	0.46
35:RA:2105:C:H2'	35:RA:2106:G:C8	2.51	0.46
35:RA:2689:U:H4'	35:RA:2690:C:H5'	1.97	0.46
51:RV:49:THR:O	51:RV:51:VAL:N	2.49	0.46
1:XA:1251:A:N3	1:XA:1369:C:O2'	2.41	0.46
1:XA:867:G:O2'	1:XA:873:A:N1	2.43	0.46
4:XD:63:LYS:HD2	4:XD:198:VAL:HG12	1.97	0.46
5:XE:76:ILE:HG13	5:XE:93:PRO:HG3	1.96	0.46
8:XH:110:ALA:HB3	8:XH:121:ASP:HB3	1.97	0.46
16:XP:43:LYS:HG2	16:XP:48:TRP:CD2	2.51	0.46
35:YA:2304:G:H22	35:YA:2312:U:H3	1.61	0.46
35:YA:2685:G:H5'	44:YO:68:GLU:OE2	2.15	0.46
55:YZ:108:PRO:HG2	55:YZ:117:LEU:HD21	1.96	0.46
1:QA:1329:A:N7	21:QU:7:ARG:NH2	2.63	0.46
35:RA:2478:A:O2'	35:RA:2536:G:N2	2.49	0.46
35:RA:521:G:H2'	35:RA:522:G:H8	1.81	0.46
1:XA:486:U:H2'	1:XA:487:A:C8	2.50	0.46
1:XA:689:C:OP1	11:XK:27:ASN:ND2	2.48	0.46
1:XA:769:G:OP2	1:XA:803:G:O2'	2.32	0.46
8:XH:33:GLU:HG2	8:XH:59:LEU:HD21	1.96	0.46
11:XK:18:ARG:NH2	11:XK:35:PRO:O	2.48	0.46
14:XN:29:ARG:HG2	14:XN:31:ARG:H	1.80	0.46
35:YA:1815:A:OP2	37:YD:54:ARG:NH2	2.42	0.46
43:YN:12:ARG:NH1	43:YN:50:ASP:OD2	2.48	0.46
35:YA:1666:G:HO2'	44:YO:6:THR:HG1	1.57	0.46
52:YW:14:PRO:HG2	52:YW:78:GLU:HG2	1.98	0.46
2:QB:68:ILE:HD12	2:QB:161:ALA:HB3	1.96	0.46
9:QI:10:ARG:NH1	9:QI:105:ASP:OD2	2.48	0.46
10:QJ:12:ASP:HB3	10:QJ:15:THR:HG22	1.98	0.46
35:RA:1084:A:H8	35:RA:1085:A:H4'	1.80	0.46
35:RA:530:G:N1	35:RA:2023:G:OP1	2.36	0.46
35:RA:2711:A:H5''	35:RA:2712(A):U:H5''	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:2788:C:OP1	38:RE:61:ARG:NH2	2.49	0.46
33:R8:7:HIS:CD2	45:RP:50:ARG:HD3	2.51	0.46
1:XA:1498:UR3:OP2	23:XX:16:A:O2'	2.32	0.46
44:YO:8:LEU:HB2	44:YO:19:ILE:HG13	1.97	0.46
46:YQ:43:THR:HG22	46:YQ:94:VAL:HG12	1.98	0.46
1:QA:824:C:H2'	1:QA:825:G:H8	1.81	0.46
35:RA:2059:A:HO2'	39:RF:69:HIS:HD1	1.63	0.46
39:RF:6:VAL:N	39:RF:22:ALA:O	2.48	0.46
41:RH:3:ARG:HE	41:RH:5:GLY:H	1.64	0.46
41:RH:7:LEU:HD22	41:RH:69:ARG:HH21	1.80	0.46
1:XA:1518:MA6:O5'	1:XA:1518:MA6:H8	2.15	0.46
28:Y3:51:ALA:HA	28:Y3:54:VAL:HG12	1.98	0.46
35:YA:630:G:N2	35:YA:633:A:OP2	2.41	0.46
37:YD:108:PRO:HA	37:YD:196:VAL:HA	1.97	0.46
1:QA:1222:G:H5''	19:QS:78:ARG:HD2	1.97	0.46
7:QG:79:ARG:HA	7:QG:84:ASN:HA	1.98	0.46
9:QI:9:ARG:HB2	9:QI:104:ARG:HE	1.81	0.46
35:RA:1007:C:H5''	43:RN:35:ARG:NH1	2.31	0.46
35:RA:2521:C:O2'	35:RA:2564:A:N3	2.45	0.46
35:RA:660:G:OP1	39:RF:99:TYR:HD2	1.99	0.46
43:RN:94:HIS:HB3	43:RN:97:ARG:HD3	1.98	0.46
35:RA:2295:C:OP1	48:RS:10:ARG:NH1	2.49	0.46
1:XA:1000:U:H2'	1:XA:1001(A):A:H8	1.78	0.46
19:XS:68:GLY:H	29:Y4:58:ARG:HH12	1.63	0.46
35:YA:1423:G:H2'	35:YA:1424:G:H8	1.81	0.46
26:R1:3:LYS:HB3	26:R1:61:ARG:HH22	1.81	0.46
35:RA:1223:G:N2	35:RA:1226:A:OP2	2.37	0.46
35:RA:776:G:N7	35:RA:793:A:O2'	2.49	0.46
39:RF:110:LEU:HD11	39:RF:181:LEU:HG	1.97	0.46
1:XA:742:G:OP2	15:XO:35:ARG:NH2	2.49	0.46
7:XG:15:ASP:OD1	7:XG:19:GLY:N	2.48	0.46
35:YA:1309:G:HO2'	35:YA:1611:C:HO2'	1.58	0.46
35:YA:1936:A:OP2	35:YA:1962:5MC:N4	2.46	0.46
1:QA:1122:U:O4	1:QA:1123:A:N6	2.49	0.45
1:QA:976:G:OP2	1:QA:1358:U:O2'	2.34	0.45
35:RA:1231:G:H2'	35:RA:1232:G:C8	2.51	0.45
35:RA:2788:C:O2'	35:RA:2809:A:N3	2.42	0.45
1:XA:148:G:H2'	1:XA:149:A:C8	2.51	0.45
1:XA:278:G:OP2	17:XQ:92:ARG:NH2	2.44	0.45
16:XP:53:VAL:HG12	16:XP:79:VAL:HG22	1.97	0.45
35:YA:1394:U:H4'	35:YA:1603:A:H4'	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1824:G:H5''	37:YD:52:ARG:HH21	1.80	0.45
37:YD:145:VAL:HB	37:YD:155:LEU:HB2	1.98	0.45
2:QB:178:ARG:HG2	8:QH:72:PRO:HA	1.98	0.45
26:R1:72:GLU:OE2	26:R1:76:ARG:HD2	2.16	0.45
1:XA:475:G:H2'	1:XA:476:G:H8	1.82	0.45
4:XD:133:VAL:HG11	4:XD:138:TYR:HD2	1.80	0.45
35:YA:2314:C:H2'	35:YA:2315:G:C8	2.52	0.45
40:YG:97:ASP:HA	40:YG:100:TRP:HD1	1.80	0.45
43:YN:71:ILE:HA	43:YN:86:PRO:HA	1.98	0.45
1:QA:1147:C:HO2'	9:QL:5:TYR:HH	1.58	0.45
35:RA:2735:G:H2'	35:RA:2736:G:H8	1.81	0.45
35:RA:276:A:H5''	35:RA:277:C:H5'	1.98	0.45
35:RA:1568:G:H5''	37:RD:61:LEU:HG	1.98	0.45
1:XA:1129:C:H2'	1:XA:1139:G:N7	2.31	0.45
4:XD:148:VAL:HG11	4:XD:158:ILE:HG21	1.99	0.45
35:YA:1541:G:OP2	35:YA:1542:A:O2'	2.31	0.45
35:YA:1567:A:H3'	37:YD:86:PRO:HG3	1.99	0.45
35:YA:1816:G:O6	37:YD:35:LYS:NZ	2.42	0.45
35:YA:956:G:OP2	46:YQ:14:ARG:NH2	2.49	0.45
36:YB:74:U:H1'	55:YZ:34:ASN:HD21	1.82	0.45
2:QB:164:VAL:HG21	2:QB:174:VAL:HG12	1.99	0.45
5:QE:145:LYS:NZ	5:QE:149:GLU:OE2	2.49	0.45
7:QG:22:LEU:HD21	7:QG:66:VAL:HG11	1.98	0.45
12:QL:70:ILE:HG12	12:QL:77:LEU:HD12	1.98	0.45
27:R2:29:LYS:HG2	27:R2:57:ILE:HD13	1.98	0.45
32:R7:34:ARG:HG3	32:R7:39:ARG:HG3	1.97	0.45
35:RA:805:G:N2	35:RA:829:A:OP1	2.50	0.45
35:RA:1798:U:OP2	37:RD:273:ARG:NH2	2.49	0.45
35:YA:220:G:O2'	35:YA:233:A:N3	2.41	0.45
35:YA:621:A:OP2	45:YP:108:LYS:NZ	2.50	0.45
43:YN:114:ARG:O	43:YN:118:LYS:NZ	2.37	0.45
5:QE:48:ALA:HB2	5:QE:57:LYS:HD3	1.98	0.45
15:QO:5:LYS:O	15:QO:9:GLN:HG2	2.17	0.45
22:QV:24:U:O2'	35:RA:1923:U:OP1	2.34	0.45
35:RA:2431:U:N3	35:RA:2434:A:OP2	2.36	0.45
35:RA:995:C:O2	43:RN:3:THR:OG1	2.32	0.45
37:RD:72:LYS:HE3	37:RD:101:GLU:HB3	1.97	0.45
39:RF:160:ASN:HB3	39:RF:163:VAL:HG12	1.98	0.45
39:RF:150:GLY:HA2	39:RF:172:TRP:CD2	2.52	0.45
54:RY:9:LYS:NZ	54:RY:28:LYS:O	2.43	0.45
17:XQ:9:VAL:HG22	17:XQ:56:VAL:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:QC:24:ALA:HB3	3:QC:29:TYR:HB2	1.98	0.45
13:QM:60:VAL:HG12	13:QM:64:TRP:HZ3	1.80	0.45
41:RH:159:GLU:HG2	41:RH:169:VAL:HG11	1.98	0.45
48:RS:35:ILE:HB	48:RS:97:ARG:HH21	1.81	0.45
50:RU:66:ASN:HD21	50:RU:70:ARG:HH21	1.65	0.45
1:XA:744:C:O2'	1:XA:851:G:N2	2.48	0.45
6:XF:35:ALA:HA	6:XF:67:MET:HB3	1.99	0.45
35:YA:1288:U:O2'	35:YA:1647:G:N2	2.48	0.45
35:YA:2133:G:O2'	35:YA:2158:A:N1	2.49	0.45
35:YA:698:C:O2'	35:YA:734:A:N6	2.50	0.45
35:YA:1035:U:OP1	41:YH:59:ARG:NH2	2.49	0.45
1:QA:1485:U:H2'	1:QA:1486:G:C8	2.52	0.45
3:QC:184:TYR:CD1	3:QC:201:TYR:CE1	3.05	0.45
35:RA:1754:C:N3	35:RA:2716:U:O2'	2.38	0.45
39:RF:178:PRO:HB2	39:RF:201:VAL:HG11	1.98	0.45
43:RN:123:TYR:HH	43:RN:130:HIS:CD2	2.30	0.45
1:XA:181:G:O2'	1:XA:183:G:N7	2.49	0.45
35:YA:1098:A:H3'	35:YA:1099:G:C8	2.52	0.45
35:YA:1853:A:N3	35:YA:2233:U:O2'	2.39	0.45
55:YZ:126:VAL:HG11	55:YZ:161:VAL:HG13	1.99	0.45
8:QH:33:GLU:OE2	8:QH:50:ARG:NE	2.47	0.45
14:QN:24:CYS:HB3	14:QN:29:ARG:H	1.81	0.45
35:RA:1312:U:O4	53:RX:60:ARG:HD3	2.17	0.45
37:RD:132:PRO:HG3	37:RD:190:TYR:CE1	2.52	0.45
54:RY:28:LYS:N	54:RY:38:ILE:O	2.44	0.45
1:XA:1192:C:O2	5:XE:25:ARG:NH2	2.50	0.45
31:Y6:37:ARG:HA	31:Y6:48:VAL:HA	1.99	0.45
35:YA:1415:U:O2'	35:YA:1417:C:OP1	2.30	0.45
35:YA:2581:G:N2	35:YA:2581:G:OP2	2.41	0.45
7:QG:27:ILE:HD12	7:QG:40:ALA:HA	1.98	0.45
1:QA:1456:G:O3'	20:QT:39:LYS:NZ	2.50	0.45
32:R7:24:THR:HG23	32:R7:27:GLY:H	1.82	0.45
46:RQ:30:GLY:N	46:RQ:105:GLU:OE2	2.48	0.45
22:XV:49:G:H1	22:XV:65:C:H42	1.63	0.45
35:YA:2352:A:N6	35:YA:2365:G:O2'	2.50	0.45
35:YA:272(L):U:P	42:YI:50:ARG:HH22	2.40	0.45
51:YV:21:ARG:CD	51:YV:91:TYR:CE2	3.00	0.45
51:YV:21:ARG:CZ	51:YV:91:TYR:HE2	2.29	0.45
4:QD:105:VAL:HG13	4:QD:110:PHE:HB2	1.99	0.45
13:QM:19:LEU:HD11	13:QM:56:LEU:HD21	1.99	0.45
20:QT:89:ARG:O	20:QT:93:GLU:HG2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RF:101:LEU:HD23	39:RF:106:ARG:HG2	2.00	0.45
35:RA:557:U:O2'	43:RN:45:ASN:O	2.35	0.45
1:XA:1073:U:O2	2:XB:104:ASN:ND2	2.50	0.45
5:XE:33:VAL:HG13	5:XE:112:LEU:HD22	1.98	0.45
5:XE:6:PHE:HD1	5:XE:36:ASP:HB3	1.82	0.45
6:XF:30:LEU:HB3	6:XF:35:ALA:HB3	1.99	0.45
9:XI:9:ARG:HG2	9:XI:14:VAL:HG12	1.99	0.45
13:XM:86:CYS:SG	13:XM:89:GLY:N	2.87	0.45
37:YD:132:PRO:HG3	37:YD:190:TYR:CE1	2.52	0.45
38:YE:84:PHE:CE2	38:YE:86:PRO:CB	3.00	0.45
35:YA:2012:G:OP1	52:YW:11:ARG:NH2	2.49	0.45
35:RA:984:A:H5''	35:RA:985:C:H5	1.81	0.44
43:RN:25:ARG:O	43:RN:29:LYS:NZ	2.45	0.44
1:XA:1309:G:P	13:XM:88:ARG:HH21	2.40	0.44
35:YA:1105:U:H2'	35:YA:1106:G:H8	1.80	0.44
38:YE:176:ILE:HB	38:YE:181:LEU:HB2	1.99	0.44
51:YV:21:ARG:HD3	51:YV:91:TYR:CE2	2.52	0.44
1:QA:447:G:O6	1:QA:485:G:O2'	2.34	0.44
1:QA:806:C:H2'	1:QA:807:A:H8	1.82	0.44
10:QJ:61:GLU:OE1	14:QN:45:ARG:NE	2.47	0.44
35:RA:1651:G:N7	47:RR:11:ASN:ND2	2.64	0.44
35:RA:1939:5MU:OP1	35:RA:2604:U:O2'	2.34	0.44
35:RA:588:U:H1'	39:RF:90:PHE:HB3	1.99	0.44
1:XA:543:C:OP2	4:XD:10:ARG:NH2	2.48	0.44
18:XR:51:LEU:HD13	18:XR:55:ARG:HG2	2.00	0.44
35:YA:30:G:O2'	35:YA:1214:A:N3	2.42	0.44
35:YA:2119:A:H61	35:YA:2168:G:H21	1.64	0.44
37:YD:183:ARG:HG3	37:YD:270:ILE:HG12	1.99	0.44
37:YD:77:ALA:HA	37:YD:97:TYR:HA	2.00	0.44
9:QI:36:TYR:HE1	9:QI:70:LYS:HE2	1.83	0.44
35:RA:1514:U:H2'	35:RA:1515:G:H8	1.82	0.44
35:RA:2441:C:OP2	35:RA:2586:C:O2'	2.28	0.44
35:RA:578:A:OP1	35:RA:1255:U:O2'	2.29	0.44
35:RA:728:G:H4'	37:RD:13:ARG:HE	1.82	0.44
37:RD:75:ILE:HG21	37:RD:99:ASP:HB2	2.00	0.44
1:XA:790:A:OP1	22:XV:38:A:O2'	2.24	0.44
5:XE:105:VAL:HG21	5:XE:128:PRO:HB3	1.99	0.44
7:XG:79:ARG:HA	7:XG:84:ASN:HA	1.99	0.44
11:XK:45:GLY:HA2	11:XK:48:ILE:HD12	2.00	0.44
35:YA:1009:A:N3	35:YA:1153:C:O2'	2.42	0.44
36:YB:87:G:N2	36:YB:90:A:OP2	2.40	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:QB:9:GLU:HG2	2:QB:11:LEU:H	1.82	0.44
5:QE:78:HIS:HA	8:QH:105:ARG:HG3	1.99	0.44
1:QA:718:G:H5'	11:QK:117:ASN:OD1	2.18	0.44
20:QT:22:ARG:O	20:QT:26:ASN:ND2	2.51	0.44
35:RA:1188:U:H2'	35:RA:1189:A:H8	1.81	0.44
35:RA:116:C:O2'	35:RA:126:A:N3	2.41	0.44
35:RA:1792:G:O2'	35:RA:1830:C:OP1	2.33	0.44
35:RA:2200:C:O2	35:RA:2226:C:N4	2.49	0.44
1:XA:978:A:O2'	1:XA:1322:C:N3	2.47	0.44
1:XA:624:C:H2'	1:XA:625:G:H8	1.82	0.44
5:XE:110:LEU:HD13	5:XE:118:ILE:HG21	1.97	0.44
32:Y7:13:ALA:HB2	32:Y7:46:VAL:HG11	1.99	0.44
35:YA:1792:G:O2'	35:YA:1830:C:OP1	2.35	0.44
40:YG:38:VAL:HG22	40:YG:93:THR:HG23	1.99	0.44
1:QA:184:G:H2'	1:QA:185:A:H8	1.81	0.44
9:QI:16:ARG:HB2	9:QI:64:THR:HG22	1.99	0.44
10:QJ:16:LEU:HD22	10:QJ:94:VAL:HG12	2.00	0.44
35:RA:463:G:N2	35:RA:466:A:OP2	2.39	0.44
35:RA:906:G:OP1	46:RQ:26:TYR:OH	2.25	0.44
1:XA:328:C:H4'	1:XA:329:A:H5'	1.99	0.44
9:XI:5:TYR:N	9:XI:87:GLN:OE1	2.50	0.44
41:YH:154:PRO:HB3	41:YH:163:TYR:CE1	2.53	0.44
47:YR:63:ARG:HG2	47:YR:80:PHE:CE2	2.53	0.44
1:QA:396:G:O2'	1:QA:398:C:OP1	2.26	0.44
43:RN:36:GLY:HA2	43:RN:38:HIS:CE1	2.53	0.44
6:XF:95:GLU:O	18:XR:32:ARG:NH1	2.50	0.44
1:XA:1368:G:OP1	9:XI:111:ARG:NH2	2.50	0.44
13:XM:17:VAL:O	13:XM:20:THR:OG1	2.27	0.44
33:Y8:64:TYR:HH	35:YA:592:G:HO2'	1.65	0.44
37:YD:108:PRO:HB3	37:YD:143:HIS:CE1	2.53	0.44
54:YY:83:THR:OG1	54:YY:84:ARG:N	2.51	0.44
1:QA:128:G:O2'	17:QQ:3:LYS:NZ	2.38	0.44
1:QA:1517:G:N3	35:RA:1919:A:O2'	2.46	0.44
35:RA:1936:A:OP2	35:RA:1962:5MC:N4	2.48	0.44
35:RA:2404:C:O3'	45:RP:77:ARG:NH2	2.51	0.44
41:RH:126:PRO:HG2	41:RH:130:ARG:HH21	1.82	0.44
45:RP:3:LEU:HD23	45:RP:6:LEU:HD12	2.00	0.44
35:RA:807:U:OP2	45:RP:41:ARG:NH2	2.51	0.44
1:XA:111:G:H5''	16:XP:27:LYS:HG2	1.99	0.44
1:XA:297:G:N2	1:XA:300:A:OP2	2.48	0.44
2:XB:207:ALA:O	2:XB:210:SER:OG	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:XB:71:VAL:HG13	2:XB:164:VAL:HA	1.99	0.44
6:XF:33:TYR:HE2	6:XF:78:GLU:HG3	1.82	0.44
9:XI:50:LEU:HD23	9:XI:85:LEU:HD11	1.98	0.44
35:YA:2377:A:O2'	48:YS:112:PHE:O	2.30	0.44
1:QA:1073:U:O2	2:QB:104:ASN:ND2	2.51	0.44
35:RA:139(A):G:H21	53:RX:41:ASN:HD21	1.66	0.44
35:RA:729:G:C5	37:RD:208:LYS:HB2	2.52	0.44
9:XI:16:ARG:HH21	9:XI:18:PHE:HZ	1.66	0.44
35:YA:956:G:H2'	35:YA:957:A:H2'	1.99	0.44
47:YR:100:LEU:HD12	47:YR:111:LEU:HB3	2.00	0.44
