



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 07:17 pm GMT

PDB ID : 3CCM
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2611U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.55 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 : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

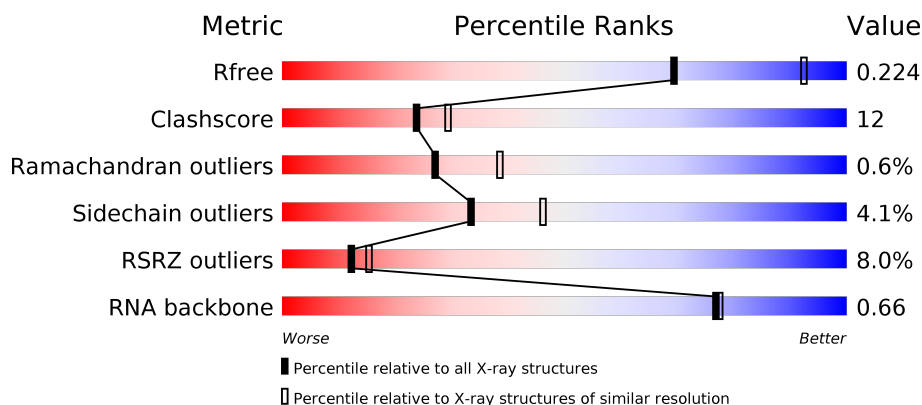
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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))
R_{free}	111664	1053 (2.56-2.52)
Clashscore	122126	1098 (2.56-2.52)
Ramachandran outliers	120053	1088 (2.56-2.52)
Sidechain outliers	120020	1088 (2.56-2.52)
RSRZ outliers	108989	1043 (2.56-2.52)
RNA backbone	2636	1015 (2.90-2.18)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>24%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>40%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>.</div> <div>21%</div> </div> </div>



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8017	-	-	-	X
32	MG	0	8038	-	-	-	X
32	MG	0	8040	-	-	-	X
32	MG	0	8082	-	-	-	X
34	SR	0	8962	-	-	-	X
34	SR	0	8987	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	0	9007	-	-	-	X
35	NA	0	8518	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8575	-	-	-	X
37	K	0	8401	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99119 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	337	Total	C	N	O	S	0	0	0
			2625	1616	493	511	5			

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	140	Total	C	N	O	S	0	0	0
			1094	685	195	210	4			

- Molecule 5 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	172	Total	C	N	O	S	0	0	0
			1357	840	224	289	4			

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	142	Total	C	N	O	S	0	0	0
			1120	696	199	222	3			

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	186	Total	C	N	O	S	0	0	0
			1445	895	262	286	2			

- Molecule 15 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	115	Total	C	N	O		0	0	0
			865	529	161	175				

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	95	Total	C	N	O		0	0	0
			735	450	141	144				

- Molecule 18 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	R	150	Total	C	N	O	S	0	0	0
			1149	713	209	223	4			

- Molecule 19 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	0
			641	389	111	138	3			

- Molecule 20 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	119	Total	C	N	O		0	0	0
			950	568	180	202				

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26348	10870	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	94	Total 94	Sr 94	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	1	Total 1	Sr 1	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	0	0
34	S	1	Total 1	Sr 1	0	0
34	F	1	Total 1	Sr 1	0	0

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	66	Total 66	Na 66	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	2	Total 2	K 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	117	Total O 117 117	0	0
38	B	139	Total O 139 139	0	0
38	C	165	Total O 165 165	0	0
38	D	48	Total O 48 48	0	0
38	E	49	Total O 49 49	0	0
38	F	25	Total O 25 25	0	0
38	G	18	Total O 18 18	0	0
38	H	71	Total O 71 71	0	0
38	I	8	Total O 8 8	0	0
38	J	55	Total O 55 55	0	0
38	K	55	Total O 55 55	0	0
38	L	79	Total O 79 79	0	0
38	M	138	Total O 138 138	0	0
38	N	58	Total O 58 58	0	0
38	O	40	Total O 40 40	0	0
38	P	61	Total O 61 61	0	0
38	Q	49	Total O 49 49	0	0
38	R	78	Total O 78 78	0	0
38	S	32	Total O 32 32	0	0
38	T	36	Total O 36 36	0	0
38	U	28	Total O 28 28	0	0
38	V	13	Total O 13 13	0	0

Continued on next page...

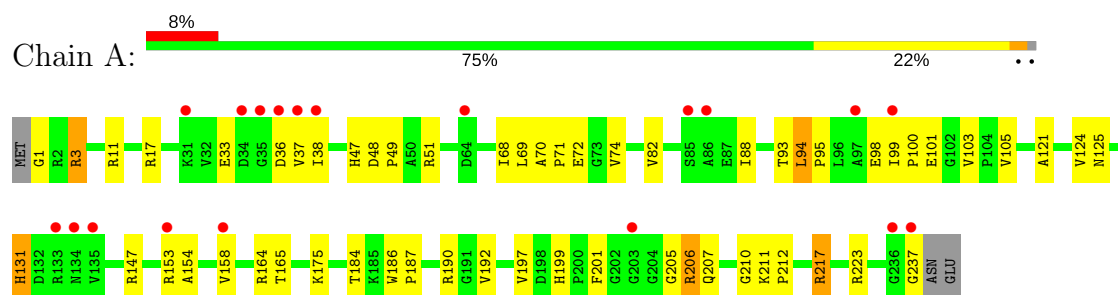
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	W	68	Total 68	O 68	0	0
38	X	24	Total 24	O 24	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	29	Total 29	O 29	0	0
38	1	51	Total 51	O 51	0	0
38	2	37	Total 37	O 37	0	0
38	3	72	Total 72	O 72	0	0
38	0	5938	Total 5938	O 5938	0	0
38	9	145	Total 145	O 145	0	0

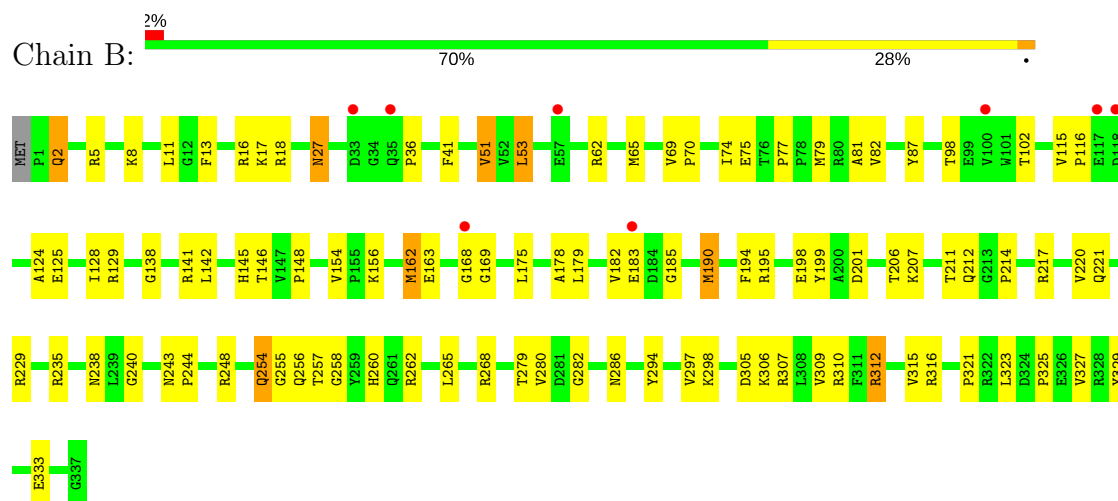
3 Residue-property plots

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

• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P



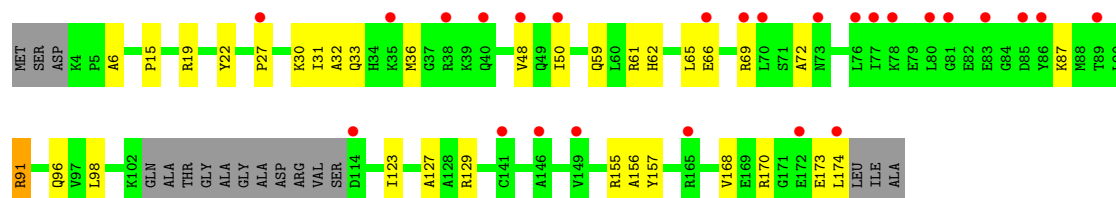
LYS
GLU
VAL
GLY
LEU
LEU
ASP
LEU
ARG
ALA
VAL
PHE
PHE
ALA
ASP
GLY
VAL
LEU
PHE
GLU
PRO
GLU
LEU
LEU
LEU
ASP
ILE
ASP
GLU
TYR
ARG
SER
ASP
ILE
GLN
ALA
ALA
ALA
GLY
ARG
ALA
PHE
ASN
LEU
SER
VAL
ASN
ALA
GLU
GLU
TYR
PRO
THR
ALA
THR
THR
ALA
PRO
THR
MET
LEU
GLN

SER
ALA
ARG
GLY
ASN
ALA
LYS
SER
LEU
LEU
ALA
LEU
SER
GLN
ALA
ASP
ALA
ILE
ASP
PRO
GLU
VAL
VAL
VAL
PRO
ASP
LEU
LEU
VAL
SER
LYS
ASP
ASP
ALA
ALA
GLN
VAL
ASP
ALA
SER
GLN
ILE
GLY
ASP
MET
GLU
ALA
LEU
ALA
PHE

PRO
THR
ASP
GLN
ASP
ASP
THR
ALA
SER
GLU
ASP
ALA
ASP
ASP
ALA
ALA
ALA
LEU
GLY
ALA
LEU
GLY
PHE

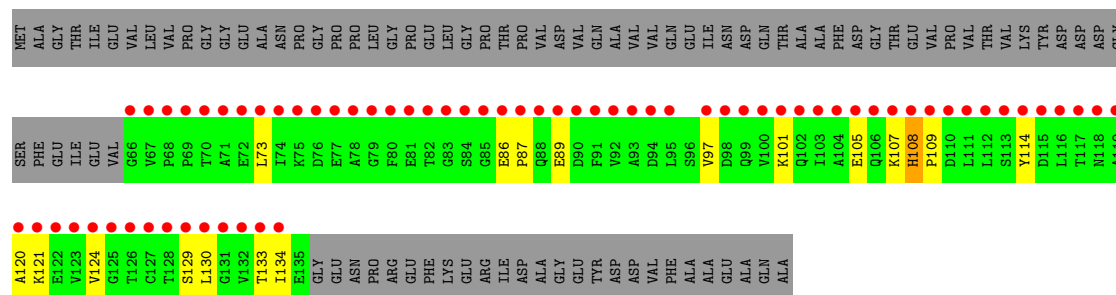
• Molecule 8: 50S ribosomal protein L10e

Chain H: 15% 72% 18% 10%



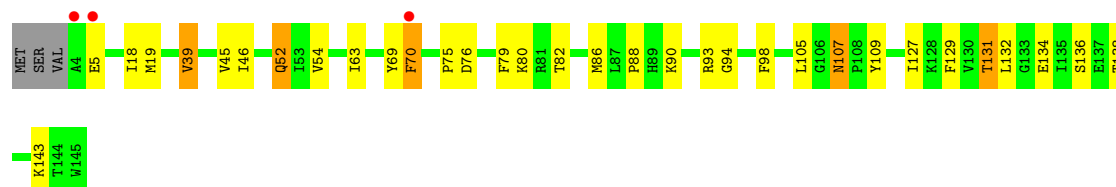
• Molecule 9: 50S ribosomal protein L11P

Chain I: 42% 32% 10% 57%



• Molecule 10: 50S ribosomal protein L13P

Chain J: 2% 75% 19%



• Molecule 11: 50S ribosomal protein L14P

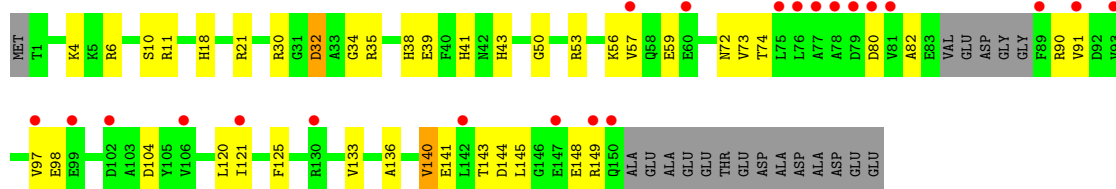
Chain K: 2% 74% 23%



V132

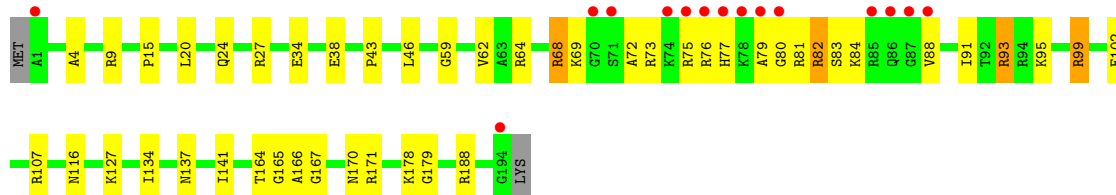
- Molecule 12: 50S ribosomal protein L15P

Chain L:



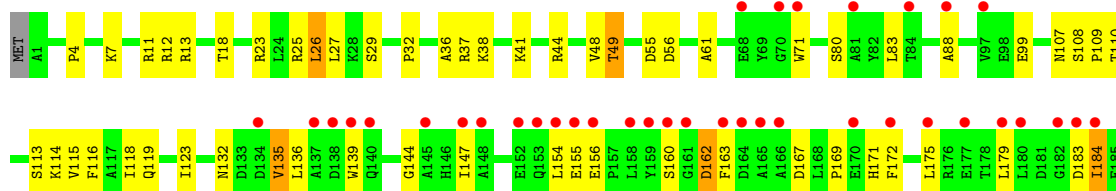
- Molecule 13: 50S ribosomal protein L15e

Chain M:



- Molecule 14: 50S ribosomal protein L18P

Chain N:



L186

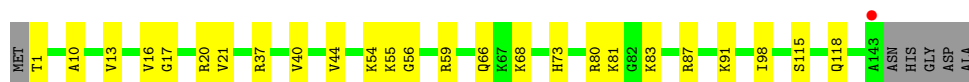
- Molecule 15: 50S ribosomal protein L18e

Chain O:



- Molecule 16: 50S ribosomal protein L19e

Chain P:



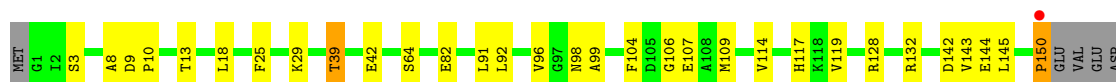
- Molecule 17: 50S ribosomal protein L21e

Chain Q: 80% 17% ..



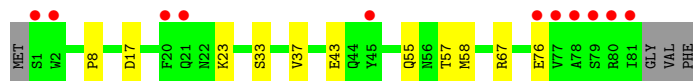
- Molecule 18: 50S ribosomal protein L22P

Chain R: 77% 19% ..



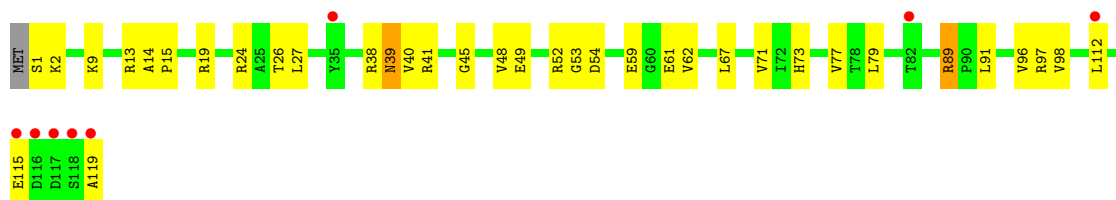
- Molecule 19: 50S ribosomal protein L23P

Chain S: 13% 82% 13% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T: 7% 69% 28% ..



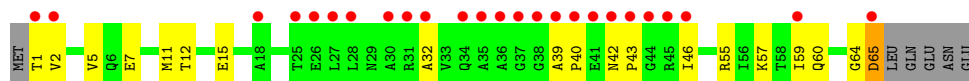
- Molecule 21: 50S ribosomal protein L24e

Chain U: 4% 52% 25% 21%

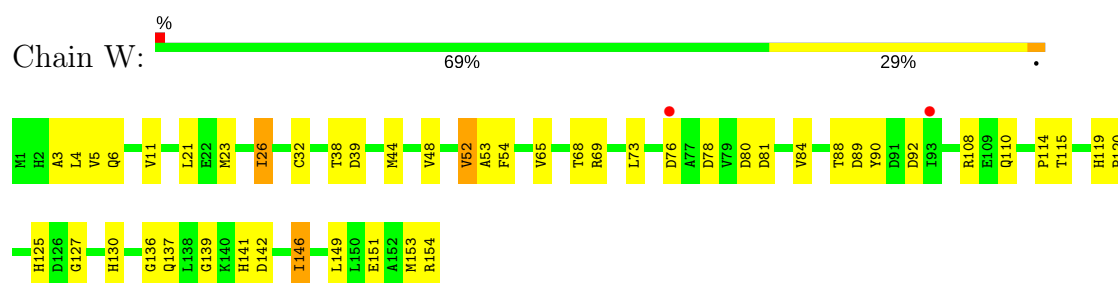


- Molecule 22: 50S ribosomal protein L29P

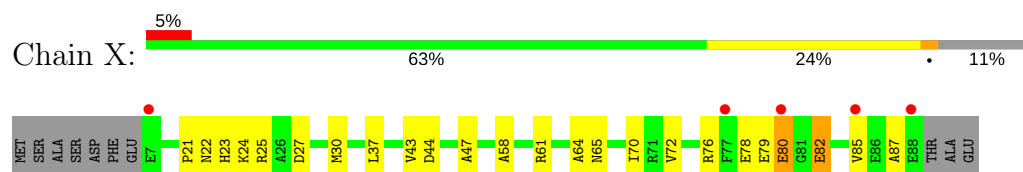
Chain V: 35% 65% 25% 8%



- Molecule 23: 50S ribosomal protein L30P



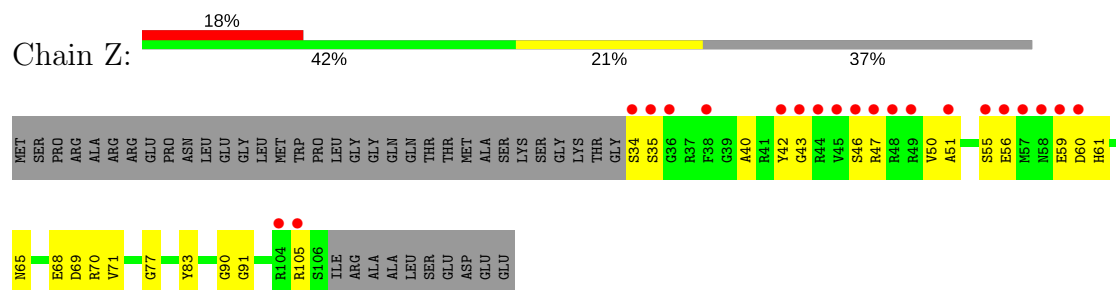
• Molecule 24: 50S ribosomal protein L31e



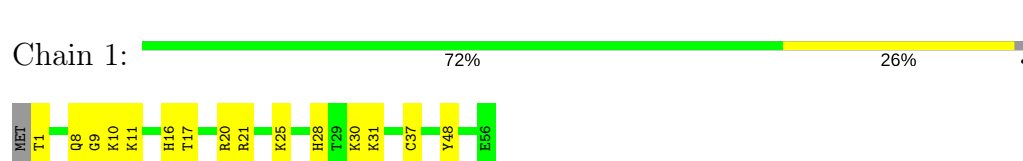
• Molecule 25: 50S ribosomal protein L32e



• Molecule 26: 50S ribosomal protein L37Ae

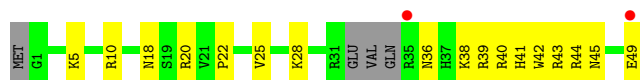


• Molecule 27: 50S ribosomal protein L37e

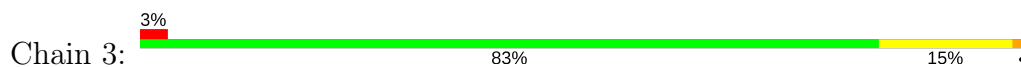


• Molecule 28: 50S ribosomal protein L39e

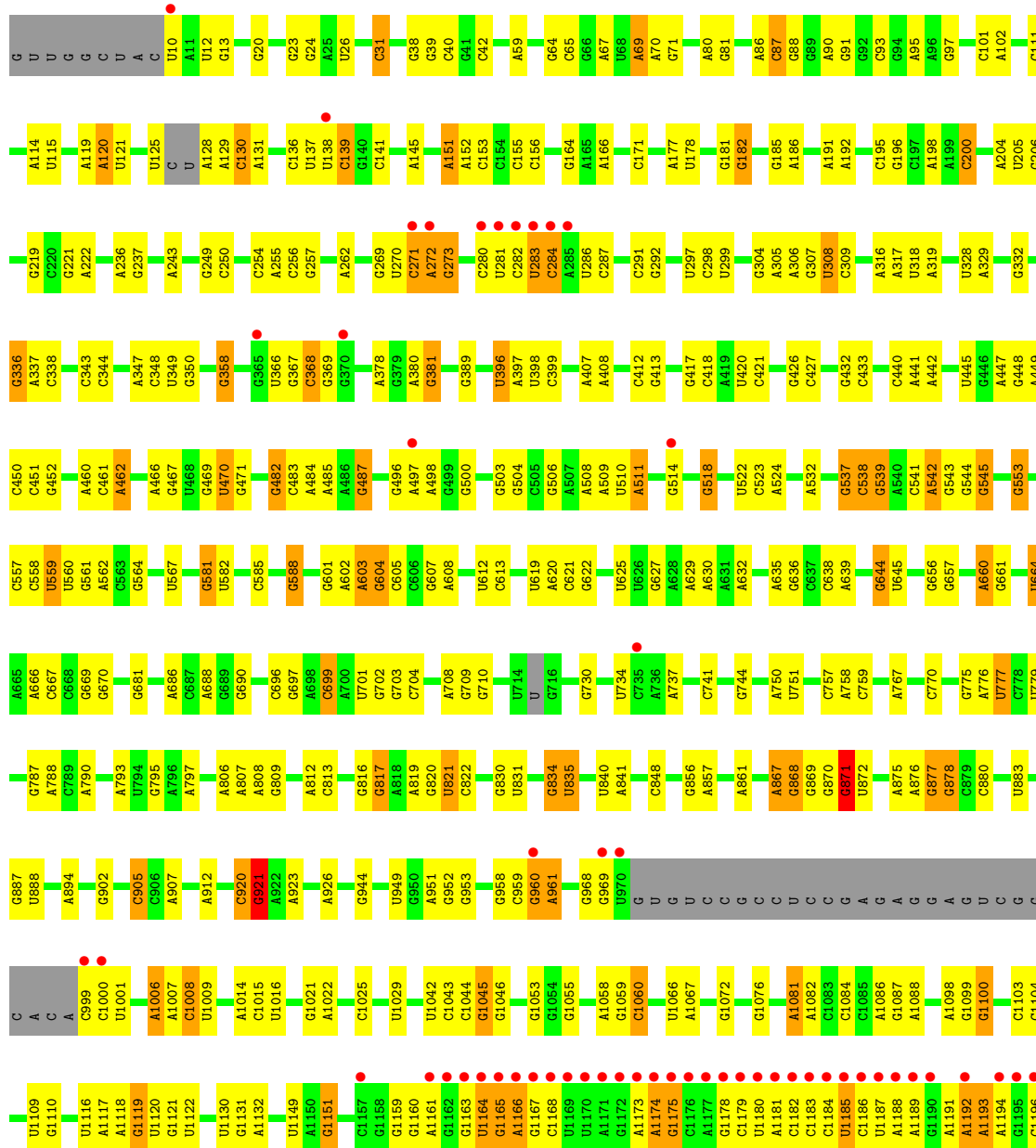




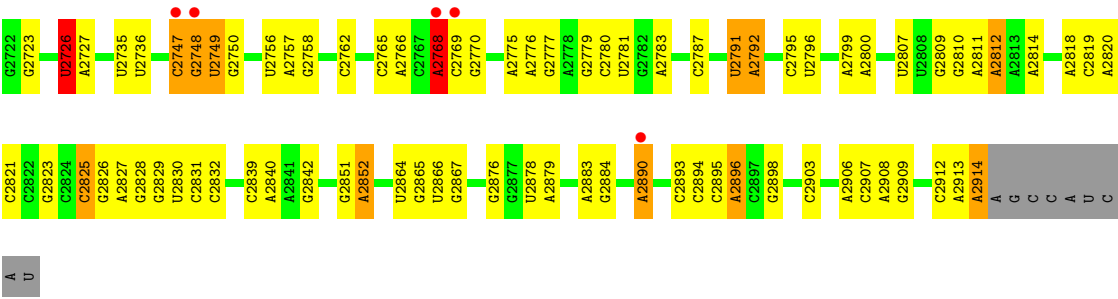
- Molecule 29: 50S ribosomal protein L44E



