



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:52 AM UTC

PDB ID : 3CME / pdb_00003cme
Title : The Structure of CA and CCA-PHE-CAP-BIO Bound to the Large Ribosomal Subunit of Haloarcula Marismortui
Authors : Simonovic, M.; Steitz, T.A.
Deposited on : 2008-03-21
Resolution : 2.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

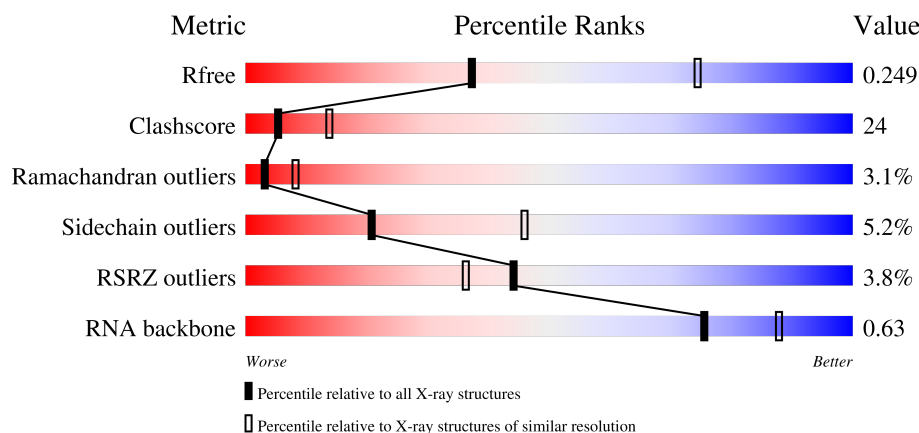
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)
RNA backbone	3983	1046 (3.16-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2% 40% 49% 8% ..
2	B	338	% 37% 54% 9%
3	C	246	2% 41% 49% 10%
4	D	177	24% 24% 47% 8% 21%

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	240	
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	
32	5	3	
33	6	3	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	MG	0	8029	-	-	-	X
34	MG	0	8045	-	-	-	X
34	MG	0	8047	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8090	-	-	-	X
35	CL	J	8801	-	-	X	-
35	CL	L	8814	-	-	X	-
36	SR	0	8994	-	-	-	X
37	NA	0	8522	-	-	-	X
37	NA	0	8558	-	-	-	X
41	ACA	6	78	-	-	-	X

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 99194 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
			1752	1072	351	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
			2624	1616	492	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
			1859	1130	344	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
			1093	685	194	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
			1356	840	223	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
			889	551	140	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
			1281	798	239	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
			518	323	80	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
			1119	696	198	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
			993	609	188	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
			1117	670	221	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
			1557	943	332	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
			1444	895	261	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
			864	529	160	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
			1135	683	228	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
			734	450	140	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
			1148	713	208	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
			640	389	110	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
			949	568	179	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
			1195	737	208	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
			653	402	128	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
			572	343	112	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
			754	458	152	137	7			

- Molecule 30 is a RNA chain called 50S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59017	26345	10873	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
			2595	1156	471	847	121			

- Molecule 32 is a RNA chain called RNA (5'-R(*C*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	5	2	Total	C	N	O	P	0	0	0
			39	19	8	11	1			

- Molecule 33 is a RNA chain called RNA (5'-R(*CP*CP*(8AN))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	6	3	Total	C	N	O	P	0	0	0
			59	28	12	17	2			

- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	3	Total	Mg	0	0
			3	3		
34	B	2	Total	Mg	0	0
			2	2		
34	C	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	K	1	Total 1	Mg 1	0	0
34	T	1	Total 1	Mg 1	0	0
34	Y	1	Total 1	Mg 1	0	0
34	2	1	Total 1	Mg 1	0	0
34	0	82	Total 82	Mg 82	0	0
34	9	1	Total 1	Mg 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	1	Total 1	Cl 1	0	0
35	B	1	Total 1	Cl 1	0	0
35	J	4	Total 4	Cl 4	0	0
35	L	2	Total 2	Cl 2	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	Q	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	Y	2	Total 2	Cl 2	0	0
35	3	1	Total 1	Cl 1	0	0
35	0	6	Total 6	Cl 6	0	0

- Molecule 36 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	A	3	Total 3 Sr 3	0	0
36	B	2	Total 2 Sr 2	0	0
36	F	1	Total 1 Sr 1	0	0
36	H	2	Total 2 Sr 2	0	0
36	L	1	Total 1 Sr 1	0	0
36	R	1	Total 1 Sr 1	0	0
36	T	2	Total 2 Sr 2	0	0
36	Y	1	Total 1 Sr 1	0	0
36	1	2	Total 2 Sr 2	0	0
36	3	3	Total 3 Sr 3	0	0
36	0	87	Total 87 Sr 87	0	0
36	9	3	Total 3 Sr 3	0	0

- Molecule 37 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	C	1	Total Na 1 1	0	0
37	H	1	Total Na 1 1	0	0
37	J	1	Total Na 1 1	0	0
37	M	1	Total Na 1 1	0	0
37	Q	1	Total Na 1 1	0	0
37	R	1	Total Na 1 1	0	0
37	S	1	Total Na 1 1	0	0
37	0	65	Total Na 65 65	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	9	3	Total 3	Na 3	0	0

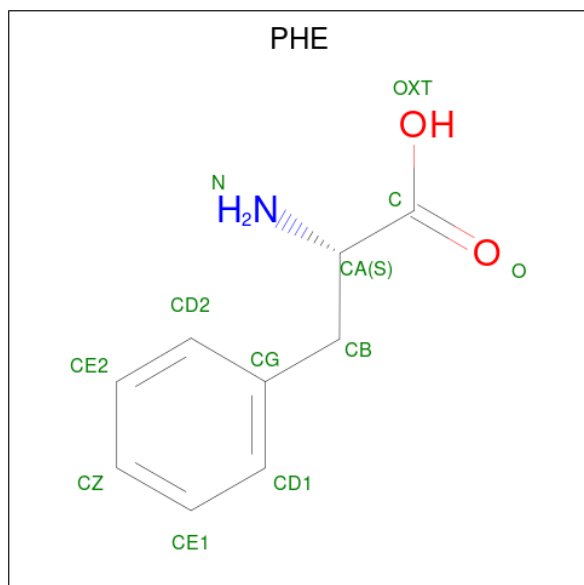
- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total 1	Cd 1	0	0
38	U	1	Total 1	Cd 1	0	0
38	Z	1	Total 1	Cd 1	0	0
38	1	1	Total 1	Cd 1	0	0
38	3	1	Total 1	Cd 1	0	0

- Molecule 39 is POTASSIUM ION (CCD ID: K) (formula: K).

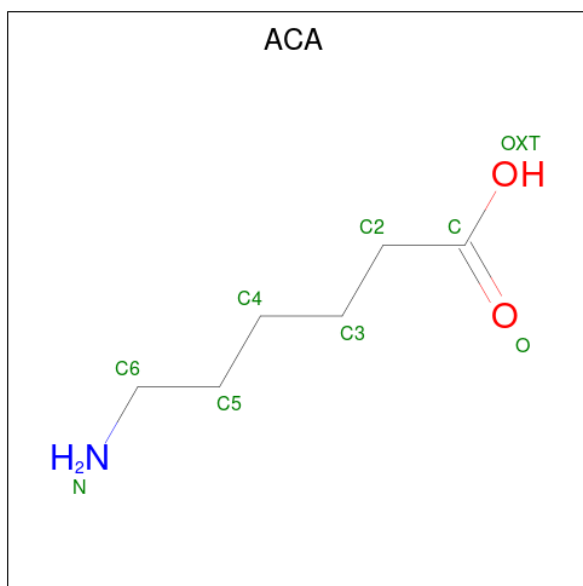
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	2	Total 2	K 2	0	0

- Molecule 40 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
40	6	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 41 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
41	6	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	A	134	Total	O	0	0
			134	134		
42	B	156	Total	O	0	0
			156	156		
42	C	168	Total	O	0	0
			168	168		
42	D	49	Total	O	0	0
			49	49		
42	E	49	Total	O	0	0
			49	49		
42	F	31	Total	O	0	0
			31	31		
42	G	20	Total	O	0	0
			20	20		
42	H	78	Total	O	0	0
			78	78		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	I	11	Total 11	O 11	0	0
42	J	58	Total 58	O 58	0	0
42	K	57	Total 57	O 57	0	0
42	L	91	Total 91	O 91	0	0
42	M	129	Total 129	O 129	0	0
42	N	68	Total 68	O 68	0	0
42	O	46	Total 46	O 46	0	0
42	P	72	Total 72	O 72	0	0
42	Q	52	Total 52	O 52	0	0
42	R	89	Total 89	O 89	0	0
42	S	35	Total 35	O 35	0	0
42	T	42	Total 42	O 42	0	0
42	U	29	Total 29	O 29	0	0
42	V	16	Total 16	O 16	0	0
42	W	75	Total 75	O 75	0	0
42	X	31	Total 31	O 31	0	0
42	Y	105	Total 105	O 105	0	0
42	Z	25	Total 25	O 25	0	0
42	1	57	Total 57	O 57	0	0
42	2	50	Total 50	O 50	0	0
42	3	66	Total 66	O 66	0	0

Continued on next page...

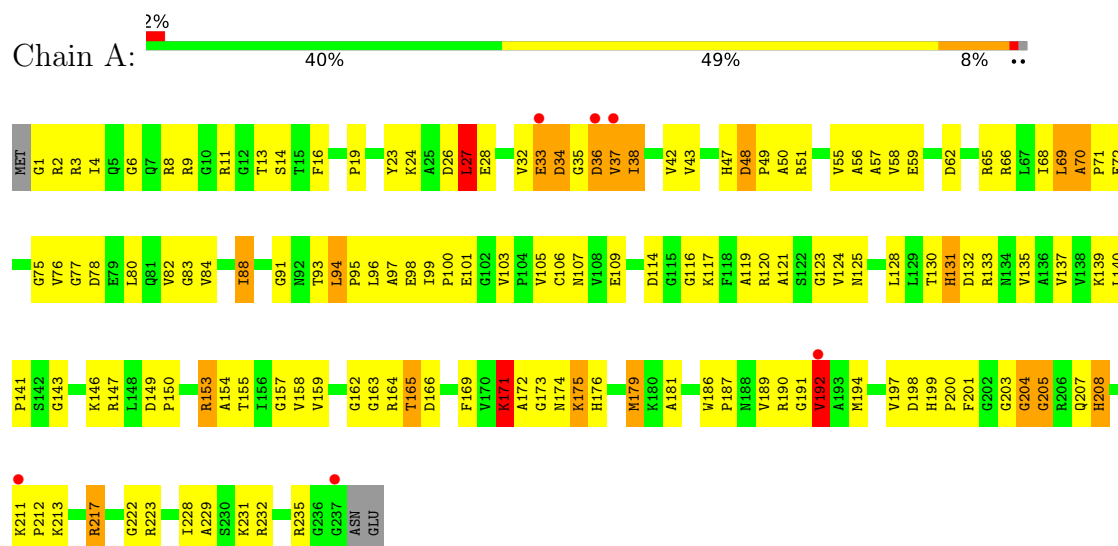
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
42	0	5775	Total 5775	O 5775	0	0
42	9	138	Total 138	O 138	0	0
42	6	6	Total 6	O 6	0	0

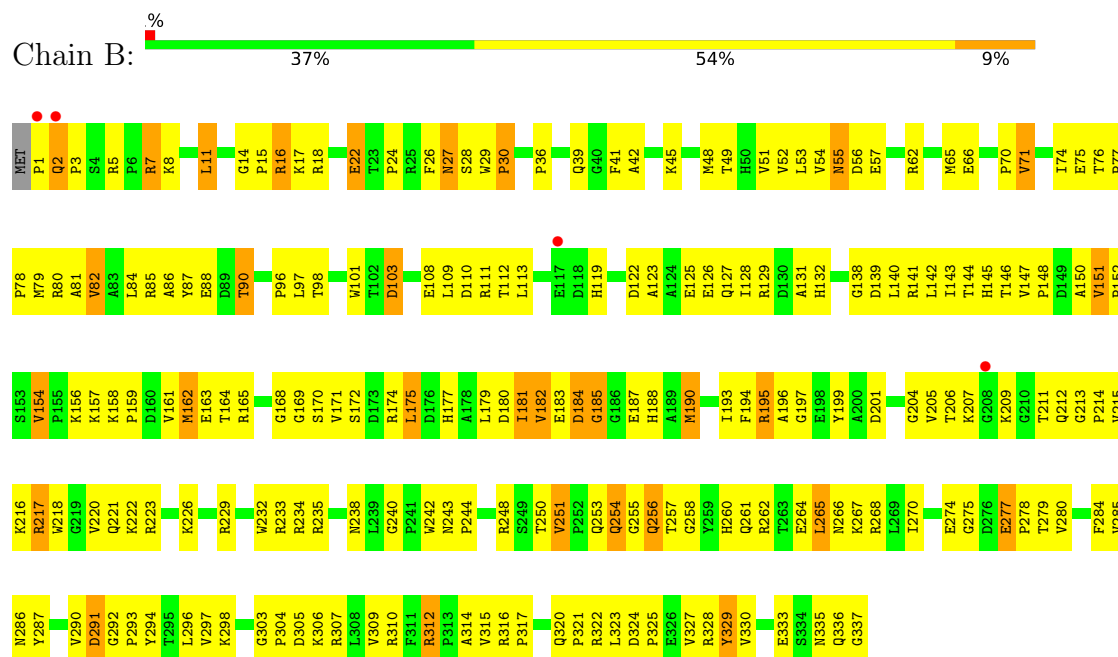
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

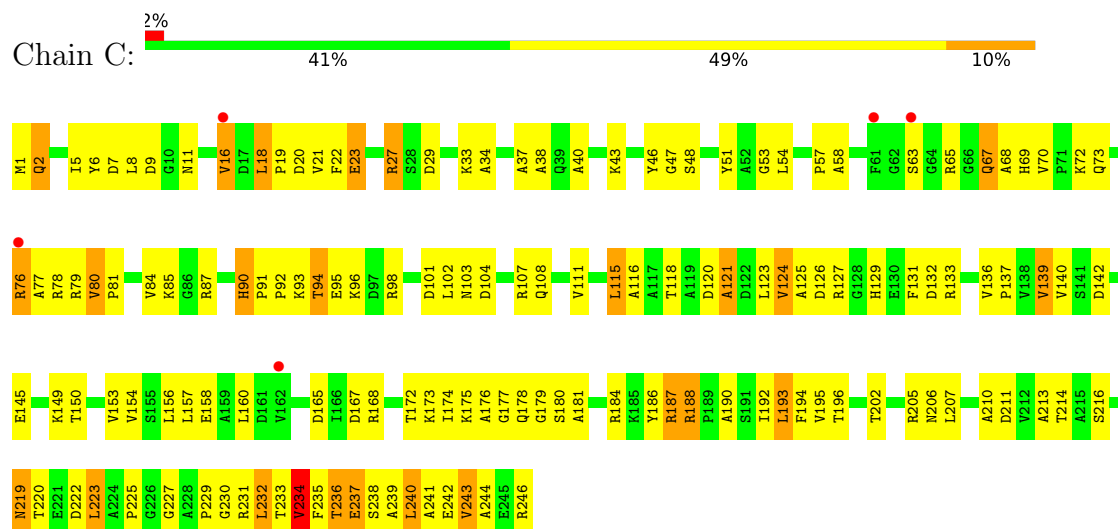
• Molecule 1: 50S ribosomal protein L2P



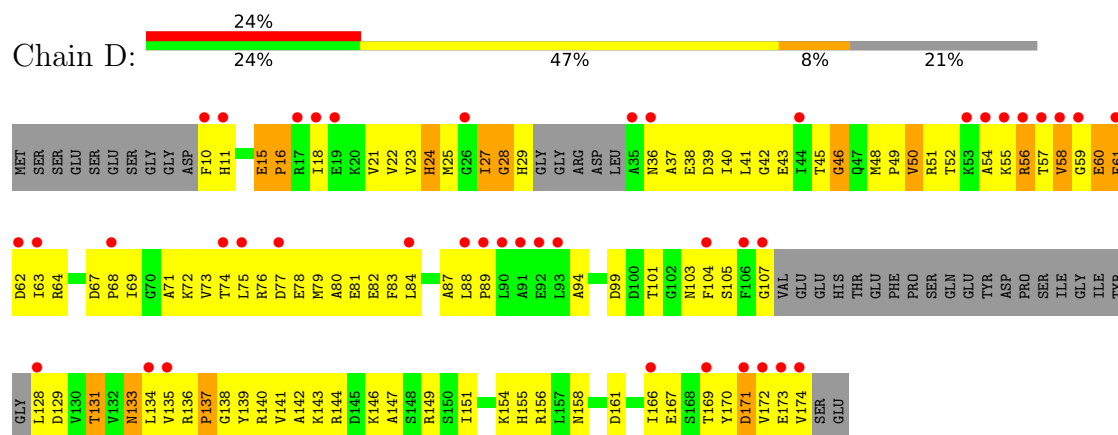
• Molecule 2: 50S ribosomal protein L3P



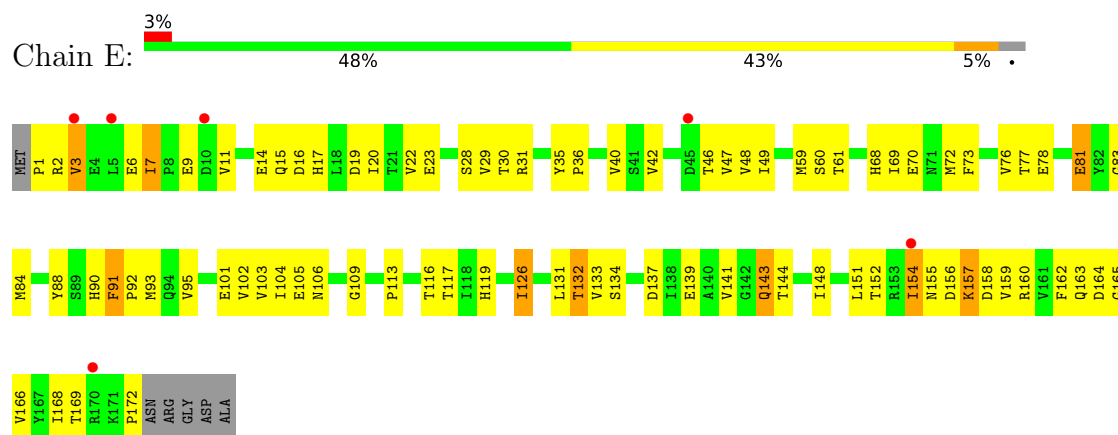
- Molecule 3: 50S ribosomal protein L4P



- Molecule 4: 50S ribosomal protein L5P

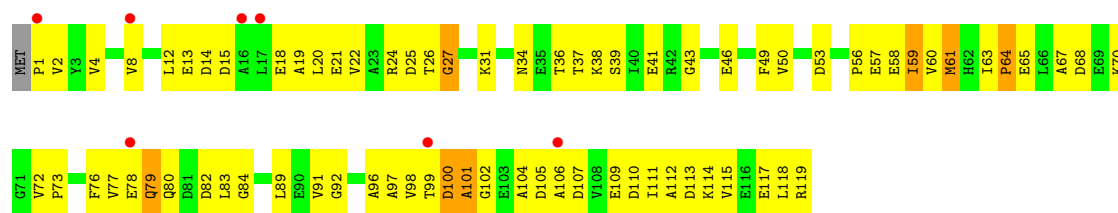


- Molecule 5: 50S ribosomal protein L6P

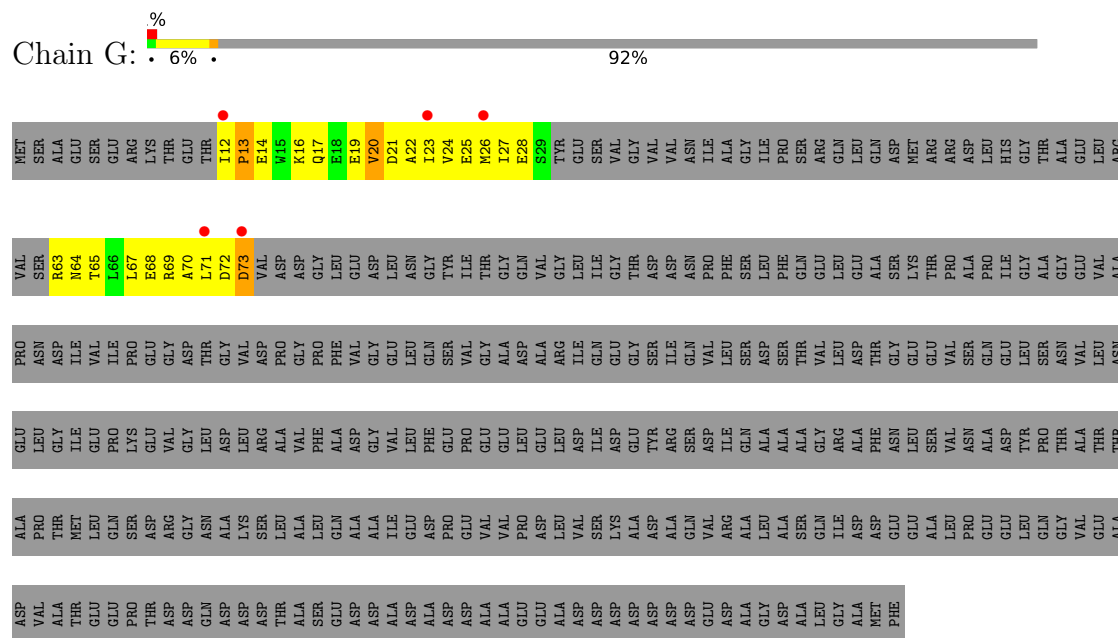


- Molecule 6: 50S ribosomal protein L7Ae

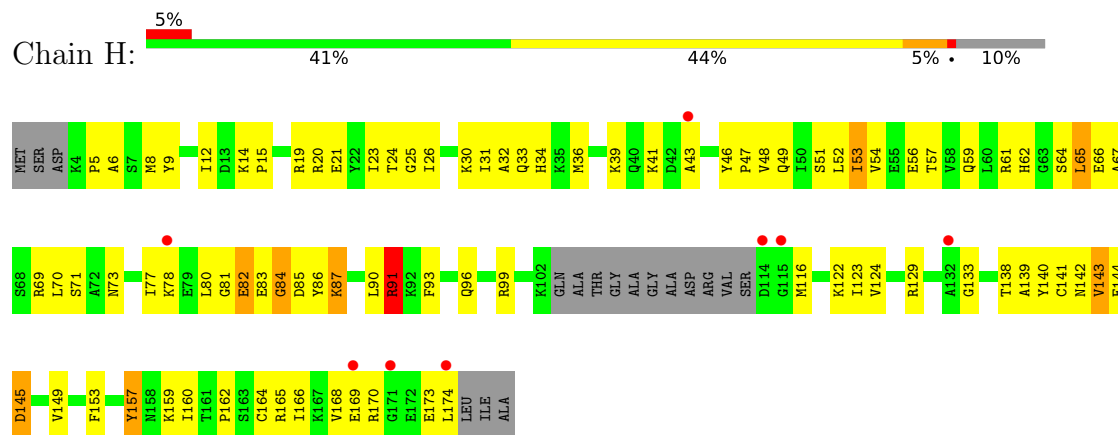




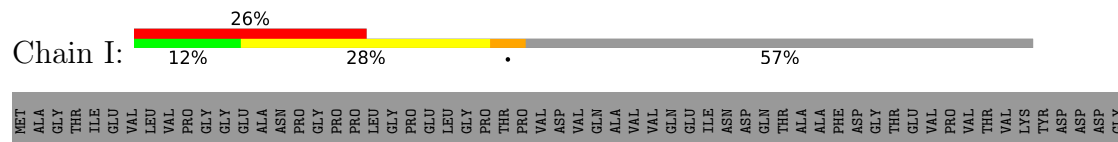
• Molecule 7: 50S ribosomal protein L10E

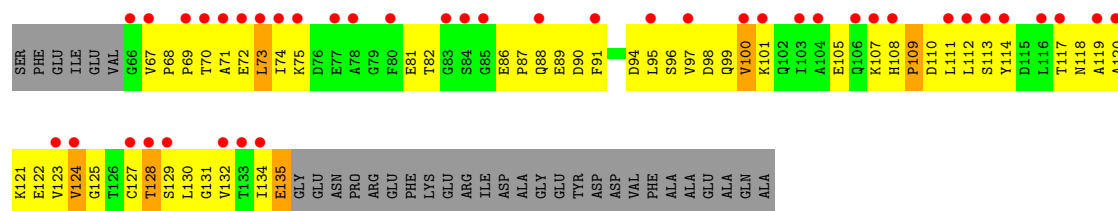


• Molecule 8: 50S ribosomal protein L10e

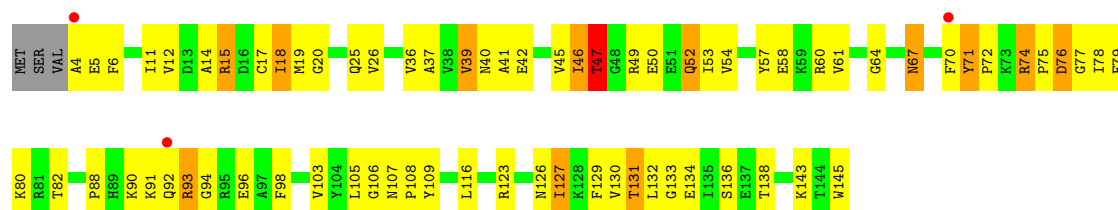


• Molecule 9: 50S ribosomal protein L11P

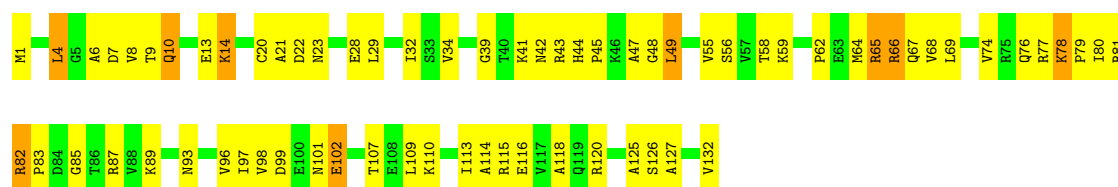




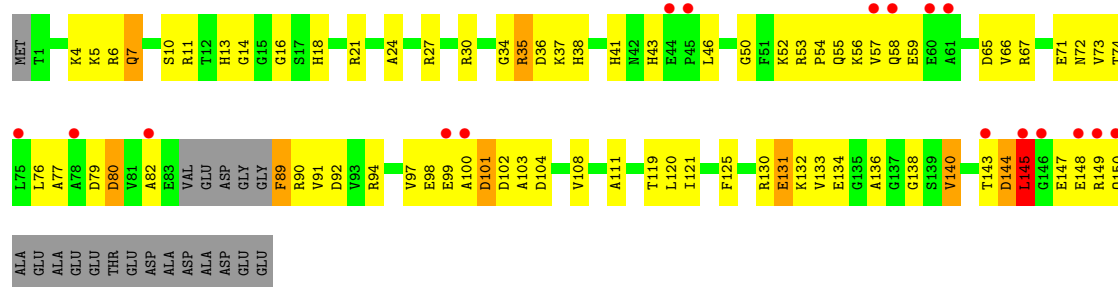
• Molecule 10: 50S ribosomal protein L13P



• Molecule 11: 50S ribosomal protein L14P

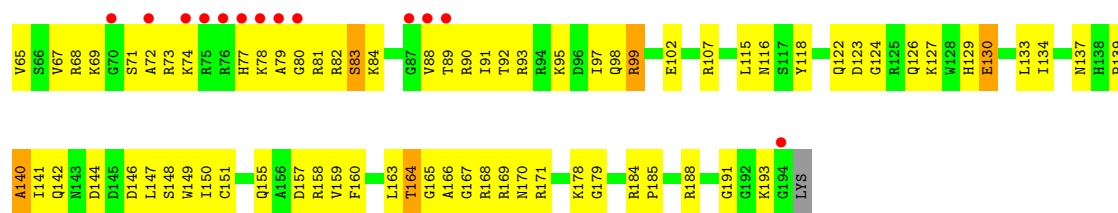


• Molecule 12: 50S ribosomal protein L15P

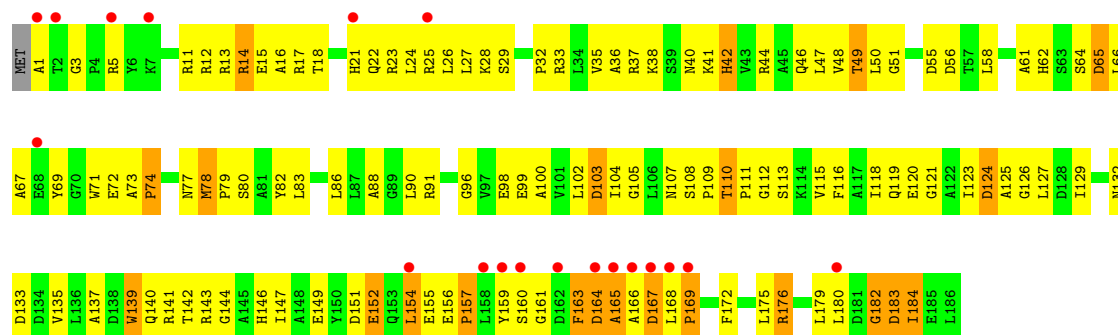


• Molecule 13: 50S ribosomal protein L15e

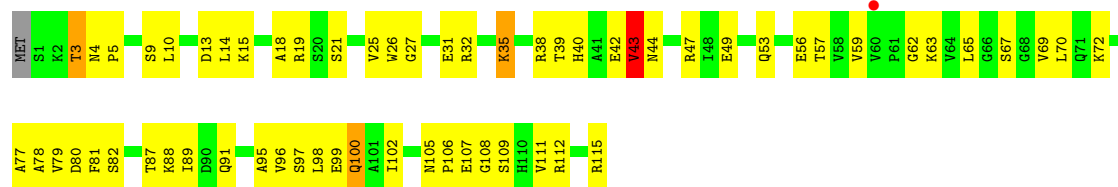




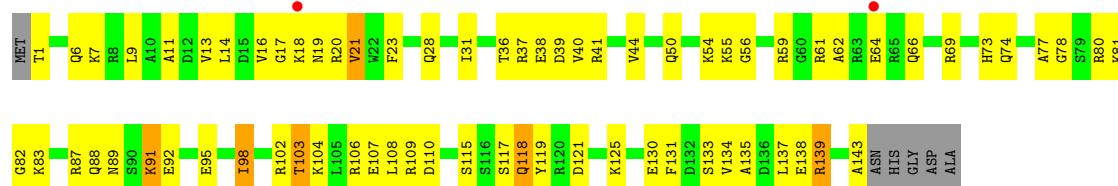
• Molecule 14: 50S ribosomal protein L18P



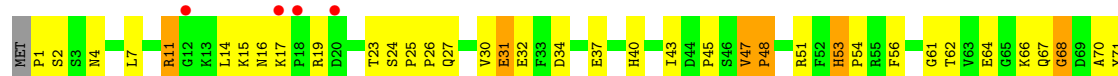
• Molecule 15: 50S ribosomal protein L18e

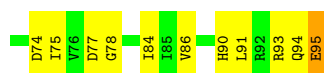


• Molecule 16: 50S ribosomal protein L19e



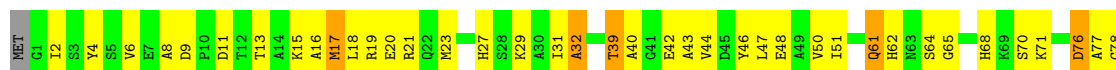
• Molecule 17: 50S ribosomal protein L21e





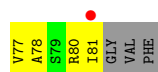
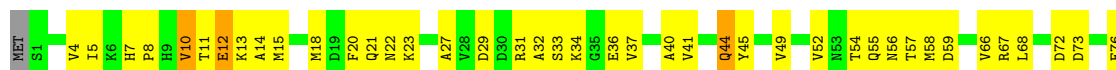
• Molecule 18: 50S ribosomal protein L22P

Chain R: 46% 46% 5%



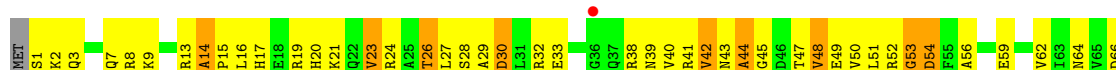
• Molecule 19: 50S ribosomal protein L23P

Chain S: 42% 49% 5%



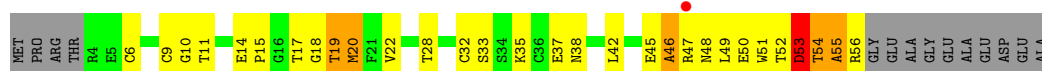
• Molecule 20: 50S ribosomal protein L24P

Chain T: 37% 52% 10%



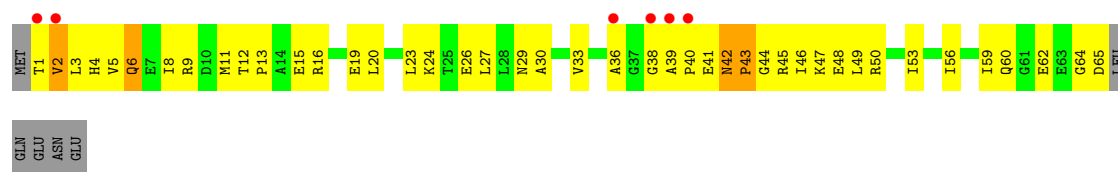
• Molecule 21: 50S ribosomal protein L24e

Chain U: 34% 36% 7% 21%



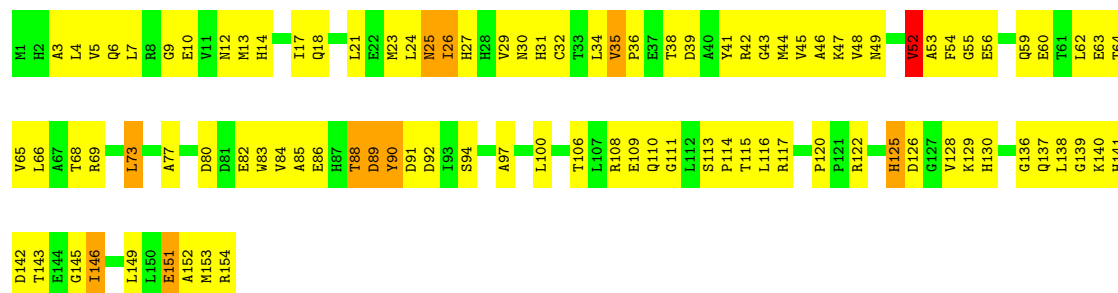
• Molecule 22: 50S ribosomal protein L29P

Chain V: 31% 55% 6% 8%



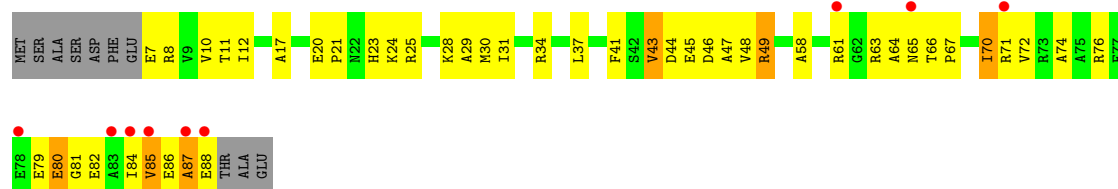
• Molecule 23: 50S ribosomal protein L30P

Chain W: 36% 56% 6%



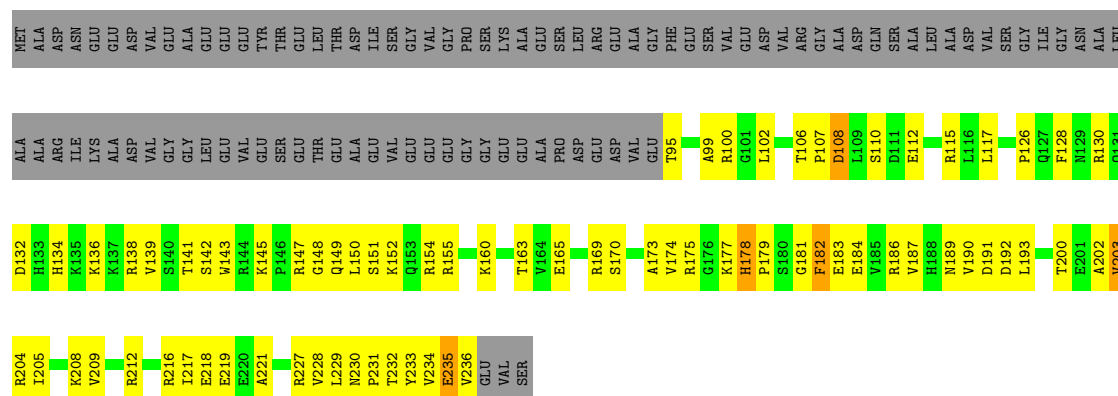
• Molecule 24: 50S ribosomal protein L31e

Chain X: 10% 39% 43% 7% 11%



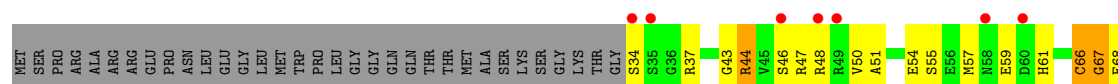
• Molecule 25: 50S ribosomal protein L32e

Chain Y: 28% 30% 41%



• Molecule 26: 50S ribosomal protein L37Ae

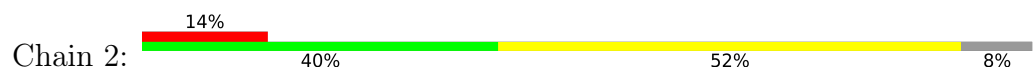
Chain Z: 8% 28% 31% 37%



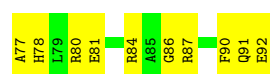
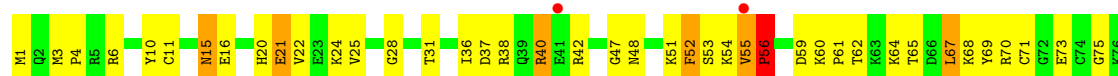
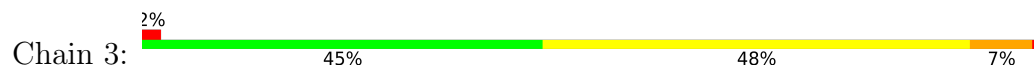
• Molecule 27: 50S ribosomal protein L37e



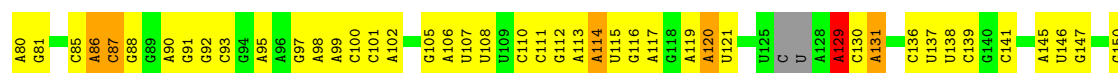
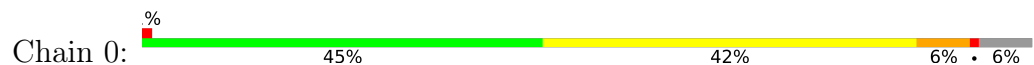
• Molecule 28: 50S ribosomal protein L39e



• Molecule 29: 50S ribosomal protein L44E

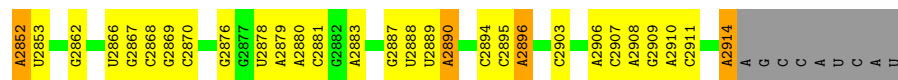


• Molecule 30: 50S RIBOSOMAL RNA

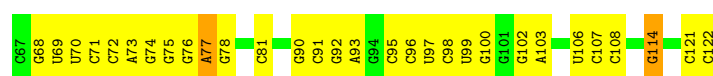
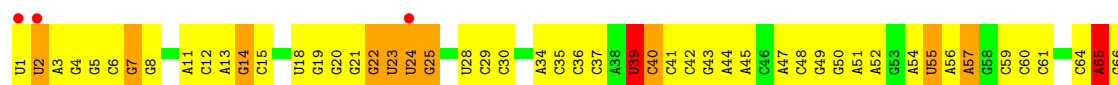


U1506	C1396	A1317	C1238	U1170	A1081	A	A907	C892	C726	U645	A566	C483	G314
C1507	U1406	A1318	GL239	A1171	A1086	G	A912	U823	C727	G646	U567	A484	G315
C1508	A1406	A1321		G1087	G1087	U		G824	C728		G588	A485	A316
C1513	A1407	G1322	C1243	A1174	A1088	C	U919	G830	G729	G652		A486	A317
C1514	U1408		C1245	A1175		G	U920	G835	U731	U653	A575	G487	U318
A1515	G1409	G1325	C1246	C1176	G1093	C	G921	U836	C732				
U1516	G1410		A1247	A1177	G1094	A	A922	U835					
U1519	G1415	A1328	A1248	G1178	U1095	C	C923	C839	C735	G656	C578	C491	C323
C1521	G1416		U1249	U1179	U1096	C999	C924	U840	C736	G657	A580	C492	G324
A1522	U1417		C1250	A1181	A1097	C	C925	U841	A737	G658	G581	U493	U325
C1523	U1418			C1182	A1098	C	A926	A844	C738	G661	U582	A495	G326
U1524	C1420		G1258	C1183	G1100	U1001	C936	A844		U662	C583	A497	A327
G1525	C1421		A1259	C1184		G1002	C937			C663	U584	A498	U328
A1526	G1340		G1260	U1185	C1103	U1003	C938	G854	C741	G664		G499	A329
C1527	A1341		A1261	C1186	C1104	A1006	G939	U855			G588	G500	G333
A1528	C1342		C1262	U1187		A1007	G940	U856	G744	G665	U589	G506	G334
G1529	C1343		C1263	A1188	U1109	C1008	G941	G857	G745		A590	A507	U335
	C1344		U1264	A1189	G1110		U942	U858	A746	G668	A591	A507	A337
	A1345			G1190		G1021	C943	C859	G747	G689	A592	A508	C338
A1533	G1433		C1267	A1191	A1114	A1022	G944	U862	A750	G671		A509	A339
C1534	G1445		C1268	A1192	U1115	A1025	U945	U863	G752	C677	G600	U510	C342
	U1446		G1269	A1193	U1116	U1026	C946	G863		G678	G601	A513	C343
G1545	U1447		U1270	A1194	A1117	C1027	U947				A602	G514	C344
C1546			A1271	G1195	A1118	G1027	G948	A867	C757	G681	A603	G514	G345
A1547	C1451			C1196	G1119	U1028	U949	G868	A758		G604	G518	U346
U1548	G1452		C1277	U1198	U1120	U1029	G950	G869	C759	A686	C605	A519	U347
			C1278	U1199	G1121	U1030	A951	G870		G687	U611	A520	C348
G1552	C1456		A1278	A1199		G1031	G952	G871	C764	G688	U612	A521	U349
	U1457		U1279	A1200	U1130	A1032	G953	U872	G765	G689	C613	U522	G350
G1555	A1458		A1280	C1201	G1131	C1033				G690	U614	U522	A351
				C1202	A1132	G1034	G956	A875	G772				A352
C1558	U1461		A1287	G1203	G1135	U1041	A957	A876	C773	A694	G615	C530	G353
A1559	C1462		U1288	C1204	U1136	U1042	G958	G877	A774		U616	A532	C355
U	U1463		C1289	U1205		C1043	C959	G878	G775	C696	U619	G535	G358
C1561	C1464		U1290	U1206	U1139	U1044	A961	C879	A776	G697	A620	A536	U359
C1562			A1291	A1207	U1140	G1045	C962	C880	U777	A698	C621	A536	A360
G1563			G1292	C1208	C1141			C881		C699	G622	A536	C361
	A1471		U1293	C1209	U1141	C1051	G969	A882	A790	C699	U623	C538	G362
C1566	C1472		C1365	G1210	C1142	U1052	U970	C883	A791	C695	U624	C539	C363
G1567	C1473		A1294	G1211		G1053		C884	G792	U701	U625	A540	U364
	C1474		C1367	C1212	U1149		U	G885	A793	G702	U626	C541	G365
A1573	U1475		U1368	C1213	U1150	U1056	G	A886		G703	U626	A542	U366
C1574	C1477		G1298	G1214	G1151	U1066	U	G887	A797	G704	G627	A542	U366
C1575			G1299	A1215	A1152	A1067	U	U888	A806	C705	A628	G543	U366
G1576	A1482		C1300	G1216	C1153	A1058	C	C889	A807	G706	A629	G544	A459
U1577	C1483		G1302	G1217		C959	C	C890	A807	C707	A630	G545	C368
	G1484		C1303	U1218	G1158	C1060	G	G891	A808	A708	A631	G553	G369
			C1304	U1219	G1159	G892	C	G892	G809	G709	A632	G554	G370
G1586	G1490		C1305	U1220	G1160	C893	C	C893		G710		G554	U371
U1587	A1496		U1306	G1221	A1161	A894	U	A894	A812	G711	A635	U559	A372
G1588	G1497		A1307	C1228	G1162	A1067	C	A895	C813		G636	C637	C376
A1590	U1308		U1309	U1229	G1163	A1067	C	C896	U	U714	C638	U559	C377
A1591	A1501		U1310	A1230	U1164	G1072	G	G896	G816	G716	A639	U560	A378
C1592	A1502				G1165	G1077	A	G902	C817		G640	G561	G379
C1593	U1503		U1314	U1234	A1166	A1078	G	U903	A818	C719	G641	A562	A380
C1594	G1595		G1315		C1167	A1078	A	U904	A819			C563	G381
U1596	U1505		G1316	U1237	C1168	A1079	G	C905	G820	G722		G564	U392
					U1169	C1080	G	C906	U821			A565	





• Molecule 31: 5S RIBOSOMAL RNA



• Molecule 32: RNA (5'-R(*C*CP*A)-3')



• Molecule 33: RNA (5'-R(*CP*CP*(8AN))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	210.79Å 297.78Å 572.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 2.95 49.82 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.82-2.95) 89.7 (49.82-2.95)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0, REFMAC	Depositor
R, R_{free}	0.198 , 0.255 0.194 , 0.249	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99194	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% 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: ACA, UR3, NA, OMG, PSU, K, 1MA, CD, MG, OMU, 8AN, CL, SR

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	0.48	0/1784	1.01	8/2403 (0.3%)
2	B	0.45	0/2687	1.08	25/3644 (0.7%)
3	C	0.47	0/1883	1.02	13/2547 (0.5%)
4	D	0.40	0/1109	0.91	2/1493 (0.1%)
5	E	0.42	0/1380	0.92	4/1875 (0.2%)
6	F	0.43	0/899	0.91	1/1219 (0.1%)
7	G	0.38	0/241	0.81	0/324
8	H	0.43	0/1300	0.98	6/1738 (0.3%)
9	I	0.36	0/524	0.84	1/711 (0.1%)
10	J	0.45	0/1134	0.95	4/1525 (0.3%)
11	K	0.48	0/1002	1.04	5/1346 (0.4%)
12	L	0.40	0/1128	1.00	3/1504 (0.2%)
13	M	0.48	1/1580 (0.1%)	0.94	3/2111 (0.1%)
14	N	0.41	0/1472	1.09	15/1994 (0.8%)
15	O	0.46	0/872	1.01	5/1176 (0.4%)
16	P	0.46	0/1145	0.94	4/1524 (0.3%)
17	Q	0.44	0/747	1.12	11/1001 (1.1%)
18	R	0.50	0/1170	0.98	5/1574 (0.3%)
19	S	0.42	0/646	0.89	2/870 (0.2%)
20	T	0.42	0/956	1.03	7/1284 (0.5%)
21	U	0.45	0/417	0.99	1/562 (0.2%)
22	V	0.39	0/502	0.96	2/675 (0.3%)
23	W	0.49	0/1217	1.28	6/1650 (0.4%)
24	X	0.47	0/662	1.01	2/890 (0.2%)
25	Y	0.47	0/1146	1.03	7/1536 (0.5%)
26	Z	0.39	0/582	0.95	0/776
27	1	0.48	0/438	0.97	2/578 (0.3%)
28	2	0.46	0/401	0.87	0/529
29	3	0.48	0/769	1.01	7/1019 (0.7%)
30	0	0.40	1/65948 (0.0%)	0.62	27/102852 (0.0%)
31	9	0.38	0/2894	0.62	2/4509 (0.0%)
32	5	0.46	0/43	0.71	0/65

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	6	0.49	0/40	0.80	0/60
All	All	0.41	2/98718 (0.0%)	0.75	180/147564 (0.1%)

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
23	W	0	1
30	0	0	39
31	9	0	2
All	All	0	42

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	1942	A	O3'-P	-5.29	1.53	1.61
13	M	13	LYS	C-O	-5.06	1.17	1.24