1:QA:1377:A:OP2	7:QG:94:ARG:NE	2.51	0.44
1:QA:127:G:HO2'	17:QQ:2:PRO:N	2.15	0.44
26:R1:11:ARG:NH2	35:RA:1365:A:O2'	2.51	0.44
35:RA:475:U:H4'	35:RA:510:C:H5'	2.00	0.44
51:RV:14:VAL:HB	51:RV:96:ILE:HG13	2.00	0.44
1:XA:1074:G:H1	1:XA:1083:U:H3	1.66	0.44
1:XA:1240:U:OP1	7:XG:119:ARG:NH2	2.46	0.44
1:XA:1316:G:N1	1:XA:1319:A:OP2	2.51	0.44
1:XA:501:C:O2	1:XA:549:C:O2'	2.29	0.44
16:XP:19:ILE:HB	16:XP:37:GLY:HA3	1.99	0.44
19:XS:68:GLY:H	29:Y4:58:ARG:NH1	2.16	0.44
35:YA:639:U:H3	35:YA:649:G:H1	1.66	0.44
35:YA:992:C:OP1	50:YU:47:TYR:OH	2.32	0.44
1:QA:189(C):C:H42	1:QA:189(J):G:H1	1.66	0.43
11:QK:20:TYR:CE1	11:QK:83:ILE:HD13	2.53	0.43
35:RA:814:C:O2'	35:RA:1224:C:N3	2.51	0.43
49:RT:9:LEU:O	49:RT:12:SER:OG	2.27	0.43
55:RZ:102:LEU:HD11	55:RZ:124:ILE:HG12	2.00	0.43
1:XA:123:C:OP1	1:XA:311:C:O2'	2.31	0.43
1:XA:96:U:H2'	1:XA:97:G:H8	1.82	0.43
6:XF:61:LEU:HD12	6:XF:63:TYR:HE1	1.83	0.43
29:Y4:11:PRO:HG3	29:Y4:25:TYR:CD2	2.53	0.43
33:Y8:12:LYS:NZ	35:YA:249:C:O2	2.35	0.43
45:YP:19:VAL:HG12	45:YP:27:HIS:HB3	2.00	0.43
11:QK:34:ASP:OD1	11:QK:38:ASN:N	2.51	0.43
18:QR:34:TYR:HD1	18:QR:34:TYR:H	1.64	0.43
32:R7:9:ARG:NH2	35:RA:1311:G:N7	2.65	0.43
41:RH:126:PRO:HG2	41:RH:130:ARG:HE	1.83	0.43
41:RH:68:THR:O	41:RH:72:ILE:HG12	2.18	0.43
42:RI:114:LEU:HD11	42:RI:128:LEU:HB3	2.00	0.43
4:XD:20:TYR:HD1	4:XD:26:CYS:HB3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:XD:59:ARG:HE	4:XD:59:ARG:HA	1.83	0.43
7:XG:16:LEU:HD11	9:XI:45:ALA:HB2	2.00	0.43
17:XQ:52:LYS:HE3	17:XQ:52:LYS:HB3	1.83	0.43
35:YA:1664:A:H61	35:YA:1996:C:H42	1.66	0.43
35:YA:2773:C:H5''	38:YE:164:ARG:HG2	2.00	0.43
55:YZ:52:SER:OG	55:YZ:53:ILE:N	2.51	0.43
1:QA:142:G:H2'	1:QA:143:A:H8	1.82	0.43
4:QD:140:VAL:HG11	4:QD:146:ILE:HD11	2.00	0.43
4:QD:10:ARG:HB2	4:QD:40:PRO:HG3	2.00	0.43
49:RT:50:ILE:HB	49:RT:99:LEU:HB2	1.99	0.43
15:XO:5:LYS:O	15:XO:9:GLN:HG2	2.19	0.43
29:Y4:43:TYR:CZ	40:YG:179:PRO:HG3	2.52	0.43
35:YA:2115:G:O2'	35:YA:2166:G:N2	2.51	0.43
39:YF:155:LEU:HD11	39:YF:176:LEU:HD12	1.99	0.43
40:YG:109:VAL:HG11	40:YG:142:PRO:HB3	2.00	0.43
1:QA:1516:G:N2	1:QA:1519:MA6:OP2	2.49	0.43
2:QB:179:LYS:HD3	8:QH:72:PRO:HG3	1.99	0.43
30:R5:7:PRO:O	35:RA:2016:U:O2'	2.31	0.43
35:RA:955:C:OP1	46:RQ:87:LYS:NZ	2.43	0.43
35:RA:956:G:OP2	46:RQ:14:ARG:NH2	2.52	0.43
49:RT:24:PRO:HA	49:RT:49:VAL:HG13	2.00	0.43
1:XA:107:G:N7	20:XT:15:ARG:NH2	2.67	0.43
1:XA:824:C:H2'	1:XA:825:G:C8	2.53	0.43
1:XA:986:A:H1'	19:XS:55:LYS:HA	1.99	0.43
13:XM:23:TYR:CE2	13:XM:71:ARG:HG2	2.52	0.43
49:YT:93:ARG:HB3	49:YT:117:ASP:HB2	2.00	0.43
49:YT:35:LYS:HA	49:YT:40:THR:HA	1.99	0.43
1:QA:1129:C:H2'	1:QA:1139:G:N7	2.33	0.43
5:QE:6:PHE:HD1	5:QE:36:ASP:HB3	1.83	0.43
8:QH:112:LEU:HB3	8:QH:133:LEU:HA	2.00	0.43
30:R5:12:SER:OG	35:RA:2021:C:OP1	2.32	0.43
35:RA:647:G:N3	35:RA:2350:C:O2'	2.51	0.43
35:RA:2572:A:H2'	38:RE:144:ARG:HD3	2.01	0.43
35:RA:2785:C:O2'	38:RE:66:HIS:ND1	2.43	0.43
35:RA:873:G:O3'	46:RQ:63:LYS:NZ	2.50	0.43
35:RA:1151:G:O2'	50:RU:77:SER:O	2.37	0.43
27:R2:36:ARG:NH2	53:RX:5:TYR:O	2.40	0.43
1:XA:601:C:H2'	1:XA:602:A:H8	1.83	0.43
1:XA:626:U:H4'	16:XP:38:TYR:CD2	2.53	0.43
4:XD:98:GLU:HG3	4:XD:194:LEU:HD11	2.01	0.43
5:XE:78:HIS:ND1	8:XH:104:ARG:HD2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Y8:23:VAL:HG22	33:Y8:49:VAL:HG22	2.01	0.43
35:YA:2164:C:H3'	35:YA:2165:G:H8	1.83	0.43
33:Y8:30:ARG:NH2	45:YP:64:LYS:O	2.52	0.43
1:QA:1005:A:O3'	1:QA:1037:C:O2'	2.37	0.43
1:QA:444:C:H2'	1:QA:445:G:H8	1.84	0.43
44:RO:8:LEU:HB2	44:RO:19:ILE:HG13	2.00	0.43
48:RS:3:ARG:HH21	48:RS:9:ARG:HH12	1.67	0.43
1:XA:1133:G:H2'	1:XA:1134:G:H8	1.82	0.43
1:XA:1133:G:H2'	1:XA:1134:G:C8	2.54	0.43
41:YH:87:LEU:HD23	41:YH:164:TYR:HA	2.00	0.43
48:YS:24:LEU:O	48:YS:86:ALA:N	2.48	0.43
1:QA:1031:G:H2'	1:QA:1032:G:C8	2.53	0.43
12:QL:71:PRO:HB2	12:QL:120:TYR:HE1	1.84	0.43
35:RA:1466:G:O2'	35:RA:1546:C:O2'	2.28	0.43
35:RA:1816:G:O6	37:RD:35:LYS:NZ	2.50	0.43
35:RA:1566:A:OP1	37:RD:211:ARG:NH1	2.51	0.43
48:RS:26:LEU:HD23	48:RS:87:PHE:HD1	1.84	0.43
49:RT:50:ILE:HA	49:RT:99:LEU:HD12	2.00	0.43
35:RA:2013:A:H2	52:RW:88:ARG:HH22	1.66	0.43
1:XA:943:U:H1'	9:XI:124:GLN:HE22	1.84	0.43
35:YA:1779:U:OP2	35:YA:1784:A:N6	2.34	0.43
35:YA:380:U:H2'	35:YA:381:G:H8	1.83	0.43
41:YH:28:GLY:HA3	41:YH:79:VAL:HB	2.01	0.43
1:QA:730:G:C5	1:QA:731:G:H1'	2.54	0.43
12:QL:70:ILE:HG13	12:QL:100:ILE:HD12	1.99	0.43
35:RA:223:A:O2'	35:RA:420:C:O2	2.33	0.43
35:RA:906:G:O2'	46:RQ:67:ARG:NH2	2.46	0.43
35:YA:1156:A:OP1	50:YU:55:ARG:HD2	2.19	0.43
22:XV:76:A:H2'	35:YA:2602:A:N6	2.33	0.43
35:YA:453:C:O2	35:YA:457:A:O2'	2.35	0.43
35:YA:1327:C:HO2'	47:YR:105:ARG:HH12	1.60	0.43
1:QA:640:A:N3	8:QH:115:SER:OG	2.40	0.43
1:QA:806:C:H2'	1:QA:807:A:C8	2.54	0.43
1:QA:985:C:H2'	1:QA:986:A:C8	2.54	0.43
1:QA:522:C:H41	12:QL:53:ARG:HH22	1.67	0.43
29:R4:14:ILE:HB	29:R4:22:ILE:HB	2.00	0.43
29:R4:34:GLU:OE1	29:R4:35:VAL:CG2	2.66	0.43
35:RA:2728:U:H2'	35:RA:2729:G:C8	2.54	0.43
40:RG:77:ILE:HG23	40:RG:80:PHE:HB2	2.01	0.43
1:XA:1030(D):G:H2'	1:XA:1030(E):A:C8	2.54	0.43
1:XA:1199:U:O2'	1:XA:1202:G:OP1	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:626:U:H5''	16:XP:38:TYR:CD2	2.52	0.43
35:YA:1453:U:O2'	35:YA:1455:G:N7	2.46	0.43
44:YO:122:LEU:HD13	49:YT:72:VAL:HG11	2.00	0.43
2:QB:54:THR:O	2:QB:58:ILE:HG12	2.19	0.43
4:QD:168:ARG:HH22	37:YD:134:ARG:NH2	2.17	0.43
35:RA:18:C:O2'	35:RA:554:U:OP1	2.37	0.43
37:RD:275:LYS:HD3	37:RD:275:LYS:HA	1.80	0.43
44:RO:2:ILE:HB	44:RO:33:ALA:HB3	2.01	0.43
35:RA:2880:C:O3'	47:RR:90:ARG:NH1	2.52	0.43
50:RU:83:LEU:HD13	50:RU:88:ILE:HB	2.01	0.43
1:XA:919:A:O2'	1:XA:1080:A:N1	2.41	0.43
2:XB:80:ILE:HG21	2:XB:211:ILE:HD12	2.01	0.43
1:XA:410:G:H3'	4:XD:25:ARG:HH22	1.84	0.43
8:XH:36:LEU:HD12	8:XH:59:LEU:HD23	2.01	0.43
7:XG:150:ALA:HB1	11:XK:57:THR:HG21	2.01	0.43
19:XS:43:GLU:N	19:XS:43:GLU:CD	2.71	0.43
31:Y6:6:ARG:HD2	31:Y6:6:ARG:HA	1.88	0.43
35:YA:2839:G:H5'	47:YR:46:GLY:HA2	2.01	0.43
40:YG:5:VAL:HG23	40:YG:8:LYS:H	1.84	0.43
35:YA:244:A:H4'	45:YP:74:GLU:HB2	2.01	0.43
35:YA:869:G:H1'	46:YQ:8:LYS:HD2	2.01	0.43
1:QA:522:C:OP2	12:QL:69:TYR:OH	2.28	0.42
3:QC:159:GLY:HA2	3:QC:193:TYR:HD2	1.75	0.42
8:QH:25:ASP:HB3	8:QH:58:TYR:HD2	1.83	0.42
26:R1:30:VAL:O	35:RA:2395:C:O2'	2.35	0.42
35:RA:1231:G:H2'	35:RA:1232:G:H8	1.84	0.42
35:RA:1980:G:O2'	35:RA:1982:C:OP2	2.34	0.42
27:R2:36:ARG:NH2	53:RX:8:ILE:O	2.51	0.42
1:XA:1131:G:OP1	9:XI:20:ARG:NH2	2.52	0.42
1:XA:148:G:H2'	1:XA:149:A:H8	1.83	0.42
1:XA:403:C:H4'	4:XD:122:ARG:HH11	1.84	0.42
1:XA:237:C:O3'	17:XQ:25:ARG:NH2	2.51	0.42
35:YA:2502:G:H5''	35:YA:2503:2MA:H5''	2.00	0.42
35:YA:2679:A:H5'	38:YE:165:VAL:HG21	2.01	0.42
39:YF:155:LEU:HB2	39:YF:189:THR:HG21	2.01	0.42
44:YO:68:GLU:HB3	44:YO:78:ARG:HB2	2.00	0.42
45:YP:20:GLY:HA2	45:YP:28:GLY:HA2	2.01	0.42
49:YT:94:ALA:HB1	49:YT:99:LEU:HD21	2.01	0.42
3:QC:37:GLN:NE2	14:QN:52:GLN:OE1	2.36	0.42
35:RA:576:U:H2'	35:RA:577:G:C8	2.54	0.42
35:RA:685:A:OP1	35:RA:686:G:N2	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:RA:1567:A:H3'	37:RD:86:PRO:HG3	2.01	0.42
38:RE:134:ILE:HA	38:RE:137:HIS:CD2	2.54	0.42
50:RU:102:GLU:HG3	51:RV:2:PHE:CZ	2.54	0.42
55:RZ:58:VAL:HA	55:RZ:68:PRO:HA	2.01	0.42
1:XA:184:G:H2'	1:XA:185:A:H8	1.84	0.42
1:XA:624:C:H2'	1:XA:625:G:C8	2.54	0.42
15:XO:3:ILE:HG22	15:XO:38:ARG:HH21	1.84	0.42
35:YA:1277:G:H2'	35:YA:1278:A:C8	2.54	0.42
35:YA:226:G:H21	35:YA:228:A:H62	1.67	0.42
35:YA:335:C:O2	54:YY:70:SER:OG	2.38	0.42
35:YA:83:G:O2'	35:YA:102:G:N2	2.51	0.42
55:YZ:30:ASN:OD1	55:YZ:33:LEU:N	2.41	0.42
1:QA:1316:G:O2'	1:QA:1318:A:N7	2.39	0.42
35:RA:743:G:O2'	35:RA:1659:U:OP1	2.32	0.42
35:RA:479:A:HO2'	35:RA:481:G:H8	1.64	0.42
35:RA:602:G:N2	35:RA:655:A:OP2	2.46	0.42
37:RD:245:PRO:HA	37:RD:246:PRO:HD3	1.94	0.42
37:RD:247:ALA:HA	37:RD:253:GLN:HA	2.00	0.42
1:XA:1286:A:N6	1:XA:1354:C:O3'	2.52	0.42
1:XA:946:A:O2'	1:XA:1333:A:N3	2.45	0.42
12:XL:117:ARG:HB2	12:XL:122:THR:HB	2.02	0.42
13:XM:4:ILE:HG13	13:XM:5:ALA:H	1.84	0.42
41:YH:149:ARG:NH2	41:YH:167:GLU:OE2	2.47	0.42
41:YH:46:GLU:OE2	41:YH:51:ARG:NH2	2.50	0.42
51:YV:52:VAL:HG21	51:YV:55:ALA:HB3	2.01	0.42
55:YZ:13:GLU:HG3	55:YZ:18:LEU:HD21	2.01	0.42
1:QA:328:C:H4'	1:QA:329:A:H5'	2.00	0.42
4:QD:61:LYS:HE2	4:QD:206:PHE:CE2	2.54	0.42
27:R2:38:GLN:HA	27:R2:41:ILE:HG12	2.01	0.42
30:R5:51:TYR:HE1	30:R5:56:LYS:HD3	1.84	0.42
35:RA:1682:G:OP2	35:RA:1699:G:N2	2.52	0.42
39:RF:161:GLU:O	39:RF:165:ARG:HB2	2.20	0.42
44:RO:68:GLU:HB3	44:RO:78:ARG:HB2	2.02	0.42
46:RQ:52:VAL:HA	46:RQ:55:VAL:HG22	2.01	0.42
50:RU:66:ASN:OD1	50:RU:70:ARG:NE	2.51	0.42
1:XA:28:G:O2'	1:XA:296:U:OP1	2.28	0.42
11:XK:20:TYR:CE1	11:XK:83:ILE:HD12	2.54	0.42
16:XP:3:LYS:HG2	16:XP:65:GLN:HB2	2.01	0.42
27:Y2:37:PHE:CD1	53:YX:11:PRO:HD3	2.55	0.42
35:YA:2328:A:H2'	35:YA:2329:G:C8	2.54	0.42
35:YA:272(R):G:H2'	35:YA:272(S):G:H8	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:414:C:H2'	35:YA:415:A:C8	2.54	0.42
35:YA:616:G:O2'	39:YF:205:ARG:NH1	2.53	0.42
35:YA:626:U:O4	45:YP:81:GLN:NE2	2.53	0.42
40:YG:78:SER:OG	40:YG:79:ASN:N	2.52	0.42
41:YH:54:ARG:HD2	41:YH:65:HIS:ND1	2.35	0.42
41:YH:86:GLU:OE2	41:YH:132:ARG:NH2	2.52	0.42
1:QA:346:G:OP1	49:RT:41:ARG:NH1	2.52	0.42
1:QA:522:C:H41	12:QL:53:ARG:NH2	2.17	0.42
1:QA:652:U:O4	1:QA:752:G:O2'	2.32	0.42
3:QC:153:VAL:HG22	3:QC:198:VAL:HG22	2.00	0.42
4:QD:18:LYS:HE3	4:QD:20:TYR:CE2	2.54	0.42
1:QA:552:U:H4'	12:QL:87:GLY:HA3	2.02	0.42
1:QA:626:U:C5'	16:QP:38:TYR:HD2	2.30	0.42
35:RA:1423:G:H2'	35:RA:1424:G:H8	1.84	0.42
35:RA:2543:G:H2'	35:RA:2544:G:C8	2.54	0.42
35:RA:698:C:O2'	35:RA:734:A:N6	2.52	0.42
45:RP:65:ARG:O	45:RP:68:GLN:NE2	2.53	0.42
53:RX:53:LYS:HB3	53:RX:82:GLN:HB3	2.01	0.42
1:XA:96:U:H2'	1:XA:97:G:C8	2.55	0.42
6:XF:30:LEU:HD23	6:XF:75:LEU:HD11	2.02	0.42
35:YA:1665:A:H1'	44:YO:1:MET:HB2	2.01	0.42
46:YQ:104:PHE:HE2	46:YQ:125:LEU:HD11	1.85	0.42
1:QA:1412:C:H2'	1:QA:1413:A:C8	2.55	0.42
2:QB:84:GLU:HB3	2:QB:219:VAL:HG21	2.02	0.42
1:QA:1106:G:H5''	3:QC:172:ARG:HG2	2.01	0.42
3:QC:19:GLU:HG2	3:QC:55:VAL:O	2.18	0.42
9:QI:4:TYR:HB2	9:QI:19:LEU:HB2	2.00	0.42
25:R0:77:ARG:NH2	35:RA:857:C:OP2	2.52	0.42
35:RA:2633:G:H5''	35:RA:2812:G:H5'	2.02	0.42
39:RF:165:ARG:HG3	39:RF:168:ARG:NH1	2.35	0.42
39:RF:184:TYR:CE2	39:RF:188:ARG:HD2	2.55	0.42
1:XA:142:G:H2'	1:XA:143:A:H8	1.84	0.42
1:XA:673:G:H4'	6:XF:87:ARG:HH12	1.84	0.42
14:YN:4:LYS:HA	14:YN:7:ILE:HG12	2.02	0.42
30:Y5:7:PRO:O	35:YA:2016:U:O2'	2.37	0.42
35:YA:200:U:O2	35:YA:386:G:N2	2.52	0.42
35:YA:78:A:H2'	35:YA:79:G:H8	1.83	0.42
13:QM:66:LEU:HD13	13:QM:66:LEU:HA	1.88	0.42
33:R8:2:PRO:O	35:RA:666:G:N2	2.52	0.42
40:RG:173:LEU:HD13	40:RG:176:LEU:HD12	2.01	0.42
40:RG:37:VAL:HG13	40:RG:94:LEU:HB2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:XA:769:G:H4'	1:XA:1513:A:H4'	2.02	0.42
17:XQ:62:SER:OG	17:XQ:72:ARG:NE	2.43	0.42
28:Y3:52:HIS:CD2	28:Y3:53:LEU:HG	2.55	0.42
35:YA:1223:G:N2	35:YA:1226:A:OP2	2.43	0.42
35:YA:2602:A:H4'	35:YA:2603:G:C5'	2.50	0.42
35:YA:1500:G:H21	37:YD:100:GLY:HA3	1.85	0.42
39:YF:178:PRO:HB2	39:YF:201:VAL:HG21	2.01	0.42
1:QA:523:A:H61	12:QL:92:0TD:CG	2.31	0.42
1:QA:981:U:O4	1:QA:1223:C:N4	2.53	0.42
2:QB:163:PHE:HA	2:QB:185:ILE:HG13	2.01	0.42
5:QE:6:PHE:CD1	5:QE:36:ASP:HB3	2.54	0.42
41:RH:3:ARG:NE	41:RH:5:GLY:H	2.18	0.42
