



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:39 am GMT

PDB ID : 1VQN
Title : The structure of CC-HPMN AND CCA-PHE-CAP-BIO bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.40 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

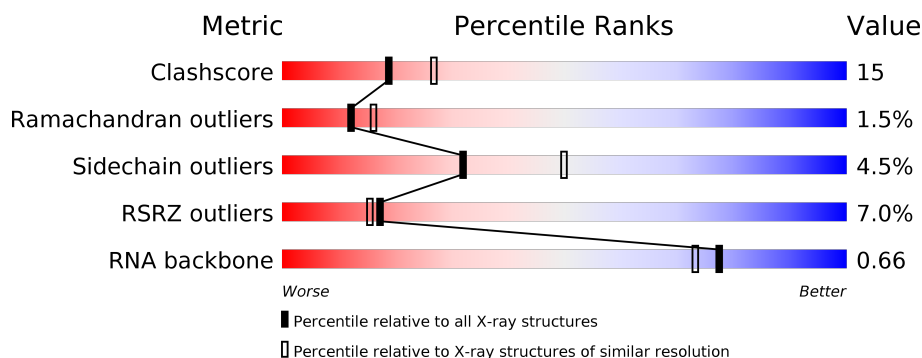
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>2%</div> <div>63%</div> <div>27%</div> <div>6%</div> </div>
2	9	122	<div> <div>5%</div> <div>57%</div> <div>33%</div> <div>10%</div> </div>
3	4	4	<div> <div>50%</div> <div>50%</div> </div>
4	5	6	<div> <div>17%</div> <div>17%</div> <div>67%</div> <div>17%</div> </div>
5	A	240	<div> <div>5%</div> <div>61%</div> <div>33%</div> <div>5%</div> </div>
6	B	338	<div> <div>3%</div> <div>57%</div> <div>39%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	C	246	
8	D	177	
9	E	178	
10	F	120	
11	G	348	
12	H	171	
13	J	145	
14	K	132	
15	L	165	
16	M	194	
17	N	187	
18	O	116	
19	P	149	
20	Q	96	
21	R	155	
22	S	85	
23	T	120	
24	U	66	
25	V	71	
26	W	154	
27	X	92	
28	Y	241	
29	Z	83	
30	1	57	
31	2	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
32	3	92	
33	I	162	

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	8001	-	-	-	X
34	MG	0	8008	-	-	-	X
34	MG	0	8012	-	-	-	X
34	MG	0	8013	-	-	-	X
34	MG	0	8021	-	-	-	X
34	MG	0	8038	-	-	-	X
34	MG	0	8052	-	-	-	X
34	MG	0	8054	-	-	-	X
34	MG	0	8056	-	-	-	X
34	MG	0	8065	-	-	-	X
34	MG	0	8080	-	-	-	X
34	MG	0	8091	-	-	-	X
34	MG	0	8101	-	-	-	X
34	MG	5	8118	-	-	-	X
35	K	0	9001	-	-	-	X
36	NA	0	9114	-	-	-	X
36	NA	0	9115	-	-	-	X
36	NA	0	9120	-	-	-	X
36	NA	0	9125	-	-	-	X
36	NA	0	9131	-	-	-	X
36	NA	0	9132	-	-	-	X
36	NA	0	9135	-	-	-	X
36	NA	0	9150	-	-	-	X
36	NA	0	9156	-	-	-	X
36	NA	0	9159	-	-	-	X
36	NA	0	9161	-	-	-	X
36	NA	0	9164	-	-	-	X
36	NA	0	9165	-	-	-	X
36	NA	0	9168	-	-	-	X
36	NA	0	9171	-	-	-	X
36	NA	0	9172	-	-	-	X
36	NA	0	9173	-	-	-	X
36	NA	0	9174	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	NA	0	9177	-	-	-	X
36	NA	0	9178	-	-	-	X
36	NA	0	9182	-	-	-	X
36	NA	9	9183	-	-	-	X
36	NA	R	9186	-	-	-	X
37	CL	0	9316	-	-	-	X
38	SR	0	9482	-	-	-	X
38	SR	B	9521	-	-	-	X

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 99077 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26350	10878	19048	2745			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*(PPU)*(LOF))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	4	Total	C	N	O	P	0	0	0
			72	39	12	19	2			

- Molecule 4 is a RNA chain called 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	5	6	Total	C	N	O	P	S	0	0	0
			93	53	15	22	2	1			

- Molecule 5 is a protein called 50S ribosomal protein L2P.

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

- Molecule 6 is a protein called 50S ribosomal protein L3P.

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

- Molecule 7 is a protein called 50S ribosomal protein L4E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 8 is a protein called 50S ribosomal protein L5P.

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

- Molecule 9 is a protein called 50S ribosomal protein L6P.

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

- Molecule 10 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 11 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 13 is a protein called 50S ribosomal protein L13P.

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

- Molecule 14 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 15 is a protein called 50S ribosomal protein L15P.

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

- Molecule 16 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 17 is a protein called 50S ribosomal protein L18P.

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

- Molecule 18 is a protein called 50S ribosomal protein L18e.

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

- Molecule 19 is a protein called 50S ribosomal protein L19E.

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

- Molecule 20 is a protein called 50S ribosomal protein L21e.

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

- Molecule 21 is a protein called 50S ribosomal protein L22P.

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

- Molecule 22 is a protein called 50S ribosomal protein L23P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24P.

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

- Molecule 24 is a protein called 50S ribosomal protein L24E.

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

- Molecule 25 is a protein called 50S ribosomal protein L29P.

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

- Molecule 26 is a protein called 50S ribosomal protein L30P.

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

- Molecule 27 is a protein called 50S ribosomal protein L31e.

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

- Molecule 28 is a protein called 50S ribosomal protein L32E.

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

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 32 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 34 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	87	Total	Mg	0	0
			87	87		
34	Y	1	Total	Mg	0	0
			1	1		
34	K	1	Total	Mg	0	0
			1	1		
34	A	1	Total	Mg	0	0
			1	1		
34	T	1	Total	Mg	0	0
			1	1		
34	5	1	Total	Mg	0	0
			1	1		
34	2	1	Total	Mg	0	0
			1	1		
34	9	1	Total	Mg	0	0
			1	1		

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	2	Total	K	0	0
			2	2		

- Molecule 36 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	66	Total	Na	0	0
			66	66		
36	J	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Q	1	Total 1	Na 1	0	0
36	D	1	Total 1	Na 1	0	0
36	C	1	Total 1	Na 1	0	0
36	R	2	Total 2	Na 2	0	0
36	9	1	Total 1	Na 1	0	0
36	S	1	Total 1	Na 1	0	0
36	M	1	Total 1	Na 1	0	0

- Molecule 37 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	10	Total 10	Cl 10	0	0
37	J	3	Total 3	Cl 3	0	0
37	B	1	Total 1	Cl 1	0	0
37	A	1	Total 1	Cl 1	0	0
37	N	1	Total 1	Cl 1	0	0
37	O	1	Total 1	Cl 1	0	0
37	R	1	Total 1	Cl 1	0	0
37	Y	1	Total 1	Cl 1	0	0
37	L	1	Total 1	Cl 1	0	0
37	3	1	Total 1	Cl 1	0	0
37	M	1	Total 1	Cl 1	0	0

- Molecule 38 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	98	Total 98	Sr 98	0	0
38	1	2	Total 2	Sr 2	0	0
38	H	1	Total 1	Sr 1	0	0
38	B	2	Total 2	Sr 2	0	0
38	3	1	Total 1	Sr 1	0	0
38	A	3	Total 3	Sr 3	0	0
38	R	1	Total 1	Sr 1	0	0
38	9	3	Total 3	Sr 3	0	0
38	L	1	Total 1	Sr 1	0	0
38	S	1	Total 1	Sr 1	0	0
38	F	1	Total 1	Sr 1	0	0

- Molecule 39 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	O	1	Total 1	Cd 1	0	0
39	Z	1	Total 1	Cd 1	0	0
39	1	1	Total 1	Cd 1	0	0
39	3	1	Total 1	Cd 1	0	0
39	U	1	Total 1	Cd 1	0	0

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	0	5727	Total 5727	O 5727	0	0
40	9	137	Total 137	O 137	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	4	1	Total 1	O 1	0	0
40	5	2	Total 2	O 2	0	0
40	A	120	Total 120	O 120	0	0
40	B	138	Total 138	O 138	0	0
40	C	180	Total 180	O 180	0	0
40	D	48	Total 48	O 48	0	0
40	E	44	Total 44	O 44	0	0
40	F	24	Total 24	O 24	0	0
40	G	14	Total 14	O 14	0	0
40	H	72	Total 72	O 72	0	0
40	J	54	Total 54	O 54	0	0
40	K	61	Total 61	O 61	0	0
40	L	83	Total 83	O 83	0	0
40	M	128	Total 128	O 128	0	0
40	N	58	Total 58	O 58	0	0
40	O	39	Total 39	O 39	0	0
40	P	61	Total 61	O 61	0	0
40	Q	51	Total 51	O 51	0	0
40	R	78	Total 78	O 78	0	0
40	S	31	Total 31	O 31	0	0
40	T	35	Total 35	O 35	0	0

Continued on next page...

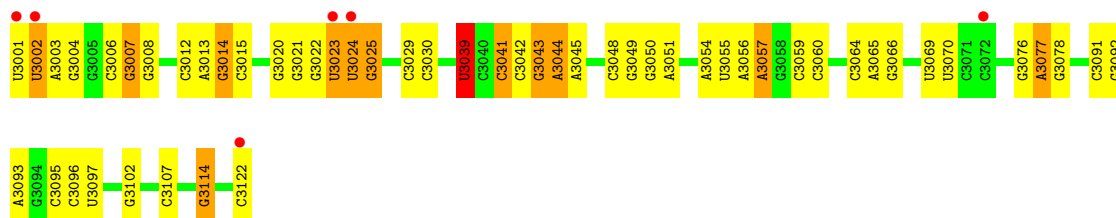
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	28	Total 28	O 28	0	0
40	V	12	Total 12	O 12	0	0
40	W	62	Total 62	O 62	0	0
40	X	21	Total 21	O 21	0	0
40	Y	93	Total 93	O 93	0	0
40	Z	34	Total 34	O 34	0	0
40	1	59	Total 59	O 59	0	0
40	2	40	Total 40	O 40	0	0
40	3	71	Total 71	O 71	0	0
40	I	10	Total 10	O 10	0	0





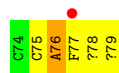
• Molecule 2: 5S ribosomal RNA



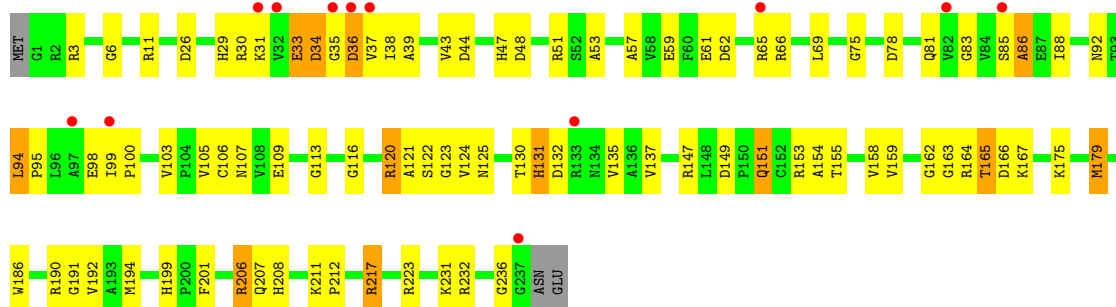
• Molecule 3: 5'-R(*CP*CP*(PPU)*(LOF))-3'



• Molecule 4: 5'-R(*CP*CP*AP*(PHE)*(ACA)*(BTN))-3'

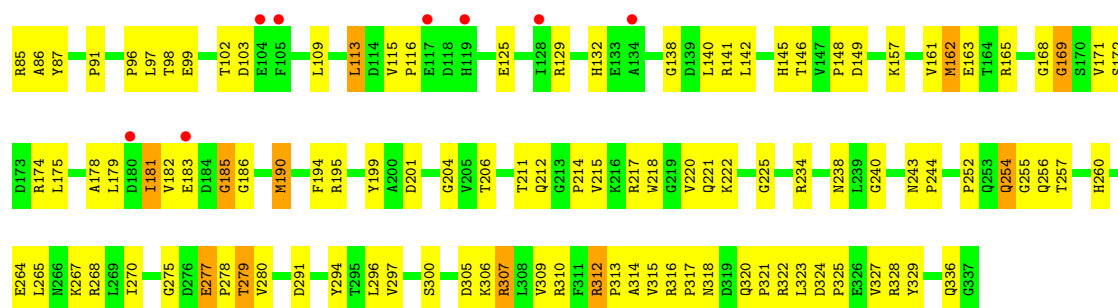


• Molecule 5: 50S ribosomal protein L2P



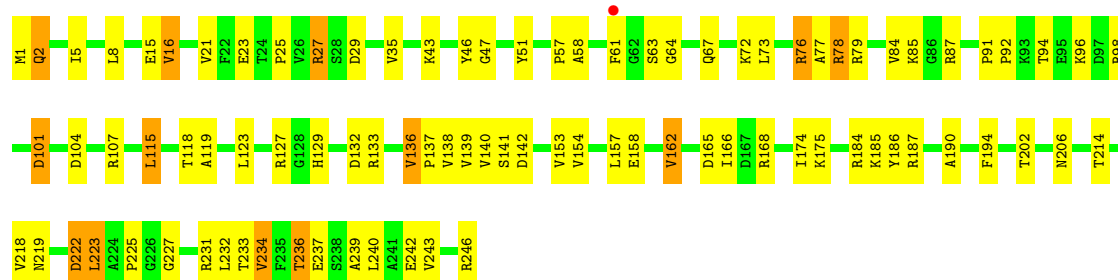
• Molecule 6: 50S ribosomal protein L3P





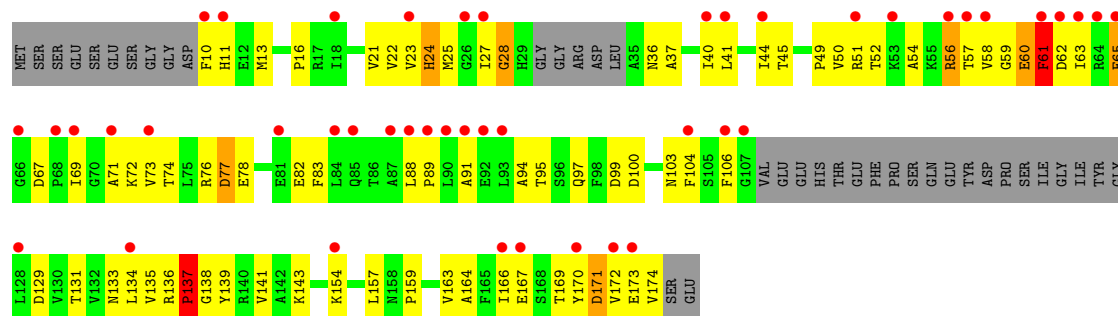
• Molecule 7: 50S ribosomal protein L4E

Chain C: 63% 31% 5%



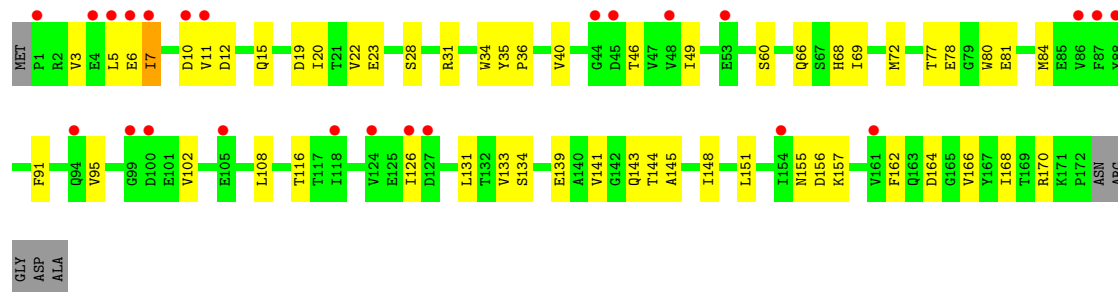
• Molecule 8: 50S ribosomal protein L5P

Chain D: 25% 36% 38% 21%

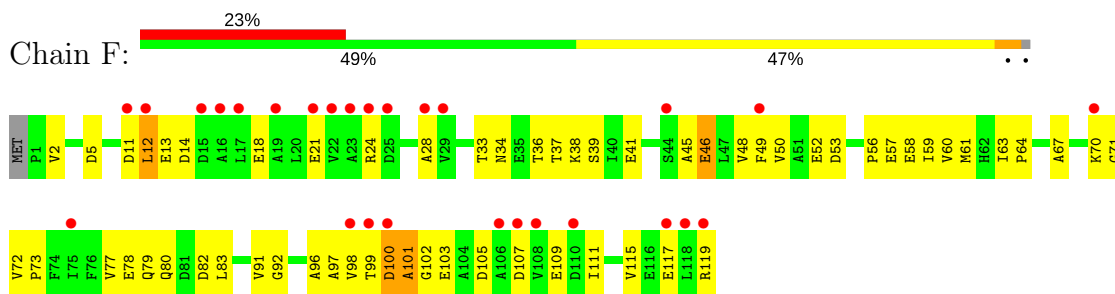


• Molecule 9: 50S ribosomal protein L6P

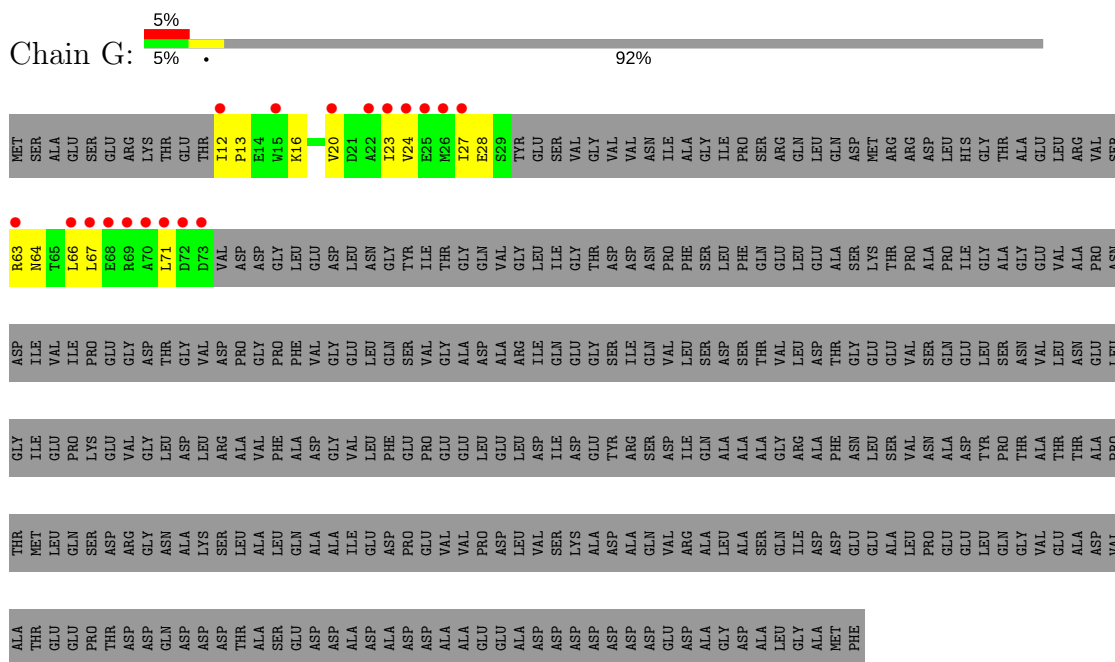
Chain E: 13% 66% 30%



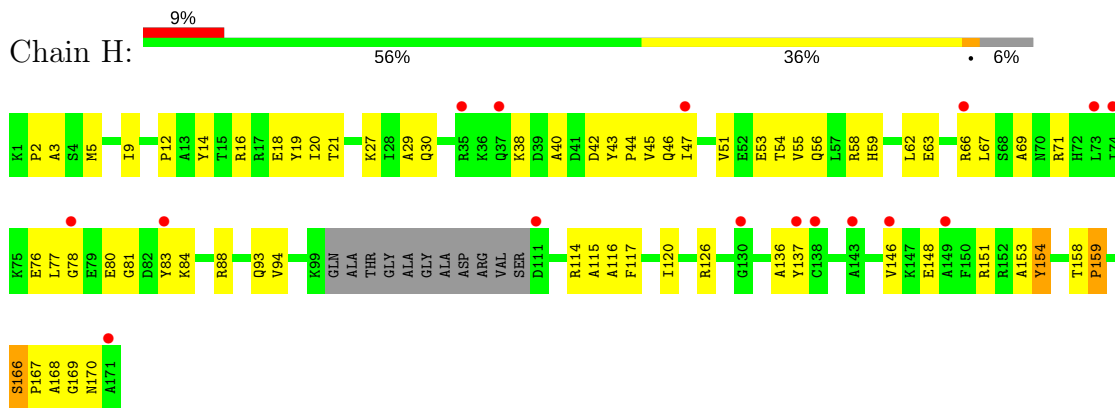
• Molecule 10: 50S ribosomal protein L7AE



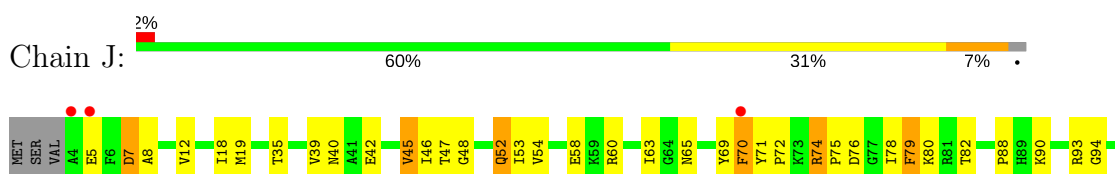
● Molecule 11: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



- Molecule 12: 50S RIBOSOMAL PROTEIN L10E

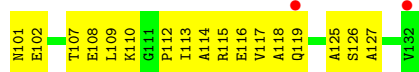


- Molecule 13: 50S ribosomal protein L13P





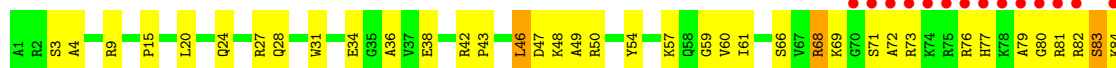
• Molecule 14: 50S ribosomal protein L14P



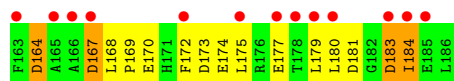
• Molecule 15: 50S ribosomal protein L15P



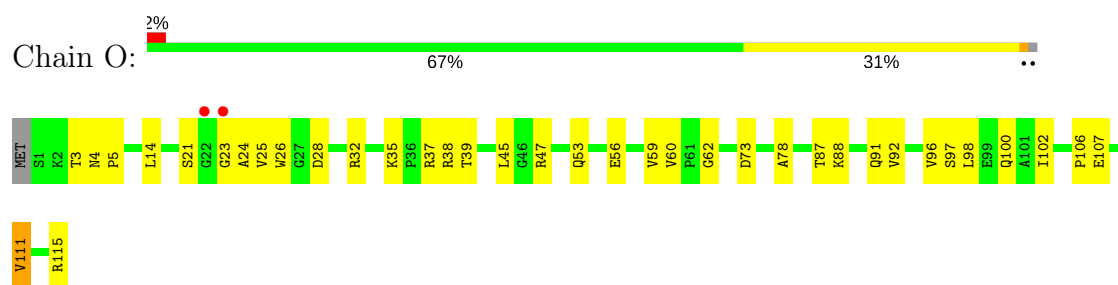
• Molecule 16: 50S Ribosomal Protein L15E



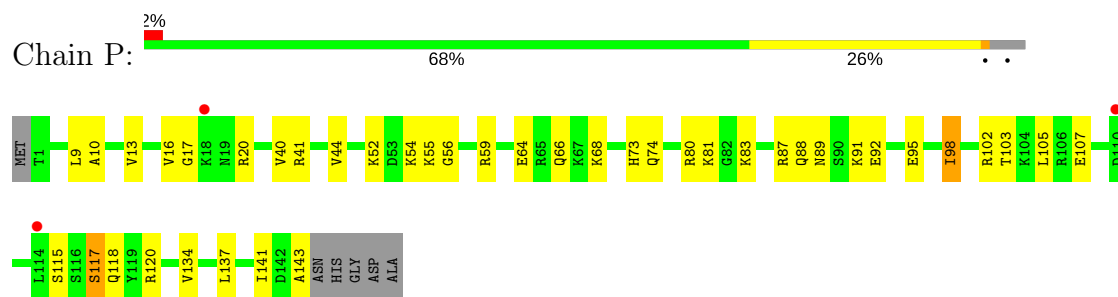
• Molecule 17: 50S ribosomal protein L18P



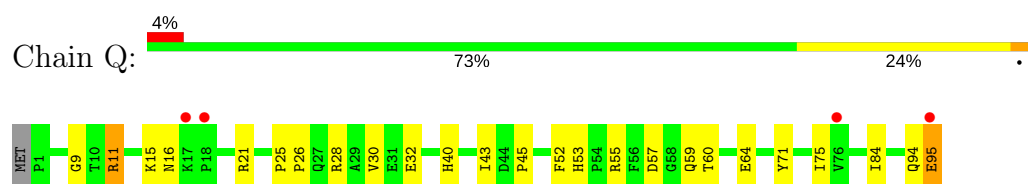
• Molecule 18: 50S ribosomal protein L18e



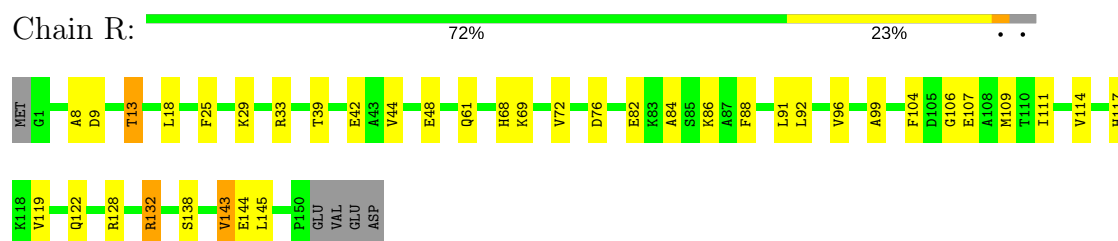
- Molecule 19: 50S ribosomal protein L19E



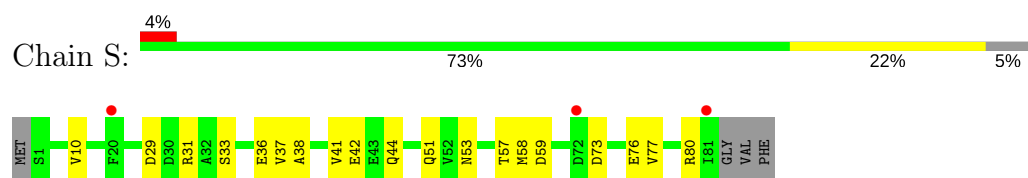
- Molecule 20: 50S ribosomal protein L21e



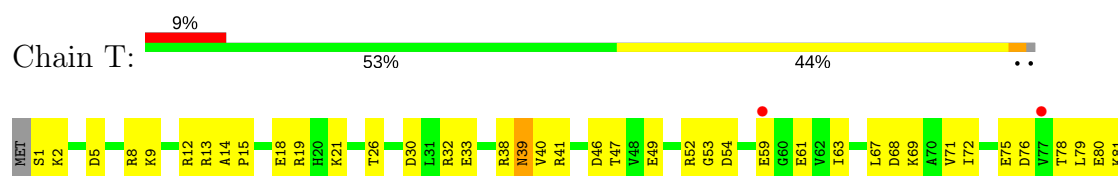
- Molecule 21: 50S ribosomal protein L22P

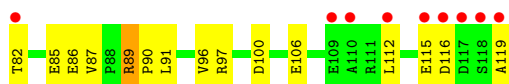


- Molecule 22: 50S ribosomal protein L23P



- Molecule 23: 50S ribosomal protein L24P

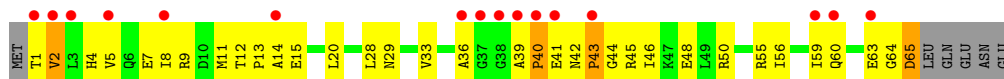




- Molecule 24: 50S ribosomal protein L24E



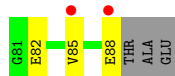
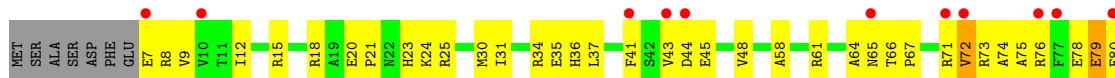
- Molecule 25: 50S ribosomal protein L29P



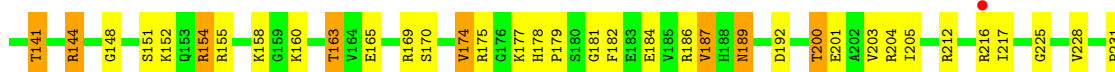
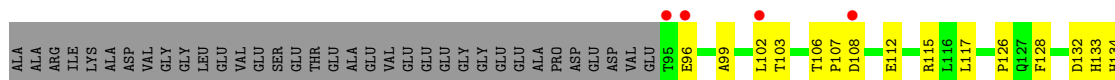
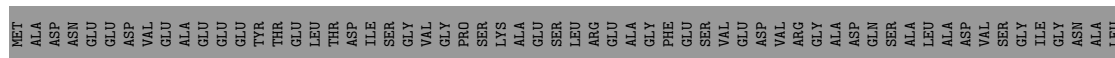
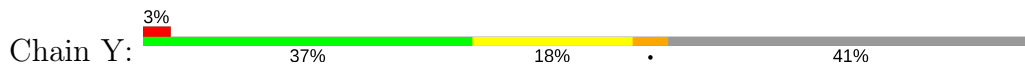
- Molecule 26: 50S ribosomal protein L30P

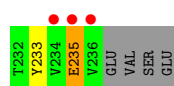


- Molecule 27: 50S ribosomal protein L31e

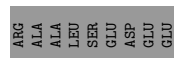
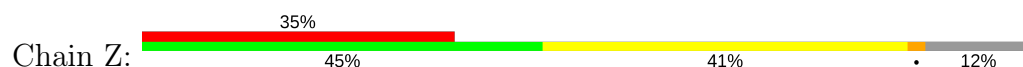


- Molecule 28: 50S ribosomal protein L32E





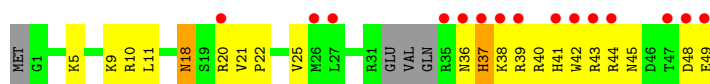
- Molecule 29: 50S ribosomal protein L37Ae



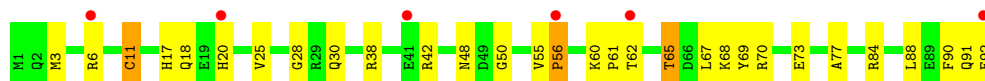
- Molecule 30: 50S ribosomal protein L37e



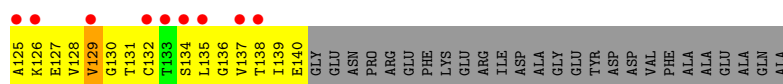
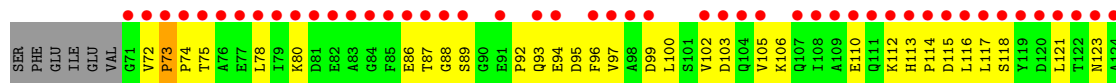
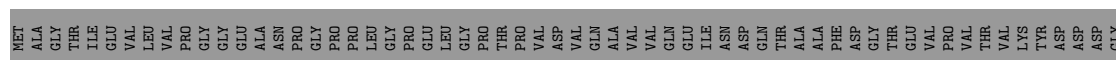
- Molecule 31: 50S ribosomal protein L39e



- Molecule 32: 50S ribosomal protein L44E



- Molecule 33: 50S RIBOSOMAL PROTEIN L11P



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.72Å 298.78Å 575.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.32 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.40) 89.2 (49.32-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.248 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99077	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% 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, OMG, PPU, CL, SR, NA, K, MG, CD, HFA, OMU, UR3, 1MA, BTN, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.70	25/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.47	0/40	0.68	0/60
4	5	0.51	0/76	0.79	0/112
5	A	0.33	0/1786	0.65	0/2408
6	B	0.34	0/2690	0.65	0/3652
7	C	0.38	0/1884	0.65	0/2551
8	D	0.29	0/1111	0.54	0/1498
9	E	0.32	0/1382	0.58	0/1880
10	F	0.33	0/901	0.54	0/1224
11	G	0.28	0/241	0.48	0/324
12	H	0.34	0/1287	0.64	0/1725
13	J	0.35	0/1136	0.62	0/1530
14	K	0.36	0/1001	0.68	0/1347
15	L	0.32	0/1130	0.64	0/1509
16	M	0.34	0/1584	0.59	0/2119
17	N	0.29	0/1474	0.61	0/1999
18	O	0.32	0/874	0.58	0/1181
19	P	0.35	0/1147	0.55	0/1528
20	Q	0.34	0/749	0.69	0/1005
21	R	0.37	0/1172	0.67	0/1578
22	S	0.32	0/648	0.56	0/875
23	T	0.31	0/958	0.63	0/1289
24	U	0.35	0/417	0.58	0/562
25	V	0.27	0/502	0.52	0/675
26	W	0.35	0/1219	0.60	0/1655
27	X	0.34	0/664	0.61	0/895
28	Y	0.37	0/1146	0.66	0/1536
29	Z	0.32	0/589	0.57	0/787
30	1	0.43	0/438	0.63	0/578
31	2	0.32	0/401	0.57	0/529
32	3	0.35	0/771	0.57	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.29	0/526	0.51	0/716
All	All	0.37	0/98808	0.67	26/147749 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	55
2	9	0	1
All	All	0	56

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.44	100.17	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
1	0	1592	G	N9-C1'-C2'	6.67	122.67	114.00
1	0	1819	G	C5'-C4'-C3'	6.40	126.24	116.00
1	0	883	U	N1-C1'-C2'	6.20	122.06	114.00
1	0	2726	U	N1-C1'-C2'	6.13	121.97	114.00
1	0	1504	A	C1'-O4'-C4'	-6.08	105.03	109.90
1	0	777	U	O4'-C1'-N1	5.98	112.98	108.20
2	9	3039	U	N1-C1'-C2'	5.95	121.73	114.00
1	0	1120	U	C5'-C4'-C3'	-5.79	106.73	116.00
1	0	2467	A	C1'-O4'-C4'	-5.79	105.27	109.90
1	0	2541	U	C2'-C3'-O3'	5.76	122.91	113.70
1	0	1819	G	C1'-O4'-C4'	-5.69	105.35	109.90
1	0	1504	A	N9-C1'-C2'	5.65	121.34	114.00
1	0	1979	G	C2'-C3'-O3'	5.55	122.58	113.70
1	0	2291	A	N9-C1'-C2'	5.45	121.09	114.00
1	0	206	G	C5'-C4'-C3'	-5.26	107.58	116.00
1	0	2313	C	C5'-C4'-O4'	5.26	115.42	109.10
1	0	841	A	C1'-O4'-C4'	-5.24	105.70	109.90
1	0	1615	A	C5'-C4'-C3'	5.20	124.33	116.00
1	0	2301	A	N9-C1'-C2'	5.12	120.66	114.00
1	0	1352	A	OP1-P-O3'	5.07	116.36	105.20
1	0	921	G	N9-C1'-C2'	5.05	120.57	114.00
1	0	1261	A	N9-C1'-C2'	5.05	120.57	114.00
1	0	457	U	C1'-O4'-C4'	-5.04	105.86	109.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	389	G	C5'-C4'-C3'	-5.00	108.00	116.00

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1080	C	Sidechain
1	0	1132	A	Sidechain
1	0	1340	G	Sidechain
1	0	1458	A	Sidechain
1	0	1491	G	Sidechain
1	0	1592	G	Sidechain
1	0	1718	G	Sidechain
1	0	1744	G	Sidechain
1	0	1777	G	Sidechain
1	0	1819	G	Sidechain
1	0	1829	A	Sidechain
1	0	1845	A	Sidechain
1	0	1863	G	Sidechain
1	0	1867	G	Sidechain
1	0	1877	G	Sidechain
1	0	1878	G	Sidechain
1	0	1885	A	Sidechain
1	0	191	A	Sidechain
1	0	1970	G	Sidechain
1	0	2115	U	Sidechain
1	0	22	U	Sidechain
1	0	2465	A	Sidechain
1	0	2493	C	Sidechain
1	0	2503	A	Sidechain
1	0	2506	A	Sidechain
1	0	2552	C	Sidechain
1	0	2599	A	Sidechain
1	0	2607	U	Sidechain
1	0	2620	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2645	U	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	2726	U	Sidechain
1	0	2842	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	507	A	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	722	G	Sidechain
1	0	771	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	868	G	Sidechain
1	0	888	U	Sidechain
1	0	952	G	Sidechain
2	9	3039	U	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	0	59021	0	29812	769	0
2	9	2600	0	1326	58	0
3	4	72	0	47	1	0
4	5	93	0	68	4	0
5	A	1753	0	1765	111	0
6	B	2625	0	2532	151	0
7	C	1859	0	1816	97	0
8	D	1094	0	1085	92	0
9	E	1357	0	1266	50	0
10	F	890	0	843	55	0
11	G	240	0	231	12	0
12	H	1266	0	1268	63	0
13	J	1120	0	1098	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	K	992	0	1031	58	0
15	L	1118	0	1076	61	0
16	M	1560	0	1568	75	0
17	N	1445	0	1401	87	0
18	O	865	0	873	42	0
19	P	1136	0	1123	42	0
20	Q	735	0	728	22	0
21	R	1149	0	1122	39	0
22	S	641	0	605	17	0
23	T	950	0	923	52	0
24	U	410	0	364	22	0
25	V	499	0	511	43	0
26	W	1196	0	1137	83	0
27	X	654	0	653	41	0
28	Y	1130	0	1133	60	0
29	Z	578	0	539	39	0
30	1	431	0	426	29	0
31	2	396	0	413	30	0
32	3	755	0	728	30	0
33	I	519	0	500	60	0
34	0	87	0	0	0	0
34	2	1	0	0	0	0
34	5	1	0	0	0	0
34	9	1	0	0	0	0
34	A	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	2	0	0	0	0
36	0	66	0	0	0	0
36	9	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	J	1	0	0	0	0
36	M	1	0	0	0	0
36	Q	1	0	0	0	0
36	R	2	0	0	0	0
36	S	1	0	0	0	0
37	0	10	0	0	0	0
37	3	1	0	0	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	J	3	0	0	1	0
37	L	1	0	0	0	0
37	M	1	0	0	0	0
37	N	1	0	0	0	0
37	O	1	0	0	0	0
37	R	1	0	0	0	0
37	Y	1	0	0	0	0
38	0	98	0	0	0	0
38	1	2	0	0	0	0
38	3	1	0	0	0	0
38	9	3	0	0	0	0
38	A	3	0	0	0	0
38	B	2	0	0	0	0
38	F	1	0	0	0	0
38	H	1	0	0	0	0
38	L	1	0	0	0	0
38	R	1	0	0	0	0
38	S	1	0	0	0	0
39	1	1	0	0	0	0
39	3	1	0	0	0	0
39	O	1	0	0	0	0
39	U	1	0	0	0	0
39	Z	1	0	0	0	0
40	0	5727	0	0	102	0
40	1	59	0	0	3	0
40	2	40	0	0	1	0
40	3	71	0	0	5	0
40	4	1	0	0	0	0
40	5	2	0	0	0	0
40	9	137	0	0	5	0
40	A	120	0	0	8	0
40	B	138	0	0	18	0
40	C	180	0	0	19	0
40	D	48	0	0	11	0
40	E	44	0	0	4	0
40	F	24	0	0	2	0
40	G	14	0	0	0	0
40	H	72	0	0	6	0
40	I	10	0	0	2	0
40	J	54	0	0	3	0
40	K	61	0	0	4	0
40	L	83	0	0	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	M	128	0	0	3	0
40	N	58	0	0	4	0
40	O	39	0	0	3	0
40	P	61	0	0	2	0
40	Q	51	0	0	5	0
40	R	78	0	0	4	0
40	S	31	0	0	1	0
40	T	35	0	0	4	0
40	U	28	0	0	3	0
40	V	12	0	0	2	0
40	W	62	0	0	6	0
40	X	21	0	0	5	0
40	Y	93	0	0	10	0
40	Z	34	0	0	2	0
All	All	99077	0	60011	2220	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 15.