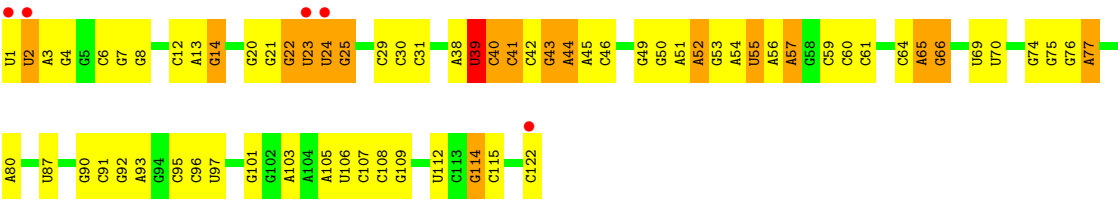
- Molecule 30: 23S RIBOSOMAL RNA



A2612	G2613	A2609	A2408	G2314	C	U	U2063	G1849	A1736	A1630	A1501	A1369	G1290	G1197
G2614	C2315	C2510	G2412	U2064	U	A	U1850	A1737	A1631	A1502	A1372	A1294	U1198	U1199
U2615	C2316	A2511	A2413	G2070	A	A	A1851	G1738	A1632	A1503	A1373	A1295	C1200	C1201
G2616	C2317	U2512	A2414	G2071	C	U	A1852	G1739	G1633	A1504	G1377	U1298	C1202	G1203
G2617	U2320	A2513	A2415	C2072	C	U	C1856	U1741	G1634	U1506	A1378	G1300	C1204	C1205
C2626	A2321	C2515	G2416	G2073	G	U	C1862	G1744	A1641	U1511	U1380	U1304	U1206	U1207
G2627	U2322	G2516	U2419	A2074	C	C	G1863	G1745	A1642	G1512	C1384	C1305	A1208	C1209
A2635	G2323	A2521	G2420	A2081	C	C	C1864	G1750	U1654	A1518	G1391	U1309	C1210	G1211
C2636	C2326	U2522	G2421	G2089	U	C	C1865	G1751	A1655	U1519	G1392	U1310	C1212	C1213
A2637	U2327	G2523	U2422	C2090	C	U	A1866	G1752	A1656	G1520	A1392	G1311	C1214	C1215
C2644	C2328	U2524	A2425	G2091	G	U	G1867	A1755	A1657	A1522	C1396	A1312	U1218	U1219
U2645	C2329	G2525	G2426	C2094	C	U	G1868	G1756	A1658	G1523	C1397	G1313	U1220	C1229
G2646	U2330	C2526	A2427	A2095	U	A	U1871	G1757	G1660	U1524	G1398	U1314	U1218	U1219
A2649	A2332	U2531	G2428	A2096	C	A	C1872	A1759	C1666	G1525	A1399	G1315	U1220	C1229
U2652	G2333	C2533	A2430	A2099	G	A	G1873	U1761	U1667	A1526	C1400	G1316	U1220	C1229
G2653	A	C2536	G2438	A2099	C	C	G1877	C1762	U1668	A1527	A1406	A1321	U1218	U1219
U2661	C	G2537	C	A2100	G	G	U1878	C1763	C1675	A1528	A1407	G1322	U1218	U1219
U2663	A	A2538	A	G2101	U	U	U1879	C1764	C1676	G1529	A1414	G1325	U1220	C1229
G2664	G	U2539	G	G2102	A	A	U1883	U1765	C1677	G1535	A1415	A1328	U1220	C1229
A	C	G2540	A	A2103	C	C	A1886	C1768	G1680	G1536	G1416	A1331	U1220	C1229
U	C	U2541	C	C2105	C	C	U1887	C1769	G1681	G1537	G1417	G1332	U1220	C1229
G2667	C2344	C2549	A2455	C2106	C	C	G1902	G1773	G1682	G1552	U1418	G1333	U1220	C1229
G2670	A2345	C2552	G2457	G2110	C	C	U1903	G1774	G1683	G1553	U1419	U1333	U1220	C1229
U2671	C2346	A2553	U2457	G2111	C	C	A1904	G1775	G1684	G1554	U1420	U1334	U1220	C1229
C2672	C2351	C2554	U2460	A2112	C	C	U1905	G1776	G1685	G1555	U1421	U1335	U1220	C1229
G2676	C2352	A2555	U2461	G2113	U	U	U1906	A1778	G1686	U	U1422	U1336	U1220	C1229
G2679	C2353	C2556	G2462	C2113	C	A	A1910	A1779	C1687	C1559	U1423	U1337	U1220	C1229
A2680	G2354	C2557	A2465	G2128	G	C	U1919	U1787	C1688	C1560	C1426	U1339	U1220	C1229
C2682	U2355	G2357	A2466	G2134	C	C	C1920	U1788	C1689	C1561	G1441	G1340	U1220	C1229
A2684	C2356	A2357	A2467	A2135	G	G	A1921	C1790	G1692	C1573	A1442	A1341	U1220	C1229
G2687	C2357	A2358	A2468	G2136	C	C	A1922	U1791	G1697	C1574	U1446	C1342	U1220	C1229
C2688	A2361	A2362	C2476	C	C	C	G1925	C1798	C1700	G1588	U1451	G1343	U1220	C1229
G2689	C2363	G2364	A2482	A	C	C	G1926	C1799	A1701	G1589	C1452	U1346	U1220	C1229
A2699	C2365	G2365	U2483	U	C	C	C1927	C1816	U1702	G1590	G1452	U1346	U1220	C1229
G2700	C2366	G2366	A2484	U	C	C	G1928	U1817	A1710	C1592	U1471	U1350	U1220	C1229
U2704	C2367	A2367	A2485	C	C	C	G1929	C1818	C1714	C1593	U1472	G1351	U1220	C1229
U2705	C2368	A2368	A2486	U	C	C	A1934	G1819	C1715	C1594	C1474	A1352	U1220	C1229
U2710	C2369	A2369	A2487	C	C	C	C1935	G1820	C1716	G1595	G1475	C1353	U1220	C1229
U2711	C2370	A2370	A2488	C	C	C	U1939	C1829	A1717	U1597	C1476	G1354	U1220	C1229
G2712	C2371	A2371	A2489	U	C	C	C1940	C1834	U1722	A1598	C1477	A1355	U1220	C1229
G2716	C2372	A2372	A2490	C	C	C	A1941	U1835	G1723	A1603	U1478	A1356	U1220	C1229
C2717	C2373	A2373	A2491	C	C	C	C1942	U1838	U1724	G1604	A1482	A1357	U1220	C1229
U2718	C2374	A2374	A2492	U	C	C	A1943	U1839	C1725	G1605	C1483	A1358	U1220	C1229
A2719	C2375	A2375	A2493	C	C	C	C1946	U1840	G1730	A1615	G1484	C1360	U1220	C1229
C2720	C2376	A2376	A2494	C	C	C	C1947	U1841	C1731	A1616	U1488	G1363	U1220	C1229
U2721	C2377	A2377	A2495	C	C	C	G1948	C1842	A1732	A1624	A1496	C1366	U1220	C1229
U2722	C2378	A2378	A2496	C	C	C	G1949	U1843	A1733	U1625	G1497	A1367	U1220	C1229
U2723	C2379	A2379	A2497	C	C	C	G1950	U1844	C1734	A1626	U1497	C1368	U1220	C1229
U2724	C2380	A2380	A2498	C	C	C	U	U1845	C1735	G1627	U1498	C1369	U1220	C1229
U2725	C2381	A2381	A2499	C	C	C	U	U1846	C1736	G1628	U1499	C1370	U1220	C1229
U2726	C2382	A2382	A2500	C	C	C	U	U1847	C1737	G1629	U1500	C1371	U1220	C1229
U2727	C2383	A2383	A2501	C	C	C	U	U1848	C1738	G1630	U1501	C1372	U1220	C1229
U2728	C2384	A2384	A2502	C	C	C	U	U1849	C1739	G1631	U1502	C1373	U1220	C1229
U2729	C2385	A2385	A2503	C	C	C	U	U1850	C1740	G1632	U1503	C1374	U1220	C1229
U2730	C2386	A2386	A2504	C	C	C	U	U1851	C1741	G1633	U1504	C1375	U1220	C1229
U2731	C2387	A2387	A2505	C	C	C	U	U1852	C1742	G1634	U1505	C1376	U1220	C1229
U2732	C2388	A2388	A2506	C	C	C	U	U1853	C1743	G1635	U1506	C1377	U1220	C1229
U2733	C2389	A2389	A2507	C	C	C	U	U1854	C1744	G1636	U1507	C1378	U1220	C1229
U2734	C2390	A2390	A2508	C	C	C	U	U1855	C1745	G1637	U1508	C1379	U1220	C1229
U2735	C2391	A2391	A2509	C	C	C	U	U1856	C1746	G1638	U1509	C1380	U1220	C1229
U2736	C2392	A2392	A2510	C	C	C	U	U1857	C1747	G1639	U1510	C1381	U1220	C1229
U2737	C2393	A2393	A2511	C	C	C	U	U1858	C1748	G1640	U1511	C1382	U1220	C1229
U2738	C2394	A2394	A2512	C	C	C	U	U1859	C1749	G1641	U1512	C1383	U1220	C1229
U2739	C2395	A2395	A2513	C	C	C	U	U1860	C1750	G1642	U1513	C1384	U1220	C1229
U2740	C2396	A2396	A2514	C	C	C	U	U1861	C1751	G1643	U1514	C1385	U1220	C1229
U2741	C2397	A2397	A2515	C	C	C	U	U1862	C1752	G1644	U1515	C1386	U1220	C1229
U2742	C2398	A2398	A2516	C	C	C	U	U1863	C1753	G1645	U1516	C1387	U1220	C1229
U2743	C2399	A2399	A2517	C	C	C	U	U1864	C1754	G1646	U1517	C1388	U1220	C1229
U2744	C2400	A2400	A2518	C	C	C	U	U1865	C1755	G1647	U1518	C1389	U1220	C1229
U2745	C2401	A2401	A2519	C	C	C	U	U1866	C1756	G1648	U1519	C1390	U1220	C1229
U2746	C2402	A2402	A2520	C	C	C	U	U1867	C1757	G1649	U1520	C1391	U1220	C1229
U2747	C2403	A2403	A2521	C	C	C	U	U1868	C1758	G1650	U1521	C1392	U1220	C1229
U2748	C2404	A2404	A2522	C	C	C	U	U1869	C1759	G1651	U1522	C1393	U1220	C1229
U2749	C2405	A2405	A2523	C	C	C	U	U1870	C1760	G1652	U1523	C1394	U1220	C1229
U2750	C2406	A2406	A2524	C	C	C	U	U1871	C1761	G1653	U1524	C1395	U1220	C1229
U2751	C2407	A2407	A2525	C	C	C	U	U1872	C1762	G1654	U1525	C1396	U1220	C1229
U2752	C2408	A2408	A2526	C	C	C	U	U1873	C1763	G1655	U1526	C1397	U1220	C1229
U2753	C2409	A2409	A2527	C	C	C	U	U1874	C1764	G1656	U1527	C1398	U1220	C1229
U2754	C2410	A2410	A2528	C	C	C	U	U1875	C1765	G1657	U1528	C1399	U1220	C1229
U2755	C2411	A2411	A2529	C	C	C	U	U1876	C1766	G1658	U1529	C1400	U1220	C1229
U2756	C2412	A2412	A2530	C	C	C	U	U1877	C1767	G1659	U1530	C1401	U1220	C1229
U2757	C2413	A2413	A2531	C	C	C	U	U1878	C1768	G1660	U1531	C1402	U1220	C1229
U2758	C2414	A2414	A2532	C	C	C	U	U1879	C1769	G1661	U1532	C1403	U1220	C1229
U2759	C2415	A2415	A2533	C	C	C	U	U1880	C1770	G1662	U1533	C1404	U1220	C1229
U2760	C2416	A2416	A2534	C	C	C	U	U1881	C1771	G1663	U1534	C1405	U1220	C1229
U2761	C2417	A2417	A2535	C	C	C	U	U1882	C1772	G1664	U1535	C1406	U1220	C1229
U2762	C2418	A2418	A2536	C	C	C	U	U1883	C1773	G1665	U1536	C1407	U1220	C1229
U2763	C2419	A2419	A2537	C	C	C	U	U1884	C1774	G1666	U1537	C1408	U1220	C1229
U2764	C2420	A2420	A2538	C	C	C	U	U1885	C1775	G1667	U1538	C1409	U1220	C1229
U2765	C2421	A2421	A2539	C	C	C	U	U1886	C1776	G1668	U1539	C1410	U1220	C1229
U2766	C2422	A2422	A2540	C	C	C	U	U1887	C1777	G1669	U1540	C1411	U1220	C1229
U2767	C2423	A2423	A2541	C	C	C	U	U1888	C1778	G1670	U1541	C1412	U1220	C1229
U2768	C2424	A2424	A2542	C	C	C	U	U1889	C1779	G1671	U1542	C1413	U1220	C1229
U2769	C2425	A2425	A2543	C	C	C	U	U1890	C1780	G1672	U1543	C1414	U1220	C1229
U2770	C2426	A2426	A2544											



● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.53Å 298.18Å 573.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.55 85.30 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.70-2.55) 90.6 (85.30-2.39)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.201 , 0.240 0.188 , 0.224	Depositor DCC
R_{free} test set	6547 reflections (0.95%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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: MG, OMG, CL, SR, NA, K, CD, OMU, UR3, 1MA, 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	A	0.33	0/1786	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.65	0/2552
4	D	0.30	0/1111	0.56	1/1498 (0.1%)
5	E	0.31	0/1382	0.56	0/1880
6	F	0.33	0/901	0.56	0/1224
7	G	0.29	0/241	0.45	0/324
8	H	0.33	0/1302	0.64	0/1743
9	I	0.29	0/526	0.47	0/716
10	J	0.36	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.66	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.35	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.63	0/1999
15	O	0.32	0/874	0.60	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.35	0/749	0.69	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.33	0/648	0.56	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.34	0/417	0.55	0/562
22	V	0.30	0/502	0.51	0/675
23	W	0.33	0/1219	0.60	0/1655
24	X	0.32	0/664	0.57	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.36	0/584	0.60	0/781
27	1	0.39	0/438	0.65	0/578
28	2	0.35	0/401	0.56	0/529
29	3	0.38	0/771	0.57	0/1024
30	0	0.35	0/65953	0.69	25/102860 (0.0%)
31	9	0.30	0/2904	0.70	1/4526 (0.0%)
All	All	0.37	7/98697 (0.0%)	0.68	33/147579 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
30	0	0	46
31	9	0	3
All	All	1	49

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	26.57	2.82	1.50
18	R	150	PRO	CA-C	-19.00	1.14	1.52
18	R	150	PRO	CG-CD	14.11	1.97	1.50
18	R	150	PRO	C-O	11.94	1.47	1.23
18	R	150	PRO	N-CA	11.60	1.67	1.47
18	R	150	PRO	N-CD	10.77	1.62	1.47
18	R	150	PRO	CA-CB	7.91	1.69	1.53

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.33	56.17	112.00
18	R	150	PRO	N-CA-C	-19.61	61.12	112.10
18	R	150	PRO	CA-N-CD	12.19	128.76	111.70
18	R	150	PRO	N-CA-CB	10.92	116.40	103.30
30	0	1942	A	C5'-C4'-C3'	8.23	129.17	116.00
18	R	150	PRO	CA-C-O	-8.07	100.83	120.20
30	0	871	G	C5'-C4'-O4'	-7.66	99.91	109.10
30	0	1942	A	C5'-C4'-O4'	6.92	117.41	109.10
30	0	1592	G	N9-C1'-C2'	6.74	122.76	114.00
30	0	1504	A	C1'-O4'-C4'	-6.26	104.89	109.90
30	0	1819	G	C5'-C4'-C3'	6.22	125.96	116.00
31	9	39	U	N1-C1'-C2'	6.17	122.03	114.00
30	0	777	U	O4'-C1'-N1	5.90	112.92	108.20
30	0	921	G	N9-C1'-C2'	5.80	121.54	114.00
30	0	1942	A	C1'-O4'-C4'	-5.80	105.26	109.90
18	R	150	PRO	CA-CB-CG	-5.79	93.00	104.00
30	0	2316	G	C5'-C4'-C3'	-5.76	106.78	116.00
30	0	1737	A	C5'-C4'-C3'	-5.68	106.91	116.00
30	0	1819	G	C1'-O4'-C4'	-5.67	105.37	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C4'-C3'-C2'	-5.63	96.97	102.60
30	0	1452	G	C5'-C4'-C3'	-5.53	107.15	116.00
30	0	1942	A	C4'-C3'-C2'	-5.52	97.08	102.60
30	0	2467	A	C1'-O4'-C4'	-5.52	105.48	109.90
30	0	206	G	C5'-C4'-C3'	-5.41	107.34	116.00
30	0	2536	C	N1-C1'-C2'	5.37	120.98	114.00
4	D	170	TYR	N-CA-C	5.32	125.35	111.00
30	0	1504	A	N9-C1'-C2'	5.28	120.87	114.00
30	0	1878	G	N9-C1'-C2'	-5.20	106.28	112.00
30	0	1615	A	C5'-C4'-C3'	5.12	124.19	116.00
30	0	1342	C	N1-C1'-C2'	-5.10	106.39	112.00
30	0	2726	U	N1-C1'-C2'	5.08	120.61	114.00
30	0	2313	C	C5'-C4'-O4'	5.07	115.18	109.10
30	0	841	A	C1'-O4'-C4'	-5.03	105.87	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1122	U	Sidechain
30	0	1237	U	Sidechain
30	0	1340	G	Sidechain
30	0	1342	C	Sidechain
30	0	1417	G	Sidechain
30	0	1488	U	Sidechain
30	0	1714	C	Sidechain
30	0	1744	G	Sidechain
30	0	1777	G	Sidechain
30	0	1819	G	Sidechain
30	0	182	G	Sidechain
30	0	1829	A	Sidechain
30	0	1863	G	Sidechain
30	0	1867	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	1979	G	Sidechain
30	0	2036	C	Sidechain
30	0	2316	G	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	2465	A	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2552	C	Sidechain
30	0	2597	U	Sidechain
30	0	2599	A	Sidechain
30	0	26	U	Sidechain
30	0	2607	U	Sidechain
30	0	270	U	Sidechain
30	0	2768	A	Sidechain
30	0	2842	G	Sidechain
30	0	332	G	Sidechain
30	0	396	U	Sidechain
30	0	460	A	Sidechain
30	0	462	A	Sidechain
30	0	469	G	Sidechain
30	0	470	U	Sidechain
30	0	471	G	Sidechain
30	0	482	G	Sidechain
30	0	518	G	Sidechain
30	0	619	U	Sidechain
30	0	664	U	Sidechain
30	0	795	G	Sidechain
30	0	817	G	Sidechain
30	0	867	A	Sidechain
30	0	868	G	Sidechain
31	9	39	U	Sidechain
31	9	87	U	Sidechain
31	9	90	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	51	0
2	B	2625	0	2533	86	0
3	C	1860	0	1813	57	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1094	0	1085	37	0
5	E	1357	0	1266	35	0
6	F	890	0	843	25	0
7	G	240	0	231	6	0
8	H	1282	0	1292	31	0
9	I	519	0	500	19	0
10	J	1120	0	1098	37	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	35	0
13	M	1558	0	1572	48	0
14	N	1445	0	1401	50	0
15	O	865	0	873	24	0
16	P	1136	0	1123	23	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	32	0
19	S	641	0	605	9	0
20	T	950	0	924	25	0
21	U	410	0	364	15	0
22	V	499	0	511	15	0
23	W	1196	0	1137	52	0
24	X	654	0	653	15	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	15	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	13	0
30	0	59017	0	29811	1046	0
31	9	2599	0	1325	78	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	1	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	94	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	1	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5938	0	0	160	0
38	1	51	0	0	1	0
38	2	37	0	0	1	0
38	3	72	0	0	4	0
38	9	145	0	0	9	0
38	A	117	0	0	8	0
38	B	139	0	0	16	0
38	C	165	0	0	10	0
38	D	48	0	0	5	0
38	E	49	0	0	1	0
38	F	25	0	0	1	0
38	G	18	0	0	1	0
38	H	71	0	0	5	0
38	I	8	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	J	55	0	0	1	0
38	K	55	0	0	2	0
38	L	79	0	0	8	0
38	M	138	0	0	3	0
38	N	58	0	0	6	0
38	O	40	0	0	0	0
38	P	61	0	0	1	0
38	Q	49	0	0	2	0
38	R	78	0	0	2	0
38	S	32	0	0	3	0
38	T	36	0	0	3	0
38	U	28	0	0	2	0
38	V	13	0	0	2	0
38	W	68	0	0	5	0
38	X	24	0	0	3	0
38	Y	97	0	0	8	0
38	Z	29	0	0	3	0
All	All	99119	0	59911	1801	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 12.

