



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:39 AM UTC

PDB ID : 1YHQ / pdb_00001yhq
Title : Crystal Structure Of Azithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-10
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

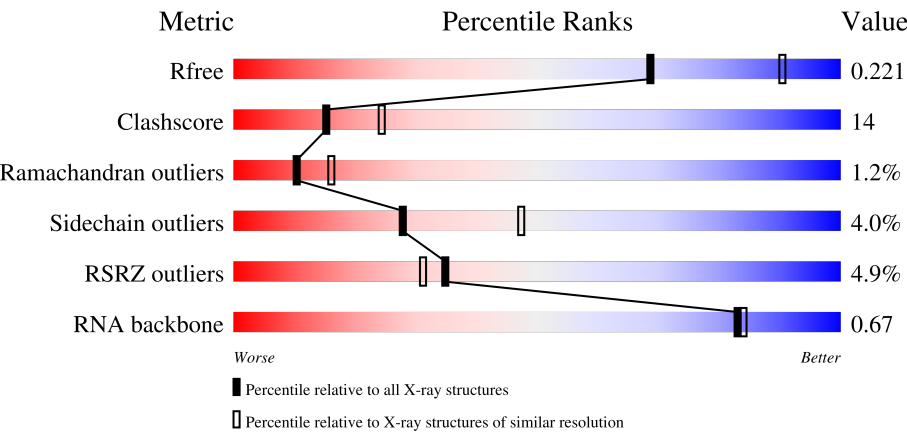
1 Overall quality at a glance i

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))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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

Mol	Chain	Length	Quality of chain
1	0	2922	3% 65%25%6%
2	9	122	3% 60%30%9%
3	A	240	4% 61%32%6%
4	B	338	% 57%38%5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	2	50	8% 50% 40% 8%
31	3	92	% 64% 34%

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99116 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
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 55229667
0	2099	A	G	engineered mutation	GB 55229667
0	2587	OMU	U	modified residue	GB 55229667
0	2588	OMG	G	modified residue	GB 55229667
0	2619	UR3	U	modified residue	GB 55229667
0	2621	PSU	U	modified residue	GB 55229667

- 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
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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

- Molecule 7 is a protein called 50S ribosomal protein L6P.

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

- Molecule 8 is a protein called 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	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 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	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 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

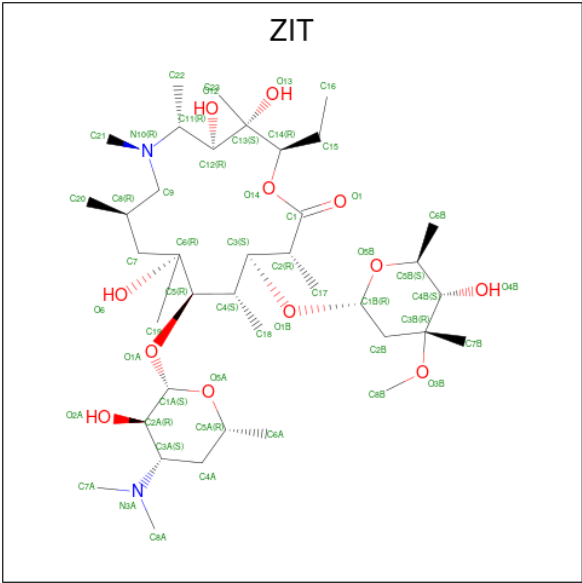
- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is AZITHROMYCIN (CCD ID: ZIT) (formula: $C_{38}H_{72}N_2O_{12}$).



- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	2	Total K 2 2	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	65	Total Na 65 65	0	0
35	9	2	Total Na 2 2	0	0
35	C	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	J	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	A	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	J	3	Total Cl 3 3	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

- Molecule 37 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	94	Total 94	Sr 94	0	0
37	9	2	Total 2	Sr 2	0	0
37	A	3	Total 3	Sr 3	0	0
37	B	2	Total 2	Sr 2	0	0
37	F	1	Total 1	Sr 1	0	0
37	H	1	Total 1	Sr 1	0	0
37	R	1	Total 1	Sr 1	0	0
37	S	1	Total 1	Sr 1	0	0
37	1	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0

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

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

Continued on next page...

Continued from previous page...

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5845	Total	O	0	0
			5845	5845		
39	9	145	Total	O	0	0
			145	145		
39	A	118	Total	O	0	0
			118	118		
39	B	151	Total	O	0	0
			151	151		
39	C	176	Total	O	0	0
			176	176		
39	D	49	Total	O	0	0
			49	49		
39	E	40	Total	O	0	0
			40	40		
39	F	26	Total	O	0	0
			26	26		
39	G	18	Total	O	0	0
			18	18		
39	H	72	Total	O	0	0
			72	72		
39	I	8	Total	O	0	0
			8	8		
39	J	59	Total	O	0	0
			59	59		
39	K	58	Total	O	0	0
			58	58		
39	L	72	Total	O	0	0
			72	72		
39	M	124	Total	O	0	0
			124	124		
39	N	61	Total	O	0	0
			61	61		
39	O	38	Total	O	0	0
			38	38		

Continued on next page...

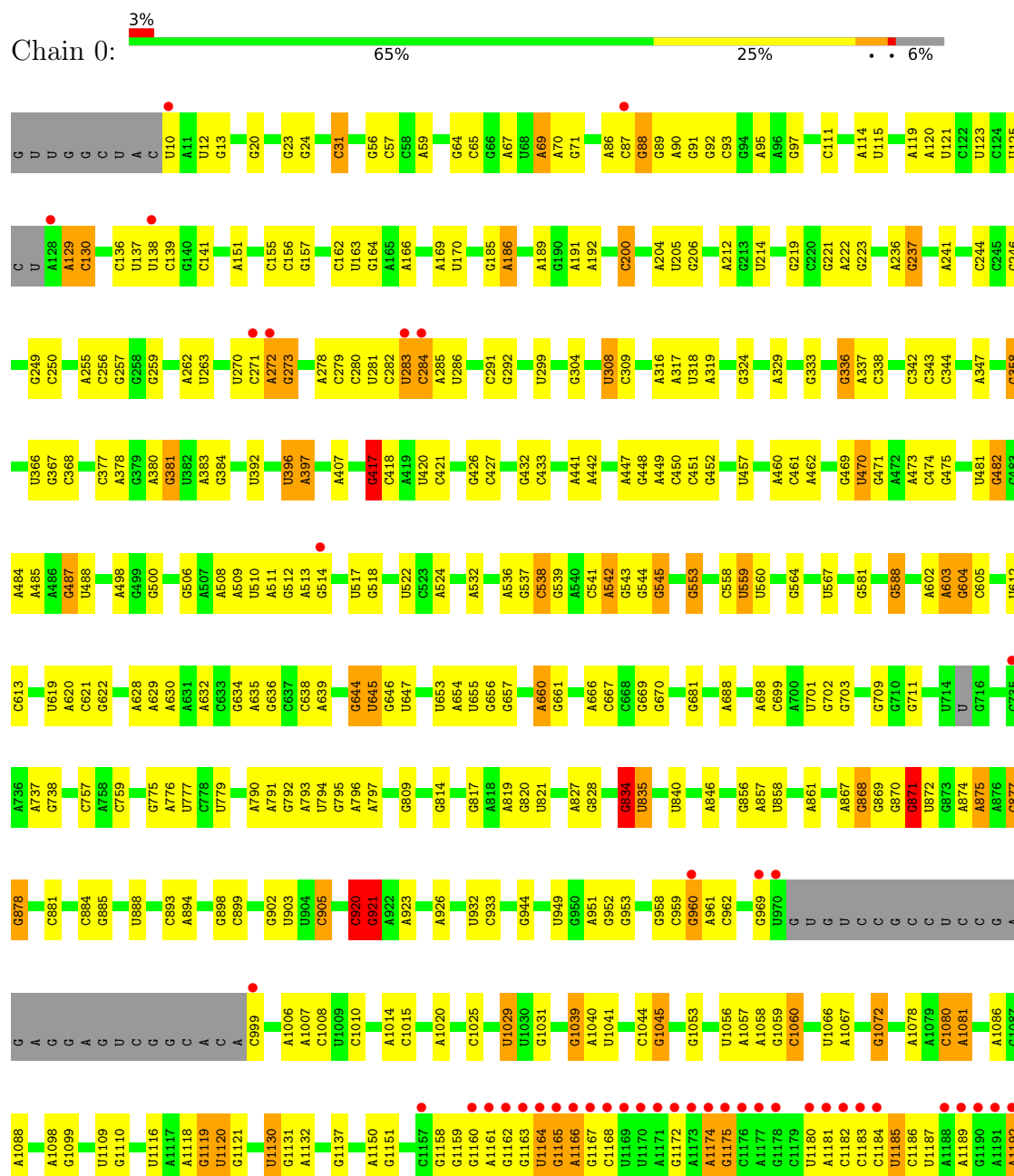
Continued from previous page...

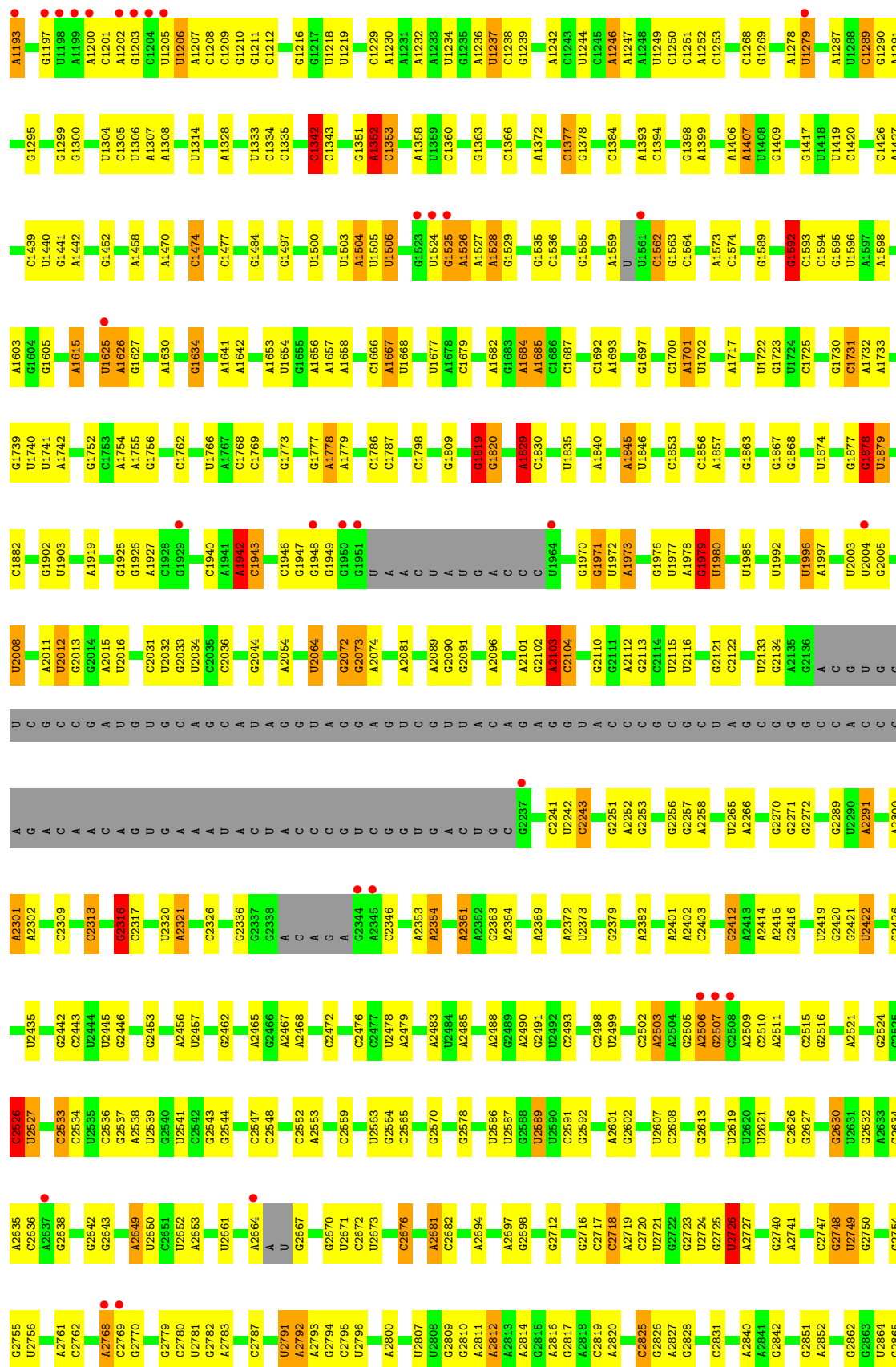
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	24	Total 24	O 24	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	32	Total 32	O 32	0	0
39	1	50	Total 50	O 50	0	0
39	2	44	Total 44	O 44	0	0
39	3	71	Total 71	O 71	0	0

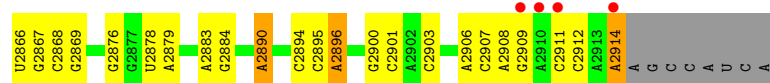
3 Residue-property plots

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

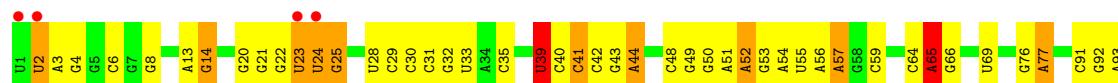
• Molecule 1: 23S Ribosomal RNA



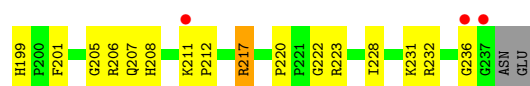
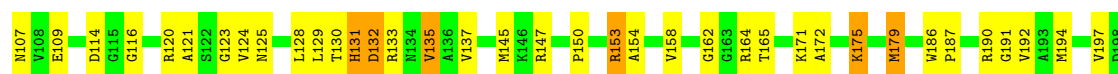
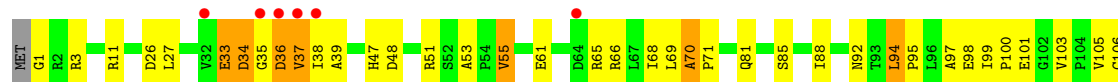




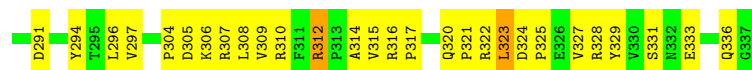
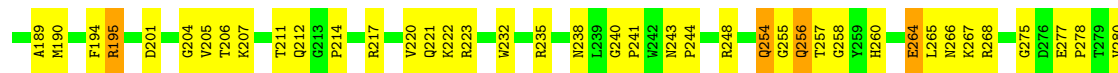
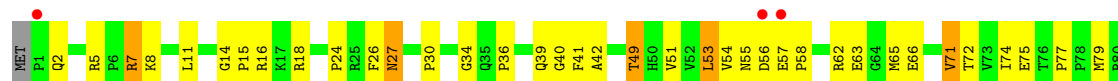
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

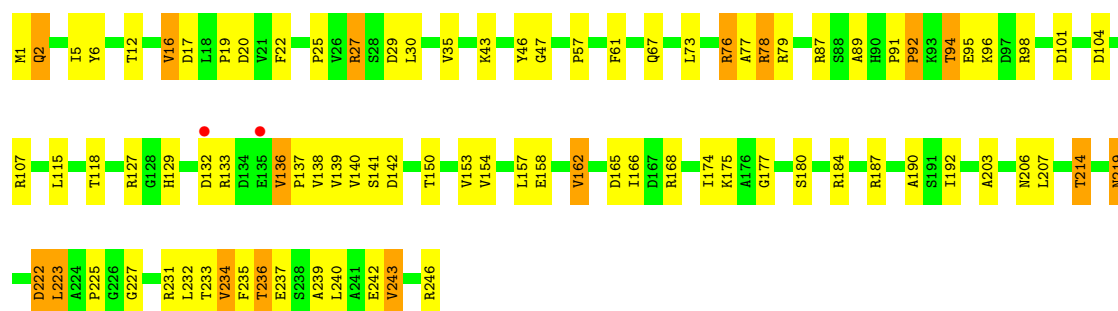


• Molecule 4: 50S ribosomal protein L3P

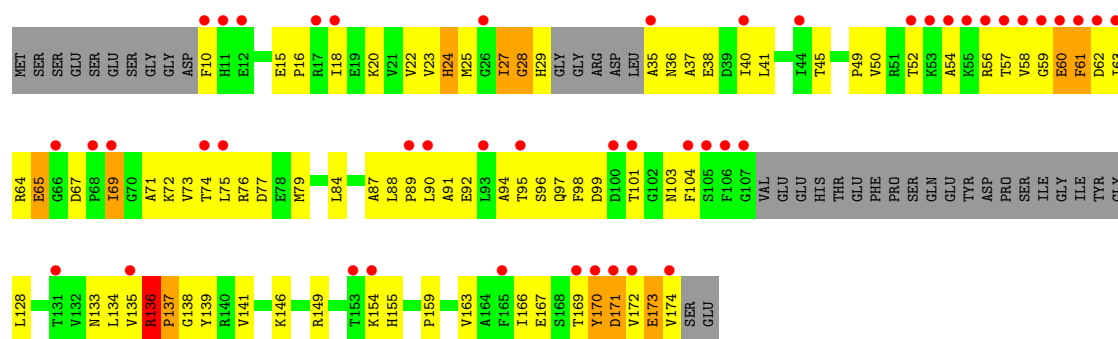


• Molecule 5: 50S ribosomal protein L4E

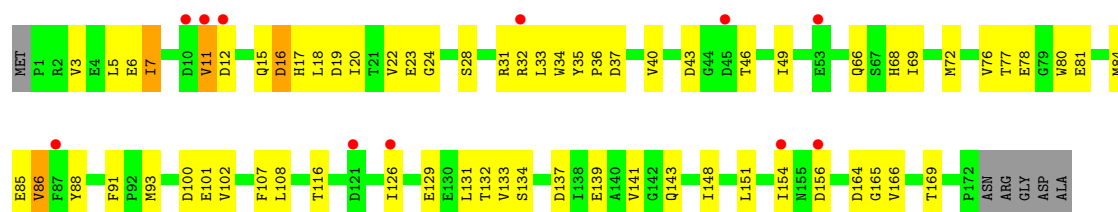




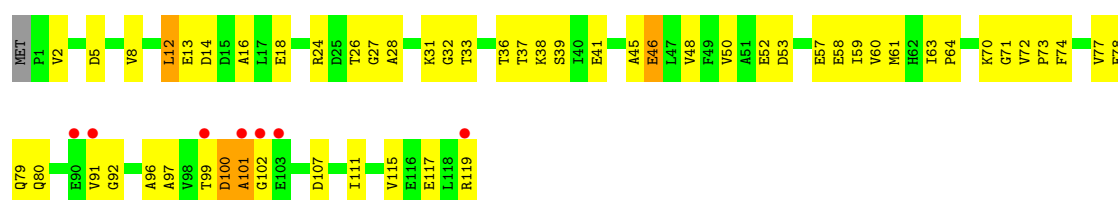
• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P