All (2220) 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)
26:W:21:LEU:HD21	26:W:48:VAL:HG11	1.35	1.08
14:K:29:LEU:HB3	14:K:55:VAL:HG11	1.33	1.07
1:O:1160:G:H5'	1:O:1161:A:H5'	1.36	1.07
27:X:37:LEU:HD13	27:X:85:VAL:HG21	1.39	1.04
2:9:3076:G:H3'	2:9:3077:A:H5''	1.36	1.04
23:T:9:LYS:HE3	23:T:13:ARG:NH1	1.73	1.04
13:J:93:ARG:HH11	13:J:93:ARG:HB3	1.21	1.02
25:V:12:THR:HG22	25:V:15:GLU:HG3	1.38	1.02
8:D:25:MET:HE2	8:D:41:LEU:HG	1.41	1.00
6:B:162:MET:HE2	6:B:310:ARG:HD3	1.44	0.99
1:O:871:G:C8	1:O:871:G:H5'	1.96	0.99
22:S:51:GLN:HE21	22:S:53:ASN:HD21	1.05	0.99
9:E:20:ILE:HD11	9:E:40:VAL:HG11	1.46	0.98
7:C:236:THR:HG22	7:C:239:ALA:H	1.24	0.98
1:O:156:C:H5''	16:M:171:ARG:HD3	1.46	0.97
5:A:211:LYS:HG2	5:A:212:PRO:HD2	1.45	0.96
7:C:127:ARG:NH2	7:C:225:PRO:HG2	1.80	0.96
10:F:91:VAL:HG12	10:F:92:GLY:H	1.26	0.96
23:T:71:VAL:HG11	23:T:90:PRO:HB3	1.46	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:78:ARG:HG3	7:C:78:ARG:HH11	1.30	0.96
1:0:1771:U:H5'	29:Z:20:ARG:HH21	1.31	0.95
1:0:871:G:H8	1:0:871:G:H5'	1.28	0.95
1:0:870:G:H2'	1:0:871:G:H5''	1.48	0.95
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.93
14:K:10:GLN:H	14:K:10:GLN:HE21	0.93	0.92
1:0:1242:A:H5'	13:J:82:THR:HG23	1.50	0.92
17:N:11:ARG:HG3	17:N:14:ARG:HH12	1.34	0.92
14:K:10:GLN:H	14:K:10:GLN:NE2	1.66	0.91
8:D:28:GLY:HA2	8:D:69:ILE:HG23	1.52	0.91
1:0:1372:A:H3'	40:0:7638:HOH:O	1.70	0.91
5:A:192:VAL:HG12	5:A:207:GLN:HB3	1.53	0.91
5:A:81:GLN:HB2	5:A:92:ASN:ND2	1.86	0.90
26:W:6:GLN:HB2	26:W:26:ILE:HD12	1.53	0.90
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.90
17:N:144:GLY:O	17:N:147:ILE:HG22	1.70	0.90
28:Y:235:GLU:H	28:Y:235:GLU:CD	1.75	0.90
6:B:238:ASN:HD22	6:B:240:GLY:H	1.18	0.90
31:2:18:ASN:HD21	31:2:40:ARG:H	1.17	0.89
14:K:74:VAL:HG13	14:K:113:ILE:HG23	1.54	0.89
6:B:307:ARG:HH11	6:B:307:ARG:HG3	1.36	0.89
12:H:29:ALA:HB3	12:H:66:ARG:HH12	1.37	0.89
7:C:1:MET:HG2	7:C:2:GLN:H	1.38	0.89
6:B:36:PRO:HA	6:B:168:GLY:HA3	1.55	0.89
8:D:58:VAL:HB	8:D:62:ASP:HB3	1.54	0.89
18:O:32:ARG:HE	18:O:35:LYS:HD2	1.36	0.88
14:K:81:ARG:HB2	14:K:87:ARG:HH11	1.37	0.88
1:0:2717:C:H2'	1:0:2718:C:H5''	1.53	0.88
14:K:74:VAL:HG11	14:K:113:ILE:HG12	1.54	0.88
1:0:289:G:H22	1:0:363:A:H2	1.21	0.87
16:M:102:GLU:OE1	16:M:164:THR:HG21	1.73	0.87
19:P:115:SER:H	19:P:118:GLN:HE21	1.20	0.87
21:R:25:PHE:CE2	21:R:29:LYS:HE2	2.09	0.87
1:0:541:C:H2'	1:0:542:A:H5''	1.57	0.86
17:N:49:THR:HG22	17:N:56:ASP:HB2	1.55	0.86
29:Z:11:SER:HB3	29:Z:23:ARG:HB2	1.55	0.86
17:N:113:SER:HB2	40:N:9354:HOH:O	1.75	0.86
17:N:83:LEU:HD13	17:N:175:LEU:HD23	1.56	0.85
7:C:5:ILE:HD11	7:C:16:VAL:HG22	1.57	0.85
5:A:192:VAL:CG1	5:A:207:GLN:HB3	2.07	0.85
1:0:1835:U:H5	1:0:1840:A:N7	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3056:A:H2'	2:9:3057:A:H5''	1.57	0.85
26:W:137:GLN:HE21	26:W:141:HIS:HE1	1.25	0.85
9:E:15:GLN:HG2	9:E:19:ASP:O	1.77	0.85
8:D:172:VAL:HG12	8:D:173:GLU:H	1.40	0.85
29:Z:37:HIS:HB2	29:Z:47:VAL:HB	1.59	0.84
16:M:99:ARG:HH21	16:M:170:ASN:HD22	1.25	0.84
21:R:8:ALA:HB1	21:R:13:THR:HG21	1.58	0.84
28:Y:200:THR:HG22	28:Y:201:GLU:HG3	1.58	0.84
14:K:10:GLN:N	14:K:10:GLN:HE21	1.74	0.84
15:L:80:ASP:HB2	15:L:90:ARG:O	1.78	0.83
2:9:3006:C:H5''	17:N:37:ARG:NH1	1.94	0.83
1:0:1116:U:HO2'	1:0:1118:A:H2	0.85	0.83
19:P:115:SER:OG	19:P:118:GLN:HG3	1.78	0.83
1:0:2506:A:O2'	1:0:2507:G:H8	1.62	0.83
5:A:192:VAL:HG22	40:A:9617:HOH:O	1.78	0.83
26:W:122:ARG:HH11	26:W:122:ARG:HG2	1.43	0.83
1:0:2717:C:C2'	1:0:2718:C:H5''	2.08	0.83
1:0:1474:C:H6	1:0:1474:C:H5'	1.43	0.82
1:0:2506:A:HO2'	1:0:2507:G:H8	0.87	0.82
1:0:2840:A:OP1	6:B:211:THR:HG23	1.77	0.82
29:Z:36:ASP:HB3	29:Z:45:ASP:HB3	1.62	0.82
12:H:56:GLN:HE22	12:H:93:GLN:HG2	1.45	0.82
14:K:39:GLY:HA2	40:K:4183:HOH:O	1.80	0.82
6:B:162:MET:CE	6:B:310:ARG:HD3	2.10	0.82
2:9:3006:C:H5''	17:N:37:ARG:HH12	1.45	0.81
21:R:99:ALA:HB1	21:R:109:MET:HE1	1.61	0.81
1:0:871:G:H8	1:0:871:G:C5'	1.94	0.81
16:M:134:ILE:HG23	16:M:141:ILE:HD13	1.63	0.81
31:2:41:HIS:H	31:2:45:ASN:HD22	1.26	0.81
1:0:288:A:H61	1:0:364:C:H42	1.29	0.80
5:A:191:GLY:HA2	5:A:194:MET:CE	2.11	0.80
8:D:134:LEU:HD11	8:D:166:ILE:HD11	1.63	0.80
14:K:107:THR:HG22	14:K:108:GLU:HG3	1.64	0.80
1:0:2851:G:C2'	1:0:2852:A:H5'	2.12	0.80
8:D:136:ARG:HH12	8:D:157:LEU:HA	1.46	0.79
6:B:179:LEU:O	6:B:183:GLU:HG2	1.81	0.79
26:W:6:GLN:HB2	26:W:26:ILE:CD1	2.13	0.79
26:W:88:THR:HB	40:W:6679:HOH:O	1.82	0.79
1:0:1160:G:C5'	1:0:1161:A:H5'	2.13	0.79
1:0:2716:G:H5''	6:B:206:THR:HG21	1.65	0.79
14:K:4:LEU:HD22	14:K:116:GLU:HB3	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:12:ILE:N	11:G:13:PRO:HD3	1.97	0.79
27:X:72:VAL:HG22	27:X:85:VAL:HG12	1.64	0.79
1:0:1603:A:H5'	1:0:1605:G:O4'	1.83	0.79
1:0:1119:G:H2'	13:J:52:GLN:NE2	1.98	0.79
14:K:98:VAL:HG13	14:K:102:GLU:HA	1.63	0.79
9:E:81:GLU:HG2	9:E:134:SER:HB3	1.64	0.79
17:N:11:ARG:HA	17:N:14:ARG:NH1	1.97	0.79
26:W:4:LEU:HD22	26:W:52:VAL:HG21	1.63	0.79
1:0:2534:C:H1'	40:0:4081:HOH:O	1.80	0.78
21:R:99:ALA:HB1	21:R:109:MET:CE	2.12	0.78
1:0:541:C:C2'	1:0:542:A:H5''	2.11	0.78
33:I:102:VAL:HG12	33:I:106:LYS:HE3	1.62	0.78
16:M:107:ARG:HH11	16:M:107:ARG:HG3	1.47	0.78
1:0:969:G:H1	1:0:999:C:H42	1.32	0.78
26:W:88:THR:HG23	26:W:110:GLN:NE2	1.99	0.78
1:0:2054:A:N3	21:R:128:ARG:NH2	2.31	0.78
1:0:1973:A:H5'	1:0:1973:A:H8	1.49	0.77
31:2:22:PRO:HG2	31:2:25:VAL:HG23	1.67	0.77
17:N:12:ARG:HD3	17:N:18:THR:OG1	1.85	0.77
1:0:2073:G:H5''	40:0:4400:HOH:O	1.83	0.77
12:H:27:LYS:H	12:H:59:HIS:HD2	1.30	0.77
1:0:1118:A:H3'	1:0:1118:A:H8	1.50	0.77
6:B:212:GLN:HB2	6:B:257:THR:HG21	1.66	0.77
5:A:199:HIS:HD2	5:A:201:PHE:H	1.32	0.76
21:R:18:LEU:HD12	21:R:143:VAL:HG11	1.68	0.76
13:J:93:ARG:NH1	13:J:93:ARG:HB3	1.99	0.76
10:F:91:VAL:HG12	10:F:92:GLY:N	2.01	0.76
40:0:5371:HOH:O	13:J:47:THR:HB	1.83	0.76
26:W:122:ARG:HH11	26:W:122:ARG:CG	1.97	0.76
26:W:125:HIS:HD2	26:W:127:GLY:H	1.30	0.76
1:0:559:U:H5'	1:0:559:U:H6	1.50	0.76
14:K:98:VAL:CG1	14:K:102:GLU:HA	2.15	0.76
1:0:560:C:H42	1:0:597:A:H61	1.33	0.76
17:N:11:ARG:HG3	17:N:14:ARG:NH1	2.01	0.76
1:0:1041:U:H5'	40:L:9491:HOH:O	1.85	0.76
8:D:57:THR:HG23	8:D:63:ILE:HA	1.67	0.76
16:M:79:ALA:HB3	16:M:81:ARG:NH1	2.00	0.76
1:0:1667:A:H8	1:0:1667:A:H5'	1.51	0.75
1:0:960:G:H4'	40:0:7866:HOH:O	1.84	0.75
2:9:3014:G:H8	2:9:3014:G:H5'	1.50	0.75
21:R:111:ILE:HG23	21:R:145:LEU:HD11	1.67	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:ASP:HA	7:C:107:ARG:HH12	1.50	0.75
13:J:93:ARG:HH11	13:J:93:ARG:CB	2.00	0.75
1:O:1119:G:N2	1:O:1246:A:C2	2.53	0.75
1:O:2533:C:H5'	1:O:2533:C:H6	1.51	0.75
6:B:195:ARG:HG2	6:B:323:LEU:HD22	1.68	0.75
1:O:506:G:H22	1:O:509:A:C5'	2.00	0.75
9:E:15:GLN:HG3	9:E:20:ILE:HG12	1.68	0.75
5:A:153:ARG:HH11	5:A:153:ARG:HB2	1.50	0.75
13:J:19:MET:HE1	13:J:132:LEU:HD21	1.69	0.75
25:V:39:ALA:N	25:V:40:PRO:HD2	2.02	0.75
26:W:13:MET:HE1	26:W:18:GLN:HA	1.67	0.75
1:O:1116:U:O2'	1:O:1118:A:H2	1.67	0.74
8:D:25:MET:HE1	8:D:37:ALA:HB1	1.67	0.74
13:J:19:MET:HE3	13:J:132:LEU:HD11	1.68	0.74
14:K:14:LYS:HB2	14:K:45:PRO:HG2	1.70	0.74
32:3:70:ARG:HG2	32:3:77:ALA:HB2	1.69	0.74
5:A:206:ARG:HD3	5:A:206:ARG:H	1.51	0.74
9:E:3:VAL:HG22	9:E:49:ILE:HB	1.69	0.74
1:O:1244:U:OP1	13:J:18:ILE:HD13	1.87	0.74
6:B:51:VAL:CG2	6:B:327:VAL:HG13	2.18	0.74
1:O:1118:A:C8	1:O:1118:A:H3'	2.22	0.74
29:Z:46:ARG:HD2	29:Z:59:TYR:HB2	1.68	0.74
1:O:281:U:H2'	1:O:282:C:O4'	1.86	0.74
9:E:84:MET:HE1	9:E:148:ILE:HD12	1.69	0.74
5:A:35:GLY:O	5:A:36:ASP:HB3	1.88	0.74
33:I:78:LEU:HD12	33:I:112:LYS:HZ2	1.53	0.74
17:N:80:SER:HB2	40:N:9333:HOH:O	1.85	0.74
8:D:54:ALA:HB2	8:D:69:ILE:HD12	1.70	0.74
21:R:39:THR:HB	21:R:42:GLU:HG3	1.69	0.74
1:O:1377:C:H6	1:O:1377:C:H5'	1.52	0.73
28:Y:154:ARG:HH12	28:Y:155:ARG:HG3	1.53	0.73
1:O:1751:G:H2'	1:O:1752:G:H5''	1.70	0.73
9:E:36:PRO:HD3	13:J:127:ILE:HD12	1.68	0.73
13:J:74:ARG:HB3	13:J:74:ARG:HH11	1.51	0.73
15:L:143:THR:HG22	15:L:144:ASP:H	1.52	0.73
26:W:88:THR:HG22	26:W:89:ASP:N	2.03	0.73
1:O:1206:U:H6	1:O:1206:U:H5'	1.52	0.73
33:I:99:ASP:OD1	33:I:138:THR:HB	1.89	0.73
22:S:57:THR:HG22	22:S:59:ASP:H	1.54	0.73
32:3:65:THR:HG22	32:3:67:LEU:HG	1.69	0.73
7:C:236:THR:HG22	7:C:239:ALA:N	2.00	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:567:U:H5''	40:W:5817:HOH:O	1.88	0.73
1:0:111:C:O2'	30:1:20:ARG:HG2	1.88	0.73
25:V:1:THR:HG23	25:V:2:VAL:H	1.54	0.73
26:W:137:GLN:HE21	26:W:141:HIS:CE1	2.07	0.73
1:0:1165:G:H4'	1:0:1174:A:O2'	1.89	0.73
23:T:49:GLU:HB3	23:T:59:GLU:HG2	1.71	0.73
16:M:69:LYS:O	16:M:73:ARG:NH2	2.22	0.72
18:O:32:ARG:HD3	18:O:32:ARG:O	1.87	0.72
1:0:506:G:H22	1:0:509:A:H5''	1.53	0.72
1:0:1118:A:H62	1:0:1244:U:H3	1.35	0.72
1:0:870:G:C2'	1:0:871:G:H5''	2.18	0.72
1:0:656:G:H5'	18:O:3:THR:HB	1.71	0.72
1:0:2890:A:H1'	24:U:56:ARG:NH2	2.04	0.72
15:L:143:THR:HG22	15:L:144:ASP:N	2.05	0.72
2:9:3039:U:H1'	2:9:3044:A:H61	1.55	0.72
7:C:104:ASP:HA	7:C:107:ARG:NH1	2.05	0.72
1:0:545:G:H8	1:0:545:G:H5'	1.55	0.71
19:P:115:SER:H	19:P:118:GLN:NE2	1.88	0.71
1:0:1700:C:H5''	1:0:1701:A:OP2	1.90	0.71
14:K:74:VAL:CG1	14:K:113:ILE:HG12	2.19	0.71
14:K:81:ARG:HB2	14:K:87:ARG:NH1	2.04	0.71
1:0:2851:G:H2'	1:0:2852:A:H5'	1.72	0.71
5:A:88:ILE:HD13	5:A:100:PRO:HD3	1.71	0.71
1:0:2005:G:H3'	1:0:2005:G:OP2	1.91	0.71
8:D:58:VAL:HG12	8:D:60:GLU:HG2	1.72	0.71
33:I:110:GLU:HA	33:I:113:HIS:NE2	2.06	0.71
10:F:58:GLU:OE1	16:M:27:ARG:NH2	2.23	0.71
10:F:50:VAL:HG13	10:F:60:VAL:HG11	1.71	0.71
13:J:74:ARG:NH1	13:J:76:ASP:HB2	2.06	0.71
14:K:29:LEU:HB3	14:K:55:VAL:CG1	2.19	0.71
1:0:544:G:H2'	1:0:545:G:H5''	1.72	0.71
5:A:191:GLY:HA2	5:A:194:MET:HE2	1.72	0.71
1:0:1299:G:O6	15:L:6:ARG:HD3	1.91	0.71
28:Y:165:GLU:HB3	40:Y:9390:HOH:O	1.90	0.71
1:0:1701:A:H4'	1:0:1702:U:H5''	1.73	0.70
40:O:7889:HOH:O	6:B:211:THR:HG21	1.91	0.70
8:D:135:VAL:HG21	8:D:139:TYR:CD1	2.26	0.70
16:M:31:TRP:HA	16:M:34:GLU:HG3	1.72	0.70
7:C:236:THR:CG2	7:C:239:ALA:H	2.04	0.70
1:0:2364:A:H5''	20:Q:15:LYS:HD3	1.73	0.70
1:0:962:C:H1'	17:N:5:ARG:NH1	2.06	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:77:VAL:HG21	10:F:83:LEU:HD13	1.74	0.70
26:W:80:ASP:O	26:W:84:VAL:HG23	1.90	0.70
10:F:96:ALA:HA	40:F:3111:HOH:O	1.91	0.70
12:H:21:THR:O	12:H:120:ILE:HD12	1.92	0.70
19:P:115:SER:N	19:P:118:GLN:HE21	1.89	0.70
27:X:74:ALA:HB2	27:X:85:VAL:HG13	1.72	0.70
16:M:79:ALA:HB3	16:M:81:ARG:HH12	1.57	0.70
7:C:132:ASP:HB3	40:C:9172:HOH:O	1.91	0.70
33:I:132:CYS:HB3	33:I:137:VAL:HB	1.74	0.70
5:A:33:GLU:CD	5:A:33:GLU:H	1.93	0.70
7:C:78:ARG:HG3	7:C:78:ARG:NH1	2.04	0.70
17:N:17:ARG:HB3	17:N:17:ARG:HH11	1.57	0.70
19:P:59:ARG:NH2	19:P:66:GLN:HE22	1.89	0.70
30:1:25:LYS:HD2	31:2:48:ASP:HA	1.72	0.70
6:B:275:GLY:O	6:B:291:ASP:HA	1.91	0.70
23:T:71:VAL:HG11	23:T:90:PRO:CB	2.21	0.70
33:I:78:LEU:HD12	33:I:112:LYS:NZ	2.07	0.69
26:W:52:VAL:HG22	26:W:53:ALA:H	1.57	0.69
1:0:1160:G:H5'	1:0:1161:A:C5'	2.18	0.69
31:2:18:ASN:HD21	31:2:40:ARG:N	1.89	0.69
30:1:28:HIS:CD2	30:1:31:LYS:HG3	2.27	0.69
10:F:37:THR:O	10:F:41:GLU:HG3	1.93	0.69
1:0:1771:U:H5'	29:Z:20:ARG:NH2	2.07	0.69
1:0:542:A:C8	1:0:542:A:H5'	2.22	0.69
1:0:481:U:H5''	40:0:6167:HOH:O	1.92	0.69
6:B:125:GLU:O	6:B:129:ARG:HG3	1.93	0.69
1:0:2491:G:H1'	40:0:7335:HOH:O	1.93	0.69
22:S:77:VAL:O	22:S:80:ARG:HG2	1.92	0.69
28:Y:212:ARG:HD2	40:Y:9398:HOH:O	1.92	0.69
5:A:51:ARG:HB2	40:A:9591:HOH:O	1.93	0.69
7:C:47:GLY:HA2	7:C:92:PRO:HB2	1.74	0.69
12:H:56:GLN:NE2	12:H:126:ARG:HE	1.90	0.69
26:W:13:MET:HE3	26:W:17:ILE:HG22	1.74	0.69
26:W:88:THR:HG22	26:W:89:ASP:H	1.57	0.69
1:0:380:A:OP2	16:M:9:ARG:HD2	1.93	0.69
8:D:172:VAL:HG12	8:D:173:GLU:N	2.07	0.69
1:0:1474:C:C6	1:0:1474:C:H5'	2.26	0.69
1:0:1641:A:H2'	1:0:1642:A:H5'	1.74	0.69
18:O:32:ARG:NE	18:O:35:LYS:HD2	2.08	0.69
1:0:2749:U:H5'	40:0:8429:HOH:O	1.92	0.68
26:W:122:ARG:NH2	26:W:154:ARG:HG2	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:76:ARG:HH11	27:X:76:ARG:HG3	1.57	0.68
1:O:871:G:C8	1:O:871:G:C5'	2.70	0.68
26:W:130:HIS:O	26:W:136:GLY:HA3	1.93	0.68
16:M:107:ARG:NH1	16:M:107:ARG:HG3	2.05	0.68
6:B:238:ASN:HD22	6:B:240:GLY:N	1.92	0.68
14:K:23:ASN:HD21	14:K:107:THR:HB	1.58	0.68
15:L:67:ARG:O	15:L:71:GLU:HG3	1.93	0.68
33:I:134:SER:O	33:I:135:LEU:HD23	1.93	0.68
21:R:18:LEU:HD12	21:R:143:VAL:CG1	2.23	0.68
26:W:137:GLN:NE2	26:W:141:HIS:HE1	1.90	0.68
26:W:81:ASP:OD1	26:W:92:ASP:HB2	1.94	0.68
7:C:2:GLN:HB3	40:C:9195:HOH:O	1.94	0.68
9:E:6:GLU:HA	9:E:46:THR:HG22	1.74	0.68
13:J:131:THR:HG22	13:J:134:GLU:H	1.56	0.68
1:O:1201:C:H2'	1:O:1202:A:H5'	1.74	0.68
12:H:56:GLN:NE2	12:H:93:GLN:HG2	2.08	0.68
14:K:81:ARG:HD3	14:K:87:ARG:NH1	2.08	0.68
19:P:91:LYS:O	19:P:95:GLU:HG3	1.93	0.68
1:O:1116:U:O2'	1:O:1118:A:C2	2.46	0.67
13:J:74:ARG:HH12	13:J:76:ASP:HB2	1.60	0.67
17:N:62:HIS:HB3	17:N:65:ASP:OD1	1.95	0.67
1:O:1182:C:H1'	1:O:1192:A:H8	1.58	0.67
6:B:62:ARG:HA	6:B:65:MET:CE	2.24	0.67
12:H:30:GLN:H	12:H:66:ARG:NH1	1.93	0.67
12:H:59:HIS:HA	12:H:62:LEU:HD23	1.76	0.67
21:R:18:LEU:HB2	21:R:143:VAL:CG1	2.24	0.67
18:O:96:VAL:HG13	18:O:100:GLN:HB2	1.75	0.67
1:O:2908:A:H2'	1:O:2909:G:O4'	1.95	0.67
1:O:1166:A:H1'	1:O:1192:A:C2	2.29	0.67
8:D:159:PRO:O	8:D:163:VAL:HG23	1.94	0.67
27:X:71:ARG:HD3	40:X:2171:HOH:O	1.95	0.67
1:O:1184:C:H1'	40:O:7899:HOH:O	1.93	0.67
1:O:2676:C:H4'	13:J:70:PHE:CE1	2.30	0.67
1:O:2676:C:H4'	13:J:70:PHE:CD1	2.30	0.67
23:T:115:GLU:HG3	23:T:116:ASP:N	2.09	0.67
24:U:5:GLU:HG2	24:U:10:GLY:O	1.95	0.67
1:O:2468:A:H61	32:3:48:ASN:HD21	1.43	0.67
1:O:883:U:H2'	1:O:883:U:O2	1.95	0.67
5:A:199:HIS:CD2	5:A:201:PHE:H	2.11	0.67
5:A:100:PRO:HG2	5:A:103:VAL:HG21	1.75	0.67
12:H:27:LYS:N	12:H:59:HIS:HD2	1.92	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:797:A:C4'	29:Z:10:ARG:N	2.57	0.67
1:0:2420:G:O2'	1:0:2421:G:H5'	1.96	0.66
26:W:21:LEU:CD2	26:W:48:VAL:HG11	2.19	0.66
1:0:1183:C:H2'	40:0:6739:HOH:O	1.94	0.66
1:0:877:G:H5'	1:0:878:G:OP1	1.95	0.66
10:F:13:GLU:OE2	10:F:78:GLU:HG2	1.95	0.66
27:X:71:ARG:HB3	27:X:88:GLU:OE1	1.95	0.66
1:0:1838:U:O2'	1:0:2644:C:H5'	1.95	0.66
1:0:2073:G:OP2	1:0:2490:A:H5'	1.94	0.66
5:A:153:ARG:NH1	5:A:153:ARG:HB2	2.10	0.66
19:P:59:ARG:HH22	19:P:66:GLN:HE22	1.42	0.66
1:0:2578:G:H5'	1:0:2578:G:H8	1.59	0.66
1:0:541:C:H2'	1:0:542:A:C5'	2.26	0.66
8:D:41:LEU:HA	8:D:44:ILE:HG22	1.76	0.66
28:Y:189:ASN:HA	28:Y:217:ILE:HD11	1.78	0.66
1:0:1666:C:H2'	1:0:1667:A:H5'	1.77	0.66
6:B:140:LEU:HA	40:B:9575:HOH:O	1.95	0.66
28:Y:144:ARG:HH11	28:Y:144:ARG:CG	2.09	0.66
1:0:2505:G:O2'	1:0:2506:A:H5'	1.96	0.66
29:Z:22:SER:O	29:Z:26:VAL:HG23	1.94	0.66
6:B:51:VAL:HG23	6:B:329:TYR:O	1.96	0.66
26:W:68:THR:HG23	26:W:69:ARG:HG2	1.78	0.66
10:F:58:GLU:CD	16:M:27:ARG:HH22	1.97	0.66
1:0:1116:U:H3	1:0:1246:A:H62	1.44	0.65
1:0:1159:G:H21	1:0:1189:A:H8	1.44	0.65
6:B:254:GLN:HG2	6:B:255:GLY:N	2.10	0.65
22:S:10:VAL:HG11	25:V:36:ALA:HA	1.78	0.65
6:B:53:LEU:HD11	6:B:327:VAL:HG22	1.77	0.65
13:J:45:VAL:HG11	13:J:121:LEU:HD22	1.79	0.65
18:O:32:ARG:HH21	18:O:35:LYS:NZ	1.94	0.65
19:P:9:LEU:O	19:P:13:VAL:HG12	1.97	0.65
23:T:41:ARG:HG2	23:T:41:ARG:HH11	1.59	0.65
1:0:1687:C:O2	30:1:9:GLY:HA2	1.97	0.65
6:B:16:ARG:NH1	40:B:9612:HOH:O	2.28	0.65
7:C:162:VAL:HG22	7:C:232:LEU:HD21	1.77	0.65
15:L:73:VAL:HG23	15:L:74:THR:H	1.62	0.65
23:T:49:GLU:OE2	23:T:97:ARG:HD2	1.95	0.65
28:Y:144:ARG:CZ	40:Y:9409:HOH:O	2.44	0.65
18:O:32:ARG:HH21	18:O:35:LYS:HZ2	1.44	0.65
23:T:32:ARG:NH1	23:T:38:ARG:HH12	1.94	0.65
1:0:1162:G:H1'	33:I:117:LEU:HD11	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:48:ASP:HB3	40:A:9591:HOH:O	1.95	0.65
12:H:166:SER:HB3	12:H:167:PRO:HD3	1.78	0.65
1:O:2661:U:H3	1:O:2812:A:H62	1.43	0.65
6:B:201:ASP:HB2	6:B:312:ARG:HD2	1.79	0.65
1:O:2521:A:OP2	12:H:3:ALA:HB3	1.96	0.65
17:N:48:VAL:CG1	17:N:55:ASP:HB3	2.27	0.65
28:Y:144:ARG:HG3	28:Y:144:ARG:HH11	1.60	0.65
1:O:1175:G:H1'	1:O:1193:A:H2'	1.78	0.65
6:B:307:ARG:NH1	6:B:307:ARG:HG3	2.05	0.65
1:O:1119:G:H22	1:O:1246:A:H2	1.41	0.64
1:O:1730:G:H5'	1:O:1731:C:C5	2.31	0.64
1:O:282:C:O2'	1:O:283:U:H5'	1.96	0.64
16:M:134:ILE:CG2	16:M:141:ILE:HD13	2.26	0.64
1:O:2896:A:H5''	40:O:6599:HOH:O	1.96	0.64
6:B:74:ILE:HD13	6:B:309:VAL:HG21	1.78	0.64
10:F:2:VAL:HG22	10:F:57:GLU:OE1	1.97	0.64
10:F:53:ASP:OD1	10:F:80:GLN:HB2	1.96	0.64
17:N:139:TRP:HA	17:N:139:TRP:CE3	2.33	0.64
26:W:88:THR:HG23	26:W:110:GLN:HE21	1.61	0.64
26:W:48:VAL:HG12	26:W:48:VAL:O	1.97	0.64
1:O:1209:C:H2'	1:O:1210:G:H8	1.61	0.64
1:O:272:A:H5'	1:O:273:G:OP2	1.97	0.64
16:M:68:ARG:NH2	16:M:73:ARG:HD3	2.13	0.64
18:O:21:SER:OG	18:O:106:PRO:HB2	1.98	0.64
23:T:112:LEU:HD23	23:T:119:ALA:HB3	1.79	0.64
29:Z:42:CYS:SG	29:Z:43:GLY:N	2.70	0.64
1:O:544:G:C2'	1:O:545:G:H5''	2.27	0.64
6:B:18:ARG:HG3	6:B:256:GLN:HG3	1.78	0.64
6:B:41:PHE:CD2	6:B:190:MET:HE3	2.32	0.64
1:O:1878:G:H1'	40:O:6620:HOH:O	1.97	0.64
1:O:381:G:H5''	40:M:9373:HOH:O	1.97	0.64
10:F:63:ILE:HB	10:F:64:PRO:HD3	1.80	0.64
12:H:46:GLN:HB3	12:H:167:PRO:HD2	1.78	0.64
13:J:75:PRO:HG2	13:J:105:LEU:HD21	1.79	0.64
24:U:45:GLU:HB2	24:U:48:ASN:ND2	2.12	0.64
31:2:18:ASN:ND2	31:2:40:ARG:H	1.93	0.64
6:B:190:MET:HE2	6:B:194:PHE:HD1	1.61	0.64
14:K:49:LEU:HD12	14:K:80:ILE:HG21	1.80	0.64
16:M:187:LEU:CD2	16:M:194:ALA:HB3	2.28	0.64
20:Q:75:ILE:HD13	20:Q:84:ILE:HD11	1.78	0.64
1:O:709:G:O2'	18:O:25:VAL:HG12	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:9:LYS:HE3	23:T:13:ARG:HH12	1.58	0.64
26:W:108:ARG:HG3	26:W:114:PRO:HG3	1.80	0.64
33:I:125:ALA:O	33:I:129:VAL:HG23	1.97	0.64
1:O:2064:U:H5'	1:O:2652:U:H4'	1.80	0.64
9:E:20:ILE:CD1	9:E:40:VAL:HG11	2.26	0.64
14:K:75:ARG:HD3	14:K:112:PRO:O	1.98	0.64
21:R:111:ILE:HG23	21:R:145:LEU:CD1	2.28	0.64
7:C:157:LEU:HD13	7:C:166:ILE:HD11	1.81	0.63
12:H:166:SER:CB	12:H:167:PRO:CD	2.75	0.63
33:I:110:GLU:HA	33:I:113:HIS:CE1	2.33	0.63
2:9:3039:U:HO2'	2:9:3042:C:H5	1.44	0.63
2:9:3056:A:C2'	2:9:3057:A:H5''	2.26	0.63
7:C:77:ALA:O	7:C:78:ARG:HG3	1.97	0.63
28:Y:126:PRO:HG2	28:Y:128:PHE:CE1	2.33	0.63
1:O:1427:A:H61	1:O:1440:U:H1'	1.62	0.63
1:O:263:U:O4'	10:F:59:ILE:HD13	1.99	0.63
5:A:36:ASP:OD2	5:A:85:SER:HB2	1.98	0.63
17:N:164:ASP:CG	17:N:167:ASP:HA	2.18	0.63
33:I:113:HIS:N	33:I:114:PRO:HD2	2.14	0.63
16:M:80:GLY:O	16:M:81:ARG:HD2	1.99	0.63
1:O:447:A:P	23:T:1:SER:HB2	2.38	0.63
1:O:2587:OMU:H5	40:O:7918:HOH:O	1.97	0.63
1:O:88:G:H2'	1:O:89:G:C8	2.34	0.63
25:V:20:LEU:HD22	25:V:60:GLN:HE22	1.63	0.63
1:O:2541:U:H4'	1:O:2542:C:OP1	1.97	0.63
14:K:55:VAL:HG12	14:K:56:SER:N	2.13	0.63
40:O:9739:HOH:O	16:M:82:ARG:HD2	1.98	0.63
2:9:3014:G:C8	2:9:3014:G:H5'	2.33	0.63
5:A:94:LEU:HG	5:A:99:ILE:HD11	1.80	0.63
1:O:2533:C:C6	1:O:2533:C:H5'	2.32	0.62
13:J:90:LYS:HB2	37:J:9302:CL:CL	2.35	0.62
30:1:25:LYS:HD2	31:2:49:GLU:H	1.64	0.62
32:3:38:ARG:HB3	32:3:42:ARG:HH12	1.64	0.62
1:O:2896:A:N3	1:O:2896:A:H2'	2.15	0.62
30:1:45:ARG:NH2	40:1:9488:HOH:O	2.31	0.62
1:O:1206:U:H2'	1:O:1207:A:O4'	2.00	0.62
1:O:1528:A:H2'	1:O:1529:G:O4'	1.98	0.62
12:H:27:LYS:H	12:H:59:HIS:CD2	2.17	0.62
12:H:40:ALA:HB1	12:H:137:TYR:CE2	2.34	0.62
31:2:22:PRO:HG2	31:2:25:VAL:CG2	2.29	0.62
16:M:164:THR:HG22	16:M:166:ALA:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:4:LEU:HD11	26:W:45:VAL:HG12	1.81	0.62
1:0:2780:C:H1'	9:E:143:GLN:HE21	1.64	0.62
1:0:524:A:H5''	21:R:29:LYS:HD3	1.82	0.62
30:1:10:LYS:HG3	40:1:9492:HOH:O	1.98	0.62
2:9:3029:C:O3'	8:D:138:GLY:HA2	2.00	0.62
9:E:23:GLU:HG2	9:E:28:SER:HB3	1.80	0.62
17:N:139:TRP:HA	17:N:139:TRP:HE3	1.65	0.62
17:N:154:LEU:HG	17:N:155:GLU:H	1.63	0.62
21:R:18:LEU:HB2	21:R:143:VAL:HG13	1.82	0.62
21:R:44:VAL:O	21:R:48:GLU:HG3	2.00	0.62
23:T:71:VAL:HG12	23:T:72:ILE:N	2.15	0.62
26:W:141:HIS:HB2	26:W:146:ILE:HG12	1.80	0.62
27:X:25:ARG:HD3	27:X:64:ALA:O	1.99	0.62
1:0:1183:C:N4	1:0:1184:C:H41	1.98	0.62
2:9:3020:G:O2'	2:9:3021:G:H5'	1.99	0.62
2:9:3051:A:H5'	17:N:160:SER:HB3	1.82	0.62
40:9:4707:HOH:O	17:N:147:ILE:HD12	1.99	0.62
19:P:80:ARG:HG2	19:P:87:ARG:CZ	2.30	0.62
1:0:1118:A:H8	1:0:1119:G:H5''	1.64	0.62
1:0:1328:A:OP1	28:Y:169:ARG:HD2	2.00	0.62
5:A:135:VAL:HG21	5:A:147:ARG:NH1	2.15	0.62
12:H:20:ILE:HG23	12:H:120:ILE:HD11	1.81	0.62
16:M:164:THR:HG22	16:M:167:GLY:H	1.65	0.62
1:0:470:U:O2'	30:1:16:HIS:HD2	1.83	0.62
2:9:3029:C:H2'	2:9:3030:C:H5'	1.81	0.62
11:G:12:ILE:N	11:G:13:PRO:CD	2.63	0.62
19:P:64:GLU:HG2	40:P:165:HOH:O	2.00	0.62
29:Z:72:GLU:OE1	29:Z:77:LYS:HE2	1.99	0.62
30:1:8:GLN:HE22	30:1:11:LYS:NZ	1.97	0.61
6:B:141:ARG:HD2	6:B:163:GLU:OE2	1.99	0.61
7:C:118:THR:HG22	7:C:137:PRO:HB3	1.81	0.61
13:J:19:MET:CE	13:J:132:LEU:HD11	2.29	0.61
14:K:109:LEU:HD13	14:K:113:ILE:HD11	1.81	0.61
1:0:2586:U:H3	1:0:2592:G:H22	1.47	0.61
6:B:225:GLY:HA3	40:B:9562:HOH:O	2.00	0.61
24:U:14:GLU:O	24:U:17:THR:HB	2.01	0.61
28:Y:112:GLU:OE1	28:Y:112:GLU:HA	2.00	0.61
28:Y:187:VAL:HG12	28:Y:205:ILE:HA	1.81	0.61
1:0:2807:U:P	6:B:27:ASN:HD21	2.24	0.61
1:0:485:A:N3	1:0:487:G:H5''	2.14	0.61
30:1:25:LYS:HD2	31:2:49:GLU:N	2.15	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:11:ARG:CG	17:N:14:ARG:HH12	2.09	0.61
24:U:52:THR:HG22	24:U:54:THR:N	2.16	0.61
1:O:289:G:N2	1:O:363:A:H2	1.94	0.61
2:9:3039:U:H1'	2:9:3044:A:N6	2.15	0.61
5:A:107:ASN:OD1	5:A:120:ARG:HD2	2.00	0.61
5:A:105:VAL:CG1	5:A:154:ALA:HB1	2.31	0.61
6:B:175:LEU:O	6:B:175:LEU:HD23	2.00	0.61
8:D:59:GLY:O	8:D:61:PHE:N	2.33	0.61
25:V:56:ILE:HG22	25:V:60:GLN:HE21	1.66	0.61
6:B:217:ARG:HG3	6:B:257:THR:HG22	1.80	0.61
27:X:43:VAL:HG12	27:X:44:ASP:N	2.16	0.61
1:O:282:C:H1'	1:O:368:C:N4	2.15	0.61
8:D:136:ARG:NH1	8:D:157:LEU:HA	2.15	0.61
9:E:35:TYR:HA	13:J:127:ILE:HD12	1.82	0.61
18:O:25:VAL:HG23	18:O:26:TRP:N	2.16	0.61
1:O:553:G:P	28:Y:204:ARG:HH22	2.23	0.61
1:O:280:C:H2'	1:O:281:U:O4'	2.01	0.61
5:A:191:GLY:HA2	5:A:194:MET:HE3	1.81	0.61
17:N:164:ASP:OD1	17:N:167:ASP:HA	2.01	0.61
20:Q:25:PRO:HB2	40:Q:4350:HOH:O	2.00	0.61
6:B:329:TYR:CE2	24:U:15:PRO:HG2	2.35	0.61
27:X:66:THR:HG23	27:X:67:PRO:HD2	1.83	0.61
5:A:69:LEU:HD23	5:A:107:ASN:HB2	1.81	0.61
1:O:263:U:O2	16:M:42:ARG:HD2	2.01	0.61
1:O:2563:U:H2'	1:O:2565:C:O5'	2.00	0.61
32:3:65:THR:HG23	32:3:88:LEU:HD22	1.83	0.61
6:B:102:THR:CG2	6:B:182:VAL:HG12	2.31	0.61
8:D:13:MET:HA	8:D:137:PRO:HG2	1.83	0.61
17:N:132:ASN:O	17:N:135:VAL:HG12	2.00	0.61
1:O:475:G:OP1	7:C:73:LEU:HD22	2.01	0.60
5:A:81:GLN:HB2	5:A:92:ASN:HD21	1.62	0.60
7:C:129:HIS:CE1	7:C:231:ARG:HA	2.36	0.60
8:D:58:VAL:CG1	8:D:60:GLU:HG2	2.30	0.60
17:N:61:ALA:HB3	17:N:88:ALA:HB2	1.83	0.60
1:O:2769:C:C2'	1:O:2770:G:H5'	2.32	0.60
5:A:123:GLY:HA3	5:A:162:GLY:HA2	1.83	0.60
7:C:136:VAL:HG22	7:C:137:PRO:HA	1.83	0.60
9:E:68:HIS:O	9:E:72:MET:HG3	2.00	0.60
1:O:902:G:N7	15:L:18:HIS:HD2	1.99	0.60
26:W:21:LEU:HD22	26:W:26:ILE:CD1	2.31	0.60
7:C:139:VAL:HG13	40:C:9254:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:I:129:VAL:O	33:I:129:VAL:HG12	2.01	0.60
33:I:92:PRO:C	33:I:94:GLU:H	2.05	0.60
16:M:71:SER:HB2	16:M:92:THR:HG22	1.83	0.60
1:0:2291:A:C8	1:0:2309:C:H5'	2.36	0.60
1:0:2426:G:H1'	40:0:6592:HOH:O	2.00	0.60
1:0:338:C:H4'	7:C:174:ILE:CD1	2.32	0.60
16:M:183:THR:HG22	16:M:194:ALA:HB1	1.82	0.60
25:V:39:ALA:N	25:V:40:PRO:CD	2.64	0.60
28:Y:187:VAL:HB	28:Y:203:VAL:HG22	1.83	0.60
1:0:2365:G:H5''	40:Q:6597:HOH:O	2.01	0.60
1:0:848:C:H5'	40:0:7714:HOH:O	2.02	0.60
5:A:105:VAL:HG11	5:A:154:ALA:HB1	1.83	0.60
7:C:27:ARG:HG3	7:C:29:ASP:OD1	2.02	0.60
8:D:94:ALA:HA	8:D:174:VAL:HA	1.83	0.60
1:0:1201:C:H5''	40:0:6728:HOH:O	2.01	0.60
1:0:156:C:H5''	16:M:171:ARG:CD	2.28	0.60
2:9:3013:A:O2'	2:9:3014:G:H5''	2.01	0.60
1:0:1943:C:H4'	5:A:211:LYS:O	2.02	0.60
10:F:58:GLU:HA	10:F:61:MET:HE2	1.82	0.60
1:0:2346:C:O2'	8:D:52:THR:HG21	2.00	0.60
2:9:3076:G:C3'	2:9:3077:A:H5''	2.24	0.60
22:S:57:THR:HG22	22:S:59:ASP:N	2.16	0.60
1:0:796:A:HO2'	29:Z:10:ARG:N	1.98	0.60
1:0:2427:C:OP2	32:3:84:ARG:HD2	2.00	0.60
2:9:3004:G:H21	17:N:44:ARG:NH1	2.00	0.60
26:W:21:LEU:HB3	26:W:26:ILE:HG12	1.83	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.60
8:D:135:VAL:HG22	8:D:136:ARG:N	2.17	0.60
8:D:23:VAL:HG21	8:D:45:THR:HG21	1.83	0.60
10:F:46:GLU:O	10:F:73:PRO:HD2	2.02	0.60
26:W:125:HIS:CD2	26:W:127:GLY:H	2.16	0.60
1:0:236:A:H8	1:0:236:A:OP1	1.84	0.60
33:I:113:HIS:CE1	33:I:121:LEU:HD22	2.36	0.60
1:0:1164:U:OP1	33:I:74:PRO:HA	2.01	0.60
14:K:113:ILE:HG22	14:K:114:ALA:N	2.16	0.60
8:D:23:VAL:HG22	8:D:73:VAL:HB	1.82	0.59
13:J:75:PRO:HD3	13:J:136:SER:OG	2.01	0.59
19:P:16:VAL:HG12	19:P:17:GLY:N	2.17	0.59
6:B:264:GLU:HG2	6:B:267:LYS:HE2	1.84	0.59
6:B:71:VAL:HG11	6:B:296:LEU:HD22	1.83	0.59
12:H:170:ASN:N	12:H:170:ASN:HD22	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:V:39:ALA:C	25:V:41:GLU:H	2.06	0.59
25:V:56:ILE:O	25:V:60:GLN:HG3	2.02	0.59
1:0:396:U:O2'	1:0:418:C:H4'	2.02	0.59
10:F:50:VAL:HG21	10:F:63:ILE:HG21	1.83	0.59
40:0:4936:HOH:O	16:M:83:SER:HB3	2.01	0.59
25:V:11:MET:HB3	25:V:15:GLU:HB2	1.84	0.59
28:Y:154:ARG:NH1	28:Y:155:ARG:HG3	2.16	0.59
5:A:153:ARG:CB	5:A:153:ARG:HH11	2.15	0.59
17:N:162:ASP:HA	40:N:9328:HOH:O	2.03	0.59
26:W:119:HIS:HD2	26:W:120:PRO:O	1.86	0.59
6:B:62:ARG:HA	6:B:65:MET:HE3	1.83	0.59
33:I:106:LYS:O	33:I:110:GLU:HG3	2.02	0.59
1:0:1555:G:H4'	1:0:1630:A:H2	1.68	0.59
1:0:1878:G:O2'	1:0:1879:U:C6	2.55	0.59
1:0:462:A:N3	31:2:37:HIS:HB3	2.18	0.59
10:F:91:VAL:CG1	10:F:92:GLY:H	2.10	0.59
33:I:105:VAL:HG11	33:I:129:VAL:HG22	1.84	0.59
23:T:38:ARG:NH1	40:T:6217:HOH:O	2.35	0.59
31:2:36:ASN:HB3	31:2:39:ARG:NE	2.17	0.59
7:C:236:THR:H	7:C:239:ALA:HB3	1.68	0.59
1:0:1946:C:H2'	1:0:1971:G:C8	2.37	0.59
5:A:33:GLU:O	5:A:34:ASP:HB2	2.02	0.59
7:C:233:THR:HG22	7:C:234:VAL:N	2.17	0.59
17:N:23:ARG:HH11	17:N:23:ARG:HG2	1.67	0.59
1:0:1187:U:HO2'	1:0:1189:A:H2	1.51	0.58
1:0:1418:U:OP1	31:2:42:TRP:HB3	2.02	0.58
1:0:1819:G:H2'	1:0:1820:G:H4'	1.85	0.58
1:0:2649:A:H5'	1:0:2649:A:H8	1.67	0.58
1:0:316:A:H5'	23:T:54:ASP:OD2	2.02	0.58
5:A:36:ASP:C	5:A:38:ILE:H	2.06	0.58
1:0:558:C:C2'	1:0:559:U:H5''	2.33	0.58
1:0:797:A:H4'	29:Z:10:ARG:N	2.18	0.58
6:B:265:LEU:HD21	6:B:316:ARG:HD3	1.85	0.58
12:H:46:GLN:HE21	12:H:137:TYR:HE2	1.51	0.58
14:K:62:PRO:HG3	14:K:65:ARG:HH21	1.66	0.58
25:V:12:THR:HG22	25:V:15:GLU:CG	2.21	0.58
1:0:343:C:O2'	1:0:344:C:H5'	2.02	0.58
6:B:254:GLN:HG2	6:B:255:GLY:H	1.68	0.58
32:3:55:VAL:HG22	40:3:9444:HOH:O	2.02	0.58
16:M:24:GLN:NE2	16:M:27:ARG:HH11	2.02	0.58
29:Z:11:SER:CB	29:Z:23:ARG:HB2	2.28	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1973:A:H5'	1:0:1973:A:C8	2.37	0.58
6:B:145:HIS:HD2	6:B:146:THR:O	1.85	0.58
9:E:116:THR:HG22	9:E:151:LEU:HD22	1.85	0.58
1:0:1163:G:H5'	33:I:115:ASP:O	2.04	0.58
14:K:109:LEU:CD1	14:K:113:ILE:HD11	2.32	0.58
15:L:148:GLU:HB2	40:L:9486:HOH:O	2.03	0.58
16:M:164:THR:HG22	16:M:166:ALA:H	1.68	0.58
17:N:143:ARG:HH21	17:N:169:PRO:HB2	1.68	0.58
17:N:78:MET:HB2	17:N:79:PRO:HD3	1.85	0.58
1:0:2769:C:O2'	1:0:2770:G:H5'	2.04	0.58
1:0:316:A:N3	1:0:336:G:O2'	2.35	0.58
6:B:87:TYR:O	6:B:138:GLY:N	2.27	0.58
8:D:54:ALA:CB	8:D:69:ILE:HD12	2.32	0.58
14:K:32:ILE:HD11	14:K:56:SER:HB3	1.86	0.58
8:D:50:VAL:O	8:D:71:ALA:HA	2.04	0.58
1:0:2081:A:H4'	13:J:69:TYR:CE1	2.39	0.58
15:L:133:VAL:HA	40:L:9470:HOH:O	2.04	0.58
24:U:47:ARG:HG3	40:U:4381:HOH:O	2.03	0.58
1:0:1187:U:O2'	1:0:1189:A:H2	1.86	0.58
1:0:1701:A:H4'	1:0:1702:U:C5'	2.32	0.58
1:0:558:C:O2'	1:0:559:U:H5''	2.04	0.58
7:C:168:ARG:NH2	7:C:190:ALA:O	2.36	0.58
12:H:58:ARG:HG3	12:H:58:ARG:HH11	1.68	0.58
1:0:119:A:H2'	1:0:120:A:H5''	1.86	0.58
1:0:69:A:H5'	1:0:69:A:C8	2.39	0.58
1:0:969:G:H1	1:0:999:C:N4	2.01	0.58
6:B:85:ARG:NH1	40:B:9629:HOH:O	2.37	0.58
13:J:47:THR:HG22	13:J:48:GLY:N	2.17	0.58
26:W:38:THR:HG22	26:W:39:ASP:N	2.19	0.58
7:C:242:GLU:HB2	40:C:9192:HOH:O	2.04	0.58
17:N:115:VAL:HG22	40:N:9354:HOH:O	2.04	0.58
1:0:681:G:N3	1:0:681:G:H5'	2.19	0.57
7:C:115:LEU:HD13	7:C:223:LEU:HD21	1.86	0.57
1:0:474:C:O3'	7:C:73:LEU:HD21	2.03	0.57
8:D:25:MET:CE	8:D:37:ALA:HB1	2.33	0.57
9:E:81:GLU:HG2	9:E:134:SER:CB	2.33	0.57
10:F:60:VAL:HG12	10:F:60:VAL:O	2.04	0.57
12:H:30:GLN:H	12:H:66:ARG:HH11	1.51	0.57
1:0:2443:C:O3'	15:L:56:LYS:HE3	2.04	0.57
32:3:60:LYS:HG3	32:3:61:PRO:HD2	1.85	0.57
6:B:5:ARG:HH11	6:B:8:LYS:HE2	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:54:VAL:HG11	13:J:138:THR:HG21	1.86	0.57
1:0:558:C:H2'	1:0:559:U:C5'	2.33	0.57
17:N:110:THR:HB	17:N:113:SER:OG	2.04	0.57
1:0:1835:U:C5	1:0:1840:A:N7	2.65	0.57
11:G:24:VAL:O	11:G:28:GLU:HB2	2.04	0.57
18:O:25:VAL:HG23	18:O:26:TRP:H	1.69	0.57
25:V:64:GLY:O	25:V:65:ASP:HB2	2.03	0.57
5:A:179:MET:HG2	5:A:186:TRP:CB	2.35	0.57
5:A:88:ILE:HG22	5:A:88:ILE:O	2.03	0.57
8:D:138:GLY:N	40:D:7597:HOH:O	2.36	0.57
1:0:1205:U:H2'	1:0:1206:U:C5'	2.35	0.57
1:0:1878:G:HO2'	1:0:1879:U:H6	1.49	0.57
1:0:2541:U:H3'	1:0:2541:U:H6	1.70	0.57
6:B:321:PRO:HA	40:B:9650:HOH:O	2.03	0.57
13:J:74:ARG:O	13:J:78:ILE:HG12	2.03	0.57
1:0:1666:C:O2'	1:0:1667:A:H5''	2.04	0.57
9:E:126:ILE:HB	9:E:131:LEU:HD23	1.86	0.57
25:V:55:ARG:O	25:V:59:ILE:HG12	2.04	0.57
27:X:37:LEU:CD1	27:X:85:VAL:HG21	2.25	0.57
6:B:17:LYS:O	6:B:260:HIS:HD2	1.87	0.57
8:D:170:TYR:O	8:D:171:ASP:HB3	2.03	0.57
26:W:139:GLY:O	26:W:141:HIS:HD2	1.87	0.57
29:Z:30:GLU:HA	29:Z:33:MET:HE3	1.87	0.57
1:0:1352:A:O2'	1:0:1353:C:OP1	2.22	0.57
5:A:165:THR:HG22	40:A:9604:HOH:O	2.05	0.57
1:0:1351:G:OP1	7:C:96:LYS:NZ	2.36	0.57
1:0:1625:U:H4'	40:0:5209:HOH:O	2.05	0.57
1:0:1919:A:H4'	40:0:5385:HOH:O	2.05	0.57
1:0:2795:C:O2'	1:0:2796:U:H5'	2.05	0.57
1:0:462:A:C2	31:2:37:HIS:HB3	2.39	0.57
2:9:3008:G:O6	17:N:11:ARG:NH1	2.33	0.57
16:M:77:HIS:HD2	16:M:79:ALA:O	1.88	0.57
9:E:126:ILE:HB	9:E:131:LEU:CD2	2.35	0.56
10:F:21:GLU:O	10:F:24:ARG:HG3	2.05	0.56
11:G:23:ILE:HD13	11:G:67:LEU:HD23	1.86	0.56
33:I:128:VAL:C	33:I:130:GLY:H	2.08	0.56
1:0:20:G:H21	21:R:117:HIS:HD2	1.53	0.56
26:W:88:THR:CG2	26:W:89:ASP:H	2.18	0.56
1:0:1684:A:H1'	31:2:43:ARG:HH22	1.70	0.56
1:0:2718:C:H6	1:0:2718:C:H5'	1.69	0.56
1:0:2824:C:H5''	1:0:2825:C:H5'	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:820:G:O2'	1:0:856:G:H4'	2.05	0.56
6:B:190:MET:HE2	6:B:194:PHE:CD1	2.39	0.56
6:B:195:ARG:HD2	6:B:324:ASP:OD1	2.04	0.56
1:0:2815:G:N7	13:J:80:LYS:NZ	2.53	0.56
16:M:60:VAL:C	16:M:61:ILE:HD12	2.25	0.56
24:U:17:THR:CG2	24:U:18:GLY:N	2.67	0.56
26:W:84:VAL:HG12	40:W:6679:HOH:O	2.04	0.56
1:0:1189:A:H1'	1:0:1209:C:O4'	2.05	0.56
1:0:2878:U:H2'	1:0:2879:A:O4'	2.04	0.56
13:J:99:GLU:HA	40:J:7377:HOH:O	2.05	0.56
14:K:114:ALA:HB3	14:K:117:VAL:HG23	1.86	0.56
21:R:9:ASP:O	21:R:13:THR:HB	2.05	0.56
28:Y:235:GLU:CD	28:Y:235:GLU:N	2.52	0.56
1:0:1426:C:H2'	40:0:3203:HOH:O	2.05	0.56
1:0:2032:U:H2'	1:0:2033:G:C5'	2.35	0.56
8:D:49:PRO:HA	8:D:73:VAL:HG22	1.87	0.56
24:U:17:THR:HG22	24:U:18:GLY:N	2.19	0.56
26:W:4:LEU:O	26:W:32:CYS:HA	2.05	0.56
28:Y:187:VAL:HB	28:Y:203:VAL:CG2	2.35	0.56
1:0:2090:G:H2'	1:0:2091:G:C8	2.41	0.56
1:0:757:C:OP1	15:L:27:ARG:HD2	2.05	0.56
8:D:22:VAL:HG22	8:D:74:THR:HG22	1.87	0.56
17:N:169:PRO:O	17:N:172:PHE:HB3	2.06	0.56
19:P:10:ALA:HA	19:P:13:VAL:CG1	2.35	0.56
26:W:122:ARG:CG	26:W:122:ARG:NH1	2.64	0.56
29:Z:29:ILE:O	29:Z:33:MET:HB2	2.06	0.56
1:0:2346:C:O5'	1:0:2346:C:H6	1.87	0.56
1:0:93:C:H5''	25:V:1:THR:HB	1.88	0.56
40:0:9699:HOH:O	6:B:214:PRO:HD2	2.04	0.56
15:L:121:ILE:HG12	15:L:141:GLU:HB2	1.87	0.56
19:P:40:VAL:O	19:P:44:VAL:HG23	2.05	0.56
1:0:1118:A:C8	1:0:1119:G:H5''	2.40	0.56
1:0:1441:G:O2'	1:0:1442:A:H5'	2.05	0.56
1:0:2649:A:H5'	1:0:2649:A:C8	2.41	0.56
1:0:506:G:H22	1:0:509:A:H5'	1.71	0.56
1:0:538:C:OP2	28:Y:134:HIS:HE1	1.89	0.56
5:A:105:VAL:HG11	5:A:154:ALA:CB	2.35	0.56
1:0:2721:U:H4'	14:K:87:ARG:HG3	1.87	0.56
40:0:3149:HOH:O	19:P:81:LYS:HG2	2.06	0.56
1:0:2866:U:H4'	1:0:2867:G:H5'	1.88	0.56
1:0:920:C:H4'	1:0:921:G:C2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:57:ALA:HB1	5:A:65:ARG:HE	1.69	0.56
8:D:103:ASN:ND2	8:D:134:LEU:H	2.03	0.56
1:0:244:C:OP2	10:F:38:LYS:HE3	2.05	0.56
40:0:8433:HOH:O	12:H:154:TYR:HB2	2.06	0.56
15:L:136:ALA:HB3	40:L:9470:HOH:O	2.06	0.56
1:0:2421:G:H1'	40:0:4280:HOH:O	2.06	0.56
1:0:1594:C:OP2	19:P:120:ARG:HD2	2.06	0.56
21:R:18:LEU:HG	21:R:91:LEU:HD13	1.88	0.56
26:W:149:LEU:HG	26:W:153:MET:CE	2.36	0.56
27:X:30:MET:HE1	27:X:58:ALA:HB3	1.88	0.56
1:0:90:A:H2'	1:0:91:G:O4'	2.05	0.56
1:0:949:U:H4'	20:Q:95:GLU:HA	1.86	0.56
8:D:135:VAL:HG21	8:D:139:TYR:CG	2.41	0.56
8:D:76:ARG:O	8:D:77:ASP:HB2	2.06	0.56
1:0:2032:U:H2'	1:0:2033:G:H5''	1.88	0.55
1:0:120:A:H5'	30:1:20:ARG:HH21	1.71	0.55
6:B:297:VAL:HB	40:B:9600:HOH:O	2.05	0.55
14:K:34:VAL:HG22	14:K:47:ALA:HB2	1.86	0.55
1:0:625:U:H5''	1:0:1044:C:N4	2.21	0.55
1:0:558:C:H2'	1:0:559:U:H5'	1.88	0.55
8:D:135:VAL:HG22	8:D:136:ARG:H	1.71	0.55
1:0:1060:C:H6	1:0:1060:C:H5'	1.72	0.55
1:0:138:U:H5''	1:0:139:C:OP2	2.06	0.55
1:0:621:C:H5'	28:Y:132:ASP:OD2	2.07	0.55
2:9:3024:U:H3'	2:9:3025:G:H5'	1.88	0.55
8:D:24:HIS:HB2	8:D:72:LYS:CB	2.35	0.55
1:0:1748:U:H4'	40:0:7953:HOH:O	2.04	0.55
1:0:2481:G:H5''	40:0:5094:HOH:O	2.05	0.55
5:A:125:ASN:HB3	5:A:158:VAL:HG12	1.88	0.55
6:B:305:ASP:O	6:B:306:LYS:HB2	2.07	0.55
25:V:1:THR:HG23	25:V:2:VAL:N	2.20	0.55
1:0:2416:G:O2'	17:N:25:ARG:HG2	2.05	0.55
1:0:2502:C:C2'	1:0:2503:A:H5'	2.37	0.55
1:0:1180:U:O2'	33:I:92:PRO:HD2	2.05	0.55
1:0:164:G:H4'	15:L:30:ARG:HD3	1.89	0.55
17:N:86:LEU:HD12	17:N:125:ALA:HB2	1.88	0.55
1:0:1205:U:H2'	1:0:1206:U:H5'	1.89	0.55
1:0:2587:OMU:H2'	1:0:2589:U:H5''	1.88	0.55
1:0:407:A:H2'	1:0:408:A:C8	2.41	0.55
12:H:166:SER:HB3	12:H:167:PRO:CD	2.35	0.55
1:0:834:G:H4'	1:0:835:U:OP2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:57:LYS:HE2	16:M:140:ALA:O	2.06	0.55
1:0:2851:G:O2'	1:0:2852:A:H5'	2.05	0.55
6:B:132:HIS:CE1	6:B:171:VAL:HG21	2.42	0.55
16:M:34:GLU:HB3	16:M:38:GLU:HG3	1.89	0.55
1:0:121:U:OP2	31:2:10:ARG:NH2	2.35	0.55
1:0:137:U:H2'	1:0:139:C:C5	2.42	0.55
9:E:31:ARG:NH1	9:E:68:HIS:CG	2.75	0.55
10:F:50:VAL:CG2	10:F:63:ILE:HG21	2.37	0.55
1:0:1168:C:H5''	33:I:87:THR:CG2	2.37	0.55
16:M:120:VAL:HG11	16:M:130:GLU:HG3	1.88	0.55
29:Z:37:HIS:O	29:Z:45:ASP:HA	2.07	0.55
1:0:2591:C:H2'	1:0:2592:G:O4'	2.06	0.55
6:B:5:ARG:NH1	6:B:8:LYS:HE2	2.22	0.55
10:F:46:GLU:OE1	10:F:100:ASP:HA	2.07	0.55
13:J:130:VAL:HG12	13:J:131:THR:N	2.22	0.55
13:J:76:ASP:HA	40:J:5907:HOH:O	2.06	0.55
15:L:10:SER:O	15:L:11:ARG:HB3	2.06	0.55
23:T:63:ILE:HD11	23:T:75:GLU:HB2	1.89	0.55
27:X:78:GLU:HG2	27:X:79:GLU:OE2	2.07	0.55
27:X:9:VAL:HG22	27:X:88:GLU:OE2	2.07	0.55
1:0:1595:G:O2'	1:0:1596:U:H5'	2.06	0.54
1:0:2270:G:H4'	5:A:223:ARG:HH12	1.72	0.54
6:B:40:GLY:HA3	40:B:9641:HOH:O	2.06	0.54
14:K:30:LYS:O	14:K:55:VAL:HG13	2.06	0.54
17:N:32:PRO:HD2	17:N:99:GLU:O	2.06	0.54
28:Y:108:ASP:N	28:Y:108:ASP:OD1	2.36	0.54
28:Y:154:ARG:HH12	28:Y:155:ARG:CG	2.20	0.54
6:B:221:GLN:HE22	14:K:42:ASN:HD22	1.55	0.54
29:Z:53:GLY:HA2	29:Z:67:GLY:O	2.06	0.54
1:0:2670:G:O2'	1:0:2671:U:H5'	2.07	0.54
8:D:24:HIS:HB2	8:D:72:LYS:HB3	1.89	0.54
14:K:4:LEU:CD2	14:K:116:GLU:HB3	2.36	0.54
28:Y:133:HIS:HD2	40:Y:9381:HOH:O	1.90	0.54
1:0:1202:A:H2'	1:0:1203:G:O4'	2.08	0.54
5:A:65:ARG:C	5:A:66:ARG:HG3	2.26	0.54
1:0:1451:C:H5'	1:0:1505:U:C5	2.43	0.54
1:0:2414:A:H2'	1:0:2415:A:C8	2.43	0.54
5:A:192:VAL:HB	40:A:9580:HOH:O	2.06	0.54
5:A:66:ARG:HH11	5:A:66:ARG:HB2	1.72	0.54
6:B:321:PRO:HG3	40:B:9595:HOH:O	2.06	0.54
7:C:1:MET:HG2	7:C:2:GLN:N	2.16	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:O:87:THR:O	18:O:91:GLN:HG3	2.07	0.54
1:O:1189:A:O2'	1:O:1208:C:H2'	2.07	0.54
2:9:3107:C:H5	40:9:3167:HOH:O	1.90	0.54
1:O:1853:C:OP1	5:A:231:LYS:HG3	2.08	0.54
9:E:144:THR:O	9:E:148:ILE:HG13	2.08	0.54
10:F:50:VAL:CG1	10:F:60:VAL:HG11	2.36	0.54
15:L:53:ARG:NH2	15:L:57:VAL:HG12	2.22	0.54
16:M:164:THR:CG2	16:M:165:GLY:N	2.70	0.54
1:O:291:C:H2'	1:O:292:G:O4'	2.08	0.54
9:E:145:ALA:HB1	9:E:168:ILE:HD11	1.88	0.54
1:O:2748:G:H2'	40:0:7972:HOH:O	2.07	0.54
1:O:95:A:H5''	1:O:97:G:O4'	2.08	0.54
40:0:7978:HOH:O	16:M:91:ILE:HG12	2.07	0.54
18:O:47:ARG:HG3	18:O:47:ARG:HH11	1.73	0.54
1:O:1773:G:C8	29:Z:16:ALA:HA	2.43	0.54
29:Z:57:CYS:SG	29:Z:59:TYR:HB3	2.48	0.54
1:O:441:A:H1'	1:O:442:A:N7	2.22	0.54
1:O:482:G:H4'	1:O:508:A:N1	2.23	0.54
8:D:44:ILE:HG12	8:D:83:PHE:HE1	1.73	0.54
18:O:97:SER:H	18:O:100:GLN:NE2	2.05	0.54
28:Y:189:ASN:HD22	28:Y:189:ASN:C	2.11	0.54
1:O:1377:C:H5'	1:O:1377:C:C6	2.38	0.54
1:O:328:U:O4'	7:C:202:THR:HG22	2.08	0.54
1:O:603:A:H5''	1:O:604:G:OP1	2.08	0.54
1:O:69:A:H5'	1:O:69:A:H8	1.73	0.54
8:D:154:LYS:HD2	8:D:154:LYS:H	1.73	0.54
33:I:113:HIS:HE1	33:I:121:LEU:HD22	1.70	0.54
16:M:187:LEU:HD23	16:M:194:ALA:HB3	1.89	0.54
23:T:32:ARG:NH1	23:T:38:ARG:NH1	2.54	0.54
1:O:1847:A:OP1	5:A:175:LYS:HG3	2.08	0.53
1:O:2837:U:H2'	40:0:7305:HOH:O	2.09	0.53
5:A:105:VAL:HG12	5:A:106:CYS:N	2.24	0.53
16:M:61:ILE:N	16:M:61:ILE:HD12	2.23	0.53
28:Y:170:SER:OG	28:Y:175:ARG:HG3	2.08	0.53
1:O:1477:C:O2'	1:O:1478:U:H5'	2.08	0.53
1:O:1730:G:C5'	1:O:1731:C:C6	2.91	0.53
5:A:217:ARG:HH11	5:A:217:ARG:CG	2.20	0.53
16:M:182:LYS:O	16:M:194:ALA:HB2	2.07	0.53
1:O:1172:G:H1'	40:0:5505:HOH:O	2.09	0.53
1:O:1766:U:O2	1:O:1778:A:H5'	2.08	0.53
1:O:475:G:H5'	7:C:73:LEU:HD23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1184:C:H4'	33:I:126:LYS:HB3	1.89	0.53
33:I:93:GLN:HA	33:I:96:PHE:HE2	1.73	0.53
19:P:103:THR:O	19:P:107:GLU:HG3	2.08	0.53
1:0:12:U:H2'	1:0:13:G:H5'	1.91	0.53
1:0:1626:A:H2'	1:0:1627:G:O4'	2.08	0.53
1:0:653:C:H2'	1:0:654:A:C8	2.43	0.53
31:2:36:ASN:HB3	31:2:39:ARG:HG3	1.90	0.53
32:3:56:PRO:HA	40:3:9486:HOH:O	2.09	0.53
6:B:102:THR:HG21	6:B:182:VAL:O	2.07	0.53
6:B:320:GLN:HE21	6:B:321:PRO:HD2	1.73	0.53
8:D:36:ASN:HA	40:D:7500:HOH:O	2.07	0.53
8:D:95:THR:OG1	8:D:174:VAL:HG22	2.08	0.53
18:O:14:LEU:CD2	18:O:102:ILE:HD11	2.38	0.53
18:O:53:GLN:HG2	18:O:56:GLU:OE1	2.08	0.53
1:0:1066:U:H2'	1:0:1067:A:C8	2.44	0.53
1:0:1838:U:H1'	1:0:2644:C:H5'	1.91	0.53
1:0:2769:C:H2'	1:0:2770:G:C5'	2.39	0.53
30:1:25:LYS:HD2	31:2:48:ASP:CA	2.38	0.53
6:B:312:ARG:HD3	6:B:315:VAL:HG13	1.89	0.53
7:C:25:PRO:HG2	40:C:9126:HOH:O	2.09	0.53
15:L:119:THR:HG23	15:L:139:SER:OG	2.08	0.53
23:T:47:THR:HB	23:T:100:ASP:HB3	1.90	0.53
1:0:1077:G:H2'	1:0:1080:C:H42	1.73	0.53
1:0:1972:U:H2'	1:0:1973:A:H5'	1.91	0.53
1:0:2883:A:H2'	1:0:2884:G:O4'	2.09	0.53
9:E:3:VAL:CG2	9:E:49:ILE:HB	2.38	0.53
1:0:2694:A:H4'	9:E:91:PHE:CE1	2.44	0.53
1:0:151:A:H2'	1:0:152:A:O4'	2.08	0.53
1:0:2812:A:C2	1:0:2814:A:N6	2.70	0.53
1:0:516:A:H5'	40:0:6167:HOH:O	2.09	0.53
1:0:775:G:OP1	30:1:16:HIS:HE1	1.91	0.53
1:0:447:A:OP2	23:T:1:SER:HB2	2.08	0.53
7:C:233:THR:HG22	7:C:234:VAL:H	1.73	0.53
26:W:88:THR:HG22	26:W:90:TYR:HD1	1.72	0.53
28:Y:112:GLU:CD	28:Y:115:ARG:NH1	2.63	0.53
1:0:1786:C:OP1	19:P:74:GLN:HG2	2.09	0.53
1:0:545:G:C8	1:0:545:G:H5'	2.42	0.53
5:A:121:ALA:O	5:A:124:VAL:HG22	2.09	0.53
6:B:41:PHE:CD1	6:B:79:MET:HE2	2.44	0.53
14:K:49:LEU:HD12	14:K:80:ILE:HD13	1.90	0.53
18:O:97:SER:OG	18:O:100:GLN:HG3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1552:G:N2	1:0:1634:G:H1'	2.24	0.53
1:0:1667:A:H2'	1:0:1668:U:C6	2.44	0.53
1:0:1741:U:H3'	40:0:3363:HOH:O	2.09	0.53
30:1:1:THR:HA	40:1:9468:HOH:O	2.08	0.53
40:0:4793:HOH:O	31:2:38:LYS:HE3	2.08	0.53
19:P:16:VAL:HG13	19:P:20:ARG:NH1	2.24	0.53
1:0:1252:A:H2'	1:0:1253:C:O4'	2.09	0.52
1:0:204:A:C2'	1:0:205:U:H5'	2.39	0.52
1:0:362:G:H2'	1:0:363:A:C8	2.44	0.52
1:0:1836:A:H1'	30:1:1:THR:O	2.09	0.52
32:3:30:GLN:HG3	40:3:9452:HOH:O	2.09	0.52
5:A:95:PRO:HG2	5:A:98:GLU:HG2	1.91	0.52
8:D:62:ASP:HA	40:D:4233:HOH:O	2.08	0.52
10:F:48:VAL:HG12	10:F:97:ALA:CB	2.39	0.52
33:I:113:HIS:N	33:I:114:PRO:CD	2.72	0.52
1:0:1730:G:H5''	1:0:1731:C:H6	1.74	0.52
1:0:2361:A:H2'	1:0:2362:A:C8	2.44	0.52
1:0:2817:G:P	40:0:8435:HOH:O	2.67	0.52
7:C:107:ARG:NH1	7:C:107:ARG:HB3	2.24	0.52
7:C:194:PHE:CD2	7:C:234:VAL:HG11	2.43	0.52
33:I:138:THR:HG22	33:I:139:ILE:N	2.24	0.52
22:S:73:ASP:OD1	22:S:76:GLU:HG3	2.09	0.52
27:X:12:ILE:HD12	27:X:36:HIS:ND1	2.24	0.52
6:B:36:PRO:HB3	6:B:174:ARG:CB	2.40	0.52
9:E:10:ASP:HA	40:E:3707:HOH:O	2.08	0.52
17:N:86:LEU:HD21	17:N:180:LEU:CD1	2.40	0.52
21:R:114:VAL:HA	21:R:144:GLU:O	2.09	0.52
26:W:88:THR:CG2	26:W:89:ASP:N	2.69	0.52
40:0:5237:HOH:O	29:Z:13:ARG:HD3	2.09	0.52
4:5:77:PHE:CE1	4:5:79:BTN:H62	2.43	0.52
7:C:236:THR:HG22	7:C:239:ALA:CB	2.40	0.52
15:L:134:GLU:HG3	40:L:9452:HOH:O	2.09	0.52
26:W:13:MET:CE	26:W:17:ILE:HG22	2.39	0.52
26:W:29:VAL:O	26:W:30:ASN:HB2	2.10	0.52
5:A:43:VAL:HG21	5:A:59:GLU:HG3	1.90	0.52
7:C:246:ARG:NH1	40:C:9180:HOH:O	2.43	0.52
12:H:63:GLU:HA	40:H:9546:HOH:O	2.08	0.52
19:P:98:ILE:HD12	19:P:102:ARG:NE	2.25	0.52
1:0:2326:U:H4'	1:0:2412:G:C4'	2.40	0.52
1:0:2644:C:O2'	1:0:2645:U:H5'	2.08	0.52
1:0:1562:C:H42	1:0:2738:G:H1	1.58	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1:28:HIS:HD2	30:1:31:LYS:H	1.57	0.52
6:B:141:ARG:HG2	6:B:165:ARG:HA	1.90	0.52
6:B:41:PHE:CG	6:B:79:MET:HE2	2.45	0.52
18:O:78:ALA:C	18:O:98:LEU:HD13	2.30	0.52
25:V:12:THR:HG23	25:V:14:ALA:H	1.73	0.52
26:W:52:VAL:HG22	26:W:53:ALA:N	2.23	0.52
1:0:2502:C:H2'	1:0:2503:A:H5'	1.91	0.52
32:3:70:ARG:HB3	40:3:9508:HOH:O	2.09	0.52
17:N:24:LEU:HD22	40:Q:2847:HOH:O	2.10	0.52
1:0:1462:C:H2'	1:0:1463:A:C8	2.45	0.52
5:A:109:GLU:HG2	5:A:116:GLY:N	2.25	0.52
23:T:40:VAL:HG22	23:T:41:ARG:N	2.25	0.52
1:0:497:A:H2'	1:0:498:A:C5'	2.40	0.52
8:D:136:ARG:HB3	8:D:137:PRO:HD2	1.91	0.52
12:H:38:LYS:HE2	12:H:42:ASP:HB2	1.92	0.52
14:K:34:VAL:CG2	14:K:47:ALA:HB2	2.39	0.52
16:M:31:TRP:CA	16:M:34:GLU:HG3	2.40	0.52
1:0:2419:U:H5''	1:0:2420:G:H5'	1.91	0.52
2:9:3069:U:OP1	17:N:4:PRO:HG3	2.10	0.52
12:H:76:GLU:O	12:H:77:LEU:HD23	2.09	0.52
16:M:107:ARG:NH1	40:M:9378:HOH:O	2.43	0.52
23:T:19:ARG:HD3	23:T:67:LEU:O	2.10	0.52
40:K:7438:HOH:O	24:U:20:MET:HE1	2.09	0.52
28:Y:184:GLU:OE1	28:Y:204:ARG:NH1	2.43	0.52
1:0:1119:G:H2'	13:J:52:GLN:HE22	1.73	0.51
6:B:41:PHE:HB3	6:B:190:MET:CE	2.40	0.51
6:B:254:GLN:HG3	40:B:9531:HOH:O	2.10	0.51
8:D:65:GLU:HA	40:D:6752:HOH:O	2.08	0.51
13:J:130:VAL:HG12	13:J:131:THR:H	1.74	0.51
15:L:36:ASP:HB2	40:L:9431:HOH:O	2.09	0.51
28:Y:187:VAL:HG23	40:Y:9369:HOH:O	2.10	0.51
1:0:2320:U:H4'	1:0:2321:A:O4'	2.10	0.51
1:0:2645:U:OP2	1:0:2645:U:C6	2.63	0.51
1:0:497:A:H2'	1:0:498:A:H5'	1.91	0.51
1:0:899:C:H5'	40:0:3792:HOH:O	2.09	0.51
6:B:58:PRO:HA	6:B:63:GLU:OE2	2.11	0.51
11:G:64:ASN:N	11:G:64:ASN:HD22	2.07	0.51
12:H:63:GLU:O	12:H:67:LEU:HB2	2.09	0.51
13:J:71:TYR:CD1	13:J:72:PRO:HD2	2.45	0.51
2:9:3051:A:H5'	17:N:160:SER:CB	2.40	0.51
23:T:49:GLU:CB	23:T:59:GLU:HG2	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1118:A:C8	1:0:1118:A:C3'	2.86	0.51
1:0:2415:A:H2'	1:0:2416:G:H5'	1.91	0.51
30:1:21:ARG:HD2	30:1:37:CYS:SG	2.51	0.51
5:A:149:ASP:OD1	5:A:151:GLN:HB2	2.10	0.51
7:C:118:THR:CG2	7:C:137:PRO:HB3	2.40	0.51
7:C:127:ARG:CZ	7:C:225:PRO:HG2	2.40	0.51
7:C:236:THR:HA	40:C:9257:HOH:O	2.10	0.51
1:0:1159:G:H1	1:0:1208:C:H42	1.57	0.51
5:A:36:ASP:O	5:A:38:ILE:N	2.44	0.51
5:A:94:LEU:HD12	5:A:98:GLU:HB2	1.91	0.51
33:I:89:SER:HB3	33:I:97:VAL:CG2	2.40	0.51
24:U:9:CYS:O	24:U:52:THR:HG23	2.10	0.51
27:X:76:ARG:NH1	27:X:76:ARG:HG3	2.24	0.51
1:0:1234:U:N3	6:B:244:PRO:HB3	2.25	0.51
7:C:129:HIS:HD2	7:C:165:ASP:OD2	1.94	0.51
8:D:49:PRO:HB3	40:D:5828:HOH:O	2.10	0.51
9:E:34:TRP:O	13:J:127:ILE:HD11	2.11	0.51
16:M:99:ARG:NH2	16:M:170:ASN:HD22	2.00	0.51
17:N:67:ALA:HA	17:N:71:TRP:HB3	1.93	0.51
1:0:1384:C:H5'	27:X:30:MET:HG2	1.92	0.51
6:B:41:PHE:HB3	6:B:190:MET:HE3	1.93	0.51
6:B:199:TYR:CE2	6:B:268:ARG:HB2	2.46	0.51
1:0:926:A:H5'	15:L:39:GLU:OE2	2.09	0.51
1:0:1189:A:H3'	40:0:8193:HOH:O	2.10	0.51
1:0:1211:G:O2'	1:0:1212:C:H5'	2.10	0.51
1:0:317:A:H5''	23:T:52:ARG:HD2	1.92	0.51
40:0:5933:HOH:O	5:A:164:ARG:CZ	2.59	0.51
18:O:106:PRO:HG2	18:O:107:GLU:OE1	2.10	0.51
23:T:112:LEU:CD2	23:T:119:ALA:HB3	2.39	0.51
1:0:1209:C:H2'	1:0:1210:G:C8	2.45	0.51
1:0:2619:UR3:H6	1:0:2619:UR3:O5'	2.11	0.51
5:A:211:LYS:CG	5:A:212:PRO:HD2	2.30	0.51
10:F:36:THR:HG23	10:F:97:ALA:HB2	1.93	0.51
33:I:78:LEU:CD1	33:I:112:LYS:HZ2	2.24	0.51
18:O:73:ASP:HA	18:O:92:VAL:O	2.11	0.51
21:R:106:GLY:HA2	21:R:109:MET:HE3	1.92	0.51
21:R:39:THR:HG22	21:R:107:GLU:O	2.10	0.51
1:0:1484:G:H2'	40:0:9725:HOH:O	2.11	0.51
1:0:1669:A:H2'	1:0:1670:G:C8	2.46	0.51
1:0:248:A:H5'	1:0:249:G:OP2	2.11	0.51
11:G:67:LEU:O	11:G:71:LEU:HG	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:35:ARG:HB2	15:L:35:ARG:NH1	2.25	0.51
1:0:1886:A:O2'	29:Z:20:ARG:HB2	2.11	0.51
1:0:1160:G:HO2'	1:0:1190:G:H8	1.59	0.51
1:0:475:G:C5'	7:C:73:LEU:HD23	2.40	0.51
1:0:2694:A:H4'	9:E:91:PHE:HE1	1.76	0.51
12:H:56:GLN:HE21	12:H:126:ARG:HE	1.56	0.51
40:0:7340:HOH:O	16:M:178:LYS:HB2	2.11	0.51
17:N:66:LEU:HD11	17:N:175:LEU:HD21	1.92	0.51
1:0:308:U:H5'	23:T:97:ARG:NH2	2.26	0.51
1:0:1077:G:H2'	1:0:1080:C:N4	2.25	0.50
1:0:1218:U:H2'	1:0:1219:U:C6	2.46	0.50
1:0:1306:U:OP1	7:C:184:ARG:HD2	2.11	0.50
1:0:1717:A:H5''	19:P:54:LYS:HB2	1.92	0.50
1:0:2421:G:H2'	40:0:4646:HOH:O	2.10	0.50
1:0:2894:C:O2'	1:0:2895:C:H5'	2.10	0.50
2:9:3054:A:H2	40:9:3535:HOH:O	1.93	0.50
2:9:3054:A:O2'	2:9:3055:U:H5'	2.11	0.50
6:B:53:LEU:HD21	6:B:270:ILE:HD12	1.92	0.50
6:B:72:THR:HB	40:B:9600:HOH:O	2.11	0.50
13:J:45:VAL:HG11	13:J:121:LEU:CD2	2.40	0.50
14:K:115:ARG:HG3	14:K:116:GLU:N	2.27	0.50
15:L:145:LEU:O	15:L:145:LEU:HD23	2.11	0.50
22:S:29:ASP:OD1	22:S:31:ARG:NH1	2.44	0.50
29:Z:30:GLU:HG2	29:Z:33:MET:HE3	1.94	0.50
1:0:2016:U:H2'	1:0:2017:U:O4'	2.10	0.50
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.50
1:0:299:U:H5'	40:0:7775:HOH:O	2.11	0.50
1:0:432:G:O2'	1:0:433:C:H5'	2.11	0.50
6:B:265:LEU:CD2	6:B:316:ARG:HD3	2.41	0.50
7:C:236:THR:HG21	40:C:9184:HOH:O	2.10	0.50
8:D:104:PHE:CE2	8:D:166:ILE:HD13	2.46	0.50
33:I:87:THR:HG22	33:I:88:GLY:N	2.25	0.50
20:Q:75:ILE:HD13	20:Q:84:ILE:CD1	2.41	0.50
26:W:21:LEU:HD22	26:W:26:ILE:HD13	1.92	0.50
1:0:2296:C:H2'	1:0:2297:U:H6	1.77	0.50
1:0:285:A:H2'	1:0:286:U:O4'	2.11	0.50
31:2:20:ARG:HG3	31:2:39:ARG:HH21	1.76	0.50
40:0:7989:HOH:O	32:3:61:PRO:HG2	2.10	0.50
17:N:179:LEU:HD23	17:N:184:ILE:HD12	1.94	0.50
19:P:115:SER:HG	19:P:118:GLN:HG3	1.76	0.50
40:0:6777:HOH:O	28:Y:158:LYS:HD3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1198:U:H2'	1:0:1200:A:OP2	2.11	0.50
1:0:1333:U:H2'	1:0:1334:C:C6	2.47	0.50
1:0:2906:A:H5'	1:0:2907:C:O4'	2.12	0.50
8:D:25:MET:HE1	8:D:37:ALA:O	2.11	0.50
9:E:133:VAL:HG12	9:E:141:VAL:HG13	1.94	0.50
21:R:92:LEU:HD23	21:R:145:LEU:HD21	1.94	0.50
1:0:177:A:H2'	1:0:178:U:O4'	2.11	0.50
1:0:1972:U:H2'	1:0:1973:A:C5'	2.42	0.50
1:0:2326:U:H4'	1:0:2412:G:H4'	1.94	0.50
1:0:2816:A:H2'	40:0:8435:HOH:O	2.12	0.50
5:A:163:GLY:HA2	5:A:166:ASP:OD2	2.12	0.50
6:B:268:ARG:NH2	6:B:325:PRO:HG3	2.25	0.50
13:J:75:PRO:HG2	13:J:105:LEU:CD2	2.41	0.50
26:W:122:ARG:CZ	40:W:5817:HOH:O	2.58	0.50
2:9:3059:C:H2'	2:9:3060:C:C6	2.46	0.50
6:B:314:ALA:HB3	6:B:317:PRO:HG3	1.92	0.50
9:E:145:ALA:HB1	9:E:168:ILE:CD1	2.42	0.50
12:H:158:THR:HB	12:H:159:PRO:HD3	1.94	0.50
13:J:74:ARG:NH1	13:J:105:LEU:HD11	2.27	0.50
1:0:1992:U:OP2	14:K:66:ARG:HD2	2.11	0.50
16:M:82:ARG:O	16:M:84:LYS:N	2.44	0.50
21:R:69:LYS:HB2	21:R:72:VAL:HG23	1.92	0.50
1:0:1714:C:O2'	1:0:1715:C:H5'	2.11	0.50
1:0:2338:G:OP1	8:D:97:GLN:HG2	2.11	0.50
10:F:48:VAL:HG12	10:F:97:ALA:HB2	1.94	0.50
1:0:155:C:OP2	16:M:188:ARG:HD3	2.11	0.50
26:W:110:GLN:NE2	26:W:110:GLN:HA	2.27	0.50
26:W:5:VAL:HG22	26:W:32:CYS:HB2	1.93	0.50
28:Y:107:PRO:HD3	28:Y:182:PHE:CE1	2.46	0.50
1:0:123:U:H5'	40:0:7132:HOH:O	2.12	0.50
1:0:2769:C:H2'	1:0:2770:G:H5'	1.92	0.50
7:C:154:VAL:O	7:C:158:GLU:HG3	2.12	0.50
29:Z:10:ARG:HA	40:Z:9215:HOH:O	2.11	0.50
1:0:1751:G:C2'	1:0:1752:G:H5''	2.40	0.50
1:0:247:A:H2'	40:0:4495:HOH:O	2.11	0.50
1:0:2827:A:H2'	1:0:2828:G:O4'	2.12	0.50
2:9:3007:G:H4'	17:N:55:ASP:OD2	2.12	0.50
2:9:3042:C:O2	8:D:76:ARG:NH1	2.45	0.50
6:B:58:PRO:HA	6:B:63:GLU:CD	2.32	0.50
8:D:28:GLY:CA	8:D:69:ILE:HG23	2.35	0.50
1:0:962:C:H1'	17:N:5:ARG:HH12	1.75	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:126:PRO:HG2	28:Y:128:PHE:CZ	2.47	0.50
1:0:1745:G:H22	1:0:2033:G:H5'	1.77	0.49
2:9:3049:G:O2'	2:9:3050:G:H5'	2.11	0.49
7:C:57:PRO:HG2	7:C:73:LEU:HD13	1.93	0.49
8:D:25:MET:SD	8:D:40:ILE:HD11	2.51	0.49
10:F:13:GLU:OE1	10:F:77:VAL:HG13	2.12	0.49
18:O:96:VAL:CG1	18:O:100:GLN:HB2	2.40	0.49
19:P:13:VAL:HG11	19:P:40:VAL:CG1	2.42	0.49
1:0:204:A:H2'	1:0:205:U:H5'	1.93	0.49
1:0:2748:G:H1'	40:0:8408:HOH:O	2.11	0.49
1:0:926:A:O2'	15:L:41:HIS:HD2	1.95	0.49
1:0:951:A:C2'	1:0:952:G:H5'	2.41	0.49
6:B:310:ARG:HD2	40:B:9586:HOH:O	2.10	0.49
6:B:51:VAL:HG23	6:B:327:VAL:HG13	1.94	0.49
7:C:185:LYS:HD3	7:C:186:TYR:CE1	2.47	0.49
33:I:131:THR:O	33:I:135:LEU:HG	2.12	0.49
13:J:19:MET:HE2	13:J:79:PHE:HA	1.92	0.49
25:V:59:ILE:O	25:V:63:GLU:HG2	2.11	0.49
1:0:820:G:H5'	1:0:821:U:H5'	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
7:C:127:ARG:HD3	7:C:129:HIS:HE1	1.76	0.49
13:J:88:PRO:O	13:J:94:GLY:HA3	2.12	0.49
15:L:143:THR:CG2	15:L:144:ASP:N	2.75	0.49
17:N:119:GLN:O	17:N:123:ILE:HG13	2.12	0.49
17:N:89:GLY:O	17:N:92:ALA:HB3	2.12	0.49
28:Y:177:LYS:HD3	28:Y:181:GLY:O	2.12	0.49
1:0:1506:U:H5'	1:0:1506:U:H6	1.78	0.49
30:1:21:ARG:HD2	30:1:39:PHE:HB2	1.95	0.49
32:3:3:MET:O	32:3:90:PHE:HA	2.12	0.49
2:9:3095:C:O2'	2:9:3096:C:H5'	2.12	0.49
11:G:20:VAL:O	11:G:24:VAL:HG23	2.13	0.49
13:J:12:VAL:HG21	13:J:116:LEU:HD11	1.94	0.49
14:K:22:ASP:O	14:K:110:LYS:HE3	2.12	0.49
14:K:55:VAL:CG1	14:K:56:SER:N	2.74	0.49
23:T:106:GLU:HG3	40:T:4913:HOH:O	2.11	0.49
23:T:38:ARG:HG3	23:T:38:ARG:HH11	1.77	0.49
27:X:61:ARG:HH11	27:X:61:ARG:HG3	1.77	0.49