All (1801) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.41
30:0:2537:G:H5''	30:0:2538:A:H5''	1.17	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.83	1.14
30:0:1205:U:H2'	30:0:1206:U:H5''	1.27	1.12
30:0:1160:G:H5'	30:0:1161:A:H5'	1.13	1.11
23:W:6:GLN:HB2	23:W:26:ILE:HD11	1.30	1.11
15:O:3:THR:HG22	30:0:656:G:H5'	1.26	1.10
14:N:37:ARG:NH1	31:9:6:C:H5''	1.67	1.09
30:0:2102:G:H21	30:0:2103:A:H2'	0.97	1.09
30:0:1160:G:C5'	30:0:1161:A:H5'	1.84	1.07
30:0:871:G:H8	30:0:871:G:H5'	1.12	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07
30:0:1165:G:H1'	30:0:1174:A:H1'	1.34	1.07
30:0:1189:A:H3'	38:0:7701:HOH:O	1.56	1.04
9:I:130:LEU:HD21	30:0:1167:G:H4'	1.40	1.04
10:J:82:THR:HG23	30:0:1242:A:H5'	1.37	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:542:A:H5'	30:0:542:A:H8	1.24	1.02
31:9:56:A:H2'	31:9:57:A:H5''	1.42	1.01
30:0:1160:G:H5'	30:0:1161:A:C5'	1.91	1.01
30:0:1166:A:H61	30:0:1180:U:H3	1.04	1.01
3:C:236:THR:HG22	3:C:239:ALA:H	1.22	1.01
30:0:2748:G:OP1	30:0:2749:U:H5''	1.58	1.00
31:9:76:G:H3'	31:9:77:A:H5''	1.41	1.00
13:M:171:ARG:HD3	30:0:156:C:H5''	1.39	0.98
30:0:2100:A:H5'	38:0:7413:HOH:O	1.63	0.98
30:0:870:G:H2'	30:0:871:G:H5''	1.42	0.98
22:V:1:THR:HB	30:0:93:C:H5''	1.43	0.97
30:0:282:C:O2'	30:0:283:U:H5'	1.64	0.96
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.11	0.96
30:0:1372:A:H3'	38:0:7215:HOH:O	1.65	0.95
30:0:1625:U:H4'	38:0:4678:HOH:O	1.67	0.95
30:0:2102:G:H1'	30:0:2103:A:C8	2.02	0.95
30:0:2541:U:H5'	30:0:2541:U:C6	2.00	0.95
30:0:2102:G:N2	30:0:2103:A:H2'	1.82	0.95
30:0:2588:OMG:H5''	38:0:7509:HOH:O	1.64	0.94
16:P:115:SER:H	16:P:118:GLN:HE21	1.09	0.94
30:0:2717:C:C2'	30:0:2718:C:H5''	1.98	0.94
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.48	0.93
30:0:2710:U:H1'	38:0:7642:HOH:O	1.66	0.93
11:K:10:GLN:H	11:K:10:GLN:HE21	1.05	0.93
30:0:2491:G:H1'	38:0:6895:HOH:O	1.68	0.93
38:B:9058:HOH:O	30:0:2672:C:H1'	1.67	0.92
30:0:1116:U:H3	30:0:1246:A:H62	1.16	0.92
30:0:1205:U:C2'	30:0:1206:U:H5''	1.99	0.92
30:0:2896:A:H5''	38:0:6127:HOH:O	1.70	0.92
30:0:2103:A:H62	30:0:2538:A:H8	1.16	0.91
30:0:2851:G:C2'	30:0:2852:A:H5'	2.01	0.91
30:0:1878:G:H1'	38:0:6149:HOH:O	1.71	0.91
30:0:1290:G:H3'	38:0:5188:HOH:O	1.70	0.90
30:0:1701:A:H4'	30:0:1702:U:H5''	1.54	0.90
30:0:2748:G:H5'	38:0:7565:HOH:O	1.71	0.90
30:0:2406:U:H1'	38:0:6728:HOH:O	1.71	0.90
30:0:2506:A:O2'	30:0:2507:G:H8	1.55	0.90
30:0:2851:G:H2'	30:0:2852:A:H5'	1.54	0.89
30:0:1118:A:H3'	30:0:1118:A:H8	1.36	0.88
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.55	0.88
30:0:1184:C:H1'	38:0:7491:HOH:O	1.73	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1835:U:H5	30:0:1840:A:N7	1.72	0.88
30:0:2812:A:H2	30:0:2814:A:H62	1.06	0.88
30:0:2541:U:H5'	30:0:2541:U:H6	1.34	0.88
30:0:2717:C:H2'	30:0:2718:C:H5''	1.54	0.88
30:0:1300:G:H1'	38:0:4694:HOH:O	1.72	0.88
30:0:2637:A:H5'	38:0:9280:HOH:O	1.73	0.87
30:0:871:G:H8	30:0:871:G:C5'	1.88	0.87
28:2:41:HIS:H	28:2:45:ASN:HD22	1.22	0.87
1:A:211:LYS:HG2	1:A:212:PRO:HD2	1.55	0.87
30:0:1118:A:H3'	30:0:1118:A:C8	2.09	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD2	1.40	0.86
30:0:2537:G:C5'	30:0:2538:A:H5''	2.03	0.86
30:0:256:C:H5''	38:0:5505:HOH:O	1.77	0.85
2:B:238:ASN:HD22	2:B:240:GLY:H	1.19	0.85
30:0:506:G:H22	30:0:509:A:C5'	1.89	0.85
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.19	0.85
30:0:1119:G:N2	30:0:1246:A:C2	2.43	0.85
30:0:545:G:H8	30:0:545:G:H5'	1.41	0.85
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.41	0.85
30:0:2004:U:H2'	30:0:2004:U:O2	1.76	0.85
30:0:1426:C:H2'	38:0:9601:HOH:O	1.76	0.84
30:0:1183:C:N4	30:0:1184:C:H41	1.75	0.84
30:0:2586:U:H3	30:0:2592:G:H22	1.24	0.84
8:H:30:LYS:H	8:H:62:HIS:HD2	1.26	0.84
15:O:3:THR:CG2	30:0:656:G:H5'	2.08	0.84
31:9:23:U:O2'	31:9:24:U:H4'	1.78	0.84
15:O:57:THR:HB	15:O:111:VAL:HG23	1.60	0.83
30:0:1632:A:H2'	30:0:1633:C:H5'	1.60	0.83
30:0:1750:C:H4'	38:0:7509:HOH:O	1.76	0.83
30:0:559:U:H5'	30:0:559:U:H6	1.42	0.83
30:0:2505:G:O2'	30:0:2506:A:H5'	1.79	0.83
30:0:1165:G:O3'	30:0:1174:A:H4'	1.78	0.82
30:0:2783:A:H3'	38:0:5253:HOH:O	1.78	0.82
30:0:1615:A:H5'	38:0:4198:HOH:O	1.76	0.82
30:0:1666:C:O2'	30:0:1667:A:H5''	1.78	0.82
30:0:960:G:H3'	30:0:960:G:N3	1.94	0.82
11:K:39:GLY:HA2	38:0:5242:HOH:O	1.79	0.82
14:N:113:SER:HB2	38:N:8854:HOH:O	1.78	0.82
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.15	0.82
30:0:1116:U:HO2'	30:0:1118:A:H2	0.82	0.82
30:0:544:G:H2'	30:0:545:G:H5''	1.62	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2506:A:HO2'	30:0:2507:G:H8	0.82	0.81
30:0:558:C:C2'	30:0:559:U:H5''	2.10	0.81
22:V:1:THR:HG23	22:V:2:VAL:H	1.43	0.81
30:0:558:C:O2'	30:0:559:U:H5''	1.81	0.81
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.28	0.81
30:0:1667:A:H8	30:0:1667:A:H5'	1.45	0.81
30:0:1183:C:H2'	38:0:6274:HOH:O	1.79	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:2005:G:H3'	30:0:2005:G:OP2	1.81	0.81
30:0:1632:A:C2'	30:0:1633:C:H5'	2.10	0.81
30:0:69:A:H5'	30:0:69:A:C8	2.16	0.81
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.16	0.80
30:0:870:G:C2'	30:0:871:G:H5''	2.09	0.80
17:Q:15:LYS:HD3	30:0:2364:A:H5''	1.62	0.80
4:D:172:VAL:HG12	4:D:173:GLU:H	1.47	0.80
30:0:272:A:H3'	38:0:7553:HOH:O	1.81	0.80
30:0:282:C:H1'	30:0:368:C:N4	1.97	0.80
31:9:56:A:C2'	31:9:57:A:H5''	2.12	0.80
30:0:1474:C:H6	30:0:1474:C:H5'	1.47	0.79
30:0:1189:A:H1'	30:0:1209:C:O4'	1.82	0.79
27:1:25:LYS:HD2	28:2:49:GLU:H	1.48	0.79
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.64	0.79
30:0:1973:A:H5'	30:0:1973:A:H8	1.46	0.79
30:0:558:C:H2'	30:0:559:U:C5'	2.13	0.79
30:0:2100:A:H1'	38:0:5670:HOH:O	1.83	0.79
2:B:206:THR:HG21	30:0:2716:G:H5''	1.65	0.79
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.64	0.79
1:A:199:HIS:HD2	1:A:201:PHE:H	1.28	0.79
30:0:1634:G:H3'	38:0:3910:HOH:O	1.82	0.78
31:9:29:C:H2'	31:9:30:C:H5'	1.65	0.78
30:0:1118:A:H62	30:0:1244:U:H3	1.31	0.78
2:B:211:THR:HG23	30:0:2840:A:OP1	1.82	0.78
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.12	0.78
30:0:381:G:H5''	38:0:4335:HOH:O	1.82	0.78
30:0:1279:U:O2	30:0:1279:U:H2'	1.83	0.78
30:0:2524:G:N2	30:0:2526:C:H41	1.82	0.78
31:9:39:U:H1'	31:9:44:A:H61	1.46	0.78
9:I:130:LEU:CD2	30:0:1167:G:H4'	2.14	0.78
30:0:1377:C:H6	30:0:1377:C:H5'	1.48	0.77
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.67	0.77
30:0:69:A:H5'	30:0:69:A:H8	1.48	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:SER:OG	30:0:2101:A:H2'	1.85	0.77
23:W:21:LEU:HD22	23:W:26:ILE:HD13	1.67	0.77
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.66	0.77
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.67	0.77
30:0:2852:A:H5''	38:0:5255:HOH:O	1.85	0.77
30:0:877:G:H5'	30:0:878:G:OP1	1.84	0.77
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.50	0.76
28:2:20:ARG:HG3	28:2:39:ARG:HH21	1.49	0.76
30:0:1175:G:H1'	30:0:1193:A:H2'	1.65	0.76
30:0:2765:C:H4'	38:0:5545:HOH:O	1.85	0.76
30:0:1730:G:H5''	30:0:1731:C:H6	1.51	0.76
30:0:2769:C:O2'	30:0:2770:G:H5'	1.86	0.76
30:0:1700:C:H5''	30:0:1701:A:OP2	1.86	0.76
23:W:88:THR:HG23	23:W:110:GLN:HE21	1.51	0.76
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.67	0.76
30:0:2537:G:H5''	30:0:2538:A:C5'	2.10	0.75
30:0:1603:A:H5'	30:0:1605:G:O4'	1.86	0.75
30:0:2769:C:C2'	30:0:2770:G:H5'	2.17	0.75
31:9:39:U:H1'	31:9:44:A:N6	2.01	0.75
30:0:1165:G:H21	30:0:1173:A:H5''	1.52	0.75
30:0:2502:C:C2'	30:0:2503:A:H5'	2.17	0.75
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.69	0.75
30:0:506:G:H22	30:0:509:A:H5''	1.50	0.75
6:F:91:VAL:HG12	6:F:92:GLY:H	1.51	0.75
30:0:1116:U:O2'	30:0:1118:A:H2	1.66	0.75
21:U:14:GLU:O	21:U:17:THR:HB	1.87	0.75
1:A:48:ASP:HB3	38:A:9069:HOH:O	1.87	0.74
30:0:2524:G:H21	30:0:2526:C:H41	1.31	0.74
30:0:1206:U:H6	30:0:1206:U:H5'	1.52	0.74
31:9:2:U:H4'	38:9:9099:HOH:O	1.88	0.74
14:N:144:GLY:O	14:N:147:ILE:HG22	1.87	0.74
23:W:88:THR:HB	38:W:6679:HOH:O	1.88	0.74
4:D:154:LYS:HD2	4:D:154:LYS:H	1.53	0.74
30:0:1552:G:N2	30:0:1634:G:H1'	2.03	0.74
30:0:1666:C:H2'	30:0:1667:A:H5'	1.69	0.74
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.68	0.74
18:R:128:ARG:NH2	30:0:2054:A:N3	2.36	0.74
30:0:1701:A:H4'	30:0:1702:U:C5'	2.17	0.74
30:0:541:C:C2'	30:0:542:A:H5''	2.17	0.74
9:I:86:GLU:HG2	30:0:1180:U:H4'	1.68	0.74
30:0:541:C:H2'	30:0:542:A:C5'	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:396:U:H1'	38:0:7649:HOH:O	1.87	0.73
30:0:871:G:C8	30:0:871:G:C5'	2.64	0.73
2:B:212:GLN:HB2	2:B:257:THR:HG21	1.69	0.73
18:R:39:THR:HG22	18:R:42:GLU:H	1.53	0.73
30:0:1209:C:H2'	30:0:1210:G:H8	1.53	0.73
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.69	0.73
30:0:2438:G:H5'	38:0:6199:HOH:O	1.87	0.73
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.71	0.73
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.69	0.73
13:M:171:ARG:CD	30:0:156:C:H5''	2.17	0.73
30:0:558:C:H2'	30:0:559:U:H5'	1.71	0.73
31:9:14:G:H5'	31:9:14:G:H8	1.53	0.73
30:0:1201:C:H5''	38:0:6263:HOH:O	1.87	0.73
30:0:542:A:H5'	30:0:542:A:C8	2.15	0.73
30:0:1165:G:C1'	30:0:1174:A:H1'	2.17	0.73
29:3:48:ASN:HD21	30:0:2468:A:H61	1.37	0.73
30:0:1166:A:N6	30:0:1180:U:H3	1.85	0.72
30:0:2502:C:H2'	30:0:2503:A:H5'	1.71	0.72
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.71	0.72
30:0:2769:C:H2'	30:0:2770:G:O4'	1.88	0.72
30:0:1476:A:O2'	30:0:1477:C:H5'	1.89	0.72
30:0:2812:A:C2	30:0:2814:A:N6	2.54	0.72
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.72
30:0:1119:G:H22	30:0:1246:A:H2	1.37	0.72
30:0:1165:G:H1'	30:0:1174:A:C1'	2.15	0.72
30:0:1730:G:H5''	30:0:1731:C:C6	2.23	0.72
30:0:2718:C:H6	30:0:2718:C:H5'	1.54	0.72
30:0:544:G:C2'	30:0:545:G:H5''	2.19	0.72
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.37	0.72
23:W:137:GLN:HE21	23:W:141:HIS:CE1	2.02	0.71
30:0:138:U:H5''	30:0:139:C:OP2	1.90	0.71
30:0:2908:A:H2'	30:0:2909:G:O4'	1.90	0.71
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.72	0.71
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.71	0.71
30:0:2635:A:O2'	30:0:2636:C:H5'	1.91	0.71
10:J:19:MET:HE3	10:J:132:LEU:HD21	1.70	0.71
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.73	0.71
3:C:139:VAL:HG13	38:C:8641:HOH:O	1.89	0.71
30:0:506:G:H22	30:0:509:A:H5'	1.55	0.71
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.21	0.71
30:0:848:C:H5'	38:0:7298:HOH:O	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2747:C:O3'	30:0:2748:G:H4'	1.90	0.71
18:R:25:PHE:CE2	18:R:29:LYS:HE2	2.26	0.71
30:0:1878:G:O2'	30:0:1879:U:C6	2.44	0.71
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.90	0.70
26:Z:35:SER:HB3	26:Z:47:ARG:HB2	1.72	0.70
30:0:2106:C:H5'	30:0:2284:G:H21	1.55	0.70
30:0:2487:C:H5	38:0:4903:HOH:O	1.74	0.70
30:0:2507:G:H2'	30:0:2510:C:H42	1.57	0.70
30:0:272:A:H5'	30:0:273:G:OP2	1.91	0.70
30:0:2578:G:H5'	30:0:2578:G:H8	1.56	0.70
30:0:282:C:C2'	30:0:283:U:H5'	2.21	0.70
30:0:1058:A:H2'	30:0:1060:C:H5''	1.73	0.70
30:0:1730:G:H5'	30:0:1731:C:C5	2.27	0.70
18:R:29:LYS:HD3	30:0:524:A:H5''	1.73	0.70
30:0:1724:U:H5''	38:0:3745:HOH:O	1.92	0.70
30:0:462:A:H2'	38:0:4898:HOH:O	1.91	0.70
30:0:1278:A:O2'	30:0:1279:U:H3'	1.92	0.69
31:9:49:G:H5''	38:9:9086:HOH:O	1.91	0.69
23:W:4:LEU:HD22	23:W:52:VAL:HG21	1.74	0.69
30:0:1165:G:H21	30:0:1173:A:C5'	2.04	0.69
30:0:280:C:H2'	30:0:281:U:O4'	1.90	0.69
30:0:1380:U:O4	30:0:2748:G:H1'	1.92	0.69
30:0:1299:G:H5'	38:0:4092:HOH:O	1.92	0.69
30:0:1666:C:C2'	30:0:1667:A:H5''	2.22	0.69
30:0:281:U:H2'	30:0:282:C:O4'	1.91	0.69
30:0:1666:C:H2'	30:0:1667:A:C5'	2.22	0.69
30:0:2748:G:C8	30:0:2748:G:H5'	2.28	0.69
13:M:99:ARG:HE	13:M:170:ASN:HD22	1.41	0.69
18:R:39:THR:HG23	18:R:107:GLU:O	1.92	0.69
30:0:2064:U:H5'	30:0:2652:U:H4'	1.75	0.69
30:0:2421:G:H4'	38:0:4795:HOH:O	1.92	0.69
30:0:2541:U:H3'	38:0:9415:HOH:O	1.93	0.69
30:0:2717:C:O2'	30:0:2718:C:H5''	1.91	0.69
30:0:681:G:N3	30:0:681:G:H5'	2.08	0.69
30:0:282:C:H1'	30:0:368:C:H42	1.58	0.69
30:0:292:G:H2'	30:0:358:G:N2	2.08	0.69
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.74	0.69
9:I:108:HIS:H	9:I:109:PRO:HD2	1.56	0.69
30:0:2533:C:H5'	30:0:2533:C:H6	1.57	0.69
1:A:199:HIS:CD2	1:A:201:PHE:H	2.09	0.69
2:B:238:ASN:HD22	2:B:240:GLY:N	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1505:U:H1'	38:0:7611:HOH:O	1.92	0.68
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
30:0:2524:G:H21	30:0:2526:C:N4	1.90	0.68
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.75	0.68
31:9:13:A:O2'	31:9:14:G:H5''	1.92	0.68
3:C:1:MET:HG2	3:C:2:GLN:H	1.59	0.68
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.90	0.68
23:W:84:VAL:HG12	38:W:6679:HOH:O	1.94	0.68
30:0:2102:G:H2'	38:0:7788:HOH:O	1.93	0.68
30:0:558:C:C2'	30:0:559:U:C5'	2.72	0.68
8:H:168:VAL:HG13	38:H:214:HOH:O	1.93	0.68
30:0:2896:A:N3	30:0:2896:A:H2'	2.08	0.68
28:2:28:LYS:O	30:0:87:C:H2'	1.93	0.68
14:N:7:LYS:HE3	17:Q:21:ARG:O	1.92	0.68
30:0:1118:A:C8	30:0:1118:A:C3'	2.73	0.67
30:0:2420:G:O2'	30:0:2421:G:H5'	1.94	0.67
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.76	0.67
30:0:2291:A:C8	30:0:2309:C:H5'	2.29	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
23:W:108:ARG:HH21	23:W:114:PRO:HG2	1.59	0.67
1:A:51:ARG:HB2	38:A:9069:HOH:O	1.94	0.67
14:N:160:SER:HB3	31:9:51:A:H5'	1.77	0.67
25:Y:235:GLU:H	25:Y:235:GLU:CD	1.96	0.67
3:C:27:ARG:NH2	30:0:657:G:OP1	2.27	0.67
6:F:96:ALA:HA	38:F:3111:HOH:O	1.94	0.67
30:0:1377:C:H5'	30:0:1377:C:C6	2.29	0.67
30:0:2661:U:H3	30:0:2812:A:H62	1.42	0.67
30:0:2505:G:C2'	30:0:2506:A:H5'	2.25	0.67
30:0:2878:U:H2'	30:0:2879:A:O4'	1.94	0.67
30:0:1641:A:H2'	30:0:1642:A:H5'	1.77	0.67
28:2:49:GLU:HB2	38:2:131:HOH:O	1.93	0.67
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.29	0.67
12:L:136:ALA:HB3	38:L:8867:HOH:O	1.95	0.67
12:L:18:HIS:HD2	30:0:902:G:N7	1.93	0.67
14:N:160:SER:CB	31:9:51:A:H5'	2.25	0.67
10:J:131:THR:HG22	10:J:134:GLU:H	1.61	0.66
14:N:37:ARG:NH1	31:9:6:C:C5'	2.53	0.66
18:R:150:PRO:O	18:R:150:PRO:CG	2.42	0.66
25:Y:200:THR:HG22	25:Y:201:GLU:HG3	1.77	0.66
30:0:182:G:H5'	38:0:5177:HOH:O	1.96	0.66
30:0:1603:A:H5''	30:0:1605:G:H5'	1.77	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2004:U:O2	30:0:2004:U:C2'	2.43	0.66
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.77	0.66
30:0:541:C:H2'	30:0:542:A:H5''	1.78	0.66
27:1:16:HIS:HD2	30:0:470:U:O2'	1.78	0.66
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.78	0.66
10:J:127:ILE:HG22	33:J:8801:CL:CL	2.33	0.66
30:0:1730:G:C5'	30:0:1731:C:C6	2.79	0.66
30:0:2426:G:H1'	38:0:6120:HOH:O	1.95	0.65
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.77	0.65
23:W:26:ILE:HB	38:W:5420:HOH:O	1.96	0.65
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.65
30:0:1187:U:H5''	38:0:6214:HOH:O	1.96	0.65
30:0:1119:G:N2	30:0:1246:A:H2	1.94	0.65
30:0:545:G:C8	30:0:545:G:H5'	2.30	0.65
2:B:211:THR:HG21	38:0:7480:HOH:O	1.96	0.65
30:0:2032:U:H2'	30:0:2033:G:C5'	2.26	0.65
30:0:299:U:H5'	38:0:7361:HOH:O	1.96	0.65
30:0:567:U:H5''	38:0:6432:HOH:O	1.96	0.65
30:0:1878:G:HO2'	30:0:1879:U:H6	1.41	0.65
30:0:2524:G:H21	30:0:2526:C:H5	1.44	0.65
24:X:61:ARG:HH11	24:X:65:ASN:HB3	1.62	0.65
2:B:51:VAL:CG1	2:B:53:LEU:HD13	2.26	0.65
12:L:140:VAL:HB	38:L:8851:HOH:O	1.96	0.65
15:O:32:ARG:HH21	15:O:35:LYS:NZ	1.94	0.65
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.89	0.65
30:0:125:U:H2'	38:0:3780:HOH:O	1.97	0.64
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.80	0.64
31:9:24:U:H3'	31:9:25:G:H5'	1.79	0.64
5:E:100:ASP:HB2	38:E:2789:HOH:O	1.97	0.64
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.78	0.64
30:0:1166:A:H1'	30:0:1192:A:C2	2.31	0.64
30:0:1187:U:H1'	30:0:1189:A:H2	1.62	0.64
30:0:1166:A:H1'	30:0:1192:A:N3	2.13	0.64
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.79	0.64
3:C:174:ILE:CD1	30:0:338:C:H4'	2.28	0.64
17:Q:25:PRO:HB2	38:9:9078:HOH:O	1.98	0.64
30:0:1451:C:H5'	30:0:1505:U:C5	2.33	0.64
30:0:196:G:H2'	38:0:6681:HOH:O	1.98	0.64
30:0:271:C:H41	30:0:378:A:H2	1.46	0.64
30:0:1187:U:HO2'	30:0:1188:A:H8	1.44	0.64
30:0:2539:U:H3'	38:0:9174:HOH:O	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:76:ASP:HA	38:J:5907:HOH:O	1.97	0.64
27:1:10:LYS:HG3	38:1:2979:HOH:O	1.98	0.64
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.78	0.64
20:T:9:LYS:HD3	38:0:3770:HOH:O	1.97	0.64
24:X:61:ARG:NH1	24:X:65:ASN:HB3	2.12	0.64
30:0:541:C:H2'	30:0:542:A:H5'	1.78	0.64
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.62	0.64
30:0:380:A:H2'	38:0:7253:HOH:O	1.97	0.63
18:R:98:ASN:HD21	30:0:500:G:H21	1.46	0.63
31:9:54:A:H2	38:9:9062:HOH:O	1.80	0.63
3:C:2:GLN:HB3	38:C:8580:HOH:O	1.97	0.63
23:W:80:ASP:O	23:W:84:VAL:HG23	1.97	0.63
6:F:91:VAL:HG12	6:F:92:GLY:N	2.13	0.63
30:0:1187:U:O2'	30:0:1188:A:H8	1.80	0.63
30:0:1666:C:C2'	30:0:1667:A:C5'	2.77	0.63
27:1:20:ARG:HG2	30:0:111:C:O2'	1.98	0.63
2:B:179:LEU:O	2:B:183:GLU:HG2	1.99	0.63
30:0:1919:A:H4'	38:0:4866:HOH:O	1.98	0.63
30:0:283:U:H5	30:0:284:C:N3	1.97	0.63
30:0:1207:A:OP2	30:0:1207:A:H8	1.81	0.63
30:0:1878:G:O2'	30:0:1879:U:H6	1.82	0.63
18:R:117:HIS:HD2	30:0:20:G:H21	1.46	0.63
24:X:25:ARG:HD2	38:X:5356:HOH:O	1.98	0.63
30:0:2670:G:O2'	30:0:2671:U:H5'	1.99	0.63
30:0:2908:A:C2'	30:0:2909:G:H5'	2.29	0.63
10:J:18:ILE:HD13	30:0:1244:U:OP1	1.99	0.63
16:P:115:SER:H	16:P:118:GLN:NE2	1.90	0.63
30:0:441:A:H1'	30:0:442:A:N7	2.13	0.62
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.81	0.62
30:0:1835:U:C5	30:0:1840:A:N7	2.62	0.62
31:9:1:U:H5''	31:9:3:A:OP1	1.99	0.62
30:0:1681:G:H5''	30:0:1682:A:H5'	1.80	0.62
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.81	0.62
25:Y:169:ARG:HD2	30:0:1328:A:OP1	2.00	0.62
30:0:2537:G:H3'	38:0:3125:HOH:O	1.98	0.62
1:A:211:LYS:O	30:0:1943:C:H4'	1.99	0.62
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.29	0.62
30:0:1359:U:C6	30:0:2537:G:N2	2.67	0.62
30:0:2112:A:H2'	30:0:2113:G:C8	2.33	0.62
30:0:42:C:H1'	38:0:4687:HOH:O	1.98	0.62
7:G:12:ILE:HG23	38:0:5483:HOH:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:HG3	26:Z:90:GLY:HA2	1.82	0.62
2:B:214:PRO:HD2	38:B:8953:HOH:O	2.00	0.62
11:K:10:GLN:N	11:K:10:GLN:HE21	1.88	0.62
22:V:5:VAL:HG23	38:V:2271:HOH:O	1.99	0.62
4:D:57:THR:HG23	4:D:63:ILE:HA	1.80	0.62
15:O:3:THR:HG22	30:0:656:G:C5'	2.16	0.62
30:0:1205:U:H2'	30:0:1206:U:C5'	2.18	0.62
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.30	0.62
23:W:65:VAL:HA	23:W:68:THR:HG22	1.81	0.62
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.81	0.62
23:W:125:HIS:HD2	23:W:127:GLY:H	1.48	0.62
30:0:1167:G:H2'	30:0:1168:C:O4'	1.99	0.61
26:Z:60:ASP:HB3	26:Z:69:ASP:HB3	1.81	0.61
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.40	0.61
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.82	0.61
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.82	0.61
30:0:1183:C:H5	30:0:1192:A:OP1	1.83	0.61
3:C:236:THR:HG22	3:C:239:ALA:N	2.05	0.61
31:9:92:G:H2'	31:9:93:A:C8	2.35	0.61
30:0:2607:U:H4'	38:0:9446:HOH:O	1.99	0.61
4:D:103:ASN:ND2	4:D:134:LEU:H	1.98	0.61
21:U:39:ASN:ND2	21:U:44:ARG:HH11	1.98	0.61
30:0:1200:A:H3'	38:0:5785:HOH:O	2.00	0.61
30:0:2748:G:H8	38:0:7565:HOH:O	1.84	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.31	0.61
12:L:6:ARG:HD3	30:0:1299:G:O6	2.00	0.61
30:0:1973:A:H5'	30:0:1973:A:C8	2.33	0.61
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.65	0.61
31:9:29:C:C2'	31:9:30:C:H5'	2.30	0.61
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.61
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.61
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.81	0.61
30:0:1187:U:O2'	30:0:1188:A:C8	2.54	0.60
30:0:558:C:H2'	30:0:559:U:H5''	1.77	0.60
3:C:140:VAL:HB	38:C:8644:HOH:O	2.00	0.60
22:V:42:ASN:HB3	38:V:7247:HOH:O	2.00	0.60
17:Q:95:GLU:HA	30:0:949:U:H4'	1.82	0.60
30:0:204:A:C2'	30:0:205:U:H5'	2.31	0.60
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.60
1:A:3:ARG:HD3	30:0:870:G:OP2	2.01	0.60
2:B:41:PHE:CD1	2:B:79:MET:HE2	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.15	0.60
31:9:54:A:O2'	31:9:55:U:H5'	2.01	0.60
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.83	0.60
2:B:254:GLN:HG2	2:B:255:GLY:N	2.16	0.60
14:N:80:SER:HB2	38:N:8834:HOH:O	2.01	0.60
30:0:1189:A:H1'	30:0:1209:C:C1'	2.31	0.60
30:0:1679:C:H5'	38:0:9330:HOH:O	2.02	0.60
17:Q:40:HIS:HE1	30:0:949:U:O2'	1.83	0.60
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.83	0.60
13:M:164:THR:HG22	13:M:166:ALA:H	1.66	0.60
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.67	0.60
13:M:83:SER:HB3	38:0:4395:HOH:O	2.01	0.60
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.29	0.60
30:0:1342:C:C2'	30:0:1343:C:H5'	2.32	0.60
30:0:254:C:O2	30:0:254:C:H2'	2.01	0.60
4:D:25:MET:SD	4:D:40:ILE:HD11	2.42	0.60
13:M:82:ARG:HD2	38:0:9124:HOH:O	2.01	0.60
25:Y:141:THR:HG23	38:Y:8888:HOH:O	2.00	0.60
30:0:1189:A:O2'	30:0:1208:C:H2'	2.02	0.60
12:L:104:ASP:HB2	38:L:8857:HOH:O	2.00	0.60
30:0:1476:A:N7	38:0:5190:HOH:O	2.32	0.60
30:0:1528:A:H2'	30:0:1529:G:O4'	2.02	0.60
30:0:1667:A:C8	30:0:1667:A:H5'	2.33	0.60
30:0:1766:U:O2	30:0:1778:A:H5'	2.02	0.60
2:B:145:HIS:HD2	2:B:146:THR:O	1.85	0.60
30:0:2769:C:H2'	30:0:2770:G:C5'	2.32	0.59
15:O:32:ARG:HD3	15:O:32:ARG:O	2.02	0.59
23:W:125:HIS:CD2	23:W:127:GLY:H	2.20	0.59
30:0:1632:A:C3'	30:0:1633:C:H5'	2.33	0.59
2:B:41:PHE:CD2	2:B:190:MET:HE3	2.37	0.59
14:N:179:LEU:HA	14:N:184:ILE:HD12	1.84	0.59
30:0:2825:C:H4'	30:0:2826:G:O5'	2.02	0.59
14:N:11:ARG:HD3	31:9:114:G:O6	2.02	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.84	0.59
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.84	0.59
30:0:1116:U:O2'	30:0:1118:A:C2	2.47	0.59
30:0:1342:C:O2'	30:0:1343:C:H5'	2.01	0.59
30:0:2073:G:OP2	30:0:2490:A:H5'	2.03	0.59
38:Z:8718:HOH:O	30:0:819:A:H5''	2.01	0.59
12:L:30:ARG:HD3	30:0:164:G:H4'	1.85	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:81:LYS:HG2	38:0:9547:HOH:O	2.02	0.59
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.84	0.59
28:2:10:ARG:NH2	30:0:121:U:OP2	2.32	0.59
30:0:2239:C:H2'	30:0:2240:U:H6	1.67	0.59
11:K:32:ILE:HD11	11:K:56:SER:HB2	1.84	0.59
17:Q:45:PRO:O	30:0:2365:G:H4'	2.03	0.59
30:0:1278:A:H4'	30:0:1279:U:C4	2.37	0.59
30:0:407:A:H3'	38:0:4474:HOH:O	2.03	0.59
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.85	0.59
3:C:214:THR:HB	38:0:9688:HOH:O	2.02	0.59
4:D:57:THR:HA	38:D:5728:HOH:O	2.01	0.59
6:F:39:SER:HB3	6:F:45:ALA:HB2	1.84	0.59
30:0:1862:C:H1'	38:0:7245:HOH:O	2.01	0.59
30:0:291:C:H2'	30:0:292:G:O4'	2.03	0.59
30:0:960:G:C3'	30:0:960:G:N3	2.66	0.59
20:T:26:THR:HA	20:T:39:ASN:HB3	1.85	0.59
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.59
3:C:174:ILE:HD11	30:0:338:C:H4'	1.85	0.59
30:0:834:G:H4'	30:0:835:U:OP2	2.03	0.59
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.85	0.59
30:0:1182:C:H1'	30:0:1192:A:C8	2.38	0.59
30:0:1819:G:H2'	30:0:1820:G:H4'	1.85	0.59
30:0:2372:A:H2'	30:0:2373:U:C6	2.38	0.59
30:0:603:A:H4'	30:0:604:G:O5'	2.03	0.59
10:J:93:ARG:HH11	10:J:93:ARG:HB3	1.68	0.59
23:W:88:THR:HG22	23:W:90:TYR:HD1	1.68	0.59
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.84	0.58
30:0:1218:U:H2'	30:0:1219:U:C6	2.38	0.58
30:0:2102:G:H21	30:0:2103:A:C2'	1.91	0.58
30:0:2894:C:O2'	30:0:2895:C:H5'	2.02	0.58
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.84	0.58
30:0:1118:A:H8	30:0:1119:G:H5''	1.68	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.03	0.58
30:0:396:U:O2'	30:0:418:C:H4'	2.03	0.58
30:0:1165:G:N2	30:0:1173:A:C5'	2.67	0.58
30:0:200:C:H2'	38:0:3459:HOH:O	2.03	0.58
30:0:2453:G:H5''	38:0:4736:HOH:O	2.04	0.58
2:B:16:ARG:NH1	38:B:9042:HOH:O	2.35	0.58
3:C:202:THR:HG22	30:0:328:U:O4'	2.04	0.58
2:B:162:MET:CE	2:B:310:ARG:HD3	2.33	0.58
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:55:LYS:HG2	16:P:56:GLY:N	2.19	0.58
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.19	0.58
12:L:39:GLU:OE2	30:0:926:A:H5'	2.02	0.58
13:M:99:ARG:HE	13:M:170:ASN:ND2	2.01	0.58
14:N:162:ASP:HA	38:N:8831:HOH:O	2.03	0.58
20:T:1:SER:HB2	30:0:447:A:P	2.44	0.58
30:0:999:C:C2'	30:0:1000:C:H5'	2.34	0.58
30:0:541:C:C2'	30:0:542:A:C5'	2.80	0.58
30:0:1595:G:O2'	30:0:1596:U:H5'	2.04	0.58
30:0:2541:U:C6	30:0:2541:U:C5'	2.82	0.58
2:B:298:LYS:HG2	38:0:5545:HOH:O	2.04	0.58
23:W:88:THR:HG23	23:W:110:GLN:NE2	2.19	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.86	0.57
30:0:1730:G:C5'	30:0:1731:C:C5	2.86	0.57
2:B:17:LYS:O	2:B:260:HIS:HD2	1.87	0.57
30:0:130:C:H5'	38:0:5234:HOH:O	2.02	0.57
30:0:2102:G:H1'	30:0:2103:A:H8	1.65	0.57
4:D:103:ASN:HD22	4:D:134:LEU:H	1.50	0.57
22:V:55:ARG:O	22:V:59:ILE:HG12	2.05	0.57
23:W:44:MET:CE	30:0:944:G:H21	2.16	0.57
30:0:1667:A:H2'	30:0:1668:U:H6	1.70	0.57
30:0:2032:U:H2'	30:0:2033:G:H5'	1.86	0.57
20:T:1:SER:HB2	30:0:447:A:OP2	2.05	0.57
30:0:951:A:C2'	30:0:952:G:H5'	2.34	0.57
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.86	0.57
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.39	0.57
30:0:2320:U:H4'	30:0:2321:A:O4'	2.05	0.57
19:S:57:THR:HG22	19:S:58:MET:N	2.20	0.57
22:V:1:THR:CB	30:0:93:C:H5''	2.28	0.57
15:O:32:ARG:NE	15:O:35:LYS:HD2	2.16	0.57
30:0:1044:C:H3'	30:0:1045:G:H5''	1.86	0.57
30:0:1355:A:H2'	38:0:4139:HOH:O	2.05	0.57
31:9:2:U:OP2	31:9:3:A:H5'	2.05	0.57
30:0:2717:C:H2'	30:0:2718:C:C5'	2.30	0.57
30:0:59:A:H5'	38:0:4347:HOH:O	2.05	0.57
11:K:29:LEU:HB3	11:K:55:VAL:HG21	1.85	0.57
30:0:1878:G:H4'	38:0:4133:HOH:O	2.05	0.57
10:J:45:VAL:HG21	10:J:129:PHE:CD1	2.39	0.57
16:P:10:ALA:HA	16:P:13:VAL:HG12	1.87	0.57
30:0:1201:C:H2'	30:0:1202:A:H5'	1.86	0.57
10:J:63:ILE:HD11	30:0:1236:A:C8	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2541:U:H6	30:0:2541:U:C5'	2.11	0.57
30:0:2827:A:H2'	30:0:2828:G:O4'	2.05	0.57
31:9:24:U:H3'	31:9:25:G:C5'	2.35	0.57
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.87	0.57
30:0:1174:A:C5	30:0:1201:C:H4'	2.39	0.56
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.40	0.56
3:C:236:THR:HG21	38:C:8570:HOH:O	2.04	0.56
26:Z:34:SER:HB3	30:0:797:A:H4'	1.86	0.56
6:F:58:GLU:HG3	6:F:61:MET:HE1	1.87	0.56
30:0:2912:C:H3'	38:0:6403:HOH:O	2.03	0.56
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.41	0.56
10:J:19:MET:CE	10:J:132:LEU:HD11	2.35	0.56
30:0:1165:G:N2	30:0:1173:A:H5''	2.17	0.56
24:X:30:MET:HG2	30:0:1384:C:H5'	1.85	0.56
30:0:2316:G:H4'	38:0:6120:HOH:O	2.05	0.56
30:0:2361:A:H2'	30:0:2362:A:C8	2.40	0.56
30:0:2866:U:H4'	30:0:2867:G:H5'	1.87	0.56
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.88	0.56
21:U:49:LEU:HG	38:U:3805:HOH:O	2.05	0.56
30:0:1474:C:C6	30:0:1474:C:H5'	2.34	0.56
30:0:1838:U:O2'	30:0:2644:C:H5'	2.05	0.56
29:3:61:PRO:HG2	38:0:7581:HOH:O	2.04	0.56
29:3:73:GLU:HB3	38:3:9055:HOH:O	2.04	0.56
38:Z:8706:HOH:O	30:0:1886:A:H4'	2.05	0.56
30:0:2697:A:H2'	30:0:2698:G:O4'	2.06	0.56
30:0:2851:G:O2'	30:0:2852:A:H5'	2.04	0.56
30:0:432:G:O2'	30:0:433:C:H5'	2.06	0.56
29:3:70:ARG:HG2	38:3:9067:HOH:O	2.05	0.56
18:R:9:ASP:O	18:R:13:THR:HG22	2.06	0.56
30:0:1921:A:C6	30:0:1922:A:C2	2.93	0.56
30:0:2032:U:O2'	30:0:2033:G:H5''	2.05	0.56
30:0:2712:G:H5'	38:0:5242:HOH:O	2.03	0.56
31:9:1:U:O3'	31:9:3:A:H5''	2.05	0.56
8:H:155:ARG:NH1	30:0:2503:A:H5''	2.21	0.56
30:0:1527:A:H1'	30:0:1528:A:C8	2.41	0.56
30:0:1667:A:H2'	30:0:1668:U:C6	2.41	0.56
30:0:349:U:O2'	30:0:350:G:H5'	2.06	0.56
30:0:1819:G:H5'	38:0:4724:HOH:O	2.04	0.56
30:0:2524:G:N2	30:0:2526:C:H5	2.04	0.56
14:N:4:PRO:HG3	31:9:69:U:OP1	2.06	0.56
1:A:47:HIS:HD2	30:0:1654:U:H2'	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.87	0.56
30:0:1166:A:P	30:0:1174:A:H4'	2.46	0.56
30:0:204:A:H2'	30:0:205:U:H5'	1.86	0.56
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.56
10:J:82:THR:HG23	30:0:1242:A:C5'	2.25	0.56
24:X:22:ASN:ND2	30:0:2726:U:O2'	2.39	0.56
30:0:602:A:O2'	30:0:605:C:H4'	2.05	0.56
3:C:115:LEU:O	3:C:118:THR:HB	2.06	0.56
11:K:74:VAL:HG12	11:K:75:ARG:HG3	1.88	0.56
18:R:99:ALA:HB1	18:R:109:MET:CE	2.34	0.56
18:R:150:PRO:CG	18:R:150:PRO:CB	2.82	0.56
30:0:2100:A:C8	30:0:2538:A:C2	2.94	0.55
3:C:214:THR:HG23	38:C:8628:HOH:O	2.05	0.55
30:0:2645:U:O2'	30:0:2646:G:P	2.65	0.55
31:9:76:G:C3'	31:9:77:A:H5''	2.27	0.55
1:A:211:LYS:CG	1:A:212:PRO:HD2	2.32	0.55
30:0:1477:C:H5'	30:0:1868:G:H5'	1.87	0.55
30:0:2101:A:O4'	30:0:2537:G:H1'	2.05	0.55
30:0:1279:U:O2	30:0:1279:U:C2'	2.53	0.55
30:0:1477:C:H5'	30:0:1868:G:C5'	2.36	0.55
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.06	0.55
13:M:69:LYS:O	13:M:73:ARG:NH2	2.39	0.55
30:0:1044:C:H5	38:0:6631:HOH:O	1.90	0.55
31:9:52:A:O2'	31:9:53:G:H5'	2.06	0.55
31:9:7:G:H5'	38:9:9096:HOH:O	2.06	0.55
5:E:143:GLN:NE2	30:0:2779:G:H21	2.05	0.55
13:M:76:ARG:HG3	13:M:88:VAL:HG21	1.89	0.55
30:0:1972:U:H2'	30:0:1973:A:C5'	2.36	0.55
30:0:2415:A:H2'	30:0:2416:G:H5'	1.87	0.55
30:0:271:C:C2	30:0:273:G:O4'	2.60	0.55
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.87	0.55
6:F:118:LEU:O	6:F:119:ARG:HB3	2.07	0.55
12:L:143:THR:HG22	12:L:144:ASP:N	2.22	0.55
14:N:110:THR:HB	14:N:113:SER:OG	2.07	0.55
26:Z:51:ALA:HA	38:Z:8715:HOH:O	2.05	0.55
30:0:1191:A:H2	30:0:1206:U:H3	1.55	0.55
30:0:1406:A:H4'	30:0:1407:A:H5''	1.87	0.55
31:9:3:A:H2'	38:9:9042:HOH:O	2.05	0.55
2:B:162:MET:HE2	2:B:310:ARG:HD3	1.87	0.55
2:B:51:VAL:HG13	2:B:53:LEU:HD13	1.89	0.55
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:LYS:O	9:I:105:GLU:HG3	2.07	0.55
30:0:1946:C:H2'	30:0:1971:G:C8	2.41	0.55
10:J:70:PHE:HD1	30:0:2676:C:H4'	1.71	0.55
13:M:9:ARG:HD2	30:0:380:A:OP2	2.07	0.55
30:0:999:C:O2'	30:0:1000:C:H5'	2.07	0.55
14:N:37:ARG:NH1	31:9:6:C:OP1	2.37	0.55
3:C:79:ARG:O	3:C:87:ARG:HG2	2.06	0.55
9:I:129:SER:HB3	30:0:1192:A:H61	1.72	0.55
30:0:2718:C:H5'	30:0:2718:C:C6	2.40	0.55
30:0:2908:A:H2'	30:0:2909:G:C4'	2.37	0.55
3:C:184:ARG:NH2	30:0:450:C:OP1	2.34	0.55
8:H:61:ARG:HG3	8:H:61:ARG:HH11	1.71	0.55
27:1:16:HIS:HE1	30:0:775:G:OP1	1.90	0.54
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.70	0.54
25:Y:133:HIS:HD2	38:Y:8882:HOH:O	1.90	0.54
26:Z:40:ALA:HA	30:0:1773:G:C8	2.41	0.54
30:0:2323:G:H5''	38:0:4795:HOH:O	2.05	0.54
30:0:271:C:H4'	30:0:272:A:OP1	2.08	0.54
31:9:42:C:H5'	31:9:43:G:OP2	2.07	0.54
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.90	0.54
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.35	0.54
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.37	0.54
30:0:1118:A:C8	30:0:1119:G:H5''	2.42	0.54
30:0:1730:G:H5'	30:0:1731:C:H5	1.70	0.54
15:O:37:ARG:HD2	30:0:656:G:OP2	2.08	0.54
2:B:212:GLN:HB2	2:B:257:THR:CG2	2.36	0.54
2:B:297:VAL:HB	38:B:9030:HOH:O	2.08	0.54
30:0:2769:C:H2'	30:0:2770:G:H5'	1.89	0.54
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.88	0.54
30:0:249:G:O2'	30:0:250:C:H5'	2.08	0.54
30:0:482:G:H4'	30:0:508:A:N1	2.22	0.54
30:0:541:C:O2'	30:0:542:A:H5''	2.07	0.54
30:0:952:G:N3	30:0:2302:A:H2'	2.22	0.54
22:V:64:GLY:O	22:V:65:ASP:HB2	2.06	0.54
30:0:1183:C:H42	30:0:1184:C:H41	1.51	0.54
30:0:1350:U:H4'	38:0:5141:HOH:O	2.06	0.54
30:0:2681:A:H4'	30:0:2682:C:H5'	1.90	0.54
31:9:52:A:H2'	31:9:53:G:O4'	2.06	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
23:W:21:LEU:O	23:W:26:ILE:HG23	2.08	0.54
30:0:1175:G:H1'	30:0:1193:A:C2'	2.34	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:37:ARG:NE	38:N:8832:HOH:O	2.36	0.54
15:O:24:ALA:HB3	30:O:710:G:OP1	2.07	0.54
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.90	0.54
23:W:48:VAL:HG12	23:W:48:VAL:O	2.07	0.54
30:O:1206:U:H2'	30:O:1207:A:O4'	2.06	0.54
3:C:43:LYS:HG2	30:O:449:A:N7	2.23	0.54
13:M:80:GLY:O	13:M:81:ARG:HD2	2.08	0.54
23:W:130:HIS:O	23:W:136:GLY:HA3	2.08	0.54
30:O:1878:G:C1'	38:O:6149:HOH:O	2.40	0.54
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.38	0.54
27:1:17:THR:HG21	30:O:120:A:C6	2.43	0.53
1:A:17:ARG:HD2	38:A:9013:HOH:O	2.08	0.53
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.53
4:D:135:VAL:HG22	4:D:136:ARG:H	1.73	0.53
8:H:30:LYS:N	8:H:62:HIS:HD2	2.02	0.53
13:M:59:GLY:HA3	13:M:141:ILE:HD12	1.89	0.53
23:W:38:THR:HB	38:W:5390:HOH:O	2.08	0.53
30:O:2102:G:N3	30:O:2103:A:C8	2.75	0.53
15:O:39:THR:O	15:O:115:ARG:NH2	2.41	0.53
25:Y:186:ARG:HG2	25:Y:186:ARG:HH11	1.72	0.53
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.08	0.53
27:1:9:GLY:HA2	30:O:1687:C:O2	2.09	0.53
30:O:2104:C:O2	30:O:2485:A:N1	2.41	0.53
30:O:2506:A:O2'	30:O:2507:G:C8	2.42	0.53
30:O:2506:A:N6	30:O:2511:A:O2'	2.40	0.53
2:B:125:GLU:O	2:B:129:ARG:HG3	2.08	0.53
4:D:169:THR:HG22	4:D:170:TYR:HD1	1.72	0.53
30:O:2766:A:H5'	38:O:9572:HOH:O	2.06	0.53
30:O:368:C:H2'	30:O:369:G:H5'	1.91	0.53
10:J:19:MET:HE2	10:J:132:LEU:HD11	1.90	0.53
31:9:39:U:C2'	31:9:40:C:OP1	2.56	0.53
3:C:64:GLY:O	30:O:2100:A:H4'	2.08	0.53
14:N:29:SER:HB3	30:O:2415:A:O2'	2.08	0.53
38:B:9058:HOH:O	30:O:2818:A:H2	1.92	0.53
30:O:307:G:H3'	38:O:6710:HOH:O	2.06	0.53
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.90	0.53
30:O:1741:U:O2'	30:O:2723:G:H4'	2.09	0.53
30:O:821:U:H2'	30:O:822:C:H6	1.73	0.53
8:H:66:GLU:HA	38:H:234:HOH:O	2.09	0.53
20:T:19:ARG:HD3	20:T:67:LEU:O	2.09	0.53
23:W:38:THR:HG22	23:W:39:ASP:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.91	0.53
30:0:2591:C:H2'	30:0:2592:G:O4'	2.09	0.53
30:0:2795:C:O2'	30:0:2796:U:H5'	2.09	0.53
13:M:178:LYS:HB2	38:0:6901:HOH:O	2.08	0.53
1:A:210:GLY:N	38:A:9052:HOH:O	2.40	0.53
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.23	0.53
23:W:5:VAL:HG11	23:W:153:MET:HE3	1.91	0.53
24:X:23:HIS:CD2	24:X:24:LYS:HG3	2.44	0.53
30:0:151:A:H2'	30:0:152:A:O4'	2.09	0.53
30:0:2112:A:H2'	30:0:2113:G:H8	1.72	0.53
30:0:2505:G:H2'	30:0:2506:A:H5'	1.91	0.53
30:0:2735:U:H2'	30:0:2736:U:C6	2.44	0.53
30:0:347:A:H2'	30:0:348:C:O4'	2.08	0.53
30:0:407:A:H5'	38:0:6054:HOH:O	2.09	0.53
30:0:1972:U:H2'	30:0:1973:A:H5'	1.91	0.52
30:0:2379:G:N7	30:0:2408:A:N1	2.57	0.52
30:0:2505:G:HO2'	30:0:2506:A:H5'	1.73	0.52
30:0:644:G:N3	30:0:644:G:H5'	2.24	0.52
12:L:41:HIS:HD2	30:0:926:A:O2'	1.91	0.52
28:2:20:ARG:HG3	28:2:39:ARG:NH2	2.23	0.52
30:0:2515:C:C2'	30:0:2516:G:H5'	2.39	0.52
30:0:2563:U:H2'	30:0:2565:C:O5'	2.09	0.52
12:L:133:VAL:HA	38:L:8867:HOH:O	2.10	0.52
23:W:119:HIS:HE1	38:0:9563:HOH:O	1.91	0.52
25:Y:204:ARG:HH22	30:0:553:G:P	2.32	0.52
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.08	0.52
30:0:559:U:C5'	30:0:559:U:H6	2.19	0.52
11:K:41:LYS:HE3	38:0:6239:HOH:O	2.08	0.52
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.91	0.52
13:M:164:THR:HG22	13:M:165:GLY:N	2.24	0.52
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.91	0.52
30:0:136:C:H2'	30:0:137:U:O4'	2.10	0.52
30:0:485:A:N3	30:0:487:G:H5''	2.24	0.52
30:0:920:C:H4'	30:0:921:G:C2	2.45	0.52
4:D:146:LYS:NZ	14:N:107:ASN:HD21	2.07	0.52
30:0:2346:C:O5'	30:0:2346:C:H6	1.92	0.52
30:0:958:G:O2'	30:0:959:C:H5'	2.10	0.52
1:A:192:VAL:HB	38:0:5683:HOH:O	2.09	0.52
2:B:53:LEU:HD11	2:B:327:VAL:HG22	1.92	0.52
4:D:50:VAL:HG13	31:9:41:C:O4'	2.10	0.52
7:G:64:ASN:N	7:G:64:ASN:HD22	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:4:PRO:HD2	38:0:6797:HOH:O	2.09	0.52
10:J:52:GLN:NE2	30:0:1119:G:H8	2.07	0.52
30:0:137:U:H2'	30:0:139:C:C5	2.44	0.52
30:0:2820:A:H2'	30:0:2821:C:C6	2.44	0.52
31:9:92:G:H2'	31:9:93:A:H8	1.74	0.52
2:B:229:ARG:HD2	38:0:9115:HOH:O	2.09	0.52
11:K:29:LEU:HB3	11:K:55:VAL:CG2	2.40	0.52
12:L:41:HIS:CD2	30:0:926:A:O2'	2.63	0.52
14:N:132:ASN:O	14:N:135:VAL:HG12	2.10	0.52
30:0:1878:G:O2'	30:0:1879:U:P	2.68	0.52
20:T:38:ARG:HH21	30:0:306:A:P	2.33	0.52
9:I:73:LEU:HD12	9:I:107:LYS:NZ	2.24	0.52
13:M:82:ARG:HB3	38:0:7854:HOH:O	2.09	0.52
14:N:11:ARG:NH1	31:9:8:G:O6	2.42	0.52
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.39	0.52
30:0:1160:G:H5'	30:0:1161:A:C4'	2.40	0.52
30:0:2070:G:H2'	30:0:2072:G:OP1	2.10	0.52
30:0:95:A:H5''	30:0:97:G:O4'	2.10	0.52
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.92	0.52
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.23	0.52
2:B:53:LEU:HD12	2:B:327:VAL:HA	1.90	0.52
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.90	0.52
30:0:1724:U:H4'	38:0:4582:HOH:O	2.09	0.52
30:0:1778:A:H2'	30:0:1779:A:H5'	1.92	0.52
30:0:2072:G:C6	30:0:2533:C:H1'	2.45	0.52
29:3:84:ARG:NE	38:3:9045:HOH:O	2.43	0.52
22:V:57:LYS:HA	22:V:60:GLN:HE21	1.73	0.52
30:0:790:A:H1'	30:0:1710:A:H2'	1.92	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.10	0.52
30:0:255:A:H2'	30:0:256:C:C6	2.45	0.52
2:B:27:ASN:HD21	30:0:2807:U:P	2.32	0.52
30:0:544:G:H2'	30:0:545:G:C5'	2.37	0.52
2:B:178:ALA:O	2:B:182:VAL:HG23	2.10	0.52
26:Z:42:TYR:HA	30:0:1829:A:N6	2.25	0.52
30:0:1164:U:O2	30:0:1166:A:H4'	2.09	0.51
30:0:2252:A:C5	30:0:2253:G:H1'	2.43	0.51
13:M:24:GLN:HE21	13:M:27:ARG:HH11	1.55	0.51
23:W:151:GLU:O	23:W:154:ARG:HB2	2.10	0.51
30:0:343:C:O2'	30:0:344:C:H5'	2.09	0.51
30:0:389:G:H5''	38:0:6487:HOH:O	2.10	0.51
27:1:25:LYS:HD2	28:2:49:GLU:N	2.21	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:3:91:GLN:O	29:3:92:GLU:HB2	2.10	0.51
10:J:69:TYR:CE1	30:0:2081:A:H4'	2.46	0.51
13:M:69:LYS:HG3	13:M:127:LYS:HG3	1.91	0.51
25:Y:144:ARG:NE	38:Y:8913:HOH:O	2.43	0.51
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.76	0.51
30:0:1209:C:H2'	30:0:1210:G:C8	2.41	0.51
30:0:2883:A:H2'	30:0:2884:G:O4'	2.10	0.51
30:0:564:G:H1'	38:0:6341:HOH:O	2.10	0.51
31:9:20:G:O2'	31:9:21:G:H5'	2.10	0.51
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.92	0.51
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.10	0.51
3:C:127:ARG:HD3	3:C:129:HIS:HE1	1.74	0.51
4:D:49:PRO:HB3	4:D:73:VAL:HG22	1.93	0.51
21:U:37:GLU:HB3	38:U:408:HOH:O	2.09	0.51
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.45	0.51
30:0:542:A:H2'	30:0:543:G:O4'	2.11	0.51
30:0:661:G:C5	30:0:686:A:C2	2.99	0.51
9:I:114:TYR:CE1	30:0:1186:C:H5''	2.45	0.51
30:0:1506:U:H5'	30:0:1506:U:H6	1.75	0.51
30:0:1909:A:N1	30:0:2128:G:H1'	2.25	0.51
30:0:856:G:C8	38:0:5452:HOH:O	2.54	0.51
1:A:206:ARG:HD3	1:A:206:ARG:H	1.75	0.51
2:B:307:ARG:NH1	2:B:307:ARG:HG3	2.17	0.51
3:C:87:ARG:NH2	30:0:894:A:N1	2.58	0.51
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.51
25:Y:174:VAL:HG22	25:Y:177:LYS:HD2	1.92	0.51
30:0:2251:G:H2'	30:0:2252:A:C8	2.46	0.51
6:F:58:GLU:HA	6:F:61:MET:HE2	1.93	0.51
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.25	0.51
20:T:24:ARG:HH21	20:T:39:ASN:HD22	1.58	0.51
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.73	0.51
30:0:1067:A:H5'	38:0:4364:HOH:O	2.10	0.51
30:0:2510:C:H5'	30:0:2511:A:OP2	2.11	0.51
30:0:2908:A:H2'	30:0:2909:G:H5'	1.92	0.51
27:1:8:GLN:HE22	27:1:11:LYS:NZ	2.08	0.51
1:A:95:PRO:HG2	1:A:98:GLU:HG2	1.92	0.51
2:B:190:MET:HE2	2:B:194:PHE:HD1	1.76	0.51
30:0:1947:G:N2	30:0:1966:U:C2	2.79	0.51
30:0:2414:A:H2'	30:0:2415:A:C8	2.46	0.51
30:0:282:C:O2'	30:0:283:U:C5'	2.48	0.51
30:0:1218:U:H2'	30:0:1219:U:H6	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:18:ASN:ND2	28:2:40:ARG:H	2.08	0.51
2:B:294:TYR:HE2	38:B:9074:HOH:O	1.94	0.51
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.11	0.51
23:W:139:GLY:O	23:W:141:HIS:HD2	1.93	0.51
26:Z:35:SER:CB	26:Z:47:ARG:HB2	2.39	0.51
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.51
30:0:1182:C:H4'	30:0:1192:A:N7	2.26	0.51
27:1:28:HIS:CD2	27:1:31:LYS:HG3	2.46	0.51
31:9:108:C:H2'	31:9:109:G:C8	2.46	0.51
3:C:153:VAL:O	3:C:157:LEU:HG	2.11	0.51
8:H:31:ILE:HG23	38:H:234:HOH:O	2.11	0.51
16:P:1:THR:O	30:0:1396:C:H1'	2.10	0.51
22:V:39:ALA:N	22:V:40:PRO:HD2	2.26	0.51
30:0:1196:C:H2'	30:0:1197:G:H5'	1.93	0.50
30:0:1739:G:H1'	30:0:2726:U:O4	2.11	0.50
30:0:440:C:H2'	30:0:441:A:C8	2.46	0.50
1:A:223:ARG:NH1	38:A:8987:HOH:O	2.44	0.50
10:J:39:VAL:HG21	10:J:107:ASN:ND2	2.25	0.50
30:0:1745:G:H22	30:0:2033:G:H5'	1.76	0.50
30:0:2515:C:H2'	30:0:2516:G:H5'	1.93	0.50
3:C:93:LYS:O	3:C:98:ARG:NH2	2.44	0.50
17:Q:21:ARG:HH12	30:0:2353:A:H1'	1.76	0.50
30:0:1948:G:H2'	30:0:1949:G:O4'	2.11	0.50
30:0:2908:A:H2'	30:0:2909:G:C5'	2.40	0.50
30:0:407:A:H2'	30:0:408:A:C8	2.47	0.50
30:0:441:A:H8	30:0:441:A:O5'	1.94	0.50
31:9:51:A:H8	31:9:51:A:OP2	1.94	0.50
11:K:10:GLN:H	11:K:10:GLN:NE2	1.90	0.50
30:0:1060:C:H6	30:0:1060:C:H5'	1.76	0.50
30:0:2769:C:C2'	30:0:2770:G:C5'	2.87	0.50
30:0:522:U:O2'	30:0:1366:C:H5'	2.12	0.50
5:E:145:ALA:HB1	5:E:168:ILE:CD1	2.41	0.50
10:J:86:MET:HE2	30:0:1241:G:H2'	1.93	0.50
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.12	0.50
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.98	0.50
30:0:1149:U:H5''	30:0:1151:G:O4'	2.11	0.50
30:0:2032:U:H2'	30:0:2033:G:H5''	1.91	0.50
30:0:2265:U:H2'	30:0:2266:A:C8	2.47	0.50
30:0:532:A:H3'	38:0:9472:HOH:O	2.11	0.50
31:9:49:G:H2'	31:9:50:G:O4'	2.12	0.50
14:N:160:SER:HB2	31:9:51:A:H5'	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.12	0.50
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.69	0.50
23:W:119:HIS:HD2	23:W:120:PRO:O	1.95	0.50
30:0:1314:U:H5''	30:0:1316:G:O4'	2.11	0.50
16:P:73:HIS:HE1	30:0:1789:G:O6	1.95	0.50
30:0:2756:U:O2	30:0:2896:A:H2	1.95	0.50
30:0:612:U:H2'	30:0:613:C:C6	2.47	0.50
30:0:830:G:O2'	30:0:831:U:H5'	2.12	0.50
8:H:48:VAL:HA	8:H:170:ARG:O	2.12	0.50
30:0:2252:A:H2'	30:0:2253:G:O4'	2.12	0.50
30:0:2587:OMU:HM23	30:0:2589:U:C6	2.47	0.50
30:0:497:A:H5''	38:0:3610:HOH:O	2.11	0.50
30:0:585:C:H5''	38:0:4886:HOH:O	2.10	0.50
30:0:920:C:H5''	30:0:921:G:O5'	2.11	0.50
31:9:49:G:O2'	31:9:50:G:H5'	2.12	0.50
20:T:61:GLU:HG2	38:T:3851:HOH:O	2.10	0.50
24:X:78:GLU:HB3	38:X:5564:HOH:O	2.12	0.50
25:Y:144:ARG:NH1	38:Y:8875:HOH:O	2.44	0.50
30:0:1131:G:C6	30:0:1230:A:C4	2.99	0.50
30:0:1193:A:C2	30:0:1194:A:N6	2.80	0.50
30:0:2649:A:H5'	30:0:2649:A:C8	2.47	0.50
30:0:2649:A:H5'	30:0:2649:A:H8	1.77	0.50
27:1:1:THR:HA	38:0:9363:HOH:O	2.11	0.50
2:B:321:PRO:HA	38:B:9081:HOH:O	2.11	0.50
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.41	0.50
12:L:145:LEU:O	12:L:148:GLU:HG3	2.12	0.50