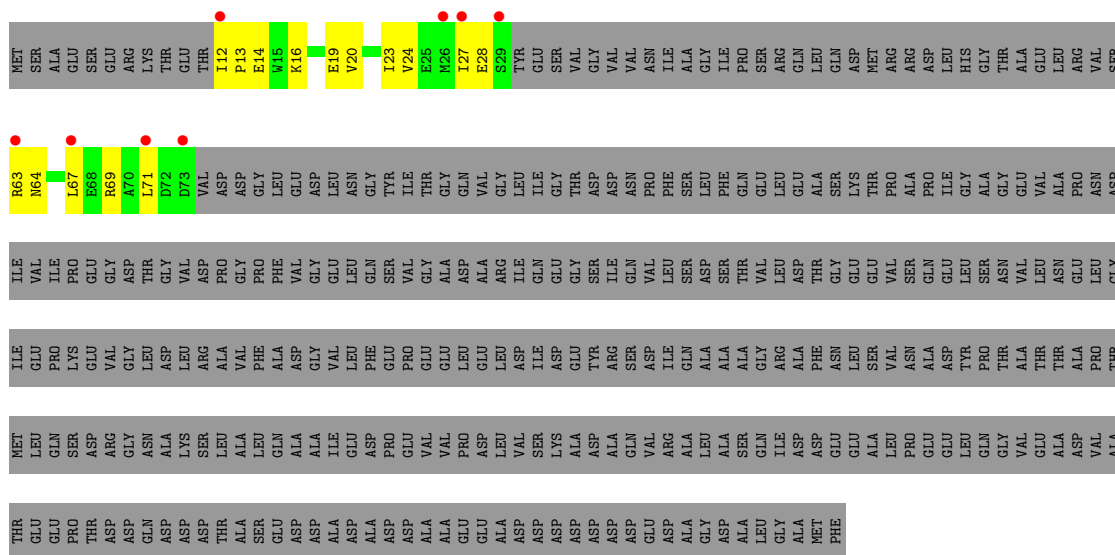


• Molecule 8: 50S ribosomal protein L7AE

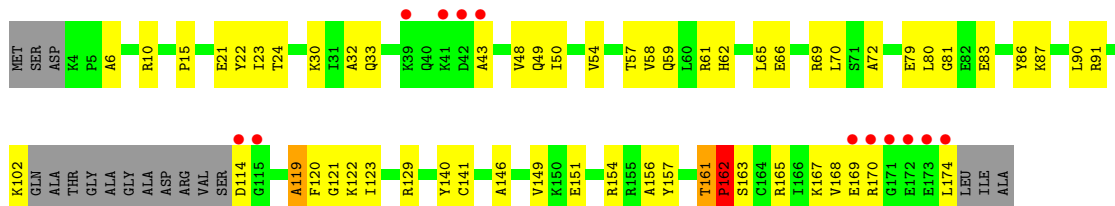


• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

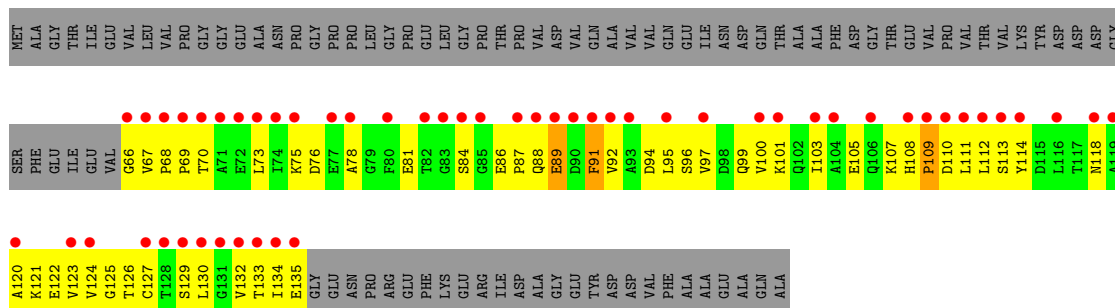




- Molecule 10: 50S RIBOSOMAL PROTEIN L10E

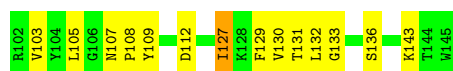


- Molecule 11: 50S RIBOSOMAL PROTEIN L11P

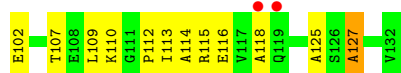


- Molecule 12: 50S ribosomal protein L13P

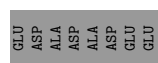




- Molecule 13: 50S ribosomal protein L14P



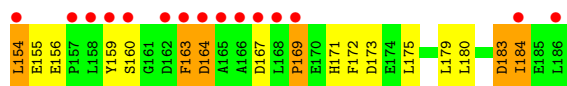
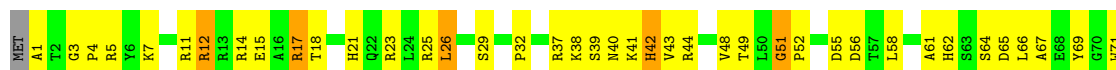
- Molecule 14: 50S ribosomal protein L15P



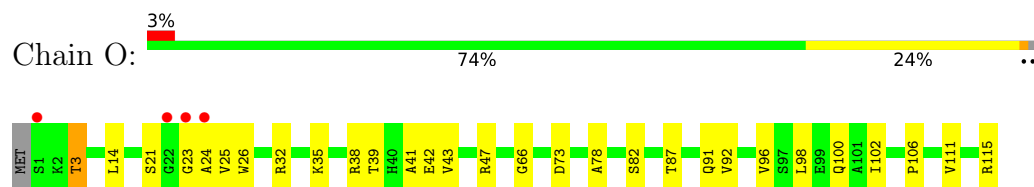
- Molecule 15: 50S Ribosomal Protein L15E



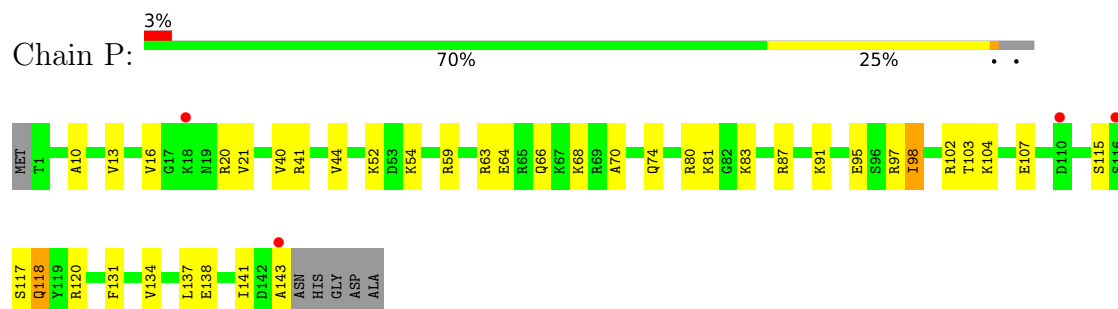
- Molecule 16: 50S ribosomal protein L18P



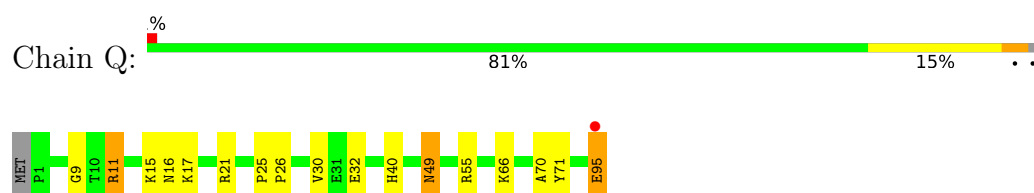
- Molecule 17: 50S ribosomal protein L18e



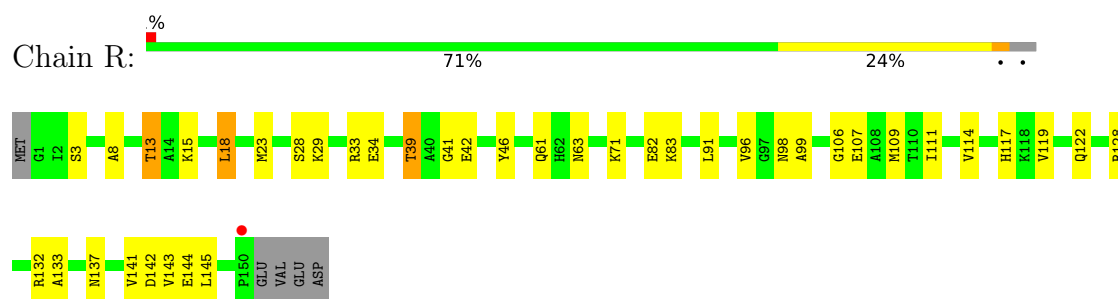
- Molecule 18: 50S ribosomal protein L19E



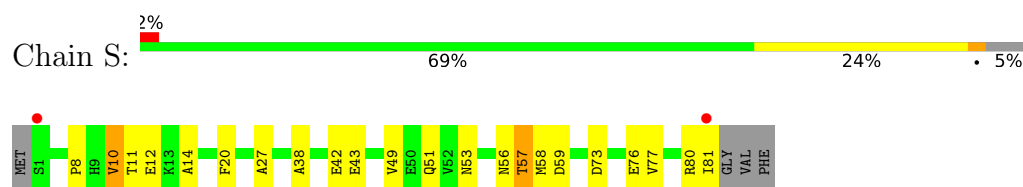
- Molecule 19: 50S ribosomal protein L21e



- Molecule 20: 50S ribosomal protein L22P

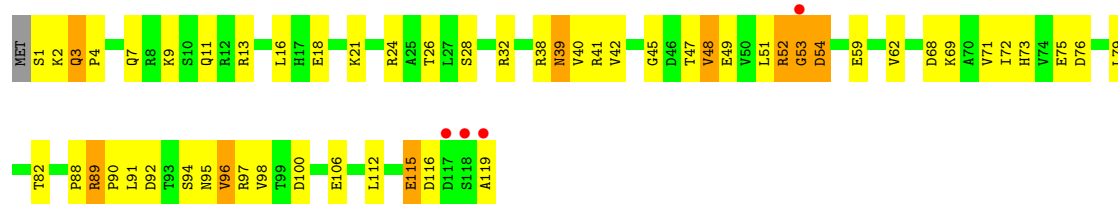


- Molecule 21: 50S ribosomal protein L23P

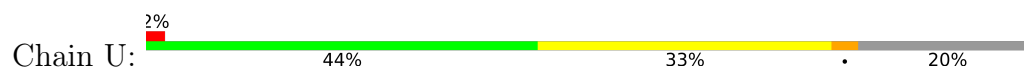


- Molecule 22: 50S ribosomal protein L24P

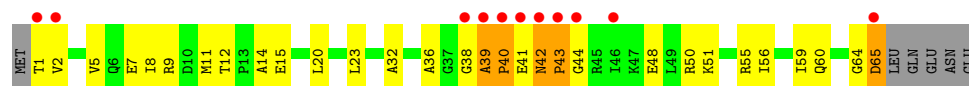




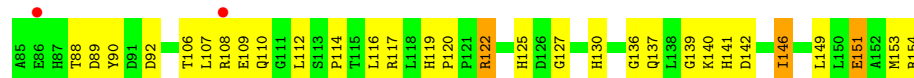
- Molecule 23: 50S ribosomal protein L24E



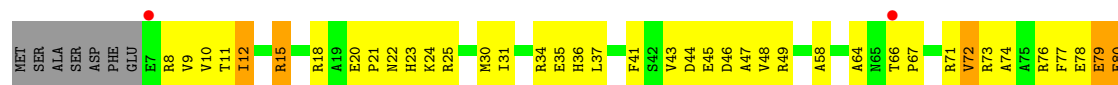
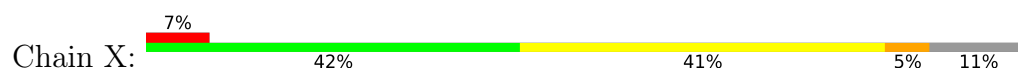
- Molecule 24: 50S ribosomal protein L29P



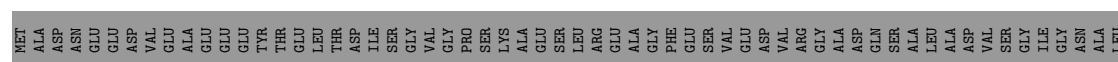
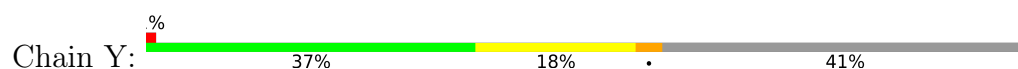
- Molecule 25: 50S ribosomal protein L30P

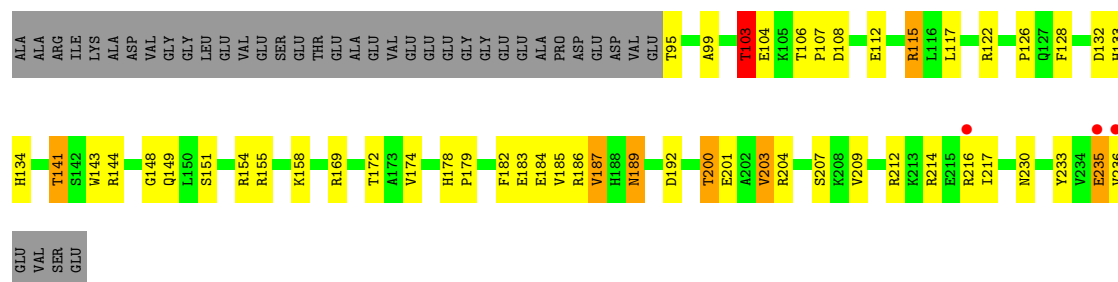


- Molecule 26: 50S ribosomal protein L31e

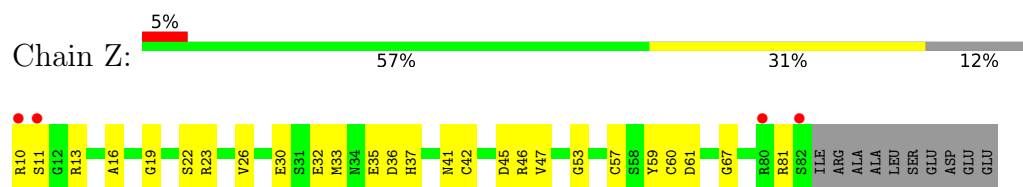


- Molecule 27: 50S ribosomal protein L32E

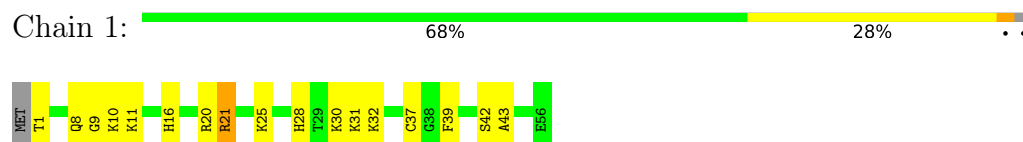




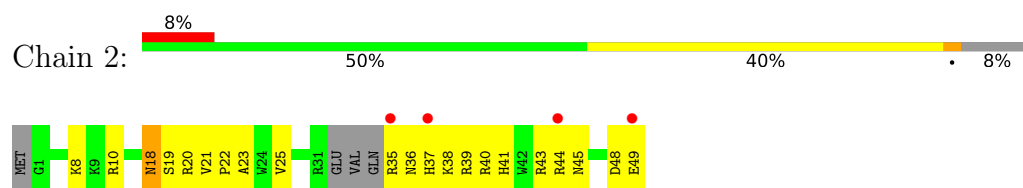
- Molecule 28: 50S ribosomal protein L37Ae



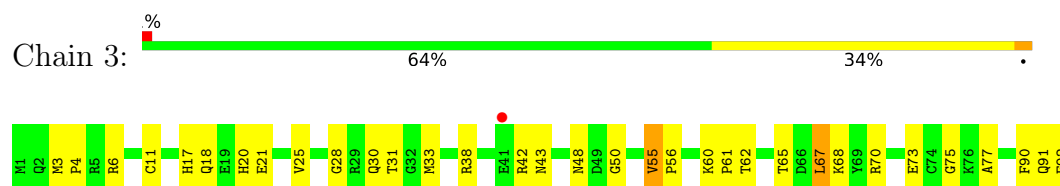
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.08Å 298.91Å 574.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 29.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.96-2.40) 90.2 (29.96-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.190 , 0.229 0.183 , 0.221	Depositor DCC
R_{free} test set	6150 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99116	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% 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: K, UR3, PSU, CD, NA, MG, SR, ZIT, OMU, OMG, CL, 1MA

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	0.37	0/65957	0.61	30/102867 (0.0%)
2	9	0.37	0/2904	0.60	3/4526 (0.1%)
3	A	0.42	0/1786	0.99	6/2408 (0.2%)
4	B	0.40	0/2690	0.98	6/3652 (0.2%)
5	C	0.45	0/1884	0.95	7/2551 (0.3%)
6	D	0.34	0/1111	0.86	5/1498 (0.3%)
7	E	0.37	0/1382	0.85	2/1880 (0.1%)
8	F	0.38	0/901	0.86	1/1224 (0.1%)
9	G	0.32	0/241	0.78	0/324
10	H	0.39	0/1302	0.95	7/1743 (0.4%)
11	I	0.35	0/526	0.91	3/716 (0.4%)
12	J	0.39	0/1136	0.91	3/1530 (0.2%)
13	K	0.39	0/1001	0.97	3/1347 (0.2%)
14	L	0.37	0/1130	1.00	6/1509 (0.4%)
15	M	0.40	0/1582	0.88	3/2117 (0.1%)
16	N	0.35	0/1474	1.01	9/1999 (0.5%)
17	O	0.41	0/874	0.91	4/1181 (0.3%)
18	P	0.39	0/1147	0.83	2/1528 (0.1%)
19	Q	0.42	0/749	1.04	2/1005 (0.2%)
20	R	0.42	0/1172	0.94	6/1578 (0.4%)
21	S	0.36	0/648	0.91	3/875 (0.3%)
22	T	0.37	0/958	0.95	5/1289 (0.4%)
23	U	0.35	0/417	0.82	1/562 (0.2%)
24	V	0.36	0/502	0.96	2/675 (0.3%)
25	W	0.44	0/1219	0.96	2/1655 (0.1%)
26	X	0.40	0/664	0.93	3/895 (0.3%)
27	Y	0.42	0/1146	0.92	5/1536 (0.3%)
28	Z	0.39	0/589	0.92	0/787
29	1	0.47	0/438	0.94	2/578 (0.3%)
30	2	0.41	0/401	0.79	0/529
31	3	0.40	0/771	0.89	4/1024 (0.4%)
All	All	0.38	0/98702	0.71	135/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	53
2	9	0	2
All	All	0	55

There are no bond length outliers.