1:XA:427:U:O2'	1:XA:541:G:OP1	2.30	0.42
7:XG:113:GLU:OE2	7:XG:122:HIS:ND1	2.38	0.42
8:XH:104:ARG:HD3	8:XH:104:ARG:HA	1.85	0.42
10:XJ:40:LEU:HB2	10:XJ:69:ASN:HB2	2.02	0.42
28:Y3:52:HIS:CG	36:YB:83:G:H4'	2.54	0.42
35:YA:1069:A:C6	35:YA:1095:A:H4'	2.55	0.42
35:YA:2679:A:OP2	38:YE:160:TYR:OH	2.27	0.42
1:QA:165:C:H2'	1:QA:166:G:H8	1.85	0.42
35:RA:1394:U:O2	53:RX:16:LYS:NZ	2.45	0.42
35:RA:411:G:OP2	35:RA:2406:U:O2'	2.37	0.42
1:XA:192:U:H5'	20:XT:101:GLY:HA3	2.01	0.42
4:XD:50:ARG:HA	4:XD:51:PRO:HD3	1.92	0.42
9:XI:42:ARG:NH2	9:XI:71:SER:OG	2.53	0.42
9:XI:73:GLN:O	9:XI:77:ILE:HG12	2.20	0.42
35:YA:2633:G:H5''	35:YA:2812:G:H5'	2.00	0.42
39:YF:31:HIS:NE2	39:YF:35:GLU:OE2	2.53	0.42
16:QP:18:ARG:NH1	16:QP:32:TYR:OH	2.53	0.42
19:QS:22:LEU:HD13	19:QS:22:LEU:HA	1.82	0.42
35:RA:1478:G:O2'	35:RA:1558:A:N7	2.50	0.42
38:RE:5:LEU:HD11	38:RE:79:ARG:HB2	2.02	0.42
41:RH:99:VAL:N	41:RH:102:ALA:O	2.51	0.42
42:RI:115:ALA:HB2	42:RI:131:LYS:HE2	2.02	0.42
46:RQ:34:LEU:HB2	46:RQ:118:LEU:HD22	2.01	0.42
50:RU:44:ASN:HD21	51:RV:75:PHE:HB3	1.84	0.42
1:XA:1356:G:H2'	1:XA:1357:A:C8	2.55	0.42
1:XA:356:A:N3	1:XA:368:U:O2'	2.37	0.42
1:XA:476:G:H2'	1:XA:477:A:H8	1.84	0.42
1:XA:779:C:H5''	11:XK:122:LYS:HG2	2.02	0.42
9:XI:9:ARG:H	9:XI:79:LEU:HD23	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:XQ:6:LEU:HD23	17:XQ:23:VAL:HG11	2.02	0.42
35:YA:1188:U:H2'	35:YA:1189:A:H8	1.84	0.42
35:YA:1790:C:H2'	35:YA:1791:A:C5	2.55	0.42
37:YD:253:GLN:HB2	37:YD:257:LEU:HD12	2.01	0.42
35:YA:1567:A:C6	37:YD:84:TYR:CD2	3.08	0.42
38:YE:34:VAL:HG12	38:YE:72:VAL:HG21	2.01	0.42
40:YG:101:ILE:HG22	40:YG:105:LYS:HE2	2.00	0.42
1:QA:1366:C:O2'	10:QJ:60:ARG:NH2	2.47	0.41
1:QA:142:G:H2'	1:QA:143:A:C8	2.54	0.41
1:QA:28:G:O2'	1:QA:296:U:OP1	2.29	0.41
1:QA:673:G:H5''	6:QF:87:ARG:NH1	2.35	0.41
31:R6:10:LEU:HD13	31:R6:19:ARG:HG2	2.02	0.41
31:R6:21:TYR:OH	35:RA:2347:C:O2'	2.33	0.41
35:RA:2503:2MA:O2'	35:RA:2505:G:OP2	2.25	0.41
41:RH:24:VAL:HG21	41:RH:72:ILE:HD12	2.02	0.41
48:RS:10:ARG:HG3	48:RS:13:ARG:HH21	1.84	0.41
1:XA:407:G:H2'	1:XA:408:A:C8	2.54	0.41
1:XA:407:G:OP1	4:XD:115:ARG:NH1	2.53	0.41
1:XA:1060:C:H5''	10:XJ:51:ARG:HG2	2.02	0.41
1:XA:684:A:O2'	11:XK:39:PRO:O	2.35	0.41
25:Y0:31:VAL:HB	25:Y0:35:ASN:HD22	1.85	0.41
35:YA:1057:A:H62	35:YA:1086:A:H3'	1.84	0.41
35:YA:557:U:O2'	43:YN:45:ASN:O	2.34	0.41
2:QB:181:PHE:CE1	8:QH:71:GLY:HA2	2.55	0.41
35:RA:1688:U:O2	35:RA:1700:A:H5'	2.20	0.41
35:RA:2857:G:N2	35:RA:2860:A:OP2	2.34	0.41
1:XA:1031:G:H2'	1:XA:1032:G:C8	2.55	0.41
28:Y3:6:VAL:HG12	28:Y3:28:LEU:HD11	2.01	0.41
40:YG:3:LEU:HD11	40:YG:101:ILE:HD11	2.01	0.41
41:YH:8:PRO:O	41:YH:69:ARG:NH2	2.46	0.41
35:YA:2405:G:H5'	45:YP:75:ILE:HD13	2.03	0.41
1:QA:749:C:H2'	1:QA:750:G:H8	1.85	0.41
14:QN:29:ARG:HG2	14:QN:31:ARG:H	1.84	0.41
35:RA:1657:C:H4'	38:RE:133:LYS:HB3	2.03	0.41
35:RA:1889:A:H2'	35:RA:1890:A:C8	2.55	0.41
1:XA:966:M2G:HM13	1:XA:967:5MC:H1'	2.02	0.41
3:XC:150:LYS:HG3	3:XC:169:ALA:HB2	2.02	0.41
4:XD:194:LEU:HB3	4:XD:196:LEU:HD12	2.01	0.41
1:XA:1149:C:P	9:XI:9:ARG:HH21	2.43	0.41
10:XJ:61:GLU:OE1	14:YN:45:ARG:NE	2.48	0.41
10:XJ:61:GLU:OE2	14:YN:49:HIS:NE2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y3:8:LEU:HA	28:Y3:54:VAL:HG23	2.01	0.41
35:YA:87:C:H5''	35:YA:88:G:H5'	2.03	0.41
39:YF:39:TRP:NE1	39:YF:99:TYR:O	2.52	0.41
2:QB:155:LEU:HD21	2:QB:159:PRO:HG3	2.03	0.41
5:QE:76:ILE:HG13	5:QE:93:PRO:HG3	2.02	0.41
11:QK:65:ALA:HB1	11:QK:98:LEU:HD12	2.03	0.41
30:R5:41:PRO:O	30:R5:44:THR:OG1	2.32	0.41
35:RA:1082:U:H2'	35:RA:1082:U:H6	1.71	0.41
35:RA:1516:C:H2'	35:RA:1517:G:H8	1.85	0.41
35:RA:272(Q):G:H2'	35:RA:272(R):G:C8	2.55	0.41
35:RA:581:C:H2'	35:RA:582:G:C8	2.55	0.41
37:RD:260:ARG:NH2	37:RD:266:SER:OG	2.53	0.41
37:RD:72:LYS:NZ	37:RD:99:ASP:OD2	2.53	0.41
46:RQ:110:THR:HG23	46:RQ:113:GLN:H	1.85	0.41
1:XA:1005:A:O2'	1:XA:1036:G:N2	2.53	0.41
1:XA:652:U:O4	1:XA:752:G:O2'	2.30	0.41
1:XA:765:G:N1	1:XA:812:C:O2'	2.37	0.41
30:Y5:4:HIS:O	35:YA:2056:G:N2	2.53	0.41
35:YA:579:G:O2'	35:YA:2019:A:OP1	2.38	0.41
35:YA:2136:C:N4	35:YA:2155:G:O6	2.52	0.41
35:YA:184:C:H1'	35:YA:217:G:H1'	2.01	0.41
25:Y0:43:THR:HG22	35:YA:2336:A:H61	1.86	0.41
35:YA:297:C:OP1	54:YY:87:LYS:NZ	2.43	0.41
45:YP:65:ARG:O	45:YP:68:GLN:NE2	2.52	0.41
1:QA:1230:C:H5'	22:QV:30:G:H5''	2.03	0.41
1:QA:521:G:N7	12:QL:53:ARG:NH1	2.67	0.41
4:QD:79:PHE:HE1	4:QD:204:ILE:HD13	1.85	0.41
8:QH:34:GLU:HB3	8:QH:118:VAL:HG21	2.01	0.41
19:QS:63:THR:OG1	19:QS:65:ASN:OD1	2.35	0.41
1:QA:1403:C:N4	23:QX:18:G:OP1	2.52	0.41
35:RA:1593:G:H2'	35:RA:1594:G:C8	2.56	0.41
35:RA:1638:C:O3'	35:RA:2709:G:N2	2.53	0.41
35:RA:1769:G:O2'	35:RA:1958:C:OP1	2.28	0.41
35:RA:442:G:N3	39:RF:48:THR:OG1	2.42	0.41
1:XA:476:G:H2'	1:XA:477:A:C8	2.55	0.41
1:XA:673:G:H2'	1:XA:674:G:C8	2.55	0.41
35:YA:1538:G:H2'	35:YA:1539:G:H8	1.86	0.41
36:YB:37:C:O2	48:YS:95:HIS:NE2	2.48	0.41
35:YA:1567:A:C6	37:YD:84:TYR:CE2	3.06	0.41
33:Y8:10:ALA:HA	45:YP:59:LEU:HD11	2.01	0.41
35:YA:483:A:O2'	54:YY:49:VAL:O	2.25	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:QA:1343:G:H4'	9:QI:122:ALA:HB3	2.02	0.41
2:QB:101:MET:HA	2:QB:108:ILE:HG21	2.02	0.41
30:R5:7:PRO:HA	35:RA:2615:U:C2	2.56	0.41
35:RA:1057:A:N6	35:RA:1087:G:OP2	2.53	0.41
35:RA:323:G:C8	39:RF:171:PRO:HG3	2.55	0.41
37:RD:13:ARG:NH1	37:RD:16:MET:SD	2.94	0.41
39:RF:182:ASN:N	39:RF:182:ASN:OD1	2.44	0.41
53:RX:55:ASN:HB2	53:RX:80:ILE:HB	2.03	0.41
9:XI:50:LEU:HB3	9:XI:56:LEU:HA	2.02	0.41
1:XA:1524:C:H5''	11:XK:120:ARG:HH12	1.85	0.41
35:YA:1243:G:O2'	45:YP:7:ARG:NH2	2.52	0.41
42:YI:114:LEU:HD23	42:YI:130:TYR:HA	2.02	0.41
2:QB:82:ARG:HG3	2:QB:92:TYR:CZ	2.55	0.41
3:QC:130:VAL:HG21	3:QC:157:ILE:HG23	2.02	0.41
3:QC:184:TYR:CD1	3:QC:201:TYR:CD1	3.08	0.41
9:QI:78:LYS:HE2	9:QI:78:LYS:HB2	1.84	0.41
1:QA:237:C:O3'	17:QQ:25:ARG:NH2	2.54	0.41
26:R1:18:ILE:HG12	26:R1:37:ILE:HG12	2.03	0.41
35:RA:451:C:OP1	39:RF:52:LYS:NZ	2.46	0.41
35:RA:2513:G:N2	38:RE:143:ASN:HD21	2.19	0.41
38:RE:34:VAL:HG12	38:RE:72:VAL:HG21	2.03	0.41
35:RA:2305:A:H5''	40:RG:134:GLY:HA3	2.02	0.41
47:RR:12:ARG:HB3	47:RR:16:HIS:HB3	2.02	0.41
52:RW:69:LEU:HB3	52:RW:107:LEU:HD23	2.03	0.41
1:XA:677:U:O2	1:XA:777:A:O2'	2.35	0.41
1:XA:84:U:O2'	1:XA:89:C:N4	2.54	0.41
5:XE:102:ALA:H	5:XE:107:ARG:HH21	1.67	0.41
13:XM:91:ARG:HH22	13:XM:103:THR:HG21	1.84	0.41
35:YA:108:U:H2'	35:YA:109:G:H8	1.86	0.41
35:YA:1889:A:H2'	35:YA:1890:A:C8	2.56	0.41
44:YO:120:GLU:OE1	49:YT:67:SER:OG	2.37	0.41
1:QA:6:G:H4'	1:QA:298:A:H4'	2.03	0.41
1:QA:444:C:H2'	1:QA:445:G:C8	2.55	0.41
1:QA:943:U:H1'	9:QI:124:GLN:HE22	1.85	0.41
2:QB:84:GLU:HG3	2:QB:215:LEU:HB3	2.02	0.41
33:R8:31:HIS:ND1	33:R8:32:LEU:HG	2.36	0.41
35:RA:252:G:OP1	45:RP:50:ARG:NH1	2.53	0.41
44:RO:34:THR:OG1	44:RO:35:VAL:N	2.54	0.41
1:XA:673:G:H4'	6:XF:87:ARG:NH1	2.36	0.41
1:XA:108:G:N1	20:XT:15:ARG:HG2	2.36	0.41
33:Y8:27:THR:HG22	45:YP:63:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1657:C:H4'	38:YE:133:LYS:HB3	2.01	0.41
55:YZ:5:LEU:HD11	55:YZ:44:PHE:HA	2.02	0.41
1:QA:9:G:H2'	1:QA:10:A:H8	1.86	0.41
2:QB:158:LEU:HA	2:QB:159:PRO:HD3	1.98	0.41
6:QF:24:GLU:O	6:QF:28:ARG:N	2.52	0.41
10:QJ:50:ILE:HB	14:QN:41:ARG:HE	1.85	0.41
17:QQ:6:LEU:HD23	17:QQ:23:VAL:HG11	2.03	0.41
35:RA:679:C:H2'	35:RA:680:G:C8	2.56	0.41
48:RS:25:ARG:NE	48:RS:88:ASP:OD2	2.50	0.41
27:R2:37:PHE:CD1	53:RX:11:PRO:HD3	2.55	0.41
1:XA:1510:U:H2'	1:XA:1511:G:C8	2.55	0.41
34:Y9:37:GLY:HA2	35:YA:1125:G:H5'	2.03	0.41
35:YA:143(A):G:H4'	53:YX:35:THR:HG21	2.02	0.41
35:YA:251:A:C5	35:YA:252:G:H1'	2.56	0.41
35:YA:2576:G:O2'	35:YA:2579:C:OP2	2.27	0.41
35:YA:321:G:O2'	35:YA:340:A:N3	2.53	0.41
35:YA:776:G:N7	35:YA:793:A:O2'	2.54	0.41
35:YA:825:C:O2	45:YP:55:ARG:NH1	2.54	0.41
1:QA:744:C:O2'	1:QA:851:G:N2	2.51	0.41
9:QI:25:LYS:N	9:QI:60:ASP:OD1	2.50	0.41
11:QK:43:SER:HB3	11:QK:68:ALA:HB2	2.03	0.41
38:RE:1:MET:HG3	38:RE:200:GLU:HB3	2.03	0.41
43:RN:123:TYR:OH	43:RN:130:HIS:NE2	2.37	0.41
7:XG:65:ALA:HB1	7:XG:127:ALA:HB3	2.03	0.41
1:XA:881:G:P	12:XL:12:ARG:HH22	2.44	0.41
18:XR:34:TYR:H	18:XR:34:TYR:HD1	1.69	0.41
19:XS:52:TYR:HB2	19:XS:57:HIS:CE1	2.56	0.41
22:XV:15:G:N2	22:XV:21:A:N3	2.69	0.41
35:YA:1082:U:H2'	35:YA:1082:U:H6	1.73	0.41
35:YA:1538:G:H2'	35:YA:1539:G:C8	2.56	0.41
35:YA:2071:A:H2'	35:YA:2072:G:H8	1.85	0.41
25:Y0:14:ARG:O	35:YA:2278:A:N6	2.54	0.41
35:YA:2513:G:N2	38:YE:143:ASN:HD21	2.19	0.41
35:YA:277:C:H4'	35:YA:278:A:H8	1.86	0.41
1:QA:1287:A:H2	1:QA:1353:G:H1'	1.86	0.41
1:QA:41:G:H2'	1:QA:42:G:H8	1.85	0.41
1:QA:986:A:N3	19:QS:52:TYR:OH	2.48	0.41
7:QG:67:GLU:HA	7:QG:70:LYS:HD3	2.01	0.41
37:RD:260:ARG:HH22	37:RD:270:ILE:HD12	1.85	0.41
55:RZ:14:LYS:HA	55:RZ:15:PRO:HD3	1.97	0.41
34:Y9:1:MET:SD	34:Y9:35:ARG:HB2	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:YA:1568:G:OP1	37:YD:63:ARG:NH1	2.42	0.41
35:YA:2144:U:HO2'	35:YA:2147:G:H1	1.66	0.41
35:YA:276:A:H5''	35:YA:277:C:H5'	2.03	0.41
35:YA:729:G:O5'	37:YD:208:LYS:NZ	2.54	0.41
35:YA:854:G:H2'	35:YA:855:G:H8	1.86	0.41
49:YT:16:ARG:HH21	49:YT:81:PRO:HA	1.86	0.41
1:QA:624:C:H2'	1:QA:625:G:C8	2.56	0.40
1:QA:924:C:H2'	1:QA:925:G:C8	2.56	0.40
7:QG:26:PHE:O	7:QG:30:ILE:HG12	2.21	0.40
8:QH:104:ARG:HD3	8:QH:104:ARG:HA	1.91	0.40
1:QA:1226:C:P	13:QM:91:ARG:HH12	2.44	0.40
35:RA:2161:C:H2'	35:RA:2162:G:H8	1.86	0.40
35:RA:2405:G:H5'	45:RP:75:ILE:HD13	2.02	0.40
35:RA:855:G:H1	35:RA:922:U:H3	1.68	0.40
38:RE:2:LYS:HG2	38:RE:200:GLU:HB2	2.03	0.40
49:RT:30:VAL:HG22	49:RT:86:ILE:HG12	2.02	0.40
1:XA:1000:U:H2'	1:XA:1001(A):A:C8	2.56	0.40
1:XA:157:G:H1	1:XA:164:U:H3	1.68	0.40
2:XB:54:THR:HG22	2:XB:199:TYR:HB3	2.02	0.40
8:XH:105:ARG:HA	8:XH:105:ARG:HD3	1.94	0.40
9:XI:48:GLU:OE2	9:XI:51:ARG:NE	2.44	0.40
35:YA:2805:G:H2'	35:YA:2807:G:C8	2.56	0.40
38:YE:21:VAL:HA	38:YE:22:PRO:HD3	1.94	0.40
41:YH:106:THR:O	41:YH:106:THR:OG1	2.31	0.40
44:YO:8:LEU:HD13	44:YO:82:ASN:HB3	2.03	0.40
1:QA:1294:G:H2'	1:QA:1295:G:H8	1.86	0.40
2:QB:177:ALA:HB1	2:QB:182:ILE:HB	2.03	0.40
3:QC:3:ASN:N	3:QC:3:ASN:OD1	2.54	0.40
7:QG:16:LEU:HD21	9:QI:45:ALA:HB2	2.02	0.40
25:R0:23:VAL:HG22	25:R0:38:VAL:HG22	2.03	0.40
30:R5:19:ARG:HH11	30:R5:19:ARG:HD3	1.78	0.40
1:QA:1484:C:O2'	35:RA:1960:A:O2'	2.24	0.40
35:RA:459:U:H2'	35:RA:460:A:H8	1.86	0.40
35:RA:535:C:O3'	50:RU:53:ARG:NH1	2.54	0.40
37:RD:133:LEU:HB3	37:RD:173:VAL:HG21	2.03	0.40
37:RD:231:HIS:CD2	37:RD:249:PRO:HG3	2.55	0.40
42:RI:72:LEU:HA	42:RI:75:LEU:HD22	2.03	0.40
46:RQ:119:ARG:O	46:RQ:123:HIS:ND1	2.50	0.40
48:RS:15:ARG:O	48:RS:19:LYS:HG2	2.21	0.40
55:RZ:151:HIS:CE1	55:RZ:153:SER:HB2	2.57	0.40
1:XA:1408:A:N1	57:XA:1794:PAR:O61	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:XM:99:ARG:HB2	13:XM:101:GLN:NE2	2.36	0.40
16:XP:20:VAL:HG21	16:XP:32:TYR:CE2	2.50	0.40
24:XY:62:C:H2'	24:XY:63:G:C8	2.57	0.40
27:Y2:55:ARG:HB3	27:Y2:59:ARG:HH12	1.87	0.40
35:YA:2441:C:OP2	35:YA:2586:C:O2'	2.35	0.40
38:YE:3:GLY:HA2	38:YE:199:ARG:HA	2.03	0.40
35:YA:323:G:C8	39:YF:171:PRO:HG3	2.56	0.40
49:YT:24:PRO:HD3	49:YT:52:ILE:HD12	2.03	0.40
1:QA:537:G:H5''	12:QL:113:ARG:HH12	1.86	0.40
1:QA:718:G:C8	11:QK:116:HIS:HB3	2.56	0.40
5:QE:50:GLU:HB2	5:QE:53:LEU:HD13	2.02	0.40
13:QM:40:ASN:HB3	13:QM:43:THR:HG23	2.02	0.40
25:R0:39:ARG:HH21	35:RA:2355:C:H1'	1.85	0.40
35:RA:1500:G:H21	37:RD:100:GLY:HA3	1.86	0.40