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.47	0.50
30:0:861:A:H4'	30:0:1697:G:H4'	1.94	0.50
30:0:282:C:C2'	30:0:283:U:C5'	2.89	0.50
5:E:81:GLU:HG2	5:E:134:SER:CB	2.42	0.50
8:H:48:VAL:HG13	38:H:214:HOH:O	2.11	0.50
13:M:188:ARG:HD3	30:0:155:C:OP2	2.11	0.50
30:0:1422:U:H2'	30:0:1423:C:C6	2.47	0.49
30:0:69:A:H8	30:0:69:A:C5'	2.23	0.49
30:0:834:G:H3'	30:0:835:U:H4'	1.94	0.49
13:M:75:ARG:HH11	30:0:1864:C:H5	1.58	0.49
30:0:2032:U:C2'	30:0:2033:G:C5'	2.89	0.49
12:L:143:THR:HG22	12:L:144:ASP:H	1.75	0.49
30:0:1168:C:H5	38:0:7521:HOH:O	1.94	0.49
30:0:603:A:H5''	30:0:604:G:OP1	2.11	0.49
31:9:64:C:C2'	31:9:65:A:H5'	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ALA:O	1:A:124:VAL:HG22	2.11	0.49
9:I:120:ALA:O	9:I:124:VAL:HG23	2.11	0.49
18:R:29:LYS:NZ	38:R:8943:HOH:O	2.46	0.49
25:Y:165:GLU:HB3	38:O:6729:HOH:O	2.12	0.49
30:O:1044:C:H5''	38:O:9029:HOH:O	2.12	0.49
30:O:1207:A:C8	30:O:1208:C:C5	3.00	0.49
30:O:1159:G:H1	30:O:1208:C:H42	1.58	0.49
31:9:105:A:H2'	31:9:106:U:H5'	1.94	0.49
30:O:912:A:C4	30:O:1294:A:C2	3.01	0.49
28:2:42:TRP:HB3	30:O:1418:U:OP1	2.12	0.49
30:O:1834:C:H2'	30:O:1840:A:N6	2.27	0.49
11:K:66:ARG:HH22	30:O:1994:A:P	2.35	0.49
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.45	0.49
2:B:280:VAL:HG13	2:B:333:GLU:O	2.12	0.49
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.94	0.49
12:L:41:HIS:HE1	38:O:9778:HOH:O	1.95	0.49
30:O:1163:G:N2	30:O:1184:C:C4	2.81	0.49
27:1:28:HIS:HE1	30:O:776:A:OP1	1.95	0.49
28:2:41:HIS:HD2	28:2:44:ARG:H	1.60	0.49
3:C:1:MET:HG2	3:C:2:GLN:N	2.25	0.49
25:Y:146:PRO:O	25:Y:154:ARG:HG3	2.13	0.49
30:O:1865:A:C2	38:O:3075:HOH:O	2.55	0.49
2:B:36:PRO:HG3	2:B:169:GLY:H	1.76	0.49
3:C:77:ALA:O	3:C:78:ARG:HD3	2.12	0.49
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.43	0.49
6:F:58:GLU:HA	6:F:61:MET:CE	2.42	0.49
13:M:59:GLY:HA3	13:M:141:ILE:CD1	2.42	0.49
20:T:53:GLY:HA3	38:T:6384:HOH:O	2.12	0.49
30:O:1562:C:N4	38:O:5891:HOH:O	2.45	0.49
30:O:1761:U:H2'	30:O:1762:C:C6	2.47	0.49
1:A:175:LYS:HG3	30:O:1847:A:OP1	2.13	0.49
30:O:1909:A:H2'	30:O:1910:A:C8	2.47	0.49
5:E:101:GLU:HB3	5:E:117:THR:HA	1.94	0.49
12:L:125:PHE:CE1	12:L:140:VAL:HG13	2.48	0.49
14:N:41:LYS:HD3	38:9:9059:HOH:O	2.12	0.49
30:O:1414:A:H2'	30:O:1415:G:O4'	2.12	0.49
30:O:2587:OMU:H6	30:O:2587:OMU:O5'	2.12	0.49
30:O:304:G:H1'	30:O:347:A:N6	2.27	0.49
30:O:426:G:H2'	30:O:427:C:O4'	2.12	0.49
2:B:195:ARG:HG2	2:B:323:LEU:HD22	1.94	0.49
2:B:87:TYR:HD1	38:B:9004:HOH:O	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:59:VAL:HG23	15:O:111:VAL:HG22	1.94	0.49
30:O:1196:C:C2'	30:O:1197:G:H5'	2.42	0.49
30:O:1755:A:H2'	30:O:1756:G:O4'	2.13	0.49
18:R:117:HIS:CD2	30:O:20:G:H21	2.30	0.49
27:1:20:ARG:HH21	30:O:120:A:H5'	1.77	0.49
29:3:60:LYS:HE2	30:O:2428:G:N7	2.27	0.49
2:B:256:GLN:HG2	38:B:9080:HOH:O	2.11	0.49
8:H:72:ALA:HB2	8:H:156:ALA:HB2	1.95	0.49
11:K:66:ARG:HD2	30:O:1992:U:OP2	2.13	0.49
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.42	0.49
30:O:1166:A:C6	30:O:1181:A:C2	3.01	0.48
30:O:1321:A:H2'	30:O:1322:G:C8	2.48	0.48
20:T:54:ASP:OD2	30:O:316:A:H5'	2.13	0.48
30:O:696:C:O2'	30:O:697:G:H5'	2.13	0.48
27:1:28:HIS:CD2	27:1:31:LYS:H	2.31	0.48
2:B:41:PHE:HB3	2:B:190:MET:CE	2.43	0.48
2:B:221:GLN:HE22	11:K:42:ASN:ND2	2.04	0.48
12:L:6:ARG:NH2	38:L:8843:HOH:O	2.45	0.48
14:N:169:PRO:O	14:N:172:PHE:HB3	2.13	0.48
23:W:4:LEU:O	23:W:32:CYS:HA	2.13	0.48
30:O:2512:U:H4'	30:O:2514:U:O4	2.13	0.48
30:O:2637:A:C5'	38:O:4944:HOH:O	2.61	0.48
25:Y:132:ASP:OD2	30:O:621:C:H5'	2.13	0.48
1:A:105:VAL:HG11	1:A:154:ALA:HB1	1.95	0.48
2:B:248:ARG:NH2	30:O:2549:C:H1'	2.28	0.48
2:B:258:GLY:H	2:B:260:HIS:CE1	2.30	0.48
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.95	0.48
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.94	0.48
30:O:221:G:H5''	38:O:5772:HOH:O	2.13	0.48
30:O:635:A:H2'	30:O:636:G:H5''	1.95	0.48
30:O:820:G:O2'	30:O:856:G:H4'	2.13	0.48
3:C:173:LYS:HE3	30:O:1311:G:O6	2.13	0.48
10:J:88:PRO:O	10:J:94:GLY:HA3	2.13	0.48
11:K:49:LEU:CD2	11:K:80:ILE:HD13	2.43	0.48
11:K:87:ARG:NH1	38:K:4066:HOH:O	2.45	0.48
13:M:107:ARG:NH2	30:O:181:G:H4'	2.27	0.48
30:O:625:U:H5''	30:O:1044:C:N4	2.28	0.48
30:O:1185:U:H2'	30:O:1186:C:C6	2.48	0.48
30:O:120:A:H2'	30:O:120:A:N3	2.28	0.48
14:N:147:ILE:HD12	38:9:9086:HOH:O	2.13	0.48
19:S:17:ASP:HB3	19:S:23:LYS:HB2	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:55:SER:O	26:Z:59:GLU:HG3	2.14	0.48
10:J:75:PRO:HD3	10:J:136:SER:OG	2.12	0.48
10:J:52:GLN:HE22	30:0:1119:G:H8	1.62	0.48
30:0:1205:U:C3'	30:0:1206:U:H5''	2.43	0.48
30:0:1205:U:H5	38:0:4455:HOH:O	1.97	0.48
30:0:1353:C:H6	30:0:1353:C:H5'	1.78	0.48
30:0:2134:G:C6	30:0:2258:A:C8	3.02	0.48
30:0:2506:A:H1'	38:0:3761:HOH:O	2.13	0.48
30:0:856:G:H2'	38:0:5452:HOH:O	2.13	0.48
6:F:91:VAL:HG11	30:0:262:A:OP2	2.14	0.48
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.43	0.48
30:0:1298:U:H2'	30:0:1299:G:C8	2.48	0.48
30:0:1790:C:H2'	30:0:1791:U:C6	2.49	0.48
30:0:1972:U:C2'	30:0:1973:A:H5''	2.44	0.48
30:0:627:G:H2'	30:0:2071:C:C4	2.48	0.48
30:0:316:A:N3	30:0:336:G:O2'	2.42	0.48
30:0:447:A:O2'	30:0:448:G:H5'	2.14	0.48
2:B:254:GLN:HG3	38:B:8960:HOH:O	2.13	0.48
2:B:305:ASP:O	2:B:306:LYS:HB2	2.14	0.48
30:0:10:U:H6	30:0:10:U:H3'	1.79	0.48
30:0:1117:A:C2	30:0:1244:U:C2	3.01	0.48
30:0:152:A:O2'	30:0:153:C:H5'	2.13	0.48
30:0:1559:A:H4'	38:0:5891:HOH:O	2.13	0.48
30:0:1632:A:H2'	30:0:1633:C:C5'	2.38	0.48
30:0:1902:G:H2'	30:0:1903:U:O4'	2.14	0.48
30:0:2101:A:H1'	30:0:2537:G:O4'	2.14	0.48
30:0:1838:U:H1'	30:0:2644:C:H5'	1.96	0.48
1:A:36:ASP:O	1:A:38:ILE:N	2.38	0.48
3:C:233:THR:HG22	3:C:234:VAL:N	2.28	0.48
30:0:1081:A:H5''	38:0:3162:HOH:O	2.14	0.48
11:K:87:ARG:NH2	30:0:2720:C:O2	2.47	0.48
30:0:697:G:H4'	30:0:730:G:O3'	2.14	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.14	0.48
25:Y:145:LYS:HE2	38:Y:8907:HOH:O	2.14	0.48
30:0:1194:A:C2	30:0:1206:U:H1'	2.48	0.48
30:0:1535:G:H2'	30:0:1536:C:C6	2.49	0.48
30:0:1555:G:H4'	30:0:1630:A:H2	1.79	0.48
30:0:2809:G:H2'	30:0:2810:G:O4'	2.14	0.48
30:0:1181:A:N1	30:0:1192:A:O2'	2.41	0.47
30:0:1333:U:H2'	30:0:1334:C:C6	2.49	0.47
30:0:1524:U:HO2'	30:0:1525:G:P	2.37	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.96	0.47
30:0:2238:A:C2	30:0:2239:C:C6	3.02	0.47
23:W:154:ARG:NH1	30:0:588:G:O6	2.47	0.47
30:0:821:U:H2'	30:0:822:C:C6	2.49	0.47
30:0:960:G:N3	30:0:960:G:C2'	2.76	0.47
2:B:102:THR:HG21	2:B:182:VAL:O	2.14	0.47
3:C:246:ARG:NE	38:C:8616:HOH:O	2.38	0.47
12:L:30:ARG:HD2	38:0:9024:HOH:O	2.14	0.47
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.28	0.47
13:M:64:ARG:HD2	38:M:8887:HOH:O	2.15	0.47
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.43	0.47
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.14	0.47
30:0:23:G:C6	30:0:24:G:N1	2.83	0.47
12:L:73:VAL:HG23	12:L:74:THR:H	1.79	0.47
14:N:155:GLU:O	14:N:156:GLU:HG3	2.14	0.47
19:S:76:GLU:HB3	38:S:7263:HOH:O	2.13	0.47
1:A:237:GLY:HA3	30:0:1939:U:H5''	1.95	0.47
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.30	0.47
14:N:114:LYS:O	14:N:118:ILE:HG13	2.14	0.47
30:0:999:C:H2'	30:0:1000:C:H5'	1.95	0.47
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.96	0.47
30:0:1182:C:C1'	30:0:1192:A:C8	2.97	0.47
30:0:1132:A:N6	30:0:1229:C:H2'	2.30	0.47
30:0:1656:A:H2'	30:0:1657:A:O4'	2.15	0.47
30:0:2001:G:O2'	30:0:2002:C:H5'	2.14	0.47
30:0:2102:G:H3'	38:0:3643:HOH:O	2.14	0.47
15:O:25:VAL:HG13	30:0:710:G:H5'	1.97	0.47
27:1:28:HIS:HD2	27:1:30:LYS:H	1.61	0.47
31:9:50:G:H2'	31:9:51:A:C8	2.48	0.47
3:C:242:GLU:HB2	38:C:8578:HOH:O	2.14	0.47
25:Y:155:ARG:NH1	38:Y:8857:HOH:O	2.47	0.47
25:Y:216:ARG:HD2	38:Y:8869:HOH:O	2.12	0.47
30:0:1406:A:H4'	30:0:1407:A:C5'	2.45	0.47
7:G:23:ILE:O	7:G:27:ILE:HG13	2.14	0.47
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.96	0.47
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.95	0.47
25:Y:144:ARG:NH1	30:0:905:C:OP1	2.48	0.47
30:0:1165:G:N2	30:0:1173:A:H5'	2.30	0.47
30:0:1477:C:H2'	30:0:1478:U:C6	2.50	0.47
30:0:2616:G:N3	30:0:2616:G:H2'	2.28	0.47
30:0:538:C:H5''	30:0:539:G:C8	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:65:A:N6	31:9:112:U:C6	2.82	0.47
2:B:262:ARG:HG3	30:0:2716:G:H5'	1.97	0.47
3:C:127:ARG:HD3	3:C:129:HIS:CE1	2.50	0.47
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.80	0.47
20:T:79:LEU:HG	20:T:89:ARG:HB2	1.96	0.47
23:W:5:VAL:HG11	23:W:153:MET:CE	2.44	0.47
26:Z:46:SER:O	26:Z:50:VAL:HG23	2.14	0.47
30:0:1178:G:C6	30:0:1179:C:N4	2.83	0.47
30:0:1925:G:O2'	30:0:1926:G:H5'	2.15	0.47
4:D:52:THR:HG21	30:0:2346:C:O2'	2.14	0.47
30:0:2502:C:H2'	30:0:2503:A:C5'	2.42	0.47
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.45	0.47
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.15	0.47
23:W:11:VAL:HG11	30:0:1086:A:C6	2.49	0.47
30:0:10:U:O4	30:0:532:A:OP2	2.32	0.47
30:0:1181:A:H2'	30:0:1182:C:H5'	1.95	0.47
30:0:1193:A:H2	30:0:1194:A:N6	2.13	0.47
30:0:2456:A:H2'	30:0:2457:U:C6	2.50	0.47
30:0:2541:U:H5''	38:0:5423:HOH:O	2.14	0.47
30:0:561:G:O2'	30:0:562:A:H5'	2.15	0.47
25:Y:148:GLY:HA3	30:0:622:G:P	2.55	0.47
30:0:999:C:H2'	30:0:1000:C:C5'	2.45	0.47
28:2:38:LYS:HE3	38:0:4243:HOH:O	2.15	0.47
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.45	0.47
10:J:39:VAL:HG22	10:J:107:ASN:HA	1.95	0.47
12:L:91:VAL:HG13	12:L:120:LEU:HD23	1.96	0.47
30:0:1014:A:H5''	31:9:101:G:O2'	2.15	0.47
30:0:1252:A:H2'	30:0:1253:C:O4'	2.15	0.47
30:0:1985:U:C2	30:0:1996:U:O4'	2.68	0.47
30:0:280:C:O2'	30:0:281:U:H5'	2.15	0.47
10:J:107:ASN:HD22	10:J:109:TYR:H	1.63	0.47
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.40	0.47
9:I:114:TYR:HE1	30:0:1186:C:H5''	1.78	0.47
30:0:1496:A:H2'	30:0:1497:G:O4'	2.15	0.47
30:0:2828:G:O2'	30:0:2829:G:H5'	2.14	0.47
31:9:95:C:O2'	31:9:96:C:H5'	2.15	0.47
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.15	0.47
10:J:52:GLN:NE2	30:0:1119:G:H2'	2.30	0.47
30:0:1163:G:N1	30:0:1184:C:N4	2.63	0.46
30:0:64:G:H2'	30:0:65:C:O4'	2.15	0.46
27:1:25:LYS:CD	28:2:49:GLU:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:20:VAL:O	7:G:24:VAL:HG23	2.15	0.46
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.46	0.46
30:0:1120:U:H5''	30:0:1120:U:C6	2.51	0.46
30:0:1160:G:H5''	30:0:1161:A:H5'	1.87	0.46
30:0:1735:C:O2'	30:0:1736:A:H5'	2.14	0.46
30:0:2247:C:H2'	30:0:2248:C:H6	1.81	0.46
31:9:60:C:O2'	31:9:61:C:H5'	2.15	0.46
2:B:258:GLY:HA2	38:0:4025:HOH:O	2.15	0.46
8:H:30:LYS:H	8:H:62:HIS:CD2	2.17	0.46
10:J:45:VAL:CG2	10:J:129:PHE:HD1	2.29	0.46
14:N:37:ARG:HH11	31:9:6:C:P	2.37	0.46
16:P:16:VAL:HG12	16:P:17:GLY:N	2.30	0.46
23:W:88:THR:CG2	23:W:90:TYR:HD1	2.28	0.46
30:0:1592:G:O2'	30:0:1593:C:O5'	2.34	0.46
2:B:282:GLY:O	30:0:2898:G:H1'	2.15	0.46
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.97	0.46
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.96	0.46
10:J:45:VAL:CG2	10:J:129:PHE:CD1	2.98	0.46
13:M:77:HIS:HD2	13:M:79:ALA:O	1.98	0.46
30:0:1120:U:H5'	30:0:1121:G:OP2	2.16	0.46
30:0:1164:U:C2	30:0:1166:A:H4'	2.50	0.46
30:0:1192:A:H3'	30:0:1193:A:H5'	1.98	0.46
30:0:1518:A:H2'	30:0:1519:U:C6	2.50	0.46
30:0:1942:A:H3'	38:0:7372:HOH:O	2.15	0.46
30:0:2241:C:O2'	30:0:2242:U:H5'	2.15	0.46
30:0:2372:A:H2'	30:0:2373:U:H6	1.80	0.46
30:0:2515:C:H2'	30:0:2516:G:C5'	2.46	0.46
30:0:690:G:H4'	30:0:741:C:O2	2.16	0.46
13:M:68:ARG:NH2	13:M:73:ARG:HD3	2.30	0.46
16:P:40:VAL:O	16:P:44:VAL:HG23	2.16	0.46
30:0:2004:U:H5''	30:0:2005:G:C8	2.50	0.46
30:0:255:A:C5	30:0:256:C:C4	3.03	0.46
30:0:703:G:O2'	30:0:704:C:H5'	2.16	0.46
27:1:48:TYR:HE2	38:0:9317:HOH:O	1.99	0.46
1:A:211:LYS:HB3	38:0:7455:HOH:O	2.15	0.46
1:A:71:PRO:HD2	1:A:74:VAL:HG21	1.98	0.46
2:B:307:ARG:HD2	38:B:9077:HOH:O	2.15	0.46
6:F:37:THR:O	6:F:41:GLU:HG3	2.15	0.46
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.97	0.46
30:0:1203:G:O2'	30:0:1204:C:H5'	2.16	0.46
30:0:2356:A:H5'	38:0:5662:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2507:G:H2'	30:0:2510:C:N4	2.27	0.46
30:0:2103:A:N6	30:0:2538:A:H8	1.97	0.46
3:C:127:ARG:CZ	3:C:225:PRO:HG2	2.45	0.46
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.97	0.46
5:E:112:ALA:HA	5:E:113:PRO:HD3	1.84	0.46
38:Q:2875:HOH:O	30:0:2392:C:H4'	2.15	0.46
30:0:816:G:C6	30:0:817:G:N1	2.84	0.46
1:A:11:ARG:HD3	38:0:9224:HOH:O	2.15	0.46
2:B:148:PRO:HD2	38:B:9005:HOH:O	2.15	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.16	0.46
30:0:1211:G:H2'	30:0:1212:C:H6	1.81	0.46
30:0:1819:G:H2'	30:0:1820:G:C4'	2.45	0.46
30:0:2072:G:H3'	30:0:2073:G:C5'	2.46	0.46
30:0:2351:C:H2'	30:0:2352:G:O4'	2.16	0.46
30:0:2587:OMU:CM2	30:0:2589:U:C6	2.99	0.46
8:H:27:PRO:HD3	8:H:123:ILE:HG22	1.98	0.46
10:J:80:LYS:HE2	10:J:98:PHE:CE1	2.51	0.46
12:L:32:ASP:HB3	30:0:222:A:H5''	1.97	0.46
18:R:3:SER:HB2	30:0:20:G:O3'	2.16	0.46
21:U:33:SER:O	21:U:37:GLU:HG3	2.15	0.46
30:0:1014:A:H2'	30:0:1015:C:H5'	1.97	0.46
30:0:1484:G:H3'	38:0:7841:HOH:O	2.16	0.46
30:0:1524:U:OP1	30:0:1524:U:H4'	2.16	0.46
30:0:1615:A:H4'	38:0:5912:HOH:O	2.16	0.46
30:0:1641:A:C2'	30:0:1642:A:H5'	2.45	0.46
30:0:1851:G:O2'	30:0:1852:A:H5'	2.16	0.46
13:M:75:ARG:NH1	30:0:1864:C:H5	2.14	0.46
30:0:1996:U:O2'	30:0:1997:A:H5'	2.16	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.47	0.46
31:9:22:G:H5'	31:9:23:U:OP1	2.16	0.46
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.46	0.46
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.98	0.46
30:0:2839:C:H2'	30:0:2840:A:H5''	1.98	0.46
30:0:407:A:H8	38:0:4474:HOH:O	1.99	0.46
30:0:830:G:H2'	30:0:831:U:C6	2.51	0.46
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.78	0.46
12:L:97:VAL:HG12	12:L:98:GLU:O	2.16	0.46
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.31	0.46
13:M:82:ARG:HA	38:M:8836:HOH:O	2.16	0.46
23:W:149:LEU:HG	23:W:153:MET:HE2	1.98	0.46
30:0:1175:G:H8	30:0:1193:A:HO2'	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2282:U:H4'	30:0:2309:C:C5	2.51	0.45
30:0:2421:G:H2'	38:0:4096:HOH:O	2.16	0.45
30:0:666:A:H2'	30:0:667:C:O4'	2.16	0.45
4:D:76:ARG:CZ	31:9:44:A:H1'	2.46	0.45
2:B:316:ARG:HB2	30:0:2768:A:C8	2.51	0.45
3:C:180:SER:HB2	38:C:8638:HOH:O	2.15	0.45
4:D:36:ASN:HB3	38:D:7502:HOH:O	2.15	0.45
30:0:2506:A:H2'	30:0:2506:A:O5'	2.16	0.45
30:0:2748:G:C5'	30:0:2748:G:C8	2.98	0.45
30:0:664:U:O4	30:0:681:G:H5''	2.16	0.45
2:B:13:PHE:HB2	2:B:16:ARG:NH1	2.31	0.45
4:D:41:LEU:HA	4:D:44:ILE:HG22	1.98	0.45
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.98	0.45
15:O:96:VAL:HG13	15:O:100:GLN:HB2	1.98	0.45
23:W:81:ASP:OD1	23:W:92:ASP:HB2	2.16	0.45
30:0:1008:C:H2'	30:0:1009:U:C6	2.51	0.45
30:0:1185:U:H5'	38:0:7491:HOH:O	2.15	0.45
30:0:1948:G:H2'	30:0:1949:G:H8	1.80	0.45
30:0:2314:G:C2'	30:0:2315:C:H5'	2.47	0.45
30:0:2906:A:H5'	30:0:2907:C:O4'	2.17	0.45
29:3:42:ARG:NH1	30:0:396:U:H5'	2.31	0.45
30:0:560:U:C2	30:0:561:G:C8	3.04	0.45
4:D:37:ALA:HA	38:D:5583:HOH:O	2.16	0.45
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.46	0.45
5:E:1:PRO:HG2	5:E:59:MET:SD	2.57	0.45
11:K:114:ALA:HB3	11:K:117:VAL:HG23	1.97	0.45
15:O:32:ARG:HH21	15:O:35:LYS:HZ3	1.62	0.45
19:S:67:ARG:HD3	38:S:3430:HOH:O	2.17	0.45
30:0:1021:G:O2'	30:0:1022:A:H5'	2.17	0.45
30:0:1335:C:H2'	30:0:1336:U:C6	2.51	0.45
30:0:1739:G:O2'	30:0:1740:U:H5'	2.16	0.45
8:H:6:ALA:HB3	30:0:2521:A:OP2	2.15	0.45
30:0:2679:G:H2'	30:0:2681:A:OP2	2.17	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.51	0.45
27:1:28:HIS:HD2	27:1:31:LYS:H	1.64	0.45
31:9:59:C:H2'	31:9:60:C:C6	2.52	0.45
3:C:150:THR:HA	3:C:203:ALA:O	2.17	0.45
9:I:129:SER:HB3	30:0:1192:A:N6	2.31	0.45
24:X:22:ASN:O	24:X:64:ALA:HA	2.17	0.45
30:0:1163:G:H2'	30:0:1164:U:C5	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1236:A:H2'	30:0:1237:U:O4'	2.16	0.45
30:0:1119:G:C5	30:0:1243:C:C4	3.04	0.45
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.45
31:9:29:C:H2'	31:9:30:C:C5'	2.43	0.45
31:9:76:G:H3'	31:9:77:A:C5'	2.30	0.45
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.44	0.45
2:B:212:GLN:HA	30:0:1733:A:H4'	1.98	0.45
30:0:2502:C:O2'	30:0:2503:A:H5'	2.17	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.99	0.45
11:K:113:ILE:HD12	11:K:128:ALA:HB2	1.98	0.45
30:0:1182:C:H1'	30:0:1192:A:H8	1.82	0.45
9:I:121:LYS:HB3	30:0:1184:C:H4'	1.98	0.45
30:0:2238:A:O2'	30:0:2239:C:H5'	2.17	0.45
30:0:2493:C:H2'	30:0:2493:C:O2	2.16	0.45
30:0:2508:C:H2'	30:0:2509:A:O5'	2.17	0.45
30:0:407:A:O2'	30:0:408:A:H5'	2.17	0.45
30:0:95:A:O5'	30:0:97:G:H5'	2.17	0.45
30:0:969:G:H1	30:0:999:C:N4	2.15	0.45
1:A:186:TRP:CG	1:A:187:PRO:HA	2.52	0.45
14:N:108:SER:HA	14:N:109:PRO:HD3	1.76	0.45
20:T:52:ARG:O	30:0:317:A:OP1	2.33	0.45
21:U:31:PHE:CG	21:U:37:GLU:HG2	2.52	0.45
23:W:3:ALA:O	23:W:54:PHE:HA	2.16	0.45
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.52	0.45
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.37	0.45
30:0:1391:G:H2'	30:0:1392:A:H5'	1.99	0.45
30:0:1419:U:H2'	30:0:1685:A:C2	2.51	0.45
1:A:192:VAL:HG12	1:A:207:GLN:HB3	1.97	0.45
9:I:108:HIS:N	9:I:109:PRO:HD2	2.29	0.45
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.45
21:U:52:THR:HG22	21:U:55:ALA:H	1.81	0.45
30:0:1714:C:O2'	30:0:1715:C:H5'	2.17	0.45
30:0:2429:A:H2'	30:0:2430:A:C8	2.52	0.45
1:A:165:THR:HG22	38:A:9083:HOH:O	2.17	0.45
3:C:218:VAL:N	38:C:8616:HOH:O	2.48	0.45
3:C:236:THR:HA	38:C:8644:HOH:O	2.16	0.45
5:E:6:GLU:HA	5:E:46:THR:HG22	1.99	0.45
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.52	0.45
21:U:52:THR:CG2	21:U:54:THR:HB	2.47	0.45
30:0:1759:A:N3	30:0:1818:C:H2'	2.32	0.45
30:0:195:C:H5''	38:0:5427:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2102:G:H1'	30:0:2103:A:N7	2.29	0.45
30:0:2509:A:OP2	30:0:2510:C:H5	2.00	0.45
30:0:2096:A:N7	30:0:2539:U:C4	2.84	0.45
4:D:23:VAL:HG11	4:D:83:PHE:CZ	2.52	0.45
17:Q:49:ASN:HB2	38:Q:5227:HOH:O	2.17	0.45
38:K:7438:HOH:O	21:U:20:MET:HE1	2.16	0.45
30:0:1198:U:C6	30:0:1200:A:OP2	2.70	0.44
30:0:1588:G:C5	30:0:1589:G:C6	3.05	0.44
16:P:68:LYS:HE2	30:0:1787:C:OP1	2.17	0.44
30:0:2775:A:C6	30:0:2799:A:C8	3.04	0.44
30:0:368:C:C2'	30:0:369:G:H5'	2.46	0.44
2:B:235:ARG:HD3	30:0:2091:G:O3'	2.16	0.44
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.37	0.44
30:0:2038:A:O2'	30:0:2039:A:H5'	2.16	0.44
30:0:2072:G:P	38:0:3107:HOH:O	2.76	0.44
30:0:2425:A:H5'	30:0:2426:G:OP2	2.18	0.44
30:0:2819:C:H2'	30:0:2820:A:C8	2.53	0.44
30:0:638:C:H2'	30:0:639:A:C8	2.52	0.44
31:9:105:A:C2'	31:9:106:U:H5'	2.46	0.44
14:N:37:ARG:HD2	31:9:6:C:OP1	2.16	0.44
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.99	0.44
4:D:173:GLU:HA	38:D:6326:HOH:O	2.17	0.44
8:H:33:GLN:H	8:H:69:ARG:NH1	2.15	0.44
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.17	0.44
30:0:1334:C:O2'	30:0:1335:C:H5'	2.17	0.44
30:0:1592:G:O2'	30:0:1593:C:O4'	2.27	0.44
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.44
30:0:2064:U:H5'	30:0:2652:U:O3'	2.17	0.44
30:0:286:U:H2'	30:0:287:C:C6	2.52	0.44
30:0:699:C:H2'	30:0:744:G:O4'	2.16	0.44
28:2:22:PRO:HG2	28:2:25:VAL:HG23	1.99	0.44
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.98	0.44
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.44
30:0:2896:A:C2'	30:0:2896:A:N3	2.78	0.44
20:T:52:ARG:HD2	30:0:317:A:H5''	1.98	0.44
30:0:319:A:H4'	30:0:338:C:C4	2.53	0.44
30:0:557:C:C2	30:0:601:G:N2	2.85	0.44
30:0:750:A:H2'	30:0:751:U:C6	2.53	0.44
30:0:876:A:N3	30:0:876:A:H2'	2.33	0.44
11:K:20:CYS:HB2	11:K:29:LEU:HG	2.00	0.44
14:N:171:HIS:CE1	38:N:8860:HOH:O	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.16	0.44
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.17	0.44
31:9:74:G:C6	31:9:75:G:N7	2.85	0.44
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.98	0.44
23:W:115:THR:HG23	38:W:5420:HOH:O	2.16	0.44
25:Y:144:ARG:NH2	38:Y:8913:HOH:O	2.51	0.44
30:0:1182:C:O2'	30:0:1192:A:H8	1.99	0.44
30:0:1588:G:C6	30:0:1589:G:N1	2.86	0.44
30:0:1790:C:H2'	30:0:1791:U:H6	1.83	0.44
30:0:1819:G:H2'	30:0:1820:G:C5'	2.48	0.44
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.17	0.44
30:0:2505:G:H2'	30:0:2506:A:C5'	2.48	0.44
20:T:2:LYS:HG2	30:0:447:A:OP1	2.17	0.44
31:9:65:A:C2'	31:9:66:G:OP2	2.65	0.44
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.17	0.44
16:P:16:VAL:CG1	16:P:20:ARG:HB2	2.47	0.44
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.33	0.44
30:0:1183:C:H41	30:0:1192:A:P	2.41	0.44
30:0:1471:A:H5'	38:0:3202:HOH:O	2.17	0.44
30:0:366:U:H2'	30:0:367:G:O4'	2.17	0.44
4:D:135:VAL:HG22	4:D:136:ARG:N	2.32	0.44
14:N:71:TRP:HB2	38:N:8837:HOH:O	2.17	0.44
23:W:88:THR:HG22	23:W:89:ASP:N	2.32	0.44
30:0:1121:G:H4'	38:0:5565:HOH:O	2.17	0.44
30:0:1367:A:H2'	30:0:1368:U:O4'	2.18	0.44
30:0:1603:A:C5'	30:0:1605:G:O4'	2.59	0.44
30:0:496:G:H3'	38:0:7689:HOH:O	2.18	0.44
33:0:8813:CL:CL	38:0:4694:HOH:O	2.58	0.44
31:9:1:U:O3'	31:9:3:A:C5'	2.66	0.44
3:C:27:ARG:HG3	3:C:29:ASP:OD1	2.17	0.44
14:N:119:GLN:O	14:N:123:ILE:HG13	2.18	0.44
22:V:12:THR:HG22	22:V:15:GLU:CG	2.48	0.44
23:W:52:VAL:HG13	23:W:53:ALA:N	2.32	0.44
25:Y:151:SER:HB3	25:Y:154:ARG:HB2	1.99	0.44
30:0:101:C:H2'	30:0:102:A:H8	1.83	0.44
30:0:1304:U:H2'	30:0:1305:C:C6	2.53	0.44
30:0:1996:U:H6	30:0:2586:U:O2	2.00	0.44
30:0:1883:U:H5'	30:0:2012:U:OP2	2.18	0.44
12:L:57:VAL:HG21	30:0:2443:C:H5'	1.99	0.44
30:0:2611:U:O2'	30:0:2614:C:OP2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:816:G:H5'	30:0:1598:A:H4'	2.00	0.44
27:1:17:THR:HG21	30:0:120:A:C5	2.52	0.44
2:B:75:GLU:C	2:B:77:PRO:HD3	2.38	0.44
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.76	0.44
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.01	0.44
30:0:1210:G:O2'	30:0:1211:G:H5'	2.17	0.43
30:0:1211:G:O2'	30:0:1212:C:H5'	2.18	0.43
30:0:2105:C:H2'	30:0:2106:C:C6	2.53	0.43
30:0:59:A:C5'	38:0:4347:HOH:O	2.64	0.43
3:C:49:ASP:HB3	3:C:52:ALA:HB2	1.99	0.43
11:K:75:ARG:HD3	11:K:112:PRO:O	2.18	0.43
13:M:95:LYS:HG2	13:M:99:ARG:HB3	2.00	0.43
14:N:116:PHE:HB3	14:N:136:LEU:HD23	2.00	0.43
19:S:8:PRO:HD2	22:V:32:ALA:HA	2.00	0.43
20:T:97:ARG:NH2	30:0:308:U:H5'	2.32	0.43
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.99	0.43
30:0:1257:C:H2'	30:0:1258:G:O4'	2.19	0.43
30:0:177:A:H2'	30:0:178:U:O4'	2.18	0.43
30:0:2369:A:C8	30:0:2371:G:C6	3.06	0.43
30:0:2617:G:N3	30:0:2617:G:H2'	2.32	0.43
30:0:2756:U:N3	30:0:2896:A:C2	2.76	0.43
30:0:445:U:H1'	38:0:7361:HOH:O	2.18	0.43
30:0:523:C:H2'	30:0:524:A:C8	2.53	0.43
10:J:107:ASN:HD21	10:J:109:TYR:HB2	1.83	0.43
12:L:21:ARG:N	38:L:8826:HOH:O	2.51	0.43
12:L:50:GLY:C	30:0:2453:G:H4'	2.38	0.43
14:N:36:ALA:HB1	14:N:118:ILE:HD12	2.01	0.43
30:0:1736:A:H1'	38:0:7607:HOH:O	2.18	0.43
30:0:776:A:H1'	30:0:779:U:O4	2.19	0.43
30:0:951:A:H2'	30:0:952:G:H5'	1.99	0.43
31:9:39:U:HO2'	31:9:42:C:H5	1.59	0.43
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.30	0.43
10:J:132:LEU:HA	10:J:132:LEU:HD23	1.80	0.43
20:T:62:VAL:N	38:T:3851:HOH:O	2.52	0.43
25:Y:208:LYS:O	30:0:1313:A:H5'	2.18	0.43
30:0:1849:G:H1'	30:0:2011:A:N1	2.34	0.43
30:0:2099:A:N6	30:0:2100:A:N6	2.66	0.43
30:0:305:A:C5	30:0:329:A:C2	3.06	0.43
30:0:542:A:C5'	30:0:542:A:C8	2.96	0.43
28:2:43:ARG:HH22	30:0:1684:A:H1'	1.83	0.43
2:B:62:ARG:HA	2:B:65:MET:CE	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:VAL:HG12	2:B:82:VAL:O	2.18	0.43
3:C:118:THR:CG2	3:C:137:PRO:HB3	2.48	0.43
5:E:159:VAL:O	5:E:163:GLN:HG2	2.18	0.43
11:K:74:VAL:HG13	11:K:113:ILE:HG23	2.00	0.43
30:0:1015:C:H2'	30:0:1016:U:H6	1.84	0.43
30:0:1098:A:H2'	30:0:1099:G:O4'	2.19	0.43
30:0:1940:C:H4'	38:0:7372:HOH:O	2.17	0.43
30:0:2004:U:H2'	30:0:2005:G:OP1	2.18	0.43
30:0:1787:C:H4'	30:0:2883:A:O4'	2.19	0.43
30:0:38:G:N2	38:0:7361:HOH:O	2.50	0.43
30:0:887:G:H2'	30:0:888:U:C6	2.53	0.43
30:0:960:G:C2'	30:0:961:A:OP2	2.66	0.43
29:3:3:MET:CG	29:3:4:PRO:HD2	2.49	0.43
31:9:96:C:H2'	31:9:97:U:C6	2.54	0.43
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.31	0.43
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.48	0.43
23:W:108:ARG:NH2	23:W:114:PRO:HG2	2.31	0.43
30:0:1183:C:H42	30:0:1184:C:N4	2.16	0.43
30:0:1377:C:C5'	30:0:1377:C:H6	2.24	0.43
30:0:1871:U:O4'	30:0:1873:G:C8	2.72	0.43
30:0:1972:U:C2'	30:0:1973:A:C5'	2.97	0.43
30:0:2329:C:O2'	30:0:2330:U:H5'	2.17	0.43
30:0:39:G:H2'	30:0:40:C:O4'	2.19	0.43
30:0:708:A:H2'	30:0:709:G:O4'	2.18	0.43
3:C:104:ASP:HA	3:C:107:ARG:HH12	1.83	0.43
3:C:104:ASP:HA	3:C:107:ARG:NH1	2.34	0.43
21:U:20:MET:CG	21:U:28:THR:HG23	2.48	0.43
30:0:1179:C:H2'	30:0:1180:U:H6	1.83	0.43
30:0:1682:A:H2'	38:0:9811:HOH:O	2.19	0.43
30:0:2004:U:H4'	38:0:5331:HOH:O	2.19	0.43
30:0:2460:A:C2	30:0:2461:U:C2	3.06	0.43
30:0:31:C:H4'	38:0:7452:HOH:O	2.19	0.43
31:9:12:C:H5'	31:9:70:U:O4'	2.18	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
2:B:286:ASN:O	2:B:306:LYS:HE3	2.18	0.43
22:V:43:PRO:O	22:V:46:ILE:HG22	2.18	0.43
24:X:80:GLU:HB3	38:X:5564:HOH:O	2.18	0.43
30:0:1280:A:H3'	30:0:1280:A:P	2.58	0.43
30:0:1588:G:C6	30:0:1589:G:C6	3.06	0.43
30:0:2252:A:H2'	30:0:2253:G:H5'	1.99	0.43
30:0:2321:A:C5	30:0:2323:G:C8	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:26:LEU:HD13	30:0:2415:A:N3	2.33	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.19	0.43
30:0:767:A:H2	30:0:2110:G:N3	2.16	0.43
1:A:164:ARG:NE	38:A:9053:HOH:O	2.47	0.43
1:A:33:GLU:CD	1:A:33:GLU:H	2.22	0.43
3:C:54:LEU:HD23	3:C:79:ARG:HG3	2.01	0.43
6:F:34:ASN:HA	13:M:4:ALA:HB2	2.01	0.43
12:L:59:GLU:HB3	38:L:8857:HOH:O	2.17	0.43
12:L:72:ASN:HB2	38:L:8876:HOH:O	2.19	0.43
9:I:86:GLU:CG	30:0:1180:U:H4'	2.43	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.19	0.43
30:0:2791:U:H1'	30:0:2792:A:H5''	2.00	0.43
15:O:25:VAL:HG12	30:0:709:G:O2'	2.19	0.43
30:0:883:U:H3'	30:0:883:U:O2	2.19	0.43
31:9:114:G:H2'	31:9:115:C:C6	2.54	0.43
31:9:45:A:C5	31:9:46:C:C4	3.06	0.43
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.54	0.43
3:C:140:VAL:HG12	3:C:141:SER:N	2.33	0.43
5:E:11:VAL:HG12	5:E:12:ASP:N	2.33	0.43
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.49	0.43
30:0:1482:A:O2'	30:0:1483:C:H5'	2.19	0.43
30:0:2456:A:H2'	30:0:2457:U:H6	1.84	0.43
30:0:2523:U:O2'	30:0:2524:G:H5'	2.19	0.43
30:0:2787:C:H5	38:0:4644:HOH:O	2.02	0.43
30:0:398:U:H2'	30:0:399:C:C6	2.54	0.43
4:D:25:MET:HE1	4:D:37:ALA:O	2.19	0.43
12:L:121:ILE:HG12	12:L:141:GLU:HB2	2.01	0.43
17:Q:9:GLY:HA2	38:0:7028:HOH:O	2.19	0.43
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.18	0.43
30:0:1188:A:H62	30:0:1189:A:N6	2.17	0.42
30:0:1503:U:H2'	30:0:1504:A:O4'	2.19	0.42
30:0:2344:G:N3	30:0:2344:G:H2'	2.34	0.42
30:0:2505:G:C2'	30:0:2506:A:C5'	2.94	0.42
30:0:2893:C:O2'	30:0:2894:C:H5'	2.19	0.42
30:0:523:C:H2'	30:0:524:A:H8	1.83	0.42
2:B:102:THR:CG2	2:B:182:VAL:HG12	2.48	0.42
2:B:198:GLU:HA	38:B:9081:HOH:O	2.18	0.42
8:H:91:ARG:HG2	8:H:91:ARG:H	1.69	0.42
9:I:133:THR:HG22	9:I:134:ILE:N	2.34	0.42
11:K:115:ARG:HG3	11:K:116:GLU:N	2.34	0.42
13:M:24:GLN:HA	13:M:24:GLN:NE2	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:96:VAL:HG13	18:R:106:GLY:HA3	2.00	0.42
18:R:18:LEU:HB2	18:R:143:VAL:HG13	2.01	0.42
23:W:38:THR:HG22	23:W:39:ASP:H	1.83	0.42
30:0:1213:C:O2'	30:0:1214:G:H5'	2.19	0.42
30:0:1249:U:H2'	30:0:1250:C:C6	2.54	0.42
30:0:1279:U:C5'	30:0:1280:A:OP2	2.68	0.42
30:0:1659:A:H2'	30:0:1660:G:O4'	2.18	0.42
30:0:1934:A:C8	30:0:1935:C:C5	3.07	0.42
30:0:2316:G:OP1	30:0:2317:C:H1'	2.19	0.42
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.54	0.42
30:0:69:A:C8	30:0:69:A:C5'	2.96	0.42
30:0:951:A:O2'	30:0:952:G:H5'	2.20	0.42
28:2:40:ARG:HG3	28:2:45:ASN:HB2	2.00	0.42
1:A:153:ARG:HH11	1:A:153:ARG:HB2	1.84	0.42
2:B:16:ARG:NH2	38:B:8982:HOH:O	2.49	0.42
30:0:1163:G:H2'	30:0:1164:U:H5	1.84	0.42
30:0:1522:A:H2'	30:0:1523:G:H5'	2.01	0.42
30:0:2486:A:H3'	38:0:4903:HOH:O	2.18	0.42
30:0:2536:C:HO2'	30:0:2537:G:P	2.42	0.42
30:0:660:A:H4'	30:0:661:G:O5'	2.20	0.42
14:N:37:ARG:HH11	31:9:6:C:H5''	1.71	0.42
2:B:102:THR:HG23	2:B:182:VAL:HG12	2.01	0.42
4:D:172:VAL:HG12	4:D:173:GLU:N	2.23	0.42
14:N:115:VAL:HG13	38:9:9105:HOH:O	2.19	0.42
22:V:1:THR:HG23	22:V:2:VAL:N	2.24	0.42
30:0:128:A:H3'	30:0:128:A:C8	2.55	0.42
30:0:2254:G:O2'	30:0:2255:A:H5'	2.19	0.42
30:0:2540:G:N2	38:0:9380:HOH:O	2.52	0.42
30:0:2829:G:O2'	30:0:2830:U:H5'	2.20	0.42
13:M:179:GLY:O	30:0:399:C:H5'	2.19	0.42
23:W:44:MET:HE2	30:0:944:G:H21	1.83	0.42
4:D:99:ASP:HB3	4:D:103:ASN:H	1.84	0.42
5:E:145:ALA:HB1	5:E:168:ILE:HD11	2.02	0.42
16:P:13:VAL:HG11	16:P:40:VAL:HG12	2.00	0.42
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.54	0.42
30:0:1099:G:H2'	30:0:1100:G:O4'	2.20	0.42
30:0:1183:C:C6	30:0:1192:A:N7	2.87	0.42
30:0:1552:G:N2	30:0:1634:G:C1'	2.80	0.42
30:0:1701:A:H4'	30:0:1702:U:O5'	2.20	0.42
30:0:2637:A:H5''	38:0:4944:HOH:O	2.18	0.42
30:0:867:A:H2	30:0:880:C:O2	2.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ALA:O	2:B:128:ILE:HG13	2.19	0.42
3:C:236:THR:H	3:C:239:ALA:HB3	1.85	0.42
5:E:101:GLU:HA	5:E:118:ILE:HG13	2.01	0.42
15:O:44:ASN:OD1	15:O:67:SER:HB2	2.20	0.42
16:P:115:SER:OG	16:P:118:GLN:HG3	2.20	0.42
23:W:88:THR:HG22	23:W:90:TYR:CD1	2.51	0.42
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.20	0.42
2:B:244:PRO:HB3	30:0:1234:U:N3	2.35	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
30:0:1972:U:H2'	30:0:1973:A:H5''	1.99	0.42
30:0:1842:A:C4	30:0:1979:G:C6	3.06	0.42
30:0:2645:U:OP2	30:0:2645:U:C6	2.72	0.42
30:0:807:A:N1	30:0:808:A:C2	2.88	0.42
3:C:168:ARG:NH2	3:C:190:ALA:O	2.53	0.42
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.45	0.42
26:Z:56:GLU:O	26:Z:61:HIS:HE1	2.03	0.42
30:0:1042:U:O2'	30:0:1043:C:H5'	2.19	0.42
30:0:138:U:OP2	30:0:139:C:H5	2.02	0.42
30:0:1520:G:H2'	30:0:1521:C:C6	2.54	0.42
30:0:1380:U:C4	30:0:2748:G:H1'	2.54	0.42
30:0:812:A:H2'	30:0:813:C:C6	2.54	0.42
3:C:87:ARG:NH2	30:0:894:A:C2	2.88	0.42
5:E:84:MET:HE1	5:E:148:ILE:HD12	2.02	0.42
7:G:63:ARG:N	38:G:2569:HOH:O	2.52	0.42
17:Q:11:ARG:HB2	38:0:7028:HOH:O	2.20	0.42
18:R:106:GLY:HA2	18:R:109:MET:HE3	2.02	0.42
18:R:92:LEU:HD23	18:R:145:LEU:HD21	2.02	0.42
19:S:33:SER:O	19:S:37:VAL:HG23	2.19	0.42
30:0:1066:U:H2'	30:0:1067:A:C8	2.54	0.42
30:0:1167:G:N2	30:0:1180:U:C2	2.88	0.42
30:0:1201:C:C2'	30:0:1202:A:H5'	2.49	0.42
30:0:1367:A:H2'	30:0:1368:U:H5'	2.02	0.42
38:A:9042:HOH:O	30:0:2271:G:H5'	2.20	0.42
30:0:2356:A:H2'	30:0:2357:G:O4'	2.19	0.42
30:0:2419:U:H5''	30:0:2420:G:H5'	2.02	0.42
30:0:2504:A:H2'	30:0:2505:G:O4'	2.20	0.42
30:0:451:C:O2'	30:0:452:G:H5'	2.19	0.42
31:9:108:C:H2'	31:9:109:G:H8	1.82	0.42
6:F:91:VAL:CG1	6:F:92:GLY:N	2.83	0.42
8:H:61:ARG:HG3	8:H:61:ARG:NH1	2.34	0.42
13:M:84:LYS:HG3	30:0:171:C:OP2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:18:LEU:HD12	18:R:143:VAL:HG11	2.01	0.42
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.55	0.42
30:0:1335:C:H2'	30:0:1336:U:H6	1.85	0.42
30:0:1626:A:H2'	30:0:1627:G:O4'	2.20	0.42
30:0:1926:G:H2'	30:0:1927:A:C8	2.54	0.42
30:0:2699:A:H2'	30:0:2700:G:O4'	2.19	0.42
30:0:629:A:H2'	30:0:630:A:O4'	2.20	0.42
30:0:90:A:H2'	30:0:91:G:O4'	2.19	0.42
31:9:38:A:H2	31:9:43:G:H5''	1.84	0.42
31:9:80:A:C2	31:9:103:A:C4	3.08	0.42
12:L:10:SER:O	12:L:11:ARG:HB3	2.19	0.42
13:M:68:ARG:HD3	13:M:68:ARG:O	2.19	0.42
19:S:43:GLU:HB3	38:S:7106:HOH:O	2.18	0.42
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	2.02	0.42
30:0:1055:G:N7	38:0:4091:HOH:O	2.51	0.42
30:0:1181:A:C2'	30:0:1182:C:H5'	2.49	0.42
30:0:1189:A:H1'	30:0:1209:C:H1'	2.02	0.42
30:0:1103:C:C2	30:0:1241:G:N2	2.88	0.42
30:0:2326:C:H4'	30:0:2412:G:C4'	2.50	0.42
30:0:2757:A:H2'	30:0:2758:G:O4'	2.20	0.42
27:1:16:HIS:CD2	30:0:470:U:O2'	2.67	0.42
30:0:734:U:O2'	30:0:737:A:N6	2.53	0.42
31:9:107:C:O2'	31:9:108:C:H5'	2.20	0.42
1:A:217:ARG:CG	1:A:217:ARG:HH11	2.31	0.42
8:H:36:MET:SD	8:H:69:ARG:HD2	2.60	0.42
14:N:13:ARG:HA	14:N:13:ARG:HD2	1.89	0.42
15:O:32:ARG:HH21	15:O:35:LYS:HZ2	1.68	0.42
15:O:87:THR:O	15:O:91:GLN:HG3	2.19	0.42
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.20	0.42
30:0:1183:C:N3	30:0:1184:C:C5	2.88	0.41
30:0:1298:U:H2'	30:0:1299:G:H8	1.85	0.41
30:0:1309:U:O2'	30:0:1310:U:H5'	2.20	0.41
30:0:2099:A:N6	30:0:2100:A:H61	2.17	0.41
30:0:2281:C:C2'	30:0:2282:U:H5'	2.49	0.41
30:0:2776:A:H2'	30:0:2777:G:O4'	2.19	0.41
30:0:506:G:N2	30:0:509:A:H5''	2.27	0.41
31:9:49:G:C2'	31:9:50:G:H5'	2.50	0.41
5:E:84:MET:HG2	5:E:168:ILE:HD13	2.02	0.41
9:I:86:GLU:HA	9:I:87:PRO:HD2	1.94	0.41
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.55	0.41
10:J:88:PRO:HD3	30:0:1104:C:H4'	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1183:C:C5	30:0:1192:A:C8	3.08	0.41
30:0:1367:A:C2'	30:0:1368:U:H5'	2.51	0.41
30:0:1641:A:C8	30:0:1702:U:O4	2.73	0.41
30:0:2011:A:H4'	30:0:2012:U:O5'	2.20	0.41
30:0:1006:A:N1	30:0:2311:A:H1'	2.35	0.41
30:0:607:G:H2'	30:0:608:A:O4'	2.21	0.41
31:9:40:C:H2'	31:9:41:C:OP1	2.20	0.41
3:C:76:ARG:HH22	30:0:1363:G:P	2.42	0.41
11:K:101:ASN:O	11:K:102:GLU:HB2	2.20	0.41
16:P:16:VAL:CG1	16:P:17:GLY:N	2.83	0.41
30:0:1878:G:O2'	30:0:1879:U:OP2	2.38	0.41
30:0:1980:U:O2'	30:0:1981:A:H5'	2.20	0.41
30:0:2089:A:C2'	30:0:2090:G:H5'	2.50	0.41
12:L:56:LYS:HE3	30:0:2443:C:H1'	2.02	0.41
30:0:537:G:O4'	30:0:538:C:C5	2.73	0.41
30:0:876:A:N3	30:0:876:A:C2'	2.83	0.41
31:9:31:C:C2	31:9:50:G:N2	2.89	0.41
2:B:243:ASN:HA	2:B:244:PRO:C	2.39	0.41
11:K:81:ARG:HB2	11:K:87:ARG:HH11	1.84	0.41
21:U:17:THR:CG2	21:U:18:GLY:N	2.83	0.41
30:0:1116:U:H3	30:0:1246:A:N6	1.98	0.41
30:0:1552:G:C6	30:0:1553:C:C4	3.08	0.41
30:0:1657:A:H2'	30:0:1658:A:C8	2.55	0.41
30:0:254:C:C2'	30:0:254:C:O2	2.64	0.41
30:0:581:G:O2'	30:0:582:U:H5'	2.21	0.41
30:0:696:C:C2'	30:0:697:G:H5'	2.51	0.41
29:3:73:GLU:HB2	38:3:9023:HOH:O	2.20	0.41
6:F:99:THR:HG23	6:F:99:THR:O	2.20	0.41
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.55	0.41
25:Y:117:LEU:HB2	25:Y:174:VAL:HG21	2.01	0.41
25:Y:174:VAL:CG2	25:Y:177:LYS:HD2	2.50	0.41
30:0:1406:A:H5'	30:0:1407:A:C8	2.56	0.41
30:0:1948:G:H2'	30:0:1949:G:C8	2.55	0.41
30:0:1971:G:H5'	38:0:7098:HOH:O	2.20	0.41
30:0:236:A:H8	30:0:236:A:OP1	2.03	0.41
30:0:2667:G:H1'	30:0:2914:A:N3	2.36	0.41
30:0:80:A:H4'	30:0:81:G:O5'	2.21	0.41
30:0:969:G:H1	30:0:999:C:H42	1.67	0.41
14:N:44:ARG:NH1	31:9:4:G:H21	2.18	0.41
31:9:64:C:H2'	31:9:65:A:H5'	2.01	0.41
3:C:19:PRO:HD2	3:C:240:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:143:GLN:OE1	30:0:2796:U:H1'	2.21	0.41
8:H:174:LEU:HD21	30:0:1220:U:H4'	2.03	0.41
8:H:22:TYR:CZ	30:0:1007:A:H2'	2.55	0.41
22:V:7:GLU:O	22:V:11:MET:HG3	2.20	0.41
30:0:1116:U:C2	30:0:1246:A:N6	2.88	0.41
30:0:1211:G:H2'	30:0:1212:C:C6	2.56	0.41
30:0:204:A:O2'	30:0:205:U:H5'	2.20	0.41
30:0:2094:G:O6	30:0:2649:A:H2	2.04	0.41
30:0:2823:G:H4'	30:0:2827:A:O4'	2.20	0.41
30:0:2864:U:O2'	30:0:2865:G:H5'	2.20	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
30:0:559:U:H5'	30:0:559:U:C6	2.34	0.41
30:0:612:U:H2'	30:0:613:C:H6	1.86	0.41
2:B:254:GLN:NE2	38:B:9014:HOH:O	2.52	0.41
2:B:69:VAL:HA	2:B:70:PRO:HD3	1.87	0.41
3:C:5:ILE:HD11	3:C:16:VAL:HG13	2.03	0.41
13:M:79:ALA:HB1	30:0:770:C:OP1	2.21	0.41
17:Q:30:VAL:O	17:Q:30:VAL:HG12	2.20	0.41
17:Q:66:LYS:HB2	17:Q:70:ALA:O	2.20	0.41
20:T:40:VAL:HG22	20:T:41:ARG:N	2.35	0.41
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.03	0.41
23:W:146:ILE:HA	23:W:146:ILE:HD13	1.83	0.41
30:0:1523:G:C6	30:0:1524:U:O4	2.74	0.41
30:0:2506:A:C2'	30:0:2506:A:O5'	2.68	0.41
30:0:2600:A:H2'	30:0:2601:A:O4'	2.21	0.41
30:0:2644:C:O2'	30:0:2645:U:O5'	2.37	0.41
30:0:466:A:H2'	30:0:467:G:O4'	2.20	0.41
30:0:503:G:H2'	30:0:504:G:H8	1.84	0.41
30:0:69:A:C8	30:0:69:A:C3'	3.04	0.41
30:0:1131:G:H4'	31:9:91:C:O4'	2.20	0.41
1:A:211:LYS:CB	38:0:7455:HOH:O	2.69	0.41
4:D:138:GLY:N	38:D:7597:HOH:O	2.53	0.41
13:M:137:ASN:ND2	30:0:145:A:H4'	2.36	0.41
13:M:68:ARG:HG3	13:M:73:ARG:HE	1.84	0.41
14:N:32:PRO:HD2	14:N:99:GLU:O	2.21	0.41
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.51	0.41
18:R:114:VAL:HA	18:R:144:GLU:O	2.21	0.41
20:T:27:LEU:HD23	20:T:98:VAL:HB	2.02	0.41
30:0:1046:G:N3	30:0:1082:A:H2	2.19	0.41
30:0:2388:C:H2'	30:0:2389:U:O4'	2.21	0.41
30:0:2597:U:H2'	30:0:2598:U:H5'	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2826:G:C5	30:0:2913:A:C6	3.08	0.41
5:E:133:VAL:HG12	5:E:141:VAL:HG13	2.02	0.41
10:J:107:ASN:HD22	10:J:107:ASN:C	2.24	0.41
12:L:4:LYS:HE2	30:0:645:U:OP2	2.20	0.41
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.41
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.89	0.41
30:0:1076:G:C2	30:0:1084:C:C2	3.09	0.41
30:0:1206:U:C5'	30:0:1206:U:H6	2.28	0.41
18:R:64:SER:OG	30:0:1369:A:H4'	2.21	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.56	0.41
30:0:2061:C:C2'	30:0:2062:A:H5'	2.51	0.41
30:0:2455:A:H2'	30:0:2456:A:O4'	2.20	0.41
2:B:81:ALA:HB1	2:B:142:LEU:HD13	2.03	0.41
8:H:98:LEU:HD11	8:H:127:ALA:HB2	2.02	0.41
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.20	0.41
14:N:23:ARG:O	14:N:27:LEU:HG	2.21	0.41
30:0:1165:G:H3'	30:0:1166:A:C5'	2.50	0.41
30:0:1441:G:O2'	30:0:1442:A:H5'	2.21	0.41
30:0:2453:G:H5'	38:0:4702:HOH:O	2.21	0.41
30:0:2526:C:H5''	38:0:7627:HOH:O	2.20	0.41
30:0:2644:C:HO2'	30:0:2645:U:P	2.44	0.41
30:0:243:A:H61	30:0:269:G:H1'	1.86	0.41
30:0:757:C:H2'	30:0:758:A:C8	2.56	0.41
2:B:87:TYR:O	2:B:138:GLY:N	2.47	0.41
3:C:118:THR:O	3:C:136:VAL:HG13	2.20	0.41
4:D:154:LYS:HD2	4:D:154:LYS:N	2.30	0.41
6:F:21:GLU:O	6:F:24:ARG:HG2	2.21	0.41
8:H:50:ILE:HG21	38:H:231:HOH:O	2.21	0.41
13:M:91:ILE:HG23	38:M:8953:HOH:O	2.20	0.41
30:0:1484:G:H2'	38:0:9110:HOH:O	2.20	0.41
30:0:1768:C:H2'	30:0:1769:C:O4'	2.21	0.41
30:0:1816:C:H2'	30:0:1817:U:O4'	2.21	0.41
30:0:2588:OMG:HM23	30:0:2617:G:N2	2.36	0.41
30:0:2645:U:H6	30:0:2645:U:H2'	1.62	0.41
15:O:25:VAL:HG13	30:0:709:G:O3'	2.20	0.41
4:D:167:GLU:C	4:D:169:THR:H	2.24	0.41
7:G:67:LEU:O	7:G:71:LEU:HG	2.21	0.41
19:S:57:THR:HG22	19:S:58:MET:H	1.84	0.41
22:V:1:THR:CG2	22:V:2:VAL:H	2.21	0.41
30:0:553:G:O4'	30:0:1325:G:H5'	2.21	0.40
30:0:12:U:C2'	30:0:13:G:H5'	2.49	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1400:C:H1'	38:0:4150:HOH:O	2.20	0.40
30:0:2748:G:P	30:0:2749:U:H5''	2.59	0.40
30:0:2831:C:C2'	30:0:2832:C:H5'	2.51	0.40
30:0:304:G:H1'	30:0:347:A:H61	1.86	0.40
30:0:336:G:H5''	38:0:3737:HOH:O	2.21	0.40
3:C:185:LYS:HD3	3:C:186:TYR:CE1	2.56	0.40
4:D:40:ILE:HG13	4:D:41:LEU:N	2.36	0.40
5:E:143:GLN:HE22	30:0:2779:G:H21	1.67	0.40
11:K:118:ALA:HA	11:K:125:ALA:HB2	2.03	0.40
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.21	0.40
18:R:9:ASP:HA	18:R:10:PRO:HD2	1.94	0.40
18:R:132:ARG:NH2	38:R:8983:HOH:O	2.54	0.40
12:L:6:ARG:NH1	30:0:1299:G:N7	2.69	0.40
30:0:1573:A:H2'	30:0:1574:C:O4'	2.21	0.40
1:A:212:PRO:HA	30:0:1943:C:O4'	2.21	0.40
30:0:2102:G:C2	30:0:2103:A:C4	3.10	0.40
30:0:2332:A:H5'	30:0:2333:G:OP2	2.20	0.40
30:0:669:G:O2'	30:0:670:G:H5'	2.21	0.40
30:0:787:G:O2'	30:0:788:A:H5'	2.20	0.40
29:3:38:ARG:HB3	29:3:42:ARG:HH12	1.85	0.40
1:A:36:ASP:C	1:A:38:ILE:H	2.21	0.40
2:B:115:VAL:HA	2:B:116:PRO:HD3	1.89	0.40
9:I:87:PRO:C	9:I:89:GLU:H	2.23	0.40
15:O:77:ALA:HA	15:O:96:VAL:O	2.20	0.40
20:T:2:LYS:HE2	38:0:7433:HOH:O	2.21	0.40
30:0:1339:G:C6	30:0:1340:G:N1	2.89	0.40
30:0:1624:A:H4'	30:0:1625:U:H5'	2.03	0.40
30:0:2250:G:H2'	30:0:2251:G:O4'	2.20	0.40
30:0:2328:U:C4	30:0:2329:C:C5	3.09	0.40
30:0:2712:G:P	38:0:5242:HOH:O	2.80	0.40
30:0:2819:C:H2'	30:0:2820:A:H8	1.87	0.40
2:B:16:ARG:NE	38:B:8982:HOH:O	2.46	0.40
6:F:30:LYS:HD3	6:F:30:LYS:HA	1.88	0.40
25:Y:186:ARG:HG2	25:Y:186:ARG:NH1	2.35	0.40
23:W:23:MET:O	30:0:1025:C:H5'	2.21	0.40
30:0:907:A:H4'	30:0:1328:A:C2	2.57	0.40
30:0:1398:G:H2'	30:0:1399:A:C8	2.56	0.40
30:0:1524:U:H3'	38:0:5355:HOH:O	2.21	0.40
30:0:1476:A:H1'	30:0:1867:G:O2'	2.21	0.40
30:0:2135:A:O4'	30:0:2243:C:N4	2.55	0.40
30:0:2482:G:H4'	30:0:2483:A:C5'	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:C8	30:0:2578:G:H5'	2.44	0.40
30:0:297:U:H2'	30:0:298:C:C6	2.55	0.40
30:0:412:C:H2'	30:0:413:G:O4'	2.21	0.40
30:0:482:G:O4'	30:0:511:A:C2	2.74	0.40
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.51	0.40
3:C:84:VAL:O	3:C:85:LYS:HB2	2.22	0.40
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.92	0.40
6:F:57:GLU:O	6:F:61:MET:HG3	2.21	0.40
10:J:90:LYS:HB2	33:J:8802:CL:CL	2.57	0.40
16:P:115:SER:HB2	38:P:4299:HOH:O	2.21	0.40
30:0:1345:A:H2'	30:0:1346:U:C6	2.55	0.40
30:0:1511:U:O2'	30:0:1512:G:H5'	2.21	0.40
30:0:1589:G:N2	30:0:1605:G:H1'	2.35	0.40
30:0:2102:G:HO2'	30:0:2103:A:P	2.44	0.40
30:0:420:U:H2'	30:0:421:C:C6	2.57	0.40
30:0:483:C:C4	30:0:484:A:C6	3.10	0.40
30:0:968:G:C2	30:0:1001:U:O2	2.75	0.40
1:A:1:GLY:HA2	1:A:197:VAL:HG23	2.04	0.40
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.88	0.40
16:P:83:LYS:HG2	30:0:793:A:H5''	2.03	0.40
18:R:104:PHE:HB3	18:R:109:MET:HE1	2.04	0.40
23:W:73:LEU:HA	23:W:73:LEU:HD12	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	
1	A	235/240 (98%)	209 (89%)	24 (10%)	2 (1%)	19	28
2	B	335/338 (99%)	315 (94%)	18 (5%)	2 (1%)	27	38
3	C	244/246 (99%)	233 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	134/177 (76%)	111 (83%)	20 (15%)	3 (2%)	7	8
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	19	28
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	149 (96%)	7 (4%)	0	100	100
9	I	68/162 (42%)	55 (81%)	12 (18%)	1 (2%)	11	16
10	J	140/145 (97%)	133 (95%)	5 (4%)	2 (1%)	12	17
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	8	8
13	M	192/196 (98%)	183 (95%)	9 (5%)	0	100	100
14	N	184/187 (98%)	171 (93%)	8 (4%)	5 (3%)	5	5
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	77 (98%)	2 (2%)	0	100	100
20	T	117/120 (98%)	113 (97%)	3 (3%)	1 (1%)	19	28
21	U	51/67 (76%)	49 (96%)	2 (4%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
24	X	80/92 (87%)	76 (95%)	2 (2%)	2 (2%)	6	6
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	12	17
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	23
All	All	3705/4472 (83%)	3486 (94%)	195 (5%)	24 (1%)	27	38