1:0:1056:U:H2'	1:0:1057:A:O4'	2.11	0.49
1:0:1503:U:H2'	1:0:1504:A:O4'	2.12	0.49
1:0:734:U:H1'	1:0:737:A:N6	2.27	0.49
32:3:25:VAL:HG22	32:3:68:LYS:HG3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:84:LEU:HD13	6:B:84:LEU:O	2.13	0.49
8:D:10:PHE:CE1	8:D:11:HIS:HB3	2.47	0.49
1:O:2333:G:P	8:D:56:ARG:HH22	2.36	0.49
8:D:56:ARG:N	40:D:6752:HOH:O	2.46	0.49
9:E:81:GLU:HA	9:E:133:VAL:O	2.12	0.49
14:K:125:ALA:C	14:K:127:ALA:H	2.14	0.49
10:F:38:LYS:NZ	16:M:3:SER:HA	2.27	0.49
1:O:1755:A:H2'	1:O:1756:G:O4'	2.12	0.49
1:O:288:A:H2'	1:O:289:G:C8	2.47	0.49
1:O:333:G:O2'	1:O:334:G:H5'	2.13	0.49
5:A:125:ASN:CB	5:A:158:VAL:HG12	2.42	0.49
24:U:39:ASN:ND2	24:U:44:ARG:HH11	2.10	0.49
25:V:1:THR:CG2	25:V:2:VAL:H	2.19	0.49
1:O:1119:G:H8	13:J:52:GLN:NE2	2.10	0.49
1:O:1878:G:O2'	1:O:1879:U:OP2	2.30	0.49
1:O:2453:G:H5''	40:L:9438:HOH:O	2.12	0.49
1:O:2531:U:O2'	1:O:2532:A:H5'	2.12	0.49
1:O:2735:U:H2'	1:O:2736:U:C6	2.47	0.49
1:O:830:G:O2'	1:O:831:U:H5'	2.13	0.49
1:O:960:G:H2'	1:O:960:G:N3	2.28	0.49
3:4:75:C:N4	3:4:76:PPU:H102	2.28	0.49
2:9:3078:G:N2	2:9:3102:G:H2'	2.28	0.49
5:A:94:LEU:HG	5:A:99:ILE:CD1	2.43	0.49
8:D:41:LEU:HA	8:D:44:ILE:CG2	2.43	0.49
10:F:34:ASN:HA	16:M:4:ALA:HB2	1.93	0.49
17:N:152:GLU:C	17:N:154:LEU:H	2.16	0.49
19:P:16:VAL:HG13	19:P:20:ARG:CZ	2.43	0.49
1:O:793:A:H5''	19:P:83:LYS:HG2	1.95	0.49
21:R:18:LEU:HB2	21:R:143:VAL:HG12	1.94	0.49
25:V:12:THR:HG23	25:V:14:ALA:N	2.27	0.49
25:V:1:THR:HG22	25:V:48:GLU:OE1	2.13	0.49
1:O:1666:C:H2'	1:O:1667:A:C5'	2.42	0.49
1:O:2032:U:C2'	1:O:2033:G:H5''	2.42	0.49
1:O:2781:U:H1'	9:E:139:GLU:OE2	2.12	0.49
1:O:669:G:O2'	1:O:670:G:H5'	2.12	0.49
5:A:94:LEU:N	5:A:94:LEU:HD23	2.28	0.49
12:H:148:GLU:HA	12:H:148:GLU:OE1	2.11	0.49
21:R:99:ALA:HB1	21:R:109:MET:HE3	1.92	0.49
23:T:41:ARG:NH1	23:T:41:ARG:HG2	2.27	0.49
23:T:69:LYS:O	23:T:71:VAL:HG23	2.13	0.49
1:O:2252:A:H2'	1:O:2253:G:O4'	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:190:ARG:NH2	5:A:207:GLN:OE1	2.46	0.49
6:B:41:PHE:CG	6:B:190:MET:HE3	2.47	0.49
8:D:172:VAL:CG1	8:D:173:GLU:H	2.18	0.49
8:D:37:ALA:O	8:D:40:ILE:HG12	2.12	0.49
9:E:11:VAL:HG12	9:E:12:ASP:N	2.26	0.49
9:E:80:TRP:O	9:E:134:SER:HA	2.13	0.49
20:Q:32:GLU:HA	20:Q:71:TYR:OH	2.13	0.49
21:R:84:ALA:O	21:R:88:PHE:HD1	1.96	0.49
26:W:122:ARG:HG3	26:W:152:ALA:O	2.13	0.49
1:O:2445:U:H2'	1:O:2446:G:C8	2.47	0.49
1:O:65:C:O2'	1:O:66:G:H5'	2.12	0.49
6:B:62:ARG:HA	6:B:65:MET:HE2	1.93	0.49
8:D:51:ARG:HD3	40:D:7636:HOH:O	2.13	0.49
12:H:69:ALA:HB2	12:H:153:ALA:HB2	1.94	0.49
17:N:155:GLU:O	17:N:156:GLU:HG3	2.12	0.49
17:N:164:ASP:OD2	17:N:167:ASP:HA	2.12	0.49
18:O:97:SER:H	18:O:100:GLN:HE21	1.59	0.49
28:Y:186:ARG:HH11	28:Y:186:ARG:HG2	1.76	0.49
1:O:1730:G:H5'	1:O:1731:C:H5	1.77	0.48
1:O:2265:U:H2'	1:O:2266:A:C8	2.48	0.48
30:1:25:LYS:HG3	31:2:49:GLU:H	1.77	0.48
12:H:170:ASN:N	12:H:170:ASN:ND2	2.61	0.48
1:O:2784:A:H1'	9:E:60:SER:OG	2.13	0.48
1:O:750:A:O3'	7:C:101:ASP:HB2	2.12	0.48
31:2:41:HIS:HD2	31:2:44:ARG:H	1.61	0.48
33:I:138:THR:HG22	33:I:139:ILE:H	1.78	0.48
14:K:28:GLU:HB3	14:K:59:LYS:HB2	1.94	0.48
16:M:99:ARG:HH21	16:M:170:ASN:ND2	2.02	0.48
5:A:167:LYS:HB2	29:Z:29:ILE:HD13	1.95	0.48
1:O:2809:G:H2'	1:O:2810:G:O4'	2.13	0.48
2:9:3024:U:H3'	2:9:3025:G:C5'	2.43	0.48
7:C:142:ASP:OD1	7:C:236:THR:HG23	2.14	0.48
8:D:99:ASP:HB3	8:D:103:ASN:H	1.77	0.48
15:L:97:VAL:HG12	15:L:98:GLU:O	2.13	0.48
1:O:2064:U:H5'	1:O:2652:U:O3'	2.13	0.48
1:O:399:C:H5'	16:M:179:GLY:O	2.13	0.48
1:O:426:G:H2'	1:O:427:C:O4'	2.13	0.48
1:O:1654:U:H2'	5:A:47:HIS:HD2	1.77	0.48
8:D:103:ASN:HD21	8:D:134:LEU:H	1.60	0.48
1:O:1242:A:C5'	13:J:82:THR:HG23	2.34	0.48
40:O:6232:HOH:O	14:K:87:ARG:CZ	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:36:ALA:HB1	40:M:9352:HOH:O	2.13	0.48
40:O:5270:HOH:O	17:N:21:HIS:HD2	1.94	0.48
20:Q:40:HIS:CD2	20:Q:60:THR:HG23	2.49	0.48
20:Q:75:ILE:CD1	20:Q:84:ILE:HD11	2.42	0.48
22:S:44:GLN:HE21	25:V:28:LEU:CD2	2.27	0.48
26:W:65:VAL:HA	26:W:68:THR:HG22	1.95	0.48
28:Y:144:ARG:NH1	40:Y:9374:HOH:O	2.46	0.48
1:O:2541:U:H3'	1:O:2541:U:C6	2.47	0.48
6:B:146:THR:C	6:B:148:PRO:HD3	2.34	0.48
8:D:134:LEU:CD1	8:D:166:ILE:HD11	2.41	0.48
10:F:117:GLU:C	10:F:119:ARG:H	2.17	0.48
21:R:96:VAL:HG13	21:R:106:GLY:HA3	1.96	0.48
1:O:1171:A:H2'	1:O:1172:G:H5'	1.94	0.48
1:O:2456:A:H2'	1:O:2457:U:C6	2.48	0.48
1:O:2779:G:H21	9:E:143:GLN:NE2	2.12	0.48
10:F:39:SER:HB3	10:F:45:ALA:HB2	1.96	0.48
12:H:3:ALA:HA	12:H:58:ARG:NH1	2.28	0.48
25:V:7:GLU:O	25:V:11:MET:HG3	2.13	0.48
27:X:61:ARG:HB2	27:X:65:ASN:O	2.14	0.48
1:O:1736:A:H1'	40:O:8069:HOH:O	2.13	0.48
30:1:28:HIS:CE1	30:1:31:LYS:HE2	2.49	0.48
32:3:42:ARG:HH11	32:3:42:ARG:HG3	1.79	0.48
13:J:39:VAL:HG11	13:J:107:ASN:CG	2.34	0.48
17:N:154:LEU:O	17:N:155:GLU:HB3	2.14	0.48
1:O:31:C:OP2	23:T:8:ARG:NH1	2.44	0.48
27:X:61:ARG:HD2	27:X:65:ASN:O	2.14	0.48
2:9:3064:C:C2'	2:9:3065:A:H5'	2.42	0.48
6:B:212:GLN:HB2	6:B:257:THR:CG2	2.38	0.48
12:H:116:ALA:O	12:H:117:PHE:C	2.52	0.48
12:H:58:ARG:O	12:H:62:LEU:HD22	2.14	0.48
23:T:61:GLU:HG3	40:T:3851:HOH:O	2.14	0.48
25:V:39:ALA:O	25:V:41:GLU:N	2.47	0.48
1:O:1044:C:H3'	1:O:1045:G:H5''	1.96	0.48
1:O:1730:G:C5'	1:O:1731:C:H6	2.26	0.48
1:O:2480:G:H3'	40:O:4750:HOH:O	2.14	0.48
1:O:241:A:C2	1:O:378:A:H4'	2.49	0.48
1:O:602:A:O2'	1:O:605:C:H4'	2.12	0.48
1:O:656:G:OP2	18:O:37:ARG:HD2	2.13	0.48
1:O:776:A:OP1	30:1:28:HIS:HE1	1.97	0.48
6:B:277:GLU:N	6:B:278:PRO:HD2	2.29	0.48
9:E:166:VAL:HG12	40:E:3134:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:47:THR:CG2	13:J:48:GLY:N	2.77	0.48
16:M:134:ILE:O	16:M:136:PRO:HD3	2.13	0.48
40:O:7242:HOH:O	17:N:4:PRO:HD2	2.12	0.48
26:W:88:THR:HG22	26:W:90:TYR:CD1	2.49	0.48
1:O:1236:A:C8	13:J:63:ILE:HD11	2.49	0.48
1:O:666:A:H2'	1:O:667:C:O4'	2.14	0.48
4:5:75:C:H2'	4:5:76:A:O4'	2.14	0.48
16:M:59:GLY:HA3	16:M:141:ILE:HD12	1.96	0.48
21:R:29:LYS:NZ	40:R:9449:HOH:O	2.47	0.48
22:S:57:THR:HG22	22:S:58:MET:N	2.28	0.48
27:X:9:VAL:HG13	27:X:88:GLU:OE1	2.14	0.48
1:O:1098:A:H2'	1:O:1099:G:O4'	2.14	0.47
1:O:1189:A:H1'	1:O:1209:C:C1'	2.44	0.47
1:O:2862:G:H4'	6:B:336:GLN:O	2.14	0.47
1:O:558:C:C2'	1:O:559:U:C5'	2.92	0.47
10:F:49:PHE:HE1	10:F:98:VAL:HG23	1.79	0.47
1:O:2504:A:H4'	12:H:71:ARG:HH11	1.80	0.47
6:B:91:PRO:O	13:J:144:THR:HG21	2.14	0.47
14:K:10:GLN:N	14:K:10:GLN:NE2	2.48	0.47
15:L:145:LEU:O	15:L:148:GLU:HG3	2.13	0.47
24:U:4:ARG:HH11	24:U:4:ARG:HG2	1.79	0.47
1:O:2253:G:O2'	1:O:2254:G:H5'	2.15	0.47
1:O:2719:A:C2	6:B:70:PRO:HG3	2.49	0.47
12:H:46:GLN:NE2	12:H:137:TYR:HE2	2.11	0.47
23:T:26:THR:HA	23:T:39:ASN:HB3	1.96	0.47
23:T:96:VAL:CG1	23:T:97:ARG:N	2.78	0.47
1:O:308:U:C4	1:O:342:C:H1'	2.49	0.47
30:1:25:LYS:CD	31:2:49:GLU:H	2.27	0.47
7:C:133:ARG:NH1	40:C:9220:HOH:O	2.47	0.47
12:H:38:LYS:HE2	12:H:42:ASP:CB	2.45	0.47
33:I:139:ILE:C	33:I:140:GLU:HG3	2.34	0.47
13:J:54:VAL:O	13:J:58:GLU:HG3	2.14	0.47
1:O:392:U:C5'	16:M:193:LYS:HB3	2.45	0.47
21:R:82:GLU:O	21:R:86:LYS:HG3	2.14	0.47
25:V:5:VAL:CG1	25:V:9:ARG:NH1	2.77	0.47
1:O:1058:A:H2'	1:O:1060:C:H5''	1.96	0.47
1:O:1149:U:H5''	1:O:1151:G:O4'	2.14	0.47
1:O:210:U:H2'	1:O:211:U:C6	2.49	0.47
1:O:2626:C:H2'	1:O:2627:G:C8	2.50	0.47
1:O:347:A:H2'	1:O:348:C:O4'	2.14	0.47
32:3:11:CYS:HB2	32:3:20:HIS:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:3076:G:H3'	2:9:3077:A:C5'	2.26	0.47
6:B:254:GLN:NE2	40:B:9587:HOH:O	2.44	0.47
9:E:31:ARG:HH12	9:E:68:HIS:CG	2.31	0.47
9:E:49:ILE:HD11	9:E:69:ILE:HD12	1.96	0.47
12:H:77:LEU:HD12	12:H:83:TYR:CD2	2.49	0.47
18:O:39:THR:O	18:O:115:ARG:NH2	2.47	0.47
21:R:119:VAL:HG12	21:R:119:VAL:O	2.13	0.47
22:S:57:THR:CG2	22:S:58:MET:N	2.77	0.47
1:0:912:A:C4	1:0:1294:A:C2	3.02	0.47
1:0:1878:G:O2'	1:0:1879:U:P	2.72	0.47
32:3:17:HIS:O	32:3:18:GLN:HG3	2.15	0.47
5:A:123:GLY:HA3	5:A:162:GLY:CA	2.44	0.47
6:B:178:ALA:O	6:B:182:VAL:HG23	2.15	0.47
7:C:157:LEU:CD1	7:C:166:ILE:HD11	2.44	0.47
17:N:15:GLU:HB3	17:N:17:ARG:HD2	1.97	0.47
26:W:64:THR:O	26:W:68:THR:HG22	2.15	0.47
1:0:29:C:C2'	1:0:30:U:H5'	2.44	0.47
1:0:329:A:OP2	7:C:206:ASN:HB2	2.15	0.47
2:9:3003:A:H2'	40:9:2430:HOH:O	2.15	0.47
6:B:87:TYR:OH	6:B:163:GLU:OE2	2.30	0.47
1:0:1167:G:H4'	33:I:135:LEU:HD22	1.96	0.47
17:N:154:LEU:O	17:N:155:GLU:CB	2.63	0.47
19:P:141:ILE:C	19:P:143:ALA:H	2.17	0.47
29:Z:32:GLU:CD	29:Z:70:LYS:HZ2	2.18	0.47
1:0:834:G:H3'	1:0:835:U:H4'	1.97	0.47
1:0:2434:A:O3'	32:3:28:GLY:HA3	2.15	0.47
32:3:20:HIS:HA	32:3:70:ARG:O	2.15	0.47
7:C:140:VAL:HB	40:C:9257:HOH:O	2.14	0.47
8:D:173:GLU:HG3	8:D:174:VAL:N	2.30	0.47
16:M:165:GLY:O	16:M:169:ARG:HG3	2.15	0.47
17:N:7:LYS:HE3	20:Q:21:ARG:O	2.13	0.47
1:0:1667:A:C8	1:0:1667:A:H5'	2.40	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.97	0.47
1:0:2379:G:N3	1:0:2418:G:H2'	2.30	0.47
1:0:635:A:H2'	1:0:636:G:H5''	1.96	0.47
1:0:999:C:H2'	1:0:1000:C:O4'	2.15	0.47
32:3:91:GLN:O	32:3:92:GLU:HB2	2.15	0.47
2:9:3048:C:H4'	17:N:141:ARG:HH21	1.79	0.47
6:B:75:GLU:C	6:B:77:PRO:HD3	2.35	0.47
10:F:14:ASP:O	10:F:18:GLU:HG3	2.14	0.47
10:F:60:VAL:O	10:F:60:VAL:CG1	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:142:ASN:O	13:J:144:THR:N	2.48	0.47
14:K:113:ILE:CG2	14:K:114:ALA:N	2.77	0.47
15:L:53:ARG:HH22	15:L:57:VAL:HG12	1.80	0.47
16:M:86:GLN:O	16:M:88:VAL:HG23	2.15	0.47
21:R:132:ARG:NH2	40:R:9489:HOH:O	2.46	0.47
22:S:38:ALA:O	22:S:42:GLU:HG3	2.15	0.47
24:U:49:LEU:HG	40:U:3805:HOH:O	2.14	0.47
25:V:64:GLY:O	25:V:65:ASP:CB	2.62	0.47
27:X:7:GLU:HA	27:X:74:ALA:O	2.15	0.47
1:0:1158:G:O2'	1:0:1159:G:H5'	2.15	0.47
1:0:1787:C:OP1	19:P:68:LYS:HE2	2.14	0.47
1:0:1921:A:O2'	1:0:1922:A:H5'	2.15	0.47
1:0:764:C:H2'	1:0:765:G:O4'	2.15	0.47
2:9:3029:C:C2'	2:9:3030:C:H5'	2.44	0.47
6:B:215:VAL:HA	6:B:220:VAL:HG22	1.97	0.47
6:B:294:TYR:HE2	40:B:9643:HOH:O	1.97	0.47
33:I:102:VAL:O	33:I:106:LYS:HG3	2.14	0.47
33:I:75:THR:HA	33:I:112:LYS:NZ	2.29	0.47
13:J:19:MET:CE	13:J:132:LEU:HD21	2.44	0.47
1:0:171:C:OP2	16:M:84:LYS:HG3	2.14	0.47
17:N:167:ASP:C	17:N:168:LEU:HG	2.35	0.47
17:N:17:ARG:HB3	17:N:17:ARG:NH1	2.27	0.47
17:N:64:SER:C	17:N:66:LEU:H	2.18	0.47
26:W:149:LEU:HG	26:W:153:MET:HE2	1.96	0.47
1:0:1681:G:H5''	1:0:1682:A:H5'	1.97	0.47
1:0:447:A:O2'	1:0:448:G:H5'	2.15	0.47
5:A:69:LEU:HD23	5:A:107:ASN:CB	2.45	0.47
40:0:5212:HOH:O	6:B:300:SER:HB3	2.15	0.47
9:E:5:LEU:HD21	9:E:66:GLN:HG3	1.95	0.47
9:E:77:THR:OG1	9:E:78:GLU:N	2.47	0.47
14:K:7:ASP:OD2	14:K:81:ARG:NH2	2.48	0.47
15:L:97:VAL:HB	15:L:100:ALA:HB2	1.97	0.47
15:L:21:ARG:N	40:L:9425:HOH:O	2.47	0.47
24:U:52:THR:HG22	24:U:54:THR:H	1.79	0.47
27:X:80:GLU:HG2	27:X:80:GLU:O	2.15	0.47
1:0:1299:G:N7	15:L:6:ARG:NH1	2.63	0.47
1:0:1634:G:H3'	40:0:4467:HOH:O	2.14	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.43	0.47
1:0:1783:A:O2'	1:0:1784:U:H5'	2.15	0.47
1:0:2506:A:O2'	1:0:2507:G:O5'	2.33	0.47
9:E:157:LYS:HD2	9:E:162:PHE:CZ	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:58:GLU:HA	10:F:61:MET:HG3	1.97	0.47
33:I:72:VAL:CG1	33:I:73:PRO:HD2	2.45	0.47
13:J:52:GLN:HG3	13:J:53:ILE:N	2.30	0.47
22:S:53:ASN:ND2	40:S:9479:HOH:O	2.49	0.47
1:0:1268:C:O2'	28:Y:169:ARG:HB2	2.15	0.47
1:0:1192:A:H3'	1:0:1193:A:H5'	1.96	0.46
1:0:1794:G:N2	1:0:1796:A:H3'	2.30	0.46
1:0:2374:A:H2'	1:0:2375:G:C8	2.51	0.46
1:0:451:C:O2'	1:0:452:G:H5'	2.15	0.46
1:0:657:G:OP1	7:C:27:ARG:NH2	2.30	0.46
7:C:153:VAL:O	7:C:157:LEU:HG	2.15	0.46
1:0:894:A:N1	7:C:87:ARG:NH2	2.63	0.46
8:D:154:LYS:HD2	8:D:154:LYS:N	2.30	0.46
8:D:65:GLU:HG3	40:D:6752:HOH:O	2.14	0.46
33:I:100:LEU:O	33:I:139:ILE:HG23	2.15	0.46
17:N:38:LYS:HD3	17:N:107:ASN:ND2	2.29	0.46
28:Y:155:ARG:NH1	40:Y:9355:HOH:O	2.49	0.46
1:0:1180:U:H1'	40:I:1549:HOH:O	2.14	0.46
1:0:136:C:H2'	1:0:137:U:O4'	2.14	0.46
1:0:1406:A:H5'	1:0:1407:A:C8	2.51	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
1:0:2270:G:H4'	5:A:223:ARG:NH1	2.30	0.46
1:0:449:A:N7	7:C:43:LYS:HG2	2.31	0.46
1:0:603:A:H1'	1:0:605:C:C2	2.50	0.46
32:3:65:THR:HG22	32:3:67:LEU:CG	2.42	0.46
7:C:35:VAL:HG21	7:C:227:GLY:HA2	1.96	0.46
8:D:166:ILE:HB	40:D:6326:HOH:O	2.14	0.46
8:D:88:LEU:HB2	8:D:89:PRO:HD3	1.97	0.46
10:F:102:GLY:O	10:F:103:GLU:HB2	2.15	0.46
33:I:112:LYS:C	33:I:114:PRO:HD2	2.35	0.46
14:K:81:ARG:HD3	14:K:87:ARG:CZ	2.44	0.46
23:T:75:GLU:O	23:T:76:ASP:HB2	2.16	0.46
1:0:56:G:H5''	25:V:50:ARG:NH1	2.31	0.46
40:0:5814:HOH:O	26:W:122:ARG:NH2	2.47	0.46
1:0:1307:A:H2'	1:0:1308:A:C8	2.49	0.46
1:0:1679:C:H5'	40:0:9938:HOH:O	2.16	0.46
5:A:65:ARG:HH11	5:A:65:ARG:HG2	1.80	0.46
8:D:60:GLU:O	8:D:60:GLU:HG3	2.15	0.46
10:F:105:ASP:O	10:F:109:GLU:HB2	2.16	0.46
10:F:56:PRO:HB2	10:F:58:GLU:OE1	2.16	0.46
15:L:57:VAL:HG12	15:L:57:VAL:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:W:88:THR:HG23	26:W:110:GLN:HB3	1.97	0.46
1:O:1799:G:H21	19:P:88:GLN:NE2	2.14	0.46
1:O:2453:G:H5'	40:O:5233:HOH:O	2.16	0.46
40:O:3854:HOH:O	6:B:222:LYS:HE2	2.16	0.46
6:B:62:ARG:HG2	6:B:65:MET:HE3	1.97	0.46
7:C:218:VAL:HG12	40:C:9232:HOH:O	2.16	0.46
8:D:172:VAL:CG1	8:D:173:GLU:N	2.78	0.46
13:J:131:THR:HG22	13:J:133:GLY:N	2.30	0.46
25:V:29:ASN:O	25:V:33:VAL:HG23	2.16	0.46
25:V:4:HIS:O	25:V:8:ILE:HG13	2.15	0.46
1:O:1435:U:H5'	40:O:3203:HOH:O	2.15	0.46
1:O:2072:G:H3'	1:O:2073:G:C5'	2.45	0.46
4:5:78:ACA:H61	4:5:79:BTN:H101	1.60	0.46
6:B:41:PHE:HA	6:B:79:MET:CE	2.45	0.46
8:D:58:VAL:N	8:D:62:ASP:O	2.45	0.46
10:F:57:GLU:O	10:F:61:MET:HG3	2.15	0.46
24:U:45:GLU:HB2	24:U:48:ASN:HD22	1.78	0.46
27:X:72:VAL:CG2	27:X:85:VAL:HG12	2.42	0.46
28:Y:102:LEU:HD11	28:Y:225:GLY:HA2	1.97	0.46
1:O:1014:A:H2'	1:O:1015:C:H5'	1.97	0.46
1:O:2587:OMU:H6	1:O:2587:OMU:O5'	2.16	0.46
1:O:702:G:O2'	1:O:703:G:H5'	2.16	0.46
30:1:56:GLU:HG2	30:1:56:GLU:OXT	2.16	0.46
6:B:14:GLY:HA2	6:B:15:PRO:C	2.36	0.46
18:O:26:TRP:N	40:O:3062:HOH:O	2.49	0.46
26:W:4:LEU:CD2	26:W:52:VAL:HG21	2.39	0.46
1:O:1636:G:O2'	1:O:1637:A:H5'	2.15	0.46
1:O:1789:G:O6	19:P:73:HIS:HE1	1.99	0.46
1:O:2511:A:H2'	1:O:2512:U:O4'	2.15	0.46
1:O:319:A:H4'	1:O:338:C:C5	2.49	0.46
6:B:215:VAL:HB	6:B:234:ARG:HH12	1.81	0.46
7:C:236:THR:O	7:C:237:GLU:C	2.53	0.46
8:D:10:PHE:CG	8:D:11:HIS:N	2.84	0.46
12:H:45:VAL:HA	12:H:167:PRO:O	2.15	0.46
12:H:58:ARG:HG3	12:H:58:ARG:NH1	2.30	0.46
33:I:103:ASP:HA	33:I:106:LYS:HD2	1.97	0.46
21:R:39:THR:CG2	21:R:107:GLU:O	2.63	0.46
23:T:71:VAL:HG13	23:T:91:LEU:O	2.16	0.46
28:Y:99:ALA:HB2	28:Y:233:TYR:CZ	2.51	0.46
29:Z:17:ARG:HD3	40:Z:9220:HOH:O	2.15	0.46
29:Z:39:CYS:SG	29:Z:41:ASN:HB3	2.55	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1778:A:H2'	1:0:1779:A:H5'	1.97	0.46
1:0:2524:G:H21	1:0:2526:C:N4	2.13	0.46
2:9:3057:A:H8	8:D:141:VAL:HG21	1.80	0.46
6:B:87:TYR:HD1	40:B:9575:HOH:O	1.99	0.46
7:C:236:THR:O	7:C:239:ALA:N	2.49	0.46
1:0:894:A:C2	7:C:87:ARG:NH2	2.83	0.46
33:I:99:ASP:O	33:I:100:LEU:HD23	2.16	0.46
13:J:71:TYR:CG	13:J:72:PRO:HD2	2.51	0.46
15:L:79:ASP:HB3	40:L:9453:HOH:O	2.15	0.46
17:N:183:ASP:O	17:N:184:ILE:O	2.34	0.46
21:R:114:VAL:HG13	21:R:114:VAL:O	2.15	0.46
26:W:142:ASP:HB2	40:W:6373:HOH:O	2.15	0.46
27:X:34:ARG:NH1	27:X:48:VAL:O	2.48	0.46
27:X:43:VAL:CG1	27:X:44:ASP:N	2.79	0.46
1:0:1015:C:H2'	1:0:1016:U:C6	2.51	0.46
1:0:2011:A:H4'	1:0:2012:U:O5'	2.16	0.46
1:0:2487:C:H5	40:0:5422:HOH:O	1.98	0.46
6:B:51:VAL:HG21	6:B:327:VAL:HG13	1.94	0.46
12:H:9:ILE:HD12	12:H:54:THR:HG22	1.97	0.46
14:K:87:ARG:NH1	40:K:4066:HOH:O	2.49	0.46
15:L:91:VAL:CG1	15:L:120:LEU:HD23	2.46	0.46
27:X:20:GLU:HG3	27:X:21:PRO:HD2	1.98	0.46
1:0:1200:A:H3'	40:0:6272:HOH:O	2.15	0.46
1:0:1298:U:H2'	1:0:1299:G:C8	2.50	0.46
1:0:1730:G:H5'	1:0:1731:C:C6	2.51	0.46
1:0:1799:G:H21	19:P:88:GLN:HE22	1.64	0.46
1:0:2372:A:H2'	1:0:2373:U:C6	2.51	0.46
1:0:2505:G:C2'	1:0:2506:A:H5'	2.46	0.46
1:0:802:G:H2'	1:0:803:C:C6	2.50	0.46
1:0:951:A:O2'	1:0:952:G:H5'	2.16	0.46
2:9:3064:C:H2'	2:9:3065:A:H5'	1.97	0.46
2:9:3092:G:H2'	2:9:3093:A:C8	2.51	0.46
1:0:1654:U:H2'	5:A:47:HIS:CD2	2.51	0.46
6:B:217:ARG:HG3	6:B:257:THR:CG2	2.46	0.46
7:C:107:ARG:NE	40:C:9266:HOH:O	2.32	0.46
10:F:107:ASP:O	10:F:111:ILE:HG13	2.16	0.46
25:V:45:ARG:HA	25:V:48:GLU:HB2	1.98	0.46
1:0:2904:U:H4'	27:X:8:ARG:NH1	2.31	0.46
28:Y:152:LYS:HB3	28:Y:160:LYS:HG3	1.98	0.46
1:0:1250:C:O2'	1:0:1251:C:H5'	2.16	0.45
1:0:1878:G:O2'	1:0:1879:U:C5	2.61	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:6:ARG:HA	32:3:20:HIS:O	2.16	0.45
5:A:217:ARG:NH1	5:A:217:ARG:CG	2.78	0.45
5:A:232:ARG:NH2	5:A:236:GLY:O	2.45	0.45
5:A:39:ALA:HB3	5:A:61:GLU:OE2	2.16	0.45
1:0:2346:C:H4'	8:D:52:THR:CG2	2.47	0.45
12:H:54:THR:O	12:H:55:VAL:HG13	2.16	0.45
14:K:101:ASN:O	14:K:102:GLU:HB2	2.17	0.45
26:W:21:LEU:HD13	26:W:26:ILE:HD11	1.99	0.45
26:W:3:ALA:O	26:W:54:PHE:HA	2.16	0.45
1:0:1067:A:H5'	40:0:4906:HOH:O	2.15	0.45
1:0:2338:G:H2'	8:D:129:ASP:OD1	2.16	0.45
6:B:42:ALA:H	6:B:79:MET:HE2	1.81	0.45
6:B:86:ALA:HA	40:B:9575:HOH:O	2.15	0.45
7:C:5:ILE:HG13	7:C:15:GLU:HA	1.99	0.45
7:C:78:ARG:CG	7:C:78:ARG:NH1	2.76	0.45
13:J:8:ALA:HA	13:J:35:THR:HG22	1.98	0.45
26:W:11:VAL:O	26:W:12:ASN:HB2	2.15	0.45
26:W:59:GLN:NE2	26:W:97:ALA:HB3	2.32	0.45
28:Y:117:LEU:HA	28:Y:174:VAL:HG11	1.98	0.45
1:0:1942:A:H3'	40:0:7785:HOH:O	2.16	0.45
1:0:1980:U:H5'	1:0:2626:C:H1'	1.98	0.45
1:0:2356:A:H2'	1:0:2357:G:O4'	2.16	0.45
5:A:130:THR:HB	5:A:137:VAL:HB	1.97	0.45
12:H:43:TYR:HA	12:H:44:PRO:HD3	1.77	0.45
17:N:110:THR:HB	17:N:113:SER:HG	1.80	0.45
19:P:10:ALA:HA	19:P:13:VAL:HG12	1.98	0.45
1:0:1182:C:H1'	1:0:1192:A:C8	2.45	0.45
1:0:1205:U:H2'	1:0:1206:U:H5''	1.99	0.45
1:0:1441:G:H1'	40:0:8275:HOH:O	2.16	0.45
1:0:1603:A:H5''	1:0:1605:G:H5'	1.98	0.45
1:0:2003:U:H4'	1:0:2004:U:H5	1.80	0.45
1:0:2072:G:C6	1:0:2533:C:H1'	2.52	0.45
1:0:558:C:H2'	1:0:559:U:H5''	1.97	0.45
1:0:737:A:H2'	1:0:738:G:O4'	2.16	0.45
6:B:168:GLY:O	6:B:169:GLY:O	2.35	0.45
8:D:167:GLU:C	8:D:169:THR:H	2.20	0.45
33:I:116:LEU:HD22	33:I:127:GLU:OE1	2.17	0.45
16:M:66:SER:HB3	16:M:128:TRP:CD1	2.51	0.45
28:Y:107:PRO:HB3	28:Y:182:PHE:CE2	2.51	0.45
1:0:2672:C:O2'	1:0:2673:U:H5'	2.16	0.45
1:0:2747:C:H4'	40:0:8429:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:27:U:H2'	1:0:28:G:O4'	2.17	0.45
1:0:447:A:OP1	23:T:2:LYS:HG2	2.16	0.45
6:B:97:LEU:HD21	40:B:9637:HOH:O	2.17	0.45
1:0:2101:A:H2'	7:C:63:SER:OG	2.16	0.45
15:L:90:ARG:NH2	15:L:121:ILE:HD11	2.32	0.45
16:M:68:ARG:O	16:M:68:ARG:HD3	2.17	0.45
17:N:154:LEU:CG	17:N:155:GLU:H	2.25	0.45
17:N:73:ALA:HB1	17:N:74:PRO:CD	2.46	0.45
1:0:1180:U:H2'	1:0:1181:A:C8	2.51	0.45
2:9:3041:C:C6	8:D:50:VAL:HG21	2.51	0.45
2:9:3045:A:H4'	8:D:143:LYS:O	2.16	0.45
9:E:95:VAL:HG11	9:E:131:LEU:HD11	1.97	0.45
9:E:31:ARG:HH12	9:E:68:HIS:CE1	2.35	0.45
9:E:69:ILE:HA	9:E:72:MET:CE	2.47	0.45
12:H:136:ALA:HB3	12:H:146:VAL:HG21	1.97	0.45
33:I:89:SER:HB2	33:I:95:ASP:HB2	1.99	0.45
13:J:131:THR:HB	13:J:134:GLU:OE1	2.16	0.45
15:L:143:THR:CG2	15:L:144:ASP:H	2.23	0.45
15:L:77:ALA:C	15:L:79:ASP:H	2.20	0.45
23:T:78:THR:HB	23:T:87:VAL:O	2.17	0.45
22:S:10:VAL:HG11	25:V:36:ALA:CA	2.45	0.45
25:V:8:ILE:HG21	25:V:59:ILE:HG13	1.98	0.45
1:0:1163:G:H2'	1:0:1164:U:C5	2.52	0.45
5:A:223:ARG:CZ	40:A:9562:HOH:O	2.64	0.45
33:I:75:THR:OG1	33:I:112:LYS:HE2	2.17	0.45
15:L:101:ASP:C	15:L:103:ALA:H	2.20	0.45
20:Q:30:VAL:HG12	20:Q:30:VAL:O	2.17	0.45
40:0:6180:HOH:O	23:T:68:ASP:HB2	2.16	0.45
23:T:85:GLU:CG	23:T:86:GLU:N	2.79	0.45
24:U:14:GLU:OE1	24:U:15:PRO:HD2	2.17	0.45
26:W:108:ARG:CG	26:W:114:PRO:HG3	2.44	0.45
26:W:85:ALA:HB2	26:W:91:ASP:O	2.17	0.45
26:W:88:THR:CG2	26:W:90:TYR:HD1	2.29	0.45
1:0:1167:G:H2'	1:0:1168:C:O4'	2.17	0.45
1:0:1201:C:C2'	1:0:1202:A:H5'	2.43	0.45
1:0:1574:C:H2'	1:0:1575:C:C6	2.52	0.45
1:0:2256:G:H2'	1:0:2257:G:H5'	1.99	0.45
1:0:962:C:H5'	40:0:7430:HOH:O	2.16	0.45
5:A:131:HIS:O	5:A:132:ASP:HB2	2.17	0.45
7:C:133:ARG:NE	7:C:138:VAL:HG22	2.30	0.45
7:C:119:ALA:HA	7:C:137:PRO:HD3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:44:ILE:HG23	8:D:45:THR:HG23	1.99	0.45
20:Q:53:HIS:CE1	20:Q:55:ARG:HB2	2.52	0.45
23:T:71:VAL:HG12	23:T:72:ILE:H	1.82	0.45
1:O:1477:C:H5'	1:O:1868:G:C5'	2.47	0.45
1:O:790:A:H1'	1:O:1710:A:H2'	1.99	0.45
1:O:2250:G:OP1	5:A:31:LYS:HD3	2.17	0.45
1:O:1168:C:H5''	33:I:87:THR:HG23	1.99	0.45
14:K:80:ILE:O	14:K:87:ARG:HA	2.16	0.45
15:L:149:ARG:O	15:L:150:GLN:HB2	2.16	0.45
16:M:46:LEU:HD22	16:M:50:ARG:HG3	1.98	0.45
20:Q:40:HIS:HD2	20:Q:60:THR:HG23	1.82	0.45
21:R:119:VAL:CG1	21:R:119:VAL:O	2.64	0.45
28:Y:187:VAL:HG23	28:Y:192:ASP:HB3	1.98	0.45
1:O:1015:C:H2'	1:O:1016:U:H6	1.81	0.45
1:O:1180:U:H2'	1:O:1181:A:O4'	2.17	0.45
1:O:2256:G:C2'	1:O:2257:G:H5'	2.47	0.45
1:O:2541:U:C6	1:O:2541:U:C3'	3.00	0.45
1:O:622:G:P	28:Y:148:GLY:HA3	2.57	0.45
1:O:816:G:H5'	1:O:1598:A:H4'	1.97	0.45
1:O:907:A:H2'	1:O:908:A:C8	2.51	0.45
5:A:206:ARG:N	5:A:206:ARG:HD3	2.27	0.45
12:H:146:VAL:HG22	40:H:9543:HOH:O	2.17	0.45
16:M:120:VAL:CG1	16:M:130:GLU:HG3	2.46	0.45
16:M:158:ARG:HB2	16:M:163:LEU:HB2	1.97	0.45
18:O:47:ARG:HG3	18:O:47:ARG:NH1	2.32	0.45
19:P:16:VAL:HG12	19:P:17:GLY:H	1.80	0.45
24:U:4:ARG:NH1	24:U:4:ARG:HG2	2.32	0.45
28:Y:144:ARG:CG	28:Y:144:ARG:NH1	2.71	0.45
5:A:167:LYS:HE3	29:Z:26:VAL:HG13	1.99	0.45
1:O:1350:U:H2'	1:O:1351:G:O4'	2.17	0.44
1:O:2724:U:H2'	1:O:2725:G:O4'	2.17	0.44
1:O:2769:C:H2'	1:O:2770:G:O4'	2.17	0.44
4:5:76:A:OP1	4:5:76:A:H4'	2.17	0.44
5:A:105:VAL:HG12	5:A:106:CYS:H	1.82	0.44
6:B:175:LEU:C	6:B:175:LEU:HD23	2.37	0.44
6:B:41:PHE:CB	6:B:190:MET:HE3	2.47	0.44
9:E:170:ARG:HE	9:E:170:ARG:HB2	1.67	0.44
10:F:33:THR:HG21	10:F:59:ILE:O	2.17	0.44
15:L:89:PHE:CD1	15:L:89:PHE:N	2.85	0.44
17:N:49:THR:HG22	17:N:56:ASP:CB	2.39	0.44
18:O:24:ALA:O	18:O:28:ASP:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2365:G:H4'	20:Q:45:PRO:O	2.17	0.44
27:X:21:PRO:HG2	27:X:24:LYS:HD3	1.98	0.44
28:Y:163:THR:HB	40:Y:9397:HOH:O	2.16	0.44
1:0:1163:G:H1	1:0:1184:C:N4	2.15	0.44
1:0:2443:C:H5'	15:L:57:VAL:HG21	1.99	0.44
1:0:603:A:H4'	1:0:604:G:O5'	2.16	0.44
2:9:3001:U:H5''	2:9:3003:A:OP1	2.17	0.44
2:9:3049:G:H2'	2:9:3050:G:O4'	2.17	0.44
2:9:3056:A:C3'	2:9:3057:A:H5''	2.47	0.44
9:E:31:ARG:NH1	40:E:5919:HOH:O	2.49	0.44
10:F:28:ALA:HB3	10:F:99:THR:O	2.18	0.44
12:H:58:ARG:HG3	40:H:9520:HOH:O	2.18	0.44
14:K:115:ARG:O	14:K:118:ALA:HB3	2.16	0.44
15:L:145:LEU:C	15:L:145:LEU:HD23	2.38	0.44
1:0:1593:C:OP1	19:P:117:SER:HB3	2.17	0.44
25:V:42:ASN:O	25:V:44:GLY:N	2.50	0.44
1:0:2726:U:O2	1:0:2749:U:O5'	2.34	0.44
1:0:656:G:H1'	40:C:9267:HOH:O	2.17	0.44
1:0:794:U:H3	1:0:819:A:H61	1.64	0.44
6:B:113:LEU:HD21	6:B:161:VAL:HG21	1.98	0.44
6:B:185:GLY:HA2	40:B:9628:HOH:O	2.16	0.44
6:B:41:PHE:HA	6:B:79:MET:HE1	1.99	0.44
6:B:8:LYS:HG3	6:B:220:VAL:HG12	1.99	0.44
7:C:107:ARG:NH1	40:C:9238:HOH:O	2.50	0.44
7:C:115:LEU:O	7:C:118:THR:HB	2.17	0.44
9:E:22:VAL:O	9:E:28:SER:HA	2.17	0.44
33:I:97:VAL:N	33:I:136:GLY:O	2.51	0.44
13:J:39:VAL:CG1	13:J:40:ASN:N	2.81	0.44
27:X:41:PHE:O	27:X:43:VAL:HG23	2.16	0.44
27:X:73:ARG:HB2	27:X:88:GLU:OE2	2.17	0.44
1:0:1380:U:O4	1:0:2043:U:H4'	2.17	0.44
5:A:179:MET:HG2	5:A:186:TRP:CG	2.52	0.44
8:D:78:GLU:O	8:D:82:GLU:HG3	2.18	0.44
10:F:5:ASP:O	10:F:119:ARG:NH1	2.50	0.44
13:J:42:GLU:O	13:J:131:THR:HG23	2.18	0.44
15:L:35:ARG:HB2	15:L:35:ARG:HH11	1.82	0.44
1:0:154:C:P	16:M:188:ARG:HH12	2.40	0.44
19:P:143:ALA:HA	40:P:164:HOH:O	2.17	0.44
1:0:2100:A:H4'	7:C:64:GLY:O	2.16	0.44
1:0:2541:U:C2	1:0:2620:U:O4	2.71	0.44
1:0:2857:C:H2'	1:0:2858:U:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:407:A:H5'	40:0:6529:HOH:O	2.18	0.44
1:0:82:C:OP1	23:T:67:LEU:HB2	2.18	0.44
2:9:3114:G:O6	17:N:11:ARG:HD3	2.17	0.44
12:H:29:ALA:C	12:H:30:GLN:HG3	2.38	0.44
1:0:1104:C:H4'	13:J:88:PRO:HD3	1.99	0.44
1:0:1185:U:H5'	40:0:7899:HOH:O	2.18	0.44
1:0:1278:A:H4'	1:0:1279:U:C4	2.52	0.44
1:0:1552:G:H2'	1:0:1553:C:C6	2.52	0.44
1:0:2019:A:H5'	40:0:5087:HOH:O	2.17	0.44
1:0:256:C:H2'	1:0:257:G:O4'	2.17	0.44
6:B:53:LEU:CD1	6:B:327:VAL:HG22	2.46	0.44
6:B:85:ARG:HB2	6:B:99:GLU:HG2	1.99	0.44
33:I:92:PRO:O	33:I:94:GLU:N	2.50	0.44
18:O:60:VAL:HG12	18:O:62:GLY:H	1.81	0.44
23:T:71:VAL:CG1	23:T:72:ILE:N	2.80	0.44
25:V:56:ILE:HG22	25:V:60:GLN:NE2	2.32	0.44
40:0:3165:HOH:O	26:W:119:HIS:HE1	2.01	0.44
1:0:1266:U:H4'	28:Y:115:ARG:HH21	1.82	0.44
1:0:1162:G:H1'	33:I:117:LEU:CD1	2.47	0.44
1:0:1666:C:C2'	1:0:1667:A:C5'	2.96	0.44
1:0:2296:C:H2'	1:0:2297:U:C6	2.52	0.44
1:0:2533:C:H6	1:0:2533:C:C5'	2.25	0.44
1:0:2748:G:H4'	1:0:2749:U:C5'	2.47	0.44
1:0:371:U:H2'	1:0:372:A:H8	1.82	0.44
31:2:5:LYS:O	31:2:9:LYS:HG3	2.17	0.44
2:9:3012:C:H5'	2:9:3070:U:O4'	2.18	0.44
6:B:217:ARG:HD3	6:B:218:TRP:NE1	2.33	0.44
6:B:66:GLU:OE1	6:B:328:ARG:HD2	2.18	0.44
6:B:96:PRO:HG3	40:B:9629:HOH:O	2.17	0.44
7:C:1:MET:HG2	7:C:2:GLN:NE2	2.33	0.44
8:D:60:GLU:O	8:D:61:PHE:C	2.55	0.44
33:I:139:ILE:HG22	33:I:140:GLU:N	2.32	0.44
1:0:645:U:OP2	15:L:4:LYS:HE2	2.18	0.44
16:M:98:GLN:O	16:M:102:GLU:HG3	2.17	0.44
16:M:82:ARG:O	16:M:83:SER:C	2.56	0.44
25:V:5:VAL:HG23	40:V:2271:HOH:O	2.18	0.44
26:W:122:ARG:NE	40:W:5817:HOH:O	2.50	0.44
27:X:18:ARG:NH1	40:X:4132:HOH:O	2.50	0.44
27:X:9:VAL:HG13	27:X:88:GLU:OE2	2.17	0.44
28:Y:203:VAL:CG1	28:Y:228:VAL:HG22	2.48	0.44
1:0:1044:C:H5''	40:0:9648:HOH:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1350:U:H1'	40:0:3273:HOH:O	2.17	0.44
1:0:2335:C:H2'	1:0:2336:G:H8	1.83	0.44
1:0:2712:G:H5'	40:K:4183:HOH:O	2.17	0.44
1:0:2895:C:H4'	40:X:4132:HOH:O	2.18	0.44
1:0:29:C:O2'	1:0:30:U:H5'	2.18	0.44
1:0:656:G:H4'	40:C:9167:HOH:O	2.18	0.44
5:A:103:VAL:O	5:A:105:VAL:HG23	2.18	0.44
1:0:1119:G:H8	13:J:52:GLN:HE22	1.66	0.44
1:0:1771:U:C4'	29:Z:20:ARG:HE	2.30	0.44
1:0:1139:U:H2'	1:0:1140:C:C6	2.53	0.44
1:0:1244:U:H2'	13:J:47:THR:HG21	1.99	0.44
1:0:1592:G:O2'	1:0:1593:C:O4'	2.34	0.44
1:0:2472:C:O2'	1:0:2634:G:H4'	2.18	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.81	0.44
6:B:71:VAL:CG1	6:B:296:LEU:HD22	2.48	0.44
12:H:55:VAL:HG12	40:H:9540:HOH:O	2.18	0.44
18:O:4:ASN:HA	18:O:5:PRO:HD3	1.90	0.44
40:0:4557:HOH:O	23:T:82:THR:HA	2.17	0.44
27:X:31:ILE:O	27:X:35:GLU:HG3	2.16	0.44
1:0:1053:G:OP1	12:H:12:PRO:HG3	2.18	0.43
1:0:2044:G:OP1	27:X:23:HIS:HE1	2.01	0.43
1:0:213:G:N2	1:0:225:G:H2'	2.33	0.43
1:0:556:C:H2'	1:0:557:C:C6	2.53	0.43
5:A:132:ASP:HB3	5:A:135:VAL:H	1.83	0.43
7:C:219:ASN:N	7:C:222:ASP:OD1	2.44	0.43
13:J:75:PRO:HB3	13:J:132:LEU:HB3	2.00	0.43
15:L:144:ASP:O	15:L:147:GLU:HB2	2.18	0.43
21:R:61:GLN:NE2	40:R:9449:HOH:O	2.50	0.43
23:T:38:ARG:HG3	23:T:38:ARG:NH1	2.32	0.43
1:0:1086:A:C6	26:W:11:VAL:HG11	2.52	0.43
27:X:61:ARG:HG3	27:X:61:ARG:NH1	2.33	0.43
29:Z:30:GLU:HA	29:Z:33:MET:HB3	1.99	0.43
1:0:157:G:H4'	16:M:95:LYS:HE2	1.99	0.43
1:0:2401:A:H2'	1:0:2402:A:C8	2.53	0.43
1:0:2503:A:OP1	12:H:151:ARG:NH2	2.42	0.43
1:0:338:C:H5''	40:C:9230:HOH:O	2.16	0.43
5:A:29:HIS:CD2	5:A:153:ARG:NH1	2.86	0.43
5:A:105:VAL:HG13	5:A:155:THR:O	2.18	0.43
6:B:279:THR:CG2	6:B:280:VAL:N	2.80	0.43
1:0:2548:C:OP2	6:B:5:ARG:NH2	2.51	0.43
19:P:55:LYS:CG	19:P:56:GLY:N	2.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Q:25:PRO:HA	20:Q:26:PRO:HD3	1.85	0.43
23:T:30:ASP:O	23:T:33:GLU:HB3	2.18	0.43
23:T:96:VAL:HG13	23:T:97:ARG:N	2.32	0.43
28:Y:106:THR:HG23	28:Y:107:PRO:HD2	1.98	0.43
28:Y:151:SER:HB3	28:Y:154:ARG:HB3	2.00	0.43
31:2:41:HIS:CD2	31:2:44:ARG:H	2.35	0.43
2:9:3057:A:C8	8:D:141:VAL:HG21	2.52	0.43
6:B:181:ILE:HG22	6:B:186:GLY:HA2	1.98	0.43
6:B:243:ASN:HA	6:B:244:PRO:C	2.37	0.43
8:D:88:LEU:N	8:D:89:PRO:CD	2.81	0.43
12:H:169:GLY:C	12:H:170:ASN:HD22	2.20	0.43
28:Y:216:ARG:HD2	40:Y:9368:HOH:O	2.16	0.43
29:Z:60:CYS:O	29:Z:61:ASP:HB2	2.18	0.43
1:0:1174:A:H62	1:0:1200:A:H2'	1.83	0.43
1:0:2568:A:H2'	1:0:2569:A:O4'	2.18	0.43
1:0:2787:C:H5	40:0:5178:HOH:O	2.01	0.43
1:0:661:G:C5	1:0:686:A:C2	3.06	0.43
5:A:123:GLY:HA2	5:A:159:VAL:O	2.18	0.43
40:0:5154:HOH:O	5:A:206:ARG:HD3	2.18	0.43
15:L:130:ARG:O	15:L:131:GLU:C	2.57	0.43
16:M:49:ALA:C	16:M:54:TYR:HB3	2.39	0.43
16:M:72:ALA:HB2	16:M:93:ARG:HG2	2.01	0.43
1:0:1289:C:O2'	1:0:1290:G:H5'	2.19	0.43
1:0:1482:A:O2'	1:0:1483:C:H5'	2.19	0.43
1:0:1928:C:C2'	1:0:1929:G:H5'	2.47	0.43
2:9:3042:C:H5'	2:9:3043:G:OP2	2.17	0.43
2:9:3044:A:O4'	8:D:76:ARG:NE	2.51	0.43
1:0:1884:G:O6	5:A:190:ARG:HD2	2.16	0.43
6:B:36:PRO:HB3	6:B:174:ARG:HB2	1.99	0.43
7:C:123:LEU:HA	7:C:123:LEU:HD23	1.86	0.43
7:C:142:ASP:CG	7:C:237:GLU:HB3	2.39	0.43
7:C:79:ARG:O	7:C:87:ARG:HG2	2.18	0.43
9:E:84:MET:CE	9:E:148:ILE:HD12	2.45	0.43
17:N:11:ARG:CG	17:N:14:ARG:NH1	2.73	0.43
17:N:71:TRP:CE3	17:N:175:LEU:HD22	2.53	0.43
20:Q:59:GLN:HB3	40:Q:6286:HOH:O	2.17	0.43
20:Q:64:GLU:OE1	20:Q:64:GLU:HA	2.18	0.43
26:W:106:THR:OG1	26:W:109:GLU:HG3	2.18	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.51	0.43
1:0:1511:U:O2'	1:0:1512:G:H5'	2.18	0.43
1:0:1657:A:H2'	1:0:1658:A:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2363:G:O3'	20:Q:11:ARG:NH1	2.51	0.43
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.43
1:0:2776:A:H2'	1:0:2777:G:O4'	2.18	0.43
1:0:415:A:O2'	1:0:416:G:H5'	2.19	0.43
1:0:588:G:O6	26:W:154:ARG:NH1	2.52	0.43
7:C:51:TYR:CD1	30:1:56:GLU:HB2	2.54	0.43
9:E:35:TYR:HB2	40:E:5715:HOH:O	2.18	0.43
10:F:11:ASP:O	10:F:14:ASP:HB2	2.17	0.43
12:H:47:ILE:HG21	40:H:9543:HOH:O	2.18	0.43
1:0:903:U:O4	15:L:18:HIS:HB2	2.17	0.43
21:R:104:PHE:HB3	21:R:109:MET:CE	2.49	0.43
26:W:110:GLN:HE21	26:W:110:GLN:HA	1.84	0.43
40:O:6985:HOH:O	28:Y:141:THR:HG23	2.19	0.43
1:0:1218:U:H2'	1:0:1219:U:H6	1.83	0.43
1:0:1878:G:O2'	1:0:1879:U:H6	1.98	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.19	0.43
30:1:53:LYS:HA	30:1:53:LYS:HD3	1.84	0.43
7:C:194:PHE:HA	7:C:234:VAL:HG13	2.01	0.43
10:F:60:VAL:HG13	10:F:63:ILE:HG13	2.01	0.43
12:H:56:GLN:HG2	12:H:126:ARG:HG2	2.00	0.43
12:H:83:TYR:C	12:H:83:TYR:CD1	2.92	0.43
33:I:132:CYS:C	33:I:134:SER:H	2.21	0.43
15:L:12:THR:HG21	15:L:16:GLY:O	2.18	0.43
16:M:107:ARG:CG	16:M:107:ARG:NH1	2.77	0.43
16:M:24:GLN:O	16:M:28:GLN:HG3	2.19	0.43
7:C:27:ARG:HD2	18:O:5:PRO:HD2	2.01	0.43
19:P:13:VAL:HG21	19:P:41:ARG:HG2	2.01	0.43
23:T:79:LEU:HG	23:T:89:ARG:HB2	2.01	0.43
26:W:146:ILE:HA	26:W:146:ILE:HD13	1.92	0.43
1:0:2856:A:P	27:X:15:ARG:HH22	2.42	0.43
1:0:1236:A:H2'	1:0:1237:U:O4'	2.19	0.43
1:0:2001:G:O2'	1:0:2002:C:H5'	2.19	0.43
1:0:2015:A:O2'	1:0:2016:U:H5'	2.19	0.43
1:0:830:G:H2'	1:0:831:U:C6	2.54	0.43
6:B:109:LEU:HD11	6:B:113:LEU:HD11	2.00	0.43
10:F:49:PHE:CB	10:F:83:LEU:HD11	2.49	0.43
10:F:52:GLU:HG3	10:F:77:VAL:O	2.19	0.43
33:I:132:CYS:C	33:I:134:SER:N	2.71	0.43
40:C:9167:HOH:O	18:O:3:THR:HG21	2.18	0.43
28:Y:112:GLU:OE2	28:Y:115:ARG:NH1	2.52	0.43
1:0:1979:G:HO2'	1:0:1980:U:P	2.41	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2676:C:H4'	13:J:70:PHE:HD1	1.83	0.43
1:0:660:A:H4'	1:0:661:G:O5'	2.19	0.43
1:0:710:G:N2	1:0:719:C:C2	2.87	0.43
1:0:907:A:H2'	1:0:908:A:H8	1.84	0.43
40:0:4966:HOH:O	5:A:11:ARG:CZ	2.67	0.43
5:A:217:ARG:HH11	5:A:217:ARG:HG3	1.84	0.43
12:H:166:SER:HB2	12:H:167:PRO:CD	2.48	0.43
1:0:1185:U:H4'	33:I:123:ASN:HB3	2.00	0.43
17:N:48:VAL:HG11	17:N:55:ASP:HB3	1.99	0.43
17:N:74:PRO:HG2	17:N:159:TYR:CE1	2.54	0.43
24:U:52:THR:CG2	24:U:54:THR:HB	2.49	0.43
26:W:108:ARG:HE	26:W:114:PRO:CG	2.32	0.43
1:0:2515:C:H2'	1:0:2516:G:O4'	2.19	0.43
1:0:821:U:H2'	1:0:822:C:H6	1.84	0.43
1:0:883:U:C2'	1:0:883:U:O2	2.65	0.43
7:C:46:TYR:CE2	7:C:98:ARG:NH1	2.87	0.43
10:F:101:ALA:HA	40:F:5413:HOH:O	2.19	0.43
12:H:2:PRO:HD2	12:H:5:MET:SD	2.58	0.43
13:J:39:VAL:HG21	13:J:107:ASN:ND2	2.34	0.43
14:K:13:GLU:OE1	14:K:44:LEU:HD12	2.19	0.43
19:P:105:LEU:CD2	19:P:137:LEU:HD21	2.49	0.43
19:P:55:LYS:HG2	19:P:56:GLY:N	2.33	0.43
25:V:5:VAL:HG11	25:V:9:ARG:NH1	2.33	0.43
28:Y:107:PRO:HB3	28:Y:182:PHE:CD2	2.54	0.43
1:0:818:A:O2'	29:Z:13:ARG:HD2	2.19	0.43
1:0:1008:C:H2'	1:0:1009:U:C6	2.54	0.42
1:0:185:G:H4'	1:0:186:A:H4'	2.00	0.42
1:0:2072:G:N2	40:0:7335:HOH:O	2.50	0.42
1:0:2088:C:H1'	1:0:2841:A:N1	2.34	0.42
1:0:2851:G:H4'	6:B:157:LYS:NZ	2.34	0.42
1:0:292:G:H2'	1:0:358:G:N2	2.33	0.42
5:A:207:GLN:O	5:A:208:HIS:HB3	2.19	0.42
6:B:102:THR:HG23	6:B:182:VAL:HG12	1.99	0.42
6:B:190:MET:CE	6:B:194:PHE:CD1	3.01	0.42
7:C:246:ARG:HB3	7:C:246:ARG:NH1	2.33	0.42
22:S:37:VAL:O	22:S:41:VAL:HG23	2.18	0.42
25:V:12:THR:OG1	25:V:13:PRO:HD2	2.19	0.42
1:0:797:A:O4'	29:Z:10:ARG:N	2.51	0.42
1:0:1151:G:OP1	11:G:63:ARG:NH1	2.52	0.42
1:0:1926:G:H2'	1:0:1927:A:C8	2.54	0.42
1:0:2748:G:H5'	40:0:7972:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:461:C:N3	1:0:479:G:H5'	2.34	0.42
1:0:920:C:H5'	1:0:921:G:C4	2.54	0.42
1:0:958:G:H2'	1:0:959:C:C6	2.53	0.42
31:2:44:ARG:HA	31:2:44:ARG:HD3	1.78	0.42
33:I:102:VAL:HG23	33:I:140:GLU:O	2.18	0.42
15:L:91:VAL:HG12	15:L:120:LEU:HD23	2.01	0.42
16:M:42:ARG:HA	16:M:43:PRO:HD3	1.87	0.42
40:9:5851:HOH:O	17:N:115:VAL:HG13	2.19	0.42
1:0:2866:U:C4	24:U:50:GLU:HB3	2.55	0.42
26:W:142:ASP:HB3	26:W:145:GLY:H	1.84	0.42
1:0:1182:C:C1'	1:0:1192:A:H8	2.30	0.42
1:0:1315:G:C4	28:Y:212:ARG:HB2	2.55	0.42
1:0:1363:G:OP1	7:C:76:ARG:NH2	2.48	0.42
1:0:1947:G:H2'	1:0:1948:G:H8	1.84	0.42
1:0:2134:G:C6	1:0:2258:A:C8	3.08	0.42
1:0:2663:U:O2	40:0:8435:HOH:O	2.22	0.42
1:0:37:A:H2'	1:0:38:G:C8	2.54	0.42
1:0:709:G:O2'	18:O:25:VAL:CG1	2.67	0.42
1:0:816:G:C6	1:0:817:G:N1	2.87	0.42
1:0:952:G:N3	1:0:2302:A:H2'	2.34	0.42
31:2:48:ASP:O	31:2:49:GLU:HB2	2.19	0.42
10:F:111:ILE:O	10:F:115:VAL:HG23	2.19	0.42
12:H:154:TYR:C	12:H:154:TYR:CD1	2.92	0.42
1:0:1819:G:H2'	1:0:1820:G:C4'	2.50	0.42
1:0:2415:A:O2'	17:N:29:SER:HB3	2.19	0.42
1:0:483:C:C4	1:0:484:A:C6	3.07	0.42
1:0:945:U:H2'	1:0:946:C:C6	2.55	0.42
32:3:18:GLN:OE1	32:3:73:GLU:HB3	2.19	0.42
6:B:69:VAL:HA	6:B:70:PRO:HD3	1.84	0.42
7:C:127:ARG:HG2	7:C:127:ARG:HH11	1.85	0.42
11:G:64:ASN:N	11:G:64:ASN:ND2	2.67	0.42
17:N:181:ASP:O	17:N:184:ILE:HG22	2.19	0.42
18:O:98:LEU:O	18:O:102:ILE:HG13	2.19	0.42
1:0:1257:C:H2'	1:0:1258:G:O4'	2.19	0.42
1:0:2064:U:H4'	1:0:2653:A:OP1	2.19	0.42
40:0:7289:HOH:O	7:C:175:LYS:HE3	2.19	0.42
13:J:132:LEU:HA	13:J:132:LEU:HD23	1.82	0.42
16:M:167:GLY:O	16:M:171:ARG:HG3	2.20	0.42
18:O:59:VAL:HG21	18:O:111:VAL:HG21	2.02	0.42
19:P:13:VAL:HG11	19:P:40:VAL:HG12	2.01	0.42
21:R:122:GLN:HB3	21:R:138:SER:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:S:33:SER:OG	22:S:36:GLU:HG3	2.19	0.42
22:S:51:GLN:HE21	22:S:53:ASN:ND2	1.90	0.42
23:T:14:ALA:HA	23:T:15:PRO:HD3	1.95	0.42
27:X:20:GLU:CG	27:X:21:PRO:HD2	2.49	0.42
29:Z:32:GLU:HA	29:Z:35:GLU:HG3	2.01	0.42
1:0:1342:C:O2'	1:0:1343:C:H5'	2.20	0.42
1:0:1574:C:H6	1:0:1574:C:O5'	2.02	0.42
1:0:2248:C:H3'	40:0:5967:HOH:O	2.18	0.42
1:0:2506:A:O2'	1:0:2507:G:P	2.77	0.42
1:0:2713:G:O2'	1:0:2714:U:H5'	2.20	0.42
1:0:2793:A:H2'	1:0:2794:G:H5'	2.00	0.42
1:0:325:U:H2'	1:0:326:G:H8	1.84	0.42
5:A:109:GLU:HG2	5:A:116:GLY:H	1.85	0.42
5:A:113:GLY:HA2	5:A:153:ARG:NH2	2.34	0.42
14:K:49:LEU:CD1	14:K:80:ILE:HD13	2.49	0.42
16:M:15:PRO:HA	16:M:20:LEU:HD23	2.02	0.42
2:9:3004:G:O2'	17:N:44:ARG:NH2	2.53	0.42
1:0:710:G:H5'	18:O:25:VAL:CG1	2.49	0.42
1:0:107:U:H2'	1:0:108:U:H5'	2.02	0.42
1:0:1298:U:H2'	1:0:1299:G:H8	1.85	0.42
1:0:1422:U:H2'	1:0:1423:C:C6	2.55	0.42
1:0:2911:C:O2'	1:0:2912:C:H5'	2.20	0.42
1:0:470:U:O2'	30:1:16:HIS:CD2	2.70	0.42
1:0:564:G:H1'	40:0:6803:HOH:O	2.18	0.42
2:9:3023:U:O2'	2:9:3024:U:H4'	2.19	0.42
7:C:133:ARG:HE	7:C:138:VAL:HG22	1.85	0.42
13:J:74:ARG:HH12	13:J:76:ASP:CB	2.30	0.42
17:N:36:ALA:HB1	17:N:118:ILE:HD12	2.02	0.42
18:O:38:ARG:NH1	40:O:7674:HOH:O	2.53	0.42
23:T:12:ARG:NH1	40:T:3035:HOH:O	2.47	0.42
25:V:1:THR:CG2	25:V:2:VAL:N	2.82	0.42
26:W:73:LEU:HA	26:W:73:LEU:HD12	1.83	0.42
1:0:1205:U:C2'	1:0:1206:U:H5''	2.50	0.42
1:0:271:C:C2	1:0:273:G:O4'	2.73	0.42
1:0:2821:C:H4'	6:B:116:PRO:HG3	2.01	0.42
1:0:64:G:H2'	1:0:65:C:O4'	2.20	0.42
2:9:3096:C:H2'	2:9:3097:U:C6	2.55	0.42
5:A:51:ARG:NH1	5:A:120:ARG:O	2.53	0.42
6:B:17:LYS:O	6:B:260:HIS:CD2	2.70	0.42
7:C:218:VAL:N	40:C:9232:HOH:O	2.52	0.42
10:F:67:ALA:HB1	10:F:72:VAL:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:14:TYR:CD2	12:H:94:VAL:HB	2.54	0.42
33:I:118:SER:HB2	33:I:123:ASN:HB2	2.02	0.42
15:L:6:ARG:NH2	40:L:9444:HOH:O	2.53	0.42
20:Q:94:GLN:O	20:Q:95:GLU:HB2	2.20	0.42
27:X:7:GLU:HA	27:X:75:ALA:HA	2.00	0.42
1:O:1733:A:H4'	6:B:212:GLN:HA	2.02	0.42
1:O:2716:G:H5''	6:B:206:THR:CG2	2.45	0.42
1:O:380:A:H2'	40:O:7673:HOH:O	2.19	0.42
1:O:695:C:H2'	1:O:696:C:C6	2.54	0.42
5:A:33:GLU:OE1	5:A:33:GLU:N	2.36	0.42
6:B:277:GLU:N	6:B:278:PRO:CD	2.82	0.42
10:F:99:THR:HG23	10:F:99:THR:O	2.19	0.42
11:G:23:ILE:O	11:G:27:ILE:HG13	2.20	0.42
12:H:51:VAL:CG1	12:H:53:GLU:O	2.67	0.42
14:K:20:CYS:HB2	14:K:29:LEU:HG	2.01	0.42
15:L:133:VAL:HB	40:L:9452:HOH:O	2.19	0.42
16:M:47:ASP:CG	16:M:48:LYS:N	2.73	0.42
17:N:173:ASP:O	17:N:177:GLU:HB2	2.20	0.42
2:9:3006:C:H4'	17:N:35:VAL:HG11	2.02	0.42
17:N:61:ALA:CB	17:N:88:ALA:HB2	2.48	0.42
22:S:51:GLN:NE2	22:S:53:ASN:HD21	1.90	0.42
29:Z:46:ARG:O	29:Z:57:CYS:HA	2.19	0.42
1:O:1314:U:H2'	40:O:6383:HOH:O	2.20	0.42
1:O:1367:A:H2'	1:O:1368:U:O4'	2.19	0.42
1:O:1940:C:H4'	40:O:7785:HOH:O	2.19	0.42
1:O:2089:A:O2'	1:O:2090:G:H5'	2.20	0.42
1:O:2456:A:H2'	1:O:2457:U:H6	1.85	0.42
1:O:2642:G:H2'	1:O:2643:G:O4'	2.20	0.42
1:O:1739:G:H1'	1:O:2726:U:O4	2.20	0.42
32:3:48:ASN:ND2	32:3:50:GLY:H	2.18	0.42
1:O:1363:G:P	7:C:76:ARG:HH22	2.43	0.42
8:D:10:PHE:CD1	8:D:11:HIS:N	2.88	0.42
11:G:63:ARG:HB2	11:G:66:LEU:HG	2.02	0.42
33:I:92:PRO:HD3	40:I:1549:HOH:O	2.19	0.42
15:L:104:ASP:HB2	40:L:9460:HOH:O	2.19	0.42
27:X:80:GLU:HB3	40:X:5564:HOH:O	2.19	0.42
1:O:1311:G:O2'	1:O:1312:G:H5'	2.20	0.41
1:O:1473:U:O2'	1:O:1474:C:H5''	2.20	0.41
1:O:226:A:H1'	1:O:393:G:C5	2.54	0.41
1:O:629:A:H2'	1:O:630:A:O4'	2.20	0.41
32:3:55:VAL:HB	32:3:56:PRO:HD2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:69:TYR:O	32:3:77:ALA:HA	2.19	0.41
5:A:122:SER:O	5:A:124:VAL:HG13	2.20	0.41
6:B:62:ARG:CA	6:B:65:MET:HE3	2.49	0.41
7:C:21:VAL:C	7:C:23:GLU:H	2.23	0.41
8:D:167:GLU:OE2	8:D:173:GLU:HB3	2.20	0.41
33:I:74:PRO:C	33:I:112:LYS:HZ1	2.23	0.41
1:0:1242:A:OP2	13:J:60:ARG:NH2	2.46	0.41
1:0:1380:U:O4	1:0:2748:G:O2'	2.28	0.41
1:0:1406:A:H4'	1:0:1407:A:H5''	2.01	0.41
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.41
1:0:2256:G:O2'	1:0:2257:G:H5'	2.21	0.41
1:0:2445:U:H2'	1:0:2446:G:H8	1.85	0.41
1:0:396:U:OP2	32:3:38:ARG:HD2	2.19	0.41
32:3:62:THR:HB	40:3:9487:HOH:O	2.20	0.41
5:A:36:ASP:O	5:A:36:ASP:CG	2.59	0.41
6:B:115:VAL:HA	6:B:116:PRO:HD3	1.93	0.41
40:0:7470:HOH:O	6:B:264:GLU:HG3	2.19	0.41
10:F:70:LYS:C	10:F:72:VAL:H	2.22	0.41
40:0:7460:HOH:O	20:Q:9:GLY:HA2	2.20	0.41
25:V:45:ARG:O	25:V:48:GLU:N	2.53	0.41
5:A:75:GLY:HA2	29:Z:64:PHE:HA	2.02	0.41
1:0:553:G:O4'	1:0:1325:G:H5'	2.20	0.41
1:0:1826:C:O2'	1:0:1827:G:H5'	2.20	0.41
1:0:195:C:H2'	1:0:196:G:H5'	2.01	0.41
6:B:171:VAL:HG23	6:B:172:SER:N	2.35	0.41
6:B:56:ASP:OD1	6:B:322:ARG:HB3	2.21	0.41
8:D:163:VAL:HA	40:D:6326:HOH:O	2.20	0.41
8:D:170:TYR:CD1	8:D:170:TYR:N	2.89	0.41
8:D:173:GLU:O	8:D:174:VAL:C	2.59	0.41
12:H:169:GLY:HA3	40:H:9557:HOH:O	2.20	0.41
33:I:80:LYS:HD3	33:I:86:GLU:O	2.20	0.41
19:P:16:VAL:CG1	19:P:17:GLY:N	2.83	0.41
26:W:38:THR:HG22	26:W:39:ASP:H	1.85	0.41
1:0:1086:A:N6	26:W:11:VAL:HG11	2.35	0.41
1:0:1120:U:H5'	1:0:1121:G:OP2	2.20	0.41
1:0:1174:A:C6	1:0:1201:C:H4'	2.55	0.41
1:0:1451:C:H5'	1:0:1505:U:C4	2.56	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.19	0.41
1:0:2362:A:H2'	1:0:2363:G:C8	2.56	0.41
16:M:81:ARG:HG2	16:M:85:ARG:O	2.19	0.41
18:O:14:LEU:HG	18:O:102:ILE:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:89:ASN:HB3	19:P:92:GLU:HB2	2.01	0.41
20:Q:28:ARG:HG2	40:Q:4350:HOH:O	2.20	0.41
24:U:47:ARG:HG2	24:U:54:THR:HG21	2.03	0.41
28:Y:154:ARG:HH11	28:Y:154:ARG:CG	2.34	0.41
1:0:1181:A:H2'	1:0:1182:C:H5'	2.03	0.41
1:0:1183:C:H5	1:0:1192:A:OP1	2.04	0.41
1:0:162:C:H2'	1:0:163:U:H5'	2.02	0.41
1:0:790:A:H1'	1:0:1710:A:O2'	2.21	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.55	0.41
1:0:20:G:H5''	1:0:510:U:O4	2.21	0.41
5:A:29:HIS:CD2	5:A:153:ARG:HH12	2.37	0.41
5:A:53:ALA:HB3	40:A:9591:HOH:O	2.20	0.41
15:L:145:LEU:C	15:L:147:GLU:H	2.23	0.41
15:L:73:VAL:HG23	15:L:74:THR:N	2.32	0.41
21:R:96:VAL:O	21:R:99:ALA:HB3	2.20	0.41
26:W:5:VAL:O	26:W:52:VAL:CG2	2.68	0.41
1:0:1524:U:HO2'	1:0:1525:G:P	2.44	0.41
1:0:1979:G:O2'	1:0:1980:U:OP1	2.30	0.41
1:0:2324:G:N2	1:0:2377:U:H1'	2.36	0.41
1:0:407:A:H8	40:0:5010:HOH:O	2.03	0.41
5:A:6:GLY:HA3	40:A:9557:HOH:O	2.20	0.41
5:A:36:ASP:HA	5:A:83:GLY:HA3	2.02	0.41
6:B:294:TYR:C	6:B:294:TYR:CD1	2.93	0.41
6:B:305:ASP:O	6:B:306:LYS:CB	2.67	0.41
6:B:81:ALA:HB1	6:B:142:LEU:HD13	2.03	0.41
33:I:110:GLU:HA	33:I:113:HIS:CD2	2.55	0.41
14:K:2:GLU:O	14:K:3:ALA:C	2.58	0.41
14:K:41:LYS:O	14:K:42:ASN:HB2	2.20	0.41
17:N:170:GLU:O	17:N:174:GLU:HG3	2.21	0.41
26:W:21:LEU:HD22	26:W:26:ILE:HD11	2.02	0.41
1:0:1535:G:H2'	1:0:1536:C:C6	2.56	0.41
1:0:2351:C:H2'	1:0:2352:G:O4'	2.21	0.41
1:0:440:C:H2'	1:0:441:A:C8	2.54	0.41
1:0:447:A:OP1	23:T:1:SER:HB2	2.21	0.41
30:1:8:GLN:HE22	30:1:11:LYS:HZ2	1.65	0.41
2:9:3039:U:O2'	2:9:3042:C:H5	2.03	0.41
5:A:30:ARG:HB3	5:A:30:ARG:HE	1.64	0.41
5:A:95:PRO:HA	5:A:153:ARG:HA	2.03	0.41
15:L:35:ARG:HD3	15:L:35:ARG:C	2.41	0.41
15:L:66:VAL:HG23	15:L:67:ARG:N	2.35	0.41
16:M:164:THR:CG2	16:M:166:ALA:H	2.32	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:N:108:SER:HA	17:N:109:PRO:HD3	1.80	0.41
18:O:45:LEU:CD1	18:O:88:LYS:HD2	2.51	0.41
29:Z:30:GLU:HG2	29:Z:33:MET:CE	2.51	0.41
1:O:1076:G:C2	1:O:1084:C:C2	3.09	0.41
1:O:1427:A:N6	1:O:1440:U:H1'	2.33	0.41
1:O:1594:C:O2'	1:O:1607:A:H4'	2.21	0.41
1:O:1849:G:H1'	1:O:2011:A:N1	2.35	0.41
1:O:2335:C:H2'	1:O:2336:G:C8	2.56	0.41
31:2:11:LEU:HA	31:2:11:LEU:HD23	1.91	0.41
31:2:39:ARG:HG2	40:2:3143:HOH:O	2.21	0.41
6:B:18:ARG:HE	6:B:256:GLN:NE2	2.19	0.41
7:C:61:PHE:HB3	40:C:9251:HOH:O	2.20	0.41
9:E:69:ILE:HA	9:E:72:MET:HE3	2.01	0.41
10:F:12:LEU:HD23	10:F:12:LEU:O	2.21	0.41
13:J:143:LYS:HA	13:J:145:TRP:CZ3	2.55	0.41
15:L:124:ASP:OD1	15:L:149:ARG:NH2	2.54	0.41
15:L:94:ARG:NH1	15:L:143:THR:HG21	2.36	0.41
16:M:76:ARG:HG3	16:M:88:VAL:HG21	2.03	0.41
40:O:3646:HOH:O	19:P:91:LYS:HA	2.21	0.41
21:R:33:ARG:NH1	40:R:9452:HOH:O	2.51	0.41
40:O:4333:HOH:O	23:T:9:LYS:HD2	2.20	0.41
25:V:43:PRO:O	25:V:46:ILE:HG22	2.19	0.41
1:O:1025:C:H5'	26:W:23:MET:O	2.21	0.41
26:W:5:VAL:O	26:W:52:VAL:HG23	2.20	0.41
29:Z:39:CYS:HA	29:Z:40:PRO:HD3	1.97	0.41
1:O:1821:A:O2'	1:O:1822:A:H5'	2.21	0.41
1:O:271:C:H41	1:O:378:A:H2	1.68	0.41
1:O:2748:G:H4'	1:O:2749:U:H5'	2.02	0.41
1:O:2819:C:O4'	6:B:96:PRO:HB2	2.21	0.41
1:O:2820:A:H2'	1:O:2821:C:C6	2.56	0.41
40:O:3421:HOH:O	6:B:252:PRO:HD3	2.21	0.41
6:B:27:ASN:H	6:B:27:ASN:HD22	1.69	0.41
6:B:41:PHE:CD1	6:B:79:MET:CE	3.04	0.41
8:D:23:VAL:O	8:D:23:VAL:HG23	2.21	0.41
10:F:79:GLN:HB2	10:F:82:ASP:OD2	2.21	0.41
33:I:92:PRO:C	33:I:94:GLU:N	2.72	0.41
33:I:93:GLN:HA	33:I:96:PHE:CE2	2.54	0.41
14:K:98:VAL:HG11	14:K:102:GLU:HA	1.99	0.41
1:O:392:U:H5''	16:M:193:LYS:HB3	2.01	0.41
19:P:134:VAL:O	19:P:137:LEU:HB3	2.21	0.41
23:T:81:LYS:HD2	23:T:87:VAL:HG11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:X:45:GLU:HG3	40:X:6178:HOH:O	2.21	0.41
1:0:1414:A:H2'	1:0:1415:G:O4'	2.20	0.41
1:0:2336:G:H1'	40:D:5675:HOH:O	2.20	0.41
1:0:284:C:H4'	1:0:285:A:H8	1.86	0.41
1:0:737:A:H3'	1:0:737:A:C8	2.56	0.41
1:0:1882:C:OP1	5:A:192:VAL:HG23	2.21	0.41
1:0:875:A:C2	5:A:194:MET:SD	3.14	0.41
5:A:65:ARG:NH1	5:A:65:ARG:HG2	2.36	0.41
5:A:66:ARG:HH11	5:A:66:ARG:CB	2.33	0.41
6:B:312:ARG:HG2	6:B:313:PRO:N	2.34	0.41
9:E:84:MET:HB2	9:E:131:LEU:HB2	2.03	0.41
1:0:1181:A:H4'	33:I:92:PRO:HG2	2.03	0.41
14:K:107:THR:HG22	14:K:108:GLU:CG	2.44	0.41
14:K:118:ALA:O	14:K:119:GLN:C	2.59	0.41
17:N:33:ARG:NH1	17:N:103:ASP:OD2	2.47	0.41
17:N:24:LEU:HD13	20:Q:26:PRO:HB3	2.02	0.41
26:W:54:PHE:CZ	26:W:140:LYS:HB2	2.55	0.41
27:X:30:MET:CE	27:X:58:ALA:HB3	2.50	0.41
29:Z:36:ASP:HB3	29:Z:45:ASP:O	2.21	0.41
1:0:1453:G:H2'	1:0:1454:U:O4'	2.21	0.41
1:0:1834:C:H2'	1:0:1840:A:N6	2.36	0.41
1:0:2767:C:OP1	6:B:318:ASN:ND2	2.54	0.41
1:0:2828:G:H2'	1:0:2829:G:O4'	2.21	0.41
1:0:791:A:H2'	1:0:792:G:O4'	2.21	0.41
30:1:28:HIS:O	30:1:32:LYS:N	2.49	0.41
31:2:20:ARG:HG3	31:2:21:VAL:H	1.86	0.41
2:9:3014:G:H2'	2:9:3015:C:H5'	2.03	0.41
15:L:120:LEU:HD12	15:L:133:VAL:HG21	2.02	0.41
18:O:14:LEU:HD23	18:O:102:ILE:HD11	2.02	0.41
18:O:60:VAL:C	18:O:62:GLY:H	2.24	0.41
21:R:68:HIS:CD2	21:R:76:ASP:HB2	2.56	0.41
24:U:17:THR:HG21	40:U:3194:HOH:O	2.21	0.41
26:W:4:LEU:HD23	26:W:54:PHE:HB3	2.03	0.41
28:Y:178:HIS:CG	28:Y:179:PRO:HD2	2.56	0.41
1:0:1724:U:H5''	40:0:4311:HOH:O	2.19	0.40
1:0:1816:C:H2'	1:0:1817:U:O4'	2.21	0.40
1:0:185:G:O3'	1:0:186:A:H4'	2.21	0.40
1:0:2720:C:O2	14:K:87:ARG:NH2	2.54	0.40
1:0:556:C:H2'	1:0:557:C:H6	1.86	0.40
1:0:932:U:H2'	1:0:933:C:C6	2.56	0.40
5:A:135:VAL:HG13	5:A:135:VAL:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:140:VAL:HG12	7:C:141:SER:N	2.36	0.40
7:C:72:LYS:HG2	7:C:77:ALA:HA	2.02	0.40
9:E:7:ILE:HD11	9:E:11:VAL:C	2.41	0.40
12:H:114:ARG:O	12:H:115:ALA:C	2.60	0.40
40:O:9644:HOH:O	15:L:30:ARG:HD2	2.20	0.40
25:V:1:THR:OG1	25:V:2:VAL:N	2.53	0.40
28:Y:186:ARG:HG2	28:Y:186:ARG:NH1	2.36	0.40
1:O:1119:G:C6	1:O:1244:U:C5	3.09	0.40
1:O:2329:C:O2'	1:O:2330:U:H5'	2.21	0.40
1:O:2361:A:H2'	1:O:2362:A:O4'	2.21	0.40
1:O:2748:G:C5'	40:O:7972:HOH:O	2.69	0.40
5:A:38:ILE:HD13	5:A:38:ILE:HA	1.92	0.40
6:B:278:PRO:HD3	6:B:294:TYR:CE2	2.56	0.40
8:D:21:VAL:HA	8:D:131:THR:O	2.21	0.40
8:D:23:VAL:CG2	8:D:73:VAL:HB	2.51	0.40
10:F:72:VAL:HA	10:F:73:PRO:HD3	1.92	0.40
17:N:37:ARG:HA	17:N:37:ARG:HD3	1.69	0.40
20:Q:43:ILE:HG13	20:Q:52:PHE:CZ	2.56	0.40
25:V:1:THR:O	25:V:2:VAL:C	2.59	0.40
26:W:4:LEU:CD1	26:W:24:LEU:HD13	2.51	0.40
1:O:120:A:H2'	1:O:120:A:N3	2.37	0.40
1:O:1589:G:N2	1:O:1605:G:H1'	2.35	0.40
1:O:1829:A:C8	1:O:1885:A:C8	3.09	0.40
1:O:2824:C:C5'	1:O:2825:C:H5'	2.51	0.40
5:A:43:VAL:O	5:A:44:ASP:HB2	2.21	0.40
5:A:81:GLN:H	5:A:92:ASN:CG	2.24	0.40
5:A:85:SER:O	5:A:86:ALA:C	2.60	0.40
6:B:81:ALA:O	6:B:186:GLY:HA3	2.22	0.40
6:B:279:THR:HG23	6:B:280:VAL:N	2.35	0.40
6:B:60:SER:HA	6:B:61:PRO:HD3	1.92	0.40
1:O:2101:A:H5'	7:C:63:SER:HB3	2.04	0.40
7:C:84:VAL:HG12	7:C:85:LYS:HG2	2.04	0.40
8:D:91:ALA:HB2	8:D:106:PHE:CD2	2.56	0.40
8:D:67:ASP:O	8:D:69:ILE:HG13	2.21	0.40
12:H:78:GLY:C	12:H:80:GLU:H	2.25	0.40
17:N:103:ASP:OD1	17:N:103:ASP:C	2.60	0.40
23:T:18:GLU:O	23:T:21:LYS:HG2	2.22	0.40
25:V:42:ASN:HB3	40:V:7247:HOH:O	2.21	0.40
25:V:8:ILE:CG2	25:V:59:ILE:HG13	2.51	0.40
28:Y:115:ARG:NE	40:Y:9353:HOH:O	2.55	0.40
28:Y:187:VAL:CG1	28:Y:205:ILE:HG12	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Y:96:GLU:O	28:Y:235:GLU:HA	2.21	0.40
1:0:1235:G:C1'	13:J:63:ILE:HG23	2.51	0.40
1:0:1299:G:N2	40:0:5226:HOH:O	2.53	0.40
1:0:1462:C:H2'	1:0:1463:A:H8	1.85	0.40
1:0:2070:G:H2'	1:0:2072:G:OP1	2.21	0.40
1:0:294:C:H2'	1:0:295:C:O4'	2.21	0.40
40:0:7989:HOH:O	32:3:60:LYS:HG3	2.21	0.40
15:L:65:ASP:CG	15:L:111:ALA:HB3	2.42	0.40
18:O:59:VAL:HG23	18:O:111:VAL:HG23	2.02	0.40
1:0:1007:A:H2'	12:H:19:TYR:CZ	2.56	0.40
1:0:1081:A:H5''	40:0:3742:HOH:O	2.21	0.40
1:0:1626:A:H2'	1:0:1627:G:C5'	2.52	0.40
1:0:2819:C:H2'	1:0:2820:A:C8	2.56	0.40
1:0:423:A:O2'	1:0:424:C:H5'	2.21	0.40
1:0:565:A:OP2	1:0:592:G:N1	2.49	0.40
30:1:25:LYS:CG	31:2:49:GLU:H	2.35	0.40
32:3:30:GLN:HE21	32:3:30:GLN:HB3	1.61	0.40
2:9:3002:U:OP2	2:9:3003:A:H5'	2.22	0.40
2:9:3008:G:OP1	17:N:23:ARG:NH1	2.51	0.40
2:9:3091:C:H2'	2:9:3092:G:O4'	2.22	0.40
1:0:1881:A:OP1	5:A:199:HIS:HE1	2.04	0.40
6:B:24:PRO:CG	6:B:204:GLY:HA2	2.52	0.40
7:C:57:PRO:HG2	7:C:73:LEU:CD1	2.51	0.40
11:G:16:LYS:O	11:G:20:VAL:HG23	2.22	0.40
13:J:103:VAL:HG12	40:J:5907:HOH:O	2.21	0.40
13:J:80:LYS:HE2	13:J:98:PHE:CZ	2.56	0.40
15:L:67:ARG:HB2	15:L:112:GLY:HA3	2.03	0.40
18:O:23:GLY:C	40:O:3062:HOH:O	2.59	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	
5	A	235/240 (98%)	207 (88%)	25 (11%)	3 (1%)	14	19
6	B	335/338 (99%)	309 (92%)	21 (6%)	5 (2%)	12	16
7	C	244/246 (99%)	223 (91%)	19 (8%)	2 (1%)	22	33
8	D	134/177 (76%)	104 (78%)	19 (14%)	11 (8%)	1	0
9	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
10	F	117/120 (98%)	103 (88%)	11 (9%)	3 (3%)	6	6
11	G	25/348 (7%)	25 (100%)	0	0	100	100
12	H	156/171 (91%)	136 (87%)	16 (10%)	4 (3%)	6	6
13	J	140/145 (97%)	130 (93%)	6 (4%)	4 (3%)	5	5
14	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	22	33
15	L	141/165 (86%)	118 (84%)	21 (15%)	2 (1%)	13	18
16	M	192/194 (99%)	178 (93%)	13 (7%)	1 (0%)	32	46
17	N	184/187 (98%)	161 (88%)	14 (8%)	9 (5%)	2	1
18	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
19	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
20	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
21	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
22	S	79/85 (93%)	73 (92%)	6 (8%)	0	100	100
23	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	11	13
24	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
25	V	63/71 (89%)	59 (94%)	1 (2%)	3 (5%)	2	1
26	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
27	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
28	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
29	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	2
30	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
31	2	42/50 (84%)	41 (98%)	0	1 (2%)	7	7
32	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	17	23
33	I	68/162 (42%)	54 (79%)	12 (18%)	2 (3%)	5	5
All	All	3705/4430 (84%)	3385 (91%)	263 (7%)	57 (2%)	12	16