All (180) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	52	VAL	CG1-CB-CG2	26.24	168.52	110.80
23	W	52	VAL	CA-CB-CG2	-20.48	75.59	110.40
20	T	54	ASP	N-CA-C	-11.31	99.13	113.16
14	N	163	PHE	N-CA-C	-11.10	97.02	112.45
2	B	157	LYS	N-CA-C	-9.08	102.59	114.31
29	3	55	VAL	CA-C-N	9.07	131.18	119.84
29	3	55	VAL	C-N-CA	9.07	131.18	119.84
1	A	222	GLY	N-CA-C	-8.96	103.99	113.58
2	B	82	VAL	N-CA-C	8.72	120.56	110.62
18	R	141	VAL	N-CA-C	7.89	119.85	108.48
2	B	242	TRP	N-CA-C	-7.88	102.77	111.36
12	L	145	LEU	N-CA-C	-7.79	102.79	111.28
19	S	27	ALA	N-CA-C	-7.76	97.04	109.76
24	X	12	ILE	N-CA-C	7.71	114.58	107.56
17	Q	17	LYS	N-CA-C	-7.58	100.53	109.93
30	0	1942	A	C5'-C4'-C3'	7.50	127.25	116.00
13	M	36	ALA	N-CA-C	-7.39	104.39	113.41
12	L	7	GLN	N-CA-C	7.37	120.25	111.33
2	B	222	LYS	N-CA-C	-7.27	101.15	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	ALA	N-CA-C	7.14	118.64	109.72
8	H	25	GLY	N-CA-C	-7.00	105.14	115.72
25	Y	202	ALA	N-CA-C	-6.90	99.44	110.14
17	Q	47	VAL	N-CA-C	6.90	114.38	107.55
14	N	51	GLY	CA-C-N	6.84	126.47	119.56
14	N	51	GLY	C-N-CA	6.84	126.47	119.56
14	N	42	HIS	N-CA-C	6.83	120.26	109.81
2	B	175	LEU	N-CA-C	-6.82	103.93	111.36
30	0	834	G	C2'-C3'-O3'	-6.82	103.47	113.70
30	0	2291	A	N9-C1'-C2'	6.75	122.13	112.00
17	Q	53	HIS	CA-C-N	6.70	128.22	119.84
17	Q	53	HIS	C-N-CA	6.70	128.22	119.84
1	A	48	ASP	CA-C-N	6.70	126.95	119.32
1	A	48	ASP	C-N-CA	6.70	126.95	119.32
25	Y	143	TRP	N-CA-C	6.61	119.87	109.96
22	V	42	ASN	CA-C-N	6.57	128.06	119.84
22	V	42	ASN	C-N-CA	6.57	128.06	119.84
18	R	137	ASN	N-CA-C	6.54	120.27	110.14
30	0	1941	A	O3'-P-O5'	6.52	113.78	104.00
12	L	144	ASP	N-CA-C	-6.51	104.26	111.36
11	K	14	LYS	N-CA-C	-6.49	100.22	109.96
25	Y	230	ASN	CA-C-N	6.45	126.41	120.03
25	Y	230	ASN	C-N-CA	6.45	126.41	120.03
2	B	213	GLY	CA-C-N	6.44	125.93	119.24
2	B	213	GLY	C-N-CA	6.44	125.93	119.24
13	M	89	THR	N-CA-C	6.41	120.19	112.38
21	U	53	ASP	N-CA-C	-6.40	104.57	112.38
2	B	90	THR	CA-C-N	6.39	126.08	119.82
2	B	90	THR	C-N-CA	6.39	126.08	119.82
30	0	2726	U	N1-C1'-C2'	6.34	121.51	112.00
29	3	40	ARG	N-CA-C	-6.31	104.03	111.03
4	D	15	GLU	CA-C-N	6.31	127.72	119.84
4	D	15	GLU	C-N-CA	6.31	127.72	119.84
30	0	2291	A	C4'-C3'-O3'	-6.28	103.58	113.00
3	C	188	ARG	N-CA-C	6.24	113.83	108.22
1	A	171	LYS	N-CA-C	6.24	119.35	109.50
1	A	133	ARG	N-CA-C	-6.16	105.41	113.17
15	O	100	GLN	N-CA-C	-6.16	104.19	111.03
10	J	71	TYR	CA-C-N	6.15	126.12	119.78
10	J	71	TYR	C-N-CA	6.15	126.12	119.78
20	T	89	ARG	CA-C-N	6.14	126.08	119.76
20	T	89	ARG	C-N-CA	6.14	126.08	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	921	G	N9-C1'-C2'	6.13	121.19	112.00
2	B	22	GLU	N-CA-C	-6.12	105.07	112.54
16	P	103	THR	N-CA-C	-6.12	104.52	111.07
17	Q	47	VAL	CA-C-N	6.09	127.46	119.84
17	Q	47	VAL	C-N-CA	6.09	127.46	119.84
27	1	51	GLN	N-CA-C	-6.09	105.61	113.16
30	0	1701	A	C5'-C4'-C3'	6.06	124.29	115.20
30	0	1979	G	N9-C1'-C2'	6.05	121.07	112.00
3	C	219	ASN	N-CA-C	6.04	118.66	109.95
10	J	67	ASN	N-CA-C	-6.04	105.17	112.54
29	3	81	GLU	N-CA-C	-6.03	102.57	110.53
11	K	82	ARG	CA-C-N	6.02	127.37	119.84
11	K	82	ARG	C-N-CA	6.02	127.37	119.84
8	H	93	PHE	CA-C-N	6.00	127.35	119.84
8	H	93	PHE	C-N-CA	6.00	127.35	119.84
3	C	192	ILE	N-CA-C	5.95	117.25	109.58
17	Q	4	ASN	N-CA-C	5.95	117.58	110.44
9	I	100	VAL	N-CA-C	-5.92	108.08	113.71
17	Q	2	SER	N-CA-C	-5.87	106.66	113.88
16	P	110	ASP	N-CA-C	-5.87	105.02	111.82
30	0	920	C	C2'-C3'-O3'	-5.85	104.93	113.70
14	N	3	GLY	CA-C-N	5.83	125.37	119.19
14	N	3	GLY	C-N-CA	5.83	125.37	119.19
25	Y	110	SER	N-CA-C	-5.80	102.83	110.43
3	C	90	HIS	CA-C-N	5.76	126.32	120.38
3	C	90	HIS	C-N-CA	5.76	126.32	120.38
30	0	1504	A	N9-C1'-C2'	5.76	120.64	112.00
14	N	13	ARG	N-CA-C	-5.74	104.47	112.45
2	B	329	TYR	N-CA-C	5.74	117.13	108.46
11	K	78	LYS	CA-C-N	5.73	125.69	119.78
11	K	78	LYS	C-N-CA	5.73	125.69	119.78
2	B	154	VAL	CA-C-N	5.73	127.00	119.84
2	B	154	VAL	C-N-CA	5.73	127.00	119.84
2	B	265	LEU	N-CA-C	5.73	117.72	110.33
14	N	169	PRO	N-CA-C	-5.70	106.26	114.18
15	O	43	VAL	N-CA-C	5.70	116.68	108.48
30	0	1819	G	C5'-C4'-C3'	5.69	124.53	116.00
30	0	2301	A	N9-C1'-C2'	5.68	120.53	112.00
18	R	17	MET	N-CA-C	5.68	117.91	108.99
23	W	113	SER	CA-C-N	5.67	126.93	119.84
23	W	113	SER	C-N-CA	5.67	126.93	119.84
30	0	2664	A	N9-C1'-C2'	5.65	120.48	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	205	ARG	N-CA-C	5.63	117.87	111.11
30	O	2313	C	C5'-C4'-C3'	5.59	124.39	116.00
10	J	47	THR	N-CA-C	5.58	118.74	110.48
2	B	217	ARG	N-CA-C	5.58	118.13	111.71
30	O	1979	G	C2'-C3'-O3'	5.53	122.00	113.70
8	H	53	ILE	N-CA-C	5.52	116.05	107.99
2	B	187	GLU	N-CA-C	5.52	117.46	108.63
15	O	35	LYS	CA-C-N	5.51	126.73	119.84
15	O	35	LYS	C-N-CA	5.51	126.73	119.84
2	B	57	GLU	CA-C-N	5.51	125.12	119.56
2	B	57	GLU	C-N-CA	5.51	125.12	119.56
8	H	116	MET	N-CA-C	-5.49	106.25	113.17
18	R	123	GLN	N-CA-C	5.47	118.22	110.50
2	B	111	ARG	N-CA-C	-5.46	106.39	113.16
3	C	186	TYR	N-CA-C	5.45	118.53	110.46
31	9	65	A	N9-C1'-C2'	5.45	120.18	112.00
23	W	25	ASN	N-CA-C	5.45	119.09	111.90
14	N	176	ARG	N-CA-C	-5.43	105.36	111.28
14	N	161	GLY	N-CA-C	-5.43	105.14	112.14
1	A	175	LYS	N-CA-C	-5.41	105.28	111.07
30	O	2673	U	N1-C1'-C2'	5.41	120.11	112.00
14	N	14	ARG	N-CA-C	-5.40	105.29	111.07
16	P	131	PHE	N-CA-C	5.40	117.21	108.41
30	O	1877	G	N9-C1'-C2'	5.40	120.10	112.00
30	O	1504	A	C4'-C3'-O3'	-5.39	104.92	113.00
5	E	157	LYS	N-CA-C	5.37	116.80	109.18
24	X	17	ALA	N-CA-C	-5.36	106.72	113.20
25	Y	173	ALA	N-CA-C	5.35	118.90	112.38
30	O	1979	G	C4'-C3'-O3'	-5.34	104.99	113.00
15	O	69	VAL	N-CA-C	5.33	115.57	108.11
3	C	167	ASP	N-CA-C	-5.31	105.61	111.71
30	O	1078	A	N9-C1'-C2'	5.29	119.93	112.00
19	S	10	VAL	N-CA-C	5.27	115.66	107.28
20	T	3	GLN	CA-C-N	5.27	125.33	119.32
20	T	3	GLN	C-N-CA	5.27	125.33	119.32
5	E	156	ASP	N-CA-C	5.27	118.49	111.75
2	B	303	GLY	CA-C-N	5.26	126.54	120.85
2	B	303	GLY	C-N-CA	5.26	126.54	120.85
13	M	140	ALA	N-CA-C	-5.26	105.96	112.38
16	P	118	GLN	N-CA-C	-5.26	106.01	112.90
1	A	149	ASP	N-CA-C	-5.26	101.91	109.48
8	H	91	ARG	N-CA-C	5.25	119.17	112.87

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	95	VAL	N-CA-C	5.25	114.31	106.85
30	0	2526	C	N1-C1'-C2'	5.25	119.88	112.00
14	N	133	ASP	N-CA-C	5.21	119.92	111.37
5	E	91	PHE	N-CA-C	5.21	116.96	109.04
30	0	2611	G	C4'-C3'-O3'	-5.21	105.19	113.00
17	Q	68	GLY	N-CA-C	-5.20	102.33	111.80
30	0	1700	C	C2'-C3'-O3'	-5.20	105.90	113.70
29	3	54	LYS	CA-C-N	-5.18	118.82	123.33
29	3	54	LYS	C-N-CA	-5.18	118.82	123.33
20	T	14	ALA	CA-C-N	5.18	125.18	119.89
20	T	14	ALA	C-N-CA	5.18	125.18	119.89
14	N	152	GLU	N-CA-C	-5.17	105.65	111.28
2	B	143	ILE	N-CA-C	-5.16	102.03	108.84
3	C	80	VAL	CA-C-N	5.15	125.19	119.32
3	C	80	VAL	C-N-CA	5.15	125.19	119.32
30	0	129	A	C2'-C3'-O3'	5.14	121.41	113.70
17	Q	24	SER	CA-C-N	5.14	125.67	120.38
17	Q	24	SER	C-N-CA	5.14	125.67	120.38
2	B	151	VAL	CA-C-N	5.14	124.64	119.19
2	B	151	VAL	C-N-CA	5.14	124.64	119.19
3	C	18	LEU	CA-C-N	5.13	125.13	119.90
3	C	18	LEU	C-N-CA	5.13	125.13	119.90
30	0	2615	U	N1-C1'-C2'	5.12	119.69	112.00
31	9	39	U	N1-C1'-C2'	5.10	119.65	112.00
29	3	67	LEU	N-CA-C	5.09	117.15	109.41
27	1	19	CYS	N-CA-C	5.08	117.04	108.96
23	W	89	ASP	N-CA-C	-5.08	106.77	113.17
2	B	193	ILE	N-CA-C	5.06	116.00	111.90
6	F	79	GLN	N-CA-C	5.06	117.54	109.65
25	Y	178	HIS	N-CA-C	-5.06	102.67	110.01
30	0	2103	A	C2'-C3'-O3'	5.05	117.07	109.50
3	C	23	GLU	N-CA-C	-5.03	107.20	113.38
14	N	78	MET	CA-C-N	5.02	124.80	119.28
14	N	78	MET	C-N-CA	5.02	124.80	119.28
18	R	122	GLN	N-CA-C	-5.02	100.33	108.41

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	1078	A	Sidechain
30	0	1237	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
30	0	1309	U	Sidechain
30	0	1340	G	Sidechain
30	0	1358	A	Sidechain
30	0	1359	U	Sidechain
30	0	1380	U	Sidechain
30	0	1417	G	Sidechain
30	0	1635	U	Sidechain
30	0	1741	U	Sidechain
30	0	1819	G	Sidechain
30	0	1829	A	Sidechain
30	0	1855	G	Sidechain
30	0	1863	G	Sidechain
30	0	1877	G	Sidechain
30	0	1878	G	Sidechain
30	0	2043	U	Sidechain
30	0	2046	G	Sidechain
30	0	2065	C	Sidechain
30	0	2316	G	Sidechain
30	0	2478	U	Sidechain
30	0	2493	C	Sidechain
30	0	2503	A	Sidechain
30	0	2506	A	Sidechain
30	0	2543	G	Sidechain
30	0	2552	C	Sidechain
30	0	2557	U	Sidechain
30	0	2673	U	Sidechain
30	0	2781	U	Sidechain
30	0	2790	C	Sidechain
30	0	2840	A	Sidechain
30	0	333	G	Sidechain
30	0	471	G	Sidechain
30	0	518	G	Sidechain
30	0	63	U	Sidechain
30	0	688	A	Sidechain
30	0	722	G	Sidechain
30	0	877	G	Sidechain
30	0	888	U	Sidechain
31	9	65	A	Sidechain
31	9	90	G	Sidechain
23	W	90	TYR	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	1752	0	1764	168	0
2	B	2624	0	2530	233	0
3	C	1859	0	1811	159	0
4	D	1093	0	1083	109	0
5	E	1356	0	1264	87	0
6	F	889	0	841	72	0
7	G	240	0	231	34	0
8	H	1281	0	1290	89	0
9	I	518	0	495	71	0
10	J	1119	0	1096	91	0
11	K	993	0	1025	81	0
12	L	1117	0	1071	91	0
13	M	1557	0	1571	134	0
14	N	1444	0	1399	142	0
15	O	864	0	868	67	0
16	P	1135	0	1120	72	0
17	Q	734	0	726	50	0
18	R	1148	0	1119	86	0
19	S	640	0	600	38	0
20	T	949	0	922	91	0
21	U	410	0	364	38	0
22	V	499	0	511	52	0
23	W	1195	0	1135	126	0
24	X	653	0	651	52	0
25	Y	1130	0	1133	85	0
26	Z	572	0	529	38	0
27	1	431	0	426	44	0
28	2	396	0	413	30	0
29	3	754	0	726	58	0
30	0	59017	0	29809	1414	0
31	9	2595	0	1322	96	0
32	5	39	0	24	3	0
33	6	59	0	35	6	0
34	0	82	0	0	0	0
34	2	1	0	0	0	0
34	9	1	0	0	0	0
34	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	K	1	0	0	0	0
34	T	1	0	0	0	0
34	Y	1	0	0	0	0
35	0	6	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	4	0	0	4	0
35	L	2	0	0	2	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	1	0
35	Q	1	0	0	1	0
35	R	1	0	0	0	0
35	Y	2	0	0	0	0
36	0	87	0	0	1	0
36	1	2	0	0	0	0
36	3	3	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	2	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	T	2	0	0	0	0
36	Y	1	0	0	0	0
37	0	65	0	0	0	0
37	9	3	0	0	0	0
37	C	1	0	0	0	0
37	H	1	0	0	0	0
37	J	1	0	0	0	0
37	M	1	0	0	0	0
37	Q	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Z	1	0	0	0	0
39	0	2	0	0	0	0
40	6	11	0	8	0	0
41	6	8	0	6	0	0
42	0	5775	0	0	197	0
42	1	57	0	0	4	0
42	2	50	0	0	2	0
42	3	66	0	0	7	0
42	6	6	0	0	4	0
42	9	138	0	0	12	0
42	A	134	0	0	19	0
42	B	156	0	0	21	0
42	C	168	0	0	21	0
42	D	49	0	0	6	0
42	E	49	0	0	5	0
42	F	31	0	0	3	0
42	G	20	0	0	2	0
42	H	78	0	0	9	0
42	I	11	0	0	3	0
42	J	58	0	0	2	0
42	K	57	0	0	3	0
42	L	91	0	0	11	0
42	M	129	0	0	5	0
42	N	68	0	0	14	0
42	O	46	0	0	6	0
42	P	72	0	0	7	0
42	Q	52	0	0	3	0
42	R	89	0	0	5	0
42	S	35	0	0	1	0
42	T	42	0	0	5	0
42	U	29	0	0	3	0
42	V	16	0	0	2	0
42	W	75	0	0	10	0
42	X	31	0	0	5	0
42	Y	105	0	0	5	0
42	Z	25	0	0	6	0
All	All	99194	0	59918	3630	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 24.