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
10	J	5	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
1	A	205	GLY
12	L	149	ARG
14	N	167	ASP
12	L	80	ASP
26	Z	105	ARG
2	B	2	GLN
2	B	185	GLY
4	D	56	ARG
20	T	45	GLY
24	X	87	ALA
4	D	137	PRO
10	J	143	LYS
12	L	82	ALA
14	N	162	ASP
4	D	27	ILE
6	F	100	ASP
24	X	70	ILE
29	3	56	PRO
9	I	108	HIS

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	
1	A	179/182 (98%)	170 (95%)	9 (5%)	27	37
2	B	282/283 (100%)	268 (95%)	14 (5%)	27	37
3	C	193/193 (100%)	178 (92%)	15 (8%)	14	18
4	D	117/148 (79%)	112 (96%)	5 (4%)	32	44
5	E	152/156 (97%)	147 (97%)	5 (3%)	41	56
6	F	93/94 (99%)	92 (99%)	1 (1%)	76	85
7	G	27/282 (10%)	26 (96%)	1 (4%)	37	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	134/145 (92%)	129 (96%)	5 (4%)	37	51
9	I	58/130 (45%)	58 (100%)	0	100	100
10	J	118/121 (98%)	111 (94%)	7 (6%)	21	29
11	K	106/106 (100%)	103 (97%)	3 (3%)	47	62
12	L	113/127 (89%)	109 (96%)	4 (4%)	39	54
13	M	158/160 (99%)	152 (96%)	6 (4%)	36	50
14	N	149/150 (99%)	145 (97%)	4 (3%)	48	64
15	O	93/94 (99%)	88 (95%)	5 (5%)	24	33
16	P	113/117 (97%)	110 (97%)	3 (3%)	48	64
17	Q	79/80 (99%)	76 (96%)	3 (4%)	36	50
18	R	117/122 (96%)	115 (98%)	2 (2%)	63	78
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	98 (93%)	7 (7%)	18	24
21	U	44/53 (83%)	43 (98%)	1 (2%)	53	69
22	V	51/57 (90%)	50 (98%)	1 (2%)	58	74
23	W	130/130 (100%)	124 (95%)	6 (5%)	29	41
24	X	66/74 (89%)	61 (92%)	5 (8%)	14	20
25	Y	120/196 (61%)	110 (92%)	10 (8%)	12	16
26	Z	60/94 (64%)	58 (97%)	2 (3%)	41	56
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	79/79 (100%)	76 (96%)	3 (4%)	36	50
All	All	3095/3646 (85%)	2968 (96%)	127 (4%)	33	46