35:RA:2572:A:O2'	38:RE:144:ARG:NH1	2.54	0.40
37:RD:16:MET:SD	37:RD:211:ARG:NH2	2.88	0.40
51:RV:62:LEU:HD11	51:RV:95:LEU:HB2	2.03	0.40
55:RZ:8:TYR:C	55:RZ:38:TYR:HD1	2.24	0.40
3:XC:108:ASN:HD21	3:XC:144:SER:HB3	1.87	0.40
28:Y3:8:LEU:HB2	28:Y3:28:LEU:HD13	2.02	0.40
35:YA:1007:C:H5''	43:YN:35:ARG:NH1	2.36	0.40
35:YA:1084:A:H8	35:YA:1085:A:H4'	1.86	0.40
35:YA:1316:U:H2'	35:YA:1317:A:H8	1.86	0.40
35:YA:1394:U:O2	53:YX:16:LYS:NZ	2.45	0.40
35:YA:1754:C:OP1	49:YT:96:ARG:NH1	2.55	0.40
35:YA:192:C:O2'	35:YA:802:A:N3	2.47	0.40
37:YD:69:ARG:HH11	37:YD:105:ILE:HG21	1.87	0.40
1:QA:1184:G:H2'	1:QA:1185:G:H8	1.86	0.40
1:QA:392:G:OP1	16:QP:8:ARG:NH2	2.51	0.40
4:QD:53:ASP:HB3	4:QD:57:ARG:NH1	2.36	0.40
11:QK:99:GLN:HG2	11:QK:105:VAL:HG21	2.04	0.40
33:R8:5:LYS:HG2	35:RA:242:G:C8	2.56	0.40
35:RA:1417:C:O2'	35:RA:1587:A:N3	2.45	0.40
35:RA:521:G:H2'	35:RA:522:G:C8	2.57	0.40
54:RY:27:VAL:HG12	54:RY:39:VAL:HG22	2.04	0.40
5:XE:6:PHE:CD1	5:XE:36:ASP:HB3	2.57	0.40
25:Y0:46:LYS:HB2	25:Y0:78:TYR:CD1	2.56	0.40
35:YA:1593:G:H2'	35:YA:1594:G:C8	2.57	0.40
1:QA:56:U:H2'	1:QA:57:G:C8	2.56	0.40
29:R4:28:LYS:HD2	29:R4:31:ILE:HD11	2.03	0.40
35:RA:614(D):A:C4	39:RF:180:GLY:HA3	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:RG:32:PRO:HB3	40:RG:163:ALA:HB2	2.03	0.40
35:RA:390:A:C6	45:RP:71:VAL:HG21	2.56	0.40
1:XA:1053:G:N7	1:XA:1200:C:H5''	2.37	0.40
1:XA:107:G:OP1	1:XA:325:A:N6	2.55	0.40
1:XA:1095:U:P	1:XA:1108:G:H1	2.44	0.40
9:XI:24:GLY:N	9:XI:60:ASP:OD1	2.37	0.40
35:YA:1400:G:H2'	35:YA:1401:G:C8	2.57	0.40
35:YA:787:U:H5''	35:YA:788:A:H5'	2.03	0.40
37:YD:206:LEU:HA	37:YD:211:ARG:HD2	2.03	0.40
37:YD:245:PRO:HA	37:YD:246:PRO:HD3	1.94	0.40
38:YE:134:ILE:HA	38:YE:137:HIS:CD2	2.57	0.40
35:YA:1012:U:C4	43:YN:25:ARG:HD3	2.56	0.40
45:YP:106:LEU:HD11	45:YP:112:LEU:HB2	2.04	0.40
46:YQ:39:PRO:HB3	46:YQ:99:PRO:HD3	2.03	0.40
55:YZ:108:PRO:HB3	55:YZ:144:LEU:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	QB	229/256 (90%)	202 (88%)	19 (8%)	8 (4%)	3	20
2	XB	229/256 (90%)	204 (89%)	22 (10%)	3 (1%)	12	42
3	QC	204/239 (85%)	197 (97%)	7 (3%)	0	100	100
3	XC	204/239 (85%)	195 (96%)	9 (4%)	0	100	100
4	QD	206/209 (99%)	195 (95%)	10 (5%)	1 (0%)	29	64
4	XD	206/209 (99%)	199 (97%)	7 (3%)	0	100	100
5	QE	146/162 (90%)	140 (96%)	6 (4%)	0	100	100
5	XE	146/162 (90%)	141 (97%)	5 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	QF	98/101 (97%)	98 (100%)	0	0	100	100
6	XF	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
7	QG	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
7	XG	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
8	QH	135/138 (98%)	132 (98%)	3 (2%)	0	100	100
8	XH	135/138 (98%)	133 (98%)	2 (2%)	0	100	100
9	QI	125/128 (98%)	110 (88%)	15 (12%)	0	100	100
9	XI	124/128 (97%)	111 (90%)	13 (10%)	0	100	100
10	QJ	95/105 (90%)	81 (85%)	11 (12%)	3 (3%)	4	22
10	XJ	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	7	30
11	QK	112/129 (87%)	107 (96%)	5 (4%)	0	100	100
11	XK	112/129 (87%)	108 (96%)	4 (4%)	0	100	100
12	QL	119/132 (90%)	105 (88%)	12 (10%)	2 (2%)	9	36
12	XL	119/132 (90%)	109 (92%)	6 (5%)	4 (3%)	3	21
13	QM	114/126 (90%)	107 (94%)	4 (4%)	3 (3%)	5	26
13	XM	112/126 (89%)	106 (95%)	6 (5%)	0	100	100
14	QN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
14	XN	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
15	QO	86/89 (97%)	82 (95%)	3 (4%)	1 (1%)	13	44
15	XO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	QP	80/88 (91%)	79 (99%)	1 (1%)	0	100	100
16	XP	80/88 (91%)	76 (95%)	4 (5%)	0	100	100
17	QQ	97/105 (92%)	90 (93%)	7 (7%)	0	100	100
17	XQ	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
18	QR	66/88 (75%)	66 (100%)	0	0	100	100
18	XR	66/88 (75%)	66 (100%)	0	0	100	100
19	QS	81/93 (87%)	78 (96%)	3 (4%)	0	100	100
19	XS	81/93 (87%)	77 (95%)	4 (5%)	0	100	100
20	QT	94/106 (89%)	91 (97%)	3 (3%)	0	100	100
20	XT	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
21	QU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	XU	21/27 (78%)	20 (95%)	1 (5%)	0	100	100
25	R0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
25	Y0	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
26	R1	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	Y1	95/98 (97%)	94 (99%)	1 (1%)	0	100	100
27	R2	68/72 (94%)	68 (100%)	0	0	100	100
27	Y2	68/72 (94%)	68 (100%)	0	0	100	100
28	R3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
28	Y3	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
29	R4	67/71 (94%)	59 (88%)	7 (10%)	1 (2%)	10	39
29	Y4	67/71 (94%)	54 (81%)	8 (12%)	5 (8%)	1	6
30	R5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
30	Y5	57/60 (95%)	56 (98%)	1 (2%)	0	100	100
31	R6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
31	Y6	51/54 (94%)	49 (96%)	2 (4%)	0	100	100
32	R7	46/49 (94%)	46 (100%)	0	0	100	100
32	Y7	46/49 (94%)	46 (100%)	0	0	100	100
33	R8	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
33	Y8	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
34	R9	35/37 (95%)	35 (100%)	0	0	100	100
34	Y9	35/37 (95%)	35 (100%)	0	0	100	100
37	RD	273/276 (99%)	263 (96%)	10 (4%)	0	100	100
37	YD	273/276 (99%)	264 (97%)	9 (3%)	0	100	100
38	RE	202/206 (98%)	195 (96%)	6 (3%)	1 (0%)	29	64
38	YE	202/206 (98%)	192 (95%)	9 (4%)	1 (0%)	29	64
39	RF	200/210 (95%)	196 (98%)	4 (2%)	0	100	100
39	YF	200/210 (95%)	198 (99%)	2 (1%)	0	100	100
40	RG	179/182 (98%)	163 (91%)	13 (7%)	3 (2%)	9	36
40	YG	179/182 (98%)	161 (90%)	16 (9%)	2 (1%)	14	46
41	RH	172/180 (96%)	166 (96%)	6 (4%)	0	100	100
41	YH	171/180 (95%)	165 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	RI	145/148 (98%)	134 (92%)	11 (8%)	0	100	100
42	YI	144/148 (97%)	140 (97%)	4 (3%)	0	100	100
43	RN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
43	YN	138/140 (99%)	133 (96%)	5 (4%)	0	100	100
44	RO	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
44	YO	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
45	RP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
45	YP	147/150 (98%)	139 (95%)	8 (5%)	0	100	100
46	RQ	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
46	YQ	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
47	RR	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
47	YR	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
48	RS	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
48	YS	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
49	RT	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
49	YT	129/146 (88%)	126 (98%)	3 (2%)	0	100	100
50	RU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
50	YU	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
51	RV	99/101 (98%)	93 (94%)	5 (5%)	1 (1%)	15	49
51	YV	99/101 (98%)	91 (92%)	7 (7%)	1 (1%)	15	49
52	RW	110/113 (97%)	107 (97%)	3 (3%)	0	100	100
52	YW	110/113 (97%)	109 (99%)	1 (1%)	0	100	100
53	RX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
53	YX	93/96 (97%)	90 (97%)	3 (3%)	0	100	100
54	RY	105/110 (96%)	102 (97%)	3 (3%)	0	100	100
54	YY	105/110 (96%)	98 (93%)	7 (7%)	0	100	100
55	RZ	176/206 (85%)	164 (93%)	11 (6%)	1 (1%)	25	59
55	YZ	175/206 (85%)	165 (94%)	8 (5%)	2 (1%)	14	46
All	All	11389/12128 (94%)	10866 (95%)	478 (4%)	45 (0%)	34	69

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QB	17	PHE
2	QB	127	ILE
4	QD	5	ILE
10	QJ	32	ALA
10	QJ	79	ARG
12	QL	48	PRO
13	QM	106	ASN
40	RG	48	GLU
40	RG	49	ASP
51	RV	50	PRO
10	XJ	79	ARG
12	XL	47	LYS
29	Y4	47	GLN
29	Y4	49	PHE
29	Y4	59	PHE
40	YG	96	ARG
55	YZ	52	SER
2	QB	9	GLU
2	QB	21	ARG
2	QB	126	GLU
10	QJ	55	LYS
12	QL	49	ASN
29	R4	56	VAL
40	RG	50	ALA
10	XJ	55	LYS
12	XL	48	PRO
29	Y4	58	ARG
2	QB	22	LYS
13	QM	107	ALA
15	QO	88	ARG
2	XB	9	GLU
2	XB	126	GLU
55	YZ	51	ALA
2	QB	8	LYS
13	QM	105	THR
55	RZ	52	SER
12	XL	46	LYS
29	Y4	48	ARG
40	YG	97	ASP
51	YV	50	PRO
38	RE	52	LEU
38	YE	52	LEU
12	XL	88	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	XB	125	PRO
2	QB	125	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	QB	191/220 (87%)	188 (98%)	3 (2%)	62	84
2	XB	187/220 (85%)	184 (98%)	3 (2%)	62	84
3	QC	144/188 (77%)	143 (99%)	1 (1%)	84	93
3	XC	140/188 (74%)	138 (99%)	2 (1%)	67	86
4	QD	171/181 (94%)	168 (98%)	3 (2%)	59	82
4	XD	172/181 (95%)	172 (100%)	0	100	100
5	QE	114/123 (93%)	113 (99%)	1 (1%)	78	91
5	XE	114/123 (93%)	113 (99%)	1 (1%)	78	91
6	QF	85/90 (94%)	85 (100%)	0	100	100
6	XF	85/90 (94%)	84 (99%)	1 (1%)	71	88
7	QG	120/127 (94%)	118 (98%)	2 (2%)	60	83
7	XG	119/127 (94%)	117 (98%)	2 (2%)	60	83
8	QH	116/119 (98%)	116 (100%)	0	100	100
8	XH	114/119 (96%)	113 (99%)	1 (1%)	78	91
9	QI	91/99 (92%)	91 (100%)	0	100	100
9	XI	88/99 (89%)	88 (100%)	0	100	100
10	QJ	68/92 (74%)	68 (100%)	0	100	100
10	XJ	68/92 (74%)	68 (100%)	0	100	100
11	QK	83/99 (84%)	83 (100%)	0	100	100
11	XK	83/99 (84%)	82 (99%)	1 (1%)	71	88
12	QL	96/108 (89%)	95 (99%)	1 (1%)	76	90
12	XL	96/108 (89%)	95 (99%)	1 (1%)	76	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	QM	90/101 (89%)	89 (99%)	1 (1%)	73	89
13	XM	87/101 (86%)	85 (98%)	2 (2%)	50	77
14	QN	49/50 (98%)	49 (100%)	0	100	100
14	XN	49/50 (98%)	49 (100%)	0	100	100
15	QO	78/80 (98%)	77 (99%)	1 (1%)	69	87
15	XO	78/80 (98%)	77 (99%)	1 (1%)	69	87
16	QP	69/74 (93%)	67 (97%)	2 (3%)	42	72
16	XP	68/74 (92%)	65 (96%)	3 (4%)	28	61
17	QQ	94/97 (97%)	94 (100%)	0	100	100
17	XQ	94/97 (97%)	94 (100%)	0	100	100
18	QR	59/77 (77%)	59 (100%)	0	100	100
18	XR	59/77 (77%)	59 (100%)	0	100	100
19	QS	68/80 (85%)	67 (98%)	1 (2%)	65	85
19	XS	67/80 (84%)	67 (100%)	0	100	100
20	QT	71/82 (87%)	71 (100%)	0	100	100
20	XT	70/82 (85%)	70 (100%)	0	100	100
21	QU	18/22 (82%)	18 (100%)	0	100	100
21	XU	18/22 (82%)	18 (100%)	0	100	100
25	R0	61/67 (91%)	59 (97%)	2 (3%)	38	69
25	Y0	61/67 (91%)	60 (98%)	1 (2%)	62	84
26	R1	79/83 (95%)	79 (100%)	0	100	100
26	Y1	81/83 (98%)	81 (100%)	0	100	100
27	R2	65/67 (97%)	64 (98%)	1 (2%)	65	85
27	Y2	66/67 (98%)	65 (98%)	1 (2%)	65	85
28	R3	51/52 (98%)	51 (100%)	0	100	100
28	Y3	50/52 (96%)	49 (98%)	1 (2%)	55	80
29	R4	58/63 (92%)	58 (100%)	0	100	100
29	Y4	54/63 (86%)	52 (96%)	2 (4%)	34	66
30	R5	51/52 (98%)	51 (100%)	0	100	100
30	Y5	50/52 (96%)	49 (98%)	1 (2%)	55	80
31	R6	51/52 (98%)	51 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	Y6	50/52 (96%)	49 (98%)	1 (2%)	55	80
32	R7	41/42 (98%)	41 (100%)	0	100	100
32	Y7	41/42 (98%)	41 (100%)	0	100	100
33	R8	54/55 (98%)	54 (100%)	0	100	100
33	Y8	54/55 (98%)	54 (100%)	0	100	100
34	R9	34/34 (100%)	34 (100%)	0	100	100
34	Y9	34/34 (100%)	34 (100%)	0	100	100
37	RD	214/218 (98%)	213 (100%)	1 (0%)	88	94
37	YD	215/218 (99%)	214 (100%)	1 (0%)	88	94
38	RE	164/166 (99%)	164 (100%)	0	100	100
38	YE	164/166 (99%)	164 (100%)	0	100	100
39	RF	160/166 (96%)	158 (99%)	2 (1%)	69	87
39	YF	159/166 (96%)	157 (99%)	2 (1%)	69	87
40	RG	144/156 (92%)	143 (99%)	1 (1%)	84	93
40	YG	142/156 (91%)	142 (100%)	0	100	100
41	RH	144/148 (97%)	144 (100%)	0	100	100
41	YH	143/148 (97%)	142 (99%)	1 (1%)	84	93
42	RI	111/124 (90%)	111 (100%)	0	100	100
42	YI	108/124 (87%)	107 (99%)	1 (1%)	78	91
43	RN	119/119 (100%)	117 (98%)	2 (2%)	60	83
43	YN	118/119 (99%)	118 (100%)	0	100	100
44	RO	100/100 (100%)	99 (99%)	1 (1%)	76	90
44	YO	100/100 (100%)	99 (99%)	1 (1%)	76	90