All (3630) 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)
23:W:21:LEU:HD21	23:W:48:VAL:HG11	1.27	1.15
3:C:236:THR:HG22	3:C:239:ALA:H	1.00	1.13
36:O:8979:SR:SR	42:O:4399:HOH:O	0.84	1.13
6:F:58:GLU:HA	6:F:61:MET:HE2	1.29	1.11
14:N:37:ARG:HH12	31:9:6:C:H5''	1.10	1.09
30:O:870:G:H2'	30:O:871:G:H5''	1.30	1.08
14:N:37:ARG:NH1	31:9:6:C:H5''	1.69	1.07
31:9:76:G:H3'	31:9:77:A:H5''	1.29	1.07
10:J:52:GLN:HE22	30:O:1119:G:H2'	0.96	1.05
4:D:25:MET:HE2	4:D:41:LEU:HG	1.39	1.05
9:I:97:VAL:HG12	9:I:101:LYS:HE3	1.39	1.05
30:O:871:G:H5'	30:O:871:G:H8	1.17	1.05
6:F:91:VAL:HG12	6:F:92:GLY:H	1.18	1.05
30:O:1160:G:H5'	30:O:1161:A:H5'	1.39	1.04
2:B:36:PRO:HA	2:B:168:GLY:HA3	1.39	1.04
22:V:1:THR:HG23	22:V:2:VAL:H	1.18	1.04
10:J:52:GLN:NE2	30:O:1119:G:H2'	1.73	1.03
24:X:28:LYS:HD2	24:X:31:ILE:HD12	1.41	1.03
10:J:82:THR:HG23	30:O:1242:A:H5'	1.40	1.03
13:M:164:THR:HG22	13:M:166:ALA:H	1.18	1.03
11:K:29:LEU:HB3	11:K:55:VAL:HG11	1.41	1.03
30:O:871:G:H5'	30:O:871:G:C8	1.93	1.02
1:A:153:ARG:HB2	1:A:153:ARG:HH11	1.18	1.02
30:O:541:C:H2'	30:O:542:A:H5''	1.42	1.02
11:K:10:GLN:NE2	11:K:10:GLN:H	1.58	1.01
3:C:1:MET:HG2	3:C:2:GLN:H	1.25	0.99
1:A:191:GLY:HA2	1:A:194:MET:HE2	1.42	0.99
16:P:115:SER:H	16:P:118:GLN:HE21	1.05	0.98
24:X:43:VAL:HG11	24:X:82:GLU:HA	1.42	0.98
10:J:19:MET:HE3	10:J:132:LEU:HD11	1.41	0.98
25:Y:189:ASN:HA	25:Y:217:ILE:HD11	1.45	0.98
1:A:179:MET:HA	1:A:179:MET:HE3	1.44	0.97
30:O:2586:U:H3	30:O:2592:G:H22	1.12	0.96
23:W:137:GLN:HE21	23:W:141:HIS:HE1	1.06	0.96
30:O:542:A:H5'	30:O:542:A:H8	1.29	0.96
11:K:74:VAL:HG13	11:K:113:ILE:HG23	1.48	0.96
2:B:36:PRO:HG3	2:B:169:GLY:H	1.30	0.95
1:A:100:PRO:HG2	1:A:103:VAL:HG21	1.43	0.95
30:O:2717:C:H2'	30:O:2718:C:H5''	1.47	0.95
14:N:144:GLY:O	14:N:147:ILE:HG22	1.66	0.95
30:O:1451:C:H5'	30:O:1505:U:C5	2.01	0.95
3:C:115:LEU:HD13	3:C:223:LEU:HD21	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:83:LEU:HD13	14:N:175:LEU:HD23	1.44	0.94
4:D:57:THR:HG23	4:D:63:ILE:HA	1.50	0.94
4:D:172:VAL:HG12	4:D:173:GLU:H	1.32	0.94
31:9:56:A:H2'	31:9:57:A:H5''	1.49	0.93
29:3:70:ARG:HG2	29:3:77:ALA:HB2	1.51	0.93
30:0:541:C:C2'	30:0:542:A:H5''	1.97	0.93
1:A:211:LYS:HB3	1:A:212:PRO:HD2	1.49	0.93
30:0:2506:A:HO2'	30:0:2507:G:H8	1.04	0.93
5:E:23:GLU:HG2	5:E:28:SER:HB3	1.49	0.92
3:C:236:THR:HG22	3:C:239:ALA:N	1.85	0.92
18:R:8:ALA:HB1	18:R:13:THR:HG21	1.50	0.91
22:V:12:THR:HG22	22:V:15:GLU:HG3	1.52	0.91
10:J:70:PHE:CE1	30:0:2676:C:H4'	2.04	0.91
18:R:39:THR:HB	18:R:42:GLU:HG3	1.50	0.90
2:B:179:LEU:O	2:B:183:GLU:HG2	1.71	0.90
30:0:506:G:H22	30:0:509:A:H5'	1.34	0.90
23:W:5:VAL:HG11	23:W:153:MET:HE1	1.54	0.90
2:B:206:THR:HG21	30:0:2716:G:H5''	1.51	0.90
8:H:30:LYS:H	8:H:62:HIS:HD2	1.17	0.89
30:0:1667:A:H8	30:0:1667:A:H5'	1.36	0.88
4:D:75:LEU:HD22	4:D:79:MET:HB3	1.53	0.88
11:K:39:GLY:HA2	42:K:4183:HOH:O	1.73	0.88
3:C:233:THR:HG22	3:C:234:VAL:H	1.38	0.88
11:K:87:ARG:HB2	21:U:19:THR:HG23	1.53	0.88
30:0:2005:G:H3'	30:0:2005:G:OP2	1.74	0.88
11:K:10:GLN:H	11:K:10:GLN:HE21	1.19	0.88
3:C:236:THR:HG21	42:C:8580:HOH:O	1.74	0.88
18:R:99:ALA:HB1	18:R:109:MET:HE1	1.56	0.88
5:E:81:GLU:HG2	5:E:134:SER:HB3	1.54	0.87
13:M:164:THR:HG22	13:M:166:ALA:N	1.89	0.87
30:0:2291:A:C8	30:0:2309:C:H5'	2.09	0.87
2:B:162:MET:HE3	2:B:310:ARG:HD2	1.56	0.87
5:E:15:GLN:HG2	5:E:19:ASP:O	1.74	0.87
1:A:153:ARG:HH11	1:A:153:ARG:CB	1.86	0.87
15:O:3:THR:HB	30:0:656:G:H5'	1.57	0.87
3:C:27:ARG:HG2	3:C:27:ARG:HH11	1.37	0.86
21:U:9:CYS:HA	21:U:52:THR:HG23	1.57	0.86
3:C:72:LYS:HG2	3:C:77:ALA:HA	1.56	0.86
26:Z:70:ARG:HD2	26:Z:83:TYR:HB2	1.57	0.86
5:E:3:VAL:HG22	5:E:49:ILE:HB	1.56	0.86
11:K:98:VAL:CG1	11:K:102:GLU:HA	2.05	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:106:GLY:HA2	18:R:109:MET:HE3	1.56	0.86
30:0:1451:C:H5'	30:0:1505:U:H5	1.34	0.86
30:0:1559:A:H1'	42:0:6702:HOH:O	1.74	0.86
30:0:870:G:C2'	30:0:871:G:H5''	2.05	0.86
15:O:32:ARG:HE	15:O:35:LYS:HD3	1.40	0.86
16:P:103:THR:HA	16:P:106:ARG:NH1	1.91	0.85
30:0:681:G:N3	30:0:681:G:H5'	1.91	0.85
1:A:109:GLU:HG2	1:A:116:GLY:H	1.42	0.85
13:M:134:ILE:HG23	13:M:141:ILE:HD13	1.56	0.85
23:W:13:MET:HE3	23:W:17:ILE:HG22	1.57	0.85
25:Y:151:SER:HB3	25:Y:154:ARG:HB3	1.58	0.85
30:0:545:G:H5'	30:0:545:G:H8	1.40	0.85
4:D:28:GLY:HA2	4:D:69:ILE:HG23	1.58	0.85
13:M:24:GLN:NE2	13:M:27:ARG:HH11	1.73	0.85
23:W:88:THR:HG23	23:W:110:GLN:HB3	1.55	0.85
29:3:25:VAL:HG22	29:3:68:LYS:HG3	1.58	0.85
10:J:70:PHE:HE1	30:0:2676:C:H4'	1.40	0.84
12:L:55:GLN:HA	12:L:58:GLN:HE21	1.38	0.84
19:S:10:VAL:HG11	22:V:36:ALA:HB2	1.59	0.84
20:T:28:SER:HA	20:T:97:ARG:HD3	1.59	0.84
1:A:153:ARG:HB2	1:A:153:ARG:NH1	1.93	0.84
30:0:2717:C:C2'	30:0:2718:C:H5''	2.07	0.84
24:X:49:ARG:HG3	24:X:49:ARG:O	1.75	0.84
28:2:41:HIS:H	28:2:45:ASN:HD22	1.20	0.84
30:0:2812:A:H2	30:0:2814:A:H62	1.22	0.84
15:O:42:GLU:HB2	42:O:2176:HOH:O	1.77	0.84
30:0:1474:C:H6	30:0:1474:C:H5'	1.41	0.84
31:9:29:C:H2'	31:9:30:C:H5'	1.59	0.84
2:B:42:ALA:HB2	2:B:162:MET:HE1	1.59	0.84
30:0:1603:A:H5'	30:0:1605:G:O4'	1.77	0.84
6:F:12:LEU:HD21	6:F:111:ILE:HG23	1.58	0.83
30:0:1116:U:O2'	30:0:1118:A:H2	1.61	0.83
42:Z:8705:HOH:O	30:0:1886:A:H4'	1.78	0.83
12:L:35:ARG:HB2	12:L:35:ARG:HH11	1.41	0.83
9:I:112:LEU:HD11	30:0:1162:G:H1'	1.60	0.83
26:Z:54:GLU:HA	26:Z:57:MET:HE2	1.60	0.83
30:0:1160:G:C5'	30:0:1161:A:H5'	2.07	0.83
1:A:33:GLU:H	1:A:33:GLU:CD	1.86	0.83
14:N:164:ASP:CG	14:N:167:ASP:HA	2.04	0.83
32:5:75:C:H3'	32:5:76:A:H8	1.42	0.83
21:U:52:THR:HG22	21:U:54:THR:H	1.44	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1184:C:H1'	42:0:9264:HOH:O	1.79	0.83
6:F:58:GLU:CD	13:M:27:ARG:HH22	1.87	0.82
2:B:190:MET:HE2	2:B:194:PHE:CD1	2.14	0.82
6:F:91:VAL:HG12	6:F:92:GLY:N	1.94	0.82
14:N:113:SER:HB2	42:N:8857:HOH:O	1.79	0.82
29:3:6:ARG:NH1	29:3:21:GLU:HG3	1.94	0.82
11:K:32:ILE:HD11	11:K:56:SER:HB3	1.62	0.82
11:K:10:GLN:HE21	11:K:10:GLN:N	1.78	0.81
11:K:109:LEU:HD13	11:K:113:ILE:HD11	1.62	0.81
29:3:48:ASN:HD21	30:0:2468:A:H61	1.28	0.81
30:0:1116:U:HO2'	30:0:1118:A:H2	0.83	0.81
10:J:52:GLN:HG3	10:J:53:ILE:N	1.94	0.81
2:B:199:TYR:HE2	2:B:268:ARG:HB2	1.43	0.81
15:O:21:SER:OG	15:O:106:PRO:HB2	1.80	0.81
3:C:127:ARG:NH2	3:C:225:PRO:HG2	1.95	0.81
30:0:1679:C:H5'	42:0:3235:HOH:O	1.78	0.81
16:P:38:GLU:HA	16:P:41:ARG:HD2	1.63	0.81
27:1:20:ARG:HG2	30:0:111:C:O2'	1.81	0.81
9:I:73:LEU:HD12	9:I:107:LYS:NZ	1.96	0.81
30:0:271:C:H41	30:0:378:A:H2	1.27	0.81
4:D:54:ALA:HB2	4:D:69:ILE:HD12	1.62	0.81
18:R:18:LEU:HB2	18:R:143:VAL:HG12	1.63	0.80
30:0:877:G:H5'	30:0:878:G:OP1	1.81	0.80
23:W:6:GLN:HB2	23:W:26:ILE:HD12	1.63	0.80
7:G:23:ILE:HD13	7:G:67:LEU:HD23	1.63	0.80
3:C:225:PRO:O	30:0:1308:A:H4'	1.82	0.80
18:R:99:ALA:HB1	18:R:109:MET:CE	2.12	0.80
2:B:201:ASP:HB2	2:B:312:ARG:HD2	1.64	0.80
30:0:1625:U:H4'	42:0:5524:HOH:O	1.80	0.80
3:C:103:ASN:ND2	30:0:663:C:H5''	1.95	0.80
5:E:154:ILE:HD11	5:E:157:LYS:HB2	1.61	0.80
20:T:71:VAL:HG11	20:T:90:PRO:HB3	1.63	0.80
5:E:20:ILE:HD11	5:E:40:VAL:HG11	1.64	0.80
30:0:1160:G:H5'	30:0:1161:A:C5'	2.12	0.80
18:R:18:LEU:HD12	18:R:143:VAL:HG11	1.63	0.80
18:R:119:VAL:HG21	18:R:142:ASP:CG	2.07	0.80
6:F:34:ASN:HA	13:M:4:ALA:HB2	1.62	0.79
30:0:2420:G:O2'	30:0:2421:G:H5'	1.82	0.79
1:A:26:ASP:HB2	42:0:4577:HOH:O	1.81	0.79
8:H:30:LYS:H	8:H:62:HIS:CD2	2.01	0.79
18:R:114:VAL:HB	18:R:145:LEU:HD12	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:73:ASP:OD1	19:S:76:GLU:HG3	1.83	0.79
27:1:16:HIS:HD2	30:0:470:U:O2'	1.65	0.79
30:0:1377:C:H5'	30:0:1377:C:H6	1.45	0.79
18:R:132:ARG:NH2	30:0:2055:A:H4'	1.98	0.79
2:B:74:ILE:HD13	2:B:309:VAL:HG21	1.64	0.79
10:J:19:MET:HE1	10:J:78:ILE:HG22	1.63	0.79
21:U:14:GLU:O	21:U:17:THR:HB	1.83	0.78
27:1:21:ARG:HD2	27:1:37:CYS:SG	2.23	0.78
30:0:2042:U:H1'	42:0:9124:HOH:O	1.82	0.78
23:W:80:ASP:O	23:W:84:VAL:HG23	1.84	0.78
13:M:171:ARG:HD3	30:0:156:C:H5''	1.64	0.78
30:0:1205:U:H2'	30:0:1206:U:H5''	1.66	0.78
1:A:192:VAL:HG13	1:A:207:GLN:HB3	1.66	0.78
22:V:50:ARG:NH1	30:0:56:G:H5''	1.99	0.78
11:K:98:VAL:HG11	11:K:102:GLU:HA	1.64	0.78
16:P:115:SER:OG	16:P:118:GLN:HG3	1.84	0.78
25:Y:187:VAL:HG23	25:Y:192:ASP:HB2	1.63	0.78
12:L:92:ASP:HA	12:L:121:ILE:HB	1.66	0.78
30:0:2506:A:O2'	30:0:2507:G:H8	1.65	0.78
1:A:199:HIS:CD2	1:A:201:PHE:H	2.02	0.78
18:R:39:THR:HG23	18:R:107:GLU:O	1.83	0.78
16:P:59:ARG:NH2	16:P:66:GLN:HE22	1.82	0.77
2:B:162:MET:CE	2:B:310:ARG:HD2	2.14	0.77
14:N:40:ASN:HD21	31:9:28:U:H5''	1.49	0.77
14:N:40:ASN:ND2	31:9:28:U:H5''	2.00	0.77
1:A:179:MET:HA	1:A:179:MET:CE	2.14	0.77
20:T:9:LYS:HE3	20:T:13:ARG:CZ	2.15	0.77
2:B:275:GLY:O	2:B:291:ASP:HA	1.84	0.77
4:D:25:MET:HE2	4:D:41:LEU:CG	2.15	0.77
3:C:27:ARG:HG2	3:C:27:ARG:NH1	1.95	0.77
23:W:137:GLN:HE21	23:W:141:HIS:CE1	1.98	0.77
26:Z:44:ARG:HH21	30:0:1771:U:H5'	1.48	0.77
3:C:115:LEU:HD21	3:C:243:VAL:HG13	1.67	0.77
14:N:67:ALA:HA	14:N:71:TRP:HB3	1.67	0.76
1:A:66:ARG:HH11	1:A:66:ARG:HB2	1.50	0.76
22:V:12:THR:HG22	22:V:15:GLU:CG	2.16	0.76
4:D:135:VAL:HG21	4:D:139:TYR:CD1	2.19	0.76
7:G:64:ASN:O	7:G:68:GLU:HG3	1.86	0.76
8:H:32:ALA:HB3	8:H:69:ARG:HH12	1.49	0.76
10:J:75:PRO:HG2	10:J:105:LEU:HD21	1.65	0.76
22:V:1:THR:HG23	22:V:2:VAL:HG23	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:541:C:H2'	30:0:542:A:C5'	2.13	0.76
30:0:1835:U:H5	30:0:1840:A:N7	1.83	0.76
2:B:267:LYS:HD3	42:0:3465:HOH:O	1.85	0.76
1:A:191:GLY:HA2	1:A:194:MET:CE	2.14	0.76
10:J:131:THR:HG22	10:J:134:GLU:H	1.51	0.76
12:L:90:ARG:HA	12:L:119:THR:HB	1.67	0.76
30:0:2661:U:H3	30:0:2812:A:H62	1.32	0.76
3:C:236:THR:H	3:C:239:ALA:HB3	1.51	0.76
2:B:329:TYR:CE2	21:U:15:PRO:HG2	2.21	0.76
30:0:1116:U:H3	30:0:1246:A:H62	1.32	0.76
13:M:80:GLY:O	13:M:81:ARG:HD2	1.86	0.75
21:U:46:ALA:HB1	21:U:52:THR:HG21	1.69	0.75
30:0:871:G:H8	30:0:871:G:C5'	1.95	0.75
30:0:1118:A:H8	30:0:1119:G:H5''	1.51	0.75
32:5:75:C:H3'	32:5:76:A:C8	2.21	0.75
1:A:192:VAL:CG1	1:A:207:GLN:HB3	2.16	0.75
2:B:81:ALA:HB1	2:B:142:LEU:HD13	1.66	0.75
24:X:43:VAL:HG12	24:X:44:ASP:H	1.51	0.75
30:0:1730:G:H5'	30:0:1731:C:C5	2.22	0.75
1:A:203:GLY:HA2	42:0:3401:HOH:O	1.87	0.75
5:E:126:ILE:HB	5:E:131:LEU:HD23	1.69	0.75
30:0:2578:G:H5'	30:0:2578:G:H8	1.50	0.75
4:D:170:TYR:O	4:D:171:ASP:HB3	1.87	0.74
30:0:542:A:H5'	30:0:542:A:C8	2.18	0.74
22:V:1:THR:HG23	22:V:2:VAL:N	1.99	0.74
15:O:57:THR:O	15:O:111:VAL:HG23	1.87	0.74
3:C:180:SER:HB2	42:C:8643:HOH:O	1.86	0.74
4:D:105:SER:HB2	4:D:131:THR:HG23	1.70	0.74
11:K:87:ARG:HG3	30:0:2721:U:H4'	1.68	0.74
20:T:49:GLU:HB3	20:T:59:GLU:HG2	1.69	0.74
30:0:530:C:H4'	30:0:612:U:H4'	1.69	0.74
30:0:625:U:H3'	42:0:4150:HOH:O	1.87	0.74
9:I:101:LYS:O	9:I:105:GLU:HG3	1.87	0.74
22:V:12:THR:HG22	22:V:15:GLU:OE2	1.87	0.74
24:X:61:ARG:HB2	24:X:65:ASN:HB2	1.69	0.74
13:M:23:LEU:HD13	13:M:27:ARG:NH2	2.02	0.74
14:N:169:PRO:O	14:N:172:PHE:HB3	1.88	0.74
30:0:292:G:H2'	30:0:358:G:N2	2.02	0.74
30:0:1206:U:H5'	30:0:1206:U:H6	1.51	0.74
2:B:199:TYR:CE2	2:B:268:ARG:HB2	2.22	0.74
7:G:12:ILE:HG23	42:0:6301:HOH:O	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:19:MET:HE3	10:J:132:LEU:CD1	2.16	0.74
25:Y:189:ASN:CA	25:Y:217:ILE:HD11	2.16	0.74
4:D:25:MET:HE3	4:D:37:ALA:HB1	1.70	0.74
14:N:86:LEU:O	14:N:90:LEU:HG	1.88	0.74
14:N:119:GLN:O	14:N:123:ILE:HG13	1.87	0.74
23:W:149:LEU:HG	23:W:153:MET:HE2	1.68	0.74
31:9:14:G:H5'	31:9:14:G:H8	1.52	0.74
30:0:1878:G:H5'	42:0:5236:HOH:O	1.87	0.73
11:K:74:VAL:CG1	11:K:113:ILE:HG12	2.18	0.73
30:0:1452:G:H1'	35:0:8803:CL:CL	2.25	0.73
10:J:19:MET:HE2	10:J:79:PHE:HA	1.69	0.73
30:0:2073:G:H5''	42:0:4699:HOH:O	1.88	0.73
2:B:27:ASN:HD21	30:0:2807:U:P	2.11	0.73
6:F:63:ILE:HB	6:F:64:PRO:HD3	1.71	0.73
8:H:59:GLN:HE22	8:H:96:GLN:HG2	1.52	0.73
25:Y:169:ARG:HD2	30:0:1328:A:OP1	1.87	0.73
18:R:82:GLU:HG3	18:R:83:LYS:N	2.04	0.73
42:M:8871:HOH:O	30:0:381:G:H5''	1.89	0.73
30:0:1119:G:N2	30:0:1246:A:C2	2.56	0.73
8:H:19:ARG:HH12	30:0:1008:C:H5''	1.53	0.73
13:M:72:ALA:HB2	13:M:93:ARG:HG2	1.70	0.72
24:X:72:VAL:HG22	24:X:85:VAL:CG1	2.19	0.72
1:A:135:VAL:HA	1:A:150:PRO:HD3	1.70	0.72
4:D:57:THR:HA	42:D:5728:HOH:O	1.89	0.72
30:0:282:C:H1'	30:0:368:C:N4	2.04	0.72
31:9:50:G:H2'	31:9:51:A:C8	2.24	0.72
4:D:84:LEU:HA	4:D:87:ALA:HB3	1.71	0.72
5:E:93:MET:HE1	5:E:165:GLY:H	1.54	0.72
14:N:110:THR:HB	14:N:113:SER:OG	1.89	0.72
14:N:112:GLY:HA2	14:N:137:ALA:H	1.54	0.72
18:R:39:THR:HB	18:R:42:GLU:CG	2.18	0.72
10:J:77:GLY:HA2	10:J:80:LYS:H	1.54	0.72
10:J:93:ARG:HB3	10:J:93:ARG:HH11	1.54	0.72
25:Y:126:PRO:HG2	25:Y:128:PHE:CE1	2.24	0.72
30:0:78:G:N2	30:0:78:G:N3	2.37	0.72
20:T:2:LYS:HG2	30:0:447:A:OP1	1.90	0.72
30:0:1118:A:H62	30:0:1244:U:H3	1.38	0.72
12:L:143:THR:HG22	12:L:145:LEU:H	1.55	0.72
27:1:1:THR:HA	42:1:435:HOH:O	1.89	0.72
30:0:558:C:H2'	30:0:559:U:H5''	1.71	0.72
28:2:41:HIS:HD2	28:2:44:ARG:H	1.35	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1973:A:H5'	30:0:1973:A:H8	1.55	0.72
2:B:140:LEU:HA	42:B:9050:HOH:O	1.90	0.72
30:0:855:U:H3'	42:0:4510:HOH:O	1.89	0.71
4:D:22:VAL:HG22	4:D:74:THR:HG22	1.71	0.71
6:F:36:THR:HG23	6:F:97:ALA:HB2	1.70	0.71
30:0:558:C:C2'	30:0:559:U:H5''	2.19	0.71
6:F:96:ALA:HA	42:F:3111:HOH:O	1.88	0.71
20:T:112:LEU:HD23	20:T:119:ALA:HB3	1.73	0.71
10:J:74:ARG:CB	10:J:74:ARG:HH11	2.04	0.71
30:0:2296:C:H2'	30:0:2297:U:H6	1.55	0.71
30:0:2356:A:H2'	30:0:2357:G:O4'	1.91	0.71
16:P:59:ARG:HH22	16:P:66:GLN:HE22	1.36	0.71
22:V:12:THR:CG2	22:V:15:GLU:HG3	2.20	0.71
30:0:119:A:H2'	30:0:120:A:H5''	1.71	0.71
30:0:1838:U:O2'	30:0:2644:C:H5'	1.90	0.71
30:0:1667:A:H5'	30:0:1667:A:C8	2.25	0.71
13:M:107:ARG:HH11	13:M:107:ARG:HG3	1.56	0.71
18:R:82:GLU:HG3	18:R:83:LYS:H	1.55	0.71
22:V:39:ALA:N	22:V:40:PRO:HD2	2.05	0.71
28:2:41:HIS:HB3	28:2:44:ARG:HB2	1.70	0.71
6:F:26:THR:HG21	6:F:102:GLY:C	2.16	0.71
18:R:6:VAL:HG21	18:R:113:HIS:CD2	2.25	0.70
22:V:1:THR:CG2	22:V:2:VAL:H	2.00	0.70
24:X:49:ARG:HG2	24:X:84:ILE:HG12	1.72	0.70
30:0:1701:A:H4'	30:0:1702:U:H5''	1.72	0.70
1:A:36:ASP:O	1:A:38:ILE:N	2.23	0.70
3:C:194:PHE:HA	3:C:234:VAL:HG13	1.73	0.70
17:Q:66:LYS:HB2	17:Q:70:ALA:O	1.91	0.70
30:0:1372:A:H3'	42:0:7993:HOH:O	1.91	0.70
14:N:164:ASP:OD1	14:N:167:ASP:HA	1.91	0.70
30:0:1474:C:H5'	30:0:1474:C:C6	2.24	0.70
25:Y:235:GLU:CD	25:Y:235:GLU:H	1.98	0.70
29:3:68:LYS:HE2	30:0:2436:U:H5'	1.71	0.70
14:N:11:ARG:HD3	31:9:114:G:O6	1.91	0.70
14:N:132:ASN:O	14:N:135:VAL:HG12	1.92	0.70
20:T:54:ASP:OD2	30:0:316:A:H5'	1.90	0.70
30:0:1183:C:N4	30:0:1184:C:H41	1.89	0.70
30:0:2851:G:O2'	30:0:2852:A:H5'	1.90	0.70
30:0:2908:A:H2'	30:0:2909:G:O4'	1.92	0.70
5:E:84:MET:HG2	5:E:168:ILE:HA	1.73	0.70
27:1:9:GLY:HA2	30:0:1687:C:O2	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:49:ILE:HD11	5:E:69:ILE:HD12	1.72	0.70
18:R:128:ARG:NH2	30:0:2054:A:N3	2.39	0.70
23:W:141:HIS:HB2	23:W:146:ILE:HG12	1.73	0.70
3:C:27:ARG:HH11	3:C:27:ARG:CG	2.05	0.70
3:C:84:VAL:HG12	3:C:85:LYS:HG2	1.72	0.69
8:H:36:MET:HB3	8:H:73:ASN:ND2	2.07	0.69
13:M:57:LYS:HE2	13:M:140:ALA:O	1.92	0.69
13:M:164:THR:CG2	13:M:166:ALA:H	2.02	0.69
24:X:37:LEU:HD13	24:X:85:VAL:HG21	1.73	0.69
31:9:56:A:C2'	31:9:57:A:H5''	2.20	0.69
30:0:951:A:C2'	30:0:952:G:H5'	2.22	0.69
9:I:127:CYS:C	9:I:129:SER:H	2.00	0.69
14:N:71:TRP:CE3	14:N:175:LEU:HD22	2.27	0.69
30:0:236:A:H4'	30:0:237:G:H5'	1.74	0.69
30:0:1829:A:H2'	30:0:1830:C:H5'	1.74	0.69
31:9:92:G:H2'	31:9:93:A:C8	2.27	0.69
2:B:62:ARG:HA	2:B:65:MET:HE2	1.72	0.69
30:0:1634:G:H3'	42:0:4766:HOH:O	1.92	0.69
3:C:233:THR:HG22	3:C:234:VAL:N	2.07	0.69
8:H:31:ILE:HA	8:H:66:GLU:OE1	1.93	0.69
18:R:18:LEU:HD12	18:R:143:VAL:CG1	2.23	0.69
26:Z:46:SER:O	26:Z:50:VAL:HG23	1.92	0.69
31:9:75:G:H1	31:9:106:U:H3	1.39	0.69
5:E:15:GLN:HG3	5:E:20:ILE:HG12	1.74	0.69
13:M:134:ILE:CG2	13:M:141:ILE:HD13	2.23	0.69
25:Y:117:LEU:HD13	25:Y:174:VAL:HG11	1.73	0.69
30:0:2637:A:H4'	30:0:2638:G:C5'	2.23	0.69
2:B:30:PRO:HB2	2:B:39:GLN:NE2	2.08	0.69
2:B:175:LEU:O	2:B:175:LEU:HD23	1.93	0.69
13:M:24:GLN:NE2	13:M:27:ARG:HD2	2.07	0.69
25:Y:234:VAL:HG12	25:Y:235:GLU:H	1.56	0.69
29:3:60:LYS:HG3	29:3:61:PRO:HD2	1.74	0.69
30:0:1205:U:H2'	30:0:1206:U:C5'	2.22	0.69
30:0:2004:U:H2'	30:0:2004:U:O2	1.93	0.69
30:0:2102:G:H2'	42:0:9555:HOH:O	1.93	0.69
30:0:2387:U:H2'	30:0:2388:C:C6	2.28	0.69
25:Y:187:VAL:HG23	25:Y:192:ASP:CB	2.22	0.69
1:A:199:HIS:HD2	1:A:201:PHE:H	1.38	0.68
2:B:162:MET:HE3	2:B:310:ARG:HH11	1.57	0.68
22:V:11:MET:HB3	22:V:15:GLU:HB2	1.73	0.68
17:Q:16:ASN:HD21	17:Q:45:PRO:HD2	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:56:ARG:NH2	30:0:2890:A:H1'	2.09	0.68
24:X:25:ARG:HD3	24:X:64:ALA:O	1.93	0.68
2:B:229:ARG:HD2	42:B:8991:HOH:O	1.93	0.68
4:D:25:MET:CE	4:D:37:ALA:HB1	2.23	0.68
20:T:9:LYS:HE3	20:T:13:ARG:NH1	2.07	0.68
3:C:118:THR:HG22	3:C:137:PRO:HB3	1.76	0.68
3:C:193:LEU:HD13	3:C:222:ASP:HB2	1.76	0.68
30:0:2247:C:H2'	30:0:2248:C:H6	1.59	0.68
1:A:139:LYS:HE2	1:A:143:GLY:HA2	1.76	0.68
1:A:211:LYS:HB3	1:A:212:PRO:CD	2.23	0.68
5:E:84:MET:HE1	5:E:148:ILE:CD1	2.23	0.68
10:J:4:ALA:O	10:J:5:GLU:HB2	1.94	0.68
16:P:139:ARG:HG3	16:P:139:ARG:HH11	1.58	0.68
20:T:71:VAL:HG11	20:T:90:PRO:CB	2.23	0.68
23:W:38:THR:HG22	23:W:39:ASP:N	2.09	0.68
30:0:304:G:H1'	30:0:347:A:N6	2.08	0.68
30:0:1300:G:H1'	42:0:5541:HOH:O	1.91	0.68
8:H:6:ALA:HB3	30:0:2521:A:OP2	1.94	0.68
14:N:5:ARG:NH1	30:0:962:C:H1'	2.09	0.68
16:P:115:SER:H	16:P:118:GLN:NE2	1.86	0.68
31:9:39:U:HO2'	31:9:42:C:H5	1.41	0.68
4:D:135:VAL:HG21	4:D:139:TYR:CG	2.28	0.68
6:F:14:ASP:O	6:F:18:GLU:HG3	1.94	0.68
11:K:125:ALA:C	11:K:127:ALA:H	2.02	0.68
30:0:2851:G:C2'	30:0:2852:A:H5'	2.24	0.68
3:C:153:VAL:O	3:C:157:LEU:HG	1.94	0.68
30:0:558:C:H2'	30:0:559:U:C5'	2.24	0.68
2:B:214:PRO:HD2	42:0:2996:HOH:O	1.92	0.68
20:T:77:VAL:HG11	20:T:91:LEU:HD11	1.75	0.68
23:W:137:GLN:NE2	23:W:141:HIS:HE1	1.87	0.68
30:0:282:C:O2'	30:0:283:U:H5'	1.93	0.68
25:Y:170:SER:OG	25:Y:175:ARG:HG3	1.94	0.67
30:0:1166:A:H1'	30:0:1192:A:C2	2.28	0.67
30:0:2505:G:O2'	30:0:2506:A:H5'	1.95	0.67
6:F:83:LEU:HD11	6:F:96:ALA:HB3	1.76	0.67
23:W:84:VAL:HG12	42:W:6679:HOH:O	1.94	0.67
30:0:1182:C:H1'	30:0:1192:A:H8	1.59	0.67
30:0:2588:OMG:HN21	32:5:76:A:H2	1.40	0.67
29:3:3:MET:HG3	29:3:4:PRO:HD2	1.76	0.67
7:G:27:ILE:HD13	7:G:71:LEU:HD23	1.76	0.67
10:J:54:VAL:O	10:J:58:GLU:HG3	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:6:ARG:HD3	30:0:1299:G:O6	1.94	0.67
18:R:117:HIS:HD2	30:0:20:G:H21	1.40	0.67
22:V:1:THR:HB	30:0:93:C:H5''	1.77	0.67
22:V:56:ILE:O	22:V:60:GLN:HG3	1.93	0.67
29:3:25:VAL:HG13	29:3:68:LYS:HE3	1.75	0.67
4:D:27:ILE:HD11	4:D:37:ALA:CB	2.25	0.67
4:D:27:ILE:HD11	4:D:37:ALA:HB3	1.76	0.67
11:K:74:VAL:HG11	11:K:113:ILE:HG12	1.75	0.67
12:L:35:ARG:C	12:L:35:ARG:HD3	2.20	0.67
21:U:11:THR:HG22	21:U:53:ASP:HB2	1.77	0.67
1:A:201:PHE:HA	42:A:9065:HOH:O	1.94	0.67
2:B:74:ILE:HG22	2:B:76:THR:HG23	1.76	0.67
2:B:321:PRO:HA	42:B:9136:HOH:O	1.94	0.67
3:C:211:ASP:HB2	3:C:231:ARG:HH22	1.60	0.67
5:E:101:GLU:HB3	5:E:117:THR:HA	1.75	0.67
8:H:48:VAL:HA	8:H:170:ARG:O	1.94	0.67
14:N:49:THR:HG22	14:N:56:ASP:HB2	1.76	0.67
16:P:80:ARG:HG2	16:P:87:ARG:CZ	2.25	0.67
30:0:2073:G:OP2	30:0:2490:A:H5'	1.94	0.67
31:9:18:U:H2'	31:9:19:G:H8	1.59	0.67
18:R:18:LEU:HB2	18:R:143:VAL:CG1	2.23	0.67
8:H:59:GLN:NE2	8:H:129:ARG:HE	1.92	0.67
11:K:20:CYS:HB2	11:K:29:LEU:HG	1.77	0.67
11:K:41:LYS:HE2	11:K:42:ASN:HD21	1.60	0.67
27:1:25:LYS:HD2	28:2:49:GLU:H	1.58	0.67
30:0:1058:A:H2'	30:0:1060:C:C5'	2.25	0.67
31:9:49:G:H5''	42:9:9086:HOH:O	1.95	0.67
1:A:103:VAL:O	1:A:105:VAL:HG23	1.95	0.67
3:C:174:ILE:CD1	30:0:338:C:H4'	2.25	0.67
13:M:24:GLN:HE22	13:M:27:ARG:HH11	1.41	0.67
30:0:1730:G:H5'	30:0:1731:C:C6	2.30	0.67
30:0:451:C:O2'	30:0:452:G:H5'	1.95	0.67
30:0:1834:C:H2'	30:0:1840:A:N6	2.10	0.67
30:0:2047:C:H5'	42:0:3722:HOH:O	1.95	0.67
23:W:122:ARG:NH2	23:W:154:ARG:HB3	2.10	0.66
26:Z:70:ARG:CD	26:Z:83:TYR:HB2	2.25	0.66
30:0:2102:G:H1'	42:0:6120:HOH:O	1.94	0.66
2:B:235:ARG:HD3	30:0:2091:G:O3'	1.95	0.66
5:E:23:GLU:HG2	5:E:28:SER:CB	2.25	0.66
18:R:16:ALA:HB1	18:R:94:ASN:HD22	1.60	0.66
30:0:1766:U:O2	30:0:1778:A:H5'	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:55:GLN:HA	12:L:58:GLN:NE2	2.07	0.66
23:W:13:MET:CE	23:W:17:ILE:HG22	2.24	0.66
27:1:16:HIS:HE1	30:0:775:G:OP1	1.79	0.66
30:0:1461:U:H2'	30:0:1462:C:C6	2.31	0.66
3:C:236:THR:CG2	3:C:239:ALA:H	1.93	0.66
4:D:131:THR:HG21	30:0:2348:C:H1'	1.77	0.66
18:R:68:HIS:CD2	18:R:76:ASP:HB2	2.30	0.66
20:T:9:LYS:HD2	42:0:4631:HOH:O	1.96	0.66
22:V:26:GLU:OE2	22:V:45:ARG:HD3	1.95	0.66
30:0:1666:C:O2'	30:0:1667:A:H5''	1.96	0.66
12:L:53:ARG:NH2	12:L:57:VAL:HG12	2.10	0.66
30:0:256:C:H2'	30:0:257:G:O4'	1.96	0.66
30:0:1159:G:H21	30:0:1189:A:H8	1.43	0.66
13:M:31:TRP:HA	13:M:34:GLU:HG3	1.78	0.66
2:B:217:ARG:HG3	2:B:257:THR:HG22	1.76	0.66
30:0:272:A:H5'	30:0:273:G:OP2	1.94	0.66
30:0:2769:C:H2'	30:0:2770:G:O4'	1.95	0.66
2:B:211:THR:HG23	30:0:2840:A:OP1	1.96	0.66
13:M:15:PRO:HA	13:M:20:LEU:HD23	1.78	0.66
14:N:36:ALA:HB1	14:N:118:ILE:HD12	1.77	0.66
21:U:45:GLU:HB2	21:U:48:ASN:HD22	1.60	0.66
24:X:80:GLU:HB3	42:X:5564:HOH:O	1.96	0.66
30:0:1171:A:H2'	30:0:1172:G:H5'	1.78	0.66
30:0:1666:C:H2'	30:0:1667:A:H5'	1.78	0.66
1:A:94:LEU:HD12	1:A:98:GLU:HB2	1.77	0.66
3:C:246:ARG:HB3	3:C:246:ARG:NH1	2.11	0.66
20:T:48:VAL:HG23	20:T:98:VAL:HA	1.78	0.66
30:0:946:C:H2'	30:0:947:U:H6	1.61	0.66
30:0:1118:A:C8	30:0:1118:A:H3'	2.30	0.66
1:A:33:GLU:O	1:A:34:ASP:HB2	1.95	0.65
3:C:111:VAL:HB	42:C:8521:HOH:O	1.95	0.65
10:J:25:GLN:HE22	10:J:116:LEU:HB3	1.61	0.65
18:R:39:THR:CB	18:R:42:GLU:HG3	2.24	0.65
26:Z:61:HIS:HB2	26:Z:71:VAL:HB	1.77	0.65
33:6:76:8AN:C2	42:6:82:HOH:O	2.44	0.65
3:C:156:LEU:O	3:C:160:LEU:HG	1.96	0.65
18:R:4:TYR:CE1	18:R:17:MET:HE2	2.31	0.65
2:B:36:PRO:CA	2:B:168:GLY:HA3	2.19	0.65
4:D:173:GLU:O	4:D:174:VAL:O	2.13	0.65
8:H:5:PRO:O	8:H:8:MET:HB2	1.95	0.65
21:U:45:GLU:HB2	21:U:48:ASN:ND2	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:8:GLN:HE22	27:1:11:LYS:NZ	1.94	0.65
31:9:23:U:O2'	31:9:24:U:H4'	1.95	0.65
1:A:194:MET:HE3	1:A:199:HIS:HB2	1.79	0.65
2:B:51:VAL:HG23	2:B:330:VAL:HG22	1.79	0.65
5:E:116:THR:HG22	5:E:151:LEU:HD22	1.79	0.65
1:A:207:GLN:HA	42:A:9036:HOH:O	1.95	0.65
3:C:242:GLU:HG3	42:C:8587:HOH:O	1.95	0.65
11:K:81:ARG:HD3	11:K:87:ARG:CZ	2.27	0.65
17:Q:75:ILE:CD1	17:Q:84:ILE:HD11	2.25	0.65
19:S:22:ASN:ND2	19:S:68:LEU:HB2	2.12	0.65
31:9:76:G:C3'	31:9:77:A:H5''	2.16	0.65
6:F:84:GLY:O	6:F:89:LEU:HB2	1.95	0.65
10:J:76:ASP:HA	42:J:5907:HOH:O	1.97	0.65
30:0:1201:C:H5''	42:0:7064:HOH:O	1.96	0.65
1:A:88:ILE:O	1:A:88:ILE:HG22	1.96	0.65
5:E:84:MET:HE1	5:E:148:ILE:HD12	1.77	0.65
8:H:6:ALA:HA	8:H:61:ARG:NH1	2.11	0.65
16:P:121:ASP:O	16:P:125:LYS:HG3	1.96	0.65
23:W:139:GLY:O	23:W:141:HIS:HD2	1.79	0.65
30:0:168:C:H5''	42:0:3347:HOH:O	1.96	0.65
14:N:78:MET:HB2	14:N:146:HIS:CE1	2.32	0.65
30:0:2387:U:H2'	30:0:2388:C:H6	1.61	0.65
2:B:175:LEU:HD23	2:B:175:LEU:C	2.22	0.65
6:F:27:GLY:HA3	6:F:101:ALA:O	1.97	0.65
6:F:46:GLU:O	6:F:73:PRO:HD2	1.97	0.65
9:I:82:THR:HG23	30:0:1168:C:H5''	1.79	0.65
30:0:506:G:H22	30:0:509:A:C5'	2.07	0.64
31:9:13:A:O2'	31:9:14:G:H5''	1.97	0.64
2:B:75:GLU:C	2:B:77:PRO:HD3	2.22	0.64
2:B:77:PRO:HA	2:B:293:PRO:HB2	1.79	0.64
11:K:4:LEU:HD22	11:K:116:GLU:HB3	1.79	0.64
13:M:34:GLU:HB3	13:M:38:GLU:HG3	1.79	0.64
30:0:545:G:H5'	30:0:545:G:C8	2.29	0.64
3:C:5:ILE:HD11	3:C:16:VAL:CG2	2.28	0.64
14:N:152:GLU:C	14:N:154:LEU:H	2.05	0.64
21:U:6:CYS:O	21:U:10:GLY:HA2	1.98	0.64
28:2:41:HIS:CD2	28:2:44:ARG:H	2.14	0.64
30:0:1118:A:H8	30:0:1118:A:H3'	1.62	0.64
30:0:1136:U:H2'	42:0:5826:HOH:O	1.96	0.64
30:0:1189:A:O2'	30:0:1208:C:H2'	1.96	0.64
2:B:24:PRO:HG3	2:B:204:GLY:HA2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:ILE:HD11	3:C:16:VAL:HG22	1.79	0.64
6:F:37:THR:O	6:F:41:GLU:HG3	1.97	0.64
14:N:182:GLY:O	14:N:184:ILE:HG22	1.97	0.64
17:Q:95:GLU:HA	30:0:949:U:H4'	1.79	0.64
20:T:48:VAL:CG2	20:T:96:VAL:HG13	2.28	0.64
27:1:28:HIS:HD2	27:1:30:LYS:H	1.45	0.64
30:0:660:A:H4'	30:0:661:G:O5'	1.98	0.64
30:0:2637:A:H4'	30:0:2638:G:H5'	1.79	0.64
6:F:57:GLU:O	6:F:61:MET:HG3	1.98	0.64
15:O:65:LEU:HD13	30:0:746:A:C6	2.32	0.64
20:T:76:ASP:C	20:T:78:THR:HG23	2.23	0.64
30:0:2540:G:O2'	30:0:2541:U:H5''	1.98	0.64
14:N:160:SER:HB3	31:9:51:A:H5'	1.80	0.64
16:P:7:LYS:HD3	16:P:23:PHE:CZ	2.32	0.64
17:Q:7:LEU:HD12	30:0:2424:U:H1'	1.80	0.64
19:S:33:SER:O	19:S:37:VAL:HG23	1.97	0.64
8:H:14:LYS:HE2	42:0:4718:HOH:O	1.98	0.64
13:M:24:GLN:NE2	13:M:27:ARG:NH1	2.45	0.64
13:M:68:ARG:O	13:M:68:ARG:HD3	1.98	0.64
14:N:77:ASN:C	14:N:80:SER:HB3	2.23	0.64
2:B:211:THR:HG21	42:0:9253:HOH:O	1.98	0.64
19:S:52:VAL:HG22	19:S:66:VAL:HG22	1.79	0.64
21:U:9:CYS:SG	21:U:11:THR:HG23	2.38	0.64
25:Y:187:VAL:HG13	25:Y:205:ILE:HA	1.79	0.64
31:9:2:U:OP2	31:9:3:A:H5'	1.96	0.64
1:A:33:GLU:CD	1:A:33:GLU:N	2.55	0.64
1:A:217:ARG:HH11	1:A:217:ARG:CG	2.11	0.64
9:I:110:ASP:O	30:0:1163:G:H5'	1.98	0.64
14:N:37:ARG:NH1	31:9:6:C:C5'	2.56	0.64
16:P:1:THR:O	30:0:1396:C:H1'	1.97	0.64
30:0:316:A:N3	30:0:336:G:O2'	2.31	0.64
2:B:62:ARG:HA	2:B:65:MET:CE	2.28	0.64
8:H:6:ALA:HA	8:H:61:ARG:HH12	1.63	0.64
22:V:50:ARG:HH12	30:0:56:G:H5''	1.60	0.64
3:C:246:ARG:HB3	3:C:246:ARG:HH11	1.63	0.63
9:I:96:SER:HB3	9:I:99:GLN:HE21	1.61	0.63
10:J:90:LYS:HB2	35:J:8802:CL:CL	2.35	0.63
20:T:16:LEU:HB2	30:0:100:C:H4'	1.80	0.63
31:9:59:C:H2'	31:9:60:C:C6	2.33	0.63
3:C:78:ARG:HH11	3:C:78:ARG:HG3	1.62	0.63
6:F:91:VAL:CG1	6:F:92:GLY:H	2.02	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:51:ILE:HD13	18:R:86:LYS:HG2	1.79	0.63
29:3:73:GLU:HB3	42:3:9050:HOH:O	1.97	0.63
31:9:29:C:C2'	31:9:30:C:H5'	2.29	0.63
1:A:11:ARG:NH1	42:A:9044:HOH:O	2.31	0.63
2:B:139:ASP:OD2	2:B:165:ARG:HD2	1.97	0.63
20:T:43:ASN:C	20:T:45:GLY:H	2.06	0.63
29:3:62:THR:HB	42:3:9041:HOH:O	1.98	0.63
30:0:2827:A:H2'	30:0:2828:G:O4'	1.98	0.63
15:O:32:ARG:O	15:O:32:ARG:HD3	1.98	0.63
3:C:34:ALA:HB3	3:C:220:THR:HG21	1.80	0.63
12:L:67:ARG:O	12:L:71:GLU:HG3	1.99	0.63
30:0:1042:U:O2'	30:0:1043:C:H5'	1.98	0.63
1:A:217:ARG:HH11	1:A:217:ARG:HG3	1.61	0.63
18:R:96:VAL:HG13	18:R:106:GLY:HA3	1.81	0.63
21:U:14:GLU:OE1	21:U:15:PRO:HD2	1.98	0.63
23:W:88:THR:HB	42:W:6679:HOH:O	1.99	0.63
30:0:1189:A:H3'	42:0:9471:HOH:O	1.98	0.63
1:A:8:ARG:HG2	42:A:9031:HOH:O	1.96	0.63
3:C:104:ASP:O	3:C:108:GLN:HG3	1.98	0.63
6:F:50:VAL:CG2	6:F:63:ILE:HG21	2.29	0.63
7:G:16:LYS:O	7:G:20:VAL:HG23	1.98	0.63
25:Y:126:PRO:HG2	25:Y:128:PHE:CZ	2.34	0.63
1:A:121:ALA:O	1:A:124:VAL:HG22	1.99	0.63
3:C:58:ALA:HA	3:C:73:GLN:HE21	1.64	0.63
3:C:129:HIS:CE1	3:C:231:ARG:HA	2.34	0.63
17:Q:64:GLU:HG3	17:Q:74:ASP:OD2	1.98	0.63
20:T:21:LYS:HA	20:T:24:ARG:HG3	1.81	0.63
30:0:1183:C:H2'	42:0:7072:HOH:O	1.99	0.63
30:0:2106:C:H5'	30:0:2284:G:H21	1.64	0.63
20:T:50:VAL:HG12	20:T:56:ALA:HA	1.81	0.63
24:X:21:PRO:HG2	24:X:24:LYS:HD3	1.81	0.63
25:Y:208:LYS:HZ3	30:0:1343:C:H1'	1.64	0.63
30:0:463:A:H5'	30:0:465:U:O4'	1.99	0.63
24:X:30:MET:HE1	24:X:58:ALA:HB3	1.81	0.62
30:0:95:A:H5''	30:0:97:G:O4'	1.99	0.62
30:0:151:A:H2'	30:0:152:A:O4'	1.99	0.62
2:B:97:LEU:O	2:B:98:THR:HG23	1.99	0.62
2:B:150:ALA:O	2:B:152:PRO:HD3	1.98	0.62
7:G:69:ARG:NH2	30:0:1150:A:N7	2.47	0.62
11:K:77:ARG:C	11:K:78:LYS:CA	2.72	0.62
30:0:858:U:H2'	30:0:859:C:H6	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:31:ARG:HH12	5:E:68:HIS:CG	2.17	0.62
13:M:171:ARG:CD	30:0:156:C:H5''	2.28	0.62
20:T:49:GLU:OE2	20:T:97:ARG:NH1	2.32	0.62
22:V:13:PRO:HA	22:V:16:ARG:NH1	2.14	0.62
23:W:46:ALA:O	23:W:49:ASN:HB2	1.99	0.62
10:J:130:VAL:HG12	10:J:131:THR:N	2.15	0.62
12:L:7:GLN:HG3	35:L:8814:CL:CL	2.37	0.62
17:Q:75:ILE:HD13	17:Q:84:ILE:HD11	1.78	0.62
24:X:47:ALA:HB1	24:X:82:GLU:HB3	1.81	0.62
30:0:281:U:H2'	30:0:282:C:O4'	1.98	0.62
30:0:603:A:H4'	30:0:604:G:O5'	2.00	0.62
30:0:871:G:C8	30:0:871:G:C5'	2.74	0.62
30:0:2362:A:H2'	30:0:2363:G:C8	2.34	0.62
20:T:48:VAL:HG21	20:T:96:VAL:HG13	1.80	0.62
27:I:9:GLY:HA3	30:0:1695:G:H1'	1.79	0.62
30:0:280:C:H2'	30:0:281:U:O4'	1.99	0.62
30:0:726:C:H2'	30:0:727:G:O4'	2.00	0.62
30:0:790:A:H1'	30:0:1710:A:H2'	1.82	0.62
30:0:1058:A:H2'	30:0:1060:C:H5''	1.80	0.62
30:0:1218:U:H2'	30:0:1219:U:C6	2.34	0.62
30:0:2266:A:H2'	30:0:2267:G:C8	2.35	0.62
31:9:98:C:H2'	31:9:99:U:H6	1.64	0.62
4:D:64:ARG:NE	4:D:67:ASP:HB3	2.15	0.62
9:I:112:LEU:CD1	30:0:1162:G:H1'	2.29	0.62
16:P:143:ALA:HA	42:P:5521:HOH:O	1.99	0.62
20:T:19:ARG:HD3	20:T:67:LEU:O	2.00	0.62
31:9:73:A:H61	31:9:108:C:H42	1.48	0.62
12:L:66:VAL:HG23	12:L:67:ARG:N	2.14	0.62
24:X:20:GLU:CD	24:X:21:PRO:HD2	2.24	0.62
30:0:204:A:H2'	30:0:205:U:H5'	1.82	0.62
5:E:47:VAL:HG11	5:E:69:ILE:HD13	1.80	0.62
5:E:84:MET:HG2	5:E:168:ILE:HD13	1.82	0.62
25:Y:169:ARG:HD3	30:0:1328:A:C8	2.35	0.62
30:0:241:A:C2	30:0:378:A:H4'	2.35	0.62
30:0:1406:A:H4'	30:0:1407:A:H5''	1.82	0.62
2:B:265:LEU:HD21	2:B:316:ARG:HD3	1.81	0.62
3:C:214:THR:HG22	3:C:216:SER:H	1.64	0.62
25:Y:235:GLU:CD	25:Y:235:GLU:N	2.58	0.62
30:0:59:A:H5'	42:0:5197:HOH:O	1.98	0.62
30:0:2106:C:H1'	30:0:2484:U:O2	2.00	0.62
2:B:77:PRO:C	2:B:78:PRO:HG3	2.25	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:PRO:HD3	10:J:127:ILE:CD1	2.30	0.62
5:E:131:LEU:HD12	5:E:166:VAL:HG11	1.81	0.62
16:P:9:LEU:O	16:P:13:VAL:HG12	2.00	0.62
24:X:76:ARG:HH11	24:X:76:ARG:HG3	1.65	0.62
27:1:25:LYS:O	27:1:25:LYS:HG2	2.00	0.62
5:E:144:THR:O	5:E:148:ILE:HG13	1.99	0.61
12:L:56:LYS:HE3	30:0:2443:C:O3'	2.00	0.61
24:X:72:VAL:HG22	24:X:85:VAL:HG12	1.80	0.61
27:1:28:HIS:CE1	27:1:31:LYS:HE2	2.35	0.61
14:N:48:VAL:CG1	14:N:55:ASP:HB3	2.29	0.61
29:3:6:ARG:HH11	29:3:21:GLU:HG3	1.65	0.61
30:0:564:G:H1'	42:0:7141:HOH:O	1.99	0.61
30:0:951:A:H2'	30:0:952:G:H5'	1.81	0.61
30:0:2766:A:H5'	42:0:3465:HOH:O	1.99	0.61
31:9:14:G:H5'	31:9:14:G:C8	2.35	0.61
23:W:6:GLN:HB2	23:W:26:ILE:CD1	2.30	0.61
30:0:946:C:H2'	30:0:947:U:C6	2.34	0.61
30:0:2866:U:H4'	30:0:2867:G:H5'	1.81	0.61
31:9:64:C:H2'	31:9:65:A:H5'	1.82	0.61
2:B:141:ARG:HG2	2:B:165:ARG:HA	1.83	0.61
3:C:101:ASP:HB2	30:0:750:A:O3'	2.01	0.61
6:F:58:GLU:OE1	13:M:27:ARG:NH2	2.33	0.61
12:L:53:ARG:HD2	30:0:2441:U:H4'	1.82	0.61
12:L:125:PHE:CZ	12:L:140:VAL:HG22	2.35	0.61
14:N:147:ILE:HD12	42:9:9086:HOH:O	2.00	0.61
30:0:589:U:H2'	30:0:590:A:H8	1.64	0.61
30:0:1976:G:O2'	30:0:1977:U:H5'	2.01	0.61
30:0:2533:C:H5'	30:0:2533:C:H6	1.65	0.61
2:B:207:LYS:HG3	30:0:2717:C:OP1	2.00	0.61
16:P:121:ASP:OD1	16:P:125:LYS:HE3	1.99	0.61
18:R:29:LYS:HB3	42:R:8939:HOH:O	1.99	0.61
30:0:247:A:H2'	42:0:4794:HOH:O	2.00	0.61
30:0:494:C:H2'	30:0:496:G:OP2	2.00	0.61
30:0:1461:U:H2'	30:0:1462:C:H6	1.65	0.61
1:A:19:PRO:HG2	1:A:23:TYR:CE2	2.35	0.61
9:I:73:LEU:HD12	9:I:107:LYS:HZ2	1.64	0.61
10:J:70:PHE:CD1	30:0:2676:C:H4'	2.35	0.61
13:M:61:ILE:HD12	13:M:61:ILE:N	2.15	0.61
20:T:41:ARG:HG2	20:T:41:ARG:HH11	1.66	0.61
25:Y:170:SER:HG	25:Y:175:ARG:HG3	1.65	0.61
29:3:65:THR:CG2	29:3:67:LEU:HG	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1205:U:C2'	30:0:1206:U:H5''	2.30	0.61
3:C:121:ALA:N	3:C:136:VAL:HG11	2.15	0.61
13:M:9:ARG:HD2	30:0:380:A:OP2	2.00	0.61
18:R:46:TYR:HD2	18:R:47:LEU:HD23	1.65	0.61
30:0:185:G:H4'	30:0:186:A:H4'	1.81	0.61
7:G:12:ILE:HG22	7:G:17:GLN:NE2	2.16	0.61
13:M:43:PRO:HG3	13:M:62:VAL:HG21	1.82	0.61
14:N:112:GLY:HA2	14:N:137:ALA:N	2.15	0.61
20:T:64:ASN:HB3	20:T:73:HIS:HB2	1.81	0.61
25:Y:148:GLY:O	25:Y:154:ARG:HD3	2.01	0.61
29:3:77:ALA:C	29:3:78:HIS:CA	2.74	0.61
30:0:1528:A:H2'	30:0:1529:G:O4'	2.00	0.61
30:0:2735:U:H2'	30:0:2736:U:C6	2.36	0.61
30:0:2896:A:N3	30:0:2896:A:H2'	2.16	0.61
31:9:64:C:C2'	31:9:65:A:H5'	2.31	0.61
3:C:51:TYR:CE1	27:1:56:GLU:HB2	2.35	0.61
3:C:235:PHE:HE2	3:C:243:VAL:HG21	1.65	0.61
4:D:58:VAL:HB	4:D:62:ASP:HB3	1.83	0.61
5:E:20:ILE:HD11	5:E:40:VAL:CG1	2.30	0.61
30:0:120:A:H2'	30:0:120:A:N3	2.15	0.61
30:0:2795:C:O2'	30:0:2796:U:H5'	2.00	0.61
4:D:58:VAL:CG1	4:D:60:GLU:HG2	2.29	0.61
10:J:127:ILE:N	35:J:8801:CL:CL	2.66	0.61
15:O:14:LEU:HG	15:O:102:ILE:HD11	1.83	0.61
5:E:35:TYR:HA	10:J:127:ILE:HD11	1.83	0.60
11:K:66:ARG:HH12	30:0:1992:U:H3'	1.66	0.60
21:U:9:CYS:HA	21:U:52:THR:CG2	2.30	0.60
23:W:48:VAL:O	23:W:48:VAL:HG12	2.00	0.60
5:E:166:VAL:HG12	42:E:3134:HOH:O	2.00	0.60
13:M:22:GLU:O	13:M:26:GLN:HG3	2.01	0.60
14:N:48:VAL:HG13	14:N:55:ASP:HB3	1.83	0.60
30:0:536:A:H3'	42:0:5901:HOH:O	2.00	0.60
30:0:2534:C:H1'	42:0:4385:HOH:O	2.00	0.60
10:J:74:ARG:HH11	10:J:74:ARG:HB3	1.65	0.60
30:0:664:U:O4	30:0:681:G:H5''	2.00	0.60
2:B:16:ARG:HD3	42:B:9081:HOH:O	2.01	0.60
2:B:279:THR:HG22	2:B:280:VAL:H	1.64	0.60
7:G:67:LEU:O	7:G:71:LEU:HG	2.01	0.60
11:K:113:ILE:HG22	11:K:114:ALA:N	2.16	0.60
1:A:130:THR:HB	1:A:137:VAL:HB	1.84	0.60
15:O:59:VAL:CG2	15:O:111:VAL:HG21	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:37:VAL:O	19:S:41:VAL:HG23	2.01	0.60
23:W:125:HIS:NE2	30:0:1097:A:H5''	2.15	0.60
30:0:1206:U:H2'	30:0:1207:A:O4'	2.01	0.60
1:A:84:VAL:O	1:A:98:GLU:HG3	2.01	0.60
21:U:17:THR:CG2	21:U:18:GLY:N	2.64	0.60
23:W:85:ALA:HB2	23:W:91:ASP:O	2.00	0.60
25:Y:152:LYS:HB3	25:Y:160:LYS:HG3	1.84	0.60
30:0:1249:U:H2'	30:0:1250:C:C6	2.36	0.60
30:0:1931:A:H2'	30:0:1932:G:H5'	1.83	0.60
2:B:42:ALA:CB	2:B:162:MET:HE1	2.31	0.60
3:C:7:ASP:OD2	3:C:9:ASP:HB2	2.01	0.60
5:E:68:HIS:O	5:E:72:MET:HG3	2.00	0.60
7:G:20:VAL:O	7:G:24:VAL:HG23	2.02	0.60
13:M:165:GLY:O	13:M:169:ARG:HB2	2.02	0.60
18:R:77:ALA:C	18:R:78:GLY:CA	2.75	0.60
31:9:20:G:O2'	31:9:21:G:H5'	2.02	0.60
3:C:78:ARG:HG3	3:C:78:ARG:NH1	2.16	0.60
10:J:75:PRO:HG2	10:J:105:LEU:CD2	2.32	0.60
11:K:14:LYS:HB2	11:K:45:PRO:HG2	1.83	0.60
30:0:1209:C:H2'	30:0:1210:G:H8	1.66	0.60
30:0:1416:G:C2'	30:0:1417:G:H5'	2.32	0.60
30:0:1909:A:N1	30:0:2128:G:H1'	2.17	0.60
30:0:2296:C:H2'	30:0:2297:U:C6	2.37	0.60
30:0:2415:A:H2'	30:0:2416:G:H5'	1.83	0.60
2:B:238:ASN:HD22	2:B:240:GLY:H	1.49	0.60
4:D:60:GLU:O	4:D:61:PHE:C	2.45	0.60
12:L:143:THR:HG22	12:L:144:ASP:N	2.17	0.60
21:U:11:THR:HG22	21:U:53:ASP:CB	2.31	0.60
22:V:29:ASN:O	22:V:33:VAL:HG23	2.02	0.60
30:0:1377:C:H5'	30:0:1377:C:C6	2.32	0.60
30:0:2472:C:O2'	30:0:2634:G:H4'	2.00	0.60
3:C:211:ASP:HB2	3:C:231:ARG:NH2	2.17	0.60
22:V:5:VAL:HG12	22:V:9:ARG:NH1	2.17	0.60
25:Y:208:LYS:NZ	30:0:1343:C:H1'	2.17	0.60
30:0:2816:A:H5''	30:0:2817:G:H5'	1.83	0.60
17:Q:32:GLU:HA	17:Q:71:TYR:OH	2.01	0.59
21:U:17:THR:HG22	21:U:18:GLY:N	2.16	0.59
30:0:2748:G:H2'	42:0:9338:HOH:O	2.01	0.59
2:B:26:PHE:HD1	2:B:310:ARG:HH21	1.50	0.59
5:E:132:THR:HB	42:E:2227:HOH:O	2.03	0.59
9:I:120:ALA:O	9:I:124:VAL:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:41:LYS:HE2	11:K:42:ASN:ND2	2.17	0.59
20:T:8:ARG:NH1	30:0:31:C:OP2	2.35	0.59
30:0:2626:C:H2'	30:0:2627:G:C8	2.37	0.59
2:B:320:GLN:HE21	2:B:321:PRO:HD2	1.67	0.59
3:C:47:GLY:HA2	3:C:92:PRO:HB2	1.83	0.59
30:0:2802:C:H2'	30:0:2803:C:H6	1.67	0.59
9:I:107:LYS:HB3	9:I:110:ASP:HB2	1.85	0.59
9:I:127:CYS:HB3	9:I:132:VAL:HB	1.84	0.59
12:L:148:GLU:HA	42:L:9037:HOH:O	2.00	0.59
30:0:336:G:H5''	42:0:4601:HOH:O	2.02	0.59
30:0:969:G:H1	30:0:999:C:H42	1.50	0.59
30:0:1883:U:H5''	30:0:2013:G:OP2	2.01	0.59
1:A:82:VAL:HG22	1:A:93:THR:HB	1.83	0.59
13:M:60:VAL:C	13:M:61:ILE:HD12	2.27	0.59
30:0:248:A:H5'	30:0:249:G:OP2	2.03	0.59
30:0:459:A:H4'	42:0:3355:HOH:O	2.03	0.59
30:0:530:C:C4'	30:0:612:U:H4'	2.32	0.59
30:0:1172:G:H1'	42:0:5831:HOH:O	2.01	0.59
30:0:1545:C:H2'	30:0:1546:G:O4'	2.02	0.59
3:C:154:VAL:O	3:C:158:GLU:HG3	2.03	0.59
9:I:108:HIS:N	9:I:109:PRO:HD2	2.17	0.59
15:O:32:ARG:HH21	15:O:35:LYS:NZ	2.00	0.59
23:W:23:MET:HE1	30:0:944:G:C8	2.38	0.59
24:X:72:VAL:HG22	24:X:85:VAL:HG11	1.84	0.59
30:0:2326:C:H4'	30:0:2412:G:C4'	2.33	0.59
5:E:152:THR:HG21	5:E:165:GLY:HA2	1.84	0.59
8:H:54:VAL:HG13	8:H:162:PRO:CG	2.32	0.59
12:L:27:ARG:NH2	12:L:30:ARG:HG2	2.17	0.59
14:N:149:GLU:HA	14:N:152:GLU:HB2	1.83	0.59
30:0:368:C:H2'	30:0:369:G:H5'	1.85	0.59
30:0:834:G:H3'	30:0:835:U:H4'	1.83	0.59
30:0:1132:A:N6	30:0:1229:C:H2'	2.18	0.59
30:0:1416:G:H2'	30:0:1417:G:H5'	1.85	0.59
30:0:1555:G:H4'	30:0:1630:A:H2	1.67	0.59
6:F:61:MET:HB3	13:M:19:GLN:OE1	2.02	0.59
12:L:35:ARG:HB2	12:L:35:ARG:NH1	2.13	0.59
12:L:71:GLU:HG2	30:0:700:A:C2	2.38	0.59
18:R:79:ARG:HB3	30:0:2050:G:OP1	2.03	0.59
25:Y:117:LEU:HD13	25:Y:174:VAL:CG1	2.33	0.59
9:I:121:LYS:HD3	30:0:1185:U:OP1	2.02	0.59
23:W:13:MET:HE2	23:W:18:GLN:CA	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:625:U:H5'	30:0:1044:C:N4	2.17	0.59
30:0:1634:G:H2'	30:0:1635:U:C6	2.38	0.59
30:0:1735:C:O2'	30:0:1736:A:H5'	2.02	0.59
4:D:38:GLU:OE2	4:D:51:ARG:NE	2.35	0.59
18:R:77:ALA:O	18:R:78:GLY:CA	2.51	0.59
23:W:13:MET:HE2	23:W:18:GLN:HA	1.84	0.59
30:0:213:G:N2	30:0:225:G:H2'	2.18	0.59
3:C:77:ALA:C	3:C:78:ARG:CA	2.76	0.58
5:E:126:ILE:HB	5:E:131:LEU:CD2	2.32	0.58
8:H:80:LEU:HD21	8:H:145:ASP:HB3	1.85	0.58
11:K:10:GLN:NE2	11:K:10:GLN:N	2.37	0.58
15:O:53:GLN:HG2	15:O:56:GLU:OE1	2.03	0.58
17:Q:25:PRO:HB2	42:9:9077:HOH:O	2.03	0.58
18:R:39:THR:HB	18:R:42:GLU:CD	2.27	0.58
24:X:43:VAL:HG22	24:X:76:ARG:NH1	2.18	0.58
28:2:25:VAL:O	28:2:29:THR:HG23	2.02	0.58
30:0:559:U:H6	30:0:559:U:H5'	1.66	0.58
14:N:71:TRP:HB2	42:N:8838:HOH:O	2.04	0.58
14:N:86:LEU:HD21	14:N:180:LEU:HD12	1.85	0.58
23:W:122:ARG:NH1	23:W:152:ALA:O	2.35	0.58
25:Y:165:GLU:HB3	42:0:7515:HOH:O	2.03	0.58
30:0:318:U:H5'	30:0:339:A:C2	2.39	0.58
1:A:66:ARG:HB2	1:A:66:ARG:NH1	2.16	0.58
3:C:1:MET:HG2	3:C:2:GLN:N	2.04	0.58
11:K:43:ARG:NH1	30:0:2712:G:OP1	2.35	0.58
17:Q:26:PRO:O	17:Q:30:VAL:HG23	2.03	0.58
30:0:958:G:O2'	30:0:959:C:H5'	2.03	0.58
1:A:55:VAL:HG23	1:A:68:ILE:O	2.03	0.58
2:B:177:HIS:O	2:B:181:ILE:HG13	2.03	0.58
2:B:268:ARG:NH2	2:B:325:PRO:HG3	2.17	0.58
9:I:127:CYS:C	9:I:129:SER:N	2.62	0.58
10:J:77:GLY:C	10:J:78:ILE:CA	2.77	0.58
14:N:96:GLY:O	14:N:98:GLU:HG3	2.04	0.58
14:N:139:TRP:HA	14:N:139:TRP:CE3	2.37	0.58
15:O:14:LEU:CD2	15:O:102:ILE:HD11	2.33	0.58
16:P:16:VAL:HG13	16:P:20:ARG:NH1	2.18	0.58
24:X:47:ALA:HB1	24:X:82:GLU:CB	2.32	0.58
25:Y:134:HIS:HE1	30:0:538:C:OP2	1.86	0.58
30:0:65:C:O2'	30:0:66:G:H5'	2.03	0.58
30:0:1067:A:H5'	42:0:5212:HOH:O	2.04	0.58
30:0:1187:U:O2'	30:0:1189:A:H2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1829:A:C2'	30:0:1830:C:H5'	2.33	0.58
30:0:2392:C:H4'	42:0:5133:HOH:O	2.03	0.58
4:D:58:VAL:HG12	4:D:60:GLU:HG2	1.86	0.58
9:I:129:SER:O	9:I:130:LEU:HD23	2.03	0.58
12:L:140:VAL:HB	42:L:9020:HOH:O	2.03	0.58
13:M:159:VAL:HG12	35:M:8818:CL:CL	2.41	0.58
22:V:50:ARG:HD3	42:V:2826:HOH:O	2.03	0.58
30:0:1527:A:H1'	30:0:1528:A:C8	2.38	0.58
2:B:262:ARG:HD2	30:0:2715:G:O2'	2.03	0.58
3:C:2:GLN:HB3	42:C:8589:HOH:O	2.02	0.58
5:E:84:MET:SD	5:E:168:ILE:HD13	2.43	0.58
12:L:59:GLU:HA	12:L:104:ASP:OD2	2.04	0.58
30:0:459:A:H5''	42:0:2968:HOH:O	2.03	0.58
30:0:1180:U:H1'	42:0:4130:HOH:O	2.04	0.58
30:0:2320:U:H4'	30:0:2321:A:O4'	2.03	0.58
30:0:2667:G:H1'	30:0:2914:A:N3	2.19	0.58
2:B:3:PRO:HG2	42:0:9686:HOH:O	2.02	0.58
4:D:18:ILE:HG12	4:D:134:LEU:HD23	1.84	0.58
4:D:52:THR:HG21	30:0:2346:C:O2'	2.03	0.58
4:D:99:ASP:HB3	4:D:103:ASN:H	1.69	0.58
14:N:61:ALA:HB3	14:N:88:ALA:HB2	1.86	0.58
14:N:139:TRP:HA	14:N:139:TRP:HE3	1.69	0.58
15:O:31:GLU:O	15:O:35:LYS:HG3	2.04	0.58
30:0:221:G:H2'	30:0:222:A:C8	2.39	0.58
30:0:264:G:H1'	30:0:265:U:H5	1.69	0.58
2:B:16:ARG:HB3	2:B:217:ARG:NH2	2.19	0.58
5:E:137:ASP:OD1	5:E:139:GLU:HB2	2.04	0.58
8:H:15:PRO:HG3	30:0:1053:G:OP1	2.03	0.58
13:M:158:ARG:HB2	13:M:163:LEU:HB2	1.86	0.58
14:N:67:ALA:HA	14:N:71:TRP:CB	2.34	0.58
22:V:64:GLY:O	22:V:65:ASP:HB2	2.04	0.58
27:1:45:ARG:HB3	42:1:988:HOH:O	2.02	0.58
30:0:150:G:H1'	42:0:4496:HOH:O	2.04	0.58
30:0:157:G:H3'	42:0:4827:HOH:O	2.03	0.58
30:0:2608:C:H2'	42:0:4456:HOH:O	2.04	0.58
30:0:2670:G:O2'	30:0:2671:U:H5'	2.03	0.58
1:A:107:ASN:OD1	1:A:120:ARG:HD2	2.04	0.58
2:B:320:GLN:NE2	2:B:321:PRO:HD2	2.19	0.58
8:H:165:ARG:HD3	42:H:9040:HOH:O	2.03	0.58
13:M:71:SER:HB2	13:M:92:THR:HG22	1.86	0.58
15:O:14:LEU:HD23	15:O:102:ILE:HD11	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:130:HIS:O	23:W:136:GLY:HA3	2.04	0.58
29:3:28:GLY:HA3	30:0:2434:A:O3'	2.04	0.58
30:0:23:G:H1'	30:0:520:A:N6	2.19	0.58
30:0:1615:A:H5'	42:0:5049:HOH:O	2.04	0.58
30:0:2089:A:O2'	30:0:2090:G:H5'	2.04	0.58
30:0:2239:C:H2'	30:0:2240:U:C6	2.38	0.58
30:0:2314:G:C2'	30:0:2315:C:H5'	2.34	0.58
4:D:40:ILE:HG13	4:D:41:LEU:N	2.19	0.58
23:W:90:TYR:N	23:W:90:TYR:CD1	2.71	0.58
30:0:31:C:H2'	42:0:9479:HOH:O	2.03	0.58
6:F:83:LEU:HD11	6:F:96:ALA:CB	2.34	0.57
13:M:99:ARG:HD2	13:M:167:GLY:HA2	1.86	0.57
14:N:143:ARG:HH21	14:N:169:PRO:HB2	1.68	0.57
25:Y:234:VAL:HG12	25:Y:235:GLU:N	2.19	0.57
30:0:2251:G:H2'	30:0:2252:A:C8	2.38	0.57
3:C:20:ASP:O	3:C:23:GLU:HB2	2.03	0.57
7:G:23:ILE:HG22	7:G:27:ILE:HD11	1.85	0.57
17:Q:32:GLU:O	17:Q:93:ARG:NH2	2.37	0.57
30:0:2312:G:H2'	30:0:2313:C:H5'	1.85	0.57
1:A:187:PRO:HB2	30:0:1845:A:O3'	2.04	0.57
1:A:194:MET:HE3	1:A:199:HIS:CB	2.34	0.57
1:A:199:HIS:HD2	1:A:201:PHE:HB2	1.69	0.57
3:C:184:ARG:NH2	30:0:450:C:OP1	2.37	0.57
6:F:4:VAL:HG13	6:F:76:PHE:CD1	2.38	0.57
28:2:11:LEU:HD22	30:0:1417:G:O2'	2.04	0.57
28:2:20:ARG:HG2	42:2:5444:HOH:O	2.04	0.57
29:3:15:ASN:O	30:0:2408:A:H4'	2.05	0.57
30:0:137:U:H2'	30:0:139:C:C5	2.38	0.57
30:0:2878:U:H2'	30:0:2879:A:O4'	2.04	0.57
2:B:14:GLY:HA2	2:B:15:PRO:C	2.28	0.57
3:C:168:ARG:NH2	3:C:190:ALA:O	2.37	0.57
10:J:107:ASN:ND2	10:J:109:TYR:H	2.02	0.57
16:P:37:ARG:HD2	30:0:1501:A:OP2	2.04	0.57
21:U:52:THR:CG2	21:U:54:THR:HB	2.34	0.57
23:W:55:GLY:HA3	23:W:146:ILE:HG13	1.86	0.57
23:W:110:GLN:HA	23:W:110:GLN:NE2	2.20	0.57
30:0:136:C:H2'	30:0:137:U:O4'	2.04	0.57
30:0:757:C:H2'	30:0:758:A:C8	2.39	0.57
30:0:2896:A:H5''	42:0:6932:HOH:O	2.04	0.57
2:B:85:ARG:NH1	42:B:9110:HOH:O	2.37	0.57
2:B:86:ALA:HA	42:B:9050:HOH:O	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:52:GLN:HG3	10:J:53:ILE:H	1.67	0.57
16:P:77:ALA:O	16:P:78:GLY:CA	2.52	0.57
23:W:35:VAL:HG22	23:W:36:PRO:O	2.05	0.57
23:W:154:ARG:NH1	30:0:588:G:O6	2.37	0.57
30:0:380:A:H2'	42:0:9039:HOH:O	2.03	0.57
11:K:74:VAL:HG13	11:K:113:ILE:CG2	2.29	0.57
12:L:34:GLY:HA3	12:L:38:HIS:CE1	2.38	0.57
12:L:92:ASP:OD1	12:L:94:ARG:HB2	2.04	0.57
14:N:23:ARG:NH1	14:N:27:LEU:HD11	2.18	0.57
23:W:108:ARG:HG3	23:W:114:PRO:HG3	1.85	0.57
25:Y:154:ARG:HH21	30:0:1293:U:H5'	1.70	0.57
26:Z:73:ARG:HG2	26:Z:75:GLY:H	1.69	0.57
30:0:12:U:H2'	30:0:13:G:H5'	1.85	0.57
30:0:619:U:H3'	42:0:4175:HOH:O	2.05	0.57
30:0:1097:A:H2'	30:0:1098:A:C8	2.39	0.57
30:0:1249:U:H2'	30:0:1250:C:H6	1.68	0.57
33:6:76:8AN:N3	42:6:80:HOH:O	2.32	0.57
1:A:105:VAL:HG12	1:A:106:CYS:N	2.20	0.57
2:B:314:ALA:HB3	2:B:317:PRO:HG3	1.87	0.57
4:D:103:ASN:ND2	4:D:134:LEU:H	2.02	0.57
13:M:92:THR:HB	30:0:401:C:O2'	2.05	0.57
23:W:64:THR:O	23:W:68:THR:HG22	2.05	0.57
30:0:1946:C:H2'	30:0:1971:G:C8	2.40	0.57
30:0:2032:U:H2'	30:0:2033:G:H5''	1.87	0.57
1:A:34:ASP:C	1:A:36:ASP:H	2.12	0.57
1:A:117:LYS:HA	42:A:9015:HOH:O	2.05	0.57
2:B:87:TYR:OH	2:B:163:GLU:OE2	2.16	0.57
6:F:13:GLU:OE1	6:F:77:VAL:HG13	2.04	0.57
9:I:69:PRO:HA	30:0:1164:U:OP1	2.05	0.57
13:M:77:HIS:C	13:M:78:LYS:CA	2.78	0.57
14:N:86:LEU:HD12	14:N:125:ALA:HB2	1.87	0.57
14:N:176:ARG:HG2	14:N:180:LEU:HD13	1.86	0.57
30:0:1165:G:O2'	30:0:1174:A:H4'	2.05	0.57
19:S:55:GLN:NE2	30:0:1446:U:H2'	2.19	0.57
19:S:57:THR:HG22	19:S:59:ASP:N	2.20	0.57
29:3:36:ILE:HG23	29:3:37:ASP:N	2.19	0.57
30:0:447:A:O2'	30:0:448:G:H5'	2.04	0.57
2:B:56:ASP:OD1	2:B:322:ARG:HB3	2.05	0.57
23:W:60:GLU:O	23:W:63:GLU:HB2	2.05	0.57
30:0:941:G:O2'	30:0:942:U:H5'	2.04	0.57
30:0:1624:A:H4'	30:0:1626:A:H5''	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2301:A:H5''	30:0:2302:A:H5'	1.86	0.57
3:C:181:ALA:HA	42:T:2331:HOH:O	2.04	0.56
9:I:123:VAL:C	9:I:125:GLY:H	2.13	0.56
15:O:14:LEU:CG	15:O:102:ILE:HD11	2.35	0.56
20:T:71:VAL:CG1	20:T:90:PRO:HB3	2.33	0.56
23:W:115:THR:HG22	23:W:116:LEU:N	2.20	0.56
23:W:122:ARG:HH12	23:W:154:ARG:N	2.03	0.56
30:0:699:C:H2'	30:0:744:G:O4'	2.05	0.56
30:0:710:G:O2'	30:0:711:G:H5'	2.05	0.56
30:0:1278:A:H4'	30:0:1279:U:C4	2.40	0.56
30:0:1342:C:O2'	30:0:1343:C:H5'	2.05	0.56
30:0:1482:A:O2'	30:0:1483:C:H5'	2.04	0.56
30:0:2011:A:H5'	30:0:2013:G:H1'	1.85	0.56
6:F:50:VAL:HG21	6:F:63:ILE:HG21	1.86	0.56
27:1:15:THR:HG1	30:0:777:U:H5	1.53	0.56
30:0:1118:A:C8	30:0:1119:G:H5''	2.37	0.56
30:0:1364:G:H1'	42:0:5657:HOH:O	2.05	0.56
2:B:8:LYS:HG3	2:B:220:VAL:HG12	1.87	0.56
2:B:141:ARG:HD2	2:B:163:GLU:OE2	2.05	0.56
2:B:162:MET:HB2	2:B:310:ARG:NH1	2.21	0.56
7:G:63:ARG:O	7:G:67:LEU:HG	2.04	0.56
13:M:102:GLU:OE1	13:M:164:THR:HG21	2.05	0.56
15:O:77:ALA:HA	15:O:96:VAL:O	2.05	0.56
19:S:57:THR:HG22	19:S:58:MET:N	2.21	0.56
30:0:255:A:H2'	30:0:256:C:C6	2.41	0.56
30:0:1419:U:H2'	30:0:1685:A:C2	2.39	0.56
4:D:167:GLU:OE2	4:D:173:GLU:HB3	2.05	0.56
11:K:109:LEU:CD1	11:K:113:ILE:HD11	2.33	0.56
13:M:82:ARG:O	13:M:84:LYS:N	2.38	0.56
16:P:83:LYS:HG2	30:0:793:A:H5''	1.88	0.56
16:P:91:LYS:O	16:P:95:GLU:HG3	2.05	0.56
30:0:499:G:O2'	30:0:500:G:H5'	2.05	0.56
30:0:1279:U:O2	30:0:1279:U:H2'	2.06	0.56
1:A:77:GLY:C	1:A:78:ASP:CA	2.79	0.56
8:H:23:ILE:HG22	8:H:123:ILE:HD11	1.88	0.56
14:N:23:ARG:NH2	31:9:7:G:H4'	2.21	0.56
16:P:82:GLY:O	30:0:1761:U:H4'	2.04	0.56
20:T:26:THR:HG23	20:T:97:ARG:HG3	1.87	0.56
30:0:334:G:H2'	30:0:335:U:O4'	2.05	0.56
30:0:1730:G:C5'	30:0:1731:C:C6	2.89	0.56
1:A:51:ARG:HD2	30:0:1874:U:OP1	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD13	1:A:100:PRO:HD3	1.88	0.56
1:A:217:ARG:HG2	1:A:229:ALA:HB2	1.88	0.56
12:L:55:GLN:CA	12:L:58:GLN:HE21	2.17	0.56
18:R:71:LYS:HE2	30:0:2831:C:O3'	2.05	0.56
30:0:69:A:H5'	30:0:69:A:C8	2.40	0.56
30:0:706:G:N2	30:0:707:C:H41	2.04	0.56
30:0:1346:U:H2'	30:0:1347:U:C6	2.41	0.56
3:C:127:ARG:HD2	3:C:229:PRO:O	2.05	0.56
6:F:50:VAL:HG13	6:F:60:VAL:HG11	1.86	0.56
13:M:60:VAL:HG22	13:M:134:ILE:HD12	1.87	0.56
18:R:40:ALA:O	18:R:43:ALA:HB3	2.05	0.56
30:0:119:A:H2'	30:0:120:A:C5'	2.36	0.56
1:A:9:ARG:HG2	1:A:16:PHE:CD2	2.41	0.56
2:B:206:THR:CG2	30:0:2716:G:H5''	2.30	0.56
2:B:243:ASN:HA	2:B:244:PRO:C	2.29	0.56
3:C:149:LYS:NZ	30:0:327:A:OP1	2.38	0.56
13:M:58:GLN:NE2	30:0:259:G:H21	2.03	0.56
24:X:23:HIS:HE1	30:0:2044:G:OP1	1.89	0.56
30:0:137:U:OP1	30:0:259:G:O2'	2.24	0.56
30:0:1342:C:C2'	30:0:1343:C:H5'	2.36	0.56
31:9:54:A:O2'	31:9:55:U:H5'	2.06	0.56
2:B:144:THR:HB	42:B:9099:HOH:O	2.03	0.56
11:K:1:MET:HE3	11:K:120:ARG:NH1	2.20	0.56
12:L:91:VAL:CG1	12:L:120:LEU:HD23	2.36	0.56
12:L:108:VAL:HB	12:L:125:PHE:CD2	2.41	0.56
14:N:24:LEU:HD13	17:Q:26:PRO:HB3	1.86	0.56
30:0:622:G:O2'	30:0:623:U:H5'	2.05	0.56
30:0:2353:A:H4'	30:0:2354:A:O5'	2.05	0.56
1:A:204:GLY:N	30:0:2634:G:OP2	2.38	0.56
8:H:61:ARG:HH11	8:H:61:ARG:HG3	1.69	0.56
10:J:25:GLN:NE2	10:J:116:LEU:HB3	2.20	0.56
10:J:93:ARG:O	10:J:96:GLU:HB2	2.06	0.56
20:T:81:LYS:HG3	20:T:87:VAL:HG13	1.88	0.56
25:Y:112:GLU:CD	25:Y:115:ARG:HH12	2.13	0.56
30:0:637:C:H2'	30:0:638:C:C6	2.41	0.56
1:A:32:VAL:HG12	1:A:34:ASP:H	1.70	0.55
2:B:132:HIS:NE2	2:B:171:VAL:HG23	2.21	0.55
8:H:34:HIS:HD2	8:H:90:LEU:O	1.88	0.55
12:L:120:LEU:HD12	12:L:133:VAL:HG21	1.87	0.55
17:Q:16:ASN:HB2	42:0:7765:HOH:O	2.06	0.55
19:S:11:THR:O	19:S:14:ALA:HB3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:187:VAL:CG1	25:Y:205:ILE:HA	2.36	0.55
30:0:612:U:H2'	30:0:613:C:C6	2.41	0.55
30:0:2439:C:H5'	42:0:6330:HOH:O	2.06	0.55
5:E:31:ARG:NH1	5:E:68:HIS:CG	2.73	0.55
6:F:53:ASP:OD1	6:F:80:GLN:HB2	2.07	0.55
12:L:13:HIS:HB3	42:L:9060:HOH:O	2.05	0.55
13:M:12:TRP:O	13:M:15:PRO:HD3	2.06	0.55
16:P:36:THR:O	16:P:40:VAL:HG23	2.05	0.55
30:0:2507:G:H2'	30:0:2510:C:H42	1.71	0.55
1:A:211:LYS:O	30:0:1943:C:H4'	2.06	0.55
4:D:60:GLU:O	4:D:60:GLU:HG3	2.07	0.55
5:E:7:ILE:HD11	5:E:11:VAL:O	2.07	0.55
5:E:36:PRO:HD3	10:J:127:ILE:HG13	1.89	0.55
7:G:63:ARG:N	42:G:2569:HOH:O	2.39	0.55
11:K:87:ARG:NH2	30:0:2720:C:O2	2.39	0.55
24:X:74:ALA:CA	24:X:85:VAL:HG13	2.37	0.55
29:3:22:VAL:HG11	29:3:67:LEU:HD13	1.88	0.55
29:3:70:ARG:HB3	42:3:9062:HOH:O	2.06	0.55
1:A:43:VAL:HG21	1:A:59:GLU:HG3	1.87	0.55
2:B:254:GLN:HG2	2:B:255:GLY:N	2.21	0.55
8:H:30:LYS:N	8:H:62:HIS:HD2	1.96	0.55
10:J:12:VAL:HG21	10:J:116:LEU:HD11	1.88	0.55
23:W:91:ASP:HB2	42:W:5425:HOH:O	2.06	0.55
30:0:553:G:H5'	42:0:4389:HOH:O	2.06	0.55
2:B:24:PRO:CG	2:B:204:GLY:HA2	2.36	0.55
2:B:274:GLU:HA	2:B:292:GLY:O	2.06	0.55
3:C:207:LEU:HB2	3:C:210:ALA:HB2	1.87	0.55
6:F:65:GLU:HB3	42:F:5163:HOH:O	2.06	0.55
8:H:69:ARG:HD3	42:H:9037:HOH:O	2.05	0.55
13:M:178:LYS:HB2	42:0:7686:HOH:O	2.06	0.55
14:N:74:PRO:HG2	14:N:159:TYR:CE1	2.42	0.55
19:S:77:VAL:C	19:S:78:ALA:CA	2.80	0.55
25:Y:174:VAL:HG13	25:Y:177:LYS:HD2	1.88	0.55
30:0:624:U:H3'	42:0:5060:HOH:O	2.07	0.55
30:0:1701:A:H4'	30:0:1702:U:C5'	2.37	0.55
2:B:98:THR:HG21	2:B:127:GLN:OE1	2.06	0.55
4:D:24:HIS:HB2	4:D:72:LYS:HA	1.88	0.55
4:D:25:MET:SD	4:D:40:ILE:HD11	2.47	0.55
6:F:19:ALA:O	6:F:22:VAL:HG22	2.07	0.55
8:H:96:GLN:NE2	8:H:129:ARG:NH2	2.55	0.55
13:M:12:TRP:CD2	13:M:45:ARG:HD2	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:11:ALA:HB1	16:P:16:VAL:O	2.06	0.55
18:R:113:HIS:HB3	18:R:146:ILE:HD12	1.89	0.55
23:W:4:LEU:HD22	23:W:52:VAL:HB	1.88	0.55
27:1:1:THR:O	30:0:1836:A:H1'	2.07	0.55
30:0:292:G:H1'	30:0:360:A:H61	1.72	0.55
30:0:2562:G:H4'	42:0:5081:HOH:O	2.07	0.55
30:0:2828:G:O5'	30:0:2828:G:H8	1.90	0.55
1:A:2:ARG:HD3	1:A:198:ASP:OD1	2.06	0.55
3:C:246:ARG:HD2	42:C:8576:HOH:O	2.07	0.55
42:C:8562:HOH:O	15:O:3:THR:HG21	2.06	0.55
5:E:77:THR:O	5:E:78:GLU:CA	2.55	0.55
13:M:146:ASP:O	13:M:147:LEU:HD23	2.06	0.55
14:N:21:HIS:HB2	42:N:8831:HOH:O	2.07	0.55
16:P:74:GLN:HG2	30:0:1786:C:OP1	2.06	0.55
23:W:88:THR:HG22	23:W:89:ASP:H	1.71	0.55
24:X:23:HIS:NE2	24:X:24:LYS:HD2	2.21	0.55
29:3:11:CYS:HB2	29:3:20:HIS:NE2	2.21	0.55
30:0:1260:G:H3'	30:0:1261:A:N7	2.21	0.55
30:0:2032:U:H2'	30:0:2033:G:C5'	2.37	0.55
30:0:2115:U:H2'	30:0:2116:U:C6	2.41	0.55
31:9:76:G:H3'	31:9:77:A:C5'	2.20	0.55
1:A:66:ARG:NH1	1:A:66:ARG:CB	2.69	0.55
22:V:20:LEU:HD22	22:V:60:GLN:HE22	1.71	0.55
30:0:2401:A:H2'	30:0:2402:A:C8	2.42	0.55
1:A:32:VAL:HG12	1:A:34:ASP:N	2.22	0.55
1:A:69:LEU:HD21	1:A:120:ARG:HB3	1.88	0.55
1:A:82:VAL:HA	1:A:93:THR:O	2.07	0.55
1:A:189:VAL:HA	30:0:1845:A:OP1	2.07	0.55
2:B:36:PRO:HA	2:B:168:GLY:CA	2.25	0.55
5:E:91:PHE:CE1	30:0:2694:A:H4'	2.42	0.55
6:F:4:VAL:HG13	6:F:76:PHE:CE1	2.42	0.55
8:H:23:ILE:CG2	8:H:123:ILE:HD11	2.37	0.55
28:2:10:ARG:NH2	30:0:121:U:OP2	2.40	0.55
1:A:65:ARG:C	1:A:66:ARG:HG3	2.32	0.55
2:B:18:ARG:HG3	2:B:256:GLN:HG3	1.89	0.55
3:C:227:GLY:O	3:C:229:PRO:HD3	2.07	0.55
4:D:172:VAL:HG12	4:D:173:GLU:N	2.13	0.55
8:H:139:ALA:HB3	8:H:149:VAL:HG21	1.88	0.55
18:R:120:GLY:HA3	42:R:8961:HOH:O	2.07	0.55
25:Y:149:GLN:HE22	30:0:1293:U:H4'	1.72	0.55
30:0:307:G:H3'	30:0:342:C:OP2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:841:A:H5''	42:0:7724:HOH:O	2.07	0.55
30:0:1529:G:H5'	42:0:9193:HOH:O	2.05	0.55
2:B:75:GLU:OE2	2:B:151:VAL:HG13	2.07	0.54
5:E:36:PRO:HD3	10:J:127:ILE:HD12	1.87	0.54
14:N:37:ARG:NE	42:N:8833:HOH:O	2.39	0.54
18:R:82:GLU:O	18:R:86:LYS:HG3	2.07	0.54
28:2:8:LYS:NZ	30:0:1677:U:OP2	2.36	0.54
10:J:80:LYS:HE2	10:J:98:PHE:CZ	2.43	0.54
12:L:14:GLY:O	30:0:1295:G:H5''	2.06	0.54
13:M:84:LYS:HE2	42:0:5258:HOH:O	2.08	0.54
23:W:4:LEU:HD22	23:W:52:VAL:HG11	1.89	0.54
30:0:107:U:H2'	30:0:108:U:H5'	1.89	0.54
30:0:905:C:H3'	42:0:6033:HOH:O	2.06	0.54
30:0:945:U:H2'	30:0:946:C:C6	2.42	0.54
30:0:1681:G:H5''	30:0:1682:A:H5'	1.88	0.54
30:0:2502:C:C2'	30:0:2503:A:H5'	2.37	0.54
1:A:95:PRO:HA	1:A:153:ARG:HA	1.90	0.54
2:B:80:ARG:HB2	2:B:145:HIS:CE1	2.42	0.54
3:C:165:ASP:O	3:C:168:ARG:HB3	2.06	0.54
15:O:63:LYS:HG3	15:O:80:ASP:O	2.07	0.54
22:V:39:ALA:N	22:V:40:PRO:CD	2.70	0.54
30:0:1198:U:H2'	30:0:1200:A:OP2	2.07	0.54
30:0:1730:G:C5'	30:0:1731:C:H6	2.20	0.54
30:0:2072:G:C6	30:0:2533:C:H1'	2.43	0.54
30:0:2783:A:H3'	42:0:6077:HOH:O	2.08	0.54
1:A:125:ASN:CB	1:A:158:VAL:HG12	2.38	0.54
3:C:80:VAL:HA	42:C:8554:HOH:O	2.08	0.54
3:C:206:ASN:HB2	30:0:329:A:OP2	2.07	0.54
5:E:81:GLU:O	5:E:172:PRO:HD3	2.07	0.54
9:I:70:THR:HG21	42:I:5331:HOH:O	2.08	0.54
9:I:114:TYR:HE1	30:0:1186:C:H4'	1.72	0.54
13:M:24:GLN:NE2	13:M:24:GLN:HA	2.23	0.54
18:R:100:ASP:C	18:R:102:GLN:H	2.16	0.54
19:S:15:MET:O	19:S:18:MET:HB3	2.07	0.54
20:T:48:VAL:HG21	20:T:96:VAL:CG1	2.37	0.54
22:V:5:VAL:HG23	42:V:2271:HOH:O	2.07	0.54
24:X:71:ARG:HD3	42:X:7542:HOH:O	2.07	0.54
30:0:666:A:H2'	30:0:667:C:O4'	2.08	0.54
30:0:1447:U:H3'	30:0:1506:U:O2	2.07	0.54
30:0:1632:A:H2'	30:0:1633:C:H5'	1.90	0.54
30:0:2326:C:H4'	30:0:2412:G:H4'	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2697:A:H2'	30:0:2698:G:O4'	2.08	0.54
2:B:2:GLN:NE2	30:0:2545:U:OP2	2.41	0.54
3:C:235:PHE:CE2	3:C:243:VAL:HG21	2.41	0.54
4:D:36:ASN:HA	42:D:7500:HOH:O	2.07	0.54
15:O:77:ALA:C	15:O:78:ALA:CA	2.81	0.54
15:O:99:GLU:HG3	42:O:6044:HOH:O	2.07	0.54
21:U:20:MET:HE2	21:U:28:THR:HG21	1.89	0.54
22:V:12:THR:HG22	22:V:15:GLU:CD	2.31	0.54
23:W:52:VAL:HG23	23:W:53:ALA:N	1.64	0.54
26:Z:105:ARG:O	26:Z:106:SER:C	2.50	0.54
28:2:48:ASP:O	28:2:49:GLU:HB2	2.08	0.54
30:0:485:A:N3	30:0:487:G:H5''	2.22	0.54
30:0:589:U:H2'	30:0:590:A:C8	2.41	0.54
30:0:631:A:C6	30:0:2074:A:H5'	2.43	0.54
30:0:1647:G:O2'	30:0:1648:G:H5'	2.08	0.54
30:0:1839:A:H5'	30:0:2643:G:H4'	1.89	0.54
31:9:30:C:H42	31:9:50:G:H1	1.55	0.54
1:A:94:LEU:HG	1:A:99:ILE:HD11	1.88	0.54
2:B:52:VAL:C	2:B:53:LEU:HD12	2.33	0.54
2:B:98:THR:HG22	30:0:2820:A:OP1	2.07	0.54
2:B:212:GLN:HA	30:0:1733:A:H4'	1.89	0.54
3:C:58:ALA:HA	3:C:73:GLN:NE2	2.22	0.54
4:D:77:ASP:C	4:D:78:GLU:CA	2.81	0.54
8:H:59:GLN:HE21	8:H:129:ARG:HG2	1.73	0.54
11:K:82:ARG:NH2	11:K:115:ARG:HG2	2.22	0.54
18:R:106:GLY:HA2	18:R:109:MET:CE	2.33	0.54
24:X:30:MET:HE1	24:X:58:ALA:CB	2.38	0.54
30:0:1189:A:H1'	30:0:1209:C:H1'	1.90	0.54
14:N:64:SER:C	14:N:66:LEU:H	2.15	0.54
18:R:98:ASN:HD22	18:R:98:ASN:N	2.06	0.54
22:V:1:THR:C	22:V:3:LEU:N	2.65	0.54
25:Y:136:LYS:HB3	25:Y:139:VAL:HG23	1.90	0.54
25:Y:203:VAL:HG12	25:Y:228:VAL:HG22	1.88	0.54
30:0:304:G:H1'	30:0:347:A:H61	1.73	0.54
30:0:1298:U:H2'	30:0:1299:G:C8	2.42	0.54
30:0:2042:U:H2'	30:0:2043:U:C6	2.42	0.54
30:0:2281:C:C2'	30:0:2282:U:H5'	2.37	0.54
14:N:37:ARG:HH12	31:9:6:C:C5'	2.00	0.54
20:T:77:VAL:C	20:T:78:THR:CA	2.81	0.54
23:W:27:HIS:CD2	30:0:1288:U:H4'	2.43	0.54
30:0:407:A:H2'	30:0:408:A:C8	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:602:A:O2'	30:0:605:C:H4'	2.07	0.54
30:0:1666:C:H2'	30:0:1667:A:C5'	2.37	0.54
30:0:2502:C:N3	30:0:2518:C:N4	2.55	0.54
18:R:132:ARG:HH21	30:0:2055:A:H4'	1.69	0.54
20:T:28:SER:CA	20:T:97:ARG:HD3	2.35	0.54
30:0:90:A:H2'	30:0:91:G:O4'	2.07	0.54
30:0:187:A:H3'	30:0:188:C:H6	1.73	0.54
30:0:2032:U:C2'	30:0:2033:G:H5''	2.38	0.54
11:K:9:THR:O	11:K:10:GLN:C	2.51	0.54
11:K:98:VAL:HG13	11:K:102:GLU:HA	1.87	0.54
13:M:122:GLN:OE1	13:M:127:LYS:HE2	2.07	0.54
16:P:77:ALA:C	16:P:78:GLY:CA	2.81	0.54
27:1:46:ARG:HA	42:0:3919:HOH:O	2.07	0.54
29:3:84:ARG:HB3	42:3:9041:HOH:O	2.08	0.54
30:0:1834:C:H2'	30:0:1840:A:H62	1.72	0.54
31:9:78:G:H1'	31:9:78:G:N3	2.22	0.54
1:A:204:GLY:O	1:A:205:GLY:C	2.51	0.53
2:B:333:GLU:HB2	21:U:14:GLU:OE2	2.09	0.53
9:I:88:GLN:HA	9:I:91:PHE:HE2	1.73	0.53
14:N:62:HIS:HB3	14:N:65:ASP:OD1	2.08	0.53
19:S:34:LYS:HG2	19:S:54:THR:HG23	1.89	0.53
30:0:877:G:H1'	42:0:3080:HOH:O	2.07	0.53
30:0:2332:A:H3'	30:0:2333:G:H8	1.73	0.53
30:0:2526:C:O2'	30:0:2527:U:H5'	2.09	0.53
30:0:2824:C:O3'	30:0:2825:C:H6	1.91	0.53
1:A:173:GLY:O	1:A:176:HIS:HB3	2.07	0.53
2:B:244:PRO:HB3	30:0:1234:U:N3	2.23	0.53
8:H:66:GLU:HA	42:H:9037:HOH:O	2.07	0.53
8:H:174:LEU:HD11	30:0:1220:U:H4'	1.90	0.53
13:M:84:LYS:HB2	30:0:170:U:OP1	2.08	0.53
17:Q:77:ASP:C	17:Q:78:GLY:CA	2.82	0.53
18:R:99:ALA:CB	18:R:109:MET:HE1	2.36	0.53
25:Y:138:ARG:NH1	30:0:638:C:OP2	2.38	0.53
30:0:812:A:H2'	30:0:813:C:C6	2.43	0.53
30:0:1940:C:H4'	42:0:9153:HOH:O	2.07	0.53
2:B:53:LEU:HD21	2:B:270:ILE:HG23	1.91	0.53
5:E:91:PHE:HE1	30:0:2694:A:H4'	1.72	0.53
18:R:9:ASP:O	18:R:13:THR:HG22	2.08	0.53
23:W:65:VAL:HA	23:W:68:THR:HG22	1.90	0.53
23:W:137:GLN:HG3	23:W:137:GLN:O	2.08	0.53
30:0:138:U:H5''	30:0:139:C:OP2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:705:C:H3'	30:0:706:G:H8	1.73	0.53
3:C:139:VAL:HG12	42:C:8645:HOH:O	2.08	0.53
5:E:81:GLU:HG2	5:E:134:SER:CB	2.33	0.53
23:W:115:THR:HB	42:W:6871:HOH:O	2.09	0.53
30:0:690:G:H4'	30:0:741:C:O2	2.09	0.53
30:0:1947:G:H2'	30:0:1948:G:H8	1.71	0.53
1:A:212:PRO:HA	30:0:1943:C:O4'	2.08	0.53
4:D:23:VAL:HG21	4:D:45:THR:HG21	1.89	0.53
6:F:20:LEU:HB2	6:F:49:PHE:CZ	2.43	0.53
9:I:91:PHE:HD2	9:I:131:GLY:HA2	1.74	0.53
16:P:89:ASN:HB3	16:P:92:GLU:HB2	1.91	0.53
23:W:39:ASP:HB2	42:W:3580:HOH:O	2.09	0.53
30:0:708:A:H2'	30:0:709:G:O4'	2.08	0.53
30:0:1118:A:C8	30:0:1118:A:C3'	2.91	0.53
30:0:1160:G:H5'	30:0:1161:A:C4'	2.38	0.53
30:0:2761:A:H2'	42:0:6484:HOH:O	2.08	0.53
30:0:2802:C:H2'	30:0:2803:C:C6	2.44	0.53
1:A:179:MET:C	1:A:181:ALA:H	2.17	0.53
1:A:194:MET:SD	30:0:875:A:C2	3.02	0.53
3:C:1:MET:HG2	3:C:2:GLN:HE21	1.74	0.53
3:C:37:ALA:O	3:C:38:ALA:C	2.51	0.53
3:C:233:THR:CG2	3:C:234:VAL:H	2.16	0.53
6:F:58:GLU:OE2	13:M:27:ARG:NH2	2.40	0.53
13:M:91:ILE:HD13	42:0:4059:HOH:O	2.08	0.53
14:N:80:SER:HB2	42:N:8835:HOH:O	2.07	0.53
23:W:55:GLY:CA	23:W:146:ILE:HG13	2.38	0.53
26:Z:54:GLU:HB2	42:Z:8712:HOH:O	2.09	0.53
30:0:78:G:N2	30:0:78:G:N1	2.56	0.53
30:0:354:A:H2'	30:0:355:C:C6	2.43	0.53
30:0:2239:C:H2'	30:0:2240:U:H6	1.74	0.53
30:0:2420:G:H4'	42:0:4965:HOH:O	2.09	0.53
30:0:2748:G:H4'	30:0:2749:U:C5'	2.39	0.53
1:A:38:ILE:HG22	1:A:38:ILE:O	2.08	0.53
1:A:179:MET:HG2	1:A:186:TRP:CB	2.38	0.53
2:B:36:PRO:HB3	2:B:174:ARG:HB3	1.90	0.53
8:H:168:VAL:HG13	42:H:9015:HOH:O	2.08	0.53
11:K:76:GLN:HA	11:K:93:ASN:HA	1.90	0.53
12:L:90:ARG:NH2	12:L:121:ILE:HD11	2.24	0.53
13:M:99:ARG:CD	13:M:167:GLY:HA2	2.39	0.53
15:O:59:VAL:HG23	15:O:111:VAL:HG21	1.91	0.53
18:R:111:ILE:HG23	18:R:145:LEU:HD11	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:10:VAL:HG11	22:V:36:ALA:CB	2.36	0.53
19:S:23:LYS:HE2	42:O:5526:HOH:O	2.09	0.53
20:T:105:ASP:OD2	20:T:107:LYS:HB2	2.08	0.53
23:W:151:GLU:O	23:W:154:ARG:HB2	2.08	0.53
30:O:855:U:H4'	30:O:856:G:O4'	2.08	0.53
30:O:2698:G:H2'	30:O:2699:A:C8	2.44	0.53
1:A:190:ARG:HD2	30:O:1884:G:O6	2.09	0.53
1:A:207:GLN:O	1:A:208:HIS:HB3	2.07	0.53
1:A:211:LYS:NZ	1:A:223:ARG:HH21	2.07	0.53
2:B:8:LYS:HB3	2:B:218:TRP:O	2.08	0.53
2:B:56:ASP:HB3	2:B:322:ARG:HH21	1.74	0.53
13:M:107:ARG:HG3	13:M:107:ARG:NH1	2.23	0.53
14:N:37:ARG:NH1	31:9:6:C:OP1	2.42	0.53
42:N:8841:HOH:O	17:Q:19:ARG:HD2	2.09	0.53
23:W:39:ASP:OD1	23:W:42:ARG:NH2	2.42	0.53
25:Y:152:LYS:CB	25:Y:160:LYS:HG3	2.38	0.53
30:O:78:G:N3	30:O:78:G:N9	2.57	0.53
30:O:820:G:O2'	30:O:856:G:H4'	2.09	0.53
30:O:839:C:H1'	42:O:6899:HOH:O	2.07	0.53
2:B:171:VAL:HG23	2:B:172:SER:N	2.24	0.53
2:B:304:PRO:HD2	2:B:307:ARG:NE	2.23	0.53
3:C:142:ASP:OD1	3:C:236:THR:HG23	2.08	0.53
9:I:130:LEU:HD22	30:O:1167:G:H4'	1.91	0.53
10:J:131:THR:HG22	10:J:133:GLY:N	2.24	0.53
15:O:3:THR:CB	30:O:656:G:H5'	2.34	0.53
42:P:6012:HOH:O	30:O:1548:U:H4'	2.07	0.53
23:W:21:LEU:HD13	23:W:26:ILE:HD11	1.91	0.53
23:W:117:ARG:HB3	23:W:117:ARG:HH11	1.74	0.53
30:O:482:G:H4'	30:O:508:A:N1	2.23	0.53
30:O:858:U:H2'	30:O:859:C:C6	2.43	0.53
30:O:1165:G:H4'	30:O:1174:A:O2'	2.08	0.53
30:O:2587:OMU:H2'	30:O:2589:U:H5''	1.90	0.53
1:A:37:VAL:HG23	42:A:9074:HOH:O	2.09	0.53
1:A:199:HIS:CD2	1:A:201:PHE:HB2	2.44	0.53
2:B:5:ARG:HD2	2:B:8:LYS:HE2	1.91	0.53
4:D:172:VAL:CG1	4:D:173:GLU:H	2.15	0.53
12:L:54:PRO:HG2	12:L:57:VAL:HG21	1.89	0.53
12:L:77:ALA:C	12:L:79:ASP:H	2.17	0.53
13:M:67:VAL:HG11	13:M:97:ILE:HG23	1.91	0.53
14:N:77:ASN:OD1	14:N:79:PRO:HD2	2.09	0.53
16:P:103:THR:HA	16:P:106:ARG:HH12	1.68	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:15:LYS:HE3	42:R:8986:HOH:O	2.09	0.53
19:S:33:SER:OG	19:S:36:GLU:HG3	2.09	0.53
30:0:1181:A:H2'	30:0:1182:C:H5'	1.91	0.53
30:0:2274:A:O2'	30:0:2275:G:H5'	2.09	0.53
30:0:2562:G:H1'	42:0:6532:HOH:O	2.09	0.53
2:B:122:ASP:O	2:B:126:GLU:HB2	2.09	0.52
2:B:294:TYR:CD1	2:B:294:TYR:C	2.87	0.52
5:E:84:MET:CG	5:E:168:ILE:HD13	2.39	0.52
6:F:99:THR:HG23	6:F:99:THR:O	2.09	0.52
8:H:14:LYS:HB3	42:H:9007:HOH:O	2.09	0.52
13:M:115:LEU:HD13	13:M:116:ASN:HB2	1.91	0.52
14:N:27:LEU:HD22	14:N:50:LEU:HD22	1.91	0.52
16:P:55:LYS:HG2	16:P:56:GLY:N	2.23	0.52
20:T:30:ASP:O	20:T:33:GLU:HB3	2.10	0.52
24:X:45:GLU:HG3	42:X:6178:HOH:O	2.09	0.52
25:Y:193:LEU:CD1	25:Y:221:ALA:HB2	2.39	0.52
29:3:80:ARG:O	30:0:2457:U:H4'	2.10	0.52
30:0:558:C:O2'	30:0:559:U:H5''	2.09	0.52
30:0:1218:U:H2'	30:0:1219:U:H6	1.73	0.52
30:0:1445:G:N2	30:0:1678:A:H1'	2.23	0.52
30:0:2414:A:H2'	30:0:2415:A:C8	2.43	0.52
30:0:2786:G:H2'	42:0:7991:HOH:O	2.10	0.52
30:0:2880:A:H2'	30:0:2881:C:H5'	1.91	0.52
3:C:236:THR:HA	42:C:8648:HOH:O	2.07	0.52
5:E:106:ASN:ND2	5:E:109:GLY:HA2	2.25	0.52
8:H:33:GLN:H	8:H:69:ARG:NH1	2.07	0.52
9:I:98:ASP:OD1	9:I:101:LYS:HD2	2.09	0.52
17:Q:77:ASP:O	17:Q:78:GLY:C	2.51	0.52
30:0:948:G:O2'	30:0:949:U:H5'	2.08	0.52
30:0:2584:G:H8	42:0:5461:HOH:O	1.91	0.52
1:A:186:TRP:CG	1:A:187:PRO:HA	2.44	0.52
2:B:171:VAL:HG23	2:B:172:SER:H	1.74	0.52
3:C:18:LEU:HD12	3:C:19:PRO:HD2	1.91	0.52
6:F:2:VAL:HG22	6:F:57:GLU:OE1	2.08	0.52
10:J:130:VAL:HG12	10:J:131:THR:H	1.72	0.52
30:0:1496:A:H2'	30:0:1497:G:O4'	2.09	0.52
30:0:1902:G:H2'	30:0:1903:U:O4'	2.10	0.52
30:0:2613:G:O2'	30:0:2614:C:H5'	2.09	0.52
1:A:96:LEU:CD2	1:A:128:LEU:HD22	2.39	0.52
3:C:123:LEU:O	3:C:126:ASP:N	2.42	0.52
4:D:21:VAL:HG23	4:D:80:ALA:HB1	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:ASP:HB3	4:D:103:ASN:HB2	1.90	0.52
4:D:136:ARG:NH1	4:D:156:ARG:O	2.41	0.52
5:E:14:GLU:O	5:E:15:GLN:HB2	2.09	0.52
10:J:14:ALA:O	10:J:17:CYS:HB2	2.10	0.52
11:K:96:VAL:HG21	11:K:109:LEU:HD22	1.92	0.52
18:R:18:LEU:HG	18:R:91:LEU:HD13	1.92	0.52
18:R:114:VAL:HB	18:R:145:LEU:CD1	2.36	0.52
19:S:57:THR:HG22	19:S:59:ASP:H	1.73	0.52
21:U:11:THR:HG22	21:U:53:ASP:CG	2.34	0.52
25:Y:107:PRO:HD3	25:Y:182:PHE:CD1	2.44	0.52
30:0:195:C:H2'	30:0:196:G:H5'	1.92	0.52
30:0:583:C:H2'	30:0:584:U:H6	1.75	0.52
30:0:2432:C:O2'	30:0:2433:A:H5'	2.10	0.52
30:0:2505:G:C2'	30:0:2506:A:H5'	2.39	0.52
30:0:2634:G:O2'	30:0:2635:A:H5'	2.09	0.52
2:B:145:HIS:HD2	2:B:146:THR:O	1.92	0.52
2:B:336:GLN:O	30:0:2862:G:H4'	2.10	0.52
4:D:99:ASP:OD2	4:D:101:THR:HB	2.08	0.52
13:M:139:PRO:HA	13:M:142:GLN:HB2	1.92	0.52
14:N:82:TYR:OH	14:N:176:ARG:NH1	2.43	0.52
20:T:66:ASP:OD1	20:T:69:LYS:N	2.34	0.52
30:0:462:A:N6	30:0:477:A:C2	2.77	0.52
30:0:578:C:H2'	30:0:579:G:O4'	2.10	0.52
30:0:1819:G:H2'	30:0:1820:G:C5'	2.40	0.52
30:0:2768:A:O2'	30:0:2769:C:H5'	2.10	0.52
1:A:217:ARG:CG	1:A:217:ARG:NH1	2.70	0.52
4:D:49:PRO:HA	4:D:73:VAL:HG22	1.90	0.52
5:E:93:MET:HE1	5:E:165:GLY:N	2.22	0.52
8:H:32:ALA:C	8:H:33:GLN:HG3	2.34	0.52
8:H:54:VAL:HG13	8:H:162:PRO:HG3	1.90	0.52
8:H:77:ILE:C	8:H:78:LYS:CA	2.83	0.52
8:H:91:ARG:O	30:0:1003:U:H4'	2.10	0.52
9:I:89:GLU:OE2	30:0:1181:A:H5'	2.10	0.52
10:J:46:ILE:HA	42:0:3802:HOH:O	2.09	0.52
23:W:35:VAL:HG23	23:W:41:TYR:CD2	2.45	0.52
24:X:74:ALA:HA	24:X:85:VAL:HG13	1.92	0.52
30:0:25:A:O2'	30:0:640:G:H5'	2.10	0.52
30:0:830:G:H5''	42:0:9420:HOH:O	2.09	0.52
30:0:1183:C:H5	30:0:1192:A:OP1	1.91	0.52
30:0:1244:U:H4'	30:0:1246:A:O4'	2.10	0.52
30:0:1314:U:H2'	42:0:6711:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1783:A:O2'	30:0:1784:U:H5'	2.08	0.52
30:0:2649:A:H2'	42:0:6965:HOH:O	2.08	0.52
1:A:14:SER:HB2	42:A:9016:HOH:O	2.09	0.52
1:A:176:HIS:CD2	30:0:857:A:H4'	2.45	0.52
2:B:36:PRO:HB3	2:B:174:ARG:CB	2.40	0.52
3:C:93:LYS:O	3:C:98:ARG:NH2	2.42	0.52
3:C:124:VAL:HG12	3:C:131:PHE:HE2	1.74	0.52
13:M:158:ARG:HA	13:M:163:LEU:HD12	1.90	0.52
19:S:57:THR:CG2	19:S:58:MET:N	2.73	0.52
20:T:66:ASP:OD1	20:T:68:ASP:N	2.42	0.52
24:X:66:THR:CG2	24:X:67:PRO:HD2	2.40	0.52
30:0:35:U:O2'	30:0:36:C:H5'	2.09	0.52
30:0:37:A:H2'	30:0:38:G:C8	2.45	0.52
30:0:336:G:H2'	42:0:4601:HOH:O	2.08	0.52
30:0:1117:A:H2'	42:0:5754:HOH:O	2.09	0.52
30:0:1809:G:N2	30:0:1811:A:H3'	2.24	0.52
2:B:258:GLY:H	2:B:260:HIS:CE1	2.28	0.52
14:N:23:ARG:NH1	42:N:8868:HOH:O	2.42	0.52
14:N:33:ARG:HH21	14:N:48:VAL:HG11	1.74	0.52
14:N:115:VAL:HG13	42:9:9103:HOH:O	2.10	0.52
15:O:32:ARG:HB2	42:O:4656:HOH:O	2.10	0.52
15:O:44:ASN:HB2	35:O:8808:CL:CL	2.47	0.52
23:W:38:THR:CG2	23:W:39:ASP:N	2.73	0.52
23:W:68:THR:HG23	23:W:69:ARG:HG2	1.91	0.52
23:W:120:PRO:HG2	30:0:1095:U:O2	2.10	0.52
23:W:142:ASP:O	23:W:143:THR:C	2.53	0.52
30:0:204:A:C2'	30:0:205:U:H5'	2.39	0.52
30:0:625:U:H5'	42:0:4081:HOH:O	2.10	0.52
30:0:627:G:H1'	42:0:5293:HOH:O	2.08	0.52
30:0:1406:A:H4'	30:0:1407:A:C5'	2.39	0.52
3:C:124:VAL:HG12	3:C:131:PHE:CE2	2.45	0.52
3:C:175:LYS:NZ	3:C:184:ARG:HB3	2.25	0.52
6:F:117:GLU:C	6:F:119:ARG:H	2.17	0.52
9:I:108:HIS:N	9:I:109:PRO:CD	2.72	0.52
10:J:54:VAL:HG11	10:J:138:THR:HG21	1.91	0.52
42:K:4183:HOH:O	30:0:2712:G:H5'	2.10	0.52
12:L:11:ARG:NH1	30:0:903:U:OP2	2.41	0.52
14:N:73:ALA:HB1	14:N:74:PRO:CD	2.39	0.52
17:Q:15:LYS:NZ	42:Q:5620:HOH:O	2.43	0.52
30:0:78:G:N3	30:0:78:G:N1	2.58	0.52
30:0:396:U:O2'	30:0:418:C:H4'	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:951:A:O2'	30:0:952:G:H5'	2.10	0.52
30:0:1574:C:O5'	30:0:1574:C:H6	1.92	0.52
30:0:1748:U:H4'	42:0:9318:HOH:O	2.10	0.52
30:0:2253:G:O2'	30:0:2254:G:H5'	2.09	0.52
30:0:2314:G:H2'	30:0:2315:C:H5'	1.92	0.52
30:0:2531:U:O2'	30:0:2532:A:H5'	2.09	0.52
30:0:2765:C:H2'	30:0:2766:A:C8	2.45	0.52
31:9:78:G:N3	31:9:78:G:N1	2.58	0.52
2:B:214:PRO:C	2:B:220:VAL:HG22	2.35	0.52
3:C:33:LYS:HE2	42:C:8564:HOH:O	2.09	0.52
7:G:22:ALA:O	7:G:25:GLU:HB3	2.10	0.52
14:N:152:GLU:C	14:N:154:LEU:N	2.67	0.52
18:R:96:VAL:O	18:R:99:ALA:HB3	2.09	0.52
21:U:49:LEU:HG	42:U:3805:HOH:O	2.10	0.52
23:W:5:VAL:HG11	23:W:153:MET:CE	2.35	0.52
26:Z:77:GLY:HA2	26:Z:91:GLY:O	2.10	0.52
27:1:28:HIS:ND1	27:1:31:LYS:HE2	2.25	0.52
30:0:2426:G:H1'	42:0:6925:HOH:O	2.09	0.52
1:A:26:ASP:O	1:A:26:ASP:CG	2.52	0.51
2:B:28:SER:HB3	30:0:2807:U:OP1	2.11	0.51
20:T:43:ASN:O	20:T:45:GLY:N	2.41	0.51
22:V:27:LEU:HA	22:V:49:LEU:HD13	1.92	0.51
25:Y:150:LEU:HB2	42:0:6295:HOH:O	2.09	0.51
1:A:132:ASP:HB3	1:A:135:VAL:H	1.75	0.51
2:B:41:PHE:CE1	2:B:79:MET:HG3	2.44	0.51
7:G:64:ASN:HD22	7:G:64:ASN:N	2.07	0.51
11:K:29:LEU:HB3	11:K:55:VAL:CG1	2.26	0.51
14:N:157:PRO:HA	42:N:8823:HOH:O	2.09	0.51
24:X:87:ALA:O	24:X:88:GLU:HB3	2.10	0.51
25:Y:177:LYS:HD3	25:Y:181:GLY:O	2.11	0.51
26:Z:66:CYS:SG	26:Z:67:GLY:N	2.81	0.51
30:0:432:G:H2'	30:0:433:C:H6	1.75	0.51
1:A:16:PHE:HB3	42:A:9032:HOH:O	2.09	0.51
2:B:145:HIS:CD2	2:B:159:PRO:HB3	2.45	0.51
4:D:173:GLU:HG3	4:D:174:VAL:HG23	1.92	0.51
7:G:27:ILE:HD12	7:G:70:ALA:HB1	1.92	0.51
9:I:111:LEU:HD23	30:0:1163:G:H4'	1.93	0.51
10:J:90:LYS:HE2	30:0:2083:A:N6	2.26	0.51
12:L:79:ASP:HB3	42:L:9021:HOH:O	2.10	0.51
15:O:32:ARG:NE	15:O:35:LYS:HD3	2.18	0.51
30:0:105:G:O2'	30:0:106:A:H5'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2247:C:H2'	30:0:2248:C:C6	2.43	0.51
4:D:23:VAL:CG2	4:D:73:VAL:HB	2.40	0.51
13:M:133:LEU:O	13:M:134:ILE:HD13	2.10	0.51
24:X:87:ALA:O	24:X:88:GLU:CB	2.57	0.51
29:3:84:ARG:HD3	42:3:9041:HOH:O	2.11	0.51
1:A:96:LEU:HD22	1:A:128:LEU:HD22	1.93	0.51
4:D:75:LEU:HD13	4:D:79:MET:O	2.10	0.51
5:E:69:ILE:HA	5:E:72:MET:HE3	1.92	0.51
16:P:125:LYS:HB3	16:P:130:GLU:HG3	1.92	0.51
16:P:139:ARG:HG3	16:P:139:ARG:NH1	2.21	0.51
23:W:142:ASP:O	23:W:145:GLY:N	2.43	0.51
25:Y:148:GLY:HA3	30:0:622:G:P	2.51	0.51
30:0:1190:G:H4'	30:0:1207:A:N1	2.24	0.51
30:0:2765:C:H2'	30:0:2766:A:H8	1.75	0.51
30:0:2842:G:H2'	30:0:2843:A:H5'	1.93	0.51
2:B:145:HIS:HD2	2:B:159:PRO:HB3	1.76	0.51
3:C:140:VAL:HB	42:C:8648:HOH:O	2.10	0.51
6:F:56:PRO:HB2	6:F:58:GLU:OE1	2.10	0.51
7:G:23:ILE:HG22	7:G:27:ILE:CD1	2.39	0.51
9:I:96:SER:OG	9:I:99:GLN:HG3	2.10	0.51
10:J:6:PHE:HB3	10:J:109:TYR:OH	2.10	0.51
12:L:18:HIS:HB3	42:L:8973:HOH:O	2.09	0.51
13:M:48:LYS:HE3	13:M:52:GLN:NE2	2.25	0.51
13:M:52:GLN:HG2	13:M:116:ASN:CG	2.36	0.51
16:P:37:ARG:NH2	30:0:1502:A:OP1	2.43	0.51
22:V:64:GLY:O	22:V:65:ASP:CB	2.58	0.51
25:Y:177:LYS:HE2	25:Y:183:GLU:OE2	2.09	0.51
28:2:36:ASN:HB3	28:2:39:ARG:HG3	1.92	0.51
30:0:146:U:O2'	30:0:147:G:H5'	2.11	0.51
30:0:1161:A:H1'	42:0:4752:HOH:O	2.11	0.51
30:0:1471:A:H2'	30:0:1472:C:C6	2.45	0.51
30:0:1746:A:H5''	42:0:6929:HOH:O	2.10	0.51
30:0:1790:C:H2'	30:0:1791:U:H6	1.75	0.51
30:0:2850:C:H1'	42:0:9168:HOH:O	2.10	0.51
2:B:316:ARG:O	2:B:316:ARG:HG3	2.11	0.51
3:C:65:ARG:HG3	3:C:67:GLN:HB2	1.93	0.51
4:D:167:GLU:C	4:D:169:THR:H	2.19	0.51
9:I:91:PHE:HA	9:I:131:GLY:HA3	1.93	0.51
11:K:101:ASN:O	11:K:102:GLU:HB2	2.10	0.51
12:L:52:LYS:NZ	30:0:215:A:OP1	2.38	0.51
12:L:56:LYS:HE3	30:0:2443:C:H1'	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:97:SER:H	15:O:100:GLN:NE2	2.08	0.51
16:P:14:LEU:O	16:P:16:VAL:HG23	2.10	0.51
20:T:24:ARG:HG2	20:T:24:ARG:HH11	1.75	0.51
20:T:40:VAL:HG23	20:T:119:ALA:OXT	2.10	0.51
23:W:77:ALA:HB3	42:W:5763:HOH:O	2.11	0.51
25:Y:203:VAL:CG1	25:Y:228:VAL:HG22	2.41	0.51
27:1:12:ASN:O	30:0:1415:G:H5'	2.11	0.51
29:3:31:THR:O	30:0:1923:G:H4'	2.11	0.51
30:0:1303:C:O2	30:0:1353:C:H1'	2.09	0.51
30:0:1700:C:OP2	42:0:6868:HOH:O	2.19	0.51
30:0:1705:C:O2	30:0:2735:U:H5''	2.11	0.51
31:9:96:C:H2'	31:9:97:U:C6	2.46	0.51
1:A:109:GLU:HG2	1:A:116:GLY:N	2.20	0.51
2:B:79:MET:HE3	2:B:144:THR:CG2	2.40	0.51
3:C:178:GLN:O	3:C:179:GLY:C	2.54	0.51
4:D:40:ILE:HA	4:D:43:GLU:OE1	2.11	0.51
5:E:159:VAL:O	5:E:163:GLN:HG2	2.11	0.51
12:L:73:VAL:HG23	12:L:74:THR:H	1.75	0.51
18:R:100:ASP:C	18:R:102:GLN:N	2.68	0.51
20:T:43:ASN:HD22	20:T:108:ARG:CZ	2.24	0.51
21:U:35:LYS:HE2	21:U:51:TRP:CH2	2.46	0.51
23:W:117:ARG:HH11	23:W:117:ARG:CB	2.23	0.51
30:0:1979:G:H2'	42:0:3192:HOH:O	2.10	0.51
30:0:2566:A:H61	30:0:2699:A:H61	1.59	0.51
1:A:51:ARG:NH1	1:A:120:ARG:O	2.44	0.51
1:A:66:ARG:HH11	1:A:66:ARG:CB	2.21	0.51
2:B:11:LEU:HD21	2:B:250:THR:HG22	1.93	0.51
4:D:154:LYS:H	4:D:154:LYS:HD2	1.75	0.51
5:E:7:ILE:HD11	5:E:11:VAL:C	2.36	0.51
8:H:87:LYS:HB2	8:H:87:LYS:NZ	2.26	0.51
9:I:134:ILE:HG22	9:I:135:GLU:N	2.26	0.51
13:M:149:TRP:C	13:M:151:CYS:H	2.18	0.51
15:O:44:ASN:CG	15:O:67:SER:HB3	2.36	0.51
30:0:1333:U:H2'	30:0:1334:C:C6	2.46	0.51
30:0:1835:U:C5	30:0:1840:A:N7	2.71	0.51
30:0:2502:C:H2'	30:0:2503:A:H5'	1.92	0.51
31:9:3:A:H2	31:9:21:G:N3	2.09	0.51
31:9:97:U:H3'	42:9:9104:HOH:O	2.11	0.51
2:B:216:LYS:HA	42:0:5933:HOH:O	2.11	0.51
4:D:10:PHE:CE1	4:D:11:HIS:HB3	2.46	0.51
8:H:20:ARG:HD3	8:H:26:ILE:HD12	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:124:GLY:HA3	30:0:2132:C:H1'	1.93	0.51
14:N:11:ARG:NH1	31:9:8:G:O6	2.43	0.51
14:N:61:ALA:CB	14:N:88:ALA:HB2	2.41	0.51
14:N:143:ARG:HG2	14:N:172:PHE:CD2	2.46	0.51
17:Q:1:PRO:HA	30:0:2299:G:O6	2.11	0.51
17:Q:7:LEU:HD12	30:0:2424:U:C1'	2.41	0.51
20:T:107:LYS:O	20:T:111:ARG:HB2	2.09	0.51
23:W:142:ASP:HB3	42:W:2729:HOH:O	2.11	0.51
30:0:1422:U:H2'	30:0:1423:C:C6	2.45	0.51
30:0:1477:C:H5'	30:0:1868:G:C5'	2.40	0.51
30:0:2735:U:H2'	30:0:2736:U:H6	1.76	0.51
30:0:2911:C:H3'	42:0:6395:HOH:O	2.11	0.51
31:9:92:G:H2'	31:9:93:A:H8	1.75	0.51
2:B:101:TRP:HB2	2:B:119:HIS:CD2	2.46	0.50
3:C:236:THR:HB	3:C:239:ALA:HB2	1.93	0.50
5:E:35:TYR:HA	10:J:127:ILE:CD1	2.41	0.50
8:H:49:GLN:OE1	8:H:169:GLU:HG2	2.11	0.50
12:L:80:ASP:HB2	12:L:90:ARG:O	2.11	0.50
14:N:86:LEU:HD21	14:N:180:LEU:CD1	2.41	0.50
16:P:107:GLU:C	16:P:109:ARG:H	2.19	0.50
20:T:49:GLU:OE2	20:T:51:LEU:HD21	2.11	0.50
23:W:24:LEU:HD21	23:W:44:MET:HE3	1.93	0.50
23:W:117:ARG:CB	23:W:117:ARG:NH1	2.74	0.50
23:W:122:ARG:CZ	23:W:154:ARG:HB3	2.40	0.50
23:W:139:GLY:O	23:W:141:HIS:CD2	2.62	0.50
25:Y:189:ASN:HD22	25:Y:191:ASP:N	2.10	0.50
29:3:84:ARG:HD2	30:0:2427:C:OP2	2.10	0.50
30:0:354:A:H2'	30:0:355:C:H6	1.76	0.50
30:0:566:A:H2'	30:0:567:U:H5'	1.91	0.50
30:0:2251:G:H2'	30:0:2252:A:H8	1.76	0.50
2:B:125:GLU:O	2:B:129:ARG:HG3	2.11	0.50
2:B:214:PRO:HB2	2:B:220:VAL:HG21	1.93	0.50
4:D:135:VAL:HG22	4:D:136:ARG:N	2.26	0.50
5:E:36:PRO:HD3	10:J:127:ILE:CG1	2.42	0.50
10:J:88:PRO:HD3	30:0:1104:C:H4'	1.92	0.50
16:P:54:LYS:HB2	30:0:1717:A:H5''	1.93	0.50
18:R:39:THR:O	18:R:40:ALA:C	2.55	0.50
20:T:43:ASN:OD1	30:0:80:A:H3'	2.11	0.50
30:0:213:G:H22	30:0:225:G:H2'	1.76	0.50
30:0:314:G:N2	30:0:316:A:H3'	2.26	0.50
30:0:561:G:O2'	30:0:562:A:H5'	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1595:G:O2'	30:0:1596:U:H5'	2.11	0.50
30:0:2819:C:H2'	30:0:2820:A:C8	2.46	0.50
2:B:76:THR:O	2:B:77:PRO:C	2.53	0.50
2:B:279:THR:HG22	2:B:280:VAL:N	2.26	0.50
3:C:168:ARG:NH1	30:0:1310:U:OP2	2.44	0.50
6:F:46:GLU:OE2	6:F:100:ASP:HA	2.10	0.50
8:H:86:TYR:C	8:H:86:TYR:CD1	2.90	0.50
10:J:71:TYR:CD1	10:J:72:PRO:HD2	2.46	0.50
22:V:23:LEU:O	22:V:24:LYS:C	2.54	0.50
25:Y:99:ALA:HB2	25:Y:233:TYR:CZ	2.47	0.50
25:Y:102:LEU:HG	42:Y:8887:HOH:O	2.11	0.50
25:Y:112:GLU:OE1	25:Y:115:ARG:NH1	2.44	0.50
1:A:146:LYS:NZ	30:0:1855:G:O3'	2.44	0.50
3:C:129:HIS:HE1	3:C:231:ARG:HA	1.75	0.50
14:N:1:ALA:HB2	31:9:14:G:O2'	2.11	0.50
16:P:134:VAL:O	16:P:138:GLU:HG3	2.11	0.50
23:W:73:LEU:HD22	23:W:111:GLY:HA2	1.94	0.50
29:3:38:ARG:NH1	30:0:396:U:OP2	2.43	0.50
30:0:1116:U:O2'	30:0:1118:A:C2	2.46	0.50
30:0:1878:G:O2'	30:0:1879:U:P	2.69	0.50
30:0:2324:G:N2	30:0:2377:U:H1'	2.26	0.50
31:9:106:U:O2'	31:9:107:C:H5'	2.11	0.50
3:C:7:ASP:O	3:C:9:ASP:N	2.44	0.50
5:E:83:GLY:O	5:E:169:THR:N	2.35	0.50
8:H:49:GLN:O	8:H:169:GLU:HB3	2.11	0.50
9:I:97:VAL:O	9:I:101:LYS:HG3	2.12	0.50
11:K:74:VAL:HG13	11:K:113:ILE:HG12	1.93	0.50
12:L:13:HIS:ND1	35:L:8814:CL:CL	2.77	0.50
14:N:183:ASP:O	14:N:184:ILE:O	2.28	0.50
22:V:39:ALA:O	22:V:41:GLU:N	2.43	0.50
24:X:10:VAL:HG12	24:X:11:THR:N	2.26	0.50
1:A:69:LEU:HD11	1:A:159:VAL:HG13	1.94	0.50
3:C:43:LYS:HG2	30:0:449:A:N7	2.27	0.50
4:D:170:TYR:O	4:D:171:ASP:CB	2.59	0.50
5:E:3:VAL:CG2	5:E:49:ILE:HB	2.35	0.50
14:N:78:MET:HB2	14:N:146:HIS:HE1	1.76	0.50
20:T:16:LEU:HB2	30:0:100:C:C4'	2.41	0.50
20:T:52:ARG:HB2	20:T:95:ASN:HB3	1.94	0.50
23:W:7:LEU:HD12	23:W:53:ALA:HB2	1.93	0.50
30:0:371:U:H2'	30:0:372:A:H8	1.76	0.50
30:0:506:G:N1	30:0:509:A:OP2	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:553:G:H2'	30:0:554:G:H5'	1.94	0.50
30:0:823:U:H3'	42:0:5310:HOH:O	2.12	0.50
30:0:1185:U:H2'	30:0:1186:C:C6	2.46	0.50
30:0:1301:C:O2'	30:0:1331:G:H4'	2.11	0.50
30:0:1309:U:H2'	30:0:1310:U:O4'	2.12	0.50
30:0:1649:G:O2'	30:0:1650:C:H5'	2.11	0.50
3:C:27:ARG:NH2	30:0:657:G:OP1	2.44	0.50
4:D:76:ARG:NE	31:9:44:A:O4'	2.45	0.50
9:I:86:GLU:HB2	9:I:90:ASP:OD2	2.12	0.50
11:K:64:MET:O	11:K:67:GLN:HB2	2.12	0.50
19:S:56:ASN:O	28:2:8:LYS:NZ	2.45	0.50
20:T:20:HIS:O	20:T:23:VAL:HG23	2.11	0.50
23:W:4:LEU:HD23	23:W:54:PHE:HB3	1.94	0.50
25:Y:112:GLU:CD	25:Y:115:ARG:NH1	2.69	0.50
29:3:3:MET:O	29:3:90:PHE:HA	2.12	0.50
29:3:22:VAL:CG1	29:3:67:LEU:HD13	2.42	0.50
30:0:303:C:H2'	30:0:304:G:O4'	2.12	0.50
30:0:1659:A:H2'	30:0:1660:G:O4'	2.11	0.50
30:0:1755:A:H2'	30:0:1756:G:O4'	2.11	0.50
30:0:1805:G:O2'	30:0:1806:G:H5'	2.12	0.50
30:0:1980:U:H5'	30:0:2626:C:H1'	1.93	0.50
2:B:7:ARG:HG2	2:B:7:ARG:HH11	1.76	0.50
2:B:42:ALA:HB2	2:B:162:MET:CE	2.35	0.50
2:B:197:GLY:HA3	2:B:323:LEU:HA	1.93	0.50
5:E:1:PRO:HG2	5:E:59:MET:SD	2.52	0.50
5:E:40:VAL:HB	42:E:2857:HOH:O	2.11	0.50
6:F:1:PRO:H3	6:F:4:VAL:HG23	1.76	0.50
8:H:41:LYS:O	8:H:87:LYS:HE2	2.11	0.50
13:M:57:LYS:HZ2	13:M:144:ASP:CG	2.20	0.50
22:V:6:GLN:HB2	42:0:7782:HOH:O	2.11	0.50
30:0:1200:A:H3'	42:0:6592:HOH:O	2.11	0.50
30:0:1590:A:H1'	30:0:1606:A:C2	2.47	0.50
30:0:1992:U:H2'	30:0:1994:A:OP2	2.12	0.50
3:C:5:ILE:HG22	3:C:6:TYR:N	2.27	0.50
3:C:124:VAL:HA	3:C:230:GLY:O	2.11	0.50
5:E:22:VAL:O	5:E:28:SER:HA	2.11	0.50
11:K:55:VAL:HG12	11:K:56:SER:N	2.27	0.50
12:L:4:LYS:HE2	30:0:645:U:OP2	2.12	0.50
12:L:10:SER:O	12:L:11:ARG:HB3	2.12	0.50
13:M:46:LEU:HD22	13:M:50:ARG:CD	2.42	0.50
14:N:151:ASP:OD1	14:N:166:ALA:HA	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:43:VAL:CG1	15:O:47:ARG:HD2	2.42	0.50
25:Y:189:ASN:HD22	25:Y:191:ASP:H	1.59	0.50
29:3:40:ARG:HD2	42:3:9047:HOH:O	2.12	0.50
30:0:162:C:H2'	30:0:163:U:H5'	1.94	0.50
30:0:445:U:O2'	30:0:446:G:H5'	2.12	0.50
30:0:1503:U:C2'	30:0:1504:A:H5'	2.42	0.50
30:0:1641:A:H2'	30:0:1642:A:H5'	1.93	0.50
30:0:1778:A:H2'	30:0:1779:A:H5'	1.94	0.50
30:0:1985:U:C5	30:0:1996:U:C2	3.00	0.50
30:0:2836:G:O2'	30:0:2838:A:N7	2.34	0.50
1:A:26:ASP:O	1:A:28:GLU:N	2.45	0.49
1:A:47:HIS:CD2	30:0:1654:U:H2'	2.46	0.49
1:A:94:LEU:HG	1:A:99:ILE:CD1	2.42	0.49
1:A:100:PRO:HG2	1:A:103:VAL:CG2	2.30	0.49
2:B:305:ASP:O	2:B:306:LYS:HB2	2.12	0.49
12:L:89:PHE:CD1	12:L:89:PHE:N	2.80	0.49
14:N:77:ASN:C	14:N:78:MET:CA	2.84	0.49
17:Q:16:ASN:ND2	17:Q:45:PRO:HB2	2.27	0.49
18:R:44:VAL:O	18:R:48:GLU:HG3	2.12	0.49
21:U:56:ARG:O	21:U:56:ARG:CD	2.60	0.49
23:W:29:VAL:O	23:W:30:ASN:HB2	2.10	0.49
25:Y:184:GLU:OE1	25:Y:204:ARG:NH1	2.45	0.49
29:3:68:LYS:HE2	30:0:2436:U:C5'	2.40	0.49
30:0:101:C:H2'	30:0:102:A:C8	2.46	0.49
30:0:412:C:H2'	30:0:413:G:O4'	2.11	0.49
30:0:875:A:H5'	30:0:876:A:N7	2.27	0.49
30:0:2001:G:O2'	30:0:2002:C:H5'	2.12	0.49
30:0:2114:C:O2'	30:0:2115:U:H5'	2.11	0.49
2:B:1:PRO:HG3	30:0:2591:C:OP1	2.11	0.49
3:C:96:LYS:NZ	30:0:1351:G:OP1	2.45	0.49
3:C:195:VAL:HA	3:C:213:ALA:O	2.12	0.49
5:E:31:ARG:NH1	42:E:5919:HOH:O	2.46	0.49
18:R:9:ASP:OD1	18:R:11:ASP:HB2	2.12	0.49
20:T:53:GLY:HA3	42:0:7613:HOH:O	2.12	0.49
30:0:1270:U:H2'	30:0:1271:A:C8	2.46	0.49
30:0:1714:C:O2'	30:0:1715:C:H5'	2.12	0.49
30:0:1773:G:H4'	42:0:4407:HOH:O	2.12	0.49
30:0:1878:G:H1'	42:0:6953:HOH:O	2.11	0.49
30:0:2252:A:H2'	30:0:2253:G:O4'	2.11	0.49
30:0:2314:G:O2'	30:0:2315:C:H5'	2.11	0.49
30:0:2839:C:H2'	30:0:2840:A:H5''	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:98:C:H2'	31:9:99:U:C6	2.44	0.49
2:B:221:GLN:HE22	11:K:42:ASN:HD22	1.59	0.49
3:C:202:THR:HG22	30:0:328:U:O4'	2.12	0.49
4:D:54:ALA:HB2	4:D:69:ILE:CD1	2.40	0.49
4:D:57:THR:HG23	4:D:63:ILE:CA	2.32	0.49
6:F:38:LYS:HA	6:F:41:GLU:OE1	2.12	0.49
9:I:87:PRO:HD3	42:0:4130:HOH:O	2.12	0.49
14:N:154:LEU:O	14:N:155:GLU:HB3	2.12	0.49
20:T:1:SER:HB2	30:0:447:A:P	2.53	0.49
42:Z:8722:HOH:O	30:0:1886:A:H5'	2.11	0.49
30:0:283:U:H5''	30:0:284:C:OP2	2.12	0.49
30:0:1165:G:H1'	30:0:1174:A:H1'	1.95	0.49
30:0:1201:C:H2'	30:0:1202:A:H5'	1.94	0.49
3:C:236:THR:O	3:C:237:GLU:C	2.55	0.49
4:D:151:ILE:CG2	4:D:155:HIS:HB3	2.43	0.49
11:K:77:ARG:O	11:K:78:LYS:CA	2.60	0.49
12:L:108:VAL:HB	12:L:125:PHE:HD2	1.77	0.49
13:M:133:LEU:HD12	13:M:133:LEU:N	2.26	0.49
16:P:138:GLU:O	16:P:139:ARG:C	2.54	0.49
19:S:40:ALA:O	19:S:44:GLN:HB2	2.12	0.49
20:T:27:LEU:HB2	20:T:32:ARG:CG	2.42	0.49
42:X:4132:HOH:O	30:0:2895:C:H4'	2.12	0.49
25:Y:212:ARG:HD2	42:Y:8907:HOH:O	2.12	0.49
26:Z:77:GLY:O	26:Z:78:ILE:CA	2.61	0.49
29:3:55:VAL:HB	29:3:56:PRO:HD2	1.94	0.49
31:9:78:G:N2	31:9:102:G:H2'	2.27	0.49
1:A:169:PHE:O	1:A:171:LYS:N	2.43	0.49
2:B:41:PHE:HB3	2:B:190:MET:CE	2.42	0.49
2:B:277:GLU:N	2:B:278:PRO:HD2	2.27	0.49
5:E:88:TYR:CE1	5:E:92:PRO:HA	2.47	0.49
13:M:80:GLY:C	13:M:81:ARG:HD2	2.37	0.49
14:N:141:ARG:HH12	31:9:35:C:H2'	1.77	0.49
14:N:176:ARG:O	14:N:180:LEU:HD13	2.12	0.49
15:O:47:ARG:HH11	15:O:47:ARG:HG3	1.77	0.49
16:P:64:GLU:HG2	42:P:2495:HOH:O	2.13	0.49
22:V:16:ARG:NH1	22:V:65:ASP:O	2.45	0.49
30:0:568:G:C6	30:0:588:G:H1'	2.48	0.49
30:0:695:C:H2'	30:0:696:C:H6	1.77	0.49
30:0:764:C:H2'	30:0:765:G:O4'	2.13	0.49
30:0:772:G:H2'	30:0:773:A:O4'	2.12	0.49
30:0:945:U:H2'	30:0:946:C:H6	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2296:C:H4'	30:0:2362:A:H2	1.78	0.49
1:A:165:THR:HG22	42:A:9096:HOH:O	2.11	0.49
2:B:161:VAL:HG12	2:B:162:MET:N	2.28	0.49
3:C:145:GLU:CD	3:C:196:THR:HB	2.38	0.49
9:I:96:SER:HB3	9:I:99:GLN:NE2	2.27	0.49
11:K:44:HIS:O	11:K:45:PRO:C	2.56	0.49
13:M:58:GLN:HG3	42:M:8907:HOH:O	2.12	0.49
15:O:26:TRP:HA	15:O:26:TRP:CE3	2.48	0.49
15:O:38:ARG:NH1	42:O:7674:HOH:O	2.45	0.49
16:P:6:GLN:HG2	16:P:31:ILE:HG22	1.93	0.49
17:Q:11:ARG:NH1	30:0:2363:G:O3'	2.45	0.49
20:T:26:THR:CG2	20:T:97:ARG:HG3	2.42	0.49
23:W:62:LEU:HD21	23:W:100:LEU:HD12	1.94	0.49
25:Y:132:ASP:OD2	30:0:621:C:H5'	2.13	0.49
25:Y:154:ARG:NH1	25:Y:155:ARG:HG3	2.28	0.49
26:Z:77:GLY:C	26:Z:78:ILE:CA	2.86	0.49
30:0:98:A:C2'	30:0:99:A:H5'	2.42	0.49
30:0:285:A:H2'	30:0:286:U:O4'	2.12	0.49
30:0:300:U:O2'	30:0:301:C:H5'	2.12	0.49
30:0:816:G:H5'	30:0:1598:A:H4'	1.95	0.49
30:0:2289:G:H21	30:0:2291:A:H2	1.57	0.49
30:0:2498:C:O2'	30:0:2499:U:H5'	2.12	0.49
31:9:18:U:H2'	31:9:19:G:C8	2.44	0.49
1:A:105:VAL:CG1	1:A:154:ALA:HB1	2.43	0.49
2:B:29:TRP:CZ3	2:B:164:THR:HG23	2.48	0.49
2:B:279:THR:HG23	2:B:290:VAL:H	1.77	0.49
9:I:118:ASN:HA	9:I:121:LYS:HD2	1.95	0.49
11:K:87:ARG:HD2	42:K:4066:HOH:O	2.12	0.49
13:M:40:ILE:HD11	13:M:62:VAL:HG12	1.94	0.49
18:R:46:TYR:O	18:R:50:VAL:HG23	2.13	0.49
19:S:5:ILE:HD12	19:S:44:GLN:HG3	1.93	0.49
24:X:25:ARG:HD2	42:X:5356:HOH:O	2.13	0.49
29:3:16:GLU:HB2	42:0:6515:HOH:O	2.12	0.49
30:0:98:A:H2'	30:0:99:A:H5'	1.95	0.49
30:0:1230:A:H8	30:0:1230:A:OP1	1.95	0.49
30:0:1314:U:H5''	30:0:1316:G:O4'	2.12	0.49
30:0:2566:A:H2	30:0:2695:C:O2	1.95	0.49
30:0:2583:A:H3'	42:0:5461:HOH:O	2.13	0.49
30:0:2909:G:O2'	30:0:2910:A:H5'	2.13	0.49
31:9:29:C:H2'	31:9:30:C:C5'	2.38	0.49
4:D:80:ALA:O	4:D:83:PHE:HB3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:96:SER:H	9:I:99:GLN:CD	2.21	0.49
10:J:18:ILE:HD13	30:0:1244:U:OP1	2.12	0.49
10:J:67:ASN:OD1	30:0:2082:G:H1'	2.12	0.49
11:K:65:ARG:C	11:K:67:GLN:H	2.19	0.49
13:M:144:ASP:O	13:M:148:SER:HB3	2.12	0.49
15:O:26:TRP:HA	15:O:26:TRP:HE3	1.78	0.49
19:S:56:ASN:HD22	30:0:1676:G:P	2.34	0.49
26:Z:54:GLU:HA	26:Z:57:MET:HB3	1.93	0.49
30:0:565:A:OP2	30:0:592:G:N1	2.42	0.49
30:0:669:G:O2'	30:0:670:G:H5'	2.13	0.49
30:0:1367:A:H2'	30:0:1368:U:O4'	2.12	0.49
30:0:2426:G:H5''	30:0:2427:C:O4'	2.11	0.49
30:0:2718:C:H6	30:0:2718:C:H5'	1.78	0.49
2:B:41:PHE:CZ	2:B:79:MET:HG3	2.48	0.49
3:C:131:PHE:CD2	3:C:232:LEU:HD22	2.47	0.49
3:C:188:ARG:NH2	42:C:8523:HOH:O	2.44	0.49
14:N:140:GLN:O	14:N:143:ARG:HB2	2.13	0.49
23:W:34:LEU:HD13	23:W:100:LEU:HD13	1.94	0.49
23:W:129:LYS:HE2	30:0:1098:A:O3'	2.12	0.49
24:X:43:VAL:HG12	24:X:44:ASP:N	2.25	0.49
24:X:63:ARG:HG2	24:X:63:ARG:O	2.13	0.49
25:Y:107:PRO:HD3	25:Y:182:PHE:CE1	2.48	0.49
28:2:20:ARG:HG3	28:2:21:VAL:N	2.28	0.49
29:3:51:LYS:HB2	42:0:5348:HOH:O	2.12	0.49
30:0:222:A:H2'	30:0:223:G:O4'	2.12	0.49
30:0:658:C:O2'	30:0:662:U:OP1	2.25	0.49
30:0:690:G:H1'	30:0:731:U:H1'	1.95	0.49
30:0:737:A:H2'	30:0:738:G:O4'	2.12	0.49
30:0:1393:A:H2'	30:0:1394:C:C6	2.48	0.49
30:0:1666:C:C2'	30:0:1667:A:C5'	2.91	0.49
1:A:211:LYS:HB2	42:A:9098:HOH:O	2.13	0.49
42:A:9044:HOH:O	30:0:871:G:H4'	2.12	0.49
2:B:128:ILE:O	2:B:131:ALA:HB3	2.12	0.49
2:B:274:GLU:HG3	2:B:292:GLY:C	2.38	0.49
3:C:87:ARG:NH2	30:0:894:A:C2	2.80	0.49
12:L:4:LYS:HD2	42:0:5885:HOH:O	2.13	0.49
15:O:87:THR:O	15:O:88:LYS:C	2.55	0.49
15:O:96:VAL:HG13	15:O:100:GLN:CD	2.37	0.49
20:T:101:LEU:HD22	20:T:108:ARG:NH2	2.27	0.49
23:W:42:ARG:HA	23:W:45:VAL:HG22	1.95	0.49
28:2:43:ARG:HH21	30:0:1685:A:H4'	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:17:G:H2'	30:0:18:C:C6	2.48	0.49
30:0:71:G:H8	42:0:4782:HOH:O	1.96	0.49
30:0:883:U:C5	30:0:888:U:H5'	2.48	0.49
30:0:1774:G:H1'	42:0:5405:HOH:O	2.13	0.49
30:0:2642:G:H2'	30:0:2643:G:O4'	2.13	0.49
4:D:52:THR:CG2	30:0:2346:C:H4'	2.43	0.48
5:E:137:ASP:O	5:E:141:VAL:HG23	2.13	0.48
6:F:50:VAL:CG1	6:F:60:VAL:HG11	2.43	0.48
6:F:100:ASP:O	6:F:101:ALA:O	2.31	0.48
10:J:52:GLN:NE2	30:0:1119:G:C2'	2.63	0.48
14:N:155:GLU:O	14:N:156:GLU:HG3	2.13	0.48
20:T:44:ALA:HA	20:T:62:VAL:HG12	1.95	0.48
21:U:33:SER:O	21:U:37:GLU:HG3	2.13	0.48
23:W:117:ARG:NH1	23:W:117:ARG:HB2	2.28	0.48
30:0:1139:U:H2'	30:0:1140:C:C6	2.48	0.48
30:0:1175:G:H1'	30:0:1193:A:H2'	1.94	0.48
30:0:2073:G:H2'	42:0:4699:HOH:O	2.13	0.48
30:0:2387:U:O2	30:0:2402:A:C2	2.66	0.48
30:0:2473:U:O3'	30:0:2474:A:H3'	2.13	0.48
2:B:280:VAL:HG13	2:B:333:GLU:O	2.14	0.48
4:D:59:GLY:O	4:D:61:PHE:N	2.46	0.48
4:D:129:ASP:OD1	30:0:2338:G:H2'	2.13	0.48
7:G:14:GLU:HB3	42:G:4173:HOH:O	2.13	0.48
12:L:6:ARG:NH2	42:L:9012:HOH:O	2.45	0.48
14:N:37:ARG:HG3	14:N:37:ARG:HH11	1.78	0.48
16:P:41:ARG:O	16:P:44:VAL:HB	2.13	0.48
25:Y:99:ALA:HB2	25:Y:233:TYR:CE2	2.48	0.48
25:Y:208:LYS:HZ1	30:0:1343:C:C2'	2.26	0.48
26:Z:54:GLU:HG2	26:Z:57:MET:CE	2.43	0.48
30:0:1121:G:H4'	42:0:6381:HOH:O	2.13	0.48
30:0:2312:G:C2'	30:0:2313:C:H5'	2.43	0.48
30:0:2688:U:H2'	30:0:2689:A:H8	1.79	0.48
31:9:28:U:H2'	31:9:29:C:C6	2.48	0.48
2:B:316:ARG:HB2	30:0:2768:A:C8	2.48	0.48
6:F:111:ILE:O	6:F:115:VAL:HG23	2.12	0.48
8:H:23:ILE:HG22	8:H:123:ILE:CD1	2.43	0.48
8:H:77:ILE:O	8:H:78:LYS:C	2.55	0.48
42:J:2219:HOH:O	30:0:1103:C:H5''	2.13	0.48
14:N:79:PRO:HG3	14:N:143:ARG:C	2.38	0.48
14:N:143:ARG:HA	14:N:172:PHE:CD2	2.49	0.48
15:O:102:ILE:HB	42:O:7481:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1:50:TRP:O	30:0:890:C:O2'	2.28	0.48
28:2:28:LYS:O	30:0:87:C:H2'	2.13	0.48
30:0:1666:C:C2'	30:0:1667:A:H5''	2.42	0.48
2:B:45:LYS:HG2	2:B:305:ASP:HA	1.94	0.48
42:B:9059:HOH:O	30:0:2819:C:H5'	2.13	0.48
8:H:122:LYS:O	8:H:124:VAL:HG13	2.13	0.48
14:N:100:ALA:HB3	14:N:129:ILE:HG12	1.95	0.48
20:T:48:VAL:HG22	20:T:97:ARG:C	2.37	0.48
21:U:45:GLU:O	21:U:46:ALA:C	2.56	0.48
21:U:52:THR:HG22	21:U:54:THR:HB	1.95	0.48
28:2:42:TRP:CZ3	28:2:43:ARG:HB2	2.48	0.48
29:3:73:GLU:C	29:3:75:GLY:N	2.69	0.48
30:0:380:A:O4'	30:0:382:U:H1'	2.13	0.48
30:0:441:A:H1'	30:0:442:A:N7	2.28	0.48
30:0:1505:U:H4'	42:0:6027:HOH:O	2.12	0.48
30:0:2607:U:H4'	42:0:3343:HOH:O	2.12	0.48
30:0:2780:C:H2'	30:0:2781:U:C6	2.49	0.48
1:A:4:ILE:HG22	1:A:198:ASP:O	2.14	0.48
4:D:23:VAL:HG21	4:D:45:THR:CG2	2.43	0.48
6:F:49:PHE:HE1	6:F:98:VAL:HG23	1.77	0.48
8:H:24:THR:O	8:H:123:ILE:HD12	2.13	0.48
9:I:81:GLU:OE1	9:I:81:GLU:N	2.46	0.48
11:K:98:VAL:CG1	11:K:99:ASP:N	2.76	0.48
22:V:1:THR:C	22:V:3:LEU:H	2.20	0.48
25:Y:193:LEU:HD13	25:Y:221:ALA:HB2	1.95	0.48
28:2:5:LYS:HD2	30:0:1675:C:H5''	1.95	0.48
30:0:1405:U:H2'	42:0:7653:HOH:O	2.14	0.48
30:0:1475:G:N3	30:0:1866:A:H2	2.11	0.48
4:D:23:VAL:HG23	4:D:23:VAL:O	2.13	0.48
4:D:45:THR:HB	4:D:75:LEU:HD11	1.96	0.48
4:D:50:VAL:O	4:D:71:ALA:HA	2.13	0.48
10:J:61:VAL:HA	42:0:3397:HOH:O	2.13	0.48
12:L:150:GLN:HB3	42:L:9035:HOH:O	2.14	0.48
14:N:82:TYR:C	14:N:82:TYR:CD2	2.92	0.48
17:Q:53:HIS:CD2	30:0:2389:U:H4'	2.48	0.48
20:T:21:LYS:HA	20:T:24:ARG:CG	2.42	0.48
22:V:27:LEU:O	22:V:30:ALA:HB3	2.13	0.48
23:W:21:LEU:HB3	23:W:26:ILE:HG12	1.96	0.48
29:3:64:LYS:HA	29:3:84:ARG:HA	1.94	0.48
30:0:368:C:C2'	30:0:369:G:H5'	2.44	0.48
30:0:694:A:H2'	30:0:695:C:H5'	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:887:G:H2'	30:0:888:U:C6	2.48	0.48
30:0:1409:G:H5'	42:0:4602:HOH:O	2.13	0.48
30:0:1876:C:H4'	30:0:1877:G:OP2	2.14	0.48
30:0:2755:G:H1'	42:0:5540:HOH:O	2.12	0.48
2:B:16:ARG:NH1	42:B:9091:HOH:O	2.45	0.48
2:B:27:ASN:C	2:B:27:ASN:ND2	2.71	0.48
3:C:7:ASP:C	3:C:9:ASP:H	2.21	0.48
5:E:81:GLU:OE2	5:E:132:THR:OG1	2.31	0.48
5:E:162:PHE:N	5:E:162:PHE:CD1	2.81	0.48
7:G:21:ASP:O	7:G:22:ALA:C	2.56	0.48
12:L:65:ASP:CG	12:L:111:ALA:HB3	2.39	0.48
12:L:97:VAL:HB	12:L:100:ALA:HB2	1.96	0.48
13:M:184:ARG:HG3	13:M:185:PRO:HA	1.96	0.48
14:N:25:ARG:HG2	30:0:2416:G:O2'	2.13	0.48
20:T:20:HIS:HB3	20:T:41:ARG:HD2	1.95	0.48
23:W:13:MET:HE3	23:W:17:ILE:CG2	2.38	0.48
25:Y:182:PHE:HD2	25:Y:200:THR:O	1.95	0.48
30:0:333:G:O2'	30:0:334:G:H5'	2.13	0.48
30:0:1394:C:H3'	30:0:1433:G:H22	1.78	0.48
30:0:2351:C:H2'	30:0:2352:G:O4'	2.14	0.48
4:D:51:ARG:HH11	4:D:68:PRO:HB3	1.78	0.48
13:M:46:LEU:HD22	13:M:50:ARG:HD2	1.96	0.48
14:N:12:ARG:HD3	14:N:18:THR:OG1	2.13	0.48
14:N:15:GLU:O	14:N:16:ALA:HB3	2.13	0.48
22:V:42:ASN:O	22:V:44:GLY:N	2.47	0.48
28:2:46:ASP:OD1	28:2:47:THR:O	2.32	0.48
30:0:111:C:C2'	30:0:112:G:H5'	2.44	0.48
30:0:746:A:H4'	30:0:747:G:H5'	1.95	0.48
30:0:1189:A:H1'	30:0:1209:C:C1'	2.43	0.48
30:0:1353:C:H5''	42:0:7423:HOH:O	2.12	0.48
1:A:57:ALA:HB1	1:A:65:ARG:HE	1.78	0.48
9:I:98:ASP:C	9:I:100:VAL:H	2.21	0.48
9:I:127:CYS:O	9:I:129:SER:N	2.47	0.48
13:M:5:TYR:CE2	13:M:50:ARG:HD3	2.49	0.48
13:M:95:LYS:CE	30:0:157:G:H4'	2.44	0.48
15:O:96:VAL:CG1	15:O:100:GLN:HB2	2.44	0.48
17:Q:86:VAL:HG11	17:Q:91:LEU:HD21	1.94	0.48
20:T:81:LYS:HE3	30:0:486:A:O5'	2.13	0.48
21:U:37:GLU:HB3	42:U:408:HOH:O	2.12	0.48
23:W:128:VAL:O	23:W:138:LEU:HD11	2.14	0.48
25:Y:117:LEU:CD1	25:Y:174:VAL:HG11	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:51:ALA:HA	42:Z:8712:HOH:O	2.13	0.48
27:1:8:GLN:HE22	27:1:11:LYS:HZ1	1.60	0.48
28:2:5:LYS:O	28:2:9:LYS:HG3	2.14	0.48
30:0:349:U:O2'	30:0:350:G:H5'	2.14	0.48
30:0:419:A:H1'	30:0:1921:A:C2	2.49	0.48
30:0:670:G:H2'	30:0:671:A:C8	2.48	0.48
30:0:696:C:O2'	30:0:731:U:OP1	2.30	0.48
30:0:1490:G:H4'	30:0:1533:A:OP1	2.14	0.48
30:0:1819:G:H2'	30:0:1820:G:H5'	1.96	0.48
2:B:264:GLU:HG3	42:B:9010:HOH:O	2.13	0.48
3:C:107:ARG:NH2	30:0:678:G:OP2	2.46	0.48
11:K:49:LEU:HD22	11:K:80:ILE:HD13	1.96	0.48
11:K:66:ARG:NH2	30:0:1994:A:P	2.87	0.48
13:M:150:ILE:HA	13:M:155:GLN:HG3	1.95	0.48
14:N:151:ASP:O	14:N:154:LEU:HD13	2.13	0.48
16:P:104:LYS:HE2	16:P:138:GLU:HG2	1.95	0.48
20:T:9:LYS:CE	20:T:13:ARG:NH1	2.76	0.48
21:U:11:THR:CG2	21:U:53:ASP:HB2	2.42	0.48
22:V:50:ARG:HH12	30:0:56:G:C5'	2.26	0.48
26:Z:73:ARG:HB2	26:Z:79:TRP:CZ3	2.49	0.48
26:Z:97:THR:O	26:Z:98:PRO:C	2.56	0.48
30:0:1457:U:O2'	30:0:1458:A:H5'	2.13	0.48
30:0:1819:G:C2'	30:0:1820:G:H5'	2.43	0.48
30:0:2045:G:H5''	42:0:9032:HOH:O	2.14	0.48
30:0:2253:G:H2'	30:0:2254:G:H8	1.78	0.48
31:9:78:G:N3	31:9:78:G:N2	2.62	0.48
2:B:123:ALA:O	2:B:126:GLU:HB3	2.14	0.47
9:I:87:PRO:HG3	30:0:1181:A:H1'	1.96	0.47
10:J:60:ARG:NH2	30:0:1242:A:OP2	2.37	0.47
12:L:53:ARG:NH2	12:L:57:VAL:CG1	2.76	0.47
14:N:82:TYR:HE1	14:N:120:GLU:HG2	1.77	0.47
15:O:26:TRP:N	42:O:3062:HOH:O	2.47	0.47
23:W:21:LEU:CD2	23:W:48:VAL:HG11	2.20	0.47
23:W:73:LEU:HD12	23:W:73:LEU:HA	1.72	0.47
27:1:53:LYS:O	27:1:54:ALA:C	2.57	0.47
30:0:559:U:H5'	30:0:559:U:C6	2.48	0.47
30:0:635:A:H2'	30:0:636:G:H5''	1.96	0.47
30:0:1057:A:H1'	30:0:2492:U:O2'	2.14	0.47
30:0:1346:U:H2'	30:0:1347:U:H6	1.79	0.47
2:B:132:HIS:CE1	2:B:171:VAL:HG21	2.50	0.47
2:B:314:ALA:CB	2:B:317:PRO:HG3	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:103:VAL:HG12	5:E:104:ILE:N	2.29	0.47
8:H:52:LEU:HD13	8:H:153:PHE:HB3	1.96	0.47
11:K:8:VAL:HG12	11:K:9:THR:N	2.29	0.47
18:R:98:ASN:N	18:R:98:ASN:ND2	2.62	0.47
18:R:136:TRP:CE2	30:0:2053:G:H4'	2.50	0.47
23:W:43:GLY:HA3	30:0:945:U:O2'	2.15	0.47
23:W:117:ARG:HB3	30:0:1263:C:OP1	2.14	0.47
26:Z:43:GLY:O	26:Z:47:ARG:HG2	2.14	0.47
27:1:37:CYS:SG	27:1:39:PHE:HB2	2.54	0.47
30:0:100:C:H2'	30:0:101:C:H6	1.80	0.47
30:0:364:U:H2'	30:0:365:G:O4'	2.14	0.47
30:0:567:U:O5'	30:0:567:U:H6	1.96	0.47
30:0:1033:C:H2'	30:0:1034:G:H5'	1.96	0.47
30:0:1159:G:H1	30:0:1208:C:H42	1.62	0.47
30:0:1167:G:H2'	30:0:1168:C:O4'	2.14	0.47
30:0:1248:A:H2'	30:0:1249:U:C6	2.49	0.47
30:0:1278:A:H2'	30:0:1280:A:C8	2.49	0.47
30:0:1790:C:H2'	30:0:1791:U:C6	2.50	0.47
30:0:1948:G:H2'	30:0:1949:G:C8	2.49	0.47
30:0:1948:G:H2'	30:0:1949:G:H8	1.79	0.47
1:A:125:ASN:HB3	1:A:158:VAL:HG12	1.96	0.47
2:B:154:VAL:HG12	2:B:156:LYS:HG2	1.96	0.47
30:0:425:U:O2'	30:0:426:G:H5'	2.14	0.47
30:0:1067:A:H3'	42:0:5158:HOH:O	2.14	0.47
30:0:1383:U:O2'	30:0:1384:C:H5'	2.14	0.47
1:A:80:LEU:HD22	1:A:91:GLY:O	2.13	0.47
3:C:53:GLY:O	3:C:79:ARG:HA	2.14	0.47
5:E:60:SER:OG	30:0:2784:A:H1'	2.15	0.47
8:H:143:VAL:HG21	8:H:173:GLU:HG2	1.96	0.47
9:I:129:SER:HB3	30:0:1192:A:N6	2.29	0.47
11:K:115:ARG:HG3	11:K:116:GLU:N	2.29	0.47
18:R:82:GLU:CG	18:R:83:LYS:N	2.77	0.47
27:1:4:GLY:O	27:1:8:GLN:HG2	2.14	0.47
27:1:8:GLN:HE22	27:1:11:LYS:HZ2	1.62	0.47
27:1:28:HIS:HE1	30:0:776:A:OP1	1.96	0.47
30:0:514:G:OP1	30:0:514:G:H3'	2.15	0.47
30:0:816:G:C6	30:0:817:G:N1	2.82	0.47
30:0:876:A:H2'	30:0:876:A:N3	2.29	0.47
30:0:1079:A:N3	30:0:2078:U:H1'	2.30	0.47
30:0:1816:C:H2'	30:0:1817:U:O4'	2.15	0.47
30:0:1819:G:H2'	30:0:1820:G:H4'	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2578:G:H5'	30:0:2578:G:C8	2.40	0.47
1:A:58:VAL:O	1:A:65:ARG:HA	2.15	0.47
1:A:95:PRO:C	1:A:97:ALA:H	2.23	0.47
2:B:17:LYS:O	2:B:260:HIS:HD2	1.97	0.47
4:D:21:VAL:CG2	4:D:80:ALA:HB1	2.45	0.47
6:F:56:PRO:HG3	13:M:44:THR:HA	1.95	0.47
7:G:19:GLU:O	7:G:20:VAL:C	2.57	0.47
7:G:65:THR:HG23	42:0:6310:HOH:O	2.15	0.47
8:H:96:GLN:HE21	8:H:129:ARG:HH21	1.62	0.47
9:I:118:ASN:HA	9:I:121:LYS:CD	2.44	0.47
10:J:74:ARG:NH1	10:J:76:ASP:HB2	2.29	0.47
12:L:101:ASP:C	12:L:103:ALA:H	2.23	0.47
42:N:8812:HOH:O	31:9:36:C:H4'	2.13	0.47
18:R:106:GLY:O	18:R:109:MET:HB2	2.14	0.47
24:X:72:VAL:HG23	24:X:86:GLU:O	2.15	0.47
30:0:78:G:N1	30:0:78:G:N7	2.62	0.47
30:0:323:C:O2'	30:0:324:G:H5'	2.14	0.47
30:0:344:C:H2'	30:0:345:G:O4'	2.13	0.47
30:0:1051:C:H2'	30:0:1052:G:O4'	2.15	0.47
30:0:1259:A:N1	30:0:1261:A:H1'	2.29	0.47
30:0:1736:A:H5'	42:0:5472:HOH:O	2.14	0.47
30:0:1973:A:H5'	30:0:1973:A:C8	2.42	0.47
30:0:2520:G:O2'	30:0:2521:A:H5'	2.14	0.47
1:A:212:PRO:HB2	42:A:9041:HOH:O	2.14	0.47
2:B:51:VAL:CG2	2:B:330:VAL:HG22	2.43	0.47
2:B:248:ARG:NH2	42:B:8995:HOH:O	2.47	0.47
2:B:285:VAL:O	2:B:286:ASN:HB2	2.13	0.47
6:F:21:GLU:O	6:F:24:ARG:CG	2.63	0.47
8:H:157:TYR:CD1	8:H:157:TYR:C	2.92	0.47
13:M:137:ASN:ND2	30:0:145:A:H4'	2.29	0.47
23:W:110:GLN:HA	23:W:110:GLN:HE21	1.78	0.47
27:1:13:THR:HG22	27:1:14:THR:N	2.30	0.47
30:0:264:G:H1'	30:0:265:U:C5	2.49	0.47
30:0:270:U:H5''	42:0:5432:HOH:O	2.14	0.47
30:0:544:G:H2'	30:0:545:G:H5''	1.97	0.47
30:0:590:A:H2'	30:0:591:A:H5'	1.97	0.47
30:0:695:C:H2'	30:0:696:C:C6	2.50	0.47
30:0:1180:U:H2'	30:0:1181:A:C8	2.50	0.47
30:0:1976:G:O2'	30:0:1977:U:C5'	2.63	0.47
1:A:83:GLY:O	1:A:94:LEU:HB3	2.14	0.47
3:C:34:ALA:CB	3:C:220:THR:HG21	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:39:LYS:HA	8:H:87:LYS:HZ1	1.78	0.47
8:H:85:ASP:OD2	8:H:142:ASN:ND2	2.37	0.47
10:J:39:VAL:HG13	10:J:106:GLY:O	2.14	0.47
13:M:57:LYS:NZ	13:M:144:ASP:HB2	2.30	0.47
14:N:24:LEU:HG	14:N:28:LYS:HE3	1.97	0.47
15:O:25:VAL:HG12	30:0:709:G:O2'	2.14	0.47
17:Q:27:GLN:NE2	31:9:8:G:H4'	2.30	0.47
17:Q:47:VAL:HA	17:Q:48:PRO:HD3	1.72	0.47
18:R:98:ASN:ND2	18:R:98:ASN:H	2.12	0.47
21:U:52:THR:HG21	21:U:54:THR:HB	1.96	0.47
23:W:13:MET:HE2	23:W:18:GLN:N	2.30	0.47
23:W:23:MET:C	23:W:25:ASN:H	2.22	0.47
30:0:352:A:H2'	30:0:353:G:C8	2.50	0.47
30:0:636:G:H5'	30:0:2059:U:OP2	2.14	0.47
30:0:970:U:O5'	30:0:970:U:H6	1.98	0.47
30:0:1309:U:O2'	30:0:1310:U:H5'	2.13	0.47
30:0:1333:U:H2'	30:0:1334:C:H6	1.79	0.47
30:0:1730:G:H5'	30:0:1731:C:H5	1.75	0.47
30:0:1972:U:H2'	30:0:1973:A:C5'	2.44	0.47
31:9:78:G:N1	31:9:78:G:N7	2.62	0.47
31:9:100:G:H3'	42:9:9133:HOH:O	2.14	0.47
1:A:231:LYS:HG3	30:0:1853:C:OP1	2.15	0.47
4:D:166:ILE:O	4:D:169:THR:N	2.48	0.47
6:F:79:GLN:HB2	6:F:82:ASP:OD2	2.14	0.47
11:K:28:GLU:HB3	11:K:59:LYS:HB2	1.95	0.47
13:M:69:LYS:HG2	13:M:127:LYS:HE3	1.95	0.47
14:N:49:THR:HB	14:N:58:LEU:HD13	1.97	0.47
25:Y:108:ASP:N	25:Y:108:ASP:OD1	2.47	0.47
30:0:187:A:H3'	30:0:188:C:C6	2.50	0.47
30:0:366:U:H2'	30:0:367:G:O4'	2.15	0.47
30:0:1158:G:O2'	30:0:1159:G:H5'	2.15	0.47
30:0:1309:U:C2'	30:0:1310:U:H5'	2.45	0.47
30:0:1519:U:H2'	30:0:1520:G:C8	2.50	0.47
30:0:1809:G:H2'	30:0:1811:A:OP2	2.15	0.47
30:0:2517:A:C2'	30:0:2518:C:H5'	2.44	0.47
1:A:6:GLY:HA3	42:0:5481:HOH:O	2.15	0.47
4:D:60:GLU:O	4:D:62:ASP:HB2	2.14	0.47
11:K:13:GLU:OE2	11:K:44:HIS:HB2	2.14	0.47
14:N:86:LEU:HA	14:N:121:GLY:O	2.14	0.47
15:O:35:LYS:O	15:O:40:HIS:NE2	2.47	0.47
16:P:69:ARG:HA	16:P:73:HIS:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:4:LEU:HD22	23:W:52:VAL:CG1	2.45	0.47
30:0:185:G:C4'	30:0:186:A:H4'	2.45	0.47
30:0:1203:G:O2'	30:0:1204:C:H5'	2.15	0.47
30:0:1682:A:H2'	42:0:3704:HOH:O	2.15	0.47
30:0:1745:G:H22	30:0:2033:G:H5'	1.80	0.47
30:0:2515:C:H2'	30:0:2516:G:O4'	2.14	0.47
2:B:36:PRO:CG	2:B:169:GLY:H	2.16	0.47
2:B:54:VAL:O	2:B:55:ASN:C	2.56	0.47
2:B:147:VAL:O	2:B:147:VAL:HG12	2.15	0.47
3:C:173:LYS:HB3	3:C:187:ARG:HG3	1.96	0.47
4:D:40:ILE:HG13	4:D:41:LEU:H	1.79	0.47
4:D:94:ALA:HA	4:D:174:VAL:C	2.40	0.47
13:M:170:ASN:HB2	42:M:8837:HOH:O	2.15	0.47
14:N:103:ASP:C	14:N:103:ASP:OD1	2.57	0.47
14:N:164:ASP:OD2	14:N:167:ASP:HA	2.15	0.47
19:S:44:GLN:HB3	19:S:45:TYR:CD1	2.50	0.47
23:W:106:THR:OG1	23:W:109:GLU:HG3	2.14	0.47
24:X:7:GLU:HG3	24:X:74:ALA:O	2.15	0.47
29:3:77:ALA:O	29:3:78:HIS:CA	2.63	0.47
30:0:308:U:H5'	30:0:309:C:OP1	2.14	0.47
30:0:400:C:H2'	30:0:401:C:C6	2.51	0.47
30:0:1347:U:H2'	30:0:1348:A:C8	2.50	0.47
30:0:1503:U:H2'	30:0:1504:A:H5'	1.96	0.47
30:0:1665:G:H2'	30:0:1666:C:O4'	2.14	0.47
30:0:2499:U:O2'	30:0:2500:C:H5'	2.14	0.47
30:0:2831:C:C2'	30:0:2832:C:H5'	2.45	0.47
3:C:238:SER:O	3:C:241:ALA:HB3	2.14	0.46
8:H:12:ILE:HD12	8:H:57:THR:CG2	2.45	0.46
13:M:68:ARG:HG2	13:M:73:ARG:CZ	2.45	0.46
13:M:84:LYS:HZ1	30:0:391:U:P	2.38	0.46
14:N:108:SER:HA	14:N:109:PRO:HD3	1.79	0.46
15:O:112:ARG:HD2	42:0:3570:HOH:O	2.15	0.46
16:P:107:GLU:C	16:P:109:ARG:N	2.73	0.46
25:Y:100:ARG:HD2	25:Y:218:GLU:OE1	2.15	0.46
29:3:51:LYS:C	29:3:53:SER:H	2.23	0.46
30:0:512:G:H1'	42:0:7627:HOH:O	2.15	0.46
30:0:583:C:H2'	30:0:584:U:C6	2.50	0.46
30:0:615:G:H2'	30:0:616:U:C6	2.50	0.46
30:0:1909:A:H2'	30:0:1910:A:C8	2.50	0.46
30:0:2554:U:H1'	42:0:6968:HOH:O	2.15	0.46
30:0:2775:A:C6	30:0:2799:A:C8	3.03	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:11:A:O2'	31:9:12:C:H3'	2.15	0.46
1:A:179:MET:HE3	1:A:179:MET:CA	2.31	0.46
3:C:48:SER:OG	3:C:91:PRO:HB2	2.16	0.46
3:C:67:GLN:O	30:0:1359:U:C4	2.68	0.46
3:C:94:THR:C	3:C:96:LYS:H	2.22	0.46
6:F:15:ASP:O	6:F:18:GLU:HB2	2.16	0.46
8:H:157:TYR:C	8:H:157:TYR:HD1	2.24	0.46
10:J:36:VAL:CG1	10:J:37:ALA:N	2.78	0.46
12:L:24:ALA:CB	12:L:30:ARG:HG3	2.46	0.46
12:L:134:GLU:HA	12:L:138:GLY:O	2.15	0.46
12:L:136:ALA:HB3	42:L:9038:HOH:O	2.15	0.46
13:M:139:PRO:C	13:M:141:ILE:N	2.71	0.46
15:O:25:VAL:CG1	30:0:710:G:H5'	2.45	0.46
23:W:130:HIS:C	23:W:136:GLY:HA3	2.40	0.46
25:Y:204:ARG:HH22	30:0:553:G:P	2.37	0.46
30:0:177:A:H2'	30:0:178:U:O4'	2.16	0.46
30:0:652:G:H2'	30:0:653:U:O4'	2.16	0.46
30:0:824:G:N2	42:0:6935:HOH:O	2.48	0.46
30:0:1077:G:H2'	30:0:1080:C:H42	1.79	0.46
30:0:1131:G:C6	30:0:1230:A:C4	3.03	0.46
30:0:1361:C:H2'	30:0:1362:U:H6	1.80	0.46
30:0:2102:G:H5''	30:0:2538:A:C2	2.51	0.46
30:0:2511:A:H2'	30:0:2512:U:O4'	2.15	0.46
30:0:2568:A:H2'	30:0:2569:A:O4'	2.14	0.46
2:B:148:PRO:HG2	2:B:158:LYS:O	2.15	0.46
2:B:175:LEU:C	2:B:175:LEU:CD2	2.88	0.46
2:B:304:PRO:HD2	2:B:307:ARG:HE	1.80	0.46
3:C:51:TYR:HA	3:C:54:LEU:HD12	1.97	0.46
11:K:21:ALA:HB1	11:K:110:LYS:O	2.14	0.46
14:N:165:ALA:C	14:N:167:ASP:H	2.22	0.46
17:Q:67:GLN:NE2	30:0:2403:C:O2	2.48	0.46
29:3:42:ARG:HH11	29:3:42:ARG:HG3	1.79	0.46
30:0:107:U:C2'	30:0:108:U:H5'	2.45	0.46
30:0:903:U:HO2'	30:0:904:U:H5	1.62	0.46
30:0:920:C:H2'	30:0:2109:U:C2	2.51	0.46
30:0:1149:U:C5	30:0:1215:A:C5	3.03	0.46
30:0:1477:C:H5'	30:0:1868:G:H5'	1.97	0.46
30:0:1931:A:C2'	30:0:1932:G:H5'	2.44	0.46
30:0:2651:C:H2'	30:0:2652:U:O4'	2.15	0.46
1:A:101:GLU:OE2	1:A:131:HIS:HB2	2.14	0.46
1:A:109:GLU:HG2	1:A:114:ASP:OD1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:248:ARG:NH2	30:0:2549:C:H1'	2.30	0.46
2:B:251:VAL:HG23	2:B:253:GLN:HG3	1.97	0.46
3:C:7:ASP:C	3:C:9:ASP:N	2.74	0.46
6:F:107:ASP:O	6:F:111:ILE:HG13	2.15	0.46
8:H:62:HIS:HA	8:H:65:LEU:HD23	1.97	0.46
8:H:87:LYS:HB2	8:H:87:LYS:HZ2	1.81	0.46
8:H:149:VAL:HG22	42:H:9034:HOH:O	2.13	0.46
11:K:62:PRO:HA	11:K:65:ARG:NH2	2.31	0.46
13:M:82:ARG:O	13:M:83:SER:C	2.59	0.46
13:M:102:GLU:CD	13:M:164:THR:HG21	2.41	0.46
13:M:157:ASP:O	13:M:158:ARG:C	2.58	0.46
17:Q:30:VAL:O	17:Q:31:GLU:C	2.59	0.46
26:Z:43:GLY:HA2	30:0:1771:U:O2	2.16	0.46
29:3:36:ILE:CG2	29:3:37:ASP:N	2.79	0.46
30:0:292:G:H1'	30:0:360:A:N6	2.29	0.46
30:0:806:A:H2'	30:0:807:A:O4'	2.16	0.46
30:0:2296:C:H4'	30:0:2362:A:C2	2.51	0.46
31:9:3:A:H2'	42:9:9043:HOH:O	2.15	0.46
1:A:35:GLY:C	1:A:37:VAL:H	2.23	0.46
1:A:42:VAL:O	1:A:76:VAL:HG13	2.14	0.46
3:C:90:HIS:HB2	42:C:8544:HOH:O	2.14	0.46
3:C:176:ALA:HB2	30:0:1343:C:C5	2.50	0.46
4:D:18:ILE:HG12	4:D:134:LEU:CD2	2.45	0.46
5:E:139:GLU:OE2	30:0:2781:U:H1'	2.15	0.46
14:N:29:SER:HB3	30:0:2415:A:O2'	2.16	0.46
16:P:88:GLN:HE22	30:0:1799:G:H21	1.63	0.46
18:R:135:ALA:O	30:0:2054:A:H4'	2.16	0.46
23:W:10:GLU:O	23:W:13:MET:HB3	2.16	0.46
24:X:66:THR:HG23	24:X:67:PRO:HD2	1.97	0.46
30:0:1410:G:H3'	42:0:6433:HOH:O	2.15	0.46
30:0:2453:G:H5'	42:0:5549:HOH:O	2.15	0.46
31:9:39:U:C2'	31:9:40:C:OP1	2.64	0.46
1:A:27:LEU:HD11	1:A:51:ARG:HE	1.79	0.46
1:A:75:GLY:HA2	26:Z:88:PHE:HA	1.98	0.46
2:B:312:ARG:HD3	2:B:315:VAL:HG13	1.97	0.46
3:C:241:ALA:O	3:C:244:ALA:HB3	2.14	0.46
4:D:39:ASP:HB2	42:D:5583:HOH:O	2.15	0.46
8:H:83:GLU:O	8:H:84:GLY:C	2.58	0.46
11:K:34:VAL:HG22	11:K:47:ALA:HB2	1.96	0.46
16:P:115:SER:C	16:P:117:SER:N	2.73	0.46
16:P:134:VAL:O	16:P:137:LEU:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:49:GLU:CB	20:T:59:GLU:HG2	2.41	0.46
22:V:45:ARG:C	22:V:47:LYS:N	2.72	0.46
30:0:129:A:O2'	30:0:131:A:OP1	2.32	0.46
30:0:574:G:H2'	30:0:575:A:O4'	2.16	0.46
30:0:699:C:H6	30:0:744:G:O4'	1.98	0.46
30:0:791:A:H2'	30:0:792:G:O4'	2.16	0.46
30:0:1001:U:O2'	30:0:1002:G:H5'	2.15	0.46
30:0:1181:A:C2'	30:0:1182:C:H5'	2.45	0.46
30:0:1791:U:H2'	30:0:1792:C:C6	2.51	0.46
30:0:1971:G:H5''	42:0:7875:HOH:O	2.14	0.46
30:0:2250:G:H2'	30:0:2251:G:O4'	2.16	0.46
30:0:2445:U:H2'	30:0:2446:G:C8	2.51	0.46
30:0:2838:A:H2'	30:0:2839:C:C6	2.51	0.46
1:A:140:LEU:HB3	1:A:141:PRO:HD2	1.98	0.46
2:B:215:VAL:HA	2:B:220:VAL:HG22	1.98	0.46
13:M:45:ARG:HB2	13:M:118:TYR:CE1	2.51	0.46
13:M:98:GLN:HB2	13:M:129:HIS:CD2	2.51	0.46
14:N:11:ARG:HG3	14:N:14:ARG:NH1	2.31	0.46
16:P:36:THR:O	16:P:39:ASP:HB2	2.16	0.46
22:V:49:LEU:O	22:V:53:ILE:HG13	2.15	0.46
30:0:558:C:H2'	30:0:559:U:H5'	1.97	0.46
30:0:566:A:C2'	30:0:567:U:H5'	2.46	0.46
30:0:566:A:N1	30:0:1093:G:O2'	2.44	0.46
30:0:1130:U:H2'	30:0:1131:G:O4'	2.16	0.46
30:0:1515:A:H2'	30:0:1516:U:C6	2.50	0.46
30:0:1596:U:H2'	30:0:1598:A:OP2	2.15	0.46
30:0:2589:U:H2'	30:0:2590:U:C6	2.51	0.46
30:0:2842:G:C2'	30:0:2843:A:H5'	2.45	0.46
2:B:109:LEU:HD22	2:B:145:HIS:CE1	2.51	0.46
2:B:238:ASN:ND2	2:B:240:GLY:H	2.11	0.46
2:B:284:PHE:HB2	2:B:287:TYR:HB3	1.96	0.46
9:I:82:THR:CG2	30:0:1168:C:H5''	2.45	0.46
11:K:81:ARG:HG3	11:K:85:GLY:O	2.15	0.46
14:N:182:GLY:O	14:N:183:ASP:C	2.59	0.46
18:R:119:VAL:HG23	18:R:142:ASP:HB2	1.98	0.46
19:S:49:VAL:HG13	19:S:66:VAL:HG13	1.96	0.46
30:0:535:G:C5	30:0:2063:U:C4	3.04	0.46
30:0:612:U:H2'	30:0:613:C:H6	1.80	0.46
30:0:1098:A:H2'	30:0:1099:G:O4'	2.15	0.46
30:0:1135:G:H5'	42:0:6761:HOH:O	2.16	0.46
30:0:1202:A:H2'	30:0:1203:G:O4'	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1657:A:H2'	30:0:1658:A:C8	2.51	0.46
31:9:39:U:H1'	31:9:44:A:H61	1.81	0.46
1:A:228:ILE:O	1:A:229:ALA:C	2.58	0.46
2:B:305:ASP:O	2:B:306:LYS:CB	2.63	0.46
3:C:139:VAL:HG13	3:C:240:LEU:HD12	1.98	0.46
6:F:49:PHE:HB2	6:F:96:ALA:HB3	1.98	0.46
10:J:45:VAL:HG23	10:J:129:PHE:HD1	1.81	0.46
11:K:23:ASN:HD21	11:K:107:THR:HB	1.80	0.46
11:K:64:MET:HA	11:K:67:GLN:HE21	1.80	0.46
13:M:40:ILE:HD11	13:M:130:GLU:HG2	1.97	0.46
14:N:164:ASP:OD1	14:N:167:ASP:OD1	2.34	0.46
15:O:19:ARG:HH11	30:0:1276:U:H3'	1.81	0.46
17:Q:25:PRO:HB3	42:9:9006:HOH:O	2.15	0.46
19:S:68:LEU:HB3	19:S:72:ASP:HB2	1.97	0.46
20:T:38:ARG:HH21	30:0:306:A:P	2.38	0.46
30:0:111:C:O2'	30:0:112:G:H5'	2.16	0.46
30:0:956:G:H5'	31:9:81:C:H4'	1.98	0.46
30:0:1260:G:H3'	30:0:1261:A:C8	2.51	0.46
30:0:1304:U:H2'	30:0:1305:C:C6	2.51	0.46
30:0:2371:G:H5'	42:0:5865:HOH:O	2.14	0.46
31:9:74:G:C6	31:9:75:G:N7	2.84	0.46
2:B:139:ASP:HB2	2:B:165:ARG:HE	1.80	0.46
2:B:337:GLY:N	42:B:9013:HOH:O	2.49	0.46
5:E:158:ASP:OD1	5:E:160:ARG:HB2	2.15	0.46
8:H:49:GLN:NE2	8:H:140:TYR:CE2	2.84	0.46
8:H:61:ARG:NH1	8:H:61:ARG:HG3	2.30	0.46
11:K:62:PRO:HG3	11:K:65:ARG:NH2	2.31	0.46
14:N:26:LEU:HD21	14:N:103:ASP:HA	1.97	0.46
24:X:23:HIS:C	24:X:24:LYS:HG3	2.41	0.46
30:0:25:A:H2'	30:0:26:U:H5'	1.98	0.46
30:0:1206:U:H5'	30:0:1206:U:C6	2.42	0.46
30:0:1607:A:H2'	30:0:1608:G:O4'	2.16	0.46
30:0:2748:G:H4'	30:0:2749:U:H5'	1.98	0.46
30:0:2760:C:H5''	42:0:6171:HOH:O	2.16	0.46
4:D:15:GLU:HA	4:D:16:PRO:HD3	1.80	0.45
6:F:8:VAL:HG13	6:F:12:LEU:HD13	1.98	0.45
6:F:13:GLU:OE2	6:F:78:GLU:HG2	2.17	0.45
42:N:8846:HOH:O	31:9:7:G:H5'	2.16	0.45
15:O:19:ARG:NH1	30:0:1276:U:H3'	2.30	0.45
16:P:104:LYS:HG2	16:P:137:LEU:HD23	1.98	0.45
16:P:115:SER:N	16:P:118:GLN:HE21	1.89	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:8:ALA:HB1	18:R:13:THR:CG2	2.35	0.45
28:2:45:ASN:HB3	28:2:46:ASP:H	1.58	0.45
30:0:37:A:C2	30:0:446:G:C2	3.04	0.45
30:0:1209:C:O2'	30:0:1210:G:H5'	2.15	0.45
30:0:1393:A:N1	30:0:1725:C:O2'	2.43	0.45
30:0:1463:U:H2'	30:0:1464:C:C6	2.51	0.45
30:0:1739:G:H1'	30:0:2726:U:O4	2.16	0.45
30:0:2269:C:H2'	30:0:2270:G:O4'	2.15	0.45
30:0:2506:A:O2'	30:0:2507:G:O5'	2.35	0.45
3:C:2:GLN:HB2	42:C:8534:HOH:O	2.16	0.45
11:K:81:ARG:HB2	11:K:87:ARG:NH1	2.31	0.45
20:T:23:VAL:O	20:T:42:VAL:HG23	2.16	0.45
20:T:29:ALA:HA	42:T:7653:HOH:O	2.16	0.45
22:V:1:THR:O	22:V:3:LEU:N	2.50	0.45
25:Y:106:THR:CG2	25:Y:107:PRO:HD2	2.46	0.45
25:Y:174:VAL:HA	25:Y:177:LYS:HE3	1.97	0.45
30:0:425:U:H4'	42:0:7746:HOH:O	2.16	0.45
30:0:544:G:C2'	30:0:545:G:H5''	2.45	0.45
30:0:820:G:H5'	30:0:821:U:C5'	2.47	0.45
30:0:2087:C:C2	30:0:2658:G:C2	3.04	0.45
30:0:2507:G:H2'	30:0:2510:C:N4	2.31	0.45
1:A:105:VAL:HG13	1:A:155:THR:O	2.16	0.45
1:A:135:VAL:HG13	1:A:135:VAL:O	2.16	0.45
3:C:193:LEU:HD23	3:C:233:THR:HG23	1.99	0.45
4:D:27:ILE:HD11	4:D:37:ALA:HB2	1.98	0.45
4:D:149:ARG:HH12	14:N:15:GLU:HA	1.79	0.45
11:K:115:ARG:O	11:K:118:ALA:HB3	2.16	0.45
18:R:64:SER:OG	30:0:1369:A:H5''	2.16	0.45
22:V:44:GLY:HA3	30:0:92:G:H4'	1.98	0.45
23:W:31:HIS:HB3	23:W:115:THR:HG21	1.98	0.45
23:W:117:ARG:HH22	30:0:1264:U:P	2.39	0.45
30:0:228:C:H2'	30:0:229:G:H5'	1.97	0.45
30:0:584:U:H3'	42:0:6928:HOH:O	2.17	0.45
30:0:644:G:H1'	42:0:7230:HOH:O	2.16	0.45
30:0:710:G:C2'	30:0:711:G:H5'	2.47	0.45
30:0:1183:C:H41	30:0:1192:A:P	2.39	0.45
30:0:1361:C:H2'	30:0:1362:U:C6	2.51	0.45
30:0:1588:G:H1'	30:0:1607:A:H61	1.81	0.45
30:0:1619:G:H2'	30:0:1620:C:O4'	2.15	0.45
30:0:1864:C:H2'	30:0:1865:A:O4'	2.16	0.45
30:0:2004:U:O2	30:0:2004:U:C2'	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2560:C:H4'	42:0:7451:HOH:O	2.17	0.45
30:0:2831:C:H2'	30:0:2832:C:H5'	1.98	0.45
33:6:76:8AN:H2	42:6:82:HOH:O	2.15	0.45
1:A:48:ASP:OD2	1:A:51:ARG:HG3	2.17	0.45
2:B:88:GLU:HB3	2:B:97:LEU:HD12	1.99	0.45
2:B:279:THR:HA	2:B:284:PHE:HE1	1.81	0.45
3:C:101:ASP:HA	42:C:8646:HOH:O	2.16	0.45
6:F:67:ALA:HB1	6:F:72:VAL:O	2.16	0.45
7:G:23:ILE:CD1	7:G:67:LEU:HD23	2.42	0.45
8:H:141:CYS:HB2	42:H:8997:HOH:O	2.15	0.45
9:I:91:PHE:CD2	9:I:131:GLY:HA2	2.50	0.45
11:K:125:ALA:O	11:K:127:ALA:N	2.50	0.45
11:K:132:VAL:HG11	21:U:22:VAL:HG22	1.98	0.45
12:L:6:ARG:NH1	30:0:1299:G:N7	2.65	0.45
12:L:125:PHE:CE1	12:L:140:VAL:HG22	2.52	0.45
13:M:8:ILE:O	13:M:11:ALA:HB3	2.17	0.45
16:P:16:VAL:HG12	16:P:17:GLY:N	2.31	0.45
16:P:73:HIS:HE1	30:0:1789:G:O6	2.00	0.45
20:T:41:ARG:NH1	20:T:42:VAL:O	2.50	0.45
20:T:43:ASN:C	20:T:45:GLY:N	2.72	0.45
20:T:52:ARG:HD2	30:0:317:A:H5''	1.97	0.45
20:T:82:THR:HA	42:0:4859:HOH:O	2.15	0.45
23:W:52:VAL:CG2	23:W:53:ALA:N	2.49	0.45
24:X:87:ALA:O	24:X:88:GLU:HG2	2.16	0.45
25:Y:130:ARG:HB2	25:Y:142:SER:O	2.16	0.45
30:0:27:U:H2'	30:0:28:G:O4'	2.17	0.45
30:0:652:G:C2	30:0:653:U:H1'	2.51	0.45
30:0:2842:G:H2'	30:0:2843:A:C5'	2.46	0.45
30:0:2846:C:H2'	30:0:2847:G:H8	1.80	0.45
30:0:2894:C:O2'	30:0:2895:C:H5'	2.16	0.45
31:9:12:C:H4'	31:9:69:U:O2	2.17	0.45
1:A:23:TYR:CD1	1:A:50:ALA:HB2	2.51	0.45
2:B:140:LEU:HD13	2:B:175:LEU:HA	1.98	0.45
6:F:21:GLU:O	6:F:24:ARG:HG2	2.17	0.45
10:J:26:VAL:HG13	10:J:36:VAL:HG11	1.98	0.45
10:J:107:ASN:C	10:J:107:ASN:HD22	2.24	0.45
14:N:72:GLU:HB3	14:N:163:PHE:CE1	2.52	0.45
14:N:73:ALA:HB1	14:N:74:PRO:HD2	1.97	0.45
19:S:11:THR:H	19:S:14:ALA:HB3	1.82	0.45
26:Z:51:ALA:O	26:Z:55:SER:HB2	2.16	0.45
28:2:21:VAL:O	28:2:22:PRO:C	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:604:G:H2'	42:0:9543:HOH:O	2.16	0.45
30:0:731:U:H2'	30:0:732:C:C6	2.52	0.45
30:0:1165:G:H21	30:0:1173:A:H5''	1.82	0.45
30:0:1181:A:H2'	30:0:1182:C:C5'	2.47	0.45
30:0:1394:C:H3'	30:0:1433:G:N2	2.32	0.45
30:0:1787:C:H4'	30:0:2883:A:O4'	2.17	0.45
30:0:1810:C:H2'	30:0:1811:A:O4'	2.17	0.45
30:0:1889:C:H2'	30:0:1890:U:O4'	2.17	0.45
1:A:199:HIS:N	42:A:9110:HOH:O	2.49	0.45
2:B:41:PHE:HB3	2:B:190:MET:HE3	1.99	0.45
2:B:185:GLY:HA2	42:B:9109:HOH:O	2.15	0.45
4:D:81:GLU:C	4:D:83:PHE:N	2.72	0.45
5:E:20:ILE:O	5:E:30:THR:HG23	2.16	0.45
7:G:64:ASN:OD1	30:0:1211:G:H5''	2.16	0.45
11:K:101:ASN:O	11:K:102:GLU:CB	2.63	0.45
19:S:73:ASP:HB3	19:S:76:GLU:OE1	2.17	0.45
20:T:43:ASN:ND2	20:T:108:ARG:CZ	2.79	0.45
27:1:15:THR:O	27:1:29:THR:N	2.46	0.45
30:0:24:G:N2	30:0:518:G:H1'	2.31	0.45
30:0:116:G:H2'	30:0:117:A:C8	2.52	0.45
30:0:168:C:H5'	30:0:2277:U:OP1	2.16	0.45
30:0:1484:G:H2'	42:0:3021:HOH:O	2.17	0.45
30:0:1833:U:O2'	30:0:1834:C:H5'	2.16	0.45
30:0:2419:U:H5''	30:0:2420:G:H5'	1.97	0.45
30:0:2506:A:O2'	30:0:2507:G:P	2.75	0.45
31:9:13:A:H3'	31:9:14:G:H5'	1.99	0.45
2:B:79:MET:HE3	2:B:144:THR:HG21	1.98	0.45
3:C:76:ARG:HB3	3:C:78:ARG:NH1	2.32	0.45
12:L:66:VAL:CG2	12:L:67:ARG:N	2.78	0.45
12:L:145:LEU:C	12:L:147:GLU:N	2.74	0.45
13:M:69:LYS:O	30:0:2263:G:H4'	2.17	0.45
14:N:102:LEU:HG	14:N:104:ILE:HG23	1.98	0.45
14:N:151:ASP:OD1	14:N:154:LEU:HD13	2.17	0.45
15:O:59:VAL:HG23	15:O:111:VAL:CG2	2.46	0.45
17:Q:14:LEU:HB3	42:Q:3971:HOH:O	2.16	0.45
20:T:17:HIS:HB3	30:0:100:C:O2	2.17	0.45
22:V:43:PRO:O	22:V:46:ILE:HG22	2.16	0.45
26:Z:81:CYS:C	26:Z:83:TYR:H	2.24	0.45
30:0:295:C:H2'	30:0:296:G:O4'	2.16	0.45
30:0:343:C:O2'	30:0:344:C:H5'	2.16	0.45
30:0:1056:U:H2'	30:0:1057:A:O4'	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1741:U:H5''	42:0:3669:HOH:O	2.17	0.45
30:0:1831:U:O4	30:0:1845:A:H2	1.99	0.45
30:0:2081:A:H2'	30:0:2082:G:O4'	2.17	0.45
2:B:141:ARG:CG	2:B:165:ARG:HA	2.47	0.45
2:B:188:HIS:HD1	2:B:188:HIS:H	1.64	0.45
3:C:193:LEU:HA	3:C:211:ASP:O	2.17	0.45
4:D:25:MET:HE1	4:D:40:ILE:HD11	1.99	0.45
4:D:88:LEU:HB2	4:D:89:PRO:HD3	1.98	0.45
8:H:9:TYR:HE2	8:H:99:ARG:O	2.00	0.45
10:J:75:PRO:HD3	10:J:136:SER:OG	2.17	0.45
12:L:130:ARG:HA	42:L:9020:HOH:O	2.17	0.45
16:P:61:ARG:NH2	30:0:2737:C:OP2	2.43	0.45
17:Q:62:THR:O	17:Q:64:GLU:HG2	2.16	0.45
20:T:27:LEU:HB2	20:T:32:ARG:HG3	1.99	0.45
23:W:122:ARG:NH2	42:0:6133:HOH:O	2.50	0.45
28:2:22:PRO:HG2	28:2:25:VAL:CG2	2.46	0.45
29:3:65:THR:HG23	29:3:67:LEU:HG	1.99	0.45
30:0:12:U:C2'	30:0:13:G:H5'	2.47	0.45
30:0:325:U:H2'	30:0:326:G:H8	1.79	0.45
30:0:750:A:H2'	30:0:751:U:C6	2.51	0.45
30:0:2011:A:H5'	30:0:2013:G:C1'	2.46	0.45
31:9:1:U:H5'	31:9:121:C:O2	2.16	0.45
31:9:60:C:H2'	31:9:61:C:H6	1.80	0.45
2:B:74:ILE:HG13	42:B:9078:HOH:O	2.16	0.45
3:C:219:ASN:O	3:C:223:LEU:HB2	2.16	0.45
5:E:84:MET:HE1	5:E:148:ILE:HD13	1.96	0.45
10:J:36:VAL:HG12	10:J:37:ALA:N	2.32	0.45
13:M:30:GLU:O	13:M:34:GLU:HG3	2.16	0.45
15:O:49:GLU:OE1	15:O:70:LEU:HD12	2.16	0.45
18:R:27:HIS:O	18:R:31:ILE:HG13	2.17	0.45
23:W:80:ASP:H	23:W:83:TRP:HB3	1.82	0.45
25:Y:142:SER:OG	30:0:1331:G:OP2	2.31	0.45
26:Z:37:ARG:HD3	42:Z:8713:HOH:O	2.16	0.45
30:0:1187:U:HO2'	30:0:1188:A:H8	1.64	0.45
30:0:1626:A:H2'	30:0:1627:G:O4'	2.17	0.45
30:0:2135:A:O4'	30:0:2243:C:N4	2.50	0.45
30:0:2443:C:H3'	42:0:4363:HOH:O	2.17	0.45
30:0:2887:G:H2'	30:0:2888:U:C6	2.52	0.45
2:B:66:GLU:OE1	2:B:328:ARG:HD2	2.17	0.45
2:B:113:LEU:HD21	2:B:161:VAL:HG21	1.97	0.45
2:B:232:TRP:CD1	2:B:235:ARG:HD2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:294:TYR:HE2	42:B:9128:HOH:O	1.99	0.45
2:B:297:VAL:HB	42:B:9078:HOH:O	2.17	0.45
4:D:141:VAL:HG13	4:D:144:ARG:NH2	2.32	0.45
8:H:91:ARG:NH1	8:H:138:THR:OG1	2.49	0.45
12:L:134:GLU:C	12:L:136:ALA:H	2.24	0.45
14:N:22:GLN:HB3	42:N:8873:HOH:O	2.17	0.45
16:P:91:LYS:NZ	30:0:816:G:OP1	2.39	0.45
17:Q:95:GLU:HA	30:0:949:U:C4'	2.46	0.45
23:W:25:ASN:OD1	30:0:1025:C:H5''	2.17	0.45
23:W:42:ARG:O	23:W:43:GLY:C	2.60	0.45
24:X:20:GLU:CG	24:X:21:PRO:HD2	2.45	0.45
26:Z:102:THR:O	26:Z:103:VAL:C	2.60	0.45
30:0:191:A:C4	30:0:237:G:N7	2.85	0.45
30:0:290:C:O2'	30:0:291:C:H5'	2.16	0.45
30:0:1985:U:C2	30:0:1996:U:O4'	2.70	0.45
30:0:2088:C:H1'	30:0:2841:A:C2	2.52	0.45
30:0:2361:A:H2'	30:0:2362:A:C8	2.51	0.45
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.87	0.44
1:A:94:LEU:HD23	1:A:94:LEU:N	2.31	0.44
5:E:9:GLU:HG2	42:E:7544:HOH:O	2.17	0.44
8:H:59:GLN:NE2	8:H:96:GLN:HG2	2.25	0.44
8:H:67:ALA:HB1	8:H:159:LYS:HD3	1.98	0.44
13:M:72:ALA:HB1	13:M:93:ARG:NE	2.32	0.44
15:O:9:SER:O	15:O:10:LEU:C	2.59	0.44
18:R:62:HIS:HB3	30:0:1370:G:O5'	2.16	0.44
30:0:297:U:H1'	42:0:4807:HOH:O	2.16	0.44
30:0:1031:G:O3'	30:0:1032:A:H8	2.00	0.44
30:0:1165:G:O2'	30:0:1174:A:C4'	2.65	0.44
30:0:1291:A:H2	42:0:6136:HOH:O	2.00	0.44
30:0:1477:C:H4'	30:0:1868:G:OP1	2.17	0.44
30:0:2072:G:H3'	30:0:2073:G:C5'	2.47	0.44
30:0:2335:C:H2'	30:0:2336:G:H8	1.82	0.44
30:0:2435:U:H1'	42:0:6273:HOH:O	2.17	0.44
31:9:73:A:H61	31:9:108:C:N4	2.13	0.44
2:B:195:ARG:HG3	2:B:196:ALA:N	2.31	0.44
2:B:261:GLN:HG2	30:0:2808:U:OP1	2.17	0.44
11:K:125:ALA:C	11:K:127:ALA:N	2.69	0.44
12:L:54:PRO:HG2	12:L:57:VAL:CG2	2.47	0.44
14:N:37:ARG:HH21	14:N:105:GLY:CA	2.30	0.44
15:O:62:GLY:O	15:O:79:VAL:HG23	2.18	0.44
17:Q:61:GLY:HA3	17:Q:74:ASP:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:97:GLY:O	18:R:98:ASN:C	2.59	0.44
23:W:9:GLY:N	30:0:1086:A:OP1	2.50	0.44
23:W:56:GLU:O	23:W:143:THR:HG23	2.17	0.44
23:W:115:THR:HG23	42:W:5420:HOH:O	2.17	0.44
23:W:126:ASP:O	23:W:136:GLY:HA2	2.16	0.44
25:Y:95:THR:N	25:Y:236:VAL:O	2.51	0.44
25:Y:95:THR:O	25:Y:95:THR:HG22	2.16	0.44
27:1:16:HIS:CD2	30:0:470:U:O2'	2.57	0.44
27:1:42:SER:HB3	30:0:1473:U:O4'	2.17	0.44
27:1:54:ALA:HB2	30:0:892:G:H5''	1.98	0.44
29:3:24:LYS:HE3	29:3:90:PHE:CE1	2.52	0.44
30:0:23:G:C6	30:0:24:G:N1	2.85	0.44
30:0:2394:A:H4'	42:0:9457:HOH:O	2.16	0.44
30:0:2869:G:H2'	30:0:2870:C:C6	2.52	0.44
2:B:209:LYS:HE2	42:B:9040:HOH:O	2.15	0.44
5:E:73:PHE:O	5:E:76:VAL:HG22	2.18	0.44
10:J:57:TYR:O	10:J:61:VAL:HG23	2.18	0.44
10:J:70:PHE:HE1	30:0:2676:C:C4'	2.19	0.44
10:J:91:LYS:O	10:J:92:GLN:C	2.58	0.44
10:J:107:ASN:HD22	10:J:109:TYR:H	1.64	0.44
12:L:73:VAL:HG23	12:L:74:THR:N	2.31	0.44
13:M:47:ASP:CG	13:M:48:LYS:N	2.76	0.44
13:M:79:ALA:HB3	13:M:81:ARG:NH1	2.33	0.44
13:M:98:GLN:HB2	13:M:129:HIS:NE2	2.32	0.44
13:M:193:LYS:HB3	30:0:392:U:C5'	2.47	0.44
18:R:39:THR:CG2	18:R:42:GLU:HG3	2.48	0.44
19:S:67:ARG:HD3	42:0:5526:HOH:O	2.16	0.44
24:X:41:PHE:HD2	24:X:76:ARG:HB2	1.81	0.44
25:Y:186:ARG:HD2	42:0:5056:HOH:O	2.17	0.44
25:Y:208:LYS:O	25:Y:209:VAL:C	2.59	0.44
30:0:34:C:H2'	30:0:35:U:C6	2.52	0.44
30:0:254:C:H2'	30:0:255:A:O4'	2.18	0.44
30:0:812:A:H2'	30:0:813:C:O4'	2.17	0.44
30:0:877:G:C2	30:0:885:G:O4'	2.70	0.44
30:0:1021:G:O2'	30:0:1022:A:H5'	2.18	0.44
30:0:1298:U:H2'	30:0:1299:G:H8	1.81	0.44
30:0:1617:C:C5	30:0:1643:C:H4'	2.53	0.44
30:0:1803:C:H2'	30:0:1804:A:C8	2.52	0.44
30:0:2323:G:H5'	42:0:7829:HOH:O	2.17	0.44
30:0:2592:G:H2'	30:0:2593:C:C6	2.52	0.44
2:B:22:GLU:HA	2:B:205:VAL:HG21	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:307:ARG:HH11	2:B:307:ARG:HG3	1.82	0.44
3:C:77:ALA:O	3:C:78:ARG:CA	2.65	0.44
12:L:36:ASP:HB2	42:0:5147:HOH:O	2.18	0.44
12:L:98:GLU:O	12:L:99:GLU:HB2	2.16	0.44
13:M:28:GLN:HA	13:M:31:TRP:HB2	1.98	0.44
13:M:122:GLN:HB2	13:M:126:GLN:O	2.18	0.44
15:O:65:LEU:HD13	30:0:746:A:N6	2.33	0.44
17:Q:25:PRO:HA	17:Q:26:PRO:HD3	1.83	0.44
18:R:104:PHE:HB3	18:R:109:MET:HE2	2.00	0.44
23:W:12:ASN:HA	30:0:1067:A:O2'	2.17	0.44
23:W:65:VAL:HA	23:W:68:THR:CG2	2.47	0.44
23:W:149:LEU:CG	23:W:153:MET:HE2	2.42	0.44
26:Z:34:SER:OG	30:0:797:A:H4'	2.18	0.44
30:0:166:A:H2'	30:0:2109:U:H5	1.83	0.44
30:0:542:A:H1'	42:0:5534:HOH:O	2.16	0.44
30:0:567:U:O2'	30:0:568:G:H5'	2.17	0.44
30:0:941:G:C5	30:0:942:U:C4	3.06	0.44
30:0:1238:C:H5'	30:0:1239:G:OP2	2.17	0.44
30:0:1558:C:O2	30:0:1563:G:N2	2.45	0.44
30:0:2846:C:H4'	42:0:5931:HOH:O	2.16	0.44
1:A:212:PRO:HA	30:0:1943:C:C4'	2.48	0.44
2:B:84:LEU:HB2	2:B:182:VAL:HG21	2.00	0.44
2:B:217:ARG:CG	2:B:257:THR:HG22	2.44	0.44
6:F:31:LYS:HD2	42:0:5661:HOH:O	2.17	0.44
8:H:39:LYS:HA	8:H:87:LYS:NZ	2.32	0.44
8:H:59:GLN:HE21	8:H:129:ARG:HE	1.63	0.44
9:I:91:PHE:HA	9:I:131:GLY:CA	2.47	0.44
10:J:41:ALA:HB2	10:J:103:VAL:CG1	2.47	0.44
13:M:179:GLY:O	30:0:399:C:H5'	2.18	0.44
13:M:188:ARG:HD3	30:0:155:C:OP2	2.18	0.44
17:Q:56:PHE:HE2	35:Q:8811:CL:CL	2.38	0.44
18:R:88:PHE:O	18:R:91:LEU:HB3	2.17	0.44
19:S:20:PHE:N	19:S:20:PHE:CD2	2.85	0.44
20:T:52:ARG:O	30:0:317:A:OP1	2.36	0.44
20:T:92:ASP:OD2	30:0:335:U:H4'	2.18	0.44
24:X:49:ARG:NH1	30:0:1385:G:O3'	2.51	0.44
29:3:24:LYS:HE3	29:3:90:PHE:HE1	1.83	0.44
30:0:255:A:C5	30:0:256:C:C4	3.05	0.44
30:0:291:C:H2'	30:0:292:G:O4'	2.17	0.44
30:0:376:C:H6	30:0:376:C:O5'	2.00	0.44
30:0:1191:A:H2	30:0:1206:U:H3	1.65	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1913:C:H2'	30:0:1914:C:C6	2.52	0.44
30:0:2285:G:H1	33:6:74:C:H42	1.65	0.44
1:A:192:VAL:HG12	42:A:9070:HOH:O	2.18	0.44
5:E:35:TYR:HB2	5:E:61:THR:HG21	2.00	0.44
8:H:6:ALA:CA	8:H:61:ARG:HH12	2.28	0.44
13:M:159:VAL:HG13	13:M:160:PHE:N	2.32	0.44
23:W:4:LEU:CD2	23:W:52:VAL:HB	2.47	0.44
30:0:362:G:O2'	30:0:363:C:H5'	2.18	0.44
30:0:462:A:N6	30:0:477:A:H2	2.15	0.44
30:0:522:U:O2'	30:0:1366:C:H5'	2.17	0.44
30:0:1457:U:H5	42:0:9660:HOH:O	2.00	0.44
30:0:1636:G:O2'	30:0:1637:A:H5'	2.17	0.44
30:0:1644:C:O2'	30:0:1645:U:H5'	2.18	0.44
30:0:1878:G:O2'	30:0:1879:U:H6	2.01	0.44
30:0:2415:A:C2'	30:0:2416:G:H5'	2.47	0.44
30:0:2889:U:H4'	30:0:2890:A:H5'	1.98	0.44
31:9:107:C:H2'	31:9:108:C:H6	1.82	0.44
1:A:88:ILE:HG21	1:A:100:PRO:HG3	1.99	0.44
1:A:157:GLY:HA2	26:Z:103:VAL:CG1	2.48	0.44
1:A:190:ARG:NH2	1:A:207:GLN:OE1	2.51	0.44
3:C:177:GLY:HA2	42:0:3551:HOH:O	2.17	0.44
4:D:104:PHE:CE2	4:D:166:ILE:HD13	2.53	0.44
8:H:54:VAL:HG12	8:H:56:GLU:O	2.17	0.44
9:I:70:THR:OG1	9:I:107:LYS:HE2	2.18	0.44
9:I:71:ALA:O	9:I:75:LYS:HE3	2.17	0.44
9:I:124:VAL:O	9:I:124:VAL:HG12	2.18	0.44
13:M:3:SER:O	13:M:4:ALA:C	2.61	0.44
13:M:46:LEU:HD11	30:0:263:U:O3'	2.17	0.44
13:M:74:LYS:HG3	42:M:8878:HOH:O	2.18	0.44
14:N:35:VAL:HG11	31:9:6:C:H4'	1.99	0.44
17:Q:45:PRO:O	30:0:2365:G:H4'	2.18	0.44
23:W:122:ARG:NH2	42:W:5817:HOH:O	2.44	0.44
25:Y:102:LEU:O	25:Y:227:ARG:HG3	2.18	0.44
25:Y:212:ARG:HB3	42:Y:8835:HOH:O	2.18	0.44
29:3:10:TYR:CD1	30:0:2408:A:H1'	2.52	0.44
30:0:371:U:H2'	30:0:372:A:C8	2.52	0.44
30:0:553:G:O4'	30:0:1325:G:H5'	2.18	0.44
30:0:844:A:C6	30:0:882:A:C6	3.06	0.44
30:0:970:U:H2'	42:0:7156:HOH:O	2.16	0.44
30:0:1174:A:C5	30:0:1201:C:H4'	2.52	0.44
30:0:1826:C:O2'	30:0:1827:G:H5'	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1894:C:N4	30:0:1939:U:H2'	2.33	0.44
1:A:71:PRO:HA	1:A:158:VAL:O	2.18	0.44
1:A:190:ARG:NE	42:A:9070:HOH:O	2.51	0.44
2:B:109:LEU:HA	2:B:159:PRO:HG2	1.99	0.44
2:B:141:ARG:CB	2:B:165:ARG:HA	2.47	0.44
2:B:251:VAL:HG22	42:0:5183:HOH:O	2.18	0.44
3:C:225:PRO:CD	3:C:231:ARG:HD2	2.48	0.44
4:D:99:ASP:CB	4:D:103:ASN:HB2	2.48	0.44
5:E:90:HIS:CD2	30:0:2694:A:H5''	2.53	0.44
5:E:105:GLU:HG2	5:E:113:PRO:HB3	2.00	0.44
7:G:64:ASN:N	7:G:64:ASN:ND2	2.65	0.44
9:I:97:VAL:CG1	9:I:101:LYS:HE3	2.28	0.44
13:M:36:ALA:O	13:M:65:VAL:HG13	2.18	0.44
13:M:164:THR:CG2	13:M:165:GLY:N	2.80	0.44
14:N:21:HIS:CD2	30:0:2369:A:H5''	2.53	0.44
17:Q:16:ASN:HD21	17:Q:45:PRO:CD	2.29	0.44
19:S:21:GLN:NE2	30:0:1508:C:H5'	2.32	0.44
20:T:14:ALA:HA	20:T:15:PRO:HD3	1.90	0.44
30:0:70:A:H4'	42:0:4782:HOH:O	2.17	0.44
30:0:138:U:OP2	30:0:139:C:H5	2.01	0.44
30:0:236:A:H8	30:0:236:A:OP1	2.00	0.44
30:0:349:U:H2'	30:0:350:G:O4'	2.17	0.44
30:0:834:G:H4'	30:0:835:U:OP2	2.18	0.44
30:0:1318:A:H4'	30:0:1343:C:H4'	2.00	0.44
30:0:1534:C:O2'	30:0:1656:A:OP1	2.24	0.44
30:0:1586:G:O2'	30:0:1587:U:H5'	2.17	0.44
30:0:2344:G:H2'	30:0:2344:G:N3	2.32	0.44
30:0:2634:G:H5'	42:0:3070:HOH:O	2.16	0.44
1:A:171:LYS:NZ	42:A:8996:HOH:O	2.51	0.44
2:B:17:LYS:O	2:B:260:HIS:CD2	2.71	0.44
2:B:77:PRO:C	2:B:78:PRO:CD	2.91	0.44
2:B:108:GLU:C	2:B:110:ASP:N	2.76	0.44
2:B:132:HIS:CE1	2:B:171:VAL:CG2	3.01	0.44
12:L:149:ARG:O	12:L:150:GLN:HB2	2.17	0.44
13:M:9:ARG:NH2	30:0:378:A:OP1	2.42	0.44
13:M:163:LEU:O	13:M:168:ARG:NH1	2.51	0.44
16:P:107:GLU:O	16:P:109:ARG:N	2.50	0.44
20:T:102:ASP:C	20:T:102:ASP:OD1	2.60	0.44
22:V:5:VAL:CG1	22:V:9:ARG:NH1	2.80	0.44
25:Y:145:LYS:O	25:Y:147:ARG:HG2	2.18	0.44
27:1:25:LYS:HD2	28:2:48:ASP:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:48:ASP:O	28:2:49:GLU:CB	2.65	0.44
30:0:491:C:H2'	30:0:492:C:C6	2.53	0.44
30:0:1242:A:O2'	30:0:1247:A:N1	2.49	0.44
30:0:1845:A:O2'	30:0:1846:U:H5'	2.17	0.44
30:0:2090:G:H2'	30:0:2091:G:C8	2.53	0.44
30:0:2379:G:N3	30:0:2418:G:H2'	2.33	0.44
31:9:56:A:C3'	31:9:57:A:H5''	2.48	0.44
2:B:74:ILE:CD1	2:B:309:VAL:HG21	2.39	0.43
2:B:232:TRP:HD1	2:B:235:ARG:HD2	1.83	0.43
3:C:51:TYR:HE1	27:1:55:GLY:O	2.00	0.43
3:C:181:ALA:HB2	30:0:30:U:OP2	2.18	0.43
3:C:242:GLU:O	3:C:243:VAL:C	2.61	0.43
4:D:103:ASN:OD1	4:D:133:ASN:ND2	2.51	0.43
4:D:146:LYS:NZ	14:N:38:LYS:HE2	2.33	0.43
5:E:119:HIS:HB2	5:E:144:THR:OG1	2.17	0.43
7:G:63:ARG:HG2	30:0:1210:G:OP1	2.18	0.43
8:H:19:ARG:HG2	42:H:8976:HOH:O	2.18	0.43
9:I:72:GLU:C	9:I:74:ILE:N	2.76	0.43
10:J:11:ILE:HD13	10:J:109:TYR:CD1	2.52	0.43
12:L:5:LYS:HE3	30:0:1354:G:O6	2.17	0.43
12:L:18:HIS:HB2	30:0:903:U:O4	2.18	0.43
12:L:66:VAL:HG23	12:L:67:ARG:H	1.80	0.43
13:M:123:ASP:OD1	13:M:126:GLN:HG2	2.17	0.43
14:N:5:ARG:HB2	42:0:7582:HOH:O	2.18	0.43
14:N:79:PRO:HG3	14:N:144:GLY:CA	2.47	0.43
14:N:124:ASP:C	14:N:126:GLY:H	2.24	0.43
15:O:47:ARG:HG3	15:O:47:ARG:NH1	2.32	0.43
16:P:18:LYS:C	16:P:20:ARG:H	2.26	0.43
24:X:28:LYS:O	24:X:29:ALA:C	2.60	0.43
26:Z:70:ARG:NH2	30:0:1602:C:OP2	2.50	0.43
27:1:5:THR:N	27:1:6:PRO:HD2	2.32	0.43
28:2:14:LEU:HD13	28:2:47:THR:CG2	2.48	0.43
29:3:1:MET:N	29:3:87:ARG:O	2.49	0.43
30:0:23:G:H1'	30:0:520:A:H61	1.83	0.43
30:0:619:U:H2'	30:0:629:A:O4'	2.18	0.43
30:0:1096:U:H5''	30:0:1258:G:O6	2.17	0.43
30:0:1267:C:O2'	30:0:1268:C:H5'	2.18	0.43
30:0:1776:A:C8	30:0:1778:A:O4'	2.71	0.43
30:0:1902:G:N2	30:0:1936:C:C2	2.86	0.43
30:0:2031:C:H2'	30:0:2032:U:C6	2.53	0.43
30:0:2059:U:H2'	30:0:2060:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2106:C:H2'	30:0:2107:U:C6	2.53	0.43
30:0:2616:G:N3	30:0:2616:G:H2'	2.33	0.43
30:0:2907:C:H2'	30:0:2908:A:O4'	2.17	0.43
1:A:11:ARG:HH12	1:A:13:THR:CG2	2.31	0.43
1:A:128:LEU:HG	42:A:9054:HOH:O	2.18	0.43
2:B:162:MET:HE3	2:B:310:ARG:NH1	2.30	0.43
3:C:7:ASP:OD1	3:C:11:ASN:O	2.36	0.43
6:F:119:ARG:OXT	6:F:119:ARG:HD3	2.18	0.43
8:H:36:MET:HB3	8:H:73:ASN:HD21	1.83	0.43
11:K:96:VAL:CG2	11:K:109:LEU:HD22	2.48	0.43
22:V:4:HIS:O	22:V:8:ILE:HG13	2.17	0.43
23:W:21:LEU:HD22	23:W:26:ILE:HD13	2.01	0.43
30:0:637:C:H2'	30:0:638:C:H6	1.83	0.43
30:0:697:G:H4'	30:0:730:G:O3'	2.19	0.43
30:0:702:G:O2'	30:0:703:G:H5'	2.18	0.43
30:0:2019:A:H5'	42:0:5405:HOH:O	2.17	0.43
30:0:2346:C:H6	30:0:2346:C:O5'	2.02	0.43
30:0:2361:A:H5'	30:0:2361:A:H8	1.83	0.43
30:0:2402:A:H1'	42:0:4055:HOH:O	2.17	0.43
30:0:2619:UR3:H2'	30:0:2620:U:C6	2.53	0.43
30:0:2704:C:H2'	30:0:2705:U:O4'	2.18	0.43
31:9:5:G:O2'	31:9:6:C:H5'	2.18	0.43
1:A:123:GLY:HA3	1:A:162:GLY:HA2	2.01	0.43
2:B:51:VAL:HG13	2:B:53:LEU:CD1	2.49	0.43
10:J:14:ALA:O	10:J:15:ARG:C	2.61	0.43
12:L:35:ARG:NE	12:L:46:LEU:CD2	2.81	0.43
12:L:56:LYS:CE	30:0:2443:C:H1'	2.48	0.43
13:M:5:TYR:O	13:M:8:ILE:N	2.51	0.43
14:N:46:GLN:NE2	31:9:5:G:N3	2.65	0.43
14:N:155:GLU:O	14:N:156:GLU:CG	2.66	0.43
20:T:47:THR:HB	20:T:100:ASP:HB3	2.00	0.43
23:W:13:MET:O	23:W:14:HIS:C	2.61	0.43
27:1:36:SER:O	27:1:46:ARG:HD3	2.17	0.43
30:0:603:A:H5''	30:0:604:G:OP1	2.18	0.43
30:0:923:A:H2'	42:0:6521:HOH:O	2.17	0.43
30:0:1667:A:H2'	30:0:1668:U:C6	2.52	0.43
30:0:1768:C:H2'	30:0:1769:C:O4'	2.18	0.43
30:0:1878:G:O2'	30:0:1879:U:C6	2.65	0.43
30:0:1914:C:H2'	30:0:1915:U:H6	1.82	0.43
30:0:2332:A:H3'	30:0:2333:G:C8	2.51	0.43
31:9:70:U:H2'	31:9:71:C:O4'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HG21	1:A:59:GLU:CG	2.48	0.43
2:B:180:ASP:O	2:B:181:ILE:C	2.62	0.43
13:M:24:GLN:HE21	13:M:27:ARG:HD2	1.83	0.43
18:R:65:GLY:HA3	42:R:9001:HOH:O	2.18	0.43
25:Y:150:LEU:HB3	42:Y:8857:HOH:O	2.17	0.43
29:3:42:ARG:HD2	42:3:9003:HOH:O	2.17	0.43
30:0:1119:G:N2	30:0:1246:A:N1	2.66	0.43
30:0:2088:C:H1'	30:0:2841:A:N1	2.33	0.43
30:0:2120:U:H2'	30:0:2121:G:O4'	2.18	0.43
30:0:2345:A:N6	42:0:6637:HOH:O	2.49	0.43
1:A:213:LYS:CE	30:0:1942:A:H5''	2.48	0.43
2:B:77:PRO:C	2:B:78:PRO:CG	2.90	0.43
2:B:77:PRO:O	2:B:78:PRO:CA	2.67	0.43
2:B:277:GLU:N	2:B:278:PRO:CD	2.81	0.43
3:C:174:ILE:HD11	30:0:338:C:H4'	2.00	0.43
5:E:77:THR:C	5:E:78:GLU:CA	2.91	0.43
5:E:91:PHE:HA	5:E:92:PRO:HD3	1.81	0.43
9:I:87:PRO:HD2	30:0:1180:U:O2'	2.18	0.43
10:J:131:THR:CG2	10:J:133:GLY:H	2.31	0.43
12:L:30:ARG:HD3	30:0:164:G:H4'	2.00	0.43
13:M:90:ARG:NH2	30:0:2266:A:OP2	2.48	0.43
18:R:114:VAL:HA	18:R:144:GLU:O	2.18	0.43
22:V:38:GLY:C	22:V:40:PRO:HD2	2.42	0.43
22:V:42:ASN:C	22:V:44:GLY:H	2.26	0.43
23:W:38:THR:HG22	23:W:39:ASP:H	1.81	0.43
23:W:110:GLN:NE2	23:W:110:GLN:CA	2.81	0.43
25:Y:100:ARG:HE	25:Y:234:VAL:HG21	1.84	0.43
28:2:35:ARG:N	42:2:2691:HOH:O	2.50	0.43
29:3:59:ASP:O	29:3:60:LYS:C	2.61	0.43
29:3:69:TYR:O	29:3:77:ALA:HA	2.17	0.43
30:0:235:C:O2'	30:0:236:A:H2'	2.18	0.43
30:0:292:G:O5'	30:0:292:G:H8	2.01	0.43
30:0:463:A:H3'	42:0:7246:HOH:O	2.19	0.43
30:0:657:G:H2'	30:0:658:C:C6	2.54	0.43
30:0:957:A:H8	30:0:957:A:O5'	2.01	0.43
30:0:960:G:H3'	30:0:960:G:N3	2.33	0.43
30:0:1006:A:N1	30:0:2311:A:H1'	2.34	0.43
30:0:1163:G:H1	30:0:1184:C:N4	2.17	0.43
30:0:1359:U:O5'	30:0:1360:C:H5''	2.17	0.43
30:0:2852:A:H4'	30:0:2853:U:H5	1.83	0.43
31:9:39:U:H3'	31:9:40:C:H5''	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:95:C:O2'	31:9:96:C:H5'	2.19	0.43
4:D:107:GLY:O	30:0:2338:G:O3'	2.37	0.43
7:G:12:ILE:HG22	7:G:17:GLN:HE21	1.81	0.43
9:I:98:ASP:HA	9:I:101:LYS:HD2	2.01	0.43
9:I:111:LEU:HD22	9:I:122:GLU:OE1	2.18	0.43
12:L:18:HIS:CD2	30:0:902:G:N7	2.87	0.43
12:L:72:ASN:O	12:L:76:LEU:HG	2.19	0.43
13:M:50:ARG:HG2	13:M:50:ARG:HH11	1.84	0.43
16:P:98:ILE:HD12	16:P:102:ARG:NE	2.34	0.43
18:R:125:ARG:HG2	42:R:8948:HOH:O	2.18	0.43
21:U:38:ASN:O	21:U:42:LEU:HG	2.18	0.43
22:V:19:GLU:HG3	22:V:56:ILE:HD11	2.01	0.43
24:X:70:ILE:HG23	24:X:70:ILE:O	2.18	0.43
27:1:7:SER:C	42:1:2979:HOH:O	2.62	0.43
27:1:15:THR:O	27:1:28:HIS:HA	2.18	0.43
30:0:29:C:O2'	30:0:30:U:H5'	2.19	0.43
30:0:1171:A:N6	30:0:1172:G:C2	2.87	0.43
30:0:1359:U:O4	30:0:2101:A:H5''	2.19	0.43
1:A:70:ALA:HA	1:A:71:PRO:HD3	1.84	0.43
1:A:82:VAL:HG13	1:A:93:THR:HB	2.00	0.43
2:B:29:TRP:CH2	2:B:164:THR:HA	2.53	0.43
2:B:87:TYR:CE2	2:B:96:PRO:HG3	2.54	0.43
2:B:183:GLU:O	2:B:184:ASP:C	2.61	0.43
3:C:236:THR:HB	3:C:239:ALA:CB	2.48	0.43
3:C:240:LEU:HD23	3:C:240:LEU:O	2.18	0.43
4:D:103:ASN:ND2	4:D:133:ASN:HD22	2.17	0.43
4:D:140:ARG:NH1	31:9:45:A:OP1	2.50	0.43
5:E:143:GLN:HE21	30:0:2780:C:H1'	1.82	0.43
6:F:99:THR:HA	42:F:3461:HOH:O	2.18	0.43
9:I:119:ALA:O	9:I:123:VAL:HG23	2.18	0.43
10:J:88:PRO:O	10:J:94:GLY:HA3	2.18	0.43
11:K:48:GLY:O	11:K:49:LEU:C	2.61	0.43
12:L:144:ASP:O	12:L:147:GLU:HB2	2.18	0.43
14:N:41:LYS:HD3	42:9:9061:HOH:O	2.18	0.43
15:O:15:LYS:HD3	15:O:19:ARG:NH2	2.34	0.43
15:O:106:PRO:HG2	15:O:107:GLU:OE2	2.18	0.43
24:X:85:VAL:HG12	24:X:86:GLU:N	2.34	0.43
25:Y:169:ARG:HB2	30:0:1268:C:O2'	2.18	0.43
30:0:581:G:O2'	30:0:582:U:H5'	2.18	0.43
30:0:854:G:H5''	30:0:855:U:OP1	2.18	0.43
30:0:936:C:H42	30:0:1034:G:H1	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1077:G:H2'	30:0:1080:C:N4	2.34	0.43
30:0:1167:G:H1	30:0:1179:C:H42	1.67	0.43
30:0:1299:G:N2	42:0:5541:HOH:O	2.52	0.43
30:0:1766:U:H2'	30:0:1776:A:N6	2.34	0.43
33:6:75:C:H5''	33:6:76:8AN:O1P	2.18	0.43
1:A:95:PRO:C	1:A:97:ALA:N	2.75	0.43
2:B:51:VAL:HG22	2:B:327:VAL:HG13	2.00	0.43
2:B:103:ASP:HB2	42:B:9064:HOH:O	2.17	0.43
5:E:2:ARG:HH21	5:E:48:VAL:HG21	1.82	0.43
5:E:6:GLU:HG2	5:E:46:THR:HG22	2.01	0.43
6:F:1:PRO:HB2	42:M:8924:HOH:O	2.17	0.43
7:G:71:LEU:O	7:G:73:ASP:N	2.52	0.43
10:J:74:ARG:HH11	10:J:74:ARG:CG	2.31	0.43
13:M:5:TYR:O	13:M:6:SER:C	2.62	0.43
14:N:72:GLU:HG2	14:N:163:PHE:HD1	1.84	0.43
20:T:21:LYS:HA	20:T:24:ARG:CD	2.49	0.43
20:T:48:VAL:HG22	20:T:97:ARG:O	2.19	0.43
20:T:101:LEU:HD13	20:T:112:LEU:HD11	2.01	0.43
27:1:48:TYR:CZ	30:0:773:A:H4'	2.54	0.43
30:0:234:A:H4'	30:0:437:A:O4'	2.19	0.43
30:0:758:A:H2'	30:0:759:C:O4'	2.19	0.43
30:0:790:A:H1'	30:0:1710:A:C2'	2.49	0.43
30:0:2569:A:H2'	30:0:2570:G:O4'	2.18	0.43
30:0:2752:C:O2'	30:0:2753:G:H5'	2.19	0.43
31:9:73:A:N6	31:9:108:C:H42	2.15	0.43
2:B:87:TYR:O	2:B:138:GLY:N	2.42	0.43
2:B:112:THR:HG23	2:B:158:LYS:HZ1	1.83	0.43
2:B:145:HIS:CD2	2:B:146:THR:O	2.72	0.43
4:D:48:MET:HE2	4:D:48:MET:HB3	1.89	0.43
4:D:81:GLU:O	4:D:82:GLU:C	2.62	0.43
6:F:22:VAL:HG23	6:F:104:ALA:HB2	2.00	0.43
6:F:105:ASP:O	6:F:106:ALA:C	2.61	0.43
8:H:8:MET:HE2	8:H:9:TYR:CZ	2.54	0.43
9:I:112:LEU:HG	42:I:6070:HOH:O	2.19	0.43
10:J:123:ARG:NH1	10:J:129:PHE:HZ	2.16	0.43
14:N:11:ARG:HG2	14:N:15:GLU:OE2	2.18	0.43
22:V:27:LEU:CA	22:V:49:LEU:HD13	2.48	0.43
25:Y:184:GLU:HG2	25:Y:229:LEU:HD11	2.01	0.43
30:0:710:G:N2	30:0:719:C:C2	2.87	0.43
30:0:812:A:H2'	30:0:813:C:H6	1.83	0.43
30:0:1473:U:O2'	30:0:1474:C:H5''	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1476:A:O2'	30:0:1477:C:H5'	2.18	0.43
30:0:1503:U:H2'	30:0:1504:A:O4'	2.18	0.43
30:0:1616:A:H5''	30:0:1617:C:OP1	2.18	0.43
30:0:2005:G:N2	30:0:2008:U:H1'	2.34	0.43
30:0:2073:G:N1	30:0:2607:U:C6	2.86	0.43
1:A:171:LYS:HG3	1:A:174:ASN:ND2	2.33	0.43
1:A:231:LYS:O	1:A:232:ARG:HB3	2.19	0.43
4:D:156:ARG:HG3	4:D:156:ARG:HH11	1.84	0.43
8:H:46:TYR:HA	8:H:47:PRO:HD3	1.80	0.43
10:J:130:VAL:CG1	10:J:131:THR:N	2.82	0.43
13:M:102:GLU:OE2	13:M:164:THR:HG21	2.19	0.43
14:N:24:LEU:CD1	17:Q:26:PRO:HB3	2.49	0.43
16:P:20:ARG:HD2	30:0:1718:G:OP2	2.19	0.43
16:P:50:GLN:HG2	42:P:6904:HOH:O	2.19	0.43
18:R:46:TYR:CD2	18:R:47:LEU:HD23	2.50	0.43
20:T:48:VAL:HG22	20:T:96:VAL:HG13	2.00	0.43
24:X:85:VAL:HG12	24:X:86:GLU:H	1.83	0.43
25:Y:216:ARG:O	25:Y:219:GLU:HG2	2.19	0.43
30:0:228:C:C2'	30:0:229:G:H5'	2.49	0.43
30:0:462:A:H2'	42:0:5741:HOH:O	2.19	0.43
30:0:1217:G:O2'	30:0:1218:U:H5'	2.19	0.43
3:C:149:LYS:NZ	30:0:328:U:OP1	2.52	0.42
8:H:81:GLY:C	8:H:83:GLU:H	2.27	0.42
8:H:87:LYS:NZ	8:H:87:LYS:CB	2.82	0.42
12:L:145:LEU:HD23	12:L:145:LEU:O	2.19	0.42
14:N:37:ARG:HA	14:N:37:ARG:HD3	1.90	0.42
15:O:49:GLU:O	15:O:72:LYS:HE3	2.19	0.42
26:Z:84:CYS:O	26:Z:85:ASP:HB2	2.18	0.42
30:0:51:G:O2'	30:0:52:A:H5'	2.19	0.42
30:0:431:G:O2'	30:0:432:G:H5'	2.19	0.42
30:0:542:A:H2'	30:0:543:G:O4'	2.19	0.42
30:0:1245:C:O5'	30:0:1245:C:H6	2.01	0.42
30:0:1724:U:H5''	42:0:4609:HOH:O	2.19	0.42
30:0:1767:A:H3'	42:0:5918:HOH:O	2.19	0.42
30:0:1819:G:H2'	30:0:1820:G:C4'	2.49	0.42
30:0:1925:G:O2'	30:0:1926:G:H5'	2.19	0.42
30:0:1972:U:H2'	30:0:1973:A:H5'	2.01	0.42
30:0:2029:C:H2'	30:0:2030:A:O4'	2.19	0.42
30:0:2241:C:O2'	30:0:2242:U:H5'	2.19	0.42
31:9:107:C:H2'	31:9:108:C:C6	2.54	0.42
33:6:75:C:H2'	42:6:80:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:MET:C	1:A:181:ALA:N	2.76	0.42
2:B:108:GLU:C	2:B:110:ASP:H	2.26	0.42
2:B:280:VAL:HG11	2:B:335:ASN:OD1	2.19	0.42
10:J:20:GLY:HA3	30:O:1242:A:O3'	2.20	0.42
10:J:93:ARG:HH11	10:J:93:ARG:CB	2.27	0.42
11:K:8:VAL:CG1	11:K:9:THR:N	2.81	0.42
12:L:16:GLY:HA2	30:O:1294:A:O3'	2.19	0.42
12:L:130:ARG:O	12:L:131:GLU:C	2.62	0.42
12:L:144:ASP:HA	12:L:147:GLU:HG3	2.01	0.42
15:O:39:THR:O	15:O:115:ARG:NH2	2.51	0.42
15:O:105:ASN:HD21	15:O:109:SER:H	1.66	0.42
16:P:104:LYS:HA	16:P:104:LYS:HD2	1.91	0.42
17:Q:43:ILE:O	17:Q:45:PRO:HD3	2.20	0.42
17:Q:86:VAL:HG13	17:Q:91:LEU:HD11	2.00	0.42
23:W:47:LYS:HE2	30:O:944:G:O3'	2.19	0.42
23:W:66:LEU:HA	23:W:66:LEU:HD23	1.87	0.42
23:W:125:HIS:CD2	23:W:125:HIS:H	2.37	0.42
30:O:67:A:H2'	42:O:5002:HOH:O	2.19	0.42
30:O:101:C:H2'	30:O:102:A:H8	1.83	0.42
30:O:639:A:H2'	30:O:640:G:C8	2.54	0.42
30:O:1503:U:H2'	30:O:1504:A:C5'	2.48	0.42
30:O:1632:A:C2'	30:O:1633:C:H5'	2.48	0.42
2:B:48:MET:O	2:B:49:THR:HG23	2.19	0.42
3:C:246:ARG:NH2	30:O:677:C:H4'	2.34	0.42
4:D:10:PHE:CD1	4:D:11:HIS:N	2.87	0.42
4:D:143:LYS:O	31:9:45:A:H4'	2.19	0.42
6:F:24:ARG:HG3	6:F:25:ASP:N	2.34	0.42
6:F:109:GLU:O	6:F:113:ASP:OD2	2.37	0.42
7:G:12:ILE:HG22	7:G:12:ILE:O	2.17	0.42
8:H:61:ARG:O	8:H:64:SER:N	2.43	0.42
10:J:45:VAL:CG2	10:J:129:PHE:CD1	3.02	0.42
12:L:143:THR:CG2	12:L:144:ASP:N	2.81	0.42
13:M:95:LYS:HE2	30:O:157:G:H4'	2.01	0.42
13:M:163:LEU:HD21	30:O:188:C:H5''	2.00	0.42
14:N:14:ARG:NH2	31:9:13:A:N3	2.66	0.42
14:N:179:LEU:HD23	14:N:184:ILE:HD12	2.01	0.42
23:W:52:VAL:H	23:W:52:VAL:HG22	1.45	0.42
25:Y:190:VAL:C	25:Y:192:ASP:H	2.27	0.42
25:Y:190:VAL:C	25:Y:192:ASP:N	2.76	0.42
27:1:28:HIS:CD2	27:1:30:LYS:HB2	2.54	0.42
27:1:45:ARG:NH2	42:1:2086:HOH:O	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:2:40:ARG:HG3	28:2:45:ASN:CB	2.49	0.42
30:0:432:G:O2'	30:0:433:C:H5'	2.19	0.42
30:0:699:C:C6	30:0:744:G:O4'	2.73	0.42
30:0:1211:G:H2'	30:0:1212:C:C6	2.53	0.42
30:0:1362:U:O2'	30:0:1363:G:H5'	2.19	0.42
30:0:1566:C:H2'	30:0:1567:G:C8	2.54	0.42
30:0:1971:G:N2	30:0:2009:G:H2'	2.34	0.42
30:0:2464:C:H5''	30:0:2465:A:OP1	2.20	0.42
30:0:2647:C:H1'	42:0:7245:HOH:O	2.19	0.42
31:9:14:G:C6	31:9:68:G:C2	3.07	0.42
1:A:69:LEU:C	1:A:69:LEU:HD12	2.44	0.42
1:A:120:ARG:HD3	42:A:9015:HOH:O	2.19	0.42
1:A:135:VAL:HG21	1:A:147:ARG:NH1	2.35	0.42
2:B:243:ASN:ND2	30:0:2607:U:OP2	2.45	0.42
3:C:27:ARG:HG2	3:C:29:ASP:OD1	2.19	0.42
3:C:40:ALA:O	3:C:43:LYS:HB2	2.19	0.42
3:C:142:ASP:CG	3:C:238:SER:HG	2.27	0.42
4:D:25:MET:HE1	4:D:37:ALA:O	2.19	0.42
6:F:58:GLU:HA	6:F:61:MET:CE	2.21	0.42
7:G:23:ILE:C	7:G:25:GLU:N	2.76	0.42
9:I:67:VAL:HG13	9:I:68:PRO:HD2	2.00	0.42
9:I:114:TYR:CD1	9:I:114:TYR:N	2.87	0.42
9:I:130:LEU:HA	42:I:7210:HOH:O	2.19	0.42
10:J:77:GLY:O	10:J:78:ILE:CA	2.68	0.42
11:K:4:LEU:HD23	11:K:4:LEU:HA	1.86	0.42
11:K:28:GLU:OE2	11:K:58:THR:HG21	2.19	0.42
13:M:71:SER:CB	13:M:92:THR:HG22	2.47	0.42
14:N:42:HIS:CG	14:N:62:HIS:HE1	2.38	0.42
14:N:119:GLN:HG2	14:N:123:ILE:HD11	2.01	0.42
15:O:18:ALA:HB2	15:O:27:GLY:N	2.34	0.42
17:Q:34:ASP:HB2	17:Q:37:GLU:HG3	2.00	0.42
21:U:56:ARG:O	21:U:56:ARG:HD2	2.20	0.42
23:W:35:VAL:HA	23:W:36:PRO:HD3	1.92	0.42
30:0:564:G:H2'	30:0:592:G:C6	2.54	0.42
30:0:611:U:H2'	30:0:612:U:C6	2.54	0.42
30:0:640:G:C6	30:0:641:G:N7	2.87	0.42
30:0:1058:A:H2'	30:0:1060:C:H5'	2.00	0.42
30:0:1342:C:H2'	30:0:1343:C:H5'	2.02	0.42
30:0:2067:A:H2'	30:0:2068:G:O4'	2.18	0.42
1:A:1:GLY:HA2	30:0:2114:C:OP1	2.19	0.42
1:A:34:ASP:C	1:A:36:ASP:N	2.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:174:ILE:HD12	30:0:338:C:H4'	1.99	0.42
7:G:63:ARG:NH1	30:0:1151:G:OP1	2.52	0.42
8:H:77:ILE:O	8:H:78:LYS:CA	2.68	0.42
11:K:68:VAL:C	11:K:69:LEU:HD23	2.44	0.42
12:L:27:ARG:HH22	12:L:30:ARG:HG2	1.81	0.42
16:P:103:THR:O	16:P:104:LYS:C	2.62	0.42
19:S:12:GLU:O	19:S:13:LYS:C	2.63	0.42
21:U:20:MET:CG	21:U:28:THR:HG23	2.50	0.42
21:U:50:GLU:HB3	30:0:2866:U:C4	2.55	0.42
23:W:82:GLU:O	23:W:86:GLU:HG3	2.19	0.42
24:X:76:ARG:HG3	24:X:76:ARG:NH1	2.31	0.42
42:Y:8878:HOH:O	30:0:1355:A:H5''	2.19	0.42
28:2:18:ASN:O	28:2:18:ASN:ND2	2.52	0.42
30:0:284:C:H4'	30:0:285:A:H8	1.84	0.42
30:0:420:U:H2'	30:0:421:C:C6	2.54	0.42
30:0:559:U:H2'	30:0:560:U:O4'	2.20	0.42
30:0:1299:G:H2'	30:0:1300:G:O4'	2.20	0.42
30:0:1821:A:O2'	30:0:1822:A:H5'	2.20	0.42
30:0:2470:A:H5''	42:0:4137:HOH:O	2.19	0.42
30:0:2604:A:H4'	42:0:9401:HOH:O	2.20	0.42
2:B:112:THR:HG23	2:B:158:LYS:NZ	2.35	0.42
3:C:46:TYR:CE1	3:C:92:PRO:HB3	2.55	0.42
3:C:68:ALA:O	3:C:70:VAL:N	2.52	0.42
4:D:140:ARG:C	4:D:142:ALA:N	2.77	0.42
5:E:16:ASP:O	5:E:17:HIS:HB2	2.19	0.42
8:H:53:ILE:HG23	8:H:133:GLY:O	2.20	0.42
11:K:74:VAL:HG21	11:K:96:VAL:HG23	2.01	0.42
13:M:193:LYS:HB3	30:0:392:U:H5''	2.01	0.42
14:N:40:ASN:HB2	42:9:9062:HOH:O	2.20	0.42
15:O:25:VAL:HG23	15:O:26:TRP:N	2.33	0.42
17:Q:27:GLN:HB2	42:9:9006:HOH:O	2.19	0.42
18:R:31:ILE:O	18:R:32:ALA:C	2.60	0.42
25:Y:231:PRO:HG2	25:Y:233:TYR:CE1	2.55	0.42
28:2:43:ARG:HH21	30:0:1685:A:C4'	2.32	0.42
30:0:370:G:O2'	30:0:371:U:H5'	2.19	0.42
30:0:2039:A:H4'	30:0:2760:C:O2'	2.20	0.42
30:0:2611:G:H5'	30:0:2613:G:C8	2.55	0.42
30:0:2791:U:C4	30:0:2794:G:O6	2.73	0.42
31:9:24:U:H3'	31:9:25:G:H5'	2.01	0.42
1:A:163:GLY:CA	1:A:166:ASP:OD2	2.68	0.42
2:B:7:ARG:CZ	2:B:11:LEU:HD13	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:52:VAL:O	2:B:53:LEU:HD12	2.19	0.42
2:B:205:VAL:O	2:B:307:ARG:NE	2.53	0.42
2:B:238:ASN:HD21	30:0:2609:G:N2	2.17	0.42
3:C:21:VAL:HG22	42:C:8598:HOH:O	2.20	0.42
5:E:88:TYR:CD1	5:E:91:PHE:O	2.71	0.42
13:M:61:ILE:N	13:M:61:ILE:CD1	2.81	0.42
13:M:78:LYS:HE2	30:0:870:G:OP1	2.19	0.42
15:O:89:ILE:HG21	15:O:95:ALA:HB2	2.01	0.42
16:P:81:LYS:HG2	42:0:3439:HOH:O	2.19	0.42
16:P:109:ARG:NH1	16:P:119:TYR:CE2	2.88	0.42
20:T:30:ASP:O	20:T:33:GLU:N	2.53	0.42
22:V:45:ARG:HA	22:V:48:GLU:HB2	2.01	0.42
23:W:13:MET:HA	42:W:4944:HOH:O	2.20	0.42
25:Y:100:ARG:HE	25:Y:234:VAL:CG2	2.32	0.42
30:0:353:G:O2'	30:0:354:A:H5'	2.19	0.42
30:0:1548:U:O2'	30:0:1798:C:O2	2.32	0.42
30:0:1684:A:H5'	30:0:1692:C:OP1	2.19	0.42
30:0:2079:G:H2'	30:0:2080:G:O4'	2.19	0.42
30:0:2355:G:H5''	30:0:2356:A:OP2	2.20	0.42
30:0:2673:U:C4	30:0:2674:G:C6	3.07	0.42
30:0:2819:C:H2'	30:0:2820:A:H8	1.84	0.42
4:D:55:LYS:O	4:D:56:ARG:HB2	2.20	0.42
4:D:88:LEU:N	4:D:89:PRO:CD	2.83	0.42
9:I:87:PRO:HB3	9:I:129:SER:O	2.19	0.42
11:K:69:LEU:HD12	11:K:97:ILE:HD13	2.02	0.42
13:M:171:ARG:HD3	30:0:156:C:C5'	2.43	0.42
14:N:175:LEU:HA	14:N:175:LEU:HD12	1.86	0.42
16:P:115:SER:O	16:P:117:SER:N	2.52	0.42
18:R:21:ARG:HB2	18:R:23:MET:HE2	2.01	0.42
18:R:82:GLU:CG	18:R:83:LYS:H	2.29	0.42
20:T:9:LYS:HE3	20:T:13:ARG:NH2	2.34	0.42
22:V:1:THR:CB	30:0:93:C:H5''	2.46	0.42
22:V:59:ILE:HA	22:V:62:GLU:HB2	2.02	0.42
24:X:30:MET:HG2	30:0:1384:C:H5'	2.00	0.42
26:Z:96:GLU:OE1	26:Z:104:ARG:NH2	2.53	0.42
29:3:42:ARG:NH1	30:0:396:U:H5'	2.35	0.42
30:0:312:U:O5'	30:0:312:U:H6	2.02	0.42
30:0:1477:C:C5'	30:0:1868:G:H5''	2.50	0.42
30:0:1504:A:O2'	30:0:1506:U:OP2	2.38	0.42
30:0:2506:A:H2'	30:0:2506:A:O5'	2.20	0.42
31:9:14:G:O2'	31:9:15:C:H5'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:72:C:H2'	31:9:73:A:H8	1.85	0.42
1:A:34:ASP:O	1:A:36:ASP:N	2.53	0.42
2:B:56:ASP:HB3	2:B:322:ARG:NH2	2.35	0.42
2:B:244:PRO:HB3	30:0:1234:U:C2	2.55	0.42
3:C:63:SER:OG	30:0:2101:A:H2'	2.20	0.42
3:C:150:THR:OG1	30:0:327:A:H2'	2.19	0.42
6:F:39:SER:O	6:F:43:GLY:N	2.53	0.42
6:F:118:LEU:O	6:F:119:ARG:OXT	2.38	0.42
8:H:59:GLN:HE21	8:H:129:ARG:CG	2.32	0.42
10:J:49:ARG:O	10:J:50:GLU:C	2.63	0.42
10:J:75:PRO:HD3	10:J:136:SER:CB	2.50	0.42
11:K:22:ASP:C	11:K:22:ASP:OD1	2.62	0.42
11:K:66:ARG:NH2	30:0:1994:A:OP2	2.42	0.42
12:L:18:HIS:HD2	30:0:902:G:N7	2.18	0.42
14:N:44:ARG:NH2	31:9:4:G:O2'	2.52	0.42
14:N:111:PRO:HD2	31:9:37:C:H4'	2.02	0.42
16:P:18:LYS:O	16:P:21:VAL:HG13	2.20	0.42
18:R:82:GLU:HB2	18:R:86:LYS:HE3	2.02	0.42
19:S:29:ASP:OD1	19:S:31:ARG:HG3	2.20	0.42
20:T:24:ARG:HG2	20:T:24:ARG:NH1	2.35	0.42
21:U:47:ARG:HG3	42:U:4381:HOH:O	2.20	0.42
24:X:49:ARG:O	24:X:49:ARG:CG	2.58	0.42
25:Y:178:HIS:CG	25:Y:179:PRO:HD2	2.55	0.42
25:Y:212:ARG:HB2	30:0:1315:G:C4	2.54	0.42
26:Z:34:SER:HB3	42:Z:8723:HOH:O	2.18	0.42
29:3:71:CYS:O	29:3:75:GLY:HA2	2.20	0.42
30:0:75:U:H2'	30:0:76:G:C8	2.55	0.42
30:0:461:C:H2'	42:0:4868:HOH:O	2.20	0.42
30:0:644:G:H5'	30:0:644:G:N3	2.34	0.42
30:0:912:A:H4'	42:0:6799:HOH:O	2.19	0.42
30:0:1044:C:H5	42:0:7418:HOH:O	2.03	0.42
30:0:1141:U:O2'	30:0:1142:C:H5'	2.19	0.42
30:0:1165:G:N2	30:0:1173:A:H5''	2.35	0.42
30:0:1603:A:H5'	30:0:1605:G:C4'	2.49	0.42
30:0:1664:A:H8	30:0:1664:A:OP1	2.03	0.42
30:0:1972:U:C2'	30:0:1973:A:H5''	2.50	0.42
30:0:2106:C:H1'	30:0:2484:U:C2	2.55	0.42
30:0:2510:C:H5'	30:0:2511:A:OP2	2.20	0.42
1:A:186:TRP:CD1	1:A:187:PRO:HA	2.55	0.42
2:B:66:GLU:HG2	42:B:9125:HOH:O	2.20	0.42
2:B:170:SER:O	2:B:171:VAL:C	2.63	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:VAL:HA	3:C:81:PRO:HD3	1.85	0.42
3:C:102:LEU:O	3:C:103:ASN:C	2.63	0.42
4:D:138:GLY:HA2	31:9:29:C:O3'	2.20	0.42
4:D:169:THR:C	4:D:170:TYR:HD1	2.28	0.42
5:E:69:ILE:O	5:E:72:MET:HB2	2.19	0.42
9:I:88:GLN:HE21	9:I:128:THR:CG2	2.33	0.42
9:I:117:THR:O	9:I:120:ALA:HB3	2.19	0.42
10:J:47:THR:HB	30:0:1244:U:C6	2.55	0.42
11:K:66:ARG:HH22	30:0:1994:A:P	2.40	0.42
12:L:66:VAL:O	12:L:67:ARG:C	2.62	0.42
12:L:133:VAL:HA	42:L:9038:HOH:O	2.20	0.42
13:M:122:GLN:HB3	13:M:127:LYS:HG2	2.02	0.42
13:M:171:ARG:NH2	30:0:189:A:OP1	2.52	0.42
14:N:32:PRO:HD2	14:N:99:GLU:O	2.20	0.42
14:N:79:PRO:HA	14:N:142:THR:O	2.20	0.42
20:T:51:LEU:O	20:T:52:ARG:HG2	2.20	0.42
21:U:6:CYS:HB2	21:U:32:CYS:HB3	2.01	0.42
23:W:4:LEU:O	23:W:32:CYS:HA	2.19	0.42
25:Y:106:THR:HG23	25:Y:107:PRO:HD2	2.01	0.42
26:Z:37:ARG:HD2	30:0:818:A:O2'	2.20	0.42
30:0:432:G:H2'	30:0:433:C:C6	2.55	0.42
30:0:696:C:O2'	30:0:697:G:H5'	2.20	0.42
30:0:1890:U:H4'	30:0:2010:A:C6	2.55	0.42
30:0:2133:U:H4'	30:0:2134:G:H5'	2.02	0.42
30:0:2462:G:O4'	30:0:2464:C:C2	2.73	0.42
30:0:2467:A:H5'	42:0:5160:HOH:O	2.19	0.42
30:0:2519:C:O2'	30:0:2520:G:H5'	2.20	0.42
1:A:56:ALA:O	1:A:68:ILE:N	2.53	0.41
2:B:217:ARG:HB2	2:B:257:THR:HG21	2.01	0.41
2:B:274:GLU:HG3	2:B:292:GLY:HA2	2.02	0.41
3:C:81:PRO:HD3	42:C:8554:HOH:O	2.20	0.41
3:C:236:THR:N	3:C:239:ALA:HB3	2.28	0.41
8:H:160:ILE:HD11	8:H:164:CYS:SG	2.60	0.41
9:I:94:ASP:O	9:I:95:LEU:HD23	2.20	0.41
10:J:42:GLU:O	10:J:131:THR:HG23	2.20	0.41
13:M:9:ARG:HG3	42:0:4079:HOH:O	2.20	0.41
13:M:31:TRP:CA	13:M:34:GLU:HG3	2.48	0.41
14:N:38:LYS:HE2	14:N:107:ASN:HD21	1.84	0.41
14:N:127:LEU:HB2	42:N:8856:HOH:O	2.19	0.41
15:O:21:SER:CB	15:O:106:PRO:HB2	2.50	0.41
16:P:133:SER:HA	42:P:1882:HOH:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:29:LYS:HD3	42:0:5581:HOH:O	2.20	0.41
18:R:61:GLN:HG2	18:R:62:HIS:CD2	2.55	0.41
18:R:122:GLN:HB3	18:R:138:SER:HB2	2.01	0.41
20:T:68:ASP:HB2	42:T:4787:HOH:O	2.20	0.41
23:W:92:ASP:OD2	23:W:94:SER:HB2	2.19	0.41
24:X:34:ARG:NH1	24:X:48:VAL:O	2.53	0.41
25:Y:112:GLU:OE1	25:Y:112:GLU:HA	2.20	0.41
29:3:6:ARG:HA	29:3:20:HIS:O	2.20	0.41
30:0:25:A:C2'	30:0:26:U:H5'	2.50	0.41
30:0:163:U:O3'	30:0:896:C:H4'	2.20	0.41
30:0:271:C:N4	30:0:378:A:H2	2.06	0.41
30:0:289:G:O2'	30:0:290:C:H5'	2.19	0.41
30:0:310:U:H2'	30:0:311:C:C6	2.54	0.41
30:0:1153:C:N3	30:0:2786:G:O6	2.52	0.41
30:0:1844:C:O5'	30:0:1844:C:H6	2.03	0.41
30:0:2896:A:N3	30:0:2896:A:C2'	2.83	0.41
30:0:2906:A:H5'	30:0:2907:C:O4'	2.20	0.41
2:B:226:LYS:NZ	30:0:1751:G:O6	2.52	0.41
3:C:184:ARG:HD2	30:0:1306:U:H5''	2.02	0.41
4:D:101:THR:O	4:D:101:THR:HG22	2.21	0.41
7:G:12:ILE:O	7:G:13:PRO:C	2.63	0.41
8:H:153:PHE:HD1	8:H:166:ILE:HG23	1.84	0.41
9:I:67:VAL:CG1	9:I:68:PRO:HD2	2.50	0.41
13:M:99:ARG:NE	13:M:167:GLY:HA2	2.35	0.41
14:N:116:PHE:O	14:N:119:GLN:HB3	2.20	0.41
15:O:81:PHE:C	15:O:82:SER:O	2.62	0.41
16:P:115:SER:C	16:P:117:SER:H	2.29	0.41
17:Q:68:GLY:HA3	30:0:2404:G:C5'	2.50	0.41
18:R:114:VAL:HG13	18:R:114:VAL:O	2.21	0.41
23:W:10:GLU:HG2	42:0:3876:HOH:O	2.19	0.41
30:0:432:G:H3'	42:0:8000:HOH:O	2.18	0.41
30:0:484:A:N1	30:0:506:G:H4'	2.35	0.41
30:0:1131:G:H5'	31:9:91:C:O4'	2.21	0.41
30:0:2072:G:O2'	30:0:2489:G:N2	2.52	0.41
30:0:2281:C:O2'	30:0:2282:U:H5'	2.20	0.41
31:9:77:A:N1	31:9:103:A:H5''	2.35	0.41
1:A:38:ILE:HD11	1:A:62:ASP:OD1	2.21	0.41
1:A:208:HIS:O	1:A:208:HIS:CG	2.74	0.41
2:B:335:ASN:HA	42:0:4561:HOH:O	2.20	0.41
3:C:22:PHE:HA	3:C:116:ALA:HA	2.01	0.41
3:C:93:LYS:HD2	30:0:646:G:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:LYS:HZ3	3:C:184:ARG:HB3	1.85	0.41
3:C:223:LEU:HD12	3:C:223:LEU:HA	1.94	0.41
4:D:23:VAL:HG22	4:D:73:VAL:HB	2.02	0.41
4:D:42:GLY:N	42:D:5828:HOH:O	2.53	0.41
10:J:52:GLN:HE21	30:0:1119:G:H5'	1.84	0.41
11:K:79:PRO:HG3	11:K:89:LYS:HB3	2.01	0.41
14:N:77:ASN:O	14:N:78:MET:CA	2.68	0.41
14:N:91:ARG:HD3	42:N:8811:HOH:O	2.20	0.41
14:N:167:ASP:C	14:N:168:LEU:HG	2.45	0.41
15:O:107:GLU:O	15:O:108:GLY:C	2.62	0.41
30:0:11:A:H2'	30:0:11:A:N3	2.36	0.41
30:0:497:A:H2'	30:0:498:A:C5'	2.51	0.41
30:0:506:G:N2	30:0:509:A:H5'	2.16	0.41
30:0:600:G:N2	30:0:601:G:H1'	2.35	0.41
30:0:921:G:H4'	30:0:924:G:C6	2.55	0.41
30:0:1741:U:H5'	30:0:1742:A:OP1	2.20	0.41
30:0:1741:U:O2'	30:0:2723:G:H4'	2.20	0.41
30:0:2398:A:O2'	30:0:2428:G:H4'	2.20	0.41
30:0:2649:A:H5'	30:0:2649:A:C8	2.55	0.41
30:0:2728:C:H4'	30:0:2894:C:HO2'	1.86	0.41
31:9:3:A:N6	31:9:22:G:H1'	2.35	0.41
1:A:72:GLU:CD	26:Z:100:GLY:HA3	2.46	0.41
2:B:266:ASN:OD1	2:B:317:PRO:HA	2.20	0.41
3:C:246:ARG:HH11	3:C:246:ARG:CB	2.32	0.41
7:G:26:MET:C	7:G:28:GLU:N	2.76	0.41
10:J:45:VAL:HG22	10:J:46:ILE:N	2.35	0.41
10:J:64:GLY:HA3	35:J:8821:CL:CL	2.57	0.41
10:J:126:ASN:HA	35:J:8801:CL:CL	2.57	0.41
12:L:41:HIS:CD2	30:0:926:A:O2'	2.73	0.41
14:N:33:ARG:NH1	14:N:103:ASP:OD2	2.53	0.41
16:P:135:ALA:HB2	42:P:4754:HOH:O	2.20	0.41
19:S:32:ALA:HA	19:S:36:GLU:OE1	2.20	0.41
24:X:74:ALA:HB2	24:X:85:VAL:HG13	2.01	0.41
30:0:287:C:H2'	30:0:288:A:C8	2.55	0.41
30:0:553:G:C2'	30:0:554:G:H5'	2.50	0.41
30:0:558:C:C2'	30:0:559:U:C5'	2.89	0.41
30:0:1416:G:H2'	30:0:1417:G:C5'	2.50	0.41
30:0:1475:G:O2'	30:0:1866:A:N1	2.50	0.41
30:0:1526:A:H4'	30:0:1527:A:C5'	2.50	0.41
30:0:1588:G:C6	30:0:1589:G:C6	3.08	0.41
30:0:2095:A:OP1	30:0:2096:A:H4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:2265:U:H2'	30:0:2266:A:C8	2.56	0.41
30:0:2783:A:H2'	30:0:2784:A:C8	2.55	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD3	1.86	0.41
1:A:105:VAL:HG11	1:A:154:ALA:CB	2.51	0.41
2:B:141:ARG:HG2	2:B:165:ARG:CA	2.49	0.41
2:B:195:ARG:HD2	2:B:324:ASP:OD1	2.20	0.41
3:C:98:ARG:NH1	42:C:8560:HOH:O	2.53	0.41
4:D:140:ARG:C	4:D:142:ALA:H	2.28	0.41
6:F:110:ASP:O	6:F:114:LYS:HG3	2.20	0.41
9:I:98:ASP:C	9:I:100:VAL:N	2.79	0.41
9:I:118:ASN:C	9:I:120:ALA:N	2.77	0.41
10:J:143:LYS:HG3	10:J:145:TRP:CE2	2.56	0.41
14:N:5:ARG:HD3	42:0:7778:HOH:O	2.20	0.41
17:Q:11:ARG:HD3	42:Q:5620:HOH:O	2.20	0.41
17:Q:47:VAL:HB	17:Q:90:HIS:CE1	2.55	0.41
17:Q:94:GLN:HG2	17:Q:95:GLU:OE1	2.21	0.41
20:T:51:LEU:O	20:T:52:ARG:NH1	2.52	0.41
23:W:9:GLY:H	30:0:1086:A:P	2.42	0.41
30:0:111:C:H2'	30:0:112:G:H5'	2.03	0.41
30:0:154:C:H2'	30:0:155:C:C6	2.55	0.41
30:0:282:C:H2'	30:0:283:U:O4'	2.20	0.41
30:0:390:G:H5''	42:0:3451:HOH:O	2.20	0.41
30:0:407:A:H5'	42:0:6858:HOH:O	2.20	0.41
30:0:867:A:N1	30:0:880:C:O2'	2.46	0.41
30:0:1212:C:H2'	30:0:1213:C:H5'	2.02	0.41
30:0:2669:U:H2'	30:0:2670:G:C8	2.55	0.41
30:0:2847:G:O2'	30:0:2848:G:H5'	2.20	0.41
2:B:321:PRO:HG3	42:B:9072:HOH:O	2.19	0.41
4:D:29:HIS:HB2	42:D:2768:HOH:O	2.20	0.41
11:K:34:VAL:CG2	11:K:47:ALA:HB2	2.51	0.41
11:K:64:MET:HA	11:K:67:GLN:NE2	2.36	0.41
12:L:98:GLU:O	12:L:99:GLU:CB	2.67	0.41
13:M:99:ARG:HD2	13:M:167:GLY:CA	2.51	0.41
15:O:13:ASP:O	15:O:14:LEU:C	2.64	0.41
20:T:92:ASP:C	20:T:94:SER:N	2.76	0.41
23:W:117:ARG:HD3	30:0:1287:A:O4'	2.20	0.41
27:1:26:SER:CB	27:1:36:SER:HB2	2.51	0.41
30:0:75:U:H2'	30:0:76:G:H8	1.86	0.41
30:0:581:G:H2'	30:0:582:U:H6	1.85	0.41
30:0:1033:C:H2'	30:0:1034:G:C5'	2.51	0.41
30:0:1513:C:H2'	30:0:1514:C:H6	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1576:G:H2'	30:0:1577:U:C6	2.55	0.41
30:0:2022:A:H5''	30:0:2023:G:OP2	2.21	0.41
30:0:2133:U:H4'	30:0:2134:G:C5'	2.51	0.41
30:0:2758:G:H2'	30:0:2759:C:C6	2.56	0.41
3:C:51:TYR:CD1	27:1:56:GLU:HB2	2.56	0.41
3:C:120:ASP:O	3:C:121:ALA:C	2.64	0.41
5:E:2:ARG:NH2	5:E:48:VAL:HG21	2.36	0.41
6:F:117:GLU:C	6:F:119:ARG:N	2.79	0.41
8:H:48:VAL:O	8:H:140:TYR:HA	2.21	0.41
8:H:143:VAL:CG2	8:H:173:GLU:HG2	2.51	0.41
11:K:113:ILE:HG22	11:K:114:ALA:H	1.86	0.41
12:L:134:GLU:C	12:L:136:ALA:N	2.78	0.41
14:N:69:TYR:N	14:N:69:TYR:CD1	2.89	0.41
17:Q:47:VAL:O	17:Q:51:ARG:NE	2.48	0.41
18:R:119:VAL:HG21	18:R:142:ASP:OD1	2.20	0.41
18:R:132:ARG:HD3	42:0:3121:HOH:O	2.20	0.41
19:S:80:ARG:HA	42:S:8538:HOH:O	2.21	0.41
20:T:32:ARG:NH1	20:T:38:ARG:NH1	2.69	0.41
20:T:94:SER:OG	30:0:334:G:N2	2.54	0.41
23:W:3:ALA:O	23:W:54:PHE:HA	2.19	0.41
30:0:111:C:H2'	30:0:112:G:C5'	2.50	0.41
30:0:293:A:P	30:0:358:G:H22	2.44	0.41
30:0:400:C:H2'	30:0:401:C:H6	1.86	0.41
30:0:532:A:N1	30:0:2660:G:O2'	2.50	0.41
30:0:1065:G:H2'	30:0:1066:U:C6	2.56	0.41
30:0:1159:G:H1	30:0:1208:C:N4	2.18	0.41
30:0:1205:U:H2'	30:0:1206:U:H5'	2.00	0.41
30:0:1592:G:H2'	30:0:1593:C:C6	2.55	0.41
30:0:1684:A:O2'	30:0:1685:A:H5''	2.20	0.41
30:0:1839:A:C5'	30:0:2643:G:H4'	2.51	0.41
30:0:2238:A:O2'	30:0:2239:C:H5'	2.21	0.41
30:0:2332:A:H5'	30:0:2333:G:OP2	2.21	0.41
3:C:123:LEU:HD11	42:C:8660:HOH:O	2.20	0.41
4:D:128:LEU:HB2	42:D:6007:HOH:O	2.19	0.41
5:E:40:VAL:HA	5:E:48:VAL:O	2.21	0.41
9:I:72:GLU:C	9:I:74:ILE:H	2.29	0.41
10:J:131:THR:HG22	10:J:134:GLU:N	2.28	0.41
12:L:27:ARG:NE	42:L:8980:HOH:O	2.39	0.41
14:N:38:LYS:HE2	14:N:107:ASN:ND2	2.35	0.41
17:Q:40:HIS:HE1	30:0:949:U:O2'	2.04	0.41
21:U:52:THR:HB	21:U:55:ALA:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:41:PHE:CZ	24:X:74:ALA:HB3	2.56	0.41
25:Y:187:VAL:HG23	25:Y:192:ASP:HB3	2.02	0.41
27:1:20:ARG:HH21	30:0:120:A:H5'	1.85	0.41
27:1:25:LYS:O	27:1:25:LYS:CG	2.67	0.41
29:3:20:HIS:CD2	29:3:71:CYS:HA	2.56	0.41
29:3:47:GLY:HA2	30:0:2121:G:H4'	2.01	0.41
30:0:52:A:C2	30:0:110:C:C2	3.08	0.41
30:0:215:A:N1	30:0:393:G:H1'	2.36	0.41
30:0:240:C:H1'	30:0:431:G:N2	2.35	0.41
30:0:537:G:H4'	30:0:538:C:O5'	2.21	0.41
30:0:705:C:H3'	30:0:706:G:C8	2.55	0.41
30:0:727:G:H5'	30:0:728:C:OP2	2.21	0.41
30:0:1170:U:O2'	30:0:1172:G:N7	2.49	0.41
30:0:1183:C:H42	30:0:1184:C:H41	1.62	0.41
30:0:1522:A:H2'	30:0:1523:G:H5'	2.03	0.41
30:0:1736:A:H1'	42:0:9381:HOH:O	2.21	0.41
30:0:2867:G:H2'	30:0:2868:C:C6	2.56	0.41
1:A:105:VAL:HG12	1:A:106:CYS:H	1.83	0.41
1:A:235:ARG:NH1	42:A:9014:HOH:O	2.53	0.41
2:B:286:ASN:O	2:B:306:LYS:HE3	2.21	0.41
3:C:123:LEU:O	3:C:125:ALA:N	2.54	0.41
3:C:194:PHE:HA	3:C:234:VAL:CG1	2.47	0.41
4:D:76:ARG:NH1	31:9:42:C:O2	2.52	0.41
4:D:158:ASN:HB2	4:D:161:ASP:HB2	2.02	0.41
5:E:84:MET:HE2	5:E:133:VAL:HG23	2.02	0.41
6:F:24:ARG:HG3	6:F:25:ASP:H	1.86	0.41
6:F:59:ILE:HD13	30:0:263:U:O4'	2.20	0.41
6:F:70:LYS:C	6:F:72:VAL:H	2.29	0.41
9:I:130:LEU:HB2	9:I:132:VAL:HG23	2.03	0.41
10:J:107:ASN:HD22	10:J:108:PRO:N	2.19	0.41
12:L:145:LEU:O	12:L:148:GLU:HG3	2.20	0.41
13:M:20:LEU:HA	13:M:23:LEU:HB2	2.03	0.41
13:M:57:LYS:HZ3	13:M:144:ASP:HB2	1.85	0.41
15:O:25:VAL:HG23	15:O:26:TRP:CE3	2.56	0.41
16:P:28:GLN:HB2	42:P:6051:HOH:O	2.20	0.41
16:P:98:ILE:HG21	30:0:1597:A:H5''	2.02	0.41
17:Q:31:GLU:HA	17:Q:31:GLU:OE1	2.21	0.41
18:R:94:ASN:ND2	30:0:500:G:O2'	2.47	0.41
19:S:81:ILE:C	19:S:81:ILE:HD12	2.45	0.41
20:T:1:SER:H3	20:T:7:GLN:HE21	1.69	0.41
20:T:52:ARG:HH22	30:0:308:U:H2'	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:31:HIS:HB3	23:W:115:THR:CG2	2.51	0.41
26:Z:81:CYS:SG	26:Z:83:TYR:HB3	2.61	0.41
29:3:60:LYS:HG3	42:0:9354:HOH:O	2.21	0.41
30:0:10:U:O4	30:0:532:A:OP2	2.39	0.41
30:0:113:A:H3'	30:0:114:A:C5'	2.50	0.41
30:0:116:G:H2'	30:0:117:A:H8	1.86	0.41
30:0:491:C:H2'	30:0:492:C:H6	1.86	0.41
30:0:919:U:H5'	30:0:2465:A:O2'	2.21	0.41
30:0:939:A:N1	30:0:1027:G:O2'	2.49	0.41
30:0:1118:A:H3'	30:0:1119:G:H5''	2.03	0.41
30:0:1211:G:H2'	30:0:1212:C:H6	1.85	0.41
30:0:1321:A:H2'	30:0:1322:G:C8	2.56	0.41
30:0:1343:C:H2'	30:0:1344:G:O5'	2.21	0.41
30:0:1358:A:N7	30:0:1360:C:C2	2.89	0.41
30:0:1421:C:H2'	30:0:1422:U:H6	1.86	0.41
30:0:1423:C:O2'	30:0:1424:A:H5'	2.21	0.41
30:0:1456:C:H2'	30:0:1457:U:C6	2.56	0.41
30:0:1573:A:N7	30:0:1574:C:C2	2.89	0.41
30:0:1617:C:C4	30:0:1643:C:H4'	2.56	0.41
30:0:1757:U:H6	30:0:1757:U:O5'	2.03	0.41
30:0:1973:A:H2'	30:0:1974:G:O4'	2.21	0.41
30:0:2096:A:H2'	30:0:2539:U:O4'	2.21	0.41
30:0:2111:G:H2'	30:0:2112:A:O4'	2.21	0.41
30:0:2305:A:H4'	30:0:2392:C:C6	2.56	0.41
30:0:2397:G:H2'	30:0:2398:A:C8	2.56	0.41
30:0:2474:A:H4'	30:0:2475:C:O5'	2.21	0.41
30:0:2531:U:C2'	30:0:2532:A:H5'	2.51	0.41
30:0:2573:G:O2'	30:0:2574:G:H5'	2.20	0.41
1:A:141:PRO:HG2	30:0:1855:G:O6	2.20	0.41
1:A:164:ARG:HB2	26:Z:92:SER:OG	2.21	0.41
2:B:71:VAL:HG11	2:B:296:LEU:HD22	2.02	0.41
2:B:221:GLN:HB2	42:B:9055:HOH:O	2.21	0.41
3:C:123:LEU:C	3:C:125:ALA:N	2.76	0.41
3:C:133:ARG:HD2	42:C:8613:HOH:O	2.21	0.41
9:I:95:LEU:HG	9:I:132:VAL:CG1	2.51	0.41
11:K:6:ALA:HB3	11:K:116:GLU:HG2	2.01	0.41
13:M:5:TYR:O	13:M:7:TYR:N	2.54	0.41
13:M:54:TYR:CG	13:M:55:LYS:N	2.89	0.41
14:N:165:ALA:HA	42:N:8823:HOH:O	2.21	0.41
15:O:4:ASN:OD1	15:O:4:ASN:C	2.64	0.41
16:P:59:ARG:O	16:P:62:ALA:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:15:LYS:HD3	30:0:2364:A:H5''	2.02	0.41
18:R:17:MET:HE1	18:R:19:ARG:NH2	2.36	0.41
18:R:84:ALA:O	18:R:88:PHE:HD1	2.04	0.41
19:S:7:HIS:HA	19:S:8:PRO:HD3	1.92	0.41
19:S:41:VAL:HG21	19:S:66:VAL:HG21	2.03	0.41
24:X:20:GLU:HG3	24:X:21:PRO:HD2	2.03	0.41
30:0:287:C:H2'	30:0:288:A:H8	1.86	0.41
30:0:544:G:H2'	30:0:545:G:C5'	2.51	0.41
30:0:574:G:O2'	30:0:575:A:H5'	2.21	0.41
30:0:629:A:H2'	30:0:630:A:O4'	2.21	0.41
30:0:907:A:H4'	30:0:1328:A:C2	2.56	0.41
30:0:1207:A:H5'	30:0:1208:C:OP2	2.21	0.41
30:0:1220:U:O2'	30:0:1221:G:H5'	2.20	0.41
30:0:2032:U:O2'	30:0:2033:G:H5''	2.21	0.41
30:0:2326:C:H4'	30:0:2412:G:O4'	2.21	0.41
30:0:2588:OMG:HM23	30:0:2617:G:C2	2.56	0.41
31:9:3:A:C2	31:9:21:G:N3	2.89	0.41
31:9:47:A:C2	31:9:48:C:C2	3.08	0.41
2:B:215:VAL:N	2:B:220:VAL:HG22	2.36	0.40
2:B:223:ARG:NE	2:B:232:TRP:HB3	2.35	0.40
2:B:233:ARG:HD2	42:0:9321:HOH:O	2.21	0.40
3:C:78:ARG:O	3:C:79:ARG:HB3	2.21	0.40
3:C:136:VAL:HG22	3:C:137:PRO:HA	2.03	0.40
4:D:45:THR:OG1	4:D:46:GLY:N	2.48	0.40
5:E:15:GLN:CG	5:E:20:ILE:HG12	2.48	0.40
6:F:111:ILE:O	6:F:112:ALA:C	2.64	0.40
8:H:170:ARG:HD2	42:H:8992:HOH:O	2.21	0.40
12:L:130:ARG:C	12:L:132:LYS:N	2.79	0.40
13:M:72:ALA:CB	13:M:93:ARG:NE	2.84	0.40
13:M:191:GLY:O	30:0:175:G:H5''	2.21	0.40
14:N:155:GLU:C	14:N:156:GLU:HG3	2.46	0.40
16:P:55:LYS:CG	16:P:56:GLY:N	2.84	0.40
16:P:81:LYS:NZ	30:0:1817:U:O2	2.36	0.40
20:T:75:GLU:HB3	42:T:4772:HOH:O	2.21	0.40
22:V:36:ALA:C	22:V:38:GLY:H	2.29	0.40
23:W:59:GLN:NE2	23:W:97:ALA:HB3	2.36	0.40
26:Z:48:ARG:O	26:Z:51:ALA:HB3	2.21	0.40
26:Z:76:THR:O	26:Z:77:GLY:C	2.64	0.40
30:0:85:C:H3'	30:0:86:A:H2'	2.03	0.40
30:0:267:G:H2'	30:0:268:U:O4'	2.20	0.40
30:0:820:G:H5'	30:0:821:U:H5'	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1065:G:H2'	30:0:1066:U:O4'	2.21	0.40
30:0:1359:U:C5	30:0:2101:A:C8	3.10	0.40
30:0:1588:G:H1'	30:0:1607:A:N6	2.37	0.40
30:0:1739:G:O2'	30:0:1740:U:H5'	2.21	0.40
30:0:1773:G:N2	30:0:1774:G:C8	2.89	0.40
30:0:1797:A:H2'	30:0:1799:G:O5'	2.21	0.40
30:0:2057:U:O5'	30:0:2057:U:H6	2.03	0.40
30:0:2656:G:O2'	30:0:2657:G:H5'	2.20	0.40
30:0:2851:G:H2'	30:0:2852:A:H5'	2.00	0.40
3:C:123:LEU:O	3:C:124:VAL:C	2.63	0.40
8:H:43:ALA:HB1	8:H:140:TYR:CE2	2.56	0.40
8:H:49:GLN:NE2	8:H:140:TYR:HE2	2.19	0.40
9:I:70:THR:O	9:I:74:ILE:HG13	2.22	0.40
9:I:132:VAL:O	9:I:132:VAL:HG12	2.21	0.40
20:T:21:LYS:HA	20:T:24:ARG:HD2	2.03	0.40
23:W:115:THR:CG2	23:W:116:LEU:N	2.84	0.40
29:3:11:CYS:HB2	29:3:20:HIS:CE1	2.56	0.40
29:3:42:ARG:HG3	29:3:42:ARG:NH1	2.36	0.40
29:3:86:GLY:HA3	30:0:2318:C:OP1	2.21	0.40
30:0:69:A:C8	30:0:69:A:C3'	3.04	0.40
30:0:233:U:H2'	30:0:234:A:O4'	2.21	0.40
30:0:297:U:H6	30:0:297:U:O5'	2.03	0.40
30:0:451:C:C2'	30:0:452:G:H5'	2.51	0.40
30:0:632:A:OP2	30:0:2534:C:O2'	2.34	0.40
30:0:1041:U:H4'	30:0:1295:G:H5'	2.02	0.40
30:0:1552:G:N2	30:0:1634:G:H1'	2.36	0.40
30:0:1724:U:H2'	42:0:5552:HOH:O	2.21	0.40
30:0:2563:U:H2'	30:0:2565:C:O5'	2.21	0.40
30:0:2800:A:H5'	30:0:2801:A:OP2	2.21	0.40
30:0:2831:C:H2'	30:0:2832:C:C5'	2.51	0.40
1:A:172:ALA:O	1:A:173:GLY:C	2.64	0.40
2:B:70:PRO:HG3	30:0:2719:A:C2	2.57	0.40
2:B:215:VAL:HG11	2:B:234:ARG:NH2	2.36	0.40
5:E:36:PRO:CD	10:J:127:ILE:HG13	2.52	0.40
5:E:70:GLU:O	5:E:73:PHE:HB2	2.21	0.40
7:G:19:GLU:C	7:G:21:ASP:N	2.80	0.40
7:G:26:MET:HE1	42:0:9290:HOH:O	2.20	0.40
8:H:142:ASN:O	8:H:144:GLU:N	2.53	0.40
10:J:47:THR:HB	30:0:1244:U:H6	1.85	0.40
14:N:143:ARG:NH2	14:N:169:PRO:HB2	2.35	0.40
15:O:87:THR:O	15:O:91:GLN:HG3	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:2:LYS:HE2	42:T:2822:HOH:O	2.21	0.40
30:0:36:C:C2	30:0:447:A:C2	3.10	0.40
30:0:39:G:H2'	30:0:40:C:O4'	2.21	0.40
30:0:80:A:H4'	30:0:81:G:O5'	2.22	0.40
30:0:190:G:O2'	30:0:204:A:N3	2.46	0.40
30:0:426:G:H5''	42:0:9419:HOH:O	2.21	0.40
30:0:653:U:H3	30:0:752:G:H1	1.70	0.40
30:0:745:G:H5''	30:0:746:A:OP1	2.20	0.40
30:0:1270:U:H2'	30:0:1271:A:H8	1.87	0.40
30:0:1445:G:H21	30:0:1678:A:H1'	1.84	0.40
30:0:2685:C:O2'	30:0:2686:C:H5'	2.22	0.40
2:B:229:ARG:NH2	30:0:1753:C:O2	2.38	0.40
2:B:267:LYS:HA	42:0:3465:HOH:O	2.22	0.40
4:D:170:TYR:N	4:D:170:TYR:CD1	2.89	0.40
6:F:26:THR:HG21	6:F:102:GLY:O	2.20	0.40
7:G:23:ILE:O	7:G:27:ILE:HG13	2.21	0.40
8:H:6:ALA:C	8:H:8:MET:N	2.78	0.40
8:H:82:GLU:O	8:H:83:GLU:HG3	2.22	0.40
10:J:40:ASN:O	10:J:41:ALA:C	2.63	0.40
12:L:130:ARG:O	12:L:132:LYS:N	2.54	0.40
15:O:4:ASN:HA	15:O:5:PRO:HD3	1.88	0.40
15:O:106:PRO:C	15:O:108:GLY:H	2.29	0.40
16:P:59:ARG:HH22	16:P:66:GLN:NE2	2.11	0.40
19:S:45:TYR:HE2	19:S:81:ILE:HG12	1.86	0.40
20:T:103:LEU:C	20:T:105:ASP:N	2.79	0.40
29:3:6:ARG:HB3	29:3:20:HIS:O	2.21	0.40
30:0:17:G:H2'	30:0:18:C:H6	1.85	0.40
30:0:168:C:O5'	30:0:168:C:H6	2.05	0.40
30:0:661:G:C5	30:0:686:A:C2	3.10	0.40
30:0:1114:A:H2'	30:0:1115:U:H6	1.86	0.40
30:0:2325:U:O2'	30:0:2411:C:H1'	2.21	0.40
30:0:2852:A:H4'	30:0:2853:U:C5	2.57	0.40
1:A:2:ARG:HG3	1:A:197:VAL:HG22	2.03	0.40
1:A:194:MET:CE	1:A:199:HIS:HB2	2.48	0.40
1:A:199:HIS:O	1:A:200:PRO:C	2.64	0.40
2:B:5:ARG:NH2	30:0:2548:C:OP2	2.54	0.40
2:B:51:VAL:HG23	2:B:329:TYR:O	2.21	0.40
2:B:298:LYS:HG2	42:0:6362:HOH:O	2.21	0.40
5:E:28:SER:C	5:E:29:VAL:HG23	2.46	0.40
5:E:84:MET:HE1	5:E:148:ILE:HG21	2.04	0.40
6:F:68:ASP:C	6:F:70:LYS:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:71:TYR:HA	10:J:72:PRO:HD2	1.89	0.40
13:M:59:GLY:C	13:M:141:ILE:HD11	2.47	0.40
14:N:41:LYS:HE3	42:9:9020:HOH:O	2.22	0.40
15:O:32:ARG:HD3	15:O:32:ARG:C	2.47	0.40
17:Q:16:ASN:ND2	17:Q:45:PRO:CG	2.84	0.40
18:R:2:ILE:HG22	30:0:21:G:H4'	2.03	0.40
18:R:43:ALA:O	18:R:46:TYR:HB3	2.22	0.40
20:T:16:LEU:HD12	30:0:100:C:H5'	2.02	0.40
23:W:54:PHE:CZ	23:W:140:LYS:HB2	2.57	0.40
25:Y:100:ARG:HD2	25:Y:232:THR:HB	2.03	0.40
26:Z:75:GLY:O	26:Z:76:THR:C	2.64	0.40
29:3:40:ARG:HG3	29:3:52:PHE:CD2	2.57	0.40
29:3:91:GLN:O	29:3:92:GLU:HB2	2.22	0.40
30:0:69:A:C8	30:0:69:A:H3'	2.56	0.40
30:0:862:U:O2'	30:0:863:G:H5'	2.21	0.40
30:0:1228:C:H2'	30:0:1229:C:O4'	2.21	0.40
30:0:1688:G:C6	30:0:1692:C:C6	3.09	0.40
30:0:2551:C:O2'	30:0:2552:C:H5'	2.21	0.40
30:0:2604:A:H5'	42:0:6629:HOH:O	2.22	0.40
30:0:2824:C:H5''	30:0:2825:C:H5'	2.04	0.40
31:9:1:U:O3'	31:9:3:A:H5''	2.21	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	233/240 (97%)	198 (85%)	25 (11%)	10 (4%)	2	4
2	B	333/338 (98%)	285 (86%)	41 (12%)	7 (2%)	5	16
3	C	242/246 (98%)	202 (84%)	32 (13%)	8 (3%)	3	7
4	D	132/177 (75%)	87 (66%)	35 (26%)	10 (8%)	1	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	168/178 (94%)	150 (89%)	17 (10%)	1 (1%)	21	45
6	F	115/120 (96%)	94 (82%)	15 (13%)	6 (5%)	1	3
7	G	25/348 (7%)	15 (60%)	7 (28%)	3 (12%)	0	0
8	H	154/177 (87%)	125 (81%)	23 (15%)	6 (4%)	2	5
9	I	66/162 (41%)	43 (65%)	18 (27%)	5 (8%)	1	1
10	J	138/145 (95%)	120 (87%)	15 (11%)	3 (2%)	5	15
11	K	128/132 (97%)	115 (90%)	8 (6%)	5 (4%)	2	5
12	L	139/165 (84%)	106 (76%)	27 (19%)	6 (4%)	2	4
13	M	190/196 (97%)	170 (90%)	16 (8%)	4 (2%)	5	16
14	N	182/187 (97%)	153 (84%)	19 (10%)	10 (6%)	1	3
15	O	111/116 (96%)	92 (83%)	19 (17%)	0	100	100
16	P	139/149 (93%)	129 (93%)	8 (6%)	2 (1%)	9	24
17	Q	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	2	4
18	R	146/155 (94%)	131 (90%)	12 (8%)	3 (2%)	5	16
19	S	77/85 (91%)	67 (87%)	9 (12%)	1 (1%)	9	26
20	T	115/120 (96%)	95 (83%)	17 (15%)	3 (3%)	4	12
21	U	51/67 (76%)	45 (88%)	4 (8%)	2 (4%)	2	5
22	V	63/71 (89%)	53 (84%)	9 (14%)	1 (2%)	7	21
23	W	150/154 (97%)	131 (87%)	19 (13%)	0	100	100
24	X	78/92 (85%)	68 (87%)	7 (9%)	3 (4%)	2	6
25	Y	140/240 (58%)	128 (91%)	11 (8%)	1 (1%)	18	40
26	Z	69/116 (60%)	51 (74%)	13 (19%)	5 (7%)	1	1
27	1	54/57 (95%)	47 (87%)	6 (11%)	1 (2%)	6	17
28	2	42/50 (84%)	34 (81%)	8 (19%)	0	100	100
29	3	88/92 (96%)	77 (88%)	9 (10%)	2 (2%)	5	14
All	All	3659/4471 (82%)	3087 (84%)	460 (13%)	112 (3%)	3	8