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1979	G	C2'-C3'-O3'	9.85	124.27	109.50
16	N	135	VAL	N-CA-C	-9.58	103.79	113.47
19	Q	17	LYS	N-CA-C	-9.53	97.73	109.83
16	N	163	PHE	N-CA-C	-9.03	102.40	113.41
1	0	1942	A	C5'-C4'-C3'	8.89	129.34	116.00
1	0	2103	A	C2'-C3'-O3'	7.58	120.86	109.50
16	N	169	PRO	N-CA-C	-7.57	104.05	114.27
24	V	42	ASN	CA-C-N	7.54	129.27	119.84
24	V	42	ASN	C-N-CA	7.54	129.27	119.84
14	L	57	VAL	N-CA-C	-7.53	105.97	113.20
26	X	22	ASN	N-CA-C	7.52	120.43	111.33
21	S	27	ALA	N-CA-C	-7.51	96.48	108.73
2	9	39	U	N1-C1'-C2'	7.32	122.97	112.00
4	B	157	LYS	N-CA-C	-7.26	105.04	114.04
4	B	222	LYS	N-CA-C	-7.14	99.95	110.52
20	R	141	VAL	N-CA-C	7.08	118.68	108.48
3	A	222	GLY	N-CA-C	-6.97	105.59	114.37
14	L	145	LEU	N-CA-C	-6.96	103.69	111.28
3	A	70	ALA	N-CA-C	6.92	118.36	109.65
6	D	170	TYR	N-CA-C	6.77	118.83	110.91
1	0	871	G	C5'-C4'-O4'	-6.76	99.66	109.80
14	L	47	GLY	N-CA-C	6.70	118.95	111.85
1	0	1592	G	N9-C1'-C2'	6.68	122.02	112.00
1	0	1559	A	C2'-C3'-O3'	6.63	123.64	113.70
31	3	55	VAL	CA-C-N	6.62	128.12	119.84
31	3	55	VAL	C-N-CA	6.62	128.12	119.84
1	0	1819	G	C5'-C4'-C3'	6.59	125.89	116.00
27	Y	143	TRP	N-CA-C	6.58	119.84	109.96
1	0	2291	A	N9-C1'-C2'	6.58	121.88	112.00
5	C	175	LYS	N-CA-C	6.56	118.77	110.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	R	137	ASN	N-CA-C	6.54	120.15	110.46
1	0	206	G	C5'-C4'-C3'	-6.52	106.22	116.00
11	I	86	GLU	CA-C-N	6.50	126.47	120.03
11	I	86	GLU	C-N-CA	6.50	126.47	120.03
22	T	54	ASP	N-CA-C	-6.42	105.42	113.18
15	M	70	GLY	N-CA-C	6.41	121.14	112.17
4	B	323	LEU	N-CA-C	6.39	118.55	110.24
1	0	2726	U	N1-C1'-C2'	6.36	121.53	112.00
13	K	127	ALA	N-CA-C	-6.30	105.06	114.64
1	0	920	C	C2'-C3'-O3'	-6.29	104.26	113.70
15	M	89	THR	N-CA-C	6.28	117.79	111.07
5	C	192	ILE	N-CA-C	6.23	117.61	109.58
19	Q	49	ASN	N-CA-C	6.20	119.58	110.59
10	H	163	SER	N-CA-C	-6.17	101.35	110.48
3	A	135	VAL	N-CA-C	6.15	116.47	108.35
1	0	2316	G	C5'-C4'-C3'	-6.11	106.04	115.20
16	N	51	GLY	CA-C-N	6.07	126.51	119.47
16	N	51	GLY	C-N-CA	6.07	126.51	119.47
27	Y	230	ASN	CA-C-N	6.07	126.26	120.31
27	Y	230	ASN	C-N-CA	6.07	126.26	120.31
20	R	122	GLN	N-CA-C	-6.06	99.33	108.96
1	0	1504	A	N9-C1'-C2'	6.03	121.05	112.00
10	H	162	PRO	N-CA-C	6.00	120.68	111.57
1	0	1120	U	C5'-C4'-C3'	-5.99	107.02	116.00
1	0	834	G	C2'-C3'-O3'	-5.99	104.72	113.70
6	D	136	ARG	CA-C-N	5.95	127.28	119.84
6	D	136	ARG	C-N-CA	5.95	127.28	119.84
16	N	3	GLY	CA-C-N	5.94	125.64	119.05
16	N	3	GLY	C-N-CA	5.94	125.64	119.05
7	E	11	VAL	N-CA-C	5.93	118.39	109.20
29	1	21	ARG	N-CA-C	5.93	118.98	111.69
17	O	24	ALA	N-CA-C	-5.83	106.51	113.97
6	D	15	GLU	CA-C-N	5.78	127.06	119.84
6	D	15	GLU	C-N-CA	5.78	127.06	119.84
25	W	68	THR	N-CA-C	5.77	117.65	111.36
22	T	52	ARG	N-CA-C	5.76	123.08	110.80
21	S	57	THR	N-CA-C	5.75	118.13	110.53
3	A	228	ILE	N-CA-C	5.67	116.59	108.93
4	B	161	VAL	N-CA-C	5.67	116.10	108.17
2	9	39	U	C4'-C3'-O3'	-5.66	104.51	113.00
5	C	20	ASP	N-CA-C	5.66	117.45	111.28
12	J	112	ASP	N-CA-C	-5.64	101.35	110.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	E	37	ASP	N-CA-C	5.63	119.45	112.58
11	I	89	GLU	N-CA-C	-5.62	106.78	113.97
5	C	89	ALA	N-CA-C	5.59	117.05	111.07
1	0	2526	C	N1-C1'-C2'	5.58	120.37	112.00
1	0	921	G	N9-C1'-C2'	5.57	120.36	112.00
31	3	67	LEU	N-CA-C	5.54	118.11	109.52
22	T	16	LEU	N-CA-C	5.54	118.03	111.33
31	3	43	ASN	N-CA-C	5.54	119.88	113.18
12	J	68	GLY	N-CA-C	5.53	119.17	112.48
1	0	1352	A	C2'-C3'-O3'	-5.53	105.41	113.70
17	O	43	VAL	N-CA-C	5.52	115.90	108.17
1	0	1452	G	C5'-C4'-C3'	-5.52	107.72	116.00
17	O	82	SER	N-CA-C	-5.49	103.28	110.53
14	L	20	ASN	N-CA-C	5.46	119.51	111.04
4	B	266	ASN	N-CA-C	5.45	118.86	111.17
1	0	874	A	C4'-C3'-O3'	-5.45	104.83	113.00
13	K	8	VAL	N-CA-C	5.44	116.32	108.48
1	0	2313	C	C5'-C4'-C3'	5.42	124.13	116.00
5	C	177	GLY	N-CA-C	5.42	118.89	112.33
12	J	44	ALA	N-CA-C	-5.41	103.40	110.53
13	K	5	GLY	N-CA-C	-5.39	107.34	115.32
1	0	129	A	C2'-C3'-O3'	5.38	121.78	113.70
1	0	1942	A	C4'-C3'-C2'	-5.37	97.23	102.60
16	N	42	HIS	N-CA-C	5.36	117.56	109.41
10	H	90	LEU	N-CA-C	-5.36	99.04	108.20
2	9	65	A	N9-C1'-C2'	5.33	120.00	112.00
18	P	70	ALA	N-CA-C	-5.33	105.64	111.82
5	C	219	ASN	N-CA-C	5.33	117.62	109.95
10	H	121	GLY	N-CA-C	5.32	119.35	112.54
18	P	118	GLN	N-CA-C	-5.31	105.57	111.36
21	S	10	VAL	N-CA-C	5.31	114.39	106.85
10	H	10	ARG	N-CA-C	5.31	117.81	111.71
3	A	208	HIS	CA-C-N	-5.23	114.57	119.85
3	A	208	HIS	C-N-CA	-5.23	114.57	119.85
10	H	161	THR	N-CA-C	5.22	121.34	109.81
1	0	1504	A	C1'-O4'-C4'	-5.19	104.71	109.90
20	R	3	SER	N-CA-C	-5.18	101.20	109.23
22	T	3	GLN	CA-C-N	5.18	125.23	119.32
22	T	3	GLN	C-N-CA	5.18	125.23	119.32
29	1	43	ALA	N-CA-C	-5.17	105.73	111.36
17	O	66	GLY	N-CA-C	5.16	125.41	113.18
16	N	152	GLU	N-CA-C	-5.15	105.74	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	L	7	GLN	N-CA-C	5.15	117.79	111.82
26	X	12	ILE	N-CA-C	5.14	112.95	107.76
1	0	1878	G	O4'-C1'-C2'	-5.12	102.48	107.60
8	F	79	GLN	N-CA-C	5.11	117.82	109.59
1	0	1615	A	C5'-C4'-C3'	5.11	123.66	116.00
10	H	119	ALA	N-CA-C	5.11	119.14	113.01
23	U	50	GLU	N-CA-C	5.11	118.28	111.75
27	Y	103	THR	N-CA-C	5.10	116.84	111.28
5	C	92	PRO	N-CA-C	-5.08	103.14	111.21
1	0	2301	A	N9-C1'-C2'	5.07	119.61	112.00
26	X	80	GLU	N-CA-C	-5.06	107.66	113.88
14	L	70	ASP	N-CA-C	5.04	116.78	111.28
15	M	74	LYS	N-CA-C	5.04	117.71	109.59
1	0	2012	U	N1-C1'-C2'	5.03	119.55	112.00
20	R	18	LEU	N-CA-C	-5.03	101.68	109.72
4	B	143	ILE	N-CA-C	-5.02	102.26	108.89
20	R	63	ASN	N-CA-C	5.02	118.94	112.41
27	Y	183	GLU	N-CA-C	-5.01	101.07	109.24
25	W	142	ASP	N-CA-C	-5.01	103.79	110.55
1	0	1878	G	C2'-C3'-O3'	-5.01	106.19	113.70
1	0	1563	G	C4'-C3'-O3'	-5.00	101.90	109.40

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	1039	G	Sidechain
1	0	1078	A	Sidechain
1	0	1237	U	Sidechain
1	0	1342	C	Sidechain
1	0	1417	G	Sidechain
1	0	1458	A	Sidechain
1	0	1592	G	Sidechain
1	0	1653	A	Sidechain
1	0	1777	G	Sidechain
1	0	1809	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	0	1878	G	Sidechain
1	0	1970	G	Sidechain
1	0	1985	U	Sidechain
1	0	221	G	Sidechain
1	0	2316	G	Sidechain
1	0	2412	G	Sidechain
1	0	246	G	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	2607	U	Sidechain
1	0	2630	G	Sidechain
1	0	2632	G	Sidechain
1	0	2681	A	Sidechain
1	0	270	U	Sidechain
1	0	2842	G	Sidechain
1	0	324	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	417	G	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain
1	0	471	G	Sidechain
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	619	U	Sidechain
1	0	792	G	Sidechain
1	0	795	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain
1	0	868	G	Sidechain
1	0	881	C	Sidechain
1	0	888	U	Sidechain
1	0	893	C	Sidechain
2	9	39	U	Sidechain
2	9	65	A	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	59020	0	29808	687	0
2	9	2599	0	1325	53	0
3	A	1753	0	1766	115	0
4	B	2625	0	2533	128	0
5	C	1859	0	1816	100	0
6	D	1094	0	1085	92	0
7	E	1357	0	1266	63	0
8	F	890	0	843	52	0
9	G	240	0	231	18	0
10	H	1282	0	1292	55	0
11	I	519	0	500	51	0
12	J	1120	0	1098	60	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	53	0
15	M	1558	0	1566	65	0
16	N	1445	0	1401	104	0
17	O	865	0	873	30	0
18	P	1136	0	1123	34	0
19	Q	735	0	728	14	0
20	R	1149	0	1122	43	0
21	S	641	0	605	21	0
22	T	950	0	923	52	0
23	U	410	0	364	24	0
24	V	499	0	511	37	0
25	W	1196	0	1137	91	0
26	X	654	0	653	43	0
27	Y	1130	0	1133	60	0
28	Z	578	0	539	19	0
29	1	431	0	426	22	0
30	2	396	0	413	26	0
31	3	755	0	728	25	0
32	0	52	0	72	0	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	94	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	2	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5845	0	0	120	0
39	1	50	0	0	2	0
39	2	44	0	0	3	0
39	3	71	0	0	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	9	145	0	0	4	0
39	A	118	0	0	21	0
39	B	151	0	0	25	0
39	C	176	0	0	24	0
39	D	49	0	0	19	0
39	E	40	0	0	6	0
39	F	26	0	0	7	0
39	G	18	0	0	2	0
39	H	72	0	0	12	0
39	I	8	0	0	2	0
39	J	59	0	0	2	0
39	K	58	0	0	5	0
39	L	72	0	0	15	0
39	M	124	0	0	8	0
39	N	61	0	0	12	0
39	O	38	0	0	6	0
39	P	66	0	0	4	0
39	Q	53	0	0	4	0
39	R	87	0	0	7	0
39	S	32	0	0	3	0
39	T	41	0	0	4	0
39	U	28	0	0	3	0
39	V	12	0	0	2	0
39	W	68	0	0	7	0
39	X	24	0	0	8	0
39	Y	95	0	0	13	0
39	Z	32	0	0	2	0
All	All	99116	0	59987	2060	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 14.