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	169	GLY
8	D	60	GLU
8	D	137	PRO
10	F	101	ALA
12	H	166	SER
13	J	143	LYS
15	L	80	ASP
17	N	154	LEU
17	N	184	ILE
29	Z	81	ARG
5	A	37	VAL
6	B	34	GLY
8	D	27	ILE
8	D	61	PHE
8	D	65	GLU
12	H	168	ALA
15	L	143	THR
16	M	83	SER
23	T	53	GLY
25	V	43	PRO
29	Z	20	ARG
31	2	37	HIS
33	I	129	VAL
5	A	86	ALA
6	B	185	GLY
8	D	28	GLY
8	D	56	ARG
8	D	164	ALA
10	F	71	GLY
17	N	183	ASP
23	T	46	ASP
5	A	34	ASP
7	C	8	LEU
7	C	58	ALA
8	D	171	ASP
12	H	16	ARG
12	H	81	GLY
13	J	5	GLU
13	J	7	ASP
17	N	65	ASP
17	N	155	GLU
17	N	162	ASP
8	D	77	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	F	100	ASP
14	K	126	SER
17	N	164	ASP
17	N	167	ASP
29	Z	42	CYS
32	3	56	PRO
6	B	2	GLN
8	D	16	PRO
13	J	65	ASN
17	N	68	GLU
25	V	40	PRO
25	V	2	VAL
6	B	181	ILE
33	I	73	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	
5	A	179/182 (98%)	165 (92%)	14 (8%)	15	23
6	B	282/283 (100%)	267 (95%)	15 (5%)	26	42
7	C	193/193 (100%)	173 (90%)	20 (10%)	8	12
8	D	117/148 (79%)	112 (96%)	5 (4%)	33	52
9	E	152/156 (97%)	146 (96%)	6 (4%)	37	56
10	F	93/94 (99%)	91 (98%)	2 (2%)	57	76
11	G	27/283 (10%)	27 (100%)	0	100	100
12	H	132/138 (96%)	127 (96%)	5 (4%)	38	58
13	J	118/121 (98%)	108 (92%)	10 (8%)	12	19
14	K	106/106 (100%)	101 (95%)	5 (5%)	30	48
15	L	113/127 (89%)	110 (97%)	3 (3%)	50	71
16	M	158/158 (100%)	153 (97%)	5 (3%)	44	65
17	N	149/150 (99%)	142 (95%)	7 (5%)	30	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	O	93/94 (99%)	92 (99%)	1 (1%)	78	90
19	P	113/117 (97%)	110 (97%)	3 (3%)	50	71
20	Q	79/80 (99%)	75 (95%)	4 (5%)	28	44
21	R	117/122 (96%)	114 (97%)	3 (3%)	51	72
22	S	71/74 (96%)	71 (100%)	0	100	100
23	T	105/106 (99%)	101 (96%)	4 (4%)	38	58
24	U	44/52 (85%)	44 (100%)	0	100	100
25	V	51/57 (90%)	50 (98%)	1 (2%)	60	79
26	W	130/130 (100%)	124 (95%)	6 (5%)	31	49
27	X	66/74 (89%)	63 (96%)	3 (4%)	32	50
28	Y	120/196 (61%)	109 (91%)	11 (9%)	11	16
29	Z	60/68 (88%)	59 (98%)	1 (2%)	66	82
30	1	46/47 (98%)	45 (98%)	1 (2%)	57	76
31	2	42/46 (91%)	41 (98%)	1 (2%)	54	74
32	3	79/79 (100%)	77 (98%)	2 (2%)	53	73
33	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2955 (96%)	138 (4%)	32	50