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	34	ASP
1	A	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	208	HIS
2	B	181	ILE
4	D	16	PRO
4	D	27	ILE
4	D	171	ASP
6	F	101	ALA
9	I	113	SER
12	L	80	ASP
13	M	83	SER
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE
24	X	87	ALA
26	Z	44	ARG
26	Z	105	ARG
29	3	56	PRO
1	A	205	GLY
2	B	291	ASP
3	C	69	HIS
6	F	27	GLY
8	H	84	GLY
9	I	124	VAL
12	L	82	ALA
14	N	165	ALA
20	T	44	ALA
20	T	53	GLY
21	U	55	ALA
22	V	43	PRO
24	X	81	GLY
26	Z	59	GLU
1	A	24	LYS
1	A	119	ALA
3	C	8	LEU
3	C	121	ALA
4	D	28	GLY
4	D	60	GLU
4	D	61	PHE
4	D	137	PRO
4	D	147	ALA
5	E	164	ASP
6	F	100	ASP
7	G	72	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	71	SER
8	H	82	GLU
9	I	128	THR
10	J	15	ARG
10	J	76	ASP
11	K	65	ARG
11	K	126	SER
12	L	21	ARG
14	N	65	ASP
14	N	74	PRO
14	N	164	ASP
14	N	167	ASP
14	N	182	GLY
16	P	19	ASN
16	P	108	LEU
17	Q	23	THR
17	Q	48	PRO
19	S	4	VAL
21	U	46	ALA
24	X	70	ILE
2	B	55	ASN
2	B	185	GLY
4	D	56	ARG
6	F	61	MET
6	F	64	PRO
8	H	70	LEU
8	H	143	VAL
8	H	145	ASP
12	L	50	GLY
12	L	102	ASP
13	M	6	SER
13	M	35	GLY
18	R	114	VAL
20	T	30	ASP
29	3	52	PHE
2	B	2	GLN
3	C	232	LEU
3	C	234	VAL
4	D	46	GLY
9	I	73	LEU
11	K	66	ARG
12	L	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	31	GLU
18	R	20	GLU
26	Z	66	CYS
27	1	54	ALA
1	A	204	GLY
2	B	182	VAL
3	C	95	GLU
6	F	59	ILE
11	K	102	GLU
13	M	88	VAL
17	Q	54	PRO
18	R	32	ALA
25	Y	182	PHE
1	A	192	VAL
3	C	124	VAL
10	J	18	ILE
26	Z	67	GLY
2	B	30	PRO
1	A	88	ILE
3	C	57	PRO
7	G	13	PRO
11	K	83	PRO
14	N	157	PRO
7	G	20	VAL
9	I	109	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	178/182 (98%)	163 (92%)	15 (8%)	10	26
2	B	281/283 (99%)	264 (94%)	17 (6%)	17	40
3	C	192/193 (100%)	174 (91%)	18 (9%)	8	22
4	D	116/148 (78%)	110 (95%)	6 (5%)	21	46
5	E	151/156 (97%)	141 (93%)	10 (7%)	15	37