All (2060) 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)
1:O:1160:G:H5'	1:O:1161:A:H5'	1.18	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.32	1.09
4:B:62:ARG:HA	4:B:65:MET:HE3	1.34	1.07
5:C:236:THR:HG22	5:C:239:ALA:H	1.10	1.06
1:O:1242:A:H5'	12:J:82:THR:HG23	1.39	1.04
20:R:99:ALA:HB1	20:R:109:MET:HE1	1.35	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:6:C:H5''	16:N:37:ARG:NH1	1.74	1.03
22:T:71:VAL:HG11	22:T:90:PRO:HB3	1.41	1.01
6:D:25:MET:HE2	6:D:41:LEU:HG	1.44	1.00
4:B:212:GLN:HB2	4:B:257:THR:HG21	1.45	0.99
3:A:191:GLY:HA2	3:A:194:MET:HE2	1.43	0.99
1:0:156:C:H5''	15:M:171:ARG:HD3	1.43	0.99
18:P:115:SER:H	18:P:118:GLN:HE21	1.09	0.99
6:D:154:LYS:H	6:D:154:LYS:HD2	1.27	0.98
1:0:871:G:C8	1:0:871:G:H5'	1.97	0.98
5:C:78:ARG:HH11	5:C:78:ARG:HG3	1.28	0.97
25:W:149:LEU:HG	25:W:153:MET:HE2	1.44	0.96
2:9:76:G:H3'	2:9:77:A:H5''	1.47	0.95
13:K:74:VAL:HG11	13:K:113:ILE:HG12	1.46	0.95
2:9:56:A:H2'	2:9:57:A:H5''	1.46	0.95
15:M:164:THR:HG22	15:M:167:GLY:H	1.32	0.95
4:B:140:LEU:HA	39:B:9048:HOH:O	1.65	0.95
5:C:127:ARG:NH2	5:C:225:PRO:HG2	1.82	0.94
25:W:137:GLN:HE21	25:W:141:HIS:HE1	1.07	0.94
4:B:86:ALA:HA	39:B:9048:HOH:O	1.68	0.93
27:Y:200:THR:HG22	27:Y:201:GLU:HG3	1.50	0.93
1:0:871:G:H5'	1:0:871:G:H8	1.30	0.93
16:N:144:GLY:O	16:N:147:ILE:HG22	1.68	0.92
15:M:102:GLU:OE1	15:M:164:THR:HG21	1.69	0.92
25:W:88:THR:HB	39:W:6679:HOH:O	1.70	0.92
1:0:541:C:H2'	1:0:542:A:H5''	1.52	0.92
13:K:10:GLN:H	13:K:10:GLN:NE2	1.67	0.91
30:2:41:HIS:H	30:2:45:ASN:HD22	1.12	0.91
6:D:57:THR:HG23	6:D:63:ILE:HA	1.52	0.91
25:W:6:GLN:HB2	25:W:26:ILE:HD12	1.52	0.91
1:0:542:A:H5'	1:0:542:A:H8	1.34	0.91
21:S:57:THR:HG22	21:S:59:ASP:H	1.36	0.90
1:0:870:G:H2'	1:0:871:G:H5''	1.51	0.90
28:Z:46:ARG:HD2	28:Z:59:TYR:HB2	1.51	0.90
1:0:2717:C:C2'	1:0:2718:C:H5''	2.02	0.90
13:K:10:GLN:HE21	13:K:10:GLN:N	1.70	0.89
1:0:2717:C:H2'	1:0:2718:C:H5''	1.54	0.89
4:B:238:ASN:HD22	4:B:240:GLY:H	1.18	0.89
13:K:39:GLY:HA2	39:K:4183:HOH:O	1.73	0.89
16:N:83:LEU:HD13	16:N:175:LEU:HD23	1.53	0.89
1:0:2812:A:H2	1:0:2814:A:H62	1.19	0.89
1:0:2270:G:H4'	3:A:223:ARG:HH12	1.36	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:28:GLY:HA2	6:D:69:ILE:HG23	1.56	0.88
22:T:9:LYS:HE3	22:T:13:ARG:NH1	1.88	0.88
3:A:35:GLY:O	3:A:36:ASP:HB3	1.71	0.88
4:B:307:ARG:HH11	4:B:307:ARG:HG3	1.38	0.88
1:O:1160:G:C5'	1:O:1161:A:H5'	2.03	0.88
7:E:20:ILE:HD11	7:E:40:VAL:HG11	1.54	0.88
1:O:1160:G:H5'	1:O:1161:A:C5'	2.04	0.87
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.54	0.87
25:W:122:ARG:NH2	25:W:154:ARG:HB3	1.90	0.87
1:O:2506:A:HO2'	1:O:2507:G:H8	0.89	0.87
2:9:6:C:H5''	16:N:37:ARG:HH12	1.37	0.87
10:H:49:GLN:HE21	10:H:140:TYR:HE2	1.21	0.87
1:O:1835:U:H5	1:O:1840:A:N7	1.73	0.86
24:V:1:THR:HG23	24:V:2:VAL:H	1.40	0.86
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.57	0.86
11:I:127:CYS:HB3	11:I:132:VAL:HB	1.58	0.86
13:K:98:VAL:CG1	13:K:102:GLU:HA	2.04	0.85
26:X:71:ARG:HD3	39:X:2171:HOH:O	1.75	0.85
1:O:960:G:H4'	39:O:7859:HOH:O	1.75	0.85
18:P:115:SER:OG	18:P:118:GLN:HG3	1.77	0.85
25:W:5:VAL:HG11	25:W:153:MET:HE1	1.58	0.85
31:3:65:THR:HG22	31:3:67:LEU:HG	1.59	0.85
3:A:199:HIS:HD2	3:A:201:PHE:H	1.23	0.85
13:K:81:ARG:HB2	13:K:87:ARG:HH11	1.39	0.84
1:O:282:C:H1'	1:O:368:C:N4	1.92	0.84
5:C:236:THR:HG22	5:C:239:ALA:N	1.92	0.84
25:W:137:GLN:HE21	25:W:141:HIS:CE1	1.95	0.84
4:B:190:MET:HE2	4:B:194:PHE:CD1	2.11	0.84
10:H:170:ARG:HD2	39:H:8989:HOH:O	1.78	0.84
12:J:19:MET:HE3	12:J:132:LEU:HD11	1.60	0.84
13:K:10:GLN:H	13:K:10:GLN:HE21	0.88	0.84
1:O:1116:U:HO2'	1:O:1118:A:H2	0.83	0.83
1:O:2716:G:H5''	4:B:206:THR:HG21	1.60	0.83
25:W:4:LEU:HD22	25:W:52:VAL:HG21	1.60	0.83
25:W:122:ARG:HG2	25:W:122:ARG:HH11	1.41	0.83
3:A:192:VAL:HG22	39:A:9095:HOH:O	1.77	0.83
17:O:42:GLU:HB2	39:O:2176:HOH:O	1.78	0.83
1:O:1667:A:H8	1:O:1667:A:H5'	1.41	0.83
1:O:1701:A:H4'	1:O:1702:U:H5''	1.60	0.83
1:O:1041:U:H5'	39:L:8881:HOH:O	1.77	0.82
1:O:506:G:H22	1:O:509:A:H5''	1.42	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:211:LYS:HB2	39:A:9081:HOH:O	1.78	0.82
24:V:12:THR:HG22	24:V:15:GLU:HG3	1.60	0.82
3:A:179:MET:HA	3:A:179:MET:HE3	1.61	0.82
1:O:1474:C:H6	1:O:1474:C:H5'	1.43	0.82
8:F:58:GLU:HA	8:F:61:MET:HE2	1.59	0.82
1:O:541:C:C2'	1:O:542:A:H5''	2.09	0.81
11:I:97:VAL:HG12	11:I:101:LYS:HE3	1.59	0.81
16:N:113:SER:HB2	39:N:8856:HOH:O	1.78	0.81
25:W:88:THR:HG23	25:W:110:GLN:HE21	1.46	0.81
1:O:1300:G:H1'	39:O:5149:HOH:O	1.79	0.81
27:Y:187:VAL:HG23	39:Y:8869:HOH:O	1.79	0.81
26:X:30:MET:HE1	26:X:58:ALA:HB3	1.62	0.81
3:A:153:ARG:HB2	3:A:153:ARG:HH11	1.45	0.81
1:O:2890:A:H1'	23:U:56:ARG:NH2	1.96	0.80
1:O:1973:A:H5'	1:O:1973:A:H8	1.45	0.80
39:9:9098:HOH:O	16:N:23:ARG:HD3	1.80	0.80
28:Z:10:ARG:HA	39:Z:8714:HOH:O	1.79	0.80
1:O:2054:A:N3	20:R:128:ARG:NH2	2.30	0.80
1:O:2840:A:OP1	4:B:211:THR:HG23	1.82	0.80
12:J:74:ARG:HB3	12:J:74:ARG:HH11	1.46	0.79
13:K:81:ARG:HB2	13:K:87:ARG:NH1	1.96	0.79
11:I:73:LEU:HD12	11:I:107:LYS:HZ2	1.47	0.79
6:D:54:ALA:HB2	6:D:69:ILE:HD12	1.63	0.79
1:O:656:G:H5'	17:O:3:THR:HG22	1.64	0.79
4:B:195:ARG:HG2	4:B:323:LEU:HD22	1.65	0.79
1:O:2586:U:H3	1:O:2592:G:H22	1.28	0.78
1:O:2488:A:H61	1:O:2534:C:H42	1.32	0.78
3:A:192:VAL:HB	39:A:9056:HOH:O	1.82	0.78
5:C:1:MET:HG2	5:C:2:GLN:H	1.46	0.78
5:C:242:GLU:HG3	39:C:8586:HOH:O	1.84	0.78
1:O:1116:U:O2'	1:O:1118:A:H2	1.65	0.78
8:F:91:VAL:HG12	8:F:92:GLY:N	1.98	0.78
14:L:133:VAL:HA	39:L:8865:HOH:O	1.84	0.78
29:1:25:LYS:HD2	30:2:49:GLU:H	1.46	0.78
11:I:73:LEU:HD12	11:I:107:LYS:NZ	1.97	0.78
25:W:88:THR:HG23	25:W:110:GLN:NE2	1.97	0.78
27:Y:235:GLU:CD	27:Y:235:GLU:H	1.92	0.78
10:H:59:GLN:HE21	10:H:129:ARG:HE	1.30	0.77
3:A:51:ARG:HB2	39:A:9068:HOH:O	1.83	0.77
12:J:76:ASP:HA	39:J:5907:HOH:O	1.85	0.77
4:B:179:LEU:O	4:B:183:GLU:HG2	1.84	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:O:5298:HOH:O	12:J:47:THR:HB	1.84	0.77
24:V:42:ASN:HB3	39:V:7247:HOH:O	1.85	0.77
25:W:13:MET:HE3	25:W:17:ILE:HG22	1.65	0.77
1:O:1116:U:H3	1:O:1246:A:H62	1.33	0.76
1:O:2506:A:O2'	1:O:2507:G:H8	1.68	0.76
7:E:100:ASP:HB2	39:E:2789:HOH:O	1.85	0.76
1:O:1878:G:H1'	39:O:6568:HOH:O	1.85	0.76
5:C:236:THR:CG2	5:C:239:ALA:H	1.95	0.76
1:O:381:G:H5''	39:O:4785:HOH:O	1.84	0.76
3:A:194:MET:HE3	3:A:199:HIS:HB2	1.67	0.76
3:A:105:VAL:CG1	3:A:154:ALA:HB1	2.15	0.76
1:O:544:G:H2'	1:O:545:G:H5''	1.67	0.76
1:O:871:G:H8	1:O:871:G:C5'	1.99	0.76
2:9:14:G:H5'	2:9:14:G:H8	1.51	0.76
5:C:115:LEU:HD21	5:C:243:VAL:HG13	1.67	0.76
8:F:91:VAL:HG12	8:F:92:GLY:H	1.48	0.76
10:H:30:LYS:H	10:H:62:HIS:HD2	1.31	0.76
1:O:559:U:H6	1:O:559:U:H5'	1.51	0.76
24:V:8:ILE:HA	24:V:11:MET:HE3	1.66	0.76
25:W:13:MET:HE2	25:W:18:GLN:HA	1.68	0.76
10:H:59:GLN:NE2	10:H:129:ARG:HE	1.83	0.75
16:N:48:VAL:CG1	16:N:55:ASP:HB3	2.16	0.75
18:P:59:ARG:NH2	18:P:66:GLN:HE22	1.83	0.75
20:R:39:THR:HB	20:R:42:GLU:HG3	1.68	0.75
4:B:201:ASP:HB2	4:B:312:ARG:HD2	1.68	0.75
16:N:164:ASP:CG	16:N:167:ASP:HA	2.11	0.75
20:R:8:ALA:HB1	20:R:13:THR:HG21	1.67	0.75
23:U:20:MET:HE2	23:U:30:HIS:NE2	2.02	0.75
4:B:41:PHE:CD1	4:B:79:MET:HE2	2.21	0.75
8:F:50:VAL:HG13	8:F:60:VAL:HG11	1.69	0.75
27:Y:212:ARG:HD2	39:Y:8899:HOH:O	1.86	0.75
1:O:870:G:C2'	1:O:871:G:H5''	2.17	0.74
4:B:162:MET:CE	4:B:310:ARG:HD3	2.17	0.74
1:O:1206:U:H5'	1:O:1206:U:H6	1.52	0.74
1:O:236:A:H4'	1:O:237:G:H5'	1.69	0.74
3:A:199:HIS:CD2	3:A:201:PHE:H	2.04	0.74
4:B:36:PRO:HA	4:B:168:GLY:HA3	1.68	0.74
21:S:57:THR:HG22	21:S:59:ASP:N	2.01	0.74
1:O:506:G:H22	1:O:509:A:C5'	2.01	0.74
5:C:140:VAL:HB	39:C:8656:HOH:O	1.88	0.74
1:O:545:G:H5'	1:O:545:G:H8	1.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:56:A:C2'	2:9:57:A:H5''	2.18	0.74
5:C:139:VAL:HG13	39:C:8653:HOH:O	1.86	0.74
1:0:1183:C:H2'	39:0:6690:HOH:O	1.87	0.74
3:A:36:ASP:OD2	3:A:85:SER:HB2	1.88	0.74
20:R:18:LEU:HD12	20:R:143:VAL:HG11	1.70	0.74
1:0:1372:A:H3'	39:0:7622:HOH:O	1.88	0.74
4:B:16:ARG:NH1	39:B:9084:HOH:O	2.20	0.74
23:U:14:GLU:OE1	23:U:15:PRO:HD2	1.88	0.73
5:C:236:THR:HG21	39:C:8579:HOH:O	1.85	0.73
5:C:5:ILE:HD11	5:C:16:VAL:CG2	2.18	0.73
7:E:3:VAL:HG22	7:E:49:ILE:HB	1.70	0.73
1:0:1819:G:H2'	1:0:1820:G:H4'	1.71	0.73
3:A:48:ASP:HB3	39:A:9068:HOH:O	1.89	0.73
20:R:18:LEU:HB2	20:R:143:VAL:HG12	1.71	0.73
1:0:93:C:H5''	24:V:1:THR:HB	1.69	0.73
39:0:6936:HOH:O	27:Y:141:THR:HG23	1.86	0.73
7:E:69:ILE:HA	7:E:72:MET:HE3	1.69	0.73
1:0:2908:A:H2'	1:0:2909:G:O4'	1.89	0.72
4:B:221:GLN:HE22	13:K:42:ASN:HD22	1.33	0.72
13:K:34:VAL:HG22	13:K:47:ALA:HB2	1.71	0.72
12:J:107:ASN:ND2	12:J:109:TYR:H	1.86	0.72
21:S:10:VAL:HG11	24:V:36:ALA:HA	1.72	0.72
1:0:2570:G:H5''	39:0:5371:HOH:O	1.88	0.72
1:0:2291:A:C8	1:0:2309:C:H5'	2.25	0.72
1:0:450:C:OP1	5:C:184:ARG:NH2	2.22	0.72
4:B:162:MET:HE2	4:B:310:ARG:HD3	1.71	0.72
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.69	0.72
1:0:1119:G:H2'	12:J:52:GLN:NE2	2.04	0.72
4:B:18:ARG:HG3	4:B:256:GLN:HG3	1.72	0.72
8:F:63:ILE:HB	8:F:64:PRO:HD3	1.71	0.72
25:W:125:HIS:HD2	25:W:127:GLY:H	1.36	0.72
7:E:84:MET:HE1	7:E:148:ILE:HD12	1.72	0.71
4:B:62:ARG:HA	4:B:65:MET:CE	2.15	0.71
1:0:2896:A:H5''	39:0:6546:HOH:O	1.89	0.71
8:F:96:ALA:HA	39:F:3111:HOH:O	1.89	0.71
13:K:74:VAL:CG1	13:K:113:ILE:HG12	2.21	0.71
17:O:32:ARG:O	17:O:32:ARG:HD3	1.90	0.71
1:0:962:C:H1'	16:N:5:ARG:NH1	2.05	0.71
1:0:1603:A:H5'	1:0:1605:G:O4'	1.91	0.71
2:9:29:C:H2'	2:9:30:C:H5'	1.73	0.71
21:S:43:GLU:HB3	39:S:8990:HOH:O	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1666:C:O2'	1:0:1667:A:H5''	1.91	0.71
25:W:6:GLN:HB2	25:W:26:ILE:CD1	2.21	0.71
1:0:111:C:O2'	29:1:20:ARG:HG2	1.92	0.70
1:0:481:U:H5''	39:0:6102:HOH:O	1.91	0.70
3:A:223:ARG:HG3	39:A:9064:HOH:O	1.91	0.70
13:K:98:VAL:HG13	13:K:102:GLU:HA	1.73	0.70
1:0:877:G:H5'	1:0:878:G:OP1	1.92	0.70
39:0:4698:HOH:O	30:2:38:LYS:HE3	1.90	0.70
4:B:275:GLY:O	4:B:291:ASP:HA	1.91	0.70
13:K:14:LYS:HB2	13:K:45:PRO:HG2	1.73	0.70
1:0:2364:A:H5''	19:Q:15:LYS:HD3	1.73	0.70
2:9:39:U:H1'	2:9:44:A:H61	1.55	0.70
3:A:164:ARG:NE	39:A:9050:HOH:O	2.24	0.70
4:B:264:GLU:HG2	4:B:267:LYS:HE2	1.73	0.70
25:W:68:THR:HG23	25:W:69:ARG:HG2	1.74	0.70
28:Z:11:SER:HB3	28:Z:23:ARG:HB2	1.73	0.70
1:0:542:A:H5'	1:0:542:A:C8	2.23	0.70
1:0:1184:C:H1'	39:0:7891:HOH:O	1.90	0.70
3:A:105:VAL:HG11	3:A:154:ALA:HB1	1.74	0.70
1:0:244:C:OP2	8:F:38:LYS:HE3	1.91	0.70
1:0:541:C:H2'	1:0:542:A:C5'	2.21	0.70
12:J:45:VAL:HG23	12:J:130:VAL:O	1.91	0.70
25:W:13:MET:HE2	25:W:18:GLN:CA	2.22	0.70
6:D:128:LEU:HB2	39:D:6007:HOH:O	1.90	0.70
13:K:74:VAL:HG13	13:K:113:ILE:HG23	1.72	0.70
1:0:1244:U:OP1	12:J:18:ILE:HD13	1.91	0.70
12:J:74:ARG:HH11	12:J:74:ARG:CB	2.05	0.70
16:N:11:ARG:HG3	16:N:14:ARG:NH1	2.06	0.70
22:T:71:VAL:HG11	22:T:90:PRO:CB	2.20	0.70
1:0:2635:A:O2'	1:0:2636:C:H5'	1.92	0.70
8:F:13:GLU:OE2	8:F:78:GLU:HG2	1.90	0.70
2:9:49:G:H5''	39:N:8845:HOH:O	1.92	0.69
1:0:796:A:HO2'	28:Z:10:ARG:N	1.90	0.69
4:B:238:ASN:HD22	4:B:240:GLY:N	1.90	0.69
24:V:39:ALA:C	24:V:41:GLU:H	1.99	0.69
1:0:281:U:H2'	1:0:282:C:O4'	1.91	0.69
10:H:32:ALA:HB3	10:H:69:ARG:HH12	1.55	0.69
10:H:102:LYS:HD3	10:H:122:LYS:HD3	1.74	0.69
1:0:1701:A:H5'	39:0:6730:HOH:O	1.90	0.69
1:0:2748:G:H2'	39:0:7963:HOH:O	1.91	0.69
20:R:39:THR:HG23	20:R:107:GLU:O	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:58:GLU:OE1	15:M:27:ARG:NH2	2.25	0.69
1:O:1593:C:OP1	18:P:117:SER:HB3	1.93	0.69
1:O:2533:C:H5'	1:O:2533:C:H6	1.58	0.69
1:O:2780:C:H1'	7:E:143:GLN:HE21	1.58	0.69
2:9:6:C:OP1	16:N:37:ARG:NH1	2.25	0.69
16:N:80:SER:HB2	39:N:8835:HOH:O	1.92	0.69
16:N:139:TRP:HA	16:N:139:TRP:CE3	2.28	0.69
27:Y:126:PRO:HG2	27:Y:128:PHE:CE1	2.28	0.69
1:O:1118:A:C8	1:O:1118:A:H3'	2.28	0.68
1:O:1118:A:H3'	1:O:1118:A:H8	1.58	0.68
1:O:2468:A:H61	31:3:48:ASN:HD21	1.40	0.68
1:O:1666:C:H2'	1:O:1667:A:H5'	1.75	0.68
3:A:33:GLU:H	3:A:33:GLU:CD	2.01	0.68
4:B:58:PRO:HA	4:B:63:GLU:OE1	1.92	0.68
14:L:148:GLU:HA	39:L:8864:HOH:O	1.93	0.68
3:A:88:ILE:HD13	3:A:100:PRO:HD3	1.76	0.68
6:D:135:VAL:HG21	6:D:139:TYR:CD1	2.29	0.68
6:D:146:LYS:NZ	16:N:107:ASN:HD21	1.92	0.68
8:F:2:VAL:HG22	8:F:57:GLU:OE1	1.94	0.68
10:H:6:ALA:HA	10:H:61:ARG:HH12	1.58	0.68
16:N:17:ARG:HB3	16:N:17:ARG:HH11	1.57	0.68
20:R:99:ALA:CB	20:R:109:MET:HE1	2.18	0.68
5:C:78:ARG:HG3	5:C:78:ARG:NH1	2.01	0.67
1:O:272:A:H3'	39:O:7953:HOH:O	1.93	0.67
1:O:1119:G:N2	1:O:1246:A:C2	2.58	0.67
24:V:12:THR:HG22	24:V:15:GLU:CG	2.24	0.67
25:W:21:LEU:HD22	25:W:26:ILE:CD1	2.25	0.67
1:O:657:G:OP1	5:C:27:ARG:NH2	2.27	0.67
1:O:2270:G:H4'	3:A:223:ARG:NH1	2.07	0.67
3:A:100:PRO:HG2	3:A:103:VAL:HG21	1.76	0.67
1:O:2081:A:H4'	12:J:69:TYR:CE1	2.30	0.67