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	3	ARG
5	A	26	ASP
5	A	33	GLU
5	A	36	ASP
5	A	62	ASP
5	A	78	ASP
5	A	94	LEU
5	A	120	ARG
5	A	131	HIS
5	A	151	GLN
5	A	165	THR
5	A	179	MET
5	A	206	ARG
5	A	217	ARG
6	B	11	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	27	ASN
6	B	82	VAL
6	B	84	LEU
6	B	98	THR
6	B	103	ASP
6	B	113	LEU
6	B	149	ASP
6	B	162	MET
6	B	190	MET
6	B	254	GLN
6	B	277	GLU
6	B	279	THR
6	B	307	ARG
6	B	312	ARG
7	C	2	GLN
7	C	16	VAL
7	C	27	ARG
7	C	67	GLN
7	C	76	ARG
7	C	78	ARG
7	C	91	PRO
7	C	94	THR
7	C	101	ASP
7	C	115	LEU
7	C	136	VAL
7	C	162	VAL
7	C	187	ARG
7	C	214	THR
7	C	222	ASP
7	C	223	LEU
7	C	234	VAL
7	C	236	THR
7	C	240	LEU
7	C	243	VAL
8	D	24	HIS
8	D	61	PHE
8	D	100	ASP
8	D	133	ASN
8	D	137	PRO
9	E	7	ILE
9	E	102	VAL
9	E	108	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	E	155	ASN
9	E	156	ASP
9	E	164	ASP
10	F	12	LEU
10	F	46	GLU
12	H	18	GLU
12	H	84	LYS
12	H	88	ARG
12	H	154	TYR
12	H	159	PRO
13	J	7	ASP
13	J	45	VAL
13	J	46	ILE
13	J	52	GLN
13	J	70	PHE
13	J	74	ARG
13	J	79	PHE
13	J	107	ASN
13	J	127	ILE
13	J	131	THR
14	K	4	LEU
14	K	10	GLN
14	K	56	SER
14	K	84	ASP
14	K	100	GLU
15	L	35	ARG
15	L	43	HIS
15	L	140	VAL
16	M	46	LEU
16	M	68	ARG
16	M	93	ARG
16	M	99	ARG
16	M	116	ASN
17	N	17	ARG
17	N	23	ARG
17	N	26	LEU
17	N	49	THR
17	N	65	ASP
17	N	139	TRP
17	N	152	GLU
18	O	111	VAL
19	P	52	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	P	98	ILE
19	P	117	SER
20	Q	11	ARG
20	Q	16	ASN
20	Q	57	ASP
20	Q	95	GLU
21	R	13	THR
21	R	132	ARG
21	R	143	VAL
23	T	5	ASP
23	T	39	ASN
23	T	80	GLU
23	T	89	ARG
25	V	65	ASP
26	W	26	ILE
26	W	35	VAL
26	W	78	ASP
26	W	122	ARG
26	W	142	ASP
26	W	146	ILE
27	X	72	VAL
27	X	79	GLU
27	X	82	GLU
28	Y	103	THR
28	Y	141	THR
28	Y	144	ARG
28	Y	154	ARG
28	Y	163	THR
28	Y	174	VAL
28	Y	187	VAL
28	Y	189	ASN
28	Y	200	THR
28	Y	231	PRO
28	Y	235	GLU
29	Z	44	GLU
30	1	47	ASP
31	2	18	ASN
32	3	11	CYS
32	3	65	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	29	HIS
5	A	199	HIS
6	B	27	ASN
6	B	145	HIS
6	B	221	GLN
6	B	238	ASN
6	B	256	GLN
6	B	260	HIS
6	B	320	GLN
6	B	332	ASN
7	C	2	GLN
7	C	39	GLN
7	C	129	HIS
8	D	47	GLN
8	D	103	ASN
8	D	133	ASN
9	E	106	ASN
9	E	143	GLN
11	G	64	ASN
12	H	56	GLN
12	H	59	HIS
12	H	70	ASN
12	H	170	ASN
13	J	52	GLN
13	J	107	ASN
14	K	10	GLN
15	L	18	HIS
15	L	41	HIS
15	L	42	ASN
16	M	24	GLN
16	M	77	HIS
16	M	170	ASN
17	N	93	GLN
17	N	107	ASN
17	N	153	GLN
18	O	100	GLN
19	P	50	GLN
19	P	66	GLN
19	P	73	HIS
19	P	88	GLN
19	P	89	ASN
19	P	118	GLN
20	Q	16	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Q	40	HIS
21	R	61	GLN
21	R	94	ASN
21	R	98	ASN
21	R	113	HIS
21	R	117	HIS
22	S	44	GLN
22	S	53	ASN
22	S	55	GLN
23	T	37	GLN
23	T	39	ASN
24	U	39	ASN
24	U	48	ASN
25	V	60	GLN
26	W	2	HIS
26	W	28	HIS
26	W	110	GLN
26	W	119	HIS
26	W	125	HIS
26	W	141	HIS
27	X	22	ASN
27	X	23	HIS
28	Y	119	GLN
28	Y	134	HIS
28	Y	149	GLN
28	Y	189	ASN
29	Z	41	ASN
30	1	8	GLN
30	1	16	HIS
30	1	28	HIS
31	2	16	ASN
31	2	18	ASN
31	2	41	HIS
31	2	45	ASN
32	3	30	GLN
32	3	48	ASN
33	I	113	HIS