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	92/94 (98%)	92 (100%)	0	100	100
7	G	27/283 (10%)	26 (96%)	1 (4%)	30	55
8	H	133/145 (92%)	127 (96%)	6 (4%)	24	50
9	I	58/130 (45%)	57 (98%)	1 (2%)	53	73
10	J	117/121 (97%)	109 (93%)	8 (7%)	14	35
11	K	105/106 (99%)	101 (96%)	4 (4%)	29	55
12	L	113/127 (89%)	106 (94%)	7 (6%)	16	39
13	M	157/160 (98%)	153 (98%)	4 (2%)	42	66
14	N	148/150 (99%)	141 (95%)	7 (5%)	23	49
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	59
16	P	113/117 (97%)	109 (96%)	4 (4%)	32	57
17	Q	79/80 (99%)	77 (98%)	2 (2%)	42	66
18	R	117/122 (96%)	112 (96%)	5 (4%)	26	52
19	S	71/74 (96%)	69 (97%)	2 (3%)	38	62
20	T	104/106 (98%)	96 (92%)	8 (8%)	12	30
21	U	44/53 (83%)	40 (91%)	4 (9%)	9	23
22	V	51/57 (90%)	49 (96%)	2 (4%)	28	54
23	W	129/130 (99%)	121 (94%)	8 (6%)	16	39
24	X	65/74 (88%)	58 (89%)	7 (11%)	6	18
25	Y	120/195 (62%)	115 (96%)	5 (4%)	26	53
26	Z	59/94 (63%)	57 (97%)	2 (3%)	32	58
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	42 (100%)	0	100	100
29	3	78/79 (99%)	75 (96%)	3 (4%)	29	55
All	All	3079/3646 (84%)	2920 (95%)	159 (5%)	21	46