45	RP	115/116 (99%)	115 (100%)	0	100	100
45	YP	115/116 (99%)	115 (100%)	0	100	100
46	RQ	111/111 (100%)	111 (100%)	0	100	100
46	YQ	111/111 (100%)	111 (100%)	0	100	100
47	RR	101/101 (100%)	101 (100%)	0	100	100
47	YR	101/101 (100%)	101 (100%)	0	100	100
48	RS	87/88 (99%)	86 (99%)	1 (1%)	73	89
48	YS	85/88 (97%)	84 (99%)	1 (1%)	71	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	RT	115/127 (91%)	113 (98%)	2 (2%)	60	83
49	YT	113/127 (89%)	112 (99%)	1 (1%)	78	91
50	RU	93/94 (99%)	91 (98%)	2 (2%)	52	78
50	YU	93/94 (99%)	91 (98%)	2 (2%)	52	78
51	RV	81/82 (99%)	80 (99%)	1 (1%)	71	88
51	YV	80/82 (98%)	79 (99%)	1 (1%)	69	87
52	RW	90/92 (98%)	90 (100%)	0	100	100
52	YW	90/92 (98%)	90 (100%)	0	100	100
53	RX	77/78 (99%)	77 (100%)	0	100	100
53	YX	77/78 (99%)	77 (100%)	0	100	100
54	RY	86/91 (94%)	86 (100%)	0	100	100
54	YY	86/91 (94%)	84 (98%)	2 (2%)	50	77
55	RZ	152/179 (85%)	149 (98%)	3 (2%)	55	80
55	YZ	148/179 (83%)	146 (99%)	2 (1%)	67	86
All	All	9329/10064 (93%)	9254 (99%)	75 (1%)	81	92

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	QB	21	ARG
2	QB	23	ARG
2	QB	212	GLN
3	QC	193	TYR
4	QD	31	CYS
4	QD	38	TYR
4	QD	209	ARG
5	QE	127	ASN
7	QG	94	ARG
7	QG	155	ARG
12	QL	89	ARG
13	QM	23	TYR
15	QO	65	ARG
16	QP	32	TYR
16	QP	38	TYR
19	QS	78	ARG
25	R0	14	ARG
25	R0	45	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	R2	65	ASN
37	RD	84	TYR
39	RF	44	ARG
39	RF	99	TYR
40	RG	181	ARG
43	RN	78	TYR
43	RN	114	ARG
44	RO	49	ARG
48	RS	25	ARG
49	RT	39	ARG
49	RT	51	ARG
50	RU	52	ARG
50	RU	55	ARG
51	RV	91	TYR
55	RZ	38	TYR
55	RZ	131	ARG
55	RZ	136	PHE
2	XB	8	LYS
2	XB	94	ASN
2	XB	96	ARG
3	XC	21	ARG
3	XC	119	ARG
5	XE	127	ASN
6	XF	50	TYR
7	XG	32	ARG
7	XG	115	ARG
8	XH	84	ARG
11	XK	117	ASN
12	XL	89	ARG
13	XM	23	TYR
13	XM	80	ARG
15	XO	65	ARG
16	XP	8	ARG
16	XP	32	TYR
16	XP	38	TYR
25	Y0	14	ARG
27	Y2	65	ASN
28	Y3	5	LYS
29	Y4	61	ARG
29	Y4	68	ARG
30	Y5	40	LYS
31	Y6	18	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
37	YD	84	TYR
39	YF	44	ARG
39	YF	62	ARG
41	YH	54	ARG
42	YI	57	ARG
44	YO	49	ARG
48	YS	25	ARG
49	YT	93	ARG
50	YU	52	ARG
50	YU	55	ARG
51	YV	91	TYR
54	YY	20	TYR
54	YY	73	ARG
55	YZ	38	TYR
55	YZ	156	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
4	QD	45	GLN
4	QD	77	ASN
4	QD	129	ASN
4	QD	161	ASN
4	QD	201	GLN
5	QE	72	GLN
5	QE	127	ASN
7	QG	68	ASN
9	QI	73	GLN
9	QI	124	GLN
10	QJ	69	ASN
12	QL	80	HIS
15	QO	37	ASN
20	QT	16	HIS
27	R2	65	ASN
38	RE	137	HIS
39	RF	40	GLN
40	RG	108	ASN
41	RH	74	ASN
52	RW	60	ASN
52	RW	61	ASN
53	RX	41	ASN
55	RZ	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	XB	113	HIS
5	XE	127	ASN
6	XF	73	ASN
7	XG	68	ASN
10	XJ	69	ASN
13	XM	106	ASN
15	XO	37	ASN
20	XT	16	HIS
37	YD	87	ASN
45	YP	70	GLN
53	YX	41	ASN
55	YZ	55	HIS
55	YZ	121	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	QA	1494/1522 (98%)	238 (15%)	15 (1%)
1	XA	1498/1522 (98%)	230 (15%)	15 (1%)
22	QV	76/77 (98%)	15 (19%)	0
22	XV	76/77 (98%)	13 (17%)	0
23	QX	17/19 (89%)	6 (35%)	1 (5%)
23	XX	17/19 (89%)	8 (47%)	1 (5%)
24	QY	75/76 (98%)	31 (41%)	0
24	XY	75/76 (98%)	33 (44%)	0
35	RA	2857/2915 (98%)	452 (15%)	16 (0%)
35	YA	2857/2915 (98%)	454 (15%)	15 (0%)
36	RB	119/122 (97%)	10 (8%)	0
36	YB	119/122 (97%)	11 (9%)	0
All	All	9280/9462 (98%)	1501 (16%)	63 (0%)

All (1501) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	QA	5	U
1	QA	6	G
1	QA	9	G
1	QA	22	G
1	QA	32	A
1	QA	39	G
1	QA	47	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	48	C
1	QA	50	A
1	QA	51	A
1	QA	52	G
1	QA	61	G
1	QA	66	G
1	QA	78	G
1	QA	101	A
1	QA	105	G
1	QA	116	A
1	QA	121	C
1	QA	129(B)	G
1	QA	131	C
1	QA	151	A
1	QA	163	C
1	QA	174	C
1	QA	182	U
1	QA	189(F)	U
1	QA	189(G)	U
1	QA	189(H)	G
1	QA	195	A
1	QA	197	A
1	QA	202	U
1	QA	203	U
1	QA	204	U
1	QA	216	G
1	QA	220	G
1	QA	247	G
1	QA	251	G
1	QA	266	G
1	QA	267	C
1	QA	289	G
1	QA	301	G
1	QA	321	A
1	QA	328	C
1	QA	332	G
1	QA	346	G
1	QA	350	G
1	QA	351	G
1	QA	352	C
1	QA	353	A
1	QA	354	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	356	A
1	QA	367	U
1	QA	372	C
1	QA	373	A
1	QA	384	G
1	QA	388	G
1	QA	397	A
1	QA	398	C
1	QA	406	G
1	QA	412	A
1	QA	413	G
1	QA	424	G
1	QA	429	U
1	QA	439	A
1	QA	452	A
1	QA	461	A
1	QA	470	C
1	QA	482	A
1	QA	484	G
1	QA	485	G
1	QA	496	A
1	QA	498	U
1	QA	508	C
1	QA	509	A
1	QA	510	A
1	QA	511	C
1	QA	518	C
1	QA	521	G
1	QA	532	A
1	QA	533	A
1	QA	547	A
1	QA	559	A
1	QA	560	U
1	QA	561	U
1	QA	564	C
1	QA	567	G
1	QA	572	A
1	QA	573	A
1	QA	576	G
1	QA	577	G
1	QA	596	C
1	QA	630	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	631	G
1	QA	653	A
1	QA	665	A
1	QA	666	G
1	QA	687	A
1	QA	688	G
1	QA	695	A
1	QA	721	G
1	QA	723	U
1	QA	731	G
1	QA	734	G
1	QA	749	C
1	QA	755	G
1	QA	760	G
1	QA	774	G
1	QA	777	A
1	QA	793	U
1	QA	794	A
1	QA	815	A
1	QA	816	A
1	QA	817	C
1	QA	821	G
1	QA	828	A
1	QA	829	G
1	QA	836	G
1	QA	840	C
1	QA	841	U
1	QA	848	C
1	QA	851	G
1	QA	902	G
1	QA	914	A
1	QA	916	G
1	QA	926	G
1	QA	927	G
1	QA	934	C
1	QA	942	G
1	QA	960	U
1	QA	961	U
1	QA	968	A
1	QA	969	A
1	QA	971	G
1	QA	974	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	975	A
1	QA	976	G
1	QA	977	A
1	QA	981	U
1	QA	982	U
1	QA	992	U
1	QA	993	G
1	QA	1002	G
1	QA	1004	A
1	QA	1005	A
1	QA	1006	C
1	QA	1009	G
1	QA	1020	U
1	QA	1022	G
1	QA	1023	G
1	QA	1025	U
1	QA	1026	G
1	QA	1027	C
1	QA	1028	C
1	QA	1029	C
1	QA	1030(B)	G
1	QA	1030(C)	C
1	QA	1031	G
1	QA	1036	G
1	QA	1044	A
1	QA	1053	G
1	QA	1054	C
1	QA	1065	U
1	QA	1066	C
1	QA	1068	G
1	QA	1070	U
1	QA	1081	G
1	QA	1094	G
1	QA	1095	U
1	QA	1101	A
1	QA	1108	G
1	QA	1117	G
1	QA	1125	U
1	QA	1129	C
1	QA	1130	A
1	QA	1136	U
1	QA	1137	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1139	G
1	QA	1146	A
1	QA	1147	C
1	QA	1152	A
1	QA	1157	A
1	QA	1159	U
1	QA	1183	A
1	QA	1187	G
1	QA	1196	U
1	QA	1197	G
1	QA	1201	A
1	QA	1211	U
1	QA	1214	C
1	QA	1224	G
1	QA	1227	A
1	QA	1228	C
1	QA	1236	A
1	QA	1238	A
1	QA	1250	A
1	QA	1256	A
1	QA	1257	U
1	QA	1258	G
1	QA	1260	C
1	QA	1270	C
1	QA	1278	U
1	QA	1279	A
1	QA	1280	A
1	QA	1282	C
1	QA	1287	A
1	QA	1300	G
1	QA	1302	U
1	QA	1303	C
1	QA	1305	G
1	QA	1320	C
1	QA	1340	A
1	QA	1346	A
1	QA	1347	G
1	QA	1353	G
1	QA	1363(A)	C
1	QA	1370	G
1	QA	1397	C
1	QA	1399	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1404	5MC
1	QA	1419	G
1	QA	1442(A)	G
1	QA	1442(B)	G
1	QA	1447	A
1	QA	1452	C
1	QA	1456	G
1	QA	1469	G
1	QA	1487	G
1	QA	1490	C
1	QA	1492	A
1	QA	1497	G
1	QA	1499	A
1	QA	1503	A
1	QA	1504	G
1	QA	1506	U
1	QA	1517	G
1	QA	1520	G
1	QA	1529	G
1	QA	1530	G
1	QA	1531	A
22	QV	3	C
22	QV	8	U
22	QV	14	A
22	QV	16	C
22	QV	17	C
22	QV	17(A)	U
22	QV	18	G
22	QV	19	G
22	QV	20	U
22	QV	21	A
22	QV	47	U
22	QV	48	C
22	QV	49	G
22	QV	65	C
22	QV	76	A
23	QX	7	G
23	QX	10	G
23	QX	11	U
23	QX	13	A
23	QX	15	A
23	QX	19	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	QY	2	G
24	QY	8	U
24	QY	9	A
24	QY	16	C
24	QY	17	U
24	QY	18	G
24	QY	19	G
24	QY	21	A
24	QY	29	U
24	QY	30	G
24	QY	43	G
24	QY	46	G
24	QY	47	U
24	QY	48	C
24	QY	49	A
24	QY	50	G
24	QY	51	C
24	QY	52	G
24	QY	55	U
24	QY	56	C
24	QY	57	G
24	QY	58	A
24	QY	61	C
24	QY	67	A
24	QY	68	G
24	QY	69	C
24	QY	71	C
24	QY	72	C
24	QY	73	A
24	QY	74	C
24	QY	75	C
35	RA	10	G
35	RA	15	G
35	RA	34	C
35	RA	45	C
35	RA	51	G
35	RA	71	A
35	RA	74	A
35	RA	75	G
35	RA	84	A
35	RA	102	G
35	RA	118	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	119	A
35	RA	120	U
35	RA	131	G
35	RA	157	U
35	RA	182	A
35	RA	188	G
35	RA	196	A
35	RA	199	A
35	RA	205	G
35	RA	214	G
35	RA	216	A
35	RA	221	A
35	RA	222	A
35	RA	229	A
35	RA	230	U
35	RA	248	G
35	RA	265	A
35	RA	272(K)	U
35	RA	272(N)	U
35	RA	273(B)	U
35	RA	273(C)	G
35	RA	278	A
35	RA	311	A
35	RA	317	G
35	RA	324	A
35	RA	329	G
35	RA	330	A
35	RA	331	A
35	RA	338	G
35	RA	342	G
35	RA	345	A
35	RA	352	G
35	RA	362	U
35	RA	363(A)	G
35	RA	372	G
35	RA	386	G
35	RA	396	G
35	RA	405	U
35	RA	411	G
35	RA	412	A
35	RA	428	A
35	RA	444	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	455	C
35	RA	457	A
35	RA	467	G
35	RA	470	A
35	RA	481	G
35	RA	491	G
35	RA	505	A
35	RA	508	G
35	RA	509	C
35	RA	530	G
35	RA	531	C
35	RA	532	A
35	RA	533	G
35	RA	563	G
35	RA	573	G
35	RA	575	A
35	RA	583	G
35	RA	586	A
35	RA	603	A
35	RA	604	G
35	RA	607	U
35	RA	614(B)	U
35	RA	614(C)	G
35	RA	615	G
35	RA	620	G
35	RA	627	A
35	RA	634	C
35	RA	637	A
35	RA	645	C
35	RA	646	A
35	RA	652(C)	A
35	RA	652(D)	G
35	RA	652(V)	G
35	RA	669	G
35	RA	686	G
35	RA	717	G
35	RA	726	G
35	RA	730	C
35	RA	734	A
35	RA	753	C
35	RA	764	A
35	RA	765	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	775	G
35	RA	776	G
35	RA	782	A
35	RA	784	A
35	RA	785	G
35	RA	788	A
35	RA	789	A
35	RA	792	G
35	RA	805	G
35	RA	812	C
35	RA	827	U
35	RA	831	G
35	RA	857	C
35	RA	859	G
35	RA	881	G
35	RA	886	C
35	RA	887	A
35	RA	888	C
35	RA	889	C
35	RA	890	A
35	RA	893	C
35	RA	896	A
35	RA	897	C
35	RA	898	C
35	RA	899	A
35	RA	907	U
35	RA	910	A
35	RA	915	C
35	RA	917	A
35	RA	932	G
35	RA	941	A
35	RA	945	A
35	RA	946	G
35	RA	953	A
35	RA	957	A
35	RA	959	A
35	RA	961	C
35	RA	974	G
35	RA	975(A)	C
35	RA	983	A
35	RA	996	A
35	RA	1005	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1012	U
35	RA	1013	C
35	RA	1022	G
35	RA	1025	G
35	RA	1026	U
35	RA	1033	U
35	RA	1045	A
35	RA	1046	A
35	RA	1047	G
35	RA	1051	G
35	RA	1052	C
35	RA	1054	A
35	RA	1058	G
35	RA	1060	U
35	RA	1063	G
35	RA	1064	C
35	RA	1065	U
35	RA	1066	U
35	RA	1067	A
35	RA	1068	G
35	RA	1070	A
35	RA	1071	G
35	RA	1073	A
35	RA	1074	G
35	RA	1076	C
35	RA	1077	A
35	RA	1079	C
35	RA	1082	U
35	RA	1083	U
35	RA	1084	A
35	RA	1085	A
35	RA	1086	A
35	RA	1088	A
35	RA	1090	U
35	RA	1092	C
35	RA	1094	U
35	RA	1096	A
35	RA	1097	U
35	RA	1098	A
35	RA	1108	U
35	RA	1109	C
35	RA	1110	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1112	G
35	RA	1128	A
35	RA	1130	U
35	RA	1135	C
35	RA	1136	G
35	RA	1155	A
35	RA	1171	G
35	RA	1188	U
35	RA	1206	G
35	RA	1211	U
35	RA	1220	A
35	RA	1236	G
35	RA	1247	A
35	RA	1250	G
35	RA	1253	A
35	RA	1256	G
35	RA	1265	A
35	RA	1271	G
35	RA	1272	A
35	RA	1273	U
35	RA	1300	U
35	RA	1301	A
35	RA	1314	C
35	RA	1341	U
35	RA	1352	U
35	RA	1359	A
35	RA	1360	A
35	RA	1365	A
35	RA	1368	G
35	RA	1379	A
35	RA	1384	A
35	RA	1385	G
35	RA	1395	A
35	RA	1416	G
35	RA	1417	C
35	RA	1419	A
35	RA	1420	U
35	RA	1421	G
35	RA	1427	A
35	RA	1428	C
35	RA	1429	G
35	RA	1445(A)	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1450(A)	G
35	RA	1455	G
35	RA	1459	G
35	RA	1460	A
35	RA	1461	G
35	RA	1467	C
35	RA	1471	A
35	RA	1482	G
35	RA	1490	A
35	RA	1493	C
35	RA	1494	A
35	RA	1497	U
35	RA	1508	A
35	RA	1509(A)	C
35	RA	1509(B)	A
35	RA	1542	A
35	RA	1543	C
35	RA	1554	A
35	RA	1558	A
35	RA	1566	A
35	RA	1569	A
35	RA	1578	U
35	RA	1580	A
35	RA	1584	C
35	RA	1586	A
35	RA	1608	A
35	RA	1609	A
35	RA	1640	C
35	RA	1648	C
35	RA	1674	G
35	RA	1696	G
35	RA	1700	A
35	RA	1701	A
35	RA	1721	G
35	RA	1722	A
35	RA	1750	G
35	RA	1756	G
35	RA	1762	A
35	RA	1763	G
35	RA	1764	G
35	RA	1773	A
35	RA	1774	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	1780	A
35	RA	1786	A
35	RA	1791	A
35	RA	1800	C
35	RA	1801	G
35	RA	1816	G
35	RA	1828	G
35	RA	1829	A
35	RA	1835	G
35	RA	1847	A
35	RA	1848	A
35	RA	1877	A
35	RA	1878	G
35	RA	1900	A
35	RA	1906	G
35	RA	1913	A
35	RA	1914	C
35	RA	1927	A
35	RA	1929	G
35	RA	1930	G
35	RA	1936	A
35	RA	1938	A
35	RA	1955	U
35	RA	1963	U
35	RA	1967	C
35	RA	1970	A
35	RA	1971	A