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	233 (8%)	0
2	9	121/122 (99%)	15 (12%)	0
3	4	1/4 (25%)	0	0
4	5	2/6 (33%)	1 (50%)	0
All	All	2869/3054 (93%)	249 (8%)	0

All (249) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G
1	0	86	A
1	0	87	C
1	0	88	G
1	0	114	A
1	0	115	U
1	0	130	C
1	0	141	C
1	0	151	A
1	0	166	A
1	0	186	A
1	0	191	A
1	0	192	A
1	0	219	G
1	0	237	G
1	0	271	C
1	0	272	A
1	0	273	G
1	0	283	U
1	0	284	C
1	0	308	U
1	0	309	C
1	0	318	C
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
1	0	497	A
1	0	498	A
1	0	510	U
1	0	511	A
1	0	514	G
1	0	537	G
1	0	538	C
1	0	539	G
1	0	542	A
1	0	545	G
1	0	553	G
1	0	559	U
1	0	581	G
1	0	588	G
1	0	604	G
1	0	620	A
1	0	632	A
1	0	644	G
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	702	G
1	0	759	C
1	0	777	U
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	875	A
1	0	877	G
1	0	878	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	905	C
1	0	920	C
1	0	921	G
1	0	923	A
1	0	953	G
1	0	960	G
1	0	961	A
1	0	1006	A
1	0	1008	C
1	0	1029	U
1	0	1045	G
1	0	1059	G
1	0	1060	C
1	0	1072	G
1	0	1081	A
1	0	1087	G
1	0	1088	A
1	0	1100	G
1	0	1109	U
1	0	1110	G
1	0	1119	G
1	0	1130	U
1	0	1164	U
1	0	1165	G
1	0	1166	A
1	0	1174	A
1	0	1175	G
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1208	C
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1378	G
1	0	1407	A
1	0	1409	G
1	0	1474	C
1	0	1505	U
1	0	1506	U
1	0	1524	U
1	0	1525	G
1	0	1528	A
1	0	1592	G
1	0	1625	U
1	0	1626	A
1	0	1633	C
1	0	1634	G
1	0	1656	A
1	0	1667	A
1	0	1682	A
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1701	A
1	0	1722	U
1	0	1723	G
1	0	1725	C
1	0	1731	C
1	0	1752	G
1	0	1778	A
1	0	1798	C
1	0	1819	G
1	0	1820	G
1	0	1829	A
1	0	1856	C
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1971	G
1	0	1973	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2006	C
1	0	2008	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2011	A
1	0	2012	U
1	0	2013	G
1	0	2033	G
1	0	2034	U
1	0	2064	U
1	0	2072	G
1	0	2073	G
1	0	2074	A
1	0	2096	A
1	0	2101	A
1	0	2102	G
1	0	2103	A
1	0	2110	G
1	0	2238	A
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C
1	0	2321	A
1	0	2354	A
1	0	2361	A
1	0	2369	A
1	0	2379	G
1	0	2422	U
1	0	2462	G
1	0	2467	A
1	0	2469	A
1	0	2476	C
1	0	2480	G
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2533	C
1	0	2537	G
1	0	2541	U
1	0	2542	C
1	0	2553	A
1	0	2564	G
1	0	2589	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2634	G
1	0	2637	A
1	0	2644	C
1	0	2645	U
1	0	2648	U
1	0	2649	A
1	0	2664	A
1	0	2681	A
1	0	2682	C
1	0	2726	U
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A
1	0	2783	A
1	0	2786	G
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2852	A
1	0	2853	U
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	3002	U
2	9	3007	G
2	9	3014	G
2	9	3022	G
2	9	3023	U
2	9	3024	U
2	9	3025	G
2	9	3041	C
2	9	3043	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	9	3044	A
2	9	3057	A
2	9	3066	G
2	9	3077	A
2	9	3114	G
2	9	3122	C
4	5	76	A