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	27	LEU
1	A	33	GLU
1	A	36	ASP
1	A	38	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	LEU
1	A	94	LEU
1	A	131	HIS
1	A	153	ARG
1	A	165	THR
1	A	171	LYS
1	A	175	LYS
1	A	179	MET
1	A	192	VAL
1	A	217	ARG
2	B	7	ARG
2	B	11	LEU
2	B	16	ARG
2	B	27	ASN
2	B	71	VAL
2	B	82	VAL
2	B	90	THR
2	B	103	ASP
2	B	162	MET
2	B	184	ASP
2	B	190	MET
2	B	195	ARG
2	B	251	VAL
2	B	254	GLN
2	B	256	GLN
2	B	277	GLU
2	B	312	ARG
3	C	2	GLN
3	C	16	VAL
3	C	27	ARG
3	C	67	GLN
3	C	76	ARG
3	C	94	THR
3	C	115	LEU
3	C	132	ASP
3	C	139	VAL
3	C	172	THR
3	C	187	ARG
3	C	193	LEU
3	C	223	LEU
3	C	234	VAL
3	C	236	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	237	GLU
3	C	240	LEU
3	C	243	VAL
4	D	24	HIS
4	D	50	VAL
4	D	58	VAL
4	D	131	THR
4	D	133	ASN
4	D	137	PRO
5	E	3	VAL
5	E	7	ILE
5	E	42	VAL
5	E	81	GLU
5	E	102	VAL
5	E	126	ILE
5	E	132	THR
5	E	143	GLN
5	E	154	ILE
5	E	155	ASN
7	G	73	ASP
8	H	21	GLU
8	H	51	SER
8	H	65	LEU
8	H	87	LYS
8	H	91	ARG
8	H	157	TYR
9	I	135	GLU
10	J	39	VAL
10	J	46	ILE
10	J	47	THR
10	J	52	GLN
10	J	74	ARG
10	J	93	ARG
10	J	127	ILE
10	J	131	THR
11	K	4	LEU
11	K	7	ASP
11	K	10	GLN
11	K	49	LEU
12	L	35	ARG
12	L	37	LYS
12	L	43	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	89	PHE
12	L	101	ASP
12	L	140	VAL
12	L	145	LEU
13	M	46	LEU
13	M	99	ARG
13	M	130	GLU
13	M	164	THR
14	N	17	ARG
14	N	47	LEU
14	N	49	THR
14	N	103	ASP
14	N	110	THR
14	N	124	ASP
14	N	139	TRP
15	O	3	THR
15	O	43	VAL
15	O	98	LEU
16	P	21	VAL
16	P	91	LYS
16	P	98	ILE
16	P	139	ARG
17	Q	11	ARG
17	Q	95	GLU
18	R	39	THR
18	R	61	GLN
18	R	70	SER
18	R	76	ASP
18	R	90	ASP
19	S	12	GLU
19	S	44	GLN
20	T	23	VAL
20	T	26	THR
20	T	39	ASN
20	T	42	VAL
20	T	48	VAL
20	T	75	GLU
20	T	89	ARG
20	T	96	VAL
21	U	19	THR
21	U	20	MET
21	U	53	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
21	U	54	THR
22	V	2	VAL
22	V	6	GLN
23	W	26	ILE
23	W	35	VAL
23	W	52	VAL
23	W	73	LEU
23	W	88	THR
23	W	125	HIS
23	W	146	ILE
23	W	151	GLU
24	X	8	ARG
24	X	43	VAL
24	X	46	ASP
24	X	49	ARG
24	X	79	GLU
24	X	80	GLU
24	X	85	VAL
25	Y	108	ASP
25	Y	141	THR
25	Y	163	THR
25	Y	203	VAL
25	Y	235	GLU
26	Z	68	GLU
26	Z	106	SER
29	3	15	ASN
29	3	21	GLU
29	3	56	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	188	ASN
1	A	199	HIS
2	B	27	ASN
2	B	94	GLN
2	B	106	HIS
2	B	145	HIS
2	B	238	ASN
2	B	260	HIS
2	B	320	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	332	ASN
3	C	2	GLN
3	C	11	ASN
3	C	39	GLN
3	C	67	GLN
3	C	73	GLN
3	C	129	HIS
3	C	163	HIS
3	C	178	GLN
4	D	47	GLN
4	D	103	ASN
4	D	133	ASN
4	D	155	HIS
5	E	90	HIS
5	E	106	ASN
5	E	143	GLN
6	F	80	GLN
7	G	64	ASN
8	H	33	GLN
8	H	34	HIS
8	H	40	GLN
8	H	59	GLN
8	H	62	HIS
8	H	75	HIS
8	H	148	HIS
9	I	88	GLN
9	I	99	GLN
10	J	25	GLN
10	J	52	GLN
10	J	107	ASN
10	J	126	ASN
11	K	10	GLN
11	K	35	HIS
11	K	42	ASN
12	L	18	HIS
12	L	20	ASN
12	L	41	HIS
12	L	42	ASN
12	L	43	HIS
12	L	58	GLN
13	M	24	GLN
13	M	52	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	58	GLN
13	M	137	ASN
14	N	22	GLN
14	N	40	ASN
14	N	93	GLN
14	N	107	ASN
14	N	119	GLN
14	N	140	GLN
14	N	153	GLN
15	O	100	GLN
16	P	50	GLN
16	P	66	GLN
16	P	73	HIS
16	P	88	GLN
16	P	118	GLN
17	Q	16	ASN
17	Q	40	HIS
18	R	61	GLN
18	R	94	ASN
18	R	98	ASN
18	R	113	HIS
18	R	117	HIS
18	R	122	GLN
18	R	140	GLN
19	S	9	HIS
19	S	21	GLN
19	S	44	GLN
19	S	53	ASN
19	S	55	GLN
20	T	7	GLN
20	T	39	ASN
20	T	73	HIS
21	U	48	ASN
22	V	60	GLN
23	W	14	HIS
23	W	28	HIS
23	W	110	GLN
23	W	119	HIS
23	W	125	HIS
23	W	141	HIS
25	Y	119	GLN
25	Y	131	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Y	133	HIS
25	Y	134	HIS
25	Y	149	GLN
25	Y	189	ASN
26	Z	74	GLN
27	1	8	GLN
27	1	16	HIS
27	1	28	HIS
28	2	16	ASN
28	2	18	ASN
28	2	41	HIS
28	2	45	ASN
29	3	48	ASN
29	3	91	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	249 (9%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	2 (1%)
32	5	1/3 (33%)	0	0
33	6	1/3 (33%)	0	0
All	All	2868/3051 (94%)	267 (9%)	32 (1%)