35	RA	1972	A
35	RA	1984	G
35	RA	1992	G
35	RA	1993	U
35	RA	1997	G
35	RA	2004	G
35	RA	2020	A
35	RA	2023	G
35	RA	2031	A
35	RA	2032	G
35	RA	2033	A
35	RA	2043	C
35	RA	2055	C
35	RA	2056	G
35	RA	2060	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2061	G
35	RA	2062	A
35	RA	2069	G
35	RA	2093	G
35	RA	2096	U
35	RA	2099	U
35	RA	2103	C
35	RA	2104	G
35	RA	2105	C
35	RA	2107	C
35	RA	2108	C
35	RA	2112	G
35	RA	2116	G
35	RA	2117	A
35	RA	2119	A
35	RA	2120	G
35	RA	2123	G
35	RA	2126	A
35	RA	2127	G
35	RA	2129	C
35	RA	2131	G
35	RA	2132	U
35	RA	2133	G
35	RA	2134	A
35	RA	2136	C
35	RA	2137	C
35	RA	2145	C
35	RA	2146	C
35	RA	2147	G
35	RA	2148	G
35	RA	2151	G
35	RA	2161	C
35	RA	2165	G
35	RA	2172	U
35	RA	2173	A
35	RA	2176	A
35	RA	2186	G
35	RA	2189	U
35	RA	2192	G
35	RA	2198	A
35	RA	2206	G
35	RA	2207	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2208	A
35	RA	2218	U
35	RA	2219	G
35	RA	2225	A
35	RA	2238	G
35	RA	2239	G
35	RA	2249	U
35	RA	2269	A
35	RA	2275	C
35	RA	2278	A
35	RA	2279	G
35	RA	2283	C
35	RA	2287	A
35	RA	2288	A
35	RA	2292	C
35	RA	2305	A
35	RA	2308	G
35	RA	2319	G
35	RA	2320	A
35	RA	2321	G
35	RA	2322	A
35	RA	2325	G
35	RA	2334	G
35	RA	2335	A
35	RA	2336	A
35	RA	2343	C
35	RA	2345	G
35	RA	2347	C
35	RA	2350	C
35	RA	2354	G
35	RA	2372	G
35	RA	2383	G
35	RA	2385	C
35	RA	2391	G
35	RA	2396	G
35	RA	2406	U
35	RA	2410	G
35	RA	2422	A
35	RA	2424	C
35	RA	2425	A
35	RA	2426	A
35	RA	2429	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2430	A
35	RA	2435	A
35	RA	2439	A
35	RA	2441	C
35	RA	2445	G
35	RA	2448	A
35	RA	2476	A
35	RA	2478	A
35	RA	2491	U
35	RA	2494	G
35	RA	2502	G
35	RA	2504	U
35	RA	2505	G
35	RA	2518	A
35	RA	2520	C
35	RA	2529	G
35	RA	2554	U
35	RA	2564	A
35	RA	2566	A
35	RA	2567	G
35	RA	2572	A
35	RA	2582	G
35	RA	2602	A
35	RA	2603	G
35	RA	2611	U
35	RA	2612	C
35	RA	2615	U
35	RA	2621	A
35	RA	2629	A
35	RA	2630	G
35	RA	2646	C
35	RA	2654	A
35	RA	2663	G
35	RA	2686	G
35	RA	2689	U
35	RA	2690	C
35	RA	2702	U
35	RA	2703	C
35	RA	2712(B)	A
35	RA	2713	A
35	RA	2714	G
35	RA	2718	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	RA	2726	U
35	RA	2732	G
35	RA	2733	A
35	RA	2748	A
35	RA	2758	A
35	RA	2765	A
35	RA	2778	A
35	RA	2818	G
35	RA	2820	A
35	RA	2821	A
35	RA	2823	A
35	RA	2833	G
35	RA	2835	A
35	RA	2839	G
35	RA	2866	U
35	RA	2872	G
35	RA	2880	C
35	RA	2892	A
35	RA	2894	G
35	RA	2896	C
35	RA	2897	U
36	RB	8	U
36	RB	9	G
36	RB	12	C
36	RB	13	A
36	RB	30	C
36	RB	33	G
36	RB	51	G
36	RB	56	G
36	RB	73	A
36	RB	110	G
1	XA	5	U
1	XA	7	G
1	XA	9	G
1	XA	31	G
1	XA	32	A
1	XA	39	G
1	XA	47	C
1	XA	48	C
1	XA	51	A
1	XA	59	A
1	XA	61	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	66	G
1	XA	88	A
1	XA	89	C
1	XA	101	A
1	XA	105	G
1	XA	116	A
1	XA	121	C
1	XA	129(B)	G
1	XA	131	C
1	XA	144	G
1	XA	151	A
1	XA	163	C
1	XA	174	C
1	XA	182	U
1	XA	189(G)	U
1	XA	189(I)	G
1	XA	195	A
1	XA	197	A
1	XA	202	U
1	XA	203	U
1	XA	204	U
1	XA	216	G
1	XA	220	G
1	XA	247	G
1	XA	250	A
1	XA	251	G
1	XA	266	G
1	XA	267	C
1	XA	289	G
1	XA	301	G
1	XA	321	A
1	XA	328	C
1	XA	332	G
1	XA	346	G
1	XA	350	G
1	XA	351	G
1	XA	352	C
1	XA	353	A
1	XA	354	G
1	XA	356	A
1	XA	367	U
1	XA	372	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	373	A
1	XA	384	G
1	XA	388	G
1	XA	397	A
1	XA	398	C
1	XA	406	G
1	XA	412	A
1	XA	413	G
1	XA	424	G
1	XA	429	U
1	XA	439	A
1	XA	452	A
1	XA	461	A
1	XA	470	C
1	XA	482	A
1	XA	484	G
1	XA	485	G
1	XA	496	A
1	XA	498	U
1	XA	509	A
1	XA	510	A
1	XA	511	C
1	XA	518	C
1	XA	521	G
1	XA	532	A
1	XA	533	A
1	XA	547	A
1	XA	559	A
1	XA	561	U
1	XA	564	C
1	XA	572	A
1	XA	573	A
1	XA	576	G
1	XA	577	G
1	XA	596	C
1	XA	630	G
1	XA	631	G
1	XA	653	A
1	XA	665	A
1	XA	666	G
1	XA	687	A
1	XA	688	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	695	A
1	XA	703	G
1	XA	721	G
1	XA	723	U
1	XA	731	G
1	XA	749	C
1	XA	755	G
1	XA	759	A
1	XA	777	A
1	XA	793	U
1	XA	794	A
1	XA	815	A
1	XA	816	A
1	XA	817	C
1	XA	821	G
1	XA	828	A
1	XA	829	G
1	XA	836	G
1	XA	840	C
1	XA	841	U
1	XA	848	C
1	XA	851	G
1	XA	891	U
1	XA	902	G
1	XA	914	A
1	XA	916	G
1	XA	926	G
1	XA	927	G
1	XA	934	C
1	XA	960	U
1	XA	961	U
1	XA	968	A
1	XA	969	A
1	XA	971	G
1	XA	974	A
1	XA	975	A
1	XA	976	G
1	XA	977	A
1	XA	992	U
1	XA	993	G
1	XA	1002	G
1	XA	1003	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1004	A
1	XA	1005	A
1	XA	1006	C
1	XA	1020	U
1	XA	1023	G
1	XA	1025	U
1	XA	1026	G
1	XA	1027	C
1	XA	1028	C
1	XA	1030(B)	G
1	XA	1030(C)	C
1	XA	1031	G
1	XA	1043	C
1	XA	1044	A
1	XA	1053	G
1	XA	1054	C
1	XA	1065	U
1	XA	1066	C
1	XA	1068	G
1	XA	1081	G
1	XA	1094	G
1	XA	1095	U
1	XA	1100	C
1	XA	1101	A
1	XA	1117	G
1	XA	1125	U
1	XA	1129	C
1	XA	1130	A
1	XA	1136	U
1	XA	1137	C
1	XA	1138	G
1	XA	1139	G
1	XA	1146	A
1	XA	1147	C
1	XA	1152	A
1	XA	1157	A
1	XA	1158	C
1	XA	1159	U
1	XA	1183	A
1	XA	1196	U
1	XA	1197	G
1	XA	1201	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1211	U
1	XA	1214	C
1	XA	1224	G
1	XA	1227	A
1	XA	1236	A
1	XA	1238	A
1	XA	1250	A
1	XA	1256	A
1	XA	1257	U
1	XA	1258	G
1	XA	1260	C
1	XA	1270	C
1	XA	1278	U
1	XA	1279	A
1	XA	1280	A
1	XA	1282	C
1	XA	1285	A
1	XA	1286	A
1	XA	1287	A
1	XA	1300	G
1	XA	1302	U
1	XA	1303	C
1	XA	1305	G
1	XA	1317	C
1	XA	1320	C
1	XA	1340	A
1	XA	1347	G
1	XA	1353	G
1	XA	1363(A)	C
1	XA	1363(B)	A
1	XA	1370	G
1	XA	1397	C
1	XA	1399	C
1	XA	1419	G
1	XA	1442(A)	G
1	XA	1442(B)	G
1	XA	1447	A
1	XA	1456	G
1	XA	1469	G
1	XA	1487	G
1	XA	1492	A
1	XA	1497	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	XA	1499	A
1	XA	1503	A
1	XA	1504	G
1	XA	1506	U
1	XA	1517	G
1	XA	1520	G
1	XA	1529	G
1	XA	1530	G
1	XA	1531	A
22	XV	3	C
22	XV	8	U
22	XV	16	C
22	XV	17(A)	U
22	XV	18	G
22	XV	19	G
22	XV	20	U
22	XV	21	A
22	XV	47	U
22	XV	48	C
22	XV	49	G
22	XV	65	C
22	XV	76	A
23	XX	7	G
23	XX	10	G
23	XX	11	U
23	XX	13	A
23	XX	14	A
23	XX	15	A
23	XX	19	G
23	XX	23	A
24	XY	2	G
24	XY	8	U
24	XY	9	A
24	XY	12	U
24	XY	16	C
24	XY	17	U
24	XY	18	G
24	XY	19	G
24	XY	21	A
24	XY	23	A
24	XY	29	U
24	XY	31	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
24	XY	43	G
24	XY	46	G
24	XY	47	U
24	XY	48	C
24	XY	49	A
24	XY	50	G
24	XY	51	C
24	XY	52	G
24	XY	54	U
24	XY	55	U
24	XY	56	C
24	XY	57	G
24	XY	58	A
24	XY	61	C
24	XY	67	A
24	XY	68	G
24	XY	69	C
24	XY	71	C
24	XY	73	A
24	XY	74	C
24	XY	75	C
35	YA	10	G
35	YA	34	C
35	YA	45	C
35	YA	51	G
35	YA	55	G
35	YA	71	A
35	YA	74	A
35	YA	75	G
35	YA	84	A
35	YA	92	A
35	YA	95	G
35	YA	102	G
35	YA	118	A
35	YA	119	A
35	YA	120	U
35	YA	131	G
35	YA	157	U
35	YA	182	A
35	YA	188	G
35	YA	196	A
35	YA	199	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	205	G
35	YA	215	G
35	YA	216	A
35	YA	221	A
35	YA	222	A
35	YA	228	A
35	YA	229	A
35	YA	230	U
35	YA	233	A
35	YA	248	G
35	YA	265	A
35	YA	272(J)	C
35	YA	272(K)	U
35	YA	272(N)	U
35	YA	273(B)	U
35	YA	273(C)	G
35	YA	277	C
35	YA	278	A
35	YA	311	A
35	YA	317	G
35	YA	324	A
35	YA	329	G
35	YA	330	A
35	YA	338	G
35	YA	342	G
35	YA	345	A
35	YA	352	G
35	YA	362	U
35	YA	363(A)	G
35	YA	372	G
35	YA	386	G
35	YA	396	G
35	YA	405	U
35	YA	411	G
35	YA	412	A
35	YA	428	A
35	YA	444	C
35	YA	455	C
35	YA	457	A
35	YA	467	G
35	YA	470	A
35	YA	481	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	505	A
35	YA	508	G
35	YA	509	C
35	YA	530	G
35	YA	531	C
35	YA	532	A
35	YA	533	G
35	YA	563	G
35	YA	573	G
35	YA	575	A
35	YA	603	A
35	YA	604	G
35	YA	607	U
35	YA	614(C)	G
35	YA	615	G
35	YA	620	G
35	YA	627	A
35	YA	634	C
35	YA	637	A
35	YA	645	C
35	YA	646	A
35	YA	652(C)	A
35	YA	652(D)	G
35	YA	652(V)	G
35	YA	669	G
35	YA	686	G
35	YA	717	G
35	YA	726	G
35	YA	730	C
35	YA	734	A
35	YA	738	G
35	YA	753	C
35	YA	764	A
35	YA	765	G
35	YA	775	G
35	YA	776	G
35	YA	782	A
35	YA	784	A
35	YA	785	G
35	YA	788	A
35	YA	789	A
35	YA	792	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	805	G
35	YA	812	C
35	YA	827	U
35	YA	831	G
35	YA	857	C
35	YA	859	G
35	YA	869	G
35	YA	881	G
35	YA	886	C
35	YA	887	A
35	YA	888	C
35	YA	889	C
35	YA	890	A
35	YA	893	C
35	YA	896	A
35	YA	897	C
35	YA	898	C
35	YA	907	U
35	YA	910	A
35	YA	915	C
35	YA	917	A
35	YA	932	G
35	YA	941	A
35	YA	945	A
35	YA	946	G
35	YA	953	A
35	YA	957	A
35	YA	959	A
35	YA	961	C
35	YA	973	A
35	YA	974	G
35	YA	975(A)	C
35	YA	983	A
35	YA	996	A
35	YA	1005	C
35	YA	1008	C
35	YA	1012	U
35	YA	1013	C
35	YA	1025	G
35	YA	1026	U
35	YA	1033	U
35	YA	1045	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1046	A
35	YA	1047	G
35	YA	1052	C
35	YA	1054	A
35	YA	1058	G
35	YA	1060	U
35	YA	1063	G
35	YA	1064	C
35	YA	1065	U
35	YA	1066	U
35	YA	1067	A
35	YA	1068	G
35	YA	1070	A
35	YA	1071	G
35	YA	1073	A
35	YA	1074	G
35	YA	1076	C
35	YA	1077	A
35	YA	1079	C
35	YA	1082	U
35	YA	1083	U
35	YA	1084	A
35	YA	1085	A
35	YA	1086	A
35	YA	1088	A
35	YA	1092	C
35	YA	1096	A
35	YA	1097	U
35	YA	1098	A
35	YA	1108	U
35	YA	1109	C
35	YA	1110	G
35	YA	1112	G
35	YA	1128	A
35	YA	1129	A
35	YA	1130	U
35	YA	1135	C
35	YA	1136	G
35	YA	1143	A
35	YA	1171	G
35	YA	1206	G
35	YA	1211	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1220	A
35	YA	1236	G
35	YA	1250	G
35	YA	1253	A
35	YA	1256	G
35	YA	1265	A
35	YA	1271	G
35	YA	1272	A
35	YA	1273	U
35	YA	1300	U
35	YA	1301	A
35	YA	1313	U
35	YA	1314	C
35	YA	1352	U
35	YA	1359	A
35	YA	1360	A
35	YA	1365	A
35	YA	1368	G
35	YA	1378	A
35	YA	1379	A
35	YA	1380	G
35	YA	1384	A
35	YA	1385	G
35	YA	1395	A
35	YA	1416	G
35	YA	1417	C
35	YA	1419	A
35	YA	1420	U
35	YA	1421	G
35	YA	1427	A
35	YA	1428	C
35	YA	1445(A)	A
35	YA	1450(A)	G
35	YA	1455	G
35	YA	1459	G
35	YA	1460	A
35	YA	1467	C
35	YA	1471	A
35	YA	1482	G
35	YA	1493	C
35	YA	1494	A
35	YA	1497	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1508	A
35	YA	1509(A)	C
35	YA	1509(B)	A
35	YA	1525	G
35	YA	1542	A
35	YA	1543	C
35	YA	1547	C
35	YA	1558	A
35	YA	1566	A
35	YA	1569	A
35	YA	1578	U
35	YA	1580	A
35	YA	1584	C
35	YA	1586	A
35	YA	1607	C
35	YA	1608	A
35	YA	1609	A
35	YA	1640	C
35	YA	1648	C
35	YA	1674	G
35	YA	1693	U
35	YA	1696	G
35	YA	1698	A
35	YA	1700	A
35	YA	1701	A
35	YA	1721	G
35	YA	1722	A
35	YA	1750	G
35	YA	1756	G
35	YA	1757	U
35	YA	1762	A
35	YA	1763	G
35	YA	1764	G
35	YA	1769	G
35	YA	1773	A
35	YA	1774	C
35	YA	1780	A
35	YA	1786	A
35	YA	1791	A
35	YA	1800	C
35	YA	1801	G
35	YA	1811	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1816	G
35	YA	1828	G
35	YA	1829	A
35	YA	1835	G
35	YA	1847	A
35	YA	1848	A
35	YA	1877	A
35	YA	1878	G
35	YA	1889	A
35	YA	1900	A
35	YA	1914	C
35	YA	1929	G
35	YA	1930	G
35	YA	1936	A
35	YA	1937	A
35	YA	1938	A
35	YA	1955	U
35	YA	1963	U
35	YA	1967	C
35	YA	1970	A
35	YA	1971	A
35	YA	1972	A
35	YA	1984	G
35	YA	1992	G
35	YA	1993	U
35	YA	1997	G
35	YA	2020	A
35	YA	2023	G
35	YA	2031	A
35	YA	2032	G
35	YA	2033	A
35	YA	2043	C
35	YA	2055	C
35	YA	2056	G
35	YA	2060	A
35	YA	2061	G
35	YA	2062	A
35	YA	2069	G
35	YA	2093	G
35	YA	2096	U
35	YA	2099	U
35	YA	2103	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2104	G
35	YA	2105	C
35	YA	2107	C
35	YA	2108	C
35	YA	2116	G
35	YA	2117	A
35	YA	2119	A
35	YA	2120	G
35	YA	2121	G
35	YA	2123	G
35	YA	2127	G
35	YA	2129	C
35	YA	2131	G
35	YA	2132	U
35	YA	2133	G
35	YA	2134	A
35	YA	2136	C
35	YA	2145	C
35	YA	2146	C
35	YA	2147	G
35	YA	2148	G
35	YA	2151	G
35	YA	2158	A
35	YA	2161	C
35	YA	2165	G
35	YA	2172	U
35	YA	2173	A
35	YA	2186	G
35	YA	2189	U
35	YA	2192	G
35	YA	2198	A
35	YA	2206	G
35	YA	2207	G
35	YA	2208	A
35	YA	2218	U
35	YA	2219	G
35	YA	2225	A
35	YA	2238	G
35	YA	2239	G