16:N:7:LYS:HE3	19:Q:21:ARG:O	1.95	0.67
1:O:1701:A:H4'	1:O:1702:U:C5'	2.25	0.67
6:D:23:VAL:HG21	6:D:45:THR:HG21	1.74	0.67
7:E:84:MET:HE2	7:E:133:VAL:CG2	2.24	0.67
25:W:122:ARG:HH11	25:W:122:ARG:CG	2.07	0.67
4:B:51:VAL:CG2	4:B:327:VAL:HG13	2.24	0.67
10:H:6:ALA:HA	10:H:61:ARG:NH1	2.09	0.67
27:Y:115:ARG:NE	39:Y:8853:HOH:O	2.27	0.67
27:Y:185:VAL:HG12	39:Y:8869:HOH:O	1.93	0.67
5:C:1:MET:HG2	5:C:2:GLN:N	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:115:LEU:HD13	5:C:223:LEU:HD21	1.76	0.67
1:O:338:C:H4'	5:C:174:ILE:CD1	2.25	0.66
15:M:164:THR:HG22	15:M:167:GLY:N	2.09	0.66
1:O:794:U:H3	1:O:819:A:H61	1.42	0.66
1:O:1679:C:H5'	39:O:9811:HOH:O	1.95	0.66
1:O:1667:A:H5'	1:O:1667:A:C8	2.29	0.66
3:A:194:MET:HE3	3:A:199:HIS:CB	2.25	0.66
25:W:13:MET:CE	25:W:17:ILE:HG22	2.24	0.66
1:O:558:C:C2'	1:O:559:U:H5''	2.26	0.66
1:O:1328:A:OP1	27:Y:169:ARG:HD2	1.96	0.66
4:B:320:GLN:HE21	4:B:321:PRO:HD2	1.61	0.66
5:C:2:GLN:HB3	39:C:8589:HOH:O	1.96	0.66
12:J:74:ARG:NH1	12:J:76:ASP:HB2	2.11	0.66
16:N:139:TRP:HA	16:N:139:TRP:HE3	1.61	0.66
4:B:212:GLN:HB2	4:B:257:THR:CG2	2.24	0.66
27:Y:144:ARG:NE	39:Y:8910:HOH:O	2.27	0.66
13:K:32:ILE:HD11	13:K:56:SER:HB3	1.76	0.66
14:L:136:ALA:HB3	39:L:8865:HOH:O	1.96	0.66
20:R:111:ILE:HG23	20:R:145:LEU:HD11	1.78	0.66
7:E:20:ILE:CD1	7:E:40:VAL:HG11	2.26	0.66
25:W:21:LEU:HD22	25:W:26:ILE:HD11	1.78	0.65
39:O:7208:HOH:O	16:N:4:PRO:HD2	1.95	0.65
7:E:15:GLN:HG2	7:E:19:ASP:O	1.96	0.65
10:H:83:GLU:HA	39:H:9037:HOH:O	1.96	0.65
1:O:2851:G:O2'	1:O:2852:A:H5'	1.96	0.65
25:W:88:THR:HG22	25:W:90:TYR:HD1	1.61	0.65
39:O:5438:HOH:O	15:M:125:ARG:HD3	1.96	0.65
4:B:185:GLY:HA2	39:B:9103:HOH:O	1.96	0.65
13:K:118:ALA:HA	13:K:125:ALA:HB2	1.79	0.65
28:Z:11:SER:CB	28:Z:23:ARG:HB2	2.27	0.65
6:D:166:ILE:HB	39:D:6326:HOH:O	1.97	0.65
15:M:107:ARG:HH11	15:M:107:ARG:HG3	1.61	0.65
25:W:21:LEU:HD21	25:W:48:VAL:CG1	2.27	0.65
1:O:513:A:N3	39:O:4140:HOH:O	2.29	0.65
1:O:1163:G:H5'	11:I:110:ASP:O	1.97	0.65
4:B:190:MET:HE2	4:B:194:PHE:HD1	1.61	0.65
16:N:132:ASN:O	16:N:135:VAL:HG12	1.97	0.65
1:O:2505:G:O2'	1:O:2506:A:H5'	1.96	0.65
10:H:114:ASP:HB2	39:H:8996:HOH:O	1.96	0.65
18:P:59:ARG:HH22	18:P:66:GLN:HE22	1.42	0.65
18:P:91:LYS:O	18:P:95:GLU:HG3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:88:THR:HG22	25:W:89:ASP:H	1.59	0.65
25:W:88:THR:HG22	25:W:89:ASP:N	2.11	0.65
1:0:1183:C:N4	1:0:1184:C:H41	1.95	0.65
5:C:236:THR:HA	39:C:8656:HOH:O	1.96	0.65
1:0:282:C:O2'	1:0:283:U:H5'	1.96	0.64
1:0:871:G:C8	1:0:871:G:C5'	2.74	0.64
15:M:60:VAL:C	15:M:61:ILE:HD12	2.22	0.64
16:N:38:LYS:HE2	16:N:107:ASN:ND2	2.12	0.64
1:0:470:U:O2'	29:1:16:HIS:HD2	1.80	0.64
1:0:797:A:C4'	28:Z:10:ARG:N	2.61	0.64
1:0:2004:U:H4'	39:0:5759:HOH:O	1.96	0.64
1:0:2783:A:H3'	39:0:5684:HOH:O	1.96	0.64
25:W:80:ASP:O	25:W:84:VAL:HG23	1.97	0.64
29:1:42:SER:HB2	39:1:8957:HOH:O	1.97	0.64
39:0:6115:HOH:O	22:T:68:ASP:HB2	1.98	0.64
6:D:25:MET:SD	6:D:40:ILE:HD11	2.37	0.64
1:0:1165:G:H4'	1:0:1174:A:O2'	1.97	0.64
1:0:1684:A:H1'	30:2:43:ARG:HH22	1.62	0.64
2:9:39:U:H1'	2:9:44:A:N6	2.11	0.64
14:L:143:THR:HG22	14:L:144:ASP:N	2.12	0.64
1:0:2827:A:H2'	1:0:2828:G:O4'	1.98	0.64
39:0:5912:HOH:O	9:G:12:ILE:HG23	1.98	0.64
4:B:62:ARG:CA	4:B:65:MET:HE3	2.20	0.64
21:S:51:GLN:HE21	21:S:53:ASN:HD21	1.44	0.64
24:V:38:GLY:C	24:V:40:PRO:HD2	2.22	0.64
25:W:151:GLU:O	25:W:154:ARG:HB2	1.98	0.64
15:M:99:ARG:HH21	15:M:170:ASN:HD22	1.45	0.64
16:N:49:THR:HG22	16:N:56:ASP:HB2	1.78	0.64
26:X:9:VAL:HG13	26:X:88:GLU:OE1	1.97	0.64
26:X:72:VAL:HG22	26:X:85:VAL:HG12	1.77	0.64
1:0:544:G:C2'	1:0:545:G:H5''	2.27	0.64
1:0:1189:A:H3'	39:0:8185:HOH:O	1.97	0.64
1:0:1641:A:H2'	1:0:1642:A:H5'	1.79	0.64
6:D:170:TYR:O	6:D:171:ASP:HB3	1.98	0.64
9:G:20:VAL:O	9:G:24:VAL:HG23	1.98	0.64
18:P:115:SER:N	18:P:118:GLN:HE21	1.88	0.64
1:0:2721:U:H4'	13:K:87:ARG:HG3	1.80	0.64
4:B:264:GLU:HG2	4:B:267:LYS:CE	2.27	0.64
4:B:305:ASP:O	4:B:306:LYS:HB2	1.98	0.64
25:W:81:ASP:OD1	25:W:92:ASP:HB2	1.97	0.64
27:Y:144:ARG:NH1	39:Y:8875:HOH:O	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:109:LEU:HD13	13:K:113:ILE:HD11	1.79	0.63
30:2:22:PRO:HG2	30:2:25:VAL:HG23	1.79	0.63
11:I:100:VAL:HG11	11:I:124:VAL:HG22	1.80	0.63
1:O:396:U:H1'	39:O:8134:HOH:O	1.99	0.63
39:O:7310:HOH:O	15:M:178:LYS:HB2	1.97	0.63
7:E:116:THR:HG22	7:E:151:LEU:HD22	1.80	0.63
27:Y:186:ARG:HG2	27:Y:186:ARG:HH11	1.64	0.63
28:Z:13:ARG:NH1	39:Z:8719:HOH:O	2.30	0.63
1:O:2816:A:H2'	39:O:8430:HOH:O	1.97	0.63
3:A:153:ARG:HH11	3:A:153:ARG:CB	2.12	0.63
7:E:5:LEU:HD21	7:E:66:GLN:HG3	1.80	0.63
18:P:10:ALA:HA	18:P:13:VAL:HG12	1.79	0.63
2:9:6:C:C5'	16:N:37:ARG:NH1	2.57	0.63
2:9:14:G:H5'	2:9:14:G:C8	2.32	0.63
7:E:81:GLU:HG2	7:E:134:SER:HB3	1.80	0.63
27:Y:106:THR:HG23	27:Y:107:PRO:HD2	1.80	0.63
1:O:1209:C:H2'	1:O:1210:G:H8	1.64	0.63
13:K:98:VAL:HG11	13:K:102:GLU:HA	1.78	0.63
26:X:66:THR:HG23	26:X:67:PRO:HD2	1.81	0.63
12:J:75:PRO:HG2	12:J:105:LEU:HD21	1.80	0.63
1:O:500:G:H21	20:R:98:ASN:HD21	1.45	0.63
1:O:2781:U:H1'	7:E:139:GLU:OE2	1.99	0.63
23:U:17:THR:HG22	23:U:18:GLY:N	2.14	0.63
25:W:65:VAL:HA	25:W:68:THR:HG22	1.80	0.63
8:F:53:ASP:OD1	8:F:80:GLN:HB2	1.98	0.62
10:H:49:GLN:HG3	10:H:140:TYR:CE2	2.34	0.62
25:W:84:VAL:HG12	39:W:6679:HOH:O	1.98	0.62
25:W:149:LEU:CG	25:W:153:MET:HE2	2.24	0.62
1:O:2426:G:H1'	39:O:6539:HOH:O	1.99	0.62
8:F:38:LYS:NZ	15:M:3:SER:HA	2.15	0.62
20:R:106:GLY:HA2	20:R:109:MET:HE3	1.81	0.62
6:D:25:MET:CE	6:D:37:ALA:HB1	2.29	0.62
7:E:68:HIS:O	7:E:72:MET:HG3	1.99	0.62
11:I:101:LYS:O	11:I:105:GLU:HG3	1.99	0.62
27:Y:189:ASN:C	27:Y:189:ASN:HD22	2.07	0.62
3:A:95:PRO:HG2	3:A:98:GLU:HG2	1.81	0.62
3:A:179:MET:HG2	3:A:186:TRP:CB	2.30	0.62
1:O:2578:G:H5'	1:O:2578:G:H8	1.64	0.62
23:U:14:GLU:O	23:U:17:THR:HB	2.00	0.62
4:B:7:ARG:HG2	4:B:7:ARG:HH11	1.65	0.62
7:E:69:ILE:HA	7:E:72:MET:CE	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:4:LEU:O	25:W:32:CYS:HA	1.99	0.62
25:W:21:LEU:HD13	25:W:26:ILE:HD11	1.81	0.62
1:0:1377:C:H5'	1:0:1377:C:H6	1.65	0.62
6:D:99:ASP:HB3	6:D:103:ASN:H	1.64	0.62
20:R:18:LEU:HD12	20:R:143:VAL:CG1	2.30	0.62
24:V:64:GLY:O	24:V:65:ASP:HB2	2.00	0.62
11:I:108:HIS:N	11:I:109:PRO:HD2	2.14	0.62
1:0:2533:C:H5'	1:0:2533:C:C6	2.34	0.61
3:A:194:MET:CE	3:A:199:HIS:HB2	2.29	0.61
1:0:2694:A:H4'	7:E:91:PHE:HE1	1.65	0.61
3:A:190:ARG:NH2	3:A:207:GLN:OE1	2.32	0.61
24:V:39:ALA:N	24:V:40:PRO:HD2	2.16	0.61
28:Z:36:ASP:HB3	28:Z:45:ASP:HB3	1.80	0.61
1:0:558:C:H2'	1:0:559:U:C5'	2.30	0.61
1:0:656:G:H5'	17:O:3:THR:CG2	2.30	0.61
1:0:2420:G:O2'	1:0:2421:G:H5'	2.00	0.61
5:C:25:PRO:HG2	39:C:8522:HOH:O	1.99	0.61
22:T:53:GLY:HA3	39:T:6384:HOH:O	2.00	0.61
26:X:9:VAL:HG22	26:X:88:GLU:OE2	1.99	0.61
1:0:1819:G:H5'	39:O:5176:HOH:O	2.01	0.61
1:0:1189:A:H1'	1:0:1209:C:C1'	2.30	0.61
4:B:307:ARG:HD2	39:B:9123:HOH:O	2.00	0.61
5:C:236:THR:H	5:C:239:ALA:HB3	1.64	0.61
6:D:91:ALA:HB1	39:D:5198:HOH:O	2.00	0.61
1:0:1168:C:H4'	39:I:5128:HOH:O	2.00	0.61
1:0:1441:G:O2'	1:0:1442:A:H5'	2.00	0.61
1:0:2414:A:H2'	1:0:2415:A:C8	2.36	0.61
1:0:2676:C:H4'	12:J:70:PHE:CE1	2.34	0.61
1:0:2769:C:C2'	1:0:2770:G:H5'	2.31	0.61
10:H:167:LYS:HE2	10:H:169:GLU:OE1	2.01	0.61
12:J:74:ARG:O	12:J:78:ILE:HG12	2.00	0.61
31:3:70:ARG:HG2	31:3:77:ALA:HB2	1.82	0.61
4:B:74:ILE:HD13	4:B:309:VAL:HG21	1.81	0.61
5:C:162:VAL:HG22	5:C:232:LEU:HD21	1.83	0.61
7:E:49:ILE:HD11	7:E:69:ILE:HD12	1.83	0.61
16:N:169:PRO:O	16:N:172:PHE:HB3	2.00	0.61
27:Y:144:ARG:NH2	39:Y:8910:HOH:O	2.33	0.61
1:0:259:G:H21	15:M:58:GLN:NE2	1.99	0.61
1:0:709:G:O2'	17:O:25:VAL:HG12	2.00	0.61
1:0:1058:A:H2'	1:0:1060:C:H5''	1.82	0.61
1:0:1189:A:H1'	1:0:1209:C:H1'	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:79:ASP:HB3	39:L:8850:HOH:O	2.01	0.61
29:1:10:LYS:HG3	39:1:8979:HOH:O	2.00	0.61
4:B:312:ARG:HB2	39:B:9118:HOH:O	2.00	0.60
20:R:23:MET:HE3	20:R:28:SER:OG	2.00	0.60
4:B:8:LYS:HG3	4:B:220:VAL:HG12	1.83	0.60
29:1:25:LYS:HD2	30:2:49:GLU:N	2.15	0.60
1:0:757:C:OP1	14:L:27:ARG:HD2	2.01	0.60
1:0:2718:C:H6	1:0:2718:C:H5'	1.67	0.60
3:A:88:ILE:O	3:A:88:ILE:HG22	2.00	0.60
18:P:115:SER:H	18:P:118:GLN:NE2	1.89	0.60
20:R:18:LEU:HB2	20:R:143:VAL:CG1	2.29	0.60
31:3:25:VAL:HG22	31:3:68:LYS:HG3	1.83	0.60
1:0:1119:G:H8	12:J:52:GLN:HE22	1.48	0.60
17:O:32:ARG:HE	17:O:35:LYS:HD2	1.65	0.60
17:O:87:THR:O	17:O:91:GLN:HG3	2.02	0.60
1:0:2064:U:H5'	1:0:2652:U:H4'	1.83	0.60
4:B:102:THR:CG2	4:B:182:VAL:HG12	2.31	0.60
4:B:145:HIS:HD2	4:B:146:THR:O	1.84	0.60
12:J:103:VAL:HG12	39:J:5907:HOH:O	2.01	0.60
31:3:55:VAL:HG22	39:3:8937:HOH:O	2.01	0.60
1:0:69:A:H5'	1:0:69:A:C8	2.36	0.60
8:F:58:GLU:HG3	8:F:61:MET:HE2	1.84	0.60
22:T:7:GLN:O	22:T:11:GLN:HG3	2.02	0.60
28:Z:37:HIS:HB2	28:Z:47:VAL:HB	1.82	0.60
1:0:90:A:H2'	1:0:91:G:O4'	2.02	0.60
1:0:1701:A:H5''	1:0:1702:U:H3'	1.82	0.60
20:R:39:THR:HG22	20:R:42:GLU:H	1.65	0.60
8:F:37:THR:O	8:F:41:GLU:HG3	2.02	0.60
16:N:12:ARG:HD3	16:N:18:THR:OG1	2.01	0.60
1:0:2005:G:H3'	1:0:2005:G:OP2	2.02	0.60
39:0:3045:HOH:O	25:W:119:HIS:HE1	1.84	0.60
13:K:62:PRO:HG3	13:K:65:ARG:HH21	1.67	0.60
14:L:145:LEU:O	14:L:148:GLU:HG3	2.02	0.60
25:W:141:HIS:HB2	25:W:146:ILE:HG12	1.82	0.60
4:B:254:GLN:HG2	4:B:255:GLY:N	2.16	0.60
31:3:17:HIS:O	31:3:18:GLN:HG3	2.02	0.60
1:0:2507:G:H2'	1:0:2510:C:H42	1.66	0.59
1:0:2768:A:H2'	1:0:2769:C:O4'	2.02	0.59
3:A:36:ASP:O	3:A:38:ILE:N	2.27	0.59
25:W:72:PRO:HG2	25:W:77:ALA:HB3	1.84	0.59
27:Y:122:ARG:NH2	39:Y:8834:HOH:O	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:105:GLU:HA	11:I:108:HIS:NE2	2.18	0.59
12:J:107:ASN:C	12:J:107:ASN:HD22	2.09	0.59
22:T:9:LYS:CE	22:T:13:ARG:NH1	2.62	0.59
1:O:2866:U:C4	23:U:50:GLU:HB3	2.37	0.59
2:9:44:A:O4'	6:D:76:ARG:NE	2.35	0.59
1:O:121:U:OP2	30:2:10:ARG:NH2	2.31	0.59
1:O:474:C:O3'	5:C:73:LEU:HD21	2.02	0.59
4:B:51:VAL:HG23	4:B:329:TYR:O	2.00	0.59
6:D:65:GLU:HA	39:D:6752:HOH:O	2.03	0.59
11:I:129:SER:O	11:I:130:LEU:HD23	2.02	0.59
14:L:80:ASP:HB2	14:L:90:ARG:O	2.03	0.59
16:N:37:ARG:NE	39:N:8832:HOH:O	2.35	0.59
21:S:73:ASP:OD1	21:S:76:GLU:HG3	2.02	0.59
26:X:74:ALA:HB2	26:X:85:VAL:HG13	1.83	0.59
6:D:159:PRO:O	6:D:163:VAL:HG23	2.02	0.59
8:F:91:VAL:CG1	8:F:92:GLY:H	2.15	0.59
15:M:34:GLU:HB3	15:M:38:GLU:HG3	1.84	0.59
20:R:39:THR:HB	20:R:42:GLU:CG	2.32	0.59
1:O:558:C:O2'	1:O:559:U:H5''	2.02	0.59
1:O:1474:C:H5'	1:O:1474:C:C6	2.32	0.59
4:B:312:ARG:HD3	4:B:315:VAL:HG13	1.84	0.59
15:M:24:GLN:NE2	15:M:27:ARG:HH11	2.01	0.59
31:3:62:THR:HB	39:3:8977:HOH:O	2.01	0.59
1:O:316:A:H5'	22:T:54:ASP:OD2	2.03	0.59
6:D:136:ARG:HB2	39:D:7597:HOH:O	2.03	0.59
18:P:80:ARG:HG2	18:P:87:ARG:CZ	2.32	0.59
31:3:6:ARG:NH1	31:3:21:GLU:HG3	2.17	0.59
4:B:102:THR:HG23	4:B:182:VAL:HG12	1.84	0.59
6:D:25:MET:HE1	6:D:37:ALA:HB1	1.85	0.59
24:V:39:ALA:N	24:V:40:PRO:CD	2.66	0.59
13:K:81:ARG:HD3	13:K:87:ARG:NH1	2.17	0.59
25:W:22:GLU:HG2	25:W:27:HIS:CD2	2.37	0.59
26:X:43:VAL:HG22	26:X:76:ARG:NH1	2.18	0.59
1:O:1080:C:H4'	1:O:1081:A:OP1	2.02	0.58
17:O:39:THR:O	17:O:115:ARG:NH2	2.36	0.58
7:E:7:ILE:HD11	7:E:11:VAL:C	2.29	0.58
9:G:23:ILE:O	9:G:27:ILE:HG13	2.03	0.58
1:O:2717:C:H2'	1:O:2718:C:C5'	2.30	0.58
2:9:114:G:O6	16:N:11:ARG:HD3	2.03	0.58
7:E:11:VAL:HG12	7:E:12:ASP:N	2.18	0.58
11:I:70:THR:OG1	11:I:107:LYS:HE2	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:131:THR:HG22	12:J:133:GLY:N	2.18	0.58
15:M:107:ARG:NH1	39:M:8876:HOH:O	2.35	0.58
1:0:603:A:H5''	1:0:604:G:OP1	2.02	0.58
1:0:1119:G:H2'	12:J:52:GLN:HE22	1.66	0.58
39:0:5912:HOH:O	9:G:12:ILE:HA	2.02	0.58
2:9:13:A:O2'	2:9:14:G:H5''	2.03	0.58
5:C:98:ARG:NH1	39:C:8561:HOH:O	2.34	0.58
7:E:166:VAL:HG12	39:E:3134:HOH:O	2.02	0.58
1:0:164:G:H4'	14:L:30:ARG:HD3	1.86	0.58
1:0:1528:A:H2'	1:0:1529:G:O4'	2.02	0.58
3:A:131:HIS:O	3:A:132:ASP:HB2	2.02	0.58
5:C:27:ARG:HG3	5:C:29:ASP:OD1	2.02	0.58
25:W:108:ARG:HE	25:W:114:PRO:HG3	1.69	0.58
6:D:54:ALA:CB	6:D:69:ILE:HD12	2.32	0.58
12:J:47:THR:HG22	12:J:48:GLY:N	2.19	0.58
26:X:25:ARG:HD3	26:X:64:ALA:O	2.04	0.58
1:0:1166:A:H61	1:0:1180:U:H3	1.51	0.58
12:J:19:MET:HE2	12:J:79:PHE:HA	1.85	0.58
17:O:47:ARG:HH11	17:O:47:ARG:HG3	1.68	0.58
24:V:12:THR:HG23	24:V:14:ALA:H	1.68	0.58
1:0:1118:A:H62	1:0:1244:U:H3	1.52	0.58
1:0:2779:G:H21	7:E:143:GLN:NE2	2.02	0.58
3:A:55:VAL:HG22	3:A:68:ILE:O	2.04	0.58
3:A:164:ARG:CZ	39:A:9050:HOH:O	2.51	0.58
6:D:50:VAL:O	6:D:71:ALA:HA	2.04	0.58
8:F:50:VAL:CG1	8:F:60:VAL:HG11	2.33	0.58
8:F:91:VAL:CG1	8:F:92:GLY:N	2.67	0.58
14:L:72:ASN:HB2	39:L:8872:HOH:O	2.03	0.58
25:W:125:HIS:CD2	25:W:127:GLY:H	2.20	0.58
1:0:125:U:H2'	39:0:4245:HOH:O	2.03	0.58
1:0:1730:G:H5'	1:0:1731:C:C5	2.38	0.58