All (267) 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	141	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	151	A
30	0	166	A
30	0	186	A
30	0	191	A
30	0	192	A
30	0	200	C
30	0	204	A
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	381	G
30	0	397	A
30	0	417	G
30	0	461	C
30	0	487	G
30	0	497	A
30	0	498	A
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	588	G
30	0	593	A
30	0	604	G
30	0	620	A
30	0	632	A
30	0	644	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	645	U
30	0	660	A
30	0	688	A
30	0	698	A
30	0	701	U
30	0	702	G
30	0	735	C
30	0	746	A
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	857	A
30	0	858	U
30	0	868	G
30	0	869	G
30	0	871	G
30	0	872	U
30	0	875	A
30	0	877	G
30	0	878	G
30	0	882	A
30	0	905	C
30	0	920	C
30	0	921	G
30	0	923	A
30	0	938	G
30	0	953	G
30	0	960	G
30	0	961	A
30	0	1006	A
30	0	1008	C
30	0	1029	U
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	1100	G
30	0	1109	U
30	0	1110	G
30	0	1119	G
30	0	1130	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	1208	C
30	0	1216	G
30	0	1237	U
30	0	1238	C
30	0	1239	G
30	0	1279	U
30	0	1289	C
30	0	1342	C
30	0	1351	G
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
30	0	1525	G
30	0	1526	A
30	0	1528	A
30	0	1559	A
30	0	1592	G
30	0	1603	A
30	0	1625	U
30	0	1626	A
30	0	1634	G
30	0	1656	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	1731	C
30	0	1752	G
30	0	1778	A
30	0	1779	A
30	0	1798	C
30	0	1819	G
30	0	1820	G
30	0	1829	A
30	0	1856	C
30	0	1873	G
30	0	1879	U
30	0	1919	A
30	0	1942	A
30	0	1943	C
30	0	1968	A
30	0	1971	G
30	0	1973	A
30	0	1980	U
30	0	1996	U
30	0	2004	U
30	0	2006	C
30	0	2008	U
30	0	2011	A
30	0	2012	U
30	0	2013	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	2101	A
30	0	2102	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2103	A
30	0	2104	C
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	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	2476	C
30	0	2480	G
30	0	2483	A
30	0	2507	G
30	0	2509	A
30	0	2511	A
30	0	2526	C
30	0	2527	U
30	0	2533	C
30	0	2536	C
30	0	2537	G
30	0	2541	U
30	0	2553	A
30	0	2564	G
30	0	2570	G
30	0	2589	U
30	0	2601	A
30	0	2602	G
30	0	2608	C
30	0	2613	G
30	0	2634	G
30	0	2637	A
30	0	2638	G
30	0	2645	U
30	0	2648	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	0	2649	A
30	0	2650	U
30	0	2664	A
30	0	2681	A
30	0	2682	C
30	0	2718	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	2786	G
30	0	2800	A
30	0	2811	A
30	0	2812	A
30	0	2825	C
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	7	G
31	9	14	G
31	9	22	G
31	9	23	U
31	9	24	U
31	9	25	G
31	9	34	A
31	9	39	U
31	9	40	C
31	9	41	C
31	9	43	G
31	9	52	A
31	9	57	A
31	9	66	G
31	9	77	A
31	9	114	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	9	122	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
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	1237	U
30	0	1352	A
30	0	1474	C
30	0	1684	A
30	0	1692	C
30	0	1730	G
30	0	1856	C
30	0	1942	A
30	0	1979	G
30	0	2011	A
30	0	2103	A
30	0	2313	C
30	0	2467	A
30	0	2526	C
30	0	2536	C
30	0	2637	A
30	0	2649	A
30	0	2681	A
30	0	2718	C
30	0	2726	U
30	0	2761	A
30	0	2852	A
31	9	55	U
31	9	65	A