There are no RNA pucker outliers to report.

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

7 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	$\# Z > 2$
1	OMU	0	2587	1	14,22,23	0.99	2 (14%)	18,31,34	3.61	2 (11%)
1	OMG	0	2588	1,3	18,26,27	1.08	2 (11%)	22,38,41	2.46	4 (18%)
1	UR3	0	2619	1,38	14,22,23	0.93	0	16,32,35	0.69	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	6.14	4 (20%)
1	1MA	0	628	1,36	16,25,26	1.01	1 (6%)	13,37,40	1.18	1 (7%)
3	PPU	4	76	1,3	17,26,41	0.67	0	17,38,60	1.03	1 (5%)
3	HFA	4	77	3	11,11,12	0.87	1 (9%)	13,13,15	0.74	1 (7%)

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
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1,38	-	0/3/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,36	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.71	1.48	1.52
1	0	2588	OMG	C8-N7	-2.12	1.30	1.34
1	0	2587	OMU	C6-C5	-2.10	1.33	1.38
3	4	77	HFA	OA-CA	2.14	1.48	1.43
1	0	2621	PSU	C2-N1	2.58	1.43	1.38
1	0	2587	OMU	C4-N3	2.63	1.37	1.33
1	0	628	1MA	C6-N6	2.92	1.34	1.27
1	0	2621	PSU	C4-N3	3.14	1.38	1.33
1	0	2588	OMG	C6-N1	3.28	1.39	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.25	114.56	128.40
1	0	2621	PSU	C5-C4-N3	-13.14	114.65	125.43
1	0	2588	OMG	C5-C6-N1	-8.29	111.69	123.48
1	0	628	1MA	C2-N3-C4	-3.64	110.83	116.41
1	0	2587	OMU	C5-C4-N3	-3.48	114.82	123.12
1	0	2588	OMG	C2-N3-C4	-2.79	111.91	115.16
1	0	2588	OMG	N3-C2-N1	-2.43	123.91	127.46
3	4	77	HFA	CB-CA-C	-2.03	107.83	111.64
1	0	2621	PSU	C6-N1-C2	2.78	119.80	115.36
3	4	76	PPU	C2-N1-C6	2.88	118.88	111.82
1	0	2588	OMG	C6-N1-C2	6.31	125.14	116.06
1	0	2621	PSU	C4-N3-C2	13.82	127.24	115.16
1	0	2587	OMU	C4-N3-C2	14.76	126.81	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	3	0
1	0	2619	UR3	1	0
3	4	76	PPU	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2922 (94%)	-0.63	62 (2%) 61 58	24, 49, 93, 153	0
2	9	122/122 (100%)	-0.24	6 (4%) 30 29	41, 69, 93, 152	0
3	4	2/4 (50%)	-1.09	0 100 100	43, 43, 43, 52	0
4	5	4/6 (66%)	-0.08	1 (25%) 1 1	55, 57, 58, 66	0
5	A	237/240 (98%)	0.33	12 (5%) 29 27	31, 54, 86, 106	0
6	B	337/338 (99%)	0.14	11 (3%) 47 45	31, 55, 79, 93	0
7	C	246/246 (100%)	-0.06	1 (0%) 92 91	27, 49, 70, 87	0
8	D	140/177 (79%)	1.71	45 (32%) 0 0	64, 96, 125, 132	0
9	E	172/178 (96%)	0.74	24 (13%) 3 3	44, 66, 86, 92	0
10	F	119/120 (99%)	1.00	27 (22%) 1 1	49, 74, 100, 112	0
11	G	29/348 (8%)	2.38	18 (62%) 0 0	74, 92, 103, 105	0
12	H	160/171 (93%)	0.60	16 (10%) 8 7	47, 65, 96, 103	0
13	J	142/145 (97%)	-0.01	3 (2%) 64 61	37, 52, 72, 93	0
14	K	132/132 (100%)	-0.15	2 (1%) 74 72	37, 48, 71, 84	0
15	L	145/165 (87%)	0.60	15 (10%) 7 6	29, 69, 112, 121	0
16	M	194/194 (100%)	0.52	20 (10%) 7 6	37, 48, 85, 93	0
17	N	186/187 (99%)	0.90	33 (17%) 2 1	49, 68, 112, 119	0
18	O	115/116 (99%)	0.15	2 (1%) 70 68	40, 59, 73, 81	0
19	P	143/149 (95%)	0.24	3 (2%) 64 61	39, 55, 66, 79	0
20	Q	95/96 (98%)	0.05	4 (4%) 37 35	42, 52, 67, 76	0
21	R	150/155 (96%)	-0.15	0 100 100	33, 47, 66, 75	0
22	S	81/85 (95%)	0.30	3 (3%) 42 41	43, 61, 84, 97	0
23	T	119/120 (99%)	0.67	11 (9%) 10 8	41, 59, 85, 110	0
24	U	53/66 (80%)	0.26	2 (3%) 41 40	42, 56, 73, 82	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	65/71 (91%)	1.61	16 (24%) 1 1	56, 78, 115, 120	0
26	W	154/154 (100%)	0.02	2 (1%) 77 75	40, 53, 74, 82	0
27	X	82/92 (89%)	0.67	13 (15%) 2 2	44, 58, 84, 103	0
28	Y	142/241 (58%)	0.11	8 (5%) 25 24	29, 45, 68, 90	0
29	Z	73/83 (87%)	1.74	29 (39%) 0 0	52, 83, 97, 105	0
30	1	56/57 (98%)	-0.43	0 100 100	31, 36, 46, 55	0
31	2	46/50 (92%)	1.45	15 (32%) 0 0	41, 68, 96, 102	0
32	3	92/92 (100%)	0.33	6 (6%) 20 18	41, 61, 73, 86	0
33	I	70/162 (43%)	5.01	57 (81%) 0 0	111, 125, 142, 144	0
All	All	6652/7484 (88%)	0.03	467 (7%) 17 15	24, 54, 100, 153	0