6:D:23:VAL:HG21	6:D:45:THR:CG2	2.33	0.58
1:0:396:U:O2'	1:0:418:C:H4'	2.04	0.58
1:0:558:C:H2'	1:0:559:U:H5''	1.85	0.58
1:0:2717:C:O2'	1:0:2718:C:H5''	2.02	0.58
7:E:35:TYR:HA	12:J:127:ILE:HD12	1.86	0.58
12:J:75:PRO:HG2	12:J:105:LEU:CD2	2.34	0.58
25:W:130:HIS:O	25:W:136:GLY:HA3	2.04	0.58
1:0:299:U:H5'	39:0:7766:HOH:O	2.03	0.57
1:0:621:C:H5'	27:Y:132:ASP:OD2	2.04	0.57
4:B:141:ARG:HD2	4:B:163:GLU:OE2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:25:MET:HE2	6:D:41:LEU:CG	2.27	0.57
6:D:95:THR:OG1	6:D:174:VAL:HG22	2.04	0.57
6:D:154:LYS:H	6:D:154:LYS:CD	2.06	0.57
15:M:134:ILE:HG23	15:M:141:ILE:HD13	1.86	0.57
23:U:11:THR:HG22	23:U:53:ASP:OD2	2.04	0.57
39:O:7854:HOH:O	22:T:9:LYS:HB2	2.03	0.57
39:9:9062:HOH:O	16:N:41:LYS:HD3	2.05	0.57
16:N:164:ASP:OD1	16:N:167:ASP:HA	2.03	0.57
25:W:38:THR:HG22	25:W:39:ASP:N	2.20	0.57
1:O:119:A:H2'	1:O:120:A:H5''	1.87	0.57
1:O:1634:G:H3'	39:O:4370:HOH:O	2.04	0.57
1:O:1766:U:O2	1:O:1778:A:H5'	2.04	0.57
1:O:2346:C:O2'	6:D:52:THR:HG21	2.04	0.57
14:L:133:VAL:HB	39:L:8849:HOH:O	2.03	0.57
1:O:1615:A:H5'	39:O:4655:HOH:O	2.03	0.57
2:9:20:G:O2'	2:9:21:G:H5'	2.04	0.57
8:F:31:LYS:HE3	39:F:2623:HOH:O	2.04	0.57
16:N:11:ARG:NH2	39:N:8817:HOH:O	2.38	0.57
1:O:588:G:O6	25:W:154:ARG:NH1	2.37	0.57
2:9:92:G:H2'	2:9:93:A:C8	2.40	0.57
5:C:107:ARG:NH1	39:C:8637:HOH:O	2.37	0.57
1:O:1175:G:H1'	1:O:1193:A:H2'	1.86	0.57
2:9:39:U:HO2'	2:9:42:C:H5	1.52	0.57
1:O:2320:U:H4'	1:O:2321:A:O4'	2.05	0.57
39:O:7881:HOH:O	4:B:211:THR:HG21	2.04	0.57
5:C:233:THR:HG22	5:C:234:VAL:N	2.18	0.57
6:D:58:VAL:CG1	6:D:60:GLU:HG2	2.33	0.57
11:I:124:VAL:O	11:I:124:VAL:HG12	2.05	0.57
14:L:148:GLU:HB2	39:L:8877:HOH:O	2.03	0.57
26:X:80:GLU:HB3	39:X:5564:HOH:O	2.04	0.57
31:3:60:LYS:HG3	31:3:61:PRO:HD2	1.85	0.57
26:X:76:ARG:HH11	26:X:76:ARG:HG3	1.70	0.57
1:O:1205:U:H2'	1:O:1206:U:C5'	2.34	0.57
8:F:101:ALA:HA	39:F:5413:HOH:O	2.04	0.57
10:H:48:VAL:HA	10:H:170:ARG:O	2.04	0.57
14:L:101:ASP:C	14:L:103:ALA:H	2.13	0.57
1:O:280:C:H2'	1:O:281:U:O4'	2.05	0.57
4:B:214:PRO:HD2	39:B:8990:HOH:O	2.05	0.57
11:I:87:PRO:C	11:I:89:GLU:H	2.12	0.57
12:J:19:MET:HE1	12:J:132:LEU:HD21	1.87	0.57
3:A:33:GLU:O	3:A:34:ASP:HB2	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:307:ARG:HG3	4:B:307:ARG:NH1	2.11	0.56
6:D:135:VAL:HG22	6:D:136:ARG:H	1.70	0.56
1:O:263:U:O4'	8:F:59:ILE:HD13	2.05	0.56
1:O:681:G:N3	1:O:681:G:H5'	2.20	0.56
1:O:1164:U:OP1	11:I:69:PRO:HA	2.05	0.56
4:B:254:GLN:HG3	39:B:9000:HOH:O	2.05	0.56
1:O:545:G:H5'	1:O:545:G:C8	2.37	0.56
1:O:949:U:O2'	19:Q:40:HIS:HE1	1.89	0.56
4:B:125:GLU:O	4:B:129:ARG:HG3	2.05	0.56
5:C:246:ARG:NH1	39:C:8575:HOH:O	2.38	0.56
39:C:8563:HOH:O	17:O:3:THR:HG21	2.05	0.56
10:H:23:ILE:HG23	10:H:123:ILE:HD11	1.88	0.56
20:R:29:LYS:HD3	39:R:8944:HOH:O	2.05	0.56
2:9:91:C:H2'	2:9:92:G:O4'	2.05	0.56
26:X:15:ARG:HB3	26:X:15:ARG:HH11	1.71	0.56
29:1:28:HIS:CE1	29:1:31:LYS:HE2	2.40	0.56
1:O:1299:G:O6	14:L:6:ARG:HD3	2.05	0.56
9:G:12:ILE:N	9:G:13:PRO:HD3	2.21	0.56
12:J:107:ASN:HD21	12:J:109:TYR:HB2	1.71	0.56
29:1:8:GLN:HE22	29:1:11:LYS:NZ	2.04	0.56
1:O:272:A:H5'	1:O:273:G:OP2	2.06	0.56
11:I:113:SER:HB2	11:I:118:ASN:HB2	1.88	0.56
1:O:1086:A:C6	25:W:11:VAL:HG11	2.40	0.56
1:O:1786:C:OP1	18:P:74:GLN:HG2	2.05	0.56
1:O:2820:A:OP1	4:B:98:THR:HG22	2.06	0.56
4:B:85:ARG:NH1	39:B:9104:HOH:O	2.38	0.56
10:H:30:LYS:N	10:H:62:HIS:HD2	2.00	0.56
17:O:38:ARG:NH1	39:O:7674:HOH:O	2.37	0.56
16:N:152:GLU:C	16:N:154:LEU:H	2.14	0.56
1:O:797:A:H4'	28:Z:10:ARG:N	2.21	0.56
5:C:132:ASP:HB3	39:C:8567:HOH:O	2.06	0.56
14:L:73:VAL:HG23	14:L:74:THR:H	1.70	0.56
16:N:61:ALA:HB3	16:N:88:ALA:HB2	1.87	0.56
16:N:86:LEU:HD21	16:N:180:LEU:CD1	2.36	0.56
22:T:71:VAL:HG12	22:T:72:ILE:N	2.21	0.56
3:A:153:ARG:HB2	3:A:153:ARG:NH1	2.17	0.56
16:N:17:ARG:HB3	16:N:17:ARG:NH1	2.21	0.56
20:R:111:ILE:HG23	20:R:145:LEU:CD1	2.36	0.56
22:T:28:SER:O	22:T:32:ARG:HG3	2.06	0.56
25:W:88:THR:HG23	25:W:110:GLN:HB3	1.88	0.56
1:O:1835:U:C5	1:O:1840:A:N7	2.65	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:VAL:CG1	3:A:207:GLN:HB3	2.37	0.55
4:B:280:VAL:HG13	4:B:333:GLU:O	2.05	0.55
17:O:73:ASP:HA	17:O:92:VAL:O	2.06	0.55
25:W:21:LEU:HB3	25:W:26:ILE:HG12	1.87	0.55
27:Y:144:ARG:CZ	39:Y:8910:HOH:O	2.54	0.55
30:2:22:PRO:HG2	30:2:25:VAL:CG2	2.35	0.55
1:0:960:G:N3	1:0:960:G:H2'	2.22	0.55
1:0:1234:U:N3	4:B:244:PRO:HB3	2.21	0.55
3:A:192:VAL:HG12	3:A:207:GLN:HB3	1.86	0.55
8:F:58:GLU:CD	15:M:27:ARG:HH22	2.14	0.55
8:F:99:THR:HA	39:F:3461:HOH:O	2.05	0.55
1:0:20:G:H21	20:R:117:HIS:HD2	1.53	0.55
1:0:417:G:P	39:0:7848:HOH:O	2.64	0.55
1:0:1120:U:H5''	1:0:1120:U:C6	2.41	0.55
1:0:1182:C:H1'	1:0:1192:A:H8	1.72	0.55
4:B:217:ARG:HG3	4:B:257:THR:HG22	1.87	0.55
16:N:58:LEU:N	16:N:58:LEU:HD12	2.20	0.55
25:W:13:MET:HE3	25:W:17:ILE:CG2	2.34	0.55
27:Y:189:ASN:HA	27:Y:217:ILE:HD11	1.87	0.55
1:0:380:A:OP2	15:M:9:ARG:HD2	2.07	0.55
1:0:447:A:P	22:T:1:SER:HB2	2.45	0.55
1:0:1363:G:OP1	5:C:76:ARG:NH2	2.39	0.55
1:0:2346:C:H6	1:0:2346:C:O5'	1.89	0.55
2:9:2:U:OP2	2:9:3:A:H5'	2.07	0.55
7:E:84:MET:HE1	7:E:148:ILE:CD1	2.36	0.55
12:J:45:VAL:HG21	12:J:129:PHE:CD1	2.41	0.55
29:1:25:LYS:CD	30:2:49:GLU:H	2.18	0.55
39:0:4235:HOH:O	22:T:9:LYS:HD3	2.06	0.55
2:9:28:U:H5''	16:N:40:ASN:ND2	2.22	0.55
11:I:97:VAL:O	11:I:101:LYS:HG3	2.06	0.55
12:J:107:ASN:HD22	12:J:109:TYR:H	1.53	0.55
16:N:147:ILE:HD12	39:N:8845:HOH:O	2.06	0.55
27:Y:151:SER:HB3	27:Y:154:ARG:HB3	1.89	0.55
27:Y:155:ARG:NH1	39:Y:8855:HOH:O	2.39	0.55
1:0:1972:U:H2'	1:0:1973:A:H5''	1.88	0.55
1:0:1973:A:H5'	1:0:1973:A:C8	2.33	0.55
39:0:9846:HOH:O	29:1:1:THR:HA	2.06	0.55
3:A:69:LEU:HD23	3:A:107:ASN:HB2	1.87	0.55
26:X:25:ARG:HG2	39:X:5356:HOH:O	2.07	0.55
1:0:319:A:H4'	1:0:338:C:C4	2.42	0.55
1:0:645:U:OP2	14:L:4:LYS:HE2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1384:C:H5'	26:X:30:MET:HG2	1.87	0.55
39:0:5193:HOH:O	16:N:21:HIS:HD2	1.90	0.55
6:D:154:LYS:HD2	6:D:154:LYS:N	2.08	0.55
13:K:82:ARG:NH2	13:K:115:ARG:HG2	2.22	0.55
25:W:139:GLY:O	25:W:141:HIS:HD2	1.88	0.55
1:0:447:A:OP2	22:T:1:SER:HB2	2.07	0.55
1:0:1116:U:O2'	1:0:1118:A:C2	2.47	0.55
3:A:129:LEU:HD12	3:A:145:MET:HE1	1.88	0.55
11:I:120:ALA:O	11:I:124:VAL:HG23	2.06	0.55
22:T:26:THR:HA	22:T:39:ASN:HB3	1.88	0.55
1:0:316:A:N3	1:0:336:G:O2'	2.40	0.55
1:0:2694:A:H4'	7:E:91:PHE:CE1	2.42	0.55
12:J:93:ARG:HB3	12:J:93:ARG:HH11	1.72	0.55
17:O:78:ALA:C	17:O:98:LEU:HD13	2.32	0.55
1:0:93:C:H5''	24:V:1:THR:CB	2.37	0.55
2:9:33:U:H2'	39:9:9068:HOH:O	2.07	0.55
2:9:51:A:H5'	16:N:160:SER:HB3	1.88	0.55
4:B:154:VAL:HG12	4:B:156:LYS:HG2	1.89	0.55
6:D:88:LEU:HB2	6:D:89:PRO:HD3	1.88	0.55
10:H:69:ARG:HD3	39:H:9031:HOH:O	2.07	0.55
24:V:42:ASN:O	24:V:44:GLY:N	2.40	0.55
28:Z:30:GLU:HA	28:Z:33:MET:HE3	1.89	0.55
1:0:475:G:H5'	5:C:73:LEU:HD23	1.88	0.54
1:0:2036:C:O4'	13:K:44:LEU:HG	2.07	0.54
2:9:23:U:O2'	2:9:24:U:H4'	2.07	0.54
5:C:115:LEU:O	5:C:118:THR:HB	2.06	0.54
16:N:49:THR:CG2	16:N:56:ASP:HB2	2.37	0.54
26:X:9:VAL:HG13	26:X:88:GLU:CD	2.32	0.54
27:Y:133:HIS:HD2	39:Y:8880:HOH:O	1.90	0.54
1:0:69:A:H5'	1:0:69:A:H8	1.72	0.54
39:0:7121:HOH:O	22:T:38:ARG:NH1	2.39	0.54
2:9:41:C:O4'	6:D:50:VAL:HG22	2.06	0.54
5:C:16:VAL:HG12	5:C:17:ASP:H	1.71	0.54
24:V:55:ARG:O	24:V:59:ILE:HG12	2.08	0.54
25:W:54:PHE:CZ	25:W:140:LYS:HB2	2.42	0.54
1:0:1201:C:H2'	1:0:1202:A:H5'	1.88	0.54
1:0:2676:C:H4'	12:J:70:PHE:HE1	1.72	0.54
15:M:99:ARG:HD2	15:M:167:GLY:HA2	1.88	0.54
16:N:183:ASP:O	16:N:184:ILE:O	2.25	0.54
20:R:132:ARG:CZ	39:R:8991:HOH:O	2.55	0.54
1:0:1278:A:H4'	1:0:1279:U:C4	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1677:U:OP2	30:2:8:LYS:NZ	2.40	0.54
5:C:214:THR:HG23	39:C:8643:HOH:O	2.07	0.54
7:E:36:PRO:HD3	12:J:127:ILE:HD12	1.89	0.54
26:X:31:ILE:O	26:X:35:GLU:HG3	2.08	0.54
4:B:66:GLU:OE1	4:B:328:ARG:HD2	2.07	0.54
1:O:1205:U:H2'	1:O:1206:U:H5''	1.89	0.54
5:C:79:ARG:O	5:C:87:ARG:HG2	2.08	0.54
6:D:22:VAL:HG22	6:D:74:THR:HG22	1.88	0.54
18:P:103:THR:O	18:P:107:GLU:HG3	2.07	0.54
1:O:1625:U:H4'	39:O:5132:HOH:O	2.07	0.54
3:A:94:LEU:HD23	3:A:94:LEU:N	2.23	0.54
5:C:129:HIS:HD2	5:C:165:ASP:OD2	1.90	0.54
7:E:31:ARG:NH1	39:E:5919:HOH:O	2.40	0.54
1:O:2769:C:H2'	1:O:2770:G:H5'	1.89	0.54
1:O:2894:C:O2'	1:O:2895:C:H5'	2.08	0.54
10:H:79:GLU:O	10:H:80:LEU:HD23	2.08	0.54
13:K:55:VAL:HG12	13:K:56:SER:N	2.22	0.54
19:Q:25:PRO:HB2	39:Q:4350:HOH:O	2.06	0.54
25:W:108:ARG:HE	25:W:114:PRO:CG	2.20	0.54
27:Y:178:HIS:CG	27:Y:179:PRO:HD2	2.43	0.54
30:2:48:ASP:O	30:2:49:GLU:HB2	2.07	0.54
1:O:1189:A:H1'	1:O:1209:C:O4'	2.08	0.54
1:O:1853:C:OP1	3:A:231:LYS:HG3	2.08	0.54
4:B:56:ASP:OD1	4:B:322:ARG:HB3	2.08	0.54
5:C:104:ASP:HA	5:C:107:ARG:HH12	1.71	0.54
26:X:25:ARG:HD2	39:X:3861:HOH:O	2.07	0.54
1:O:2862:G:H4'	4:B:336:GLN:O	2.07	0.54
6:D:58:VAL:HG12	6:D:60:GLU:HG2	1.89	0.54
8:F:14:ASP:O	8:F:18:GLU:HG3	2.08	0.54
13:K:66:ARG:HD3	39:K:2777:HOH:O	2.07	0.54
15:M:80:GLY:O	15:M:81:ARG:HD3	2.08	0.54
1:O:338:C:H4'	5:C:174:ILE:HD11	1.89	0.53
1:O:902:G:N7	14:L:18:HIS:HD2	2.06	0.53
1:O:2878:U:H2'	1:O:2879:A:O4'	2.08	0.53
39:O:3028:HOH:O	18:P:81:LYS:HG2	2.07	0.53
4:B:329:TYR:CE2	23:U:15:PRO:HG2	2.43	0.53
5:C:2:GLN:HB3	39:C:8535:HOH:O	2.08	0.53
6:D:23:VAL:HG22	6:D:73:VAL:HB	1.89	0.53
15:M:107:ARG:HG3	15:M:107:ARG:NH1	2.22	0.53
1:O:200:C:H2'	39:O:3929:HOH:O	2.07	0.53
1:O:485:A:N3	1:O:487:G:H5''	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1314:U:H2'	39:0:6326:HOH:O	2.07	0.53
2:9:29:C:C2'	2:9:30:C:H5'	2.38	0.53
3:A:121:ALA:O	3:A:124:VAL:HG22	2.07	0.53
6:D:134:LEU:HD11	6:D:166:ILE:HD11	1.89	0.53
6:D:163:VAL:HA	39:D:6326:HOH:O	2.06	0.53
13:K:62:PRO:HG3	13:K:65:ARG:NH2	2.23	0.53
29:1:21:ARG:HD2	29:1:37:CYS:SG	2.48	0.53
1:0:538:C:OP2	27:Y:134:HIS:HE1	1.91	0.53
1:0:2670:G:O2'	1:0:2671:U:H5'	2.08	0.53
4:B:82:VAL:O	4:B:82:VAL:HG12	2.07	0.53
7:E:126:ILE:HB	7:E:131:LEU:CD2	2.38	0.53
10:H:169:GLU:C	39:H:8993:HOH:O	2.51	0.53
11:I:94:ASP:OD1	11:I:133:THR:HB	2.09	0.53
16:N:43:VAL:HG13	16:N:118:ILE:HD11	1.91	0.53
16:N:62:HIS:HB3	16:N:65:ASP:OD1	2.09	0.53
1:0:10:U:O4	1:0:532:A:OP2	2.26	0.53
1:0:1268:C:O2'	27:Y:169:ARG:HB2	2.08	0.53
1:0:1594:C:OP2	18:P:120:ARG:HD2	2.08	0.53
39:0:7836:HOH:O	22:T:2:LYS:HE2	2.07	0.53
3:A:65:ARG:C	3:A:66:ARG:HG3	2.32	0.53
3:A:101:GLU:OE2	3:A:131:HIS:HB2	2.07	0.53
13:K:34:VAL:CG2	13:K:47:ALA:HB2	2.38	0.53
16:N:154:LEU:O	16:N:155:GLU:HB3	2.08	0.53
24:V:1:THR:HG23	24:V:2:VAL:N	2.19	0.53
26:X:8:ARG:NH1	39:X:2479:HOH:O	2.40	0.53
30:2:23:ALA:HB3	39:2:6863:HOH:O	2.08	0.53
1:0:905:C:OP1	27:Y:144:ARG:NH1	2.42	0.53
30:2:39:ARG:HG2	39:2:3143:HOH:O	2.09	0.53
30:2:41:HIS:HD2	30:2:44:ARG:H	1.56	0.53
3:A:66:ARG:HH11	3:A:66:ARG:HB2	1.74	0.53
6:D:65:GLU:HG3	39:D:6752:HOH:O	2.07	0.53
12:J:19:MET:CE	12:J:132:LEU:HD11	2.35	0.53
22:T:69:LYS:O	22:T:71:VAL:HG23	2.08	0.53
1:0:536:A:H3'	39:0:5504:HOH:O	2.09	0.53
1:0:2243:C:H5''	39:0:4230:HOH:O	2.09	0.53
2:9:69:U:OP1	16:N:4:PRO:HG3	2.09	0.53
16:N:48:VAL:HG11	16:N:55:ASP:HB3	1.90	0.53
23:U:52:THR:HG22	23:U:54:THR:N	2.23	0.53
1:0:156:C:H5''	15:M:171:ARG:CD	2.29	0.53
1:0:1187:U:O2'	1:0:1189:A:H2	1.92	0.53
1:0:1972:U:C2'	1:0:1973:A:H5''	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:94:LEU:HG	3:A:99:ILE:HD11	1.91	0.53
4:B:321:PRO:HA	39:B:9127:HOH:O	2.09	0.53
6:D:24:HIS:HB2	6:D:72:LYS:CB	2.39	0.53
8:F:26:THR:HG21	8:F:102:GLY:C	2.34	0.53
1:O:1201:C:H5''	39:O:6679:HOH:O	2.09	0.53
1:O:2419:U:H5''	1:O:2420:G:H5'	1.90	0.53
5:C:107:ARG:NE	39:C:8661:HOH:O	2.20	0.53
10:H:165:ARG:HD2	39:H:9034:HOH:O	2.08	0.53
26:X:43:VAL:HG12	26:X:44:ASP:N	2.24	0.53
27:Y:112:GLU:OE2	27:Y:115:ARG:NH1	2.42	0.53
1:O:820:G:O2'	1:O:856:G:H4'	2.09	0.52
1:O:2812:A:C2	1:O:2814:A:N6	2.68	0.52
1:O:2817:G:P	39:O:8430:HOH:O	2.67	0.52
2:9:14:G:O2'	16:N:1:ALA:HB2	2.08	0.52
5:C:118:THR:O	5:C:136:VAL:HG13	2.08	0.52
12:J:80:LYS:HE3	12:J:101:VAL:O	2.08	0.52
14:L:134:GLU:HG3	39:L:8849:HOH:O	2.08	0.52
16:N:32:PRO:HD2	16:N:99:GLU:O	2.09	0.52
17:O:25:VAL:HG23	17:O:26:TRP:N	2.23	0.52
1:O:1162:G:H1'	11:I:112:LEU:HD11	1.91	0.52
1:O:2044:G:OP1	26:X:23:HIS:HE1	1.92	0.52
1:O:2712:G:H5'	39:K:4183:HOH:O	2.09	0.52
21:S:81:ILE:HG23	39:S:8984:HOH:O	2.10	0.52
25:W:64:THR:O	25:W:68:THR:HG22	2.09	0.52
26:X:18:ARG:NH1	39:X:4132:HOH:O	2.40	0.52
4:B:265:LEU:HD21	4:B:316:ARG:HD3	1.91	0.52
1:O:870:G:OP2	3:A:3:ARG:HD3	2.09	0.52
1:O:1119:G:H22	1:O:1246:A:H2	1.51	0.52
5:C:162:VAL:CG2	5:C:232:LEU:HD21	2.40	0.52
7:E:154:ILE:HG13	7:E:156:ASP:OD1	2.10	0.52
11:I:96:SER:H	11:I:99:GLN:NE2	2.07	0.52
13:K:125:ALA:C	13:K:127:ALA:H	2.17	0.52
17:O:96:VAL:HG13	17:O:100:GLN:HB2	1.90	0.52