35	YA	2249	U
35	YA	2269	A
35	YA	2275	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2278	A
35	YA	2279	G
35	YA	2283	C
35	YA	2287	A
35	YA	2288	A
35	YA	2305	A
35	YA	2308	G
35	YA	2309	A
35	YA	2312	U
35	YA	2319	G
35	YA	2320	A
35	YA	2321	G
35	YA	2322	A
35	YA	2325	G
35	YA	2334	G
35	YA	2335	A
35	YA	2336	A
35	YA	2343	C
35	YA	2347	C
35	YA	2350	C
35	YA	2354	G
35	YA	2372	G
35	YA	2383	G
35	YA	2385	C
35	YA	2391	G
35	YA	2396	G
35	YA	2406	U
35	YA	2410	G
35	YA	2422	A
35	YA	2424	C
35	YA	2425	A
35	YA	2427	C
35	YA	2428	G
35	YA	2429	G
35	YA	2430	A
35	YA	2435	A
35	YA	2439	A
35	YA	2441	C
35	YA	2445	G
35	YA	2448	A
35	YA	2476	A
35	YA	2491	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2494	G
35	YA	2502	G
35	YA	2504	U
35	YA	2505	G
35	YA	2518	A
35	YA	2520	C
35	YA	2529	G
35	YA	2554	U
35	YA	2564	A
35	YA	2566	A
35	YA	2567	G
35	YA	2582	G
35	YA	2586	C
35	YA	2602	A
35	YA	2604	U
35	YA	2609	U
35	YA	2611	U
35	YA	2612	C
35	YA	2615	U
35	YA	2629	A
35	YA	2630	G
35	YA	2633	G
35	YA	2646	C
35	YA	2654	A
35	YA	2663	G
35	YA	2673	G
35	YA	2686	G
35	YA	2689	U
35	YA	2690	C
35	YA	2691	C
35	YA	2702	U
35	YA	2703	C
35	YA	2712(B)	A
35	YA	2713	A
35	YA	2714	G
35	YA	2726	U
35	YA	2732	G
35	YA	2733	A
35	YA	2748	A
35	YA	2758	A
35	YA	2764	A
35	YA	2765	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	2766	G
35	YA	2778	A
35	YA	2818	G
35	YA	2820	A
35	YA	2821	A
35	YA	2833	G
35	YA	2835	A
35	YA	2866	U
35	YA	2872	G
35	YA	2892	A
35	YA	2894	G
35	YA	2896	C
35	YA	2897	U
36	YB	8	U
36	YB	9	G
36	YB	12	C
36	YB	13	A
36	YB	24	G
36	YB	30	C
36	YB	33	G
36	YB	51	G
36	YB	56	G
36	YB	73	A
36	YB	110	G

All (63) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	QA	60	A
1	QA	65	U
1	QA	115	G
1	QA	266	G
1	QA	509	A
1	QA	560	U
1	QA	687	A
1	QA	748	C
1	QA	840	C
1	QA	913	A
1	QA	991	U
1	QA	992	U
1	QA	1065	U
1	QA	1067	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	QA	1442(A)	G
23	QX	18	G
35	RA	272(M)	G
35	RA	277	C
35	RA	752	A
35	RA	827	U
35	RA	856	C
35	RA	1057	A
35	RA	1065	U
35	RA	1073	A
35	RA	1210	A
35	RA	1992	G
35	RA	2126	A
35	RA	2171	A
35	RA	2172	U
35	RA	2406	U
35	RA	2601	C
35	RA	2689	U
1	XA	60	A
1	XA	65	U
1	XA	115	G
1	XA	266	G
1	XA	509	A
1	XA	560	U
1	XA	687	A
1	XA	748	C
1	XA	840	C
1	XA	913	A
1	XA	991	U
1	XA	992	U
1	XA	1065	U
1	XA	1067	A
1	XA	1442(A)	G
23	XX	18	G
35	YA	272(M)	G
35	YA	277	C
35	YA	752	A
35	YA	827	U
35	YA	856	C
35	YA	1057	A
35	YA	1065	U
35	YA	1073	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	YA	1210	A
35	YA	1992	G
35	YA	2126	A
35	YA	2171	A
35	YA	2172	U
35	YA	2406	U
35	YA	2689	U

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
35	PSU	YA	1917	56,35	17,21,22	1.69	5 (29%)	20,30,33	3.05	5 (25%)
35	5MC	YA	1962	56,35	15,22,23	1.21	1 (6%)	19,32,35	1.28	3 (15%)
1	2MG	QA	1207	1	19,26,27	1.13	2 (10%)	21,38,41	2.21	7 (33%)
1	4OC	XA	1402	1	16,23,24	0.85	1 (6%)	17,32,35	1.39	1 (5%)
35	PSU	RA	2605	35	17,21,22	1.69	5 (29%)	20,30,33	3.10	6 (30%)
1	2MG	XA	1207	1	19,26,27	1.07	2 (10%)	21,38,41	2.22	7 (33%)
35	5MU	RA	1939	35	15,22,23	1.08	2 (13%)	16,32,35	1.74	2 (12%)
1	PSU	QA	516	1	17,21,22	1.76	5 (29%)	20,30,33	3.25	5 (25%)
35	PSU	YA	1911	35	17,21,22	1.61	5 (29%)	20,30,33	3.07	5 (25%)
35	5MC	YA	1942	35	15,22,23	1.22	1 (6%)	19,32,35	1.31	2 (10%)
1	5MC	XA	1404	1	15,22,23	1.21	1 (6%)	19,32,35	1.34	3 (15%)
35	OMC	YA	1920	35	15,22,23	0.94	1 (6%)	17,31,34	1.62	4 (23%)
35	2MA	YA	2503	56,35	17,25,26	1.22	2 (11%)	19,37,40	2.13	3 (15%)
1	MA6	QA	1518	1	19,26,27	0.97	1 (5%)	18,38,41	1.81	4 (22%)
1	G7M	QA	527	1,56	20,26,27	2.60	4 (20%)	20,39,42	2.02	5 (25%)
12	0TD	XL	92	12	4,9,10	0.57	0	3,11,13	1.85	1 (33%)
1	M2G	XA	966	1	20,27,28	1.17	3 (15%)	22,40,43	2.09	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	M2G	QA	966	1	20,27,28	1.26	3 (15%)	22,40,43	2.02	6 (27%)
35	5MC	RA	1942	35	15,22,23	1.26	1 (6%)	19,32,35	1.29	3 (15%)
35	PSU	RA	1911	35	17,21,22	1.76	5 (29%)	20,30,33	3.00	6 (30%)
35	OMC	RA	1920	35	15,22,23	0.83	0	17,31,34	1.69	3 (17%)
1	MA6	XA	1518	1	19,26,27	0.99	1 (5%)	18,38,41	1.90	4 (22%)
1	5MC	XA	1400	1	15,22,23	1.23	1 (6%)	19,32,35	1.44	3 (15%)
12	0TD	QL	92	12	4,9,10	0.56	0	3,11,13	1.85	1 (33%)
1	5MC	QA	1404	1	15,22,23	1.21	1 (6%)	19,32,35	1.28	3 (15%)
35	PSU	RA	1917	56,35	17,21,22	1.67	5 (29%)	20,30,33	3.11	5 (25%)
35	5MU	YA	1915	35	15,22,23	1.03	2 (13%)	16,32,35	2.01	2 (12%)
35	OMU	RA	2552	56,35	14,22,23	1.06	1 (7%)	14,31,34	0.92	1 (7%)
35	OMG	YA	2251	56,22,35	18,26,27	1.11	2 (11%)	20,38,41	2.04	6 (30%)
1	4OC	QA	1402	1	16,23,24	0.81	1 (6%)	17,32,35	1.39	1 (5%)
1	PSU	XA	516	1	17,21,22	1.62	5 (29%)	20,30,33	3.02	6 (30%)
1	5MC	QA	1407	1	15,22,23	1.23	1 (6%)	19,32,35	1.44	2 (10%)
1	G7M	XA	527	1,56	20,26,27	2.61	4 (20%)	20,39,42	2.08	5 (25%)
1	5MC	QA	967	1	15,22,23	1.32	1 (6%)	19,32,35	1.25	2 (10%)
35	5MU	RA	1915	35	15,22,23	1.03	2 (13%)	16,32,35	2.01	2 (12%)
1	5MC	QA	1400	1	15,22,23	1.23	1 (6%)	19,32,35	1.37	3 (15%)
35	2MA	RA	2503	56,35	17,25,26	1.26	1 (5%)	19,37,40	2.15	3 (15%)
1	MA6	QA	1519	1	19,26,27	0.90	1 (5%)	18,38,41	1.85	6 (33%)
1	UR3	XA	1498	1	14,22,23	0.92	1 (7%)	15,32,35	0.69	0
35	OMG	RA	2251	56,22,35	18,26,27	1.09	2 (11%)	20,38,41	2.05	6 (30%)
35	5MU	YA	1939	35	15,22,23	1.12	2 (13%)	16,32,35	1.80	2 (12%)
35	PSU	YA	2605	35	17,21,22	1.63	5 (29%)	20,30,33	2.99	5 (25%)
1	UR3	QA	1498	1	14,22,23	0.75	0	15,32,35	0.67	0
1	5MC	XA	967	1	15,22,23	1.15	1 (6%)	19,32,35	1.35	3 (15%)
35	5MC	RA	1962	56,35	15,22,23	1.15	1 (6%)	19,32,35	1.41	3 (15%)
35	OMU	YA	2552	56,35	14,22,23	1.03	2 (14%)	14,31,34	0.82	1 (7%)
1	5MC	XA	1407	1	15,22,23	1.13	1 (6%)	19,32,35	1.39	2 (10%)
1	MA6	XA	1519	1	19,26,27	0.90	1 (5%)	18,38,41	1.96	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	YA	1917	56,35	-	0/7/25/26	0/2/2/2
35	5MC	YA	1962	56,35	-	1/5/25/26	0/2/2/2
1	2MG	QA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	XA	1402	1	-	2/9/29/30	0/2/2/2
35	PSU	RA	2605	35	-	0/7/25/26	0/2/2/2
1	2MG	XA	1207	1	-	0/5/27/28	0/3/3/3
35	5MU	RA	1939	35	-	0/5/25/26	0/2/2/2
1	PSU	QA	516	1	-	0/7/25/26	0/2/2/2
35	PSU	YA	1911	35	-	0/7/25/26	0/2/2/2
35	5MC	YA	1942	35	-	0/5/25/26	0/2/2/2
1	5MC	XA	1404	1	-	0/5/25/26	0/2/2/2
35	OMC	YA	1920	35	-	0/7/27/28	0/2/2/2
35	2MA	YA	2503	56,35	-	1/3/25/26	0/3/3/3
1	MA6	QA	1518	1	-	3/7/29/30	0/3/3/3
1	G7M	QA	527	1,56	-	2/3/25/26	0/3/3/3
12	0TD	XL	92	12	-	1/3/12/14	-
1	M2G	XA	966	1	-	0/7/29/30	0/3/3/3
1	M2G	QA	966	1	-	2/7/29/30	0/3/3/3
35	5MC	RA	1942	35	-	0/5/25/26	0/2/2/2
35	PSU	RA	1911	35	-	0/7/25/26	0/2/2/2
35	OMC	RA	1920	35	-	0/7/27/28	0/2/2/2
1	MA6	XA	1518	1	-	3/7/29/30	0/3/3/3
1	5MC	XA	1400	1	-	2/5/25/26	0/2/2/2
12	0TD	QL	92	12	-	1/3/12/14	-
1	5MC	QA	1404	1	-	2/5/25/26	0/2/2/2
35	PSU	RA	1917	56,35	-	0/7/25/26	0/2/2/2
35	5MU	YA	1915	35	-	0/5/25/26	0/2/2/2
35	OMU	RA	2552	56,35	-	1/7/27/28	0/2/2/2
35	OMG	YA	2251	56,22,35	-	0/5/27/28	0/3/3/3
1	4OC	QA	1402	1	-	3/9/29/30	0/2/2/2
1	PSU	XA	516	1	-	0/7/25/26	0/2/2/2
1	5MC	QA	1407	1	-	0/5/25/26	0/2/2/2
1	G7M	XA	527	1,56	-	3/3/25/26	0/3/3/3
1	5MC	QA	967	1	-	0/5/25/26	0/2/2/2
35	5MU	RA	1915	35	-	0/5/25/26	0/2/2/2
1	5MC	QA	1400	1	-	2/5/25/26	0/2/2/2
35	2MA	RA	2503	56,35	-	1/3/25/26	0/3/3/3
1	MA6	QA	1519	1	-	3/7/29/30	0/3/3/3
1	UR3	XA	1498	1	-	0/5/25/26	0/2/2/2
35	OMG	RA	2251	56,22,35	-	0/5/27/28	0/3/3/3
35	5MU	YA	1939	35	-	0/5/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	YA	2605	35	-	0/7/25/26	0/2/2/2
1	UR3	QA	1498	1	-	0/5/25/26	0/2/2/2
1	5MC	XA	967	1	-	0/5/25/26	0/2/2/2
35	5MC	RA	1962	56,35	-	1/5/25/26	0/2/2/2
35	OMU	YA	2552	56,35	-	0/7/27/28	0/2/2/2
1	5MC	XA	1407	1	-	0/5/25/26	0/2/2/2
1	MA6	XA	1519	1	-	3/7/29/30	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	QA	527	G7M	C8-N9	7.12	1.46	1.33
1	XA	527	G7M	C8-N9	7.09	1.46	1.33
1	QA	527	G7M	C8-N7	6.53	1.45	1.33
1	XA	527	G7M	C8-N7	6.25	1.44	1.33
1	XA	527	G7M	C5-C4	5.50	1.47	1.39
1	QA	527	G7M	C5-C4	5.08	1.46	1.39
35	RA	1911	PSU	C5-C1'	-5.08	1.47	1.52
1	QA	516	PSU	C5-C1'	-4.88	1.48	1.52
35	RA	2605	PSU	C5-C1'	-4.53	1.48	1.52
1	QA	967	5MC	C5-C4	4.48	1.48	1.41
35	YA	1917	PSU	C5-C1'	-4.45	1.48	1.52
1	XA	516	PSU	C5-C1'	-4.30	1.48	1.52
35	RA	1942	5MC	C5-C4	4.28	1.48	1.41
35	RA	1917	PSU	C5-C1'	-4.27	1.48	1.52
35	RA	2503	2MA	C6-C5	4.22	1.47	1.41
1	XA	1400	5MC	C5-C4	4.12	1.47	1.41
35	YA	2605	PSU	C5-C1'	-4.11	1.48	1.52
35	YA	1942	5MC	C5-C4	4.08	1.47	1.41
1	QA	1400	5MC	C5-C4	4.05	1.47	1.41
35	YA	2503	2MA	C6-C5	3.96	1.47	1.41
1	QA	1207	2MG	C6-C5	3.94	1.48	1.41
1	QA	966	M2G	C6-C5	3.93	1.48	1.41
1	QA	1404	5MC	C5-C4	3.93	1.47	1.41
35	YA	1962	5MC	C5-C4	3.89	1.47	1.41
1	QA	1407	5MC	C5-C4	3.87	1.47	1.41
35	YA	1911	PSU	C5-C1'	-3.86	1.49	1.52
1	XA	1207	2MG	C6-C5	3.78	1.47	1.41
35	RA	1962	5MC	C5-C4	3.73	1.47	1.41
1	XA	1404	5MC	C5-C4	3.70	1.47	1.41
35	YA	2251	OMG	C6-C5	3.65	1.47	1.41
1	XA	527	G7M	C6-C5	3.64	1.47	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	XA	967	5MC	C5-C4	3.61	1.47	1.41
1	XA	966	M2G	C6-C5	3.59	1.47	1.41
1	QA	527	G7M	C6-C5	3.58	1.47	1.41
35	RA	2251	OMG	C6-C5	3.55	1.47	1.41
1	XA	1407	5MC	C5-C4	3.37	1.46	1.41
35	YA	1911	PSU	C4-C5	3.33	1.48	1.41
1	QA	516	PSU	C4-C5	3.31	1.48	1.41
35	RA	1917	PSU	C4-C5	3.23	1.48	1.41
35	RA	1911	PSU	C4-C5	3.10	1.48	1.41
35	YA	1917	PSU	C4-C5	3.09	1.48	1.41
1	XA	516	PSU	C4-C5	3.08	1.48	1.41
35	YA	2605	PSU	C4-C5	2.93	1.47	1.41
35	RA	2605	PSU	C4-C5	2.89	1.47	1.41
35	RA	1939	5MU	C4-C5	2.86	1.47	1.41
35	RA	1915	5MU	C4-C5	2.79	1.47	1.41
35	YA	1915	5MU	C4-C5	2.75	1.47	1.41
35	YA	1939	5MU	C4-C5	2.74	1.47	1.41
1	QA	966	M2G	C2-N2	2.66	1.39	1.34
35	YA	1939	5MU	C2-N3	-2.62	1.33	1.38
1	XA	966	M2G	C2-N2	2.58	1.39	1.34
35	RA	1939	5MU	C2-N3	-2.53	1.33	1.38
1	QA	1518	MA6	C5-C4	2.48	1.47	1.40
1	QA	516	PSU	O4'-C1'	-2.41	1.41	1.44
35	YA	2605	PSU	C2-N1	-2.40	1.33	1.38
35	YA	1920	OMC	C6-N1	-2.37	1.32	1.35
1	XA	1518	MA6	C5-C4	2.34	1.47	1.40
35	RA	2605	PSU	C2-N1	-2.33	1.33	1.38
1	QA	1519	MA6	C5-C4	2.33	1.47	1.40
35	YA	1917	PSU	C2-N3	-2.33	1.33	1.38
35	YA	1917	PSU	O4'-C1'	-2.32	1.41	1.44
1	XA	1498	UR3	C6-N1	-2.32	1.33	1.35
35	YA	1911	PSU	C2-N3	-2.31	1.33	1.38
35	YA	1911	PSU	C2-N1	-2.31	1.33	1.38
35	YA	1917	PSU	C2-N1	-2.31	1.33	1.38
35	YA	2605	PSU	C2-N3	-2.31	1.33	1.38
1	XA	516	PSU	O4'-C1'	-2.31	1.41	1.44
1	QA	966	M2G	C5-C4	2.30	1.47	1.40
35	RA	1917	PSU	O4'-C1'	-2.30	1.41	1.44
35	RA	1915	5MU	C2-N3	-2.30	1.33	1.38
35	YA	2251	OMG	C5-C4	2.28	1.47	1.40
35	RA	2605	PSU	C2-N3	-2.28	1.33	1.38
35	RA	1917	PSU	C2-N1	-2.27	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	YA	1915	5MU	C2-N3	-2.27	1.33	1.38
1	XA	516	PSU	C2-N3	-2.26	1.33	1.38
35	YA	2552	OMU	C2-N3	-2.26	1.33	1.38
35	RA	1911	PSU	C2-N3	-2.26	1.33	1.38
35	RA	1917	PSU	C2-N3	-2.25	1.33	1.38
1	QA	516	PSU	C2-N1	-2.20	1.33	1.38
35	RA	2605	PSU	O4'-C1'	-2.19	1.41	1.44
1	QA	1207	2MG	C5-C4	2.19	1.46	1.40
35	RA	2552	OMU	C2-N3	-2.18	1.33	1.38
35	RA	1911	PSU	C2-N1	-2.17	1.33	1.38
35	YA	2605	PSU	O4'-C1'	-2.17	1.41	1.44
1	XA	1519	MA6	C5-C4	2.17	1.46	1.40
35	RA	2251	OMG	C5-C4	2.17	1.46	1.40
35	RA	1911	PSU	O4'-C1'	-2.16	1.41	1.44
1	XA	516	PSU	C2-N1	-2.16	1.33	1.38
35	YA	1911	PSU	O4'-C1'	-2.16	1.41	1.44
1	XA	1402	4OC	C6-N1	-2.09	1.33	1.35
1	QA	516	PSU	C2-N3	-2.05	1.34	1.38
35	YA	2503	2MA	C5-C4	2.04	1.46	1.40
35	YA	2552	OMU	C6-N1	-2.04	1.33	1.35