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	68	ILE
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	147	ARG
1	A	184	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	ARG
1	A	217	ARG
2	B	2	GLN
2	B	5	ARG
2	B	11	LEU
2	B	27	ASN
2	B	51	VAL
2	B	53	LEU
2	B	98	THR
2	B	162	MET
2	B	175	LEU
2	B	190	MET
2	B	254	GLN
2	B	265	LEU
2	B	279	THR
2	B	312	ARG
3	C	2	GLN
3	C	27	ARG
3	C	76	ARG
3	C	78	ARG
3	C	94	THR
3	C	101	ASP
3	C	115	LEU
3	C	136	VAL
3	C	187	ARG
3	C	211	ASP
3	C	214	THR
3	C	223	LEU
3	C	234	VAL
3	C	236	THR
3	C	243	VAL
4	D	24	HIS
4	D	36	ASN
4	D	39	ASP
4	D	50	VAL
4	D	149	ARG
5	E	7	ILE
5	E	86	VAL
5	E	102	VAL
5	E	132	THR
5	E	154	ILE
6	F	12	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	73	ASP
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
8	H	173	GLU
10	J	39	VAL
10	J	46	ILE
10	J	52	GLN
10	J	70	PHE
10	J	79	PHE
10	J	107	ASN
10	J	131	THR
11	K	4	LEU
11	K	10	GLN
11	K	55	VAL
12	L	32	ASP
12	L	35	ARG
12	L	43	HIS
12	L	140	VAL
13	M	46	LEU
13	M	68	ARG
13	M	82	ARG
13	M	93	ARG
13	M	99	ARG
13	M	116	ASN
14	N	26	LEU
14	N	49	THR
14	N	135	VAL
14	N	163	PHE
15	O	3	THR
15	O	25	VAL
15	O	38	ARG
15	O	43	VAL
15	O	111	VAL
16	P	21	VAL
16	P	91	LYS
16	P	98	ILE
17	Q	11	ARG
17	Q	16	ASN
17	Q	95	GLU
18	R	39	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	82	GLU
20	T	39	ASN
20	T	48	VAL
20	T	71	VAL
20	T	73	HIS
20	T	89	ARG
20	T	96	VAL
20	T	115	GLU
21	U	17	THR
22	V	65	ASP
23	W	26	ILE
23	W	52	VAL
23	W	76	ASP
23	W	78	ASP
23	W	142	ASP
23	W	146	ILE
24	X	27	ASP
24	X	72	VAL
24	X	79	GLU
24	X	80	GLU
24	X	82	GLU
25	Y	103	THR
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	172	THR
25	Y	174	VAL
25	Y	189	ASN
25	Y	200	THR
25	Y	203	VAL
25	Y	235	GLU
26	Z	65	ASN
26	Z	68	GLU
29	3	18	GLN
29	3	56	PRO
29	3	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	199	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	27	ASN
2	B	145	HIS
2	B	221	GLN
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN
2	B	332	ASN
3	C	39	GLN
3	C	73	GLN
3	C	129	HIS
3	C	151	GLN
3	C	163	HIS
4	D	103	ASN
4	D	133	ASN
5	E	106	ASN
5	E	143	GLN
7	G	64	ASN
8	H	34	HIS
8	H	59	GLN
8	H	62	HIS
8	H	73	ASN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
11	K	10	GLN
11	K	44	HIS
12	L	18	HIS
12	L	41	HIS
12	L	116	HIS
13	M	24	GLN
13	M	58	GLN
13	M	77	HIS
13	M	137	ASN
13	M	170	ASN
14	N	21	HIS
14	N	107	ASN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
19	S	44	GLN
19	S	51	GLN
19	S	53	ASN
20	T	37	GLN
20	T	39	ASN
21	U	39	ASN
21	U	48	ASN
22	V	60	GLN
23	W	87	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
24	X	22	ASN
24	X	23	HIS
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	15	ASN
29	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	3 (2%)
All	All	2866/3045 (94%)	259 (9%)	31 (1%)