1:O:711:G:H1'	39:O:7530:HOH:O	2.09	0.52
1:O:1120:U:H5'	1:O:1121:G:OP2	2.08	0.52
1:O:2491:G:H1'	39:O:7304:HOH:O	2.09	0.52
21:S:77:VAL:O	21:S:80:ARG:HG2	2.09	0.52
1:O:564:G:H1'	39:O:6756:HOH:O	2.08	0.52
1:O:1972:U:H2'	1:O:1973:A:C5'	2.39	0.52
3:A:53:ALA:HB3	39:A:9068:HOH:O	2.10	0.52
15:M:134:ILE:CG2	15:M:141:ILE:HD13	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:O:32:ARG:HH21	17:O:35:LYS:NZ	2.07	0.52
26:X:34:ARG:NH1	26:X:48:VAL:O	2.36	0.52
27:Y:154:ARG:NH1	27:Y:155:ARG:HG3	2.24	0.52
31:3:3:MET:HG3	31:3:4:PRO:HD2	1.92	0.52
1:O:1666:C:H2'	1:O:1667:A:C5'	2.38	0.52
39:O:6731:HOH:O	27:Y:158:LYS:HD3	2.10	0.52
7:E:84:MET:HB2	7:E:131:LEU:HB2	1.91	0.52
11:I:108:HIS:N	11:I:109:PRO:CD	2.72	0.52
14:L:67:ARG:O	14:L:71:GLU:HG3	2.10	0.52
16:N:78:MET:HB2	16:N:79:PRO:HD3	1.90	0.52
23:U:17:THR:CG2	23:U:18:GLY:N	2.73	0.52
24:V:56:ILE:O	24:V:60:GLN:HG3	2.10	0.52
1:O:31:C:H4'	39:O:7854:HOH:O	2.10	0.52
1:O:1119:G:H8	12:J:52:GLN:NE2	2.08	0.52
1:O:1730:G:C5'	1:O:1731:C:C6	2.93	0.52
17:O:26:TRP:N	39:O:3062:HOH:O	2.42	0.52
22:T:24:ARG:HH21	22:T:39:ASN:HD22	1.56	0.52
30:2:41:HIS:H	30:2:45:ASN:ND2	1.95	0.52
1:O:449:A:N7	5:C:43:LYS:HG2	2.25	0.52
1:O:949:U:H4'	19:Q:95:GLU:HA	1.90	0.52
3:A:81:GLN:HB2	3:A:92:ASN:ND2	2.24	0.52
4:B:314:ALA:HB3	4:B:317:PRO:HG3	1.92	0.52
6:D:135:VAL:HG22	6:D:136:ARG:N	2.25	0.52
8:F:27:GLY:HA3	8:F:101:ALA:O	2.10	0.52
11:I:133:THR:HG22	11:I:134:ILE:N	2.24	0.52
13:K:29:LEU:HB3	13:K:55:VAL:CG1	2.35	0.52
1:O:407:A:H5'	39:O:6477:HOH:O	2.10	0.52
1:O:1700:C:H5''	1:O:1701:A:OP2	2.09	0.52
3:A:37:VAL:HG13	39:A:9072:HOH:O	2.10	0.52
5:C:27:ARG:HG2	5:C:30:LEU:HD12	1.91	0.52
5:C:129:HIS:CE1	5:C:231:ARG:HA	2.45	0.52
7:E:15:GLN:NE2	7:E:40:VAL:O	2.43	0.52
9:G:64:ASN:HD22	9:G:64:ASN:N	2.08	0.52
10:H:62:HIS:HA	10:H:65:LEU:HD23	1.92	0.52
13:K:20:CYS:HB2	13:K:29:LEU:HG	1.92	0.52
16:N:49:THR:CG2	16:N:58:LEU:HD11	2.40	0.52
17:O:23:GLY:C	39:O:3062:HOH:O	2.52	0.52
25:W:122:ARG:CG	25:W:122:ARG:NH1	2.71	0.52
1:O:1730:G:H5''	1:O:1731:C:H6	1.74	0.51
3:A:232:ARG:NH2	3:A:236:GLY:O	2.34	0.51
6:D:35:ALA:C	6:D:37:ALA:H	2.18	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:174:LEU:HA	39:H:9021:HOH:O	2.10	0.51
27:Y:187:VAL:HB	27:Y:203:VAL:HG22	1.92	0.51
39:O:6168:HOH:O	13:K:87:ARG:CZ	2.57	0.51
8:F:38:LYS:HZ3	15:M:3:SER:HA	1.75	0.51
12:J:75:PRO:HD3	12:J:136:SER:OG	2.09	0.51
16:N:110:THR:HB	16:N:113:SER:OG	2.11	0.51
17:O:14:LEU:CD2	17:O:102:ILE:HD11	2.41	0.51
23:U:9:CYS:HA	23:U:52:THR:HG23	1.92	0.51
1:O:653:U:H2'	1:O:654:A:C8	2.44	0.51
1:O:2643:G:H5''	39:O:4401:HOH:O	2.09	0.51
20:R:106:GLY:HA2	20:R:109:MET:CE	2.41	0.51
29:1:8:GLN:HE22	29:1:11:LYS:HZ1	1.56	0.51
1:O:775:G:OP1	29:1:16:HIS:HE1	1.94	0.51
1:O:2289:G:H21	1:O:2291:A:H2	1.54	0.51
10:H:119:ALA:O	10:H:120:PHE:C	2.54	0.51
12:J:74:ARG:HH12	12:J:76:ASP:HB2	1.74	0.51
25:W:65:VAL:HG12	25:W:116:LEU:HD13	1.92	0.51
3:A:105:VAL:HG12	3:A:106:CYS:N	2.24	0.51
4:B:72:THR:HB	39:B:9073:HOH:O	2.10	0.51
4:B:141:ARG:HG2	4:B:165:ARG:HA	1.91	0.51
11:I:97:VAL:CG1	11:I:101:LYS:HE3	2.35	0.51
22:T:115:GLU:HG3	22:T:116:ASP:N	2.25	0.51
25:W:106:THR:OG1	25:W:109:GLU:HG3	2.11	0.51
27:Y:186:ARG:HG2	27:Y:186:ARG:NH1	2.25	0.51
1:O:136:C:H2'	1:O:137:U:O4'	2.10	0.51
1:O:834:G:H4'	1:O:835:U:OP2	2.11	0.51
1:O:1242:A:C5'	12:J:82:THR:HG23	2.27	0.51
1:O:1947:G:H2'	1:O:1948:G:H8	1.75	0.51
1:O:2661:U:H3	1:O:2812:A:H62	1.59	0.51
2:9:35:C:H5''	39:9:9078:HOH:O	2.09	0.51
3:A:97:ALA:HB2	3:A:150:PRO:HB2	1.93	0.51
3:A:109:GLU:HG2	3:A:116:GLY:N	2.26	0.51
6:D:58:VAL:HB	6:D:62:ASP:HB3	1.93	0.51
6:D:136:ARG:HD2	6:D:155:HIS:O	2.10	0.51
7:E:93:MET:HE1	7:E:165:GLY:N	2.26	0.51
24:V:20:LEU:HD22	24:V:60:GLN:HE22	1.75	0.51
1:O:123:U:H5'	39:O:7091:HOH:O	2.10	0.51
1:O:1159:G:H1	1:O:1208:C:H42	1.58	0.51
1:O:2748:G:H5'	39:O:7963:HOH:O	2.11	0.51
1:O:2795:C:O2'	1:O:2796:U:H5'	2.10	0.51
2:9:54:A:O2'	2:9:55:U:H5'	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:166:ILE:CD1	5:C:207:LEU:HD13	2.41	0.51
7:E:84:MET:HE2	7:E:133:VAL:HG23	1.93	0.51
16:N:154:LEU:HG	16:N:155:GLU:H	1.76	0.51
18:P:10:ALA:HA	18:P:13:VAL:CG1	2.40	0.51
1:0:162:C:H2'	1:0:163:U:H5'	1.93	0.51
1:0:1351:G:OP1	5:C:96:LYS:NZ	2.37	0.51
1:0:1595:G:O2'	1:0:1596:U:H5'	2.11	0.51
1:0:2563:U:H2'	1:0:2565:C:O5'	2.11	0.51
16:N:179:LEU:HD23	16:N:184:ILE:HD12	1.93	0.51
26:X:21:PRO:HG2	26:X:24:LYS:HD3	1.91	0.51
27:Y:184:GLU:OE1	27:Y:204:ARG:NH1	2.44	0.51
28:Z:26:VAL:O	28:Z:30:GLU:HG3	2.11	0.51
1:0:474:C:O3'	5:C:73:LEU:CD2	2.59	0.51
1:0:1118:A:H8	1:0:1119:G:H5''	1.76	0.51
10:H:50:ILE:HG21	39:H:9028:HOH:O	2.11	0.51
11:I:84:SER:HB3	11:I:92:VAL:CG2	2.41	0.51
1:0:262:A:OP2	8:F:91:VAL:HG11	2.10	0.51
1:0:392:U:O2'	15:M:182:LYS:HE2	2.11	0.51
1:0:2073:G:OP2	1:0:2490:A:H5'	2.11	0.51
1:0:2301:A:H5''	1:0:2302:A:H5'	1.93	0.51
3:A:125:ASN:HB3	3:A:158:VAL:HG12	1.91	0.51
3:A:129:LEU:CD1	3:A:145:MET:HE1	2.41	0.51
5:C:61:PHE:HB3	39:C:8650:HOH:O	2.10	0.51
5:C:136:VAL:HG22	5:C:137:PRO:HA	1.93	0.51
16:N:116:PHE:HB3	16:N:136:LEU:HD23	1.93	0.51
22:T:32:ARG:NH1	22:T:38:ARG:HH12	2.09	0.51
23:U:4:ARG:HG2	23:U:4:ARG:HH11	1.74	0.51
1:0:92:G:H4'	24:V:44:GLY:HA3	1.93	0.50
1:0:1244:U:H2'	12:J:47:THR:HG21	1.92	0.50
1:0:2456:A:H5'	39:O:6149:HOH:O	2.10	0.50
2:9:64:C:H2'	2:9:65:A:H5'	1.93	0.50
4:B:258:GLY:H	4:B:260:HIS:CE1	2.29	0.50
4:B:297:VAL:HB	39:B:9073:HOH:O	2.11	0.50
12:J:131:THR:HG22	12:J:133:GLY:H	1.76	0.50
13:K:28:GLU:HB3	13:K:59:LYS:HB2	1.92	0.50
31:3:18:GLN:OE1	31:3:73:GLU:HB3	2.11	0.50
2:9:48:C:H4'	16:N:141:ARG:HH21	1.76	0.50
23:U:39:ASN:ND2	23:U:44:ARG:HH11	2.08	0.50
26:X:37:LEU:CD1	26:X:85:VAL:HG21	2.23	0.50
30:2:20:ARG:HG3	30:2:21:VAL:H	1.77	0.50
1:0:2472:C:O2'	1:0:2634:G:H4'	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2502:C:C2'	1:0:2503:A:H5'	2.40	0.50
2:9:76:G:C3'	2:9:77:A:H5''	2.31	0.50
4:B:14:GLY:HA2	4:B:15:PRO:C	2.36	0.50
15:M:47:ASP:CG	15:M:48:LYS:N	2.69	0.50
16:N:164:ASP:OD2	16:N:167:ASP:HA	2.10	0.50
20:R:132:ARG:NH2	39:R:8991:HOH:O	2.45	0.50
21:S:10:VAL:HG11	24:V:36:ALA:CA	2.40	0.50
1:0:1289:C:O2'	1:0:1290:G:H5'	2.11	0.50
1:0:1470:A:OP1	15:M:93:ARG:HD2	2.12	0.50
1:0:2089:A:O2'	1:0:2090:G:H5'	2.11	0.50
3:A:105:VAL:HG11	3:A:154:ALA:CB	2.41	0.50
7:E:108:LEU:HD11	7:E:164:ASP:HB2	1.94	0.50
25:W:122:ARG:NH2	39:W:5817:HOH:O	2.44	0.50
1:0:558:C:H2'	1:0:559:U:H5'	1.93	0.50
1:0:1118:A:C8	1:0:1118:A:C3'	2.90	0.50
1:0:1181:A:C2'	1:0:1182:C:H5'	2.42	0.50
1:0:1250:C:O2'	1:0:1251:C:H5'	2.12	0.50
4:B:51:VAL:HG21	4:B:327:VAL:HG13	1.92	0.50
6:D:23:VAL:CG2	6:D:73:VAL:HB	2.41	0.50
10:H:30:LYS:H	10:H:62:HIS:CD2	2.21	0.50
12:J:19:MET:HE1	12:J:78:ILE:HG22	1.93	0.50
23:U:46:ALA:HB1	23:U:52:THR:HG21	1.92	0.50
24:V:64:GLY:O	24:V:65:ASP:CB	2.59	0.50
1:0:1299:G:H5'	39:0:4547:HOH:O	2.12	0.50
1:0:2638:G:H1'	39:0:8261:HOH:O	2.11	0.50
1:0:2769:C:H2'	1:0:2770:G:C5'	2.41	0.50
6:D:103:ASN:ND2	6:D:134:LEU:H	2.08	0.50
1:0:1163:G:H5''	11:I:110:ASP:HB3	1.94	0.50
1:0:1666:C:C2'	1:0:1667:A:C5'	2.89	0.50
39:0:3115:HOH:O	8:F:38:LYS:HE2	2.11	0.50
39:0:8211:HOH:O	5:C:94:THR:HG21	2.12	0.50
14:L:89:PHE:N	39:L:8863:HOH:O	2.45	0.50
20:R:119:VAL:HG21	20:R:142:ASP:CG	2.37	0.50
25:W:48:VAL:CG1	25:W:48:VAL:O	2.60	0.50
1:0:2756:U:H3	1:0:2896:A:H2	1.50	0.50
39:0:3724:HOH:O	11:I:87:PRO:HD3	2.11	0.50
39:0:9515:HOH:O	14:L:30:ARG:HD2	2.10	0.50
5:C:77:ALA:O	5:C:78:ARG:HG3	2.11	0.50
8:F:46:GLU:OE1	8:F:100:ASP:HA	2.12	0.50
21:S:81:ILE:HG12	39:S:8984:HOH:O	2.11	0.50
27:Y:187:VAL:HG22	27:Y:192:ASP:CB	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:64:C:C2'	2:9:65:A:H5'	2.41	0.49
5:C:246:ARG:NE	39:C:8630:HOH:O	2.26	0.49
6:D:146:LYS:HZ3	16:N:107:ASN:HD21	1.59	0.49
11:I:126:THR:HG22	11:I:126:THR:O	2.11	0.49
13:K:115:ARG:HG3	13:K:116:GLU:N	2.26	0.49
25:W:38:THR:HG22	39:W:3580:HOH:O	2.11	0.49
26:X:71:ARG:HB3	26:X:88:GLU:OE1	2.11	0.49
28:Z:57:CYS:SG	28:Z:59:TYR:HB3	2.52	0.49
1:0:776:A:OP1	29:1:28:HIS:HE1	1.95	0.49
1:0:1377:C:H5'	1:0:1377:C:C6	2.45	0.49
1:0:2363:G:O3'	19:Q:11:ARG:NH1	2.45	0.49
1:0:2415:A:H2'	1:0:2416:G:H5'	1.93	0.49
6:D:96:SER:C	6:D:98:PHE:H	2.20	0.49
9:G:16:LYS:O	9:G:20:VAL:HG23	2.13	0.49
22:T:41:ARG:HG2	22:T:41:ARG:HH11	1.76	0.49
25:W:88:THR:CG2	25:W:90:TYR:HD1	2.25	0.49
27:Y:126:PRO:HG2	27:Y:128:PHE:CZ	2.47	0.49
30:2:20:ARG:CG	30:2:21:VAL:N	2.76	0.49
1:0:343:C:O2'	1:0:344:C:H5'	2.11	0.49
1:0:1200:A:H3'	39:0:6208:HOH:O	2.13	0.49
1:0:2791:U:H1'	1:0:2792:A:H5''	1.94	0.49
1:0:2812:A:H1'	39:0:6244:HOH:O	2.12	0.49
1:0:2825:C:H4'	1:0:2826:G:O5'	2.12	0.49
3:A:192:VAL:HG13	39:A:9022:HOH:O	2.12	0.49
4:B:74:ILE:HG13	39:B:9073:HOH:O	2.12	0.49
4:B:149:ASP:HB2	39:B:9049:HOH:O	2.13	0.49
6:D:23:VAL:HG23	6:D:23:VAL:O	2.13	0.49
10:H:6:ALA:CA	10:H:61:ARG:HH12	2.22	0.49
10:H:43:ALA:HB1	10:H:140:TYR:CE2	2.47	0.49
13:K:55:VAL:CG1	13:K:56:SER:N	2.75	0.49
14:L:125:PHE:CE1	14:L:140:VAL:HG13	2.48	0.49
15:M:31:TRP:HA	15:M:34:GLU:HG3	1.93	0.49
25:W:26:ILE:O	25:W:26:ILE:HG13	2.12	0.49
27:Y:209:VAL:HG12	27:Y:214:ARG:HG3	1.94	0.49
1:0:920:C:H5''	1:0:921:G:O5'	2.13	0.49
1:0:1306:U:OP1	5:C:184:ARG:HD2	2.13	0.49
3:A:1:GLY:HA2	3:A:197:VAL:HG23	1.95	0.49
4:B:49:THR:HG21	4:B:331:SER:O	2.13	0.49
4:B:223:ARG:HG3	4:B:232:TRP:O	2.11	0.49
5:C:133:ARG:NH1	39:C:8616:HOH:O	2.45	0.49
6:D:29:HIS:HB2	39:D:2768:HOH:O	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:P:141:ILE:C	18:P:143:ALA:H	2.19	0.49
19:Q:26:PRO:O	19:Q:30:VAL:HG23	2.12	0.49
25:W:108:ARG:HG3	25:W:114:PRO:HG3	1.94	0.49
26:X:74:ALA:CB	26:X:85:VAL:HG22	2.42	0.49
31:3:48:ASN:ND2	31:3:50:GLY:H	2.10	0.49
1:0:638:C:H2'	1:0:639:A:C8	2.47	0.49
1:0:899:C:H5'	39:0:3690:HOH:O	2.11	0.49
1:0:1151:G:OP1	9:G:63:ARG:NH1	2.45	0.49
1:0:2270:G:C4'	3:A:223:ARG:HH12	2.18	0.49
3:A:179:MET:HA	3:A:179:MET:CE	2.38	0.49
6:D:104:PHE:CE2	6:D:166:ILE:HD13	2.47	0.49
8:F:39:SER:HB3	8:F:45:ALA:HB2	1.95	0.49
16:N:147:ILE:HB	39:N:8845:HOH:O	2.12	0.49
22:T:73:HIS:CD2	22:T:88:PRO:HG3	2.48	0.49
25:W:31:HIS:HB3	39:W:5420:HOH:O	2.12	0.49
4:B:268:ARG:NH2	4:B:325:PRO:HG3	2.28	0.49
5:C:19:PRO:HG2	5:C:22:PHE:CE1	2.48	0.49
8:F:16:ALA:HA	8:F:111:ILE:HD13	1.94	0.49
14:L:73:VAL:HG21	14:L:116:HIS:CD2	2.48	0.49
25:W:41:TYR:HA	25:W:44:MET:HE3	1.94	0.49
25:W:65:VAL:HA	25:W:68:THR:CG2	2.42	0.49
27:Y:235:GLU:CD	27:Y:235:GLU:N	2.66	0.49
30:2:35:ARG:HB2	39:2:2691:HOH:O	2.11	0.49
1:0:1181:A:H2'	1:0:1182:C:H5'	1.94	0.49
1:0:1778:A:H2'	1:0:1779:A:H5'	1.95	0.49
6:D:18:ILE:HG12	6:D:134:LEU:CD2	2.43	0.49
16:N:154:LEU:C	16:N:156:GLU:H	2.20	0.49
22:T:62:VAL:HB	39:T:3851:HOH:O	2.13	0.49
22:T:112:LEU:HD23	22:T:119:ALA:HB3	1.95	0.49
1:0:793:A:H5''	18:P:83:LYS:HG2	1.95	0.49
1:0:1426:C:H2'	39:0:3083:HOH:O	2.11	0.49
3:A:34:ASP:OD1	3:A:35:GLY:N	2.39	0.49
4:B:102:THR:HG21	4:B:182:VAL:O	2.13	0.49
10:H:61:ARG:HH11	10:H:61:ARG:HG3	1.77	0.49
18:P:98:ILE:HD12	18:P:102:ARG:NE	2.28	0.49
1:0:1205:U:C2'	1:0:1206:U:H5''	2.43	0.49
1:0:2521:A:OP2	10:H:6:ALA:HB3	2.13	0.49
1:0:2697:A:H2'	1:0:2698:G:O4'	2.13	0.49
3:A:81:GLN:HG3	3:A:92:ASN:HD21	1.77	0.49
14:L:130:ARG:HA	39:L:8849:HOH:O	2.12	0.49
15:M:99:ARG:HE	15:M:170:ASN:HD22	1.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Y:103:THR:HG22	27:Y:104:GLU:OE2	2.13	0.49
1:0:291:C:H2'	1:0:292:G:O4'	2.13	0.49
1:0:475:G:C5'	5:C:73:LEU:HD23	2.43	0.49
1:0:602:A:O2'	1:0:605:C:H4'	2.12	0.49
6:D:35:ALA:C	6:D:37:ALA:N	2.71	0.49
13:K:22:ASP:O	13:K:110:LYS:HE3	2.13	0.49
31:3:56:PRO:N	39:3:8976:HOH:O	2.45	0.49
1:0:1525:G:H5'	1:0:1526:A:OP2	2.13	0.48
1:0:1996:U:O2'	1:0:1997:A:H5'	2.13	0.48
1:0:2667:G:H1'	1:0:2914:A:N3	2.27	0.48
2:9:92:G:H2'	2:9:93:A:H8	1.78	0.48
6:D:36:ASN:HA	39:D:7500:HOH:O	2.12	0.48
12:J:130:VAL:HG12	12:J:131:THR:N	2.28	0.48
15:M:58:GLN:HG3	39:M:8905:HOH:O	2.11	0.48
27:Y:107:PRO:HB3	27:Y:182:PHE:CE2	2.47	0.48
27:Y:216:ARG:HD2	39:Y:8868:HOH:O	2.13	0.48
28:Z:32:GLU:HA	28:Z:35:GLU:HG3	1.95	0.48
1:0:138:U:H5''	1:0:139:C:OP2	2.14	0.48
1:0:666:A:H2'	1:0:667:C:O4'	2.14	0.48
1:0:2672:C:H1'	39:B:9104:HOH:O	2.12	0.48
39:0:7653:HOH:O	3:A:11:ARG:HA	2.13	0.48
6:D:167:GLU:C	6:D:169:THR:H	2.21	0.48
8:F:36:THR:HG23	8:F:97:ALA:HB2	1.94	0.48
20:R:132:ARG:HG2	20:R:133:ALA:N	2.28	0.48
24:V:12:THR:HG23	24:V:14:ALA:N	2.28	0.48
29:1:28:HIS:HD2	29:1:30:LYS:H	1.60	0.48
1:0:304:G:H1'	1:0:347:A:N6	2.28	0.48
1:0:656:G:C5'	17:O:3:THR:HG22	2.40	0.48
1:0:1477:C:H5'	1:0:1868:G:C5'	2.43	0.48
1:0:1741:U:H5'	1:0:1742:A:OP1	2.13	0.48
1:0:1942:A:H3'	39:0:7777:HOH:O	2.13	0.48
6:D:35:ALA:N	39:D:5576:HOH:O	2.46	0.48
7:E:85:GLU:HG3	7:E:169:THR:OG1	2.13	0.48
15:M:164:THR:HG23	15:M:165:GLY:N	2.26	0.48