1	XA	1207	2MG	C5-C4	2.04	1.46	1.40
1	QA	1402	4OC	C6-N1	-2.02	1.33	1.35
1	XA	966	M2G	C5-C4	2.00	1.46	1.40

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	QA	516	PSU	N1-C2-N3	-9.00	121.28	128.43
35	RA	2605	PSU	N1-C2-N3	-8.90	121.36	128.43
35	RA	1917	PSU	N1-C2-N3	-8.67	121.54	128.43
35	YA	1911	PSU	N1-C2-N3	-8.54	121.64	128.43
35	YA	1917	PSU	N1-C2-N3	-8.46	121.71	128.43
1	XA	516	PSU	N1-C2-N3	-8.32	121.81	128.43
35	YA	2605	PSU	N1-C2-N3	-8.28	121.84	128.43
35	RA	1911	PSU	N1-C2-N3	-8.06	122.02	128.43
1	QA	516	PSU	C4-N3-C2	7.50	121.47	115.14
35	RA	2503	2MA	C2-N3-C4	7.33	121.48	115.52
35	RA	1915	5MU	C4-N3-C2	7.16	121.19	115.14
35	YA	2503	2MA	C2-N3-C4	7.09	121.28	115.52
35	RA	1917	PSU	C4-N3-C2	6.99	121.05	115.14
35	YA	1915	5MU	C4-N3-C2	6.96	121.02	115.14
1	XA	516	PSU	C4-N3-C2	6.76	120.85	115.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	1917	PSU	C4-N3-C2	6.69	120.79	115.14
35	YA	1911	PSU	C4-N3-C2	6.66	120.77	115.14
35	RA	2605	PSU	C4-N3-C2	6.61	120.72	115.14
35	YA	2605	PSU	C4-N3-C2	6.52	120.64	115.14
35	RA	1911	PSU	C4-N3-C2	6.31	120.47	115.14
35	YA	1939	5MU	C4-N3-C2	5.86	120.09	115.14
1	QA	516	PSU	C5-C4-N3	-5.65	118.08	125.36
35	RA	1939	5MU	C4-N3-C2	5.54	119.82	115.14
1	XA	527	G7M	C5-C6-N1	-5.46	115.97	123.43
35	YA	1917	PSU	C5-C4-N3	-5.25	118.59	125.36
1	XA	1207	2MG	C2-N3-C4	5.22	121.20	115.28
35	RA	1917	PSU	C5-C4-N3	-5.21	118.65	125.36
35	RA	1911	PSU	C5-C4-N3	-5.18	118.69	125.36
1	XA	966	M2G	C6-N1-C2	5.09	122.24	116.18
1	XA	516	PSU	C5-C4-N3	-5.09	118.81	125.36
35	YA	1911	PSU	C5-C4-N3	-5.07	118.83	125.36
1	QA	966	M2G	C6-N1-C2	5.02	122.16	116.18
35	YA	2251	OMG	C2-N3-C4	5.02	121.09	115.36
35	YA	2605	PSU	C5-C4-N3	-4.96	118.97	125.36
1	QA	527	G7M	C5-C6-N1	-4.96	116.65	123.43
35	RA	2251	OMG	C2-N3-C4	4.87	120.91	115.36
1	QA	1207	2MG	C2-N3-C4	4.75	120.67	115.28
1	QA	1518	MA6	C4-C5-N7	-4.73	104.47	109.40
35	RA	2605	PSU	C5-C4-N3	-4.71	119.30	125.36
1	XA	1518	MA6	C4-C5-N7	-4.70	104.50	109.40
1	XA	1402	4OC	CM4-N4-C4	-4.60	119.02	122.97
1	QA	1407	5MC	C2-N3-C4	4.58	121.54	116.02
1	XA	966	M2G	C2-N3-C4	4.54	120.43	115.28
1	QA	966	M2G	C5-C6-N1	-4.52	117.25	123.43
35	RA	1920	OMC	C2-N3-C4	4.48	120.89	116.34
35	YA	2503	2MA	C5-C6-N1	-4.48	118.36	123.06
1	QA	527	G7M	C2-N3-C4	4.47	120.46	115.36
1	QA	1402	4OC	CM4-N4-C4	-4.45	119.15	122.97
1	XA	1407	5MC	C2-N3-C4	4.26	121.17	116.02
35	RA	2503	2MA	C5-C6-N1	-4.26	118.59	123.06
35	RA	2605	PSU	C6-N1-C2	4.23	122.34	115.36
35	YA	1911	PSU	C6-N1-C2	4.22	122.32	115.36
1	XA	966	M2G	C5-C6-N1	-4.21	117.67	123.43
1	QA	1207	2MG	CM2-N2-C2	-4.21	118.51	123.59
1	QA	966	M2G	C2-N3-C4	4.17	120.01	115.28
35	RA	1911	PSU	C5-C6-N1	-4.14	119.35	124.44
1	XA	527	G7M	C6-N1-C2	4.13	122.49	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	YA	2251	OMG	C5-C6-N1	-4.09	117.83	123.43
35	RA	1911	PSU	C6-N1-C2	4.09	122.10	115.36
35	YA	1917	PSU	C6-N1-C2	4.08	122.09	115.36
1	XA	527	G7M	C2-N3-C4	4.06	119.99	115.36
1	QA	1207	2MG	C5-C6-N1	-4.05	117.90	123.43
1	QA	516	PSU	C6-N1-C2	4.04	122.03	115.36
35	RA	1917	PSU	C6-N1-C2	4.04	122.02	115.36
35	YA	2605	PSU	C6-N1-C2	4.01	121.97	115.36
1	QA	527	G7M	C6-N1-C2	3.94	122.19	115.93
1	XA	516	PSU	C6-N1-C2	3.92	121.83	115.36
1	XA	1207	2MG	CM2-N2-C2	-3.92	118.86	123.59
35	RA	2251	OMG	C5-C6-N1	-3.90	118.10	123.43
1	XA	1207	2MG	C5-C6-N1	-3.87	118.14	123.43
35	YA	1920	OMC	C2-N3-C4	3.86	120.25	116.34
35	RA	2605	PSU	C5-C6-N1	-3.82	119.74	124.44
35	YA	1917	PSU	C5-C6-N1	-3.80	119.77	124.44
35	RA	2251	OMG	C6-N1-C2	3.79	121.95	115.93
35	YA	1911	PSU	C5-C6-N1	-3.78	119.80	124.44
35	YA	2605	PSU	C5-C6-N1	-3.72	119.86	124.44
1	XA	516	PSU	C5-C6-N1	-3.72	119.87	124.44
1	XA	966	M2G	C6-C5-C4	-3.72	117.25	120.80
1	QA	1519	MA6	C4-C5-N7	-3.69	105.55	109.40
1	XA	1207	2MG	C6-N1-C2	3.66	121.73	115.18
35	YA	2251	OMG	C6-N1-C2	3.64	121.71	115.93
1	XA	1518	MA6	C10-N6-C9	-3.60	104.53	116.12
35	RA	1917	PSU	C5-C6-N1	-3.57	120.06	124.44
1	QA	1207	2MG	C6-N1-C2	3.56	121.56	115.18
1	QA	516	PSU	C5-C6-N1	-3.56	120.06	124.44
1	XA	1519	MA6	C10-N6-C9	-3.56	104.66	116.12
35	YA	1920	OMC	N4-C4-N3	3.54	122.08	116.49
1	QA	967	5MC	C2-N3-C4	3.52	120.26	116.02
1	XA	1518	MA6	N3-C2-N1	-3.51	123.19	128.68
1	XA	1519	MA6	N3-C2-N1	-3.51	123.19	128.68
35	RA	1920	OMC	N4-C4-N3	3.48	121.99	116.49
35	YA	1942	5MC	C2-N3-C4	3.48	120.21	116.02
1	XA	1404	5MC	C2-N3-C4	3.46	120.19	116.02
1	QA	1207	2MG	C6-C5-C4	-3.46	117.49	120.80
1	XA	967	5MC	C2-N3-C4	3.46	120.19	116.02
35	RA	2251	OMG	C6-C5-C4	-3.43	117.53	120.80
1	QA	1519	MA6	C10-N6-C9	-3.41	105.13	116.12
1	XA	1519	MA6	C4-C5-N7	-3.40	105.86	109.40
1	XA	1518	MA6	C9-N6-C6	-3.40	109.22	119.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	XA	1207	2MG	C6-C5-C4	-3.38	117.57	120.80
1	QA	1518	MA6	C10-N6-C9	-3.35	105.33	116.12
35	RA	1962	5MC	N4-C4-N3	3.34	121.75	117.03
1	QA	1519	MA6	N3-C2-N1	-3.32	123.50	128.68
1	QA	1404	5MC	C2-N3-C4	3.31	120.02	116.02
1	QA	1518	MA6	C9-N6-C6	-3.30	109.51	119.51
1	XA	527	G7M	CN7-N7-C8	-3.29	109.61	125.43
1	XA	1400	5MC	C2-N3-C4	3.26	119.95	116.02
35	RA	1939	5MU	C5-C6-N1	-3.25	118.69	122.19
35	YA	1939	5MU	C5-C6-N1	-3.23	118.71	122.19
1	QA	966	M2G	C6-C5-C4	-3.23	117.71	120.80
1	XA	1519	MA6	N1-C6-N6	3.21	120.44	117.06
1	QA	1207	2MG	C4-C5-N7	-3.14	106.13	109.40
1	XA	1407	5MC	N4-C4-N3	3.11	121.43	117.03
1	QA	1400	5MC	C2-N3-C4	3.11	119.77	116.02
1	XA	1519	MA6	C10-N6-C6	-3.11	110.11	119.51
35	RA	1942	5MC	C2-N3-C4	3.10	119.76	116.02
1	QA	1518	MA6	N3-C2-N1	-3.10	123.84	128.68
1	QA	1519	MA6	C10-N6-C6	-3.08	110.19	119.51
1	XA	1519	MA6	C9-N6-C6	-3.06	110.26	119.51
1	XA	1207	2MG	C4-C5-N7	-3.06	106.21	109.40
35	YA	1915	5MU	C6-N1-C1'	-3.02	112.44	119.24
1	XA	1404	5MC	N4-C4-N3	2.98	121.25	117.03
35	RA	1962	5MC	C5-C6-N1	-2.98	118.98	122.19
35	RA	2251	OMG	N3-C2-N1	-2.94	123.30	127.22
12	XL	92	0TD	O-C-CA	-2.93	117.11	124.78
1	QA	527	G7M	CN7-N7-C8	-2.92	111.39	125.43
35	YA	1962	5MC	C5-C6-N1	-2.91	119.06	122.19
1	QA	1400	5MC	N4-C4-N3	2.90	121.13	117.03
35	RA	2503	2MA	C4-C5-N7	-2.88	106.40	109.40
1	XA	1400	5MC	C5-C6-N1	-2.87	119.10	122.19
12	QL	92	0TD	O-C-CA	-2.87	117.26	124.78
35	YA	1962	5MC	C2-N3-C4	2.87	119.48	116.02
1	XA	1400	5MC	N4-C4-N3	2.83	121.04	117.03
1	XA	967	5MC	N4-C4-N3	2.83	121.04	117.03
1	QA	1400	5MC	C5-C6-N1	-2.75	119.23	122.19
35	RA	1962	5MC	C2-N3-C4	2.70	119.28	116.02
35	RA	1915	5MU	C6-N1-C1'	-2.69	113.20	119.24
35	YA	1942	5MC	N4-C4-N3	2.69	120.83	117.03
35	YA	2251	OMG	N3-C2-N1	-2.67	123.66	127.22
1	QA	1519	MA6	N1-C6-N6	2.66	119.86	117.06
35	YA	2251	OMG	C4-C5-N7	-2.60	106.69	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	RA	1911	PSU	C5-C1'-C2'	-2.57	110.72	115.32
35	YA	2503	2MA	C4-C5-N7	-2.57	106.72	109.40
35	RA	1942	5MC	C5-C6-N1	-2.55	119.44	122.19
1	QA	1207	2MG	N2-C2-N1	2.54	119.40	116.96
1	QA	966	M2G	C4-C5-N7	-2.54	106.75	109.40
35	RA	1942	5MC	N4-C4-N3	2.52	120.60	117.03
35	YA	2251	OMG	C6-C5-C4	-2.52	118.39	120.80
1	QA	527	G7M	N3-C2-N1	-2.50	123.89	127.22
1	XA	966	M2G	C4-C5-N7	-2.50	106.79	109.40
1	QA	1404	5MC	N4-C4-N3	2.49	120.56	117.03
35	RA	2251	OMG	C4-C5-N7	-2.35	106.95	109.40
1	QA	967	5MC	C5-C6-N1	-2.34	119.67	122.19
35	YA	1962	5MC	N4-C4-N3	2.31	120.31	117.03
1	XA	527	G7M	N3-C2-N1	-2.31	124.14	127.22
35	YA	1920	OMC	C5-C4-N4	-2.28	117.17	121.14
1	QA	1519	MA6	C9-N6-C6	-2.28	112.61	119.51
1	XA	1404	5MC	C5-C6-N1	-2.27	119.75	122.19
35	YA	2552	OMU	C5-C4-N3	-2.23	118.39	123.31
1	QA	1407	5MC	N4-C4-N3	2.20	120.15	117.03
35	RA	1920	OMC	C6-N1-C2	-2.11	117.84	121.20
1	XA	967	5MC	C5-C6-N1	-2.11	119.92	122.19
1	QA	1404	5MC	C5-C6-N1	-2.10	119.93	122.19
35	YA	1920	OMC	C6-N1-C2	-2.10	117.86	121.20
35	RA	2552	OMU	C5-C4-N3	-2.09	118.71	123.31
1	XA	516	PSU	O4'-C1'-C2'	2.09	108.04	104.66
1	XA	1207	2MG	N2-C2-N1	2.06	118.94	116.96
1	QA	966	M2G	CM2-N2-C2	-2.05	119.34	121.29
35	RA	2605	PSU	C5-C1'-C2'	-2.04	111.68	115.32

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	QA	1518	MA6	C5-C6-N6-C9
1	QA	1518	MA6	C5-C6-N6-C10
12	XL	92	0TD	CG-CB-SB-CSB
1	XA	1518	MA6	C5-C6-N6-C9
1	XA	1518	MA6	C5-C6-N6-C10
12	QL	92	0TD	CG-CB-SB-CSB
1	QA	1519	MA6	O4'-C4'-C5'-O5'
35	RA	1962	5MC	O4'-C1'-N1-C6
1	XA	1519	MA6	O4'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	QA	1402	4OC	O4'-C4'-C5'-O5'
1	QA	1519	MA6	C3'-C4'-C5'-O5'
1	XA	1519	MA6	C3'-C4'-C5'-O5'
1	XA	1402	4OC	O4'-C4'-C5'-O5'
1	XA	1400	5MC	O4'-C4'-C5'-O5'
1	QA	1518	MA6	N1-C6-N6-C9
1	XA	1518	MA6	N1-C6-N6-C9
1	XA	1400	5MC	C3'-C4'-C5'-O5'
1	QA	1402	4OC	C3'-C4'-C5'-O5'
1	XA	527	G7M	C3'-C4'-C5'-O5'
1	XA	1519	MA6	C5-C6-N6-C9
1	XA	527	G7M	O4'-C4'-C5'-O5'
1	QA	1400	5MC	O4'-C4'-C5'-O5'
1	QA	1402	4OC	C5-C4-N4-CM4
1	QA	1404	5MC	C3'-C4'-C5'-O5'
1	QA	1519	MA6	C5-C6-N6-C9
1	QA	1404	5MC	O4'-C4'-C5'-O5'
35	RA	2552	OMU	O4'-C4'-C5'-O5'
1	QA	527	G7M	C4'-C5'-O5'-P
1	XA	527	G7M	C4'-C5'-O5'-P
1	XA	1402	4OC	C3'-C4'-C5'-O5'
1	QA	1400	5MC	C3'-C4'-C5'-O5'
1	QA	966	M2G	N3-C2-N2-CM2
1	QA	527	G7M	C3'-C4'-C5'-O5'
1	QA	966	M2G	N1-C2-N2-CM2
35	YA	2503	2MA	O4'-C4'-C5'-O5'
35	YA	1962	5MC	O4'-C4'-C5'-O5'
35	RA	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	YA	1962	5MC	1	0
35	RA	1939	5MU	1	0
35	YA	2503	2MA	2	0
1	QA	1518	MA6	1	0
1	XA	966	M2G	1	0
1	XA	1518	MA6	1	0
12	QL	92	0TD	1	0
35	RA	2503	2MA	2	0
1	QA	1519	MA6	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	XA	1498	UR3	1	0
1	XA	967	5MC	1	0
35	RA	1962	5MC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2027 ligands modelled in this entry, 2023 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	QD	302	-	0,12,12	0.00	-	-		
57	PAR	XA	1794	-	45,45,45	0.66	0	64,67,67	1.23	6 (9%)
57	PAR	QA	1821	-	45,45,45	0.68	0	64,67,67	1.49	11 (17%)
58	SF4	XD	301	-	0,12,12	0.00	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	SF4	QD	302	-	-	-	0/6/5/5
57	PAR	XA	1794	-	-	3/18/94/94	0/4/4/4
57	PAR	QA	1821	-	-	4/18/94/94	0/4/4/4
58	SF4	XD	301	-	-	-	0/6/5/5

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	QA	1821	PAR	C44-C34-C24	4.78	119.30	111.07
57	QA	1821	PAR	O52-C13-C23	3.44	115.09	107.96
57	XA	1794	PAR	C13-O52-C52	-3.34	109.70	117.96
57	QA	1821	PAR	C13-O52-C52	-3.33	109.73	117.96
57	XA	1794	PAR	C14-O33-C33	-2.90	110.79	117.96
57	XA	1794	PAR	C11-O51-C51	2.74	119.07	113.69
57	QA	1821	PAR	O62-C62-C12	-2.59	105.07	109.81
57	QA	1821	PAR	C14-C24-N24	-2.54	105.63	110.20
57	QA	1821	PAR	O11-C42-C32	-2.44	103.35	109.18
57	QA	1821	PAR	C62-C12-N12	-2.42	106.19	110.97
57	QA	1821	PAR	O34-C34-C44	-2.41	104.77	110.35
57	QA	1821	PAR	C14-O33-C33	-2.26	112.38	117.96
57	QA	1821	PAR	O52-C13-O43	-2.24	109.00	111.43
57	XA	1794	PAR	O11-C42-C32	-2.21	103.90	109.18
57	XA	1794	PAR	O33-C33-C23	-2.18	104.30	111.32
57	QA	1821	PAR	O54-C14-C24	-2.13	105.26	110.06
57	XA	1794	PAR	O11-C11-C21	-2.10	104.61	108.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	QA	1821	PAR	O51-C51-C61-O61
57	QA	1821	PAR	C41-C51-C61-O61
57	QA	1821	PAR	C23-C33-O33-C14
57	XA	1794	PAR	O54-C14-O33-C33
57	QA	1821	PAR	C52-C42-O11-C11
57	XA	1794	PAR	C23-C33-O33-C14
57	XA	1794	PAR	C43-C33-O33-C14

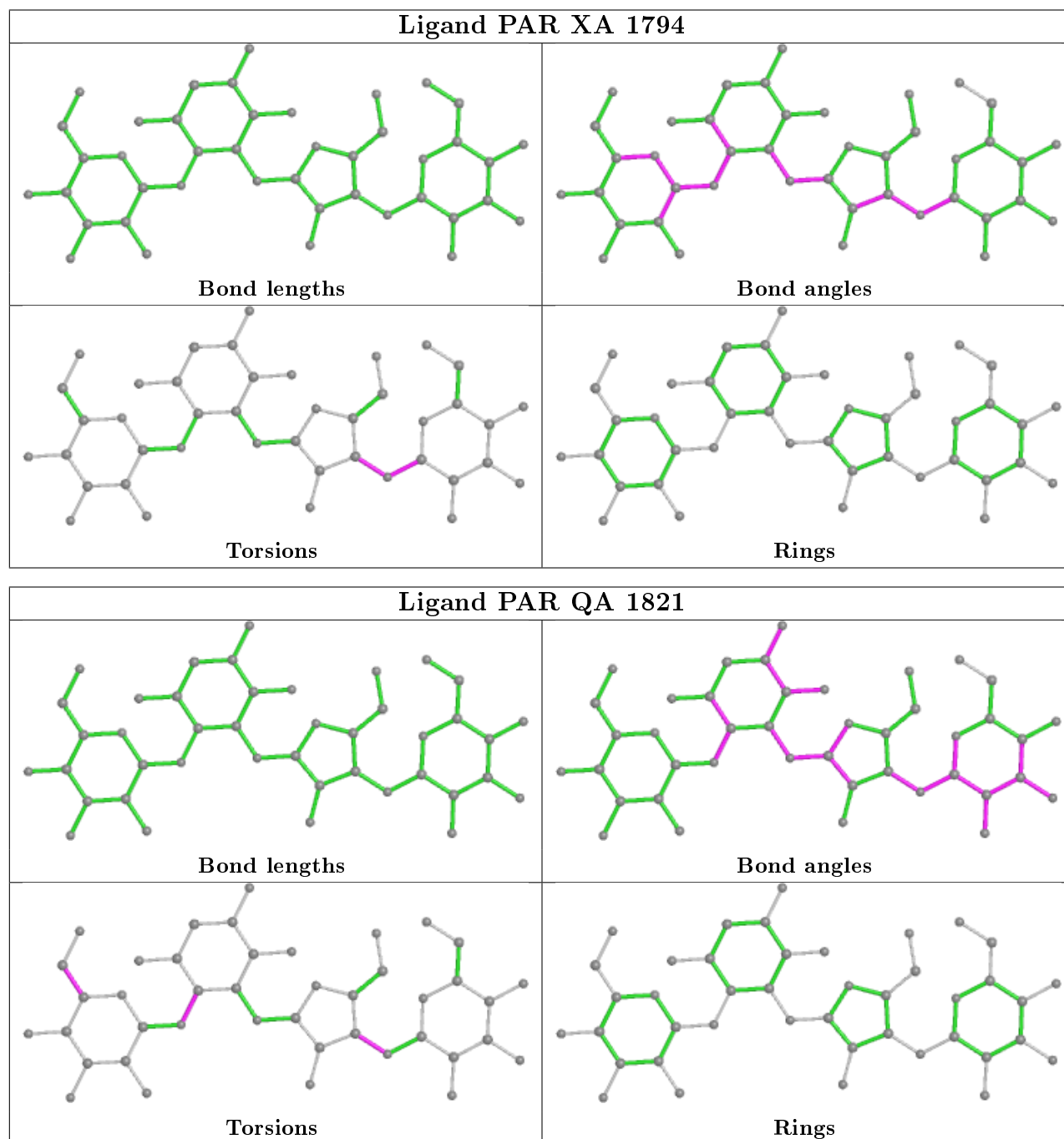
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	XA	1794	PAR	1	0
57	QA	1821	PAR	1	0
58	XD	301	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.