All (259) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G
30	0	86	A
30	0	87	C
30	0	88	G
30	0	114	A
30	0	115	U
30	0	120	A
30	0	130	C
30	0	131	A
30	0	139	C
30	0	141	C
30	0	151	A
30	0	166	A
30	0	185	G
30	0	186	A
30	0	191	A
30	0	192	A
30	0	198	A
30	0	200	C
30	0	219	G
30	0	237	G
30	0	271	C
30	0	272	A
30	0	273	G
30	0	283	U
30	0	284	C
30	0	308	U
30	0	309	C
30	0	318	U
30	0	336	G
30	0	337	A
30	0	358	G
30	0	368	C
30	0	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	498	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	510	U
30	0	511	A
30	0	514	G
30	0	537	G
30	0	538	C
30	0	539	G
30	0	542	A
30	0	545	G
30	0	553	G
30	0	559	U
30	0	581	G
30	0	588	G
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G
30	0	660	A
30	0	688	A
30	0	701	U
30	0	702	G
30	0	759	C
30	0	777	U
30	0	809	G
30	0	821	U
30	0	835	U
30	0	840	U
30	0	868	G
30	0	869	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1045	G
30	0	1059	G
30	0	1060	C
30	0	1072	G
30	0	1081	A
30	0	1087	G
30	0	1088	A
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	U
30	0	1151	G
30	0	1164	U
30	0	1165	G
30	0	1166	A
30	0	1174	A
30	0	1175	G
30	0	1185	U
30	0	1192	A
30	0	1193	A
30	0	1206	U
30	0	1207	A
30	0	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1280	A
30	0	1289	C
30	0	1342	C
30	0	1353	C
30	0	1357	A
30	0	1360	C
30	0	1377	C
30	0	1378	G
30	0	1407	A
30	0	1474	C
30	0	1505	U
30	0	1506	U
30	0	1524	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1562	C
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1633	C
30	0	1634	G
30	0	1656	A
30	0	1667	A
30	0	1682	A
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1701	A
30	0	1722	U
30	0	1723	G
30	0	1725	C
30	0	1730	G
30	0	1731	C
30	0	1752	G
30	0	1778	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1971	G
30	0	1973	A
30	0	1979	G
30	0	1996	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2033	G
30	0	2034	U
30	0	2064	U
30	0	2072	G
30	0	2073	G
30	0	2074	A
30	0	2096	A
30	0	2100	A
30	0	2101	A
30	0	2102	G
30	0	2103	A
30	0	2110	G
30	0	2238	A
30	0	2243	C
30	0	2258	A
30	0	2271	G
30	0	2272	G
30	0	2291	A
30	0	2317	C
30	0	2320	U
30	0	2321	A
30	0	2354	A
30	0	2361	A
30	0	2369	A
30	0	2379	G
30	0	2422	U
30	0	2462	G
30	0	2467	A
30	0	2476	C
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2533	C
30	0	2537	G
30	0	2539	U
30	0	2540	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2611	U
30	0	2613	G
30	0	2644	C
30	0	2645	U
30	0	2649	A
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2719	A
30	0	2726	U
30	0	2727	A
30	0	2747	C
30	0	2748	G
30	0	2749	U
30	0	2750	G
30	0	2762	C
30	0	2768	A
30	0	2792	A
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
30	0	2852	A
30	0	2876	G
30	0	2890	A
30	0	2896	A
30	0	2903	C
30	0	2914	A
31	9	2	U
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	44	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G
31	9	122	C

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	69	A
30	0	129	A
30	0	603	A
30	0	644	G
30	0	699	C
30	0	834	G
30	0	857	A
30	0	871	G
30	0	877	G
30	0	1232	A
30	0	1237	U
30	0	1246	A
30	0	1352	A
30	0	1506	U
30	0	1684	A
30	0	1685	A
30	0	1692	C
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2313	C
30	0	2467	A
30	0	2541	U
30	0	2649	A
30	0	2718	C
30	0	2726	U
30	0	2748	G
30	0	2791	U
31	9	43	G
31	9	55	U
31	9	65	A

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

5 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
30	OMU	0	2587	30	14,22,23	1.01	1 (7%)	18,31,34	3.65	2 (11%)
30	OMG	0	2588	30	19,26,27	1.10	2 (10%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	13,22,23	0.75	0	15,32,35	0.72	0
30	PSU	0	2621	30	16,21,22	1.76	3 (18%)	20,30,33	5.38	5 (25%)
30	1MA	0	628	30,35	16,25,26	0.98	1 (6%)	12,37,40	1.23	1 (8%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.50	1.47	1.52
30	0	2588	OMG	C8-N7	-2.03	1.30	1.34
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2587	OMU	C4-N3	2.74	1.38	1.33
30	0	628	1MA	C6-N6	2.86	1.33	1.27
30	0	2621	PSU	C4-N3	2.89	1.38	1.33
30	0	2588	OMG	C6-N1	3.50	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.32	114.49	128.41
30	0	2588	OMG	C5-C6-N1	-8.38	111.55	123.47
30	0	2621	PSU	C5-C4-N3	-8.12	114.90	125.36
30	0	628	1MA	C2-N3-C4	-3.74	110.79	116.51
30	0	2587	OMU	C5-C4-N3	-3.70	114.57	123.17
30	0	2588	OMG	C2-N3-C4	-2.68	112.03	115.16
30	0	2588	OMG	N3-C2-N1	-2.40	123.89	127.41
30	0	2588	OMG	C6-C5-C4	-2.17	118.72	120.85
30	0	2621	PSU	C5-C1'-C2'	-2.13	111.52	115.32
30	0	2621	PSU	C6-N1-C2	2.94	120.06	115.36
30	0	2588	OMG	C6-N1-C2	6.32	125.15	116.06
30	0	2621	PSU	C4-N3-C2	13.76	126.86	115.14
30	0	2587	OMU	C4-N3-C2	14.87	126.94	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	3	0
30	0	2588	OMG	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	0.52	19 (8%) 12 15	20, 40, 77, 100	0
2	B	337/338 (99%)	0.34	8 (2%) 59 66	21, 44, 73, 83	0
3	C	246/246 (100%)	0.37	9 (3%) 41 48	17, 36, 60, 73	0
4	D	140/177 (79%)	2.33	71 (50%) 0 0	48, 89, 116, 126	0
5	E	172/178 (96%)	0.60	11 (6%) 19 22	34, 59, 79, 85	0
6	F	119/120 (99%)	1.31	31 (26%) 0 0	34, 61, 91, 105	0
7	G	29/348 (8%)	2.64	17 (58%) 0 0	70, 87, 96, 98	0
8	H	160/177 (90%)	0.96	26 (16%) 1 1	32, 50, 85, 91	0
9	I	70/162 (43%)	6.43	68 (97%) 0 0	124, 138, 156, 156	0
10	J	142/145 (97%)	0.17	3 (2%) 63 71	27, 41, 63, 89	0
11	K	132/132 (100%)	0.08	2 (1%) 73 79	23, 39, 63, 72	0
12	L	145/165 (87%)	1.08	22 (15%) 2 2	18, 55, 103, 118	0
13	M	194/196 (98%)	0.43	15 (7%) 13 16	23, 34, 54, 59	0
14	N	186/187 (99%)	1.16	37 (19%) 1 1	34, 52, 104, 112	0
15	O	115/116 (99%)	0.31	1 (0%) 84 89	31, 45, 61, 69	0
16	P	143/149 (95%)	0.10	1 (0%) 87 91	28, 43, 56, 68	0
17	Q	95/96 (98%)	0.16	0 100 100	29, 37, 55, 66	0
18	R	150/155 (96%)	0.20	1 (0%) 87 91	23, 36, 57, 71	0
19	S	81/85 (95%)	0.73	11 (13%) 3 3	33, 48, 70, 81	0
20	T	119/120 (99%)	0.64	8 (6%) 18 21	29, 46, 74, 101	0
21	U	53/67 (79%)	0.62	3 (5%) 24 28	33, 46, 65, 74	0
22	V	65/71 (91%)	2.37	25 (38%) 0 0	41, 63, 106, 113	0
23	W	154/154 (100%)	0.30	2 (1%) 77 82	26, 42, 59, 71	0
24	X	82/92 (89%)	0.57	5 (6%) 21 24	34, 49, 77, 92	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.10	5 (3%) 44 51	19, 34, 58, 80	0
26	Z	73/116 (62%)	1.43	21 (28%) 0 0	36, 55, 72, 89	0
27	1	56/57 (98%)	0.43	0 100 100	18, 24, 34, 41	0
28	2	46/50 (92%)	0.54	2 (4%) 35 41	25, 49, 74, 86	0
29	3	92/92 (100%)	0.44	3 (3%) 46 54	27, 45, 60, 74	0
30	0	2749/2923 (94%)	-0.14	103 (3%) 41 48	14, 35, 77, 154	0
31	9	122/122 (100%)	-0.05	5 (4%) 37 43	29, 54, 76, 138	0
All	All	6646/7517 (88%)	0.36	535 (8%) 12 15	14, 41, 89, 156	0