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

6 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	PSU	0	2621	30	18,21,22	1.57	2 (11%)	21,30,33	1.40	3 (14%)
30	UR3	0	2619	30	19,22,23	0.58	0	26,32,35	0.67	1 (3%)
33	8AN	6	76	30,33	21,24,25	0.97	1 (4%)	26,35,38	1.22	3 (11%)
30	OMG	0	2588	30,32	23,26,27	0.38	0	32,38,41	0.43	0
30	1MA	0	628	37,30	21,25,26	0.75	1 (4%)	30,37,40	1.01	3 (10%)
30	OMU	0	2587	30	19,22,23	0.36	0	25,31,34	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
33	8AN	6	76	30,33	-	3/7/25/26	0/3/3/3
30	OMG	0	2588	30,32	-	0/9/27/28	0/3/3/3
30	1MA	0	628	37,30	-	2/7/25/26	0/3/3/3
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	5.35	1.43	1.36
30	0	2621	PSU	C6-C5	2.82	1.38	1.35
30	0	628	1MA	C6-N6	2.52	1.34	1.28
33	6	76	8AN	C3'-N3'	-2.19	1.44	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.68	120.66	118.17
33	6	76	8AN	O2'-C2'-C3'	3.64	121.22	111.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	76	8AN	O4'-C4'-C3'	3.41	109.19	104.22
30	0	628	1MA	CM1-N1-C6	3.32	125.29	120.15
30	0	2621	PSU	O2-C2-N1	2.85	125.72	122.79
30	0	628	1MA	N1-C2-N3	2.82	129.35	126.00
30	0	2621	PSU	C6-N1-C2	-2.80	120.09	122.69
30	0	2619	UR3	C4-N3-C2	2.58	126.66	124.58
33	6	76	8AN	C2'-C1'-N9	2.48	119.47	113.30
30	0	628	1MA	CM1-N1-C2	-2.07	116.25	120.50

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	6	76	8AN	O4'-C4'-C5'-O5'
33	6	76	8AN	C4'-C5'-O5'-P
33	6	76	8AN	C3'-C4'-C5'-O5'
30	0	628	1MA	C2'-C1'-N9-C8
30	0	628	1MA	C2'-C1'-N9-C4

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	1	0
33	6	76	8AN	4	0
30	0	2588	OMG	2	0
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 307 ligands modelled in this entry, 305 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	PHE	6	77	-	10,11,12	1.47	2 (20%)	8,13,15	0.63	0
41	ACA	6	78	-	6,7,8	1.89	2 (33%)	5,6,8	1.31	1 (20%)

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
40	PHE	6	77	-	-	2/5/6/8	0/1/1/1
41	ACA	6	78	-	-	4/5/5/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	6	78	ACA	C3-C2	-3.77	1.36	1.52
40	6	77	PHE	CE1-CD1	3.09	1.44	1.38
40	6	77	PHE	CA-N	-2.43	1.41	1.48
41	6	78	ACA	C5-C6	2.20	1.62	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	6	78	ACA	C5-C4-C3	-2.34	102.56	114.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
40	6	77	PHE	C-CA-CB-CG
41	6	78	ACA	O-C-C2-C3
41	6	78	ACA	C3-C4-C5-C6
41	6	78	ACA	C2-C3-C4-C5
40	6	77	PHE	N-CA-CB-CG
41	6	78	ACA	C4-C5-C6-N

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%)	0.24	6 (2%) 58 50	24, 46, 80, 105	0
2	B	337/338 (99%)	0.26	4 (1%) 76 71	26, 49, 75, 88	0
3	C	246/246 (100%)	0.10	5 (2%) 65 57	24, 45, 69, 80	0
4	D	140/177 (79%)	1.64	42 (30%) 1 1	64, 93, 124, 135	0
5	E	172/178 (96%)	0.42	6 (3%) 47 40	41, 62, 84, 92	0
6	F	119/120 (99%)	0.71	7 (5%) 28 23	50, 73, 100, 114	0
7	G	29/348 (8%)	1.11	5 (17%) 4 3	75, 95, 109, 113	0
8	H	160/177 (90%)	0.42	8 (5%) 34 28	39, 58, 93, 99	0
9	I	70/162 (43%)	2.52	42 (60%) 0 0	141, 152, 166, 168	0
10	J	142/145 (97%)	0.17	3 (2%) 63 55	35, 47, 66, 86	0
11	K	132/132 (100%)	-0.11	0 100 100	28, 41, 63, 73	0
12	L	145/165 (87%)	0.66	17 (11%) 9 8	22, 67, 105, 121	0
13	M	194/196 (98%)	0.37	13 (6%) 24 20	25, 46, 68, 82	0
14	N	186/187 (99%)	0.82	19 (10%) 12 11	42, 63, 116, 124	0
15	O	115/116 (99%)	0.37	1 (0%) 81 76	39, 55, 67, 75	0
16	P	143/149 (95%)	0.14	2 (1%) 73 67	35, 51, 62, 68	0
17	Q	95/96 (98%)	0.31	4 (4%) 40 33	35, 49, 66, 75	0
18	R	150/155 (96%)	-0.02	0 100 100	22, 42, 62, 69	0
19	S	81/85 (95%)	0.34	1 (1%) 76 71	44, 56, 81, 94	0
20	T	119/120 (99%)	0.42	5 (4%) 40 33	38, 54, 84, 116	0
21	U	53/67 (79%)	0.11	1 (1%) 66 58	38, 49, 73, 86	0
22	V	65/71 (91%)	0.73	6 (9%) 14 13	55, 78, 115, 122	0
23	W	154/154 (100%)	0.17	0 100 100	37, 48, 72, 86	0
24	X	82/92 (89%)	0.61	9 (10%) 10 9	39, 55, 80, 103	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/240 (59%)	0.10	0 100 100	25, 44, 64, 90	0
26	Z	73/116 (62%)	0.92	9 (12%) 8 8	48, 67, 87, 96	0
27	1	56/57 (98%)	-0.27	0 100 100	22, 32, 39, 51	0
28	2	46/50 (92%)	0.90	7 (15%) 5 5	29, 61, 76, 89	0
29	3	92/92 (100%)	0.41	2 (2%) 62 54	33, 58, 71, 81	0
30	0	2749/2923 (94%)	-0.33	23 (0%) 82 78	16, 45, 92, 179	0
31	9	122/122 (100%)	0.10	3 (2%) 58 50	36, 65, 92, 148	0
32	5	2/3 (66%)	2.84	2 (100%) 0 0	100, 100, 100, 102	0
33	6	2/3 (66%)	3.04	2 (100%) 0 0	96, 96, 96, 104	0
All	All	6650/7522 (88%)	0.11	254 (3%) 44 36	16, 50, 99, 179	0

All (254) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	100	VAL	6.3
9	I	132	VAL	5.8
28	2	49	GLU	5.6
4	D	90	LEU	5.5
9	I	66	GLY	5.3
9	I	70	THR	5.2
24	X	88	GLU	5.2
4	D	57	THR	5.1
22	V	1	THR	5.1
9	I	128	THR	5.0
14	N	154	LEU	5.0
26	Z	34	SER	4.9
4	D	174	VAL	4.9
26	Z	35	SER	4.8
4	D	63	ILE	4.7
14	N	168	LEU	4.6
9	I	71	ALA	4.5
12	L	78	ALA	4.5
4	D	18	ILE	4.5
4	D	10	PHE	4.5
24	X	65	ASN	4.5
1	A	237	GLY	4.4
9	I	74	ILE	4.3
31	9	1	U	4.2
13	M	78	LYS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	113	SER	4.2
9	I	72	GLU	4.2
4	D	134	LEU	4.1
9	I	73	LEU	4.1
9	I	120	ALA	4.1
26	Z	46	SER	4.1
4	D	44	ILE	4.1
9	I	134	ILE	4.1
9	I	133	THR	4.1
30	0	514	G	4.0
8	H	174	LEU	3.9
22	V	2	VAL	3.9
4	D	107	GLY	3.9
4	D	55	LYS	3.9
9	I	124	VAL	3.8
30	0	1199	A	3.8
28	2	35	ARG	3.7
30	0	2637	A	3.7
2	B	2	GLN	3.7
9	I	69	PRO	3.6
32	5	76	A	3.6
13	M	194	GLY	3.6
4	D	17	ARG	3.5
24	X	87	ALA	3.5
29	3	55	VAL	3.5
16	P	18	LYS	3.5
30	0	271	C	3.5
22	V	39	ALA	3.5
9	I	103	ILE	3.5
31	9	2	U	3.5
26	Z	106	SER	3.5
3	C	61	PHE	3.5
12	L	146	GLY	3.5
9	I	97	VAL	3.4
33	6	74	C	3.4
13	M	70	GLY	3.4
20	T	117	ASP	3.4
29	3	41	GLU	3.4
1	A	36	ASP	3.4
26	Z	58	ASN	3.3
1	A	37	VAL	3.3
30	0	2748	G	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	106	PHE	3.2
9	I	85	GLY	3.2
4	D	59	GLY	3.2
4	D	62	ASP	3.2
4	D	84	LEU	3.2
4	D	88	LEU	3.2
4	D	61	PHE	3.2
9	I	123	VAL	3.2
12	L	150	GLN	3.2
2	B	208	GLY	3.2
14	N	2	THR	3.2
21	U	47	ARG	3.1
12	L	148	GLU	3.1
13	M	74	LYS	3.1
6	F	78	GLU	3.1
22	V	40	PRO	3.1
9	I	111	LEU	3.0
9	I	104	ALA	3.0
9	I	116	LEU	3.0
17	Q	18	PRO	3.0
19	S	81	ILE	3.0
14	N	162	ASP	3.0
24	X	83	ALA	3.0
24	X	85	VAL	2.9
17	Q	12	GLY	2.9
4	D	54	ALA	2.9
14	N	1	ALA	2.9
14	N	165	ALA	2.9
14	N	166	ALA	2.9
10	J	70	PHE	2.9
12	L	45	PRO	2.8
3	C	76	ARG	2.8
12	L	82	ALA	2.8
12	L	149	ARG	2.8
28	2	39	ARG	2.8
2	B	1	PRO	2.8
4	D	91	ALA	2.8
7	G	12	ILE	2.8
9	I	78	ALA	2.8
9	I	83	GLY	2.8
13	M	72	ALA	2.7
4	D	75	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	95	LEU	2.7
30	0	1951	G	2.7
9	I	67	VAL	2.7
12	L	145	LEU	2.7
9	I	101	LYS	2.7
4	D	74	THR	2.7
26	Z	49	ARG	2.7
26	Z	77	GLY	2.7
30	0	1196	C	2.7
12	L	44	GLU	2.7
24	X	78	GLU	2.7
20	T	114	SER	2.7
12	L	100	ALA	2.6
4	D	56	ARG	2.6
33	6	75	C	2.6
8	H	115	GLY	2.6
4	D	53	LYS	2.6
4	D	77	ASP	2.6
14	N	180	LEU	2.6
15	O	60	VAL	2.6
7	G	23	ILE	2.6
8	H	171	GLY	2.6
9	I	117	THR	2.6
4	D	172	VAL	2.6
30	0	2237	G	2.6
13	M	75	ARG	2.6
30	0	1200	A	2.6
14	N	169	PRO	2.6
4	D	93	LEU	2.6
2	B	117	GLU	2.6
28	2	48	ASP	2.6
30	0	497	A	2.5
12	L	75	LEU	2.5
12	L	58	GLN	2.5
4	D	36	ASN	2.5
3	C	63	SER	2.5
30	0	10	U	2.5
4	D	89	PRO	2.5
9	I	77	GLU	2.5
4	D	35	ALA	2.5
5	E	45	ASP	2.5
14	N	158	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
24	X	84	ILE	2.5
30	O	960	G	2.5
14	N	7	LYS	2.5
8	H	114	ASP	2.5
12	L	61	ALA	2.5
26	Z	48	ARG	2.5
4	D	166	ILE	2.4
7	G	26	MET	2.4
30	O	1172	G	2.4
13	M	76	ARG	2.4
8	H	169	GLU	2.4
13	M	77	HIS	2.4
4	D	104	PHE	2.4
8	H	132	ALA	2.4
9	I	91	PHE	2.4
13	M	79	ALA	2.4
9	I	114	TYR	2.4
4	D	128	LEU	2.4
5	E	10	ASP	2.3
12	L	60	GLU	2.3
12	L	99	GLU	2.3
6	F	99	THR	2.3
6	F	16	ALA	2.3
14	N	21	HIS	2.3
13	M	89	THR	2.3
4	D	58	VAL	2.3
6	F	8	VAL	2.3
30	O	1929	G	2.3
9	I	108	HIS	2.3
14	N	160	SER	2.3
13	M	88	VAL	2.3
30	O	999	C	2.3
13	M	80	GLY	2.3
4	D	19	GLU	2.3
8	H	43	ALA	2.3
4	D	171	ASP	2.3
7	G	73	ASP	2.3
14	N	167	ASP	2.3
1	A	211	LYS	2.3
17	Q	17	LYS	2.3
4	D	11	HIS	2.3
30	O	1165	G	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	I	84	SER	2.3
14	N	25	ARG	2.3
4	D	135	VAL	2.3
7	G	71	LEU	2.2
9	I	112	LEU	2.2
17	Q	20	ASP	2.2
20	T	118	SER	2.2
30	O	1195	G	2.2
8	H	78	LYS	2.2
24	X	61	ARG	2.2
4	D	173	GLU	2.2
6	F	17	LEU	2.2
9	I	107	LYS	2.2
22	V	36	ALA	2.2
30	O	1173	A	2.2
26	Z	60	ASP	2.2
6	F	1	PRO	2.2
9	I	129	SER	2.2
14	N	159	TYR	2.2
22	V	38	GLY	2.2
20	T	119	ALA	2.2
5	E	154	ILE	2.2
24	X	71	ARG	2.2
9	I	106	GLN	2.2
28	2	17	GLN	2.2
1	A	192	VAL	2.2
4	D	68	PRO	2.2
12	L	57	VAL	2.2
4	D	26	GLY	2.2
9	I	88	GLN	2.1
4	D	169	THR	2.1
13	M	87	GLY	2.1
30	O	2747	C	2.1
9	I	127	CYS	2.1
6	F	106	ALA	2.1
10	J	4	ALA	2.1
14	N	5	ARG	2.1
3	C	16	VAL	2.1
12	L	143	THR	2.1
9	I	119	ALA	2.1
14	N	68	GLU	2.1
16	P	64	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	3	VAL	2.1
9	I	75	LYS	2.1
5	E	5	LEU	2.1
1	A	33	GLU	2.1
30	0	1177	A	2.1
3	C	162	VAL	2.1
10	J	92	GLN	2.0
32	5	75	C	2.0
5	E	170	ARG	2.0
9	I	80	PHE	2.0
30	0	1160	G	2.0
31	9	24	U	2.0
4	D	92	GLU	2.0
28	2	44	ARG	2.0
20	T	36	GLY	2.0
30	0	735	C	2.0
14	N	164	ASP	2.0
28	2	38	LYS	2.0
30	0	1175	G	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
33	8AN	6	76	22/23	0.87	0.17	87,92,94,95	0
30	UR3	0	2619	21/22	0.95	0.09	40,41,44,47	0
30	OMG	0	2588	24/25	0.96	0.10	30,34,35,37	0
30	OMU	0	2587	21/22	0.97	0.08	30,33,38,38	0
30	PSU	0	2621	20/21	0.97	0.07	36,38,42,42	0
30	1MA	0	628	23/24	0.97	0.08	36,40,42,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	MG	B	8042	1/1	0.52	0.38	103,103,103,103	0
37	NA	0	8573	1/1	0.54	0.34	79,79,79,79	0
36	SR	0	8979	1/1	0.56	0.36	184,184,184,184	0
37	NA	9	8543	1/1	0.56	0.29	65,65,65,65	0
36	SR	0	9001	1/1	0.59	0.23	190,190,190,190	0
34	MG	0	8065	1/1	0.60	0.40	102,102,102,102	0
37	NA	0	8571	1/1	0.60	0.38	85,85,85,85	0
34	MG	0	8038	1/1	0.65	0.15	97,97,97,97	0
36	SR	0	8983	1/1	0.66	0.26	169,169,169,169	0
34	MG	0	8063	1/1	0.66	0.28	69,69,69,69	0
37	NA	0	8557	1/1	0.66	0.39	82,82,82,82	0
37	NA	S	8510	1/1	0.67	0.18	80,80,80,80	0
39	K	0	8401	1/1	0.67	0.29	82,82,82,82	0
34	MG	0	8091	1/1	0.69	0.20	76,76,76,76	0
37	NA	9	8572	1/1	0.72	0.37	96,96,96,96	0
37	NA	0	8535	1/1	0.72	0.36	75,75,75,75	0
36	SR	0	8994	1/1	0.73	0.43	200,200,200,200	0
37	NA	H	8518	1/1	0.74	0.26	69,69,69,69	0
34	MG	0	8049	1/1	0.75	0.32	103,103,103,103	0
37	NA	0	8558	1/1	0.76	0.40	67,67,67,67	0
36	SR	0	8971	1/1	0.76	0.14	191,191,191,191	0
41	ACA	6	78	8/9	0.76	0.41	88,90,91,91	0
34	MG	0	8047	1/1	0.77	0.46	92,92,92,92	0
37	NA	0	8522	1/1	0.78	0.42	72,72,72,72	0
34	MG	0	8045	1/1	0.78	0.65	119,119,119,119	0
34	MG	0	8090	1/1	0.78	0.72	130,130,130,130	0
34	MG	0	8016	1/1	0.78	0.40	131,131,131,131	0
36	SR	0	8990	1/1	0.78	0.31	177,177,177,177	0
34	MG	0	8029	1/1	0.79	0.43	83,83,83,83	0
36	SR	0	8942	1/1	0.79	0.27	155,155,155,155	0
36	SR	0	8920	1/1	0.80	0.41	200,200,200,200	0
37	NA	0	8559	1/1	0.80	0.29	64,64,64,64	0
36	SR	0	8944	1/1	0.81	0.15	155,155,155,155	0
37	NA	0	8564	1/1	0.81	0.22	35,35,35,35	0
37	NA	0	8529	1/1	0.81	0.07	24,24,24,24	0
36	SR	0	9006	1/1	0.81	0.52	198,198,198,198	0
37	NA	0	8546	1/1	0.81	0.37	97,97,97,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	NA	9	8544	1/1	0.81	0.44	73,73,73,73	0
37	NA	0	8547	1/1	0.81	0.30	78,78,78,78	0
34	MG	0	8085	1/1	0.81	0.27	92,92,92,92	0
36	SR	L	8969	1/1	0.81	0.32	175,175,175,175	0
37	NA	0	8508	1/1	0.82	0.10	27,27,27,27	0
37	NA	0	8569	1/1	0.82	0.12	32,32,32,32	0
37	NA	0	8516	1/1	0.82	0.39	65,65,65,65	0
37	NA	0	8502	1/1	0.83	0.39	60,60,60,60	0
37	NA	0	8536	1/1	0.83	0.26	63,63,63,63	0
34	MG	0	8066	1/1	0.83	0.49	98,98,98,98	0
37	NA	0	8509	1/1	0.83	0.36	80,80,80,80	0
37	NA	0	8523	1/1	0.84	0.31	61,61,61,61	0
34	MG	0	8037	1/1	0.84	0.22	64,64,64,64	0
37	NA	0	8531	1/1	0.84	0.19	41,41,41,41	0
37	NA	0	8514	1/1	0.84	0.35	83,83,83,83	0
34	MG	0	8071	1/1	0.84	0.45	88,88,88,88	0
37	NA	0	8567	1/1	0.84	0.30	61,61,61,61	0
34	MG	0	8081	1/1	0.84	0.40	91,91,91,91	0
34	MG	A	8044	1/1	0.85	0.09	51,51,51,51	0
37	NA	0	8550	1/1	0.85	0.19	51,51,51,51	0
36	SR	0	8996	1/1	0.85	0.16	158,158,158,158	0
37	NA	Q	8540	1/1	0.85	0.16	66,66,66,66	0
39	K	0	8402	1/1	0.85	0.33	117,117,117,117	0
36	SR	0	8961	1/1	0.85	0.19	185,185,185,185	0
37	NA	0	8519	1/1	0.86	0.24	71,71,71,71	0
37	NA	0	8545	1/1	0.86	0.18	64,64,64,64	0
36	SR	0	8933	1/1	0.86	0.20	126,126,126,126	0
34	MG	0	8017	1/1	0.86	0.39	123,123,123,123	0
37	NA	0	8525	1/1	0.86	0.20	53,53,53,53	0
37	NA	0	8528	1/1	0.86	0.14	55,55,55,55	0
34	MG	0	8046	1/1	0.86	0.25	72,72,72,72	0
34	MG	0	8064	1/1	0.86	0.20	53,53,53,53	0
37	NA	0	8562	1/1	0.86	0.34	55,55,55,55	0
34	MG	0	8036	1/1	0.86	0.22	50,50,50,50	0
37	NA	0	8506	1/1	0.87	0.12	50,50,50,50	0
34	MG	0	8040	1/1	0.87	0.26	70,70,70,70	0
37	NA	0	8520	1/1	0.87	0.25	58,58,58,58	0
34	MG	0	8039	1/1	0.87	0.14	40,40,40,40	0
37	NA	0	8533	1/1	0.87	0.34	64,64,64,64	0
37	NA	0	8556	1/1	0.87	0.21	75,75,75,75	0
36	SR	B	8987	1/1	0.87	0.39	199,199,199,199	0
37	NA	0	8513	1/1	0.88	0.18	53,53,53,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8070	1/1	0.88	0.15	63,63,63,63	0
36	SR	0	9007	1/1	0.88	0.38	195,195,195,195	0
37	NA	0	8504	1/1	0.88	0.11	31,31,31,31	0
37	NA	0	8565	1/1	0.88	0.11	48,48,48,48	0
34	MG	0	8035	1/1	0.89	0.19	84,84,84,84	0
35	CL	L	8810	1/1	0.89	0.13	56,56,56,56	0
37	NA	0	8507	1/1	0.89	0.12	29,29,29,29	0
36	SR	0	8985	1/1	0.89	0.12	142,142,142,142	0
37	NA	0	8552	1/1	0.89	0.26	86,86,86,86	0
36	SR	9	9003	1/1	0.89	0.11	144,144,144,144	0
37	NA	0	8511	1/1	0.89	0.10	35,35,35,35	0
34	MG	0	8010	1/1	0.89	0.13	78,78,78,78	0
34	MG	0	8088	1/1	0.89	0.13	40,40,40,40	0
34	MG	0	8072	1/1	0.89	0.08	55,55,55,55	0
40	PHE	6	77	11/12	0.89	0.27	88,88,90,90	0
36	SR	0	9000	1/1	0.89	0.14	147,147,147,147	0
34	MG	0	8062	1/1	0.90	0.22	41,41,41,41	0
37	NA	0	8534	1/1	0.90	0.19	68,68,68,68	0
37	NA	M	8539	1/1	0.90	0.14	33,33,33,33	0
36	SR	0	8989	1/1	0.90	0.28	200,200,200,200	0
35	CL	N	8807	1/1	0.90	0.12	70,70,70,70	0
36	SR	0	8955	1/1	0.90	0.10	127,127,127,127	0
34	MG	A	8051	1/1	0.90	0.12	82,82,82,82	0
36	SR	0	8962	1/1	0.90	0.11	104,104,104,104	0
37	NA	0	8524	1/1	0.90	0.14	52,52,52,52	0
34	MG	0	8033	1/1	0.90	0.06	44,44,44,44	0
36	SR	0	8976	1/1	0.90	0.11	117,117,117,117	0
34	MG	0	8056	1/1	0.90	0.33	94,94,94,94	0
34	MG	0	8078	1/1	0.90	0.43	115,115,115,115	0
37	NA	0	8561	1/1	0.90	0.36	66,66,66,66	0
36	SR	0	9004	1/1	0.91	0.11	121,121,121,121	0
37	NA	0	8526	1/1	0.91	0.11	55,55,55,55	0
37	NA	0	8570	1/1	0.91	0.28	48,48,48,48	0
34	MG	0	8076	1/1	0.91	0.19	72,72,72,72	0
35	CL	Y	8817	1/1	0.91	0.10	55,55,55,55	0
37	NA	0	8517	1/1	0.91	0.14	36,36,36,36	0
36	SR	9	8980	1/1	0.91	0.10	132,132,132,132	0
34	MG	0	8048	1/1	0.91	0.14	49,49,49,49	0
37	NA	0	8521	1/1	0.91	0.22	51,51,51,51	0
35	CL	B	8819	1/1	0.91	0.24	62,62,62,62	0
36	SR	0	8959	1/1	0.91	0.06	120,120,120,120	0
34	MG	0	8079	1/1	0.91	0.18	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	NA	0	8527	1/1	0.92	0.27	73,73,73,73	0
37	NA	0	8548	1/1	0.92	0.17	26,26,26,26	0
37	NA	0	8549	1/1	0.92	0.10	36,36,36,36	0
36	SR	0	8982	1/1	0.92	0.09	116,116,116,116	0
34	MG	0	8092	1/1	0.92	0.16	76,76,76,76	0
37	NA	C	8503	1/1	0.92	0.14	31,31,31,31	0
34	MG	0	8052	1/1	0.92	0.10	42,42,42,42	0
34	MG	0	8030	1/1	0.92	0.34	167,167,167,167	0
36	SR	0	8981	1/1	0.92	0.12	117,117,117,117	0
37	NA	R	8532	1/1	0.92	0.11	25,25,25,25	0
36	SR	0	8991	1/1	0.92	0.09	148,148,148,148	0
37	NA	0	8563	1/1	0.92	0.16	51,51,51,51	0
36	SR	0	8992	1/1	0.92	0.17	122,122,122,122	0
34	MG	0	8093	1/1	0.93	0.07	27,27,27,27	0
36	SR	Y	9002	1/1	0.93	0.10	124,124,124,124	0
36	SR	0	8915	1/1	0.93	0.09	84,84,84,84	0
37	NA	0	8560	1/1	0.93	0.26	134,134,134,134	0
37	NA	0	8501	1/1	0.93	0.29	107,107,107,107	0
34	MG	0	8075	1/1	0.93	0.05	38,38,38,38	0
35	CL	J	8816	1/1	0.93	0.19	80,80,80,80	0
35	CL	J	8802	1/1	0.93	0.10	69,69,69,69	0
34	MG	0	8069	1/1	0.93	0.28	120,120,120,120	0
35	CL	M	8818	1/1	0.93	0.10	46,46,46,46	0
36	SR	0	8956	1/1	0.93	0.11	111,111,111,111	0
34	MG	2	8060	1/1	0.93	0.18	45,45,45,45	0
37	NA	0	8512	1/1	0.93	0.28	46,46,46,46	0
35	CL	Q	8811	1/1	0.93	0.14	86,86,86,86	0
37	NA	0	8575	1/1	0.93	0.13	44,44,44,44	0
34	MG	0	8015	1/1	0.93	0.11	41,41,41,41	0
36	SR	0	8970	1/1	0.93	0.08	99,99,99,99	0
35	CL	3	8804	1/1	0.93	0.10	60,60,60,60	0
35	CL	0	8803	1/1	0.93	0.11	51,51,51,51	0
35	CL	0	8822	1/1	0.93	0.29	66,66,66,66	0
36	SR	A	8929	1/1	0.93	0.13	114,114,114,114	0
34	MG	0	8024	1/1	0.93	0.19	69,69,69,69	0
36	SR	0	8997	1/1	0.94	0.09	116,116,116,116	0
36	SR	0	8998	1/1	0.94	0.11	113,113,113,113	0
36	SR	0	8975	1/1	0.94	0.07	125,125,125,125	0
34	MG	B	8043	1/1	0.94	0.14	29,29,29,29	0
34	MG	0	8020	1/1	0.94	0.20	24,24,24,24	0
36	SR	0	8945	1/1	0.94	0.09	104,104,104,104	0
36	SR	0	8946	1/1	0.94	0.08	98,98,98,98	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	9	8968	1/1	0.94	0.08	117,117,117,117	0
34	MG	Y	8086	1/1	0.94	0.08	48,48,48,48	0
37	NA	0	8566	1/1	0.94	0.21	54,54,54,54	0
36	SR	F	9005	1/1	0.94	0.10	98,98,98,98	0
37	NA	0	8568	1/1	0.94	0.20	18,18,18,18	0
37	NA	0	8541	1/1	0.94	0.23	103,103,103,103	0
35	CL	O	8808	1/1	0.94	0.08	75,75,75,75	0
34	MG	0	8080	1/1	0.94	0.09	45,45,45,45	0
37	NA	J	8538	1/1	0.94	0.14	31,31,31,31	0
34	MG	0	8034	1/1	0.94	0.10	30,30,30,30	0
34	MG	0	8027	1/1	0.94	0.09	28,28,28,28	0
36	SR	0	8993	1/1	0.94	0.10	146,146,146,146	0
37	NA	0	8551	1/1	0.94	0.06	32,32,32,32	0
34	MG	0	8050	1/1	0.94	0.34	152,152,152,152	0
37	NA	0	8553	1/1	0.94	0.21	100,100,100,100	0
37	NA	0	8555	1/1	0.94	0.18	52,52,52,52	0
36	SR	0	8973	1/1	0.94	0.08	98,98,98,98	0
37	NA	0	8515	1/1	0.95	0.07	26,26,26,26	0
34	MG	0	8032	1/1	0.95	0.05	21,21,21,21	0
37	NA	0	8537	1/1	0.95	0.05	21,21,21,21	0
35	CL	J	8801	1/1	0.95	0.11	62,62,62,62	0
34	MG	0	8059	1/1	0.95	0.14	88,88,88,88	0
36	SR	H	8972	1/1	0.95	0.11	132,132,132,132	0
36	SR	0	8951	1/1	0.95	0.06	105,105,105,105	0
34	MG	0	8061	1/1	0.95	0.11	17,17,17,17	0
34	MG	0	8003	1/1	0.95	0.08	14,14,14,14	0
37	NA	0	8505	1/1	0.95	0.28	29,29,29,29	0
36	SR	0	8957	1/1	0.95	0.09	124,124,124,124	0
36	SR	0	8984	1/1	0.95	0.09	92,92,92,92	0
37	NA	0	8574	1/1	0.95	0.31	43,43,43,43	0
36	SR	0	8901	1/1	0.95	0.07	48,48,48,48	0
37	NA	0	8554	1/1	0.95	0.12	42,42,42,42	0
35	CL	0	8812	1/1	0.95	0.08	50,50,50,50	0
35	CL	0	8815	1/1	0.95	0.10	69,69,69,69	0
37	NA	0	8530	1/1	0.95	0.12	49,49,49,49	0
36	SR	0	8965	1/1	0.95	0.09	95,95,95,95	0
36	SR	0	8967	1/1	0.95	0.07	103,103,103,103	0
34	MG	0	8089	1/1	0.95	0.07	31,31,31,31	0
36	SR	0	8958	1/1	0.96	0.07	77,77,77,77	0
34	MG	0	8053	1/1	0.96	0.15	33,33,33,33	0
34	MG	0	8041	1/1	0.96	0.07	33,33,33,33	0
34	MG	0	8026	1/1	0.96	0.13	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8964	1/1	0.96	0.07	102,102,102,102	0
34	MG	0	8073	1/1	0.96	0.17	58,58,58,58	0
36	SR	0	9008	1/1	0.96	0.09	90,90,90,90	0
36	SR	3	8953	1/1	0.96	0.10	110,110,110,110	0
35	CL	R	8806	1/1	0.96	0.06	44,44,44,44	0
36	SR	0	8914	1/1	0.96	0.13	88,88,88,88	0
34	MG	9	8074	1/1	0.96	0.23	52,52,52,52	0
36	SR	0	8916	1/1	0.96	0.06	64,64,64,64	0
35	CL	Y	8820	1/1	0.96	0.08	48,48,48,48	0
36	SR	0	8924	1/1	0.96	0.15	80,80,80,80	0
36	SR	0	8926	1/1	0.96	0.12	87,87,87,87	0
36	SR	0	8928	1/1	0.96	0.07	92,92,92,92	0
36	SR	0	8931	1/1	0.96	0.11	80,80,80,80	0
34	MG	0	8082	1/1	0.96	0.14	70,70,70,70	0
36	SR	0	8941	1/1	0.96	0.10	77,77,77,77	0
36	SR	0	8986	1/1	0.96	0.08	108,108,108,108	0
34	MG	0	8084	1/1	0.96	0.10	27,27,27,27	0
34	MG	A	8025	1/1	0.96	0.09	39,39,39,39	0
37	NA	0	8542	1/1	0.96	0.08	31,31,31,31	0
35	CL	0	8813	1/1	0.96	0.07	63,63,63,63	0
34	MG	0	8031	1/1	0.96	0.05	41,41,41,41	0
35	CL	J	8821	1/1	0.96	0.09	64,64,64,64	0
38	CD	O	8705	1/1	0.96	0.08	111,111,111,111	0
34	MG	0	8077	1/1	0.96	0.15	41,41,41,41	0
36	SR	0	8995	1/1	0.96	0.09	98,98,98,98	0
36	SR	A	8930	1/1	0.96	0.12	78,78,78,78	0
35	CL	L	8814	1/1	0.96	0.12	62,62,62,62	0
36	SR	0	8954	1/1	0.97	0.08	82,82,82,82	0
34	MG	0	8023	1/1	0.97	0.10	25,25,25,25	0
36	SR	0	8919	1/1	0.97	0.07	92,92,92,92	0
35	CL	A	8809	1/1	0.97	0.19	51,51,51,51	0
36	SR	0	8923	1/1	0.97	0.12	72,72,72,72	0
34	MG	0	8005	1/1	0.97	0.10	25,25,25,25	0
36	SR	0	8960	1/1	0.97	0.07	98,98,98,98	0
36	SR	0	8925	1/1	0.97	0.10	70,70,70,70	0
36	SR	T	8911	1/1	0.97	0.06	58,58,58,58	0
36	SR	0	8927	1/1	0.97	0.11	70,70,70,70	0
34	MG	T	8057	1/1	0.97	0.15	31,31,31,31	0
36	SR	0	8966	1/1	0.97	0.11	85,85,85,85	0
36	SR	1	8952	1/1	0.97	0.07	67,67,67,67	0
34	MG	0	8087	1/1	0.97	0.22	107,107,107,107	0
36	SR	0	8935	1/1	0.97	0.06	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	0	8936	1/1	0.97	0.09	67,67,67,67	0
36	SR	0	8974	1/1	0.97	0.08	125,125,125,125	0
36	SR	3	8932	1/1	0.97	0.08	74,74,74,74	0
36	SR	3	8999	1/1	0.97	0.06	69,69,69,69	0
36	SR	0	8943	1/1	0.97	0.09	88,88,88,88	0
34	MG	0	8068	1/1	0.97	0.10	50,50,50,50	0
36	SR	0	8903	1/1	0.97	0.11	55,55,55,55	0
36	SR	B	8950	1/1	0.97	0.06	98,98,98,98	0
36	SR	0	8947	1/1	0.97	0.10	91,91,91,91	0
35	CL	0	8805	1/1	0.97	0.06	60,60,60,60	0
34	MG	0	8067	1/1	0.98	0.12	33,33,33,33	0
36	SR	H	8907	1/1	0.98	0.06	48,48,48,48	0
36	SR	0	8988	1/1	0.98	0.06	114,114,114,114	0
36	SR	0	8918	1/1	0.98	0.10	53,53,53,53	0
36	SR	0	8948	1/1	0.98	0.08	65,65,65,65	0
36	SR	0	8949	1/1	0.98	0.08	62,62,62,62	0
34	MG	0	8021	1/1	0.98	0.11	24,24,24,24	0
36	SR	0	8934	1/1	0.98	0.09	71,71,71,71	0
36	SR	A	8977	1/1	0.98	0.10	95,95,95,95	0
36	SR	0	8921	1/1	0.98	0.05	58,58,58,58	0
36	SR	0	8937	1/1	0.98	0.05	69,69,69,69	0
36	SR	0	8978	1/1	0.98	0.08	71,71,71,71	0
36	SR	0	8938	1/1	0.98	0.09	95,95,95,95	0
34	MG	K	8054	1/1	0.98	0.07	15,15,15,15	0
36	SR	T	8939	1/1	0.98	0.06	70,70,70,70	0
36	SR	0	8905	1/1	0.98	0.14	61,61,61,61	0
34	MG	0	8083	1/1	0.98	0.08	29,29,29,29	0
34	MG	0	8018	1/1	0.99	0.13	3,3,3,3	0
34	MG	0	8019	1/1	0.99	0.07	1,1,1,1	0
34	MG	0	8009	1/1	0.99	0.16	1,1,1,1	0
36	SR	0	8902	1/1	0.99	0.07	39,39,39,39	0
34	MG	C	8012	1/1	0.99	0.15	17,17,17,17	0
36	SR	0	8904	1/1	0.99	0.12	55,55,55,55	0
36	SR	0	8963	1/1	0.99	0.07	74,74,74,74	0
34	MG	0	8022	1/1	0.99	0.12	11,11,11,11	0
36	SR	0	8906	1/1	0.99	0.11	56,56,56,56	0
36	SR	0	8908	1/1	0.99	0.08	64,64,64,64	0
36	SR	0	8909	1/1	0.99	0.07	56,56,56,56	0
36	SR	0	8940	1/1	0.99	0.08	51,51,51,51	0
36	SR	0	8910	1/1	0.99	0.06	47,47,47,47	0
34	MG	0	8011	1/1	0.99	0.04	4,4,4,4	0
34	MG	0	8013	1/1	0.99	0.05	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	MG	0	8055	1/1	0.99	0.14	26,26,26,26	0
36	SR	0	8917	1/1	0.99	0.09	67,67,67,67	0
36	SR	R	8912	1/1	0.99	0.07	64,64,64,64	0
34	MG	0	8014	1/1	0.99	0.10	16,16,16,16	0
34	MG	0	8002	1/1	0.99	0.15	19,19,19,19	0
34	MG	0	8028	1/1	0.99	0.12	1,1,1,1	0
38	CD	U	8701	1/1	0.99	0.01	57,57,57,57	0
38	CD	3	8704	1/1	0.99	0.02	52,52,52,52	0
36	SR	0	8922	1/1	0.99	0.04	61,61,61,61	0
36	SR	1	8913	1/1	0.99	0.09	54,54,54,54	0
34	MG	0	8007	1/1	0.99	0.08	30,30,30,30	0
34	MG	0	8008	1/1	0.99	0.05	9,9,9,9	0
38	CD	1	8702	1/1	1.00	0.03	57,57,57,57	0
34	MG	0	8001	1/1	1.00	0.13	7,7,7,7	0
34	MG	0	8006	1/1	1.00	0.06	8,8,8,8	0
34	MG	0	8004	1/1	1.00	0.08	21,21,21,21	0
34	MG	0	8058	1/1	1.00	0.14	1,1,1,1	0
38	CD	Z	8703	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.