All (467) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	I	71	GLY	15.2
25	V	1	THR	14.1
33	I	79	ILE	12.3
33	I	76	ALA	12.2
33	I	133	THR	11.8
8	D	63	ILE	11.6
29	Z	11	SER	11.4
23	T	119	ALA	10.9
2	9	3001	U	10.1
33	I	85	PHE	10.0
17	N	166	ALA	9.5
8	D	57	THR	9.1
16	M	70	GLY	9.1
31	2	49	GLU	8.9
29	Z	22	SER	8.8
25	V	40	PRO	8.5
33	I	88	GLY	8.5
25	V	39	ALA	8.2
33	I	121	LEU	8.2
33	I	81	ASP	8.1
33	I	75	THR	8.1
33	I	77	GLU	7.9
33	I	116	LEU	7.9
33	I	137	VAL	7.9
33	I	91	GLU	7.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
33	I	105	VAL	7.7
16	M	79	ALA	7.7
33	I	129	VAL	7.5
33	I	118	SER	7.4
33	I	109	ALA	7.3
33	I	87	THR	7.2
33	I	96	PHE	7.1
8	D	90	LEU	7.1
33	I	78	LEU	7.0
33	I	126	LYS	6.9
5	A	37	VAL	6.8
31	2	48	ASP	6.7
33	I	113	HIS	6.4
2	9	3024	U	6.4
33	I	132	CYS	6.3
5	A	237	GLY	6.2
33	I	89	SER	6.2
1	0	282	C	6.1
29	Z	20	ARG	5.9
33	I	93	GLN	5.9
33	I	108	ILE	5.8
23	T	118	SER	5.8
31	2	39	ARG	5.8
29	Z	45	ASP	5.7
33	I	74	PRO	5.6
8	D	69	ILE	5.5
33	I	111	GLN	5.5
25	V	38	GLY	5.5
16	M	74	LYS	5.4
33	I	107	GLN	5.4
8	D	64	ARG	5.3
27	X	88	GLU	5.3
2	9	3023	U	5.2
33	I	83	ALA	5.2
29	Z	18	TYR	5.1
31	2	41	HIS	5.1
33	I	104	GLN	5.1
33	I	80	LYS	5.0
29	Z	12	GLY	5.0
16	M	75	ARG	5.0
27	X	80	GLU	5.0
14	K	132	VAL	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
17	N	155	GLU	5.0
33	I	98	ALA	5.0
11	G	26	MET	5.0
29	Z	25	ARG	4.9
11	G	69	ARG	4.9
16	M	86	GLN	4.9
29	Z	32	GLU	4.8
8	D	61	PHE	4.8
1	0	1199	A	4.8
25	V	41	GLU	4.8
1	0	1951	G	4.8
29	Z	21	VAL	4.8
16	M	71	SER	4.7
17	N	68	GLU	4.7
33	I	125	ALA	4.7
29	Z	14	PHE	4.6
33	I	138	THR	4.6
16	M	87	GLY	4.6
29	Z	23	ARG	4.6
15	L	81	VAL	4.6
11	G	23	ILE	4.6
31	2	47	THR	4.5
11	G	71	LEU	4.5
31	2	44	ARG	4.5
33	I	86	GLU	4.5
8	D	66	GLY	4.4
33	I	102	VAL	4.4
17	N	175	LEU	4.4
17	N	163	PHE	4.4
8	D	170	TYR	4.3
23	T	117	ASP	4.3
1	0	1172	G	4.3
1	0	2237	G	4.3
2	9	3002	U	4.3
1	0	497	A	4.3
1	0	1169	U	4.3
1	0	1177	A	4.3
17	N	147	ILE	4.2
11	G	27	ILE	4.2
9	E	10	ASP	4.2
11	G	66	LEU	4.2
33	I	114	PRO	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	H	138	CYS	4.2
27	X	77	PHE	4.2
23	T	116	ASP	4.2
8	D	44	ILE	4.1
9	E	45	ASP	4.1
1	0	2004	U	4.1
29	Z	37	HIS	4.1
12	H	74	ILE	4.1
12	H	73	LEU	4.0
1	0	2508	C	4.0
29	Z	34	ASN	4.0
8	D	26	GLY	4.0
15	L	80	ASP	4.0
1	0	280	C	4.0
12	H	78	GLY	4.0
28	Y	216	ARG	3.9
33	I	112	LYS	3.9
15	L	93	VAL	3.9
10	F	28	ALA	3.9
31	2	38	LYS	3.9
28	Y	235	GLU	3.9
8	D	134	LEU	3.9
33	I	122	THR	3.8
29	Z	24	ARG	3.8
10	F	107	ASP	3.8
27	X	41	PHE	3.7
15	L	76	LEU	3.7
8	D	92	GLU	3.7
5	A	31	LYS	3.7
5	A	133	ARG	3.7
8	D	56	ARG	3.7
1	0	285	A	3.7
29	Z	33	MET	3.6
16	M	78	LYS	3.6
1	0	2511	A	3.6
25	V	59	ILE	3.6
8	D	154	LYS	3.6
33	I	119	TYR	3.6
8	D	73	VAL	3.6
25	V	37	GLY	3.5
16	M	77	HIS	3.5
29	Z	31	SER	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	E	100	ASP	3.5
12	H	146	VAL	3.5
31	2	42	TRP	3.5
33	I	134	SER	3.5
1	0	970	U	3.5
1	0	1173	A	3.5
8	D	10	PHE	3.5
9	E	87	PHE	3.5
29	Z	19	GLY	3.5
10	F	117	GLU	3.5
8	D	40	ILE	3.5
17	N	185	GLU	3.4
25	V	36	ALA	3.4
9	E	86	VAL	3.4
8	D	166	ILE	3.4
33	I	84	GLY	3.4
31	2	35	ARG	3.4
27	X	7	GLU	3.4
17	N	178	THR	3.4
8	D	128	LEU	3.4
33	I	99	ASP	3.4
15	L	97	VAL	3.4
1	0	1198	U	3.4
8	D	88	LEU	3.4
15	L	100	ALA	3.4
1	0	1202	A	3.4
25	V	63	GLU	3.3
23	T	82	THR	3.3
5	A	36	ASP	3.3
32	3	92	GLU	3.3
1	0	960	G	3.3
1	0	1948	G	3.3
22	S	81	ILE	3.3
15	L	91	VAL	3.3
25	V	8	ILE	3.3
1	0	2645	U	3.3
16	M	72	ALA	3.3
16	M	81	ARG	3.3
17	N	95	ALA	3.3
1	0	514	G	3.3
8	D	18	ILE	3.3
5	A	35	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	D	27	ILE	3.3
10	F	16	ALA	3.2
29	Z	29	ILE	3.2
22	S	20	PHE	3.2
1	0	2238	A	3.2
33	I	117	LEU	3.2
1	0	1966	U	3.2
17	N	184	ILE	3.2
1	0	1163	G	3.2
8	D	68	PRO	3.2
17	N	134	ASP	3.2
1	0	272	A	3.2
8	D	41	LEU	3.2
8	D	62	ASP	3.2
29	Z	30	GLU	3.2
27	X	85	VAL	3.2
1	0	1965	C	3.1
10	F	100	ASP	3.1
33	I	120	ASP	3.1
16	M	80	GLY	3.1
33	I	123	ASN	3.1
9	E	124	VAL	3.1
15	L	120	LEU	3.1
8	D	172	VAL	3.1
15	L	145	LEU	3.1
31	2	27	LEU	3.1
6	B	104	GLU	3.1
17	N	2	THR	3.1
15	L	60	GLU	3.1
33	I	73	PRO	3.1
8	D	53	LYS	3.1
12	H	171	ALA	3.1
13	J	70	PHE	3.1
31	2	26	MET	3.1
10	F	17	LEU	3.1
17	N	139	TRP	3.1
16	M	76	ARG	3.1
29	Z	10	ARG	3.1
17	N	180	LEU	3.1
8	D	11	HIS	3.1
1	0	1950	G	3.0
20	Q	95	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	A	65	ARG	3.0
9	E	127	ASP	3.0
5	A	32	VAL	3.0
6	B	2	GLN	3.0
1	0	716	G	3.0
1	0	735	C	3.0
9	E	88	TYR	3.0
8	D	107	GLY	3.0
33	I	82	GLU	3.0
11	G	22	ALA	3.0
1	0	1180	U	2.9
10	F	49	PHE	2.9
1	0	284	C	2.9
28	Y	95	THR	2.9
31	2	37	HIS	2.9
15	L	102	ASP	2.9
10	F	44	SER	2.9
1	0	1168	C	2.9
1	0	358	G	2.9
33	I	72	VAL	2.9
33	I	94	GLU	2.9
12	H	149	ALA	2.9
17	N	179	LEU	2.9
8	D	173	GLU	2.9
9	E	6	GLU	2.9
10	F	22	VAL	2.9
12	H	47	ILE	2.9
8	D	85	GLN	2.9
29	Z	59	TYR	2.9
10	F	106	ALA	2.9
11	G	73	ASP	2.8
1	0	1981	A	2.8
25	V	3	LEU	2.8
24	U	47	ARG	2.8
11	G	72	ASP	2.8
10	F	119	ARG	2.8
10	F	99	THR	2.8
33	I	115	ASP	2.8
29	Z	26	VAL	2.8
8	D	51	ARG	2.8
11	G	63	ARG	2.8
17	N	67	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
29	Z	36	ASP	2.8
29	Z	16	ALA	2.8
24	U	43	GLY	2.8
9	E	4	GLU	2.8
32	3	41	GLU	2.8
19	P	18	LYS	2.8
8	D	89	PRO	2.8
16	M	82	ARG	2.8
1	0	1200	A	2.8
10	F	110	ASP	2.8
17	N	138	ASP	2.8
1	0	281	U	2.8
8	D	106	PHE	2.8
8	D	93	LEU	2.8
23	T	112	LEU	2.8
17	N	156	GLU	2.7
1	0	138	U	2.7
1	0	1171	A	2.7
10	F	12	LEU	2.7
1	0	1170	U	2.7
11	G	12	ILE	2.7
13	J	5	GLU	2.7
1	0	999	C	2.7
8	D	91	ALA	2.7
17	N	165	ALA	2.7
17	N	71	TRP	2.7
6	B	117	GLU	2.7
10	F	108	VAL	2.7
6	B	180	ASP	2.7
1	0	1625	U	2.7
11	G	67	LEU	2.7
17	N	1	ALA	2.7
17	N	160	SER	2.7
1	0	1164	U	2.7
27	X	71	ARG	2.7
12	H	130	GLY	2.7
8	D	167	GLU	2.6
11	G	24	VAL	2.6
25	V	2	VAL	2.6
27	X	10	VAL	2.6
16	M	89	THR	2.6
1	0	10	U	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	E	11	VAL	2.6
25	V	14	ALA	2.6
1	0	1967	U	2.6
10	F	25	ASP	2.6
12	H	143	ALA	2.6
9	E	99	GLY	2.6
1	0	1192	A	2.6
10	F	21	GLU	2.6
12	H	37	GLN	2.6
28	Y	102	LEU	2.6
16	M	73	ARG	2.6
10	F	98	VAL	2.6
11	G	25	GLU	2.6
33	I	97	VAL	2.6
20	Q	18	PRO	2.6
10	F	70	LYS	2.6
16	M	84	LYS	2.6
17	N	172	PHE	2.6
17	N	159	TYR	2.6
25	V	43	PRO	2.5
7	C	61	PHE	2.5
5	A	85	SER	2.5
28	Y	234	VAL	2.5
9	E	118	ILE	2.5
8	D	65	GLU	2.5
10	F	75	ILE	2.5
19	P	114	LEU	2.5
17	N	137	ALA	2.5
1	0	2769	C	2.5
6	B	183	GLU	2.5
6	B	1	PRO	2.5
1	0	1525	G	2.5
9	E	44	GLY	2.5
13	J	4	ALA	2.5
20	Q	76	VAL	2.4
8	D	104	PHE	2.4
1	0	370	G	2.4
33	I	135	LEU	2.4
23	T	77	VAL	2.4
27	X	43	VAL	2.4
5	A	97	ALA	2.4
10	F	29	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	283	U	2.4
9	E	126	ILE	2.4
15	L	79	ASP	2.4
11	G	15	TRP	2.4
11	G	70	ALA	2.4
17	N	65	ASP	2.4
12	H	66	ARG	2.4
1	0	288	A	2.4
23	T	109	GLU	2.4
28	Y	96	GLU	2.4
6	B	128	ILE	2.4
9	E	5	LEU	2.4
9	E	48	VAL	2.3
5	A	99	ILE	2.3
9	E	154	ILE	2.3
33	I	103	ASP	2.3
32	3	62	THR	2.3
8	D	84	LEU	2.3
1	0	2748	G	2.3
2	9	3072	C	2.3
29	Z	35	GLU	2.3
8	D	81	GLU	2.3
29	Z	28	GLU	2.3
20	Q	17	LYS	2.3
1	0	1947	G	2.3
31	2	36	ASN	2.3
33	I	124	ALA	2.3
31	2	43	ARG	2.3
10	F	15	ASP	2.3
1	0	1929	G	2.3
16	M	85	ARG	2.3
31	2	20	ARG	2.3
27	X	72	VAL	2.3
17	N	158	LEU	2.3
1	0	1203	G	2.3
6	B	105	PHE	2.3
9	E	94	GLN	2.3
12	H	35	ARG	2.2
1	0	362	G	2.2
17	N	167	ASP	2.2
22	S	72	ASP	2.2
23	T	115	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
27	X	65	ASN	2.2
17	N	161	GLY	2.2
28	Y	108	ASP	2.2
28	Y	236	VAL	2.2
11	G	68	GLU	2.2
6	B	134	ALA	2.2
16	M	132	ILE	2.2
27	X	76	ARG	2.2
17	N	106	LEU	2.2
9	E	1	PRO	2.2
12	H	83	TYR	2.2
6	B	57	GLU	2.2
12	H	111	ASP	2.2
8	D	87	ALA	2.2
14	K	119	GLN	2.2
9	E	161	VAL	2.2
23	T	110	ALA	2.2
17	N	183	ASP	2.2
10	F	24	ARG	2.2
15	L	105	TYR	2.2
5	A	82	VAL	2.2
10	F	19	ALA	2.2
4	5	77	PHE	2.2
15	L	75	LEU	2.2
18	O	23	GLY	2.2
32	3	6	ARG	2.2
17	N	152	GLU	2.2
26	W	86	GLU	2.2
6	B	119	HIS	2.2
1	0	359	U	2.2
29	Z	27	ALA	2.2
2	9	3122	C	2.2
29	Z	15	GLY	2.2
1	0	2344	G	2.1
25	V	5	VAL	2.1
27	X	44	ASP	2.1
10	F	118	LEU	2.1
10	F	11	ASP	2.1
1	0	371	U	2.1
8	D	58	VAL	2.1
18	O	22	GLY	2.1
25	V	60	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
15	L	148	GLU	2.1
9	E	7	ILE	2.1
1	0	1181	A	2.1
1	0	2345	A	2.1
9	E	105	GLU	2.1
17	N	177	GLU	2.1
23	T	59	GLU	2.1
19	P	110	ASP	2.1
29	Z	44	GLU	2.1
33	I	110	GLU	2.1
1	0	2747	C	2.0
8	D	71	ALA	2.0
10	F	23	ALA	2.0
32	3	20	HIS	2.0
9	E	53	GLU	2.0
26	W	78	ASP	2.0
32	3	56	PRO	2.0
1	0	2239	C	2.0
8	D	23	VAL	2.0
11	G	20	VAL	2.0
16	M	88	VAL	2.0
12	H	137	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	PSU	0	2621	20/21	0.98	0.14	-	36,38,43,43	0
1	1MA	0	628	23/24	0.98	0.12	-	32,35,37,38	0
1	OMG	0	2588	24/25	0.98	0.13	-	31,34,39,41	0
3	PPU	4	76	24/38	0.98	0.13	-	41,44,45,49	0
1	OMU	0	2587	21/22	0.98	0.13	-	32,37,40,40	0
3	HFA	4	77	11/12	0.95	0.19	-	42,44,47,48	0
1	UR3	0	2619	21/22	0.97	0.15	-	39,42,45,48	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
36	NA	0	9125	1/1	0.95	0.82	77.79	92,92,92,92	0
36	NA	0	9164	1/1	0.87	0.56	60.98	61,61,61,61	0
36	NA	0	9161	1/1	0.85	0.72	43.33	68,68,68,68	0
36	NA	0	9135	1/1	0.72	0.30	35.12	55,55,55,55	0
36	NA	0	9171	1/1	0.93	0.31	20.63	61,61,61,61	0
38	SR	B	9521	1/1	0.59	0.63	18.92	200,200,200,200	0
34	MG	0	8013	1/1	0.84	0.34	18.68	25,25,25,25	0
34	MG	0	8052	1/1	0.83	0.25	18.55	99,99,99,99	0
36	NA	0	9178	1/1	0.96	0.46	16.82	54,54,54,54	0
38	SR	0	9482	1/1	0.90	0.35	15.85	135,135,135,135	0
36	NA	0	9177	1/1	0.91	0.35	13.20	77,77,77,77	0
35	K	0	9001	1/1	0.88	0.31	13.00	74,74,74,74	0
36	NA	9	9183	1/1	0.76	0.38	12.87	75,75,75,75	0
36	NA	0	9182	1/1	0.62	0.40	12.50	90,90,90,90	0
36	NA	R	9186	1/1	0.83	0.39	12.42	80,80,80,80	0
34	MG	5	8118	1/1	0.88	0.34	11.85	45,45,45,45	0
36	NA	0	9173	1/1	0.93	0.34	10.94	69,69,69,69	0
36	NA	0	9159	1/1	0.93	0.35	10.57	58,58,58,58	0
36	NA	0	9174	1/1	0.91	0.38	10.49	65,65,65,65	0
34	MG	0	8038	1/1	0.99	0.25	10.45	25,25,25,25	0
34	MG	0	8101	1/1	0.62	0.28	10.41	80,80,80,80	0
36	NA	0	9150	1/1	0.94	0.21	9.56	47,47,47,47	0
36	NA	0	9172	1/1	0.83	0.35	9.54	76,76,76,76	0
36	NA	0	9168	1/1	0.90	0.17	9.19	69,69,69,69	0
34	MG	0	8012	1/1	0.97	0.22	7.62	39,39,39,39	0
36	NA	0	9120	1/1	0.93	0.21	7.11	61,61,61,61	0
36	NA	0	9132	1/1	0.86	0.23	5.52	68,68,68,68	0
34	MG	0	8001	1/1	0.97	0.19	4.99	22,22,22,22	0
34	MG	0	8008	1/1	0.99	0.19	4.76	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9165	1/1	0.89	0.30	4.41	45,45,45,45	0
34	MG	0	8065	1/1	0.81	0.35	4.36	107,107,107,107	0
36	NA	0	9115	1/1	0.96	0.18	4.21	41,41,41,41	0
34	MG	0	8054	1/1	0.93	0.16	4.16	63,63,63,63	0
34	MG	0	8056	1/1	0.98	0.23	3.85	44,44,44,44	0
34	MG	0	8091	1/1	0.89	0.15	3.78	64,64,64,64	0
36	NA	0	9114	1/1	0.75	0.20	3.64	65,65,65,65	0
37	CL	0	9316	1/1	0.97	0.26	3.56	78,78,78,78	0
34	MG	0	8080	1/1	0.98	0.17	2.85	57,57,57,57	0
36	NA	0	9131	1/1	0.90	0.14	2.58	47,47,47,47	0
36	NA	0	9156	1/1	0.96	0.16	2.35	57,57,57,57	0
34	MG	0	8021	1/1	0.95	0.17	2.28	56,56,56,56	0
37	CL	B	9319	1/1	0.99	0.16	1.43	54,54,54,54	0
36	NA	0	9162	1/1	0.96	0.15	1.40	52,52,52,52	0
34	MG	0	8107	1/1	0.84	0.17	1.24	65,65,65,65	0
34	MG	0	8017	1/1	0.98	0.14	1.07	31,31,31,31	0
36	NA	0	9124	1/1	0.93	0.19	1.03	50,50,50,50	0
38	SR	0	9475	1/1	0.98	0.13	1.01	83,83,83,83	0
38	SR	0	9410	1/1	0.99	0.14	1.00	41,41,41,41	0
34	MG	0	8074	1/1	0.99	0.18	0.89	27,27,27,27	0
34	MG	0	8020	1/1	0.98	0.16	0.87	36,36,36,36	0
38	SR	0	9515	1/1	0.99	0.14	0.86	100,100,100,100	0
38	SR	0	9406	1/1	1.00	0.13	0.66	35,35,35,35	0
34	MG	0	8057	1/1	0.94	0.20	0.62	77,77,77,77	0
36	NA	M	9147	1/1	0.93	0.18	0.52	42,42,42,42	0
38	SR	0	9407	1/1	1.00	0.13	0.50	47,47,47,47	0
38	SR	0	9509	1/1	0.92	0.15	0.38	95,95,95,95	0
38	SR	0	9490	1/1	0.96	0.13	0.37	116,116,116,116	0
34	MG	0	8070	1/1	0.96	0.14	0.31	24,24,24,24	0
38	SR	0	9451	1/1	0.99	0.12	0.30	60,60,60,60	0
38	SR	0	9534	1/1	0.97	0.14	0.16	111,111,111,111	0
35	K	0	9002	1/1	0.76	0.18	0.13	88,88,88,88	0
38	SR	H	9486	1/1	0.95	0.15	0.08	125,125,125,125	0
38	SR	F	9595	1/1	0.96	0.16	-0.02	109,109,109,109	0
34	MG	0	8097	1/1	0.94	0.13	-0.04	57,57,57,57	0
36	NA	C	9104	1/1	0.95	0.16	-0.36	33,33,33,33	0
38	SR	0	9424	1/1	1.00	0.16	-0.56	49,49,49,49	0
37	CL	M	9318	1/1	0.95	0.17	-0.57	41,41,41,41	0
36	NA	0	9143	1/1	0.89	0.14	-0.62	40,40,40,40	0
36	NA	0	9139	1/1	0.95	0.10	-0.80	43,43,43,43	0
38	SR	0	9455	1/1	0.98	0.09	-0.87	88,88,88,88	0
39	CD	Z	9203	1/1	0.75	0.13	-0.90	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	J	9146	1/1	0.79	0.11	-1.01	55,55,55,55	0
37	CL	J	9321	1/1	0.96	0.11	-1.04	66,66,66,66	0
38	SR	0	9504	1/1	0.91	0.11	-1.25	108,108,108,108	0
37	CL	0	9312	1/1	0.99	0.10	-1.32	57,57,57,57	0
34	MG	A	8066	1/1	0.97	0.11	-1.33	57,57,57,57	0
36	NA	0	9166	1/1	0.89	0.09	-1.37	74,74,74,74	0
34	MG	0	8004	1/1	0.95	0.10	-1.42	35,35,35,35	0
39	CD	U	9201	1/1	1.00	0.09	-1.45	53,53,53,53	0
36	NA	0	9117	1/1	0.93	0.07	-1.45	51,51,51,51	0
34	MG	Y	8109	1/1	0.96	0.12	-1.58	45,45,45,45	0
37	CL	O	9308	1/1	0.98	0.09	-1.61	67,67,67,67	0
34	MG	0	8028	1/1	0.99	0.13	-1.63	37,37,37,37	0
38	SR	0	9450	1/1	0.99	0.07	-1.71	72,72,72,72	0
34	MG	T	8073	1/1	0.94	0.11	-1.76	43,43,43,43	0
36	NA	Q	9148	1/1	0.98	0.09	-1.84	49,49,49,49	0
34	MG	0	8015	1/1	0.99	0.09	-1.89	35,35,35,35	0
36	NA	0	9127	1/1	0.96	0.10	-2.14	60,60,60,60	0
39	CD	3	9204	1/1	0.99	0.04	-2.19	64,64,64,64	0
36	NA	0	9138	1/1	0.97	0.07	-2.20	62,62,62,62	0
36	NA	R	9137	1/1	0.96	0.08	-2.25	36,36,36,36	0
38	SR	1	9419	1/1	0.99	0.09	-2.38	40,40,40,40	0
38	SR	0	9428	1/1	0.99	0.07	-2.38	55,55,55,55	0
34	MG	0	8003	1/1	0.95	0.13	-2.52	35,35,35,35	0
38	SR	3	9439	1/1	0.99	0.05	-2.54	72,72,72,72	0
38	SR	0	9456	1/1	0.98	0.10	-2.54	67,67,67,67	0
38	SR	0	9468	1/1	0.91	0.05	-2.75	128,128,128,128	0
37	CL	3	9304	1/1	0.96	0.07	-2.79	61,61,61,61	0
34	MG	0	8067	1/1	0.95	0.11	-2.80	40,40,40,40	0
34	MG	0	8002	1/1	0.97	0.09	-3.00	34,34,34,34	0
38	SR	A	9436	1/1	0.97	0.06	-3.02	60,60,60,60	0
34	MG	0	8060	1/1	0.96	0.08	-3.10	82,82,82,82	0
34	MG	0	8096	1/1	0.98	0.06	-3.40	41,41,41,41	0
34	MG	0	8032	1/1	0.92	0.10	-3.48	48,48,48,48	0
38	SR	L	9409	1/1	0.99	0.07	-3.52	37,37,37,37	0
38	SR	0	9532	1/1	0.90	0.05	-3.54	120,120,120,120	0
37	CL	0	9305	1/1	0.97	0.07	-3.55	61,61,61,61	0
34	MG	0	8110	1/1	0.97	0.11	-3.71	45,45,45,45	0
39	CD	1	9202	1/1	0.99	0.05	-3.76	54,54,54,54	0
38	SR	0	9457	1/1	0.98	0.08	-4.14	51,51,51,51	0
36	NA	0	9105	1/1	0.96	0.09	-4.22	44,44,44,44	0
34	MG	0	8044	1/1	0.97	0.07	-4.61	35,35,35,35	0
38	SR	0	9416	1/1	1.00	0.08	-4.74	43,43,43,43	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8112	1/1	0.96	0.06	-4.79	46,46,46,46	0
38	SR	0	9444	1/1	0.99	0.05	-5.06	55,55,55,55	0
34	MG	0	8019	1/1	0.92	0.06	-5.38	51,51,51,51	0
38	SR	0	9483	1/1	0.94	0.06	-5.71	77,77,77,77	0
37	CL	0	9315	1/1	0.97	0.09	-5.89	52,52,52,52	0
38	SR	0	9442	1/1	0.97	0.10	-6.28	66,66,66,66	0
36	NA	0	9123	1/1	0.99	0.09	-6.29	52,52,52,52	0
38	SR	0	9473	1/1	0.99	0.03	-6.47	82,82,82,82	0
38	SR	0	9453	1/1	0.99	0.06	-6.87	72,72,72,72	0
38	SR	0	9498	1/1	0.99	0.05	-7.61	63,63,63,63	0
38	SR	0	9506	1/1	0.98	0.04	-9.14	68,68,68,68	0
38	SR	0	9425	1/1	0.99	0.15	-	56,56,56,56	0
34	MG	0	8039	1/1	0.98	0.17	-	49,49,49,49	0
36	NA	0	9155	1/1	0.95	0.18	-	60,60,60,60	0
34	MG	0	8037	1/1	0.84	0.10	-	46,46,46,46	0
38	SR	0	9405	1/1	0.97	0.16	-	59,59,59,59	0
36	NA	0	9107	1/1	0.95	0.39	-	71,71,71,71	0
38	SR	B	9458	1/1	0.99	0.05	-	82,82,82,82	0
34	MG	0	8058	1/1	0.90	0.21	-	41,41,41,41	0
38	SR	0	9477	1/1	0.98	0.10	-	86,86,86,86	0
38	SR	0	9421	1/1	0.98	0.10	-	78,78,78,78	0
34	MG	0	8014	1/1	0.90	0.39	-	73,73,73,73	0
38	SR	R	9418	1/1	0.99	0.15	-	57,57,57,57	0
34	MG	0	8061	1/1	0.86	0.19	-	87,87,87,87	0
38	SR	0	9466	1/1	0.97	0.06	-	96,96,96,96	0
36	NA	0	9154	1/1	0.98	0.14	-	54,54,54,54	0
34	MG	0	8092	1/1	0.82	0.34	-	77,77,77,77	0
34	MG	9	8095	1/1	0.92	0.35	-	55,55,55,55	0
36	NA	0	9170	1/1	0.89	0.29	-	77,77,77,77	0
38	SR	0	9501	1/1	0.65	0.20	-	159,159,159,159	0
38	SR	0	9547	1/1	0.52	0.39	-	194,194,194,194	0
34	MG	0	8043	1/1	0.91	0.06	-	52,52,52,52	0
38	SR	0	9415	1/1	1.00	0.10	-	56,56,56,56	0
34	MG	0	8083	1/1	0.95	0.11	-	53,53,53,53	0
34	MG	2	8076	1/1	0.95	0.17	-	64,64,64,64	0
36	NA	0	9157	1/1	0.94	0.18	-	47,47,47,47	0
36	NA	0	9179	1/1	0.91	0.59	-	121,121,121,121	0
34	MG	K	8069	1/1	0.97	0.17	-	25,25,25,25	0
38	SR	0	9448	1/1	1.00	0.07	-	63,63,63,63	0
38	SR	0	9469	1/1	0.98	0.05	-	85,85,85,85	0
38	SR	0	9413	1/1	0.99	0.12	-	49,49,49,49	0
38	SR	0	9522	1/1	0.96	0.04	-	114,114,114,114	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9136	1/1	0.98	0.12	-	34,34,34,34	0
37	CL	N	9307	1/1	0.96	0.16	-	65,65,65,65	0
34	MG	0	8084	1/1	0.97	0.40	-	89,89,89,89	0
34	MG	0	8108	1/1	0.68	0.14	-	103,103,103,103	0
38	SR	0	9440	1/1	0.96	0.05	-	72,72,72,72	0
36	NA	0	9175	1/1	0.93	0.34	-	55,55,55,55	0
38	SR	0	9464	1/1	0.98	0.05	-	81,81,81,81	0
36	NA	0	9102	1/1	0.87	0.22	-	63,63,63,63	0
34	MG	0	8114	1/1	0.97	0.47	-	83,83,83,83	0
34	MG	0	8094	1/1	0.92	0.50	-	72,72,72,72	0
36	NA	0	9169	1/1	0.86	0.39	-	116,116,116,116	0
38	SR	0	9517	1/1	0.95	0.06	-	110,110,110,110	0
37	CL	J	9301	1/1	0.93	0.18	-	60,60,60,60	0
38	SR	0	9626	1/1	0.91	0.25	-	154,154,154,154	0
38	SR	0	9435	1/1	0.98	0.08	-	76,76,76,76	0
34	MG	0	8031	1/1	0.98	0.12	-	49,49,49,49	0
38	SR	0	9443	1/1	0.98	0.10	-	63,63,63,63	0
36	NA	0	9128	1/1	0.90	0.15	-	49,49,49,49	0
38	SR	0	9478	1/1	0.99	0.06	-	77,77,77,77	0
38	SR	0	9454	1/1	0.98	0.10	-	82,82,82,82	0
34	MG	0	8099	1/1	0.91	0.14	-	75,75,75,75	0
34	MG	0	8116	1/1	0.95	0.10	-	64,64,64,64	0
36	NA	0	9122	1/1	0.58	0.40	-	90,90,90,90	0
38	SR	0	9484	1/1	0.32	0.14	-	149,149,149,149	0
38	SR	0	9430	1/1	0.99	0.10	-	49,49,49,49	0
34	MG	0	8042	1/1	0.96	0.11	-	48,48,48,48	0
38	SR	0	9568	1/1	0.97	0.07	-	80,80,80,80	0
34	MG	0	8102	1/1	0.85	0.12	-	68,68,68,68	0
36	NA	0	9163	1/1	0.94	0.16	-	73,73,73,73	0
34	MG	0	8025	1/1	0.90	0.42	-	27,27,27,27	0
38	SR	0	9417	1/1	0.99	0.08	-	63,63,63,63	0
38	SR	0	9441	1/1	0.98	0.07	-	68,68,68,68	0
36	NA	0	9181	1/1	0.72	0.16	-	54,54,54,54	0
37	CL	0	9303	1/1	0.99	0.13	-	53,53,53,53	0
38	SR	0	9462	1/1	0.98	0.10	-	74,74,74,74	0
34	MG	0	8090	1/1	0.80	0.36	-	68,68,68,68	0
38	SR	9	9503	1/1	0.91	0.05	-	122,122,122,122	0
36	NA	0	9167	1/1	0.91	0.10	-	65,65,65,65	0
38	SR	0	9500	1/1	0.88	1.54	-	200,200,200,200	0
34	MG	0	8103	1/1	0.89	0.17	-	67,67,67,67	0
34	MG	0	8050	1/1	0.88	0.22	-	89,89,89,89	0
38	SR	0	9474	1/1	0.99	0.08	-	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	NA	0	9149	1/1	0.94	0.29	-	49,49,49,49	0
38	SR	0	9629	1/1	0.98	0.08	-	75,75,75,75	0
38	SR	0	9459	1/1	0.91	0.10	-	103,103,103,103	0
38	SR	0	9449	1/1	0.99	0.09	-	67,67,67,67	0
36	NA	0	9152	1/1	0.77	1.03	-	83,83,83,83	0
34	MG	0	8046	1/1	0.97	0.06	-	39,39,39,39	0
34	MG	0	8117	1/1	0.97	0.12	-	46,46,46,46	0
38	SR	0	9461	1/1	0.98	0.06	-	82,82,82,82	0
38	SR	0	9411	1/1	0.99	0.14	-	43,43,43,43	0
38	SR	0	9480	1/1	0.98	0.05	-	93,93,93,93	0
38	SR	0	9429	1/1	0.99	0.10	-	72,72,72,72	0
34	MG	0	8051	1/1	0.90	0.21	-	36,36,36,36	0
38	SR	0	9495	1/1	0.95	0.14	-	111,111,111,111	0
36	NA	0	9129	1/1	0.79	0.13	-	72,72,72,72	0
38	SR	0	9422	1/1	0.99	0.10	-	58,58,58,58	0
34	MG	0	8072	1/1	0.89	0.65	-	89,89,89,89	0
36	NA	0	9158	1/1	0.85	0.43	-	66,66,66,66	0
36	NA	0	9116	1/1	0.77	0.36	-	52,52,52,52	0
36	NA	0	9118	1/1	0.98	0.21	-	66,66,66,66	0
38	SR	0	9570	1/1	0.94	0.07	-	111,111,111,111	0
34	MG	0	8026	1/1	0.99	0.14	-	30,30,30,30	0
37	CL	0	9313	1/1	0.99	0.10	-	59,59,59,59	0
34	MG	0	8079	1/1	0.95	0.13	-	33,33,33,33	0
36	NA	0	9108	1/1	0.97	0.10	-	34,34,34,34	0
36	NA	0	9141	1/1	0.75	0.13	-	73,73,73,73	0
38	SR	0	9423	1/1	1.00	0.05	-	64,64,64,64	0
34	MG	0	8106	1/1	0.88	0.09	-	51,51,51,51	0
38	SR	0	9412	1/1	0.99	0.13	-	45,45,45,45	0
34	MG	0	8055	1/1	0.91	0.31	-	97,97,97,97	0
38	SR	A	9497	1/1	0.98	0.09	-	96,96,96,96	0
34	MG	0	8085	1/1	0.93	0.21	-	63,63,63,63	0
34	MG	0	8059	1/1	0.83	0.42	-	84,84,84,84	0
34	MG	0	8045	1/1	0.95	0.26	-	72,72,72,72	0
34	MG	0	8104	1/1	0.84	0.13	-	57,57,57,57	0
36	NA	0	9101	1/1	0.92	0.13	-	46,46,46,46	0
34	MG	0	8041	1/1	0.97	0.09	-	55,55,55,55	0
38	SR	0	9447	1/1	0.97	0.07	-	73,73,73,73	0
36	NA	D	9151	1/1	0.70	0.23	-	68,68,68,68	0
37	CL	0	9311	1/1	0.97	0.15	-	71,71,71,71	0
38	SR	0	9590	1/1	0.90	0.12	-	131,131,131,131	0
38	SR	0	9426	1/1	0.97	0.08	-	71,71,71,71	0
38	SR	0	9434	1/1	0.99	0.14	-	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	MG	0	8009	1/1	0.97	0.10	-	21,21,21,21	0
37	CL	Y	9320	1/1	0.96	0.08	-	47,47,47,47	0
38	SR	0	9431	1/1	0.98	0.13	-	65,65,65,65	0
38	SR	0	9585	1/1	0.96	0.08	-	94,94,94,94	0
34	MG	0	8047	1/1	0.55	0.55	-	107,107,107,107	0
36	NA	0	9110	1/1	0.94	0.32	-	46,46,46,46	0
34	MG	0	8082	1/1	0.95	0.20	-	82,82,82,82	0
38	SR	0	9438	1/1	0.97	0.09	-	70,70,70,70	0
38	SR	0	9505	1/1	0.95	0.07	-	106,106,106,106	0
34	MG	0	8040	1/1	0.90	0.21	-	92,92,92,92	0
38	SR	A	9437	1/1	0.97	0.10	-	70,70,70,70	0
37	CL	L	9310	1/1	0.92	0.12	-	58,58,58,58	0
38	SR	0	9539	1/1	0.88	0.38	-	157,157,157,157	0
38	SR	0	9445	1/1	0.98	0.09	-	57,57,57,57	0
38	SR	0	9488	1/1	0.99	0.11	-	86,86,86,86	0
34	MG	0	8036	1/1	0.94	0.11	-	65,65,65,65	0
36	NA	0	9184	1/1	0.41	0.41	-	87,87,87,87	0
38	SR	9	9588	1/1	0.59	0.15	-	143,143,143,143	0
34	MG	0	8005	1/1	0.98	0.06	-	29,29,29,29	0
34	MG	0	8093	1/1	0.79	0.13	-	49,49,49,49	0
36	NA	0	9111	1/1	0.91	0.31	-	63,63,63,63	0
36	NA	0	9113	1/1	0.94	0.12	-	60,60,60,60	0
34	MG	0	8022	1/1	0.85	0.93	-	112,112,112,112	0
38	SR	0	9432	1/1	0.97	0.14	-	68,68,68,68	0
38	SR	0	9581	1/1	0.87	0.08	-	130,130,130,130	0
38	SR	0	9529	1/1	-0.08	0.27	-	131,131,131,131	0
38	SR	0	9414	1/1	0.98	0.12	-	57,57,57,57	0
38	SR	0	9452	1/1	0.94	0.16	-	106,106,106,106	0
38	SR	1	9460	1/1	1.00	0.10	-	52,52,52,52	0
34	MG	0	8024	1/1	0.88	0.41	-	86,86,86,86	0
37	CL	0	9314	1/1	0.99	0.06	-	51,51,51,51	0
34	MG	0	8113	1/1	0.88	0.12	-	52,52,52,52	0
38	SR	S	9470	1/1	0.99	0.16	-	101,101,101,101	0
38	SR	0	9489	1/1	0.98	0.11	-	94,94,94,94	0
34	MG	0	8075	1/1	0.98	0.07	-	47,47,47,47	0
38	SR	0	9465	1/1	0.92	0.10	-	107,107,107,107	0
38	SR	9	9481	1/1	0.98	0.08	-	89,89,89,89	0
37	CL	0	9322	1/1	0.95	0.38	-	61,61,61,61	0
34	MG	0	8068	1/1	0.95	0.14	-	48,48,48,48	0
37	CL	0	9317	1/1	0.95	0.06	-	52,52,52,52	0
34	MG	0	8027	1/1	0.97	0.24	-	36,36,36,36	0
38	SR	0	9537	1/1	0.50	0.23	-	157,157,157,157	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
39	CD	O	9205	1/1	0.94	0.05	-	132,132,132,132	0
37	CL	J	9302	1/1	0.96	0.07	-	53,53,53,53	0
38	SR	0	9467	1/1	0.99	0.10	-	86,86,86,86	0
36	NA	0	9185	1/1	0.85	0.61	-	54,54,54,54	0
38	SR	0	9601	1/1	0.98	0.05	-	119,119,119,119	0
38	SR	0	9560	1/1	0.95	0.08	-	101,101,101,101	0
38	SR	0	9427	1/1	0.98	0.13	-	56,56,56,56	0
34	MG	0	8089	1/1	0.88	0.17	-	61,61,61,61	0
38	SR	0	9530	1/1	0.96	0.11	-	72,72,72,72	0
36	NA	0	9126	1/1	0.78	0.12	-	63,63,63,63	0
34	MG	0	8063	1/1	0.92	0.10	-	65,65,65,65	0
36	NA	0	9106	1/1	0.93	0.44	-	44,44,44,44	0
34	MG	0	8115	1/1	0.93	0.09	-	59,59,59,59	0
38	SR	0	9446	1/1	0.97	0.07	-	88,88,88,88	0
36	NA	0	9130	1/1	0.98	0.15	-	50,50,50,50	0
34	MG	0	8088	1/1	0.97	0.11	-	28,28,28,28	0
36	NA	S	9112	1/1	0.87	0.25	-	80,80,80,80	0
38	SR	0	9420	1/1	1.00	0.17	-	70,70,70,70	0
36	NA	0	9160	1/1	0.97	0.17	-	46,46,46,46	0
38	SR	0	9433	1/1	0.96	0.12	-	75,75,75,75	0
34	MG	0	8098	1/1	0.95	0.07	-	45,45,45,45	0
37	CL	A	9309	1/1	0.92	0.19	-	66,66,66,66	0
34	MG	0	8030	1/1	0.87	0.08	-	37,37,37,37	0
34	MG	0	8029	1/1	0.95	0.22	-	35,35,35,35	0
38	SR	0	9545	1/1	0.97	0.06	-	85,85,85,85	0
36	NA	0	9134	1/1	0.97	0.10	-	47,47,47,47	0
36	NA	0	9140	1/1	0.89	0.15	-	57,57,57,57	0
38	SR	0	9566	1/1	0.98	0.04	-	80,80,80,80	0
37	CL	R	9306	1/1	0.97	0.10	-	45,45,45,45	0
38	SR	0	9508	1/1	0.94	0.08	-	97,97,97,97	0
38	SR	0	9408	1/1	0.99	0.12	-	36,36,36,36	0

6.5 Other polymers

There are no such residues in this entry.