All (535) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	63	ILE	17.7
22	V	1	THR	16.7
22	V	39	ALA	15.1
9	I	91	PHE	14.0
9	I	74	ILE	11.6
30	0	2101	A	11.6
14	N	166	ALA	11.3
9	I	132	VAL	11.3
9	I	128	THR	11.0
9	I	70	THR	10.9
22	V	40	PRO	10.8
9	I	108	HIS	10.8
9	I	100	VAL	10.5
9	I	104	ALA	10.2
9	I	80	PHE	10.1
9	I	88	GLN	9.8
9	I	103	ILE	9.7
9	I	116	LEU	9.5
9	I	97	VAL	9.5
4	D	10	PHE	9.0
20	T	119	ALA	8.8
4	D	57	THR	8.7
7	G	23	ILE	8.6
9	I	72	GLU	8.5
9	I	111	LEU	8.5
9	I	120	ALA	8.4
9	I	127	CYS	8.4
1	A	37	VAL	8.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	82	THR	8.3
9	I	133	THR	8.2
9	I	66	GLY	8.1
30	0	2537	G	8.1
26	Z	35	SER	8.0
4	D	61	PHE	7.9
30	0	2102	G	7.8
19	S	81	ILE	7.8
1	A	35	GLY	7.8
9	I	71	ALA	7.6
9	I	113	SER	7.6
30	0	1951	G	7.5
9	I	92	VAL	7.5
9	I	121	LYS	7.5
9	I	73	LEU	7.4
9	I	98	ASP	7.2
9	I	106	GLN	7.2
9	I	69	PRO	7.2
30	0	2103	A	7.2
9	I	117	THR	7.2
30	0	1177	A	7.2
26	Z	46	SER	7.0
9	I	83	GLY	7.0
1	A	237	GLY	7.0
20	T	118	SER	6.9
9	I	112	LEU	6.9
9	I	109	PRO	6.8
30	0	1202	A	6.6
9	I	76	ASP	6.6
12	L	75	LEU	6.6
30	0	1163	G	6.5
9	I	118	ASN	6.5
9	I	122	GLU	6.5
26	Z	45	VAL	6.4
30	0	1172	G	6.3
9	I	123	VAL	6.2
9	I	90	ASP	6.2
7	G	24	VAL	6.1
30	0	1198	U	6.1
9	I	81	GLU	6.1
4	D	64	ARG	6.1
31	9	1	U	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1948	G	6.0
4	D	90	LEU	6.0
24	X	88	GLU	5.9
9	I	78	ALA	5.9
30	0	1199	A	5.8
30	0	1965	C	5.8
4	D	11	HIS	5.8
1	A	31	LYS	5.8
30	0	2100	A	5.8
20	T	117	ASP	5.8
30	0	1164	U	5.8
22	V	38	GLY	5.8
14	N	160	SER	5.7
30	0	2538	A	5.7
9	I	94	ASP	5.7
9	I	86	GLU	5.6
30	0	2769	C	5.6
9	I	131	GLY	5.6
9	I	130	LEU	5.5
28	2	49	GLU	5.5
14	N	163	PHE	5.5
9	I	102	GLN	5.4
4	D	166	ILE	5.4
26	Z	49	ARG	5.4
30	0	2540	G	5.3
26	Z	34	SER	5.2
9	I	101	LYS	5.2
9	I	105	GLU	5.2
13	M	79	ALA	5.2
4	D	93	LEU	5.2
20	T	116	ASP	5.1
13	M	75	ARG	5.0
30	0	1192	A	5.0
30	0	1173	A	5.0
22	V	2	VAL	5.0
9	I	99	GLN	4.9
9	I	129	SER	4.9
1	A	85	SER	4.9
30	0	1179	C	4.8
30	0	272	A	4.8
22	V	46	ILE	4.8
19	S	77	VAL	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	92	GLU	4.7
30	0	1966	U	4.7
4	D	170	TYR	4.7
30	0	2539	U	4.7
30	0	1171	A	4.7
26	Z	55	SER	4.6
4	D	134	LEU	4.6
7	G	26	MET	4.6
5	E	45	ASP	4.6
5	E	100	ASP	4.6
30	0	1200	A	4.6
8	H	141	CYS	4.6
9	I	110	ASP	4.6
30	0	2237	G	4.5
6	F	117	GLU	4.5
13	M	71	SER	4.5
14	N	165	ALA	4.5
30	0	282	C	4.5
30	0	970	U	4.5
30	0	1170	U	4.5
6	F	25	ASP	4.5
30	0	1176	C	4.5
9	I	89	GLU	4.4
11	K	118	ALA	4.4
30	0	2645	U	4.4
30	0	1175	G	4.4
9	I	93	ALA	4.4
30	0	10	U	4.4
6	F	110	ASP	4.4
30	0	1180	U	4.3
31	9	23	U	4.3
13	M	70	GLY	4.3
9	I	114	TYR	4.3
12	L	91	VAL	4.3
30	0	514	G	4.2
6	F	22	VAL	4.2
9	I	125	GLY	4.2
26	Z	58	ASN	4.2
22	V	45	ARG	4.2
7	G	69	ARG	4.2
14	N	164	ASP	4.2
30	0	1189	A	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	1525	G	4.2
4	D	40	ILE	4.1
8	H	81	GLY	4.1
4	D	69	ILE	4.1
31	9	24	U	4.1
12	L	99	GLU	4.1
19	S	78	ALA	4.1
30	0	1178	G	4.1
4	D	73	VAL	4.1
13	M	194	GLY	4.1
26	Z	48	ARG	4.1
14	N	81	ALA	4.0
8	H	174	LEU	4.0
4	D	157	LEU	4.0
30	0	1950	G	4.0
1	A	36	ASP	4.0
4	D	104	PHE	4.0
7	G	71	LEU	4.0
30	0	1181	A	4.0
8	H	86	TYR	4.0
22	V	27	LEU	4.0
8	H	40	GLN	4.0
12	L	77	ALA	4.0
30	0	999	C	3.9
30	0	1208	C	3.9
5	E	6	GLU	3.9
6	F	12	LEU	3.9
22	V	35	ALA	3.9
9	I	107	LYS	3.9
30	0	2004	U	3.9
12	L	97	VAL	3.9
13	M	80	GLY	3.9
30	0	1162	G	3.9
13	M	74	LYS	3.9
22	V	37	GLY	3.8
26	Z	60	ASP	3.8
30	0	1184	C	3.8
30	0	1190	G	3.8
6	F	106	ALA	3.8
12	L	150	GLN	3.8
9	I	87	PRO	3.8
30	0	1196	C	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	130	VAL	3.8
4	D	56	ARG	3.8
30	0	1967	U	3.8
4	D	62	ASP	3.7
6	F	16	ALA	3.7
26	Z	38	PHE	3.7
4	D	66	GLY	3.7
6	F	26	THR	3.7
4	D	160	ALA	3.7
1	A	38	ILE	3.7
4	D	77	ASP	3.7
12	L	60	GLU	3.7
14	N	175	LEU	3.7
22	V	42	ASN	3.7
30	0	1947	G	3.6
4	D	135	VAL	3.6
5	E	87	PHE	3.6
30	0	1169	U	3.6
12	L	80	ASP	3.6
9	I	126	THR	3.6
10	J	70	PHE	3.6
14	N	147	ILE	3.6
26	Z	43	GLY	3.6
4	D	85	GLN	3.6
14	N	159	TYR	3.6
9	I	119	ALA	3.6
9	I	124	VAL	3.6
8	H	73	ASN	3.6
31	9	2	U	3.6
14	N	139	TRP	3.6
1	A	134	ASN	3.6
9	I	115	ASP	3.6
4	D	81	GLU	3.6
24	X	80	GLU	3.6
30	0	1197	G	3.6
9	I	79	GLY	3.6
4	D	23	VAL	3.6
14	N	155	GLU	3.5
30	0	2238	A	3.5
19	S	76	GLU	3.5
21	U	47	ARG	3.5
4	D	86	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	25	GLU	3.5
4	D	91	ALA	3.5
30	0	283	U	3.5
9	I	95	LEU	3.5
30	0	1201	C	3.5
30	0	1165	G	3.5
14	N	172	PHE	3.4
16	P	143	ALA	3.4
4	D	18	ILE	3.4
30	0	2637	A	3.4
7	G	21	ASP	3.4
4	D	107	GLY	3.4
7	G	22	ALA	3.4
14	N	145	ALA	3.4
7	G	73	ASP	3.4
6	F	107	ASP	3.3
22	V	31	ARG	3.3
4	D	99	ASP	3.3
8	H	70	LEU	3.3
30	0	1166	A	3.3
30	0	1174	A	3.3
30	0	138	U	3.3
30	0	1203	G	3.3
14	N	183	ASP	3.3
22	V	28	LEU	3.3
26	Z	36	GLY	3.3
13	M	87	GLY	3.3
1	A	97	ALA	3.2
26	Z	104	ARG	3.2
30	0	284	C	3.2
2	B	183	GLU	3.2
9	I	67	VAL	3.2
4	D	53	LYS	3.2
12	L	93	VAL	3.2
1	A	99	ILE	3.2
12	L	147	GLU	3.2
8	H	149	VAL	3.2
15	O	23	GLY	3.2
4	D	162	ALA	3.2
4	D	68	PRO	3.2
14	N	70	GLY	3.2
6	F	23	ALA	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	77	ILE	3.2
30	0	1964	U	3.2
3	C	135	GLU	3.2
4	D	74	THR	3.1
26	Z	42	TYR	3.1
9	I	68	PRO	3.1
19	S	80	ARG	3.1
4	D	95	THR	3.1
22	V	32	ALA	3.1
30	0	1168	C	3.1
7	G	66	LEU	3.1
22	V	44	GLY	3.1
30	0	1183	C	3.1
14	N	152	GLU	3.1
22	V	36	ALA	3.1
4	D	172	VAL	3.1
2	B	57	GLU	3.0
13	M	76	ARG	3.0
4	D	165	PHE	3.0
14	N	68	GLU	3.0
14	N	180	LEU	3.0
8	H	69	ARG	3.0
13	M	78	LYS	3.0
7	G	68	GLU	3.0
14	N	97	VAL	3.0
9	I	75	LYS	3.0
8	H	80	LEU	3.0
2	B	168	GLY	3.0
30	0	1625	U	3.0
28	2	35	ARG	3.0
30	0	960	G	2.9
4	D	17	ARG	2.9
4	D	84	LEU	2.9
1	A	34	ASP	2.9
24	X	85	VAL	2.9
30	0	2508	C	2.9
6	F	72	VAL	2.9
3	C	63	SER	2.9
1	A	236	GLY	2.9
30	0	280	C	2.9
24	X	77	PHE	2.9
30	0	1185	U	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	72	ASP	2.9
8	H	85	ASP	2.9
30	0	1188	A	2.9
8	H	38	ARG	2.9
14	N	153	GLN	2.9
12	L	81	VAL	2.8
14	N	154	LEU	2.8
4	D	171	ASP	2.8
1	A	203	GLY	2.8
19	S	1	SER	2.8
4	D	21	VAL	2.8
14	N	184	ILE	2.8
30	0	1182	C	2.8
2	B	117	GLU	2.8
12	L	102	ASP	2.8
4	D	51	ARG	2.8
13	M	86	GLN	2.8
30	0	1157	C	2.8
8	H	50	ILE	2.8
5	E	10	ASP	2.8
4	D	132	VAL	2.7
30	0	1929	G	2.7
30	0	2748	G	2.7
6	F	18	GLU	2.7
5	E	118	ILE	2.7
6	F	49	PHE	2.7
4	D	88	LEU	2.7
25	Y	234	VAL	2.7
23	W	93	ILE	2.7
14	N	134	ASP	2.7
30	0	1161	A	2.7
4	D	173	GLU	2.7
3	C	244	ALA	2.7
22	V	59	ILE	2.7
22	V	43	PRO	2.7
1	A	86	ALA	2.7
13	M	1	ALA	2.7
30	0	1206	U	2.7
7	G	67	LEU	2.7
26	Z	56	GLU	2.7
8	H	27	PRO	2.7
29	3	57	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	10	ALA	2.7
6	F	45	ALA	2.7
8	H	89	THR	2.7
30	0	969	G	2.7
26	Z	57	MET	2.7
6	F	100	ASP	2.7
26	Z	44	ARG	2.6
4	D	22	VAL	2.6
12	L	78	ALA	2.6
30	0	1194	A	2.6
30	0	2511	A	2.6
4	D	38	GLU	2.6
12	L	57	VAL	2.6
24	X	7	GLU	2.6
4	D	128	LEU	2.6
7	G	12	ILE	2.6
2	B	118	ASP	2.6
4	D	94	ALA	2.6
4	D	142	ALA	2.6
14	N	148	ALA	2.6
30	0	1187	U	2.6
6	F	111	ILE	2.6
12	L	121	ILE	2.6
30	0	1949	G	2.6
8	H	35	LYS	2.6
30	0	1000	C	2.6
22	V	25	THR	2.6
20	T	112	LEU	2.6
1	A	64	ASP	2.6
30	0	365	G	2.6
30	0	1167	G	2.6
30	0	1195	G	2.6
6	F	99	THR	2.5
8	H	114	ASP	2.5
9	I	85	GLY	2.5
25	Y	98	GLN	2.5
25	Y	236	VAL	2.5
8	H	76	LEU	2.5
11	K	27	ARG	2.5
4	D	129	ASP	2.5
19	S	79	SER	2.5
22	V	41	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
7	G	20	VAL	2.5
30	O	285	A	2.5
9	I	84	SER	2.5
6	F	14	ASP	2.5
5	E	169	THR	2.5
30	O	1526	A	2.5
14	N	138	ASP	2.5
6	F	24	ARG	2.4
8	H	78	LYS	2.4
26	Z	47	ARG	2.4
30	O	2768	A	2.4
4	D	52	THR	2.4
8	H	48	VAL	2.4
19	S	20	PHE	2.4
25	Y	235	GLU	2.4
12	L	130	ARG	2.4
30	O	1186	C	2.4
2	B	100	VAL	2.4
10	J	5	GLU	2.4
26	Z	51	ALA	2.4
1	A	133	ARG	2.4
30	O	2890	A	2.4
19	S	2	TRP	2.4
22	V	34	GLN	2.4
8	H	172	GLU	2.4
20	T	115	GLU	2.4
4	D	167	GLU	2.4
14	N	179	LEU	2.4
14	N	182	GLY	2.3
4	D	44	ILE	2.3
4	D	106	PHE	2.3
7	G	70	ALA	2.3
8	H	146	ALA	2.3
5	E	42	VAL	2.3
4	D	89	PRO	2.3
6	F	95	ALA	2.3
3	C	62	GLY	2.3
4	D	26	GLY	2.3
6	F	114	LYS	2.3
14	N	88	ALA	2.3
20	T	82	THR	2.3
1	A	135	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	0	370	G	2.3
12	L	79	ASP	2.3
4	D	43	GLU	2.3
4	D	48	MET	2.3
30	0	281	U	2.3
9	I	77	GLU	2.3
13	M	88	VAL	2.3
5	E	156	ASP	2.3
30	0	271	C	2.3
31	9	122	C	2.3
1	A	153	ARG	2.2
30	0	1970	G	2.2
4	D	54	ALA	2.2
12	L	106	VAL	2.2
22	V	26	GLU	2.2
6	F	119	ARG	2.2
12	L	149	ARG	2.2
14	N	177	GLU	2.2
30	0	1279	U	2.2
6	F	28	ALA	2.2
21	U	55	ALA	2.2
21	U	54	THR	2.2
30	0	2289	G	2.2
29	3	92	GLU	2.2
3	C	143	ASP	2.2
29	3	22	VAL	2.2
4	D	80	ALA	2.2
9	I	134	ILE	2.2
30	0	497	A	2.2
6	F	98	VAL	2.2
8	H	66	GLU	2.2
22	V	18	ALA	2.2
5	E	43	ASP	2.2
22	V	65	ASP	2.2
4	D	75	LEU	2.2
8	H	165	ARG	2.2
14	N	156	GLU	2.2
19	S	45	TYR	2.1
10	J	4	ALA	2.1
14	N	137	ALA	2.1
25	Y	216	ARG	2.1
14	N	170	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
20	T	35	TYR	2.1
23	W	76	ASP	2.1
18	R	150	PRO	2.1
12	L	142	LEU	2.1
2	B	33	ASP	2.1
13	M	85	ARG	2.1
4	D	25	MET	2.1
4	D	133	ASN	2.1
4	D	87	ALA	2.1
14	N	71	TRP	2.1
6	F	76	PHE	2.1
12	L	76	LEU	2.1
14	N	158	LEU	2.1
1	A	158	VAL	2.1
2	B	35	GLN	2.1
3	C	139	VAL	2.1
6	F	101	ALA	2.1
3	C	126	ASP	2.1
6	F	43	GLY	2.1
30	O	735	C	2.1
3	C	68	ALA	2.1
7	G	65	THR	2.1
30	O	1524	U	2.1
4	D	24	HIS	2.1
12	L	89	PHE	2.1
26	Z	59	GLU	2.1
14	N	84	THR	2.1
4	D	37	ALA	2.0
22	V	30	ALA	2.0
13	M	77	HIS	2.0
6	F	19	ALA	2.0
4	D	101	THR	2.0
19	S	21	GLN	2.0
30	O	1527	A	2.0
6	F	11	ASP	2.0
8	H	83	GLU	2.0
4	D	154	LYS	2.0
14	N	161	GLY	2.0
26	Z	105	ARG	2.0
5	E	20	ILE	2.0
30	O	2747	C	2.0
3	C	61	PHE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	F	105	ASP	2.0
30	0	1919	A	2.0
14	N	140	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.96	0.15	43,48,52,56	0
30	1MA	0	628	23/24	0.97	0.19	20,23,25,25	0
30	OMG	0	2588	24/25	0.97	0.14	23,29,30,31	0
30	PSU	0	2621	20/21	0.97	0.16	29,31,42,42	0
30	OMU	0	2587	21/22	0.98	0.14	23,27,29,29	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	SR	0	8979	1/1	0.07	0.20	193,193,193,193	0
34	SR	0	9006	1/1	0.20	0.60	199,199,199,199	0
34	SR	0	8971	1/1	0.41	0.14	153,153,153,153	0
34	SR	0	9004	1/1	0.42	0.68	182,182,182,182	0
35	NA	0	8562	1/1	0.42	0.58	61,61,61,61	0
32	MG	0	8040	1/1	0.43	0.55	81,81,81,81	0
34	SR	0	8983	1/1	0.47	0.22	151,151,151,151	0
34	SR	0	8994	1/1	0.48	0.51	173,173,173,173	0
34	SR	0	9007	1/1	0.48	1.11	178,178,178,178	0
32	MG	0	8038	1/1	0.56	0.40	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8575	1/1	0.56	0.54	78,78,78,78	0
32	MG	0	8082	1/1	0.61	0.49	63,63,63,63	0
35	NA	0	8518	1/1	0.69	0.63	81,81,81,81	0
37	K	0	8401	1/1	0.69	0.44	97,97,97,97	0
34	SR	0	8962	1/1	0.71	1.21	165,165,165,165	0
35	NA	9	8543	1/1	0.71	0.16	60,60,60,60	0
32	MG	0	8067	1/1	0.72	0.37	55,55,55,55	0
34	SR	0	8987	1/1	0.73	0.66	199,199,199,199	0
35	NA	R	8532	1/1	0.73	0.13	32,32,32,32	0
34	SR	9	8980	1/1	0.74	0.14	144,144,144,144	0
34	SR	0	8991	1/1	0.75	0.25	171,171,171,171	0
32	MG	0	8044	1/1	0.75	0.23	62,62,62,62	0
35	NA	0	8516	1/1	0.77	0.38	50,50,50,50	0
32	MG	0	8017	1/1	0.78	0.41	67,67,67,67	0
32	MG	0	8037	1/1	0.78	0.35	77,77,77,77	0
32	MG	0	8085	1/1	0.79	0.21	90,90,90,90	0
35	NA	0	8526	1/1	0.79	0.12	43,43,43,43	0
35	NA	0	8525	1/1	0.80	0.20	57,57,57,57	0
32	MG	0	8010	1/1	0.80	0.30	69,69,69,69	0
32	MG	0	8081	1/1	0.80	0.30	65,65,65,65	0
32	MG	0	8048	1/1	0.80	0.27	55,55,55,55	0
35	NA	0	8536	1/1	0.80	0.17	62,62,62,62	0
34	SR	0	8902	1/1	0.81	0.57	112,112,112,112	0
35	NA	0	8534	1/1	0.82	0.36	56,56,56,56	0
32	MG	0	8049	1/1	0.82	0.41	78,78,78,78	0
32	MG	0	8076	1/1	0.82	0.22	52,52,52,52	0
35	NA	0	8512	1/1	0.82	0.63	63,63,63,63	0
34	SR	0	8955	1/1	0.83	0.21	140,140,140,140	0
32	MG	0	8056	1/1	0.83	0.21	66,66,66,66	0
32	MG	0	8071	1/1	0.83	0.23	73,73,73,73	0
34	SR	0	8957	1/1	0.83	0.33	149,149,149,149	0
35	NA	0	8559	1/1	0.83	0.27	67,67,67,67	0
34	SR	0	8990	1/1	0.84	0.13	132,132,132,132	0
32	MG	0	8047	1/1	0.84	0.33	66,66,66,66	0
34	SR	0	8959	1/1	0.84	0.10	129,129,129,129	0
35	NA	0	8569	1/1	0.84	0.53	61,61,61,61	0
35	NA	0	8567	1/1	0.84	0.53	59,59,59,59	0
35	NA	0	8504	1/1	0.85	0.28	34,34,34,34	0
34	SR	0	8919	1/1	0.85	0.19	167,167,167,167	0
34	SR	0	9002	1/1	0.85	0.17	141,141,141,141	0
35	NA	0	8557	1/1	0.85	0.10	63,63,63,63	0
32	MG	0	8070	1/1	0.85	0.18	50,50,50,50	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8542	1/1	0.85	0.40	44,44,44,44	0
32	MG	0	8025	1/1	0.86	0.12	40,40,40,40	0
32	MG	0	8050	1/1	0.86	0.50	63,63,63,63	0
35	NA	0	8564	1/1	0.86	0.16	49,49,49,49	0
34	SR	0	8922	1/1	0.86	0.54	164,164,164,164	0
32	MG	0	8084	1/1	0.86	0.17	59,59,59,59	0
32	MG	B	8042	1/1	0.86	0.26	75,75,75,75	0
35	NA	0	8554	1/1	0.87	0.47	55,55,55,55	0
32	MG	0	8068	1/1	0.87	0.17	50,50,50,50	0
32	MG	0	8065	1/1	0.87	0.99	68,68,68,68	0
32	MG	0	8059	1/1	0.88	0.09	31,31,31,31	0
35	NA	0	8573	1/1	0.88	0.19	69,69,69,69	0
32	MG	0	8078	1/1	0.88	0.25	52,52,52,52	0
32	MG	0	8079	1/1	0.88	0.31	52,52,52,52	0
35	NA	M	8539	1/1	0.88	0.18	34,34,34,34	0
34	SR	0	8938	1/1	0.88	0.19	102,102,102,102	0
32	MG	0	8089	1/1	0.88	0.20	48,48,48,48	0
35	NA	0	8517	1/1	0.88	0.43	68,68,68,68	0
35	NA	9	8572	1/1	0.88	0.12	66,66,66,66	0
34	SR	0	8989	1/1	0.88	0.24	149,149,149,149	0
32	MG	0	8075	1/1	0.89	0.11	37,37,37,37	0
32	MG	0	8018	1/1	0.89	0.28	13,13,13,13	0
32	MG	0	8013	1/1	0.89	0.14	41,41,41,41	0
34	SR	0	8969	1/1	0.89	0.16	115,115,115,115	0
35	NA	0	8549	1/1	0.89	0.43	73,73,73,73	0
32	MG	0	8066	1/1	0.89	0.33	67,67,67,67	0
32	MG	0	8080	1/1	0.89	0.13	54,54,54,54	0
34	SR	0	8993	1/1	0.89	0.08	154,154,154,154	0
35	NA	0	8556	1/1	0.89	0.26	38,38,38,38	0
32	MG	0	8090	1/1	0.89	0.10	51,51,51,51	0
34	SR	9	8968	1/1	0.89	0.14	96,96,96,96	0
32	MG	0	8073	1/1	0.89	0.30	72,72,72,72	0
35	NA	0	8553	1/1	0.89	0.33	61,61,61,61	0
32	MG	0	8007	1/1	0.89	0.29	53,53,53,53	0
32	MG	0	8063	1/1	0.89	0.32	74,74,74,74	0
35	NA	J	8538	1/1	0.90	0.15	47,47,47,47	0
35	NA	0	8535	1/1	0.90	0.30	55,55,55,55	0
35	NA	0	8509	1/1	0.90	0.26	60,60,60,60	0
35	NA	0	8522	1/1	0.90	0.20	52,52,52,52	0
37	K	0	8402	1/1	0.90	0.26	77,77,77,77	0
34	SR	0	9001	1/1	0.90	0.05	142,142,142,142	0
32	MG	0	8088	1/1	0.90	0.09	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8035	1/1	0.90	0.10	63,63,63,63	0
35	NA	0	8563	1/1	0.90	0.51	64,64,64,64	0
35	NA	0	8521	1/1	0.90	0.53	70,70,70,70	0
35	NA	0	8571	1/1	0.90	0.12	83,83,83,83	0
32	MG	0	8072	1/1	0.90	0.15	36,36,36,36	0
32	MG	0	8069	1/1	0.90	0.27	75,75,75,75	0
32	MG	0	8041	1/1	0.91	0.26	52,52,52,52	0
34	SR	0	8992	1/1	0.91	0.09	108,108,108,108	0
32	MG	0	8052	1/1	0.91	0.10	29,29,29,29	0
35	NA	T	8537	1/1	0.91	0.09	26,26,26,26	0
34	SR	0	8944	1/1	0.91	0.16	117,117,117,117	0
35	NA	0	8508	1/1	0.91	0.19	36,36,36,36	0
35	NA	0	8533	1/1	0.91	0.19	57,57,57,57	0
32	MG	0	8026	1/1	0.91	0.11	44,44,44,44	0
34	SR	0	8998	1/1	0.92	0.14	99,99,99,99	0
32	MG	0	8016	1/1	0.92	0.30	75,75,75,75	0
34	SR	0	8981	1/1	0.92	0.15	115,115,115,115	0
32	MG	0	8002	1/1	0.92	0.16	33,33,33,33	0
35	NA	0	8560	1/1	0.92	0.30	67,67,67,67	0
34	SR	9	9003	1/1	0.92	0.06	122,122,122,122	0
32	MG	0	8062	1/1	0.92	0.29	46,46,46,46	0
32	MG	0	8031	1/1	0.92	0.09	39,39,39,39	0
35	NA	0	8555	1/1	0.92	0.92	59,59,59,59	0
34	SR	0	8976	1/1	0.92	0.29	122,122,122,122	0
34	SR	0	8963	1/1	0.92	0.13	135,135,135,135	0
33	CL	J	8802	1/1	0.92	0.13	49,49,49,49	0
33	CL	0	8822	1/1	0.92	0.11	46,46,46,46	0
33	CL	0	8811	1/1	0.92	0.17	54,54,54,54	0
34	SR	0	9000	1/1	0.93	0.16	125,125,125,125	0
34	SR	0	8972	1/1	0.93	0.17	121,121,121,121	0
35	NA	0	8511	1/1	0.93	0.25	61,61,61,61	0
32	MG	0	8039	1/1	0.93	0.33	42,42,42,42	0
32	MG	0	8029	1/1	0.93	0.12	35,35,35,35	0
35	NA	0	8545	1/1	0.93	0.30	40,40,40,40	0
35	NA	0	8558	1/1	0.93	0.29	39,39,39,39	0
34	SR	0	8949	1/1	0.93	0.50	184,184,184,184	0
32	MG	0	8027	1/1	0.93	0.09	36,36,36,36	0
32	MG	0	8015	1/1	0.93	0.20	50,50,50,50	0
34	SR	0	8956	1/1	0.93	0.10	111,111,111,111	0
32	MG	0	8091	1/1	0.93	0.11	50,50,50,50	0
35	NA	0	8561	1/1	0.93	0.39	67,67,67,67	0
34	SR	S	8961	1/1	0.93	0.10	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8520	1/1	0.93	0.24	49,49,49,49	0
34	SR	0	8995	1/1	0.93	0.17	94,94,94,94	0
32	MG	Y	8086	1/1	0.93	0.13	30,30,30,30	0
32	MG	0	8043	1/1	0.93	0.12	51,51,51,51	0
35	NA	0	8547	1/1	0.93	0.28	49,49,49,49	0
34	SR	0	8986	1/1	0.93	0.17	136,136,136,136	0
34	SR	0	8951	1/1	0.94	0.07	99,99,99,99	0
34	SR	0	8988	1/1	0.94	0.11	110,110,110,110	0
35	NA	0	8523	1/1	0.94	0.21	48,48,48,48	0
35	NA	0	8552	1/1	0.94	0.28	51,51,51,51	0
35	NA	0	8565	1/1	0.94	0.09	39,39,39,39	0
34	SR	0	8985	1/1	0.94	0.19	98,98,98,98	0
32	MG	0	8001	1/1	0.94	0.20	9,9,9,9	0
32	MG	0	8020	1/1	0.94	0.18	22,22,22,22	0
34	SR	0	8996	1/1	0.94	0.29	173,173,173,173	0
33	CL	0	8816	1/1	0.94	0.12	49,49,49,49	0
32	MG	0	8045	1/1	0.94	0.20	40,40,40,40	0
34	SR	0	8960	1/1	0.94	0.09	100,100,100,100	0
35	NA	0	8570	1/1	0.94	0.18	35,35,35,35	0
32	MG	A	8051	1/1	0.94	0.34	51,51,51,51	0
35	NA	0	8528	1/1	0.94	0.25	67,67,67,67	0
33	CL	A	8809	1/1	0.94	0.14	51,51,51,51	0
35	NA	0	8505	1/1	0.94	0.22	37,37,37,37	0
34	SR	0	8975	1/1	0.94	0.15	114,114,114,114	0
35	NA	S	8510	1/1	0.94	0.07	32,32,32,32	0
35	NA	0	8506	1/1	0.95	0.14	44,44,44,44	0
32	MG	0	8060	1/1	0.95	0.13	41,41,41,41	0
32	MG	0	8008	1/1	0.95	0.19	27,27,27,27	0
32	MG	0	8011	1/1	0.95	0.23	26,26,26,26	0
35	NA	0	8514	1/1	0.95	0.19	34,34,34,34	0
32	MG	0	8003	1/1	0.95	0.15	24,24,24,24	0
34	SR	0	8982	1/1	0.95	0.15	116,116,116,116	0
35	NA	C	8503	1/1	0.95	0.26	19,19,19,19	0
32	MG	0	8092	1/1	0.95	0.11	53,53,53,53	0
32	MG	0	8024	1/1	0.95	0.14	45,45,45,45	0
34	SR	0	8970	1/1	0.95	0.12	73,73,73,73	0
34	SR	0	8974	1/1	0.95	0.34	119,119,119,119	0
32	MG	0	8077	1/1	0.95	0.14	34,34,34,34	0
35	NA	0	8546	1/1	0.95	0.40	51,51,51,51	0
32	MG	T	8057	1/1	0.95	0.15	32,32,32,32	0
35	NA	0	8530	1/1	0.95	0.22	41,41,41,41	0
35	NA	0	8513	1/1	0.95	0.21	32,32,32,32	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CL	B	8819	1/1	0.95	0.26	57,57,57,57	0
35	NA	0	8574	1/1	0.95	0.31	47,47,47,47	0
35	NA	0	8527	1/1	0.96	0.18	35,35,35,35	0
35	NA	0	8566	1/1	0.96	0.41	37,37,37,37	0
32	MG	0	8030	1/1	0.96	0.28	51,51,51,51	0
32	MG	9	8074	1/1	0.96	0.28	42,42,42,42	0
35	NA	Q	8540	1/1	0.96	0.09	39,39,39,39	0
35	NA	0	8551	1/1	0.96	0.18	40,40,40,40	0
32	MG	0	8064	1/1	0.96	0.20	54,54,54,54	0
32	MG	0	8033	1/1	0.96	0.10	45,45,45,45	0
34	SR	0	8945	1/1	0.96	0.10	71,71,71,71	0
36	CD	O	8705	1/1	0.96	0.05	88,88,88,88	0
35	NA	0	8550	1/1	0.96	0.17	37,37,37,37	0
32	MG	0	8032	1/1	0.96	0.21	42,42,42,42	0
32	MG	0	8022	1/1	0.97	0.15	7,7,7,7	0
34	SR	0	8939	1/1	0.97	0.10	62,62,62,62	0
34	SR	0	8997	1/1	0.97	0.22	115,115,115,115	0
35	NA	0	8531	1/1	0.97	0.10	17,17,17,17	0
33	CL	J	8821	1/1	0.97	0.22	52,52,52,52	0
33	CL	N	8807	1/1	0.97	0.11	43,43,43,43	0
32	MG	0	8009	1/1	0.97	0.32	1,1,1,1	0
33	CL	O	8808	1/1	0.97	0.10	52,52,52,52	0
32	MG	0	8014	1/1	0.97	0.18	23,23,23,23	0
33	CL	0	8813	1/1	0.97	0.10	34,34,34,34	0
34	SR	0	8958	1/1	0.97	0.10	57,57,57,57	0
34	SR	0	8946	1/1	0.97	0.18	75,75,75,75	0
32	MG	0	8036	1/1	0.97	0.16	37,37,37,37	0
35	NA	0	8501	1/1	0.97	0.16	30,30,30,30	0
34	SR	0	8965	1/1	0.97	0.12	80,80,80,80	0
34	SR	0	8933	1/1	0.97	0.06	54,54,54,54	0
32	MG	0	8087	1/1	0.97	0.15	33,33,33,33	0
32	MG	0	8083	1/1	0.97	0.07	35,35,35,35	0
35	NA	0	8502	1/1	0.97	0.30	52,52,52,52	0
35	NA	0	8568	1/1	0.97	0.15	33,33,33,33	0
32	MG	K	8054	1/1	0.97	0.14	20,20,20,20	0
32	MG	0	8093	1/1	0.97	0.17	29,29,29,29	0
34	SR	0	8967	1/1	0.97	0.10	86,86,86,86	0
34	SR	A	8977	1/1	0.97	0.13	88,88,88,88	0
35	NA	0	8544	1/1	0.97	0.15	53,53,53,53	0
34	SR	A	8929	1/1	0.97	0.11	78,78,78,78	0
34	SR	0	9008	1/1	0.97	0.14	59,59,59,59	0
34	SR	0	8928	1/1	0.97	0.09	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	CL	3	8804	1/1	0.97	0.09	48,48,48,48	0
35	NA	0	8507	1/1	0.97	0.22	19,19,19,19	0
33	CL	L	8810	1/1	0.97	0.14	43,43,43,43	0
34	SR	0	8914	1/1	0.98	0.21	67,67,67,67	0
34	SR	0	8953	1/1	0.98	0.07	76,76,76,76	0
34	SR	B	8950	1/1	0.98	0.14	83,83,83,83	0
34	SR	0	8984	1/1	0.98	0.09	75,75,75,75	0
35	NA	0	8515	1/1	0.98	0.20	28,28,28,28	0
34	SR	0	8964	1/1	0.98	0.09	76,76,76,76	0
34	SR	0	8948	1/1	0.98	0.10	57,57,57,57	0
34	SR	0	8973	1/1	0.98	0.13	79,79,79,79	0
33	CL	R	8806	1/1	0.98	0.16	28,28,28,28	0
32	MG	0	8004	1/1	0.98	0.20	13,13,13,13	0
34	SR	0	8907	1/1	0.98	0.20	50,50,50,50	0
32	MG	0	8019	1/1	0.98	0.26	18,18,18,18	0
34	SR	0	8947	1/1	0.98	0.21	73,73,73,73	0
33	CL	0	8803	1/1	0.98	0.14	38,38,38,38	0
34	SR	0	8954	1/1	0.98	0.12	60,60,60,60	0
35	NA	0	8529	1/1	0.98	0.10	29,29,29,29	0
35	NA	0	8548	1/1	0.98	0.30	41,41,41,41	0
34	SR	0	8978	1/1	0.98	0.10	47,47,47,47	0
32	MG	0	8021	1/1	0.98	0.12	24,24,24,24	0
32	MG	0	8058	1/1	0.98	0.16	3,3,3,3	0
35	NA	0	8541	1/1	0.98	0.24	33,33,33,33	0
32	MG	0	8055	1/1	0.98	0.27	12,12,12,12	0
34	SR	0	8941	1/1	0.98	0.14	60,60,60,60	0
33	CL	J	8801	1/1	0.98	0.10	42,42,42,42	0
34	SR	0	8911	1/1	0.98	0.11	48,48,48,48	0
34	SR	0	8915	1/1	0.98	0.11	58,58,58,58	0
32	MG	0	8005	1/1	0.98	0.15	29,29,29,29	0
32	MG	0	8061	1/1	0.98	0.22	17,17,17,17	0
33	CL	0	8814	1/1	0.98	0.14	35,35,35,35	0
32	MG	0	8034	1/1	0.98	0.11	25,25,25,25	0
34	SR	0	8942	1/1	0.98	0.12	55,55,55,55	0
34	SR	0	8940	1/1	0.98	0.11	62,62,62,62	0
34	SR	0	8966	1/1	0.98	0.10	68,68,68,68	0
34	SR	F	9005	1/1	0.98	0.11	77,77,77,77	0
32	MG	0	8053	1/1	0.98	0.13	45,45,45,45	0
34	SR	0	8927	1/1	0.99	0.17	58,58,58,58	0
35	NA	0	8519	1/1	0.99	0.14	29,29,29,29	0
34	SR	0	8910	1/1	0.99	0.24	60,60,60,60	0
36	CD	1	8702	1/1	0.99	0.13	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8918	1/1	0.99	0.22	45,45,45,45	0
34	SR	0	8904	1/1	0.99	0.08	20,20,20,20	0
34	SR	0	8931	1/1	0.99	0.11	61,61,61,61	0
34	SR	1	8913	1/1	0.99	0.15	32,32,32,32	0
34	SR	0	8923	1/1	0.99	0.10	54,54,54,54	0
34	SR	0	8921	1/1	0.99	0.15	46,46,46,46	0
34	SR	0	8906	1/1	0.99	0.20	50,50,50,50	0
34	SR	0	8924	1/1	0.99	0.12	50,50,50,50	0
33	CL	0	8805	1/1	0.99	0.10	39,39,39,39	0
34	SR	A	8930	1/1	0.99	0.12	57,57,57,57	0
34	SR	0	8926	1/1	0.99	0.16	69,69,69,69	0
32	MG	0	8028	1/1	0.99	0.29	1,1,1,1	0
34	SR	0	8903	1/1	0.99	0.18	36,36,36,36	0
32	MG	0	8046	1/1	0.99	0.16	1,1,1,1	0
34	SR	0	8943	1/1	0.99	0.08	49,49,49,49	0
36	CD	Z	8703	1/1	0.99	0.20	67,67,67,67	0
34	SR	0	8916	1/1	0.99	0.11	45,45,45,45	0
34	SR	0	8908	1/1	0.99	0.15	46,46,46,46	0
34	SR	0	8934	1/1	0.99	0.10	52,52,52,52	0
32	MG	0	8012	1/1	0.99	0.25	4,4,4,4	0
32	MG	0	8006	1/1	0.99	0.32	1,1,1,1	0
34	SR	0	8925	1/1	0.99	0.13	55,55,55,55	0
33	CL	Y	8820	1/1	0.99	0.09	27,27,27,27	0
33	CL	M	8818	1/1	0.99	0.14	22,22,22,22	0
34	SR	0	8909	1/1	0.99	0.14	44,44,44,44	0
34	SR	3	8932	1/1	0.99	0.08	65,65,65,65	0
35	NA	0	8524	1/1	0.99	0.16	27,27,27,27	0
34	SR	3	8999	1/1	0.99	0.10	63,63,63,63	0
32	MG	0	8023	1/1	0.99	0.12	30,30,30,30	0
33	CL	0	8815	1/1	0.99	0.12	38,38,38,38	0
36	CD	U	8701	1/1	0.99	0.17	62,62,62,62	0
34	SR	0	8920	1/1	0.99	0.07	63,63,63,63	0
33	CL	0	8812	1/1	0.99	0.14	43,43,43,43	0
33	CL	0	8817	1/1	0.99	0.08	33,33,33,33	0
34	SR	0	8936	1/1	0.99	0.12	44,44,44,44	0
34	SR	0	8917	1/1	0.99	0.14	46,46,46,46	0
34	SR	0	8935	1/1	1.00	0.09	54,54,54,54	0
34	SR	0	8905	1/1	1.00	0.25	43,43,43,43	0
34	SR	0	8937	1/1	1.00	0.16	53,53,53,53	0
36	CD	3	8704	1/1	1.00	0.14	63,63,63,63	0
34	SR	R	8912	1/1	1.00	0.15	55,55,55,55	0
34	SR	1	8952	1/1	1.00	0.15	47,47,47,47	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8901	1/1	1.00	0.17	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.