25:W:88:THR:HG22	25:W:90:TYR:CD1	2.46	0.48
27:Y:189:ASN:ND2	27:Y:192:ASP:H	2.11	0.48
1:0:57:C:H5''	39:0:7195:HOH:O	2.12	0.48
1:0:462:A:H2'	39:0:5343:HOH:O	2.14	0.48
1:0:1120:U:H5''	1:0:1120:U:H6	1.78	0.48
1:0:1166:A:H1'	1:0:1192:A:C2	2.48	0.48
1:0:2064:U:H5'	1:0:2652:U:O3'	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2769:C:O2'	1:0:2770:G:H5'	2.13	0.48
22:T:49:GLU:HB3	22:T:59:GLU:HG2	1.95	0.48
24:V:23:LEU:HD12	24:V:56:ILE:HD12	1.95	0.48
25:W:48:VAL:O	25:W:48:VAL:HG12	2.13	0.48
28:Z:60:CYS:O	28:Z:61:ASP:HB2	2.12	0.48
1:0:558:C:C2'	1:0:559:U:C5'	2.90	0.48
10:H:66:GLU:HA	39:H:9031:HOH:O	2.13	0.48
18:P:13:VAL:HG21	18:P:41:ARG:HG2	1.94	0.48
25:W:139:GLY:O	25:W:141:HIS:CD2	2.65	0.48
1:0:1053:G:OP1	10:H:15:PRO:HG3	2.13	0.48
2:9:30:C:OP1	6:D:137:PRO:O	2.31	0.48
5:C:168:ARG:NH2	5:C:190:ALA:O	2.47	0.48
5:C:180:SER:HB2	39:C:8651:HOH:O	2.13	0.48
6:D:155:HIS:NE2	39:D:7597:HOH:O	2.31	0.48
7:E:133:VAL:HG12	7:E:141:VAL:HG13	1.96	0.48
9:G:23:ILE:HD13	9:G:67:LEU:HD23	1.96	0.48
10:H:141:CYS:HB2	39:H:8994:HOH:O	2.14	0.48
12:J:13:ASP:OD1	12:J:15:ARG:HB3	2.14	0.48
20:R:99:ALA:HB1	20:R:109:MET:CE	2.26	0.48
1:0:292:G:H2'	1:0:358:G:N2	2.29	0.48
1:0:377:C:H5	39:0:3795:HOH:O	1.97	0.48
1:0:447:A:OP1	22:T:2:LYS:HG2	2.13	0.48
1:0:1010:C:H4'	16:N:4:PRO:HB2	1.95	0.48
1:0:1427:A:H61	1:0:1440:U:H1'	1.79	0.48
6:D:149:ARG:NH2	39:D:3066:HOH:O	2.45	0.48
7:E:137:ASP:OD1	7:E:139:GLU:HB2	2.13	0.48
15:M:64:ARG:HD2	39:M:8884:HOH:O	2.14	0.48
22:T:40:VAL:HG22	22:T:41:ARG:N	2.29	0.48
27:Y:149:GLN:NE2	39:Y:8900:HOH:O	2.41	0.48
1:0:1185:U:H2'	1:0:1186:C:C6	2.49	0.48
1:0:1874:U:H2'	3:A:120:ARG:HG3	1.96	0.48
1:0:1878:G:O2'	1:0:1879:U:OP2	2.31	0.48
1:0:2036:C:C1'	13:K:44:LEU:HG	2.43	0.48
6:D:37:ALA:O	6:D:40:ILE:HG12	2.13	0.48
19:Q:32:GLU:HA	19:Q:71:TYR:OH	2.14	0.48
20:R:34:GLU:HG2	20:R:46:TYR:OH	2.14	0.48
21:S:57:THR:CG2	21:S:58:MET:N	2.76	0.48
1:0:814:G:H4'	39:0:3620:HOH:O	2.12	0.48
39:0:5740:HOH:O	25:W:122:ARG:NH2	2.46	0.48
2:9:8:G:O6	16:N:11:ARG:NH1	2.46	0.48
3:A:36:ASP:HB2	3:A:85:SER:H	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:195:ARG:HD2	4:B:324:ASP:OD1	2.13	0.48
6:D:75:LEU:HD22	6:D:79:MET:HB3	1.96	0.48
7:E:80:TRP:O	7:E:134:SER:HA	2.13	0.48
19:Q:66:LYS:HB2	19:Q:70:ALA:O	2.14	0.48
23:U:52:THR:CG2	23:U:54:THR:HB	2.44	0.48
1:0:644:G:H5'	1:0:644:G:N3	2.29	0.48
1:0:654:A:OP2	17:O:38:ARG:HD3	2.14	0.48
1:0:1132:A:N6	1:0:1229:C:H2'	2.29	0.48
39:O:7437:HOH:O	19:Q:9:GLY:HA2	2.13	0.48
4:B:24:PRO:CG	4:B:204:GLY:HA2	2.44	0.48
5:C:127:ARG:CZ	5:C:225:PRO:HG2	2.42	0.48
13:K:30:LYS:O	13:K:55:VAL:HG13	2.14	0.48
18:P:97:ARG:HD2	39:P:162:HOH:O	2.13	0.48
24:V:5:VAL:CG1	24:V:9:ARG:NH1	2.77	0.48
1:0:1527:A:H1'	1:0:1528:A:C8	2.48	0.47
1:0:2456:A:H2'	1:0:2457:U:C6	2.49	0.47
39:O:7978:HOH:O	31:3:60:LYS:HG3	2.13	0.47
2:9:49:G:H2'	2:9:50:G:O4'	2.14	0.47
3:A:94:LEU:HD12	3:A:98:GLU:HB2	1.95	0.47
5:C:104:ASP:HA	5:C:107:ARG:NH1	2.29	0.47
6:D:40:ILE:HG13	6:D:41:LEU:N	2.29	0.47
7:E:101:GLU:HB2	7:E:116:THR:O	2.13	0.47
8:F:70:LYS:C	8:F:72:VAL:H	2.21	0.47
18:P:104:LYS:HE2	18:P:138:GLU:OE2	2.14	0.47
24:V:39:ALA:O	24:V:41:GLU:N	2.47	0.47
1:0:951:A:C2'	1:0:952:G:H5'	2.44	0.47
1:0:1014:A:H2'	1:0:1015:C:H5'	1.95	0.47
1:0:1730:G:C5'	1:0:1731:C:H6	2.27	0.47
1:0:1787:C:OP1	18:P:68:LYS:HE2	2.14	0.47
1:0:1819:G:H2'	1:0:1820:G:C4'	2.41	0.47
1:0:1878:G:O2'	1:0:1879:U:C6	2.63	0.47
1:0:1882:C:OP1	3:A:192:VAL:HG23	2.14	0.47
1:0:2443:C:O3'	14:L:56:LYS:HE3	2.13	0.47
1:0:2809:G:H2'	1:0:2810:G:O4'	2.15	0.47
11:I:105:GLU:HA	11:I:108:HIS:CE1	2.49	0.47
22:T:32:ARG:NH1	22:T:38:ARG:NH1	2.62	0.47
29:1:25:LYS:HD2	30:2:48:ASP:HA	1.96	0.47
1:0:396:U:OP2	31:3:38:ARG:HD2	2.15	0.47
1:0:1503:U:H2'	1:0:1504:A:O4'	2.14	0.47
4:B:71:VAL:HG11	4:B:296:LEU:HD22	1.96	0.47
10:H:81:GLY:C	10:H:83:GLU:H	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:63:GLU:HG2	39:K:6344:HOH:O	2.14	0.47
23:U:6:CYS:HB2	23:U:32:CYS:HB3	1.95	0.47
24:V:44:GLY:O	24:V:48:GLU:HG2	2.14	0.47
31:3:3:MET:O	31:3:90:PHE:HA	2.14	0.47
1:0:1056:U:H2'	1:0:1057:A:O4'	2.13	0.47
1:0:1441:G:H1'	39:0:8267:HOH:O	2.15	0.47
1:0:1641:A:C2'	1:0:1642:A:H5'	2.44	0.47
1:0:2787:C:H5	39:0:5098:HOH:O	1.96	0.47
3:A:130:THR:HB	3:A:137:VAL:HB	1.95	0.47
3:A:220:PRO:HD2	3:A:223:ARG:HD3	1.96	0.47
5:C:142:ASP:OD1	5:C:236:THR:HG23	2.14	0.47
6:D:24:HIS:HB2	6:D:72:LYS:HB3	1.97	0.47
11:I:123:VAL:C	11:I:125:GLY:H	2.22	0.47
16:N:65:ASP:HB3	39:N:8821:HOH:O	2.14	0.47
26:X:9:VAL:HG13	26:X:88:GLU:OE2	2.14	0.47
27:Y:187:VAL:HG22	27:Y:192:ASP:HB2	1.95	0.47
29:1:28:HIS:CD2	29:1:31:LYS:HG3	2.49	0.47
1:0:185:G:H4'	1:0:186:A:H4'	1.96	0.47
1:0:1342:C:O2'	1:0:1343:C:H5'	2.14	0.47
1:0:1926:G:H2'	1:0:1927:A:C8	2.49	0.47
8:F:48:VAL:CG2	8:F:74:PHE:HB3	2.44	0.47
1:0:1167:G:H2'	1:0:1168:C:O4'	2.15	0.47
1:0:1667:A:H2'	1:0:1668:U:C6	2.50	0.47
1:0:2133:U:H4'	1:0:2134:G:H5'	1.95	0.47
1:0:2896:A:N3	1:0:2896:A:H2'	2.29	0.47
6:D:170:TYR:O	6:D:171:ASP:CB	2.61	0.47
14:L:125:PHE:CZ	14:L:140:VAL:HG13	2.49	0.47
23:U:44:ARG:HB3	39:U:3805:HOH:O	2.15	0.47
1:0:282:C:H1'	1:0:368:C:H42	1.79	0.47
1:0:553:G:P	27:Y:204:ARG:HH22	2.37	0.47
1:0:737:A:H2'	1:0:738:G:O4'	2.15	0.47
1:0:1086:A:N6	25:W:11:VAL:HG11	2.30	0.47
1:0:1206:U:H2'	1:0:1207:A:O4'	2.15	0.47
1:0:1291:A:H2	39:0:5743:HOH:O	1.97	0.47
1:0:1419:U:H5'	1:0:1420:C:OP2	2.14	0.47
1:0:1943:C:O4'	3:A:212:PRO:HA	2.15	0.47
1:0:2251:G:H2'	1:0:2252:A:C8	2.50	0.47
4:B:85:ARG:HB2	4:B:99:GLU:HG2	1.95	0.47
4:B:205:VAL:O	4:B:307:ARG:NE	2.46	0.47
6:D:172:VAL:HG12	6:D:173:GLU:N	2.29	0.47
15:M:59:GLY:HA3	15:M:141:ILE:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:98:GLN:O	15:M:102:GLU:HG3	2.14	0.47
15:M:169:ARG:NH1	39:M:8871:HOH:O	2.47	0.47
16:N:171:HIS:CE1	39:N:8863:HOH:O	2.68	0.47
22:T:52:ARG:HB2	22:T:95:ASN:HB3	1.97	0.47
24:V:5:VAL:HG23	39:V:2271:HOH:O	2.14	0.47
26:X:78:GLU:HG2	26:X:79:GLU:H	1.79	0.47
4:B:81:ALA:O	4:B:186:GLY:HA3	2.14	0.47
6:D:84:LEU:HA	6:D:87:ALA:HB3	1.97	0.47
11:I:67:VAL:HG13	11:I:68:PRO:HD2	1.97	0.47
11:I:87:PRO:O	11:I:89:GLU:HG3	2.15	0.47
19:Q:25:PRO:HA	19:Q:26:PRO:HD3	1.80	0.47
1:O:285:A:H2'	1:O:286:U:O4'	2.15	0.47
1:O:553:G:OP2	27:Y:204:ARG:NH2	2.47	0.47
1:O:1593:C:OP1	18:P:117:SER:CB	2.63	0.47
1:O:2587:OMU:H2'	1:O:2589:U:H5''	1.96	0.47
1:O:2672:C:O2'	1:O:2673:U:H5'	2.15	0.47
2:9:51:A:H5'	16:N:160:SER:CB	2.45	0.47
4:B:243:ASN:HA	4:B:244:PRO:C	2.39	0.47
6:D:92:GLU:HB2	39:D:3862:HOH:O	2.14	0.47
25:W:125:HIS:HE1	39:W:3071:HOH:O	1.97	0.47
1:O:157:G:H4'	15:M:95:LYS:HE2	1.97	0.47
1:O:1159:G:H21	1:O:1189:A:H8	1.63	0.47
1:O:1506:U:H6	1:O:1506:U:H5'	1.80	0.47
1:O:2505:G:C2'	1:O:2506:A:H5'	2.44	0.47
1:O:2591:C:H2'	1:O:2592:G:O4'	2.15	0.47
39:O:6693:HOH:O	23:U:56:ARG:HD3	2.15	0.47
5:C:12:THR:HB	39:C:8646:HOH:O	2.14	0.47
5:C:118:THR:CG2	5:C:137:PRO:HB3	2.44	0.47
9:G:14:GLU:HB3	39:G:4173:HOH:O	2.14	0.47
10:H:161:THR:HB	10:H:162:PRO:HD3	1.97	0.47
11:I:75:LYS:HD3	11:I:81:GLU:O	2.15	0.47
25:W:4:LEU:HD23	25:W:54:PHE:HB3	1.97	0.47
1:O:12:U:H2'	1:O:13:G:H5'	1.97	0.46
1:O:255:A:H2'	1:O:256:C:C6	2.50	0.46
1:O:1130:U:H2'	1:O:1131:G:O4'	2.15	0.46
1:O:1535:G:H2'	1:O:1536:C:C6	2.50	0.46
1:O:1992:U:OP2	13:K:66:ARG:HD2	2.15	0.46
1:O:2506:A:O2'	1:O:2507:G:O5'	2.34	0.46
1:O:2507:G:H2'	1:O:2510:C:N4	2.30	0.46
1:O:2769:C:H2'	1:O:2770:G:O4'	2.15	0.46
4:B:238:ASN:ND2	4:B:240:GLY:H	2.00	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:142:ASP:OD1	5:C:237:GLU:HB3	2.15	0.46
16:N:152:GLU:OE1	16:N:152:GLU:HA	2.15	0.46
25:W:6:GLN:CB	25:W:26:ILE:HD12	2.34	0.46
25:W:76:ASP:O	25:W:77:ALA:C	2.57	0.46
1:O:1185:U:OP1	11:I:121:LYS:HD3	2.15	0.46
1:O:1666:C:C2'	1:O:1667:A:H5''	2.44	0.46
1:O:2851:G:C2'	1:O:2852:A:H5'	2.45	0.46
3:A:97:ALA:C	3:A:131:HIS:HE2	2.22	0.46
4:B:162:MET:HE3	4:B:310:ARG:HD3	1.93	0.46
4:B:241:PRO:HD2	39:B:9125:HOH:O	2.15	0.46
7:E:81:GLU:HG2	7:E:134:SER:CB	2.45	0.46
13:K:113:ILE:HG22	13:K:114:ALA:N	2.29	0.46
16:N:64:SER:C	16:N:66:LEU:H	2.22	0.46
16:N:143:ARG:NH1	16:N:173:ASP:OD2	2.48	0.46
1:O:2716:G:H5''	4:B:206:THR:CG2	2.41	0.46
3:A:109:GLU:HG2	3:A:116:GLY:H	1.81	0.46
5:C:236:THR:HG22	5:C:239:ALA:CB	2.46	0.46
14:L:114:VAL:HG11	39:L:8865:HOH:O	2.14	0.46
15:M:167:GLY:O	15:M:171:ARG:HG3	2.15	0.46
26:X:76:ARG:O	26:X:77:PHE:HB3	2.15	0.46
1:O:317:A:H4'	39:O:4251:HOH:O	2.16	0.46
1:O:2265:U:H2'	1:O:2266:A:C8	2.51	0.46
1:O:2453:G:H4'	14:L:50:GLY:C	2.40	0.46
1:O:2807:U:P	4:B:27:ASN:HD21	2.39	0.46
5:C:153:VAL:O	5:C:157:LEU:HG	2.16	0.46
6:D:60:GLU:O	6:D:61:PHE:C	2.57	0.46
6:D:94:ALA:HA	6:D:174:VAL:O	2.15	0.46
8:F:117:GLU:C	8:F:119:ARG:H	2.22	0.46
14:L:65:ASP:CG	14:L:111:ALA:HB3	2.40	0.46
16:N:179:LEU:HA	16:N:184:ILE:HD12	1.97	0.46
17:O:14:LEU:HD23	17:O:102:ILE:HD11	1.98	0.46
21:S:38:ALA:O	21:S:42:GLU:HG3	2.16	0.46
27:Y:189:ASN:HD22	27:Y:192:ASP:H	1.63	0.46
28:Z:53:GLY:HA2	28:Z:67:GLY:O	2.15	0.46
1:O:1172:G:H1'	39:O:5430:HOH:O	2.15	0.46
1:O:1211:G:O2'	1:O:1212:C:H5'	2.15	0.46
1:O:1333:U:H2'	1:O:1334:C:C6	2.51	0.46
1:O:1500:U:P	18:P:41:ARG:HH22	2.38	0.46
1:O:1687:C:O2	29:1:9:GLY:HA2	2.16	0.46
2:9:6:C:C5'	16:N:37:ARG:HH12	2.19	0.46
5:C:140:VAL:HG12	5:C:141:SER:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:21:ARG:N	39:L:8826:HOH:O	2.47	0.46
14:L:143:THR:HG22	14:L:144:ASP:H	1.76	0.46
15:M:166:ALA:HA	15:M:169:ARG:NH1	2.30	0.46
20:R:82:GLU:HG3	20:R:83:LYS:N	2.30	0.46
1:0:426:G:H2'	1:0:427:C:O4'	2.16	0.46
1:0:2256:G:H2'	1:0:2257:G:C5'	2.46	0.46
1:0:2526:C:O2'	1:0:2527:U:H5'	2.16	0.46
11:I:87:PRO:HB3	11:I:129:SER:C	2.41	0.46
12:J:19:MET:CE	12:J:132:LEU:HD21	2.46	0.46
22:T:71:VAL:HG13	22:T:91:LEU:O	2.15	0.46
25:W:38:THR:HG22	25:W:39:ASP:H	1.80	0.46
1:0:894:A:C2	5:C:87:ARG:NH2	2.83	0.46
1:0:1419:U:H2'	1:0:1685:A:C2	2.51	0.46
3:A:51:ARG:NH1	3:A:120:ARG:O	2.49	0.46
7:E:34:TRP:O	12:J:127:ILE:HD11	2.15	0.46
10:H:49:GLN:HG3	10:H:140:TYR:CD2	2.51	0.46
10:H:86:TYR:CD1	10:H:86:TYR:C	2.93	0.46
12:J:107:ASN:ND2	12:J:107:ASN:C	2.73	0.46
25:W:21:LEU:HB3	25:W:26:ILE:CG1	2.46	0.46
1:0:317:A:H5''	22:T:52:ARG:HD2	1.98	0.46
1:0:475:G:OP1	5:C:73:LEU:HD22	2.16	0.46
1:0:1279:U:O2	1:0:1279:U:H2'	2.15	0.46
1:0:1603:A:H5''	1:0:1605:G:H5'	1.96	0.46
6:D:173:GLU:O	6:D:174:VAL:C	2.59	0.46
8:F:46:GLU:O	8:F:73:PRO:HD2	2.16	0.46
11:I:87:PRO:C	11:I:89:GLU:N	2.74	0.46
20:R:39:THR:HG22	20:R:41:GLY:N	2.30	0.46
1:0:470:U:O2'	29:I:16:HIS:CD2	2.65	0.46
1:0:484:A:N1	1:0:506:G:H4'	2.31	0.46
1:0:1025:C:H5'	25:W:23:MET:O	2.16	0.46
1:0:1497:G:H4'	1:0:1627:G:O2'	2.16	0.46
1:0:1625:U:H5''	39:O:6473:HOH:O	2.16	0.46
1:0:2300:A:H4'	1:0:2301:A:O5'	2.16	0.46
1:0:2626:C:H2'	1:0:2627:G:C8	2.51	0.46
1:0:2911:C:H2'	1:0:2912:C:C6	2.51	0.46
5:C:19:PRO:HG2	5:C:22:PHE:CD1	2.51	0.46
12:J:88:PRO:O	12:J:94:GLY:HA3	2.16	0.46
15:M:69:LYS:HG2	15:M:127:LYS:HG3	1.98	0.46
17:O:26:TRP:HB2	39:O:3062:HOH:O	2.15	0.46
26:X:20:GLU:CD	26:X:21:PRO:HD2	2.41	0.46
26:X:45:GLU:HG3	39:X:6178:HOH:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:420:U:H2'	1:0:421:C:C6	2.51	0.46
1:0:1044:C:H5''	39:0:9520:HOH:O	2.15	0.46
1:0:1295:G:H5''	14:L:14:GLY:O	2.16	0.46
1:0:1717:A:H5''	18:P:54:LYS:HB2	1.97	0.46
1:0:2256:G:H2'	1:0:2257:G:H5'	1.98	0.46
4:B:75:GLU:C	4:B:77:PRO:HD3	2.41	0.46
4:B:162:MET:HE1	4:B:308:LEU:HD21	1.98	0.46
5:C:95:GLU:H	5:C:95:GLU:CD	2.24	0.46
11:I:94:ASP:O	11:I:95:LEU:HD23	2.16	0.46
14:L:73:VAL:HG23	14:L:74:THR:N	2.30	0.46
14:L:97:VAL:HG12	14:L:98:GLU:O	2.16	0.46
16:N:163:PHE:HZ	16:N:171:HIS:HD1	1.64	0.46
17:O:47:ARG:HG3	17:O:47:ARG:NH1	2.31	0.46
1:0:2266:A:OP2	15:M:90:ARG:NH2	2.49	0.45
1:0:2502:C:H2'	1:0:2503:A:H5'	1.98	0.45
1:0:2720:C:O2	13:K:87:ARG:NH2	2.50	0.45
3:A:81:GLN:HB2	3:A:92:ASN:HD22	1.81	0.45
6:D:101:THR:HG22	39:D:7400:HOH:O	2.15	0.45
7:E:31:ARG:NH1	7:E:68:HIS:CG	2.84	0.45
11:I:124:VAL:HG13	11:I:134:ILE:HD11	1.99	0.45
13:K:87:ARG:NH1	39:K:4066:HOH:O	2.49	0.45
14:L:145:LEU:O	14:L:145:LEU:HD23	2.16	0.45
25:W:38:THR:O	25:W:42:ARG:HB2	2.15	0.45
1:0:629:A:H2'	1:0:630:A:O4'	2.16	0.45
1:0:875:A:C2	3:A:194:MET:SD	3.10	0.45
1:0:1741:U:O2'	1:0:2723:G:H4'	2.16	0.45
2:9:49:G:O2'	2:9:50:G:H5'	2.16	0.45
4:B:24:PRO:HG3	4:B:204:GLY:HA2	1.98	0.45
5:C:118:THR:HG23	39:C:8504:HOH:O	2.15	0.45
22:T:32:ARG:HH12	22:T:38:ARG:HH12	1.64	0.45
23:U:47:ARG:HG2	39:U:4381:HOH:O	2.15	0.45
24:V:7:GLU:O	24:V:11:MET:HG3	2.16	0.45
25:W:110:GLN:NE2	25:W:110:GLN:HA	2.31	0.45
1:0:2415:A:O2'	16:N:29:SER:HB3	2.17	0.45
1:0:2421:G:H3'	1:0:2422:U:H5''	1.98	0.45
39:0:6804:HOH:O	3:A:205:GLY:HA3	2.16	0.45
3:A:94:LEU:HG	3:A:99:ILE:CD1	2.47	0.45
4:B:41:PHE:HA	4:B:79:MET:CE	2.46	0.45
4:B:294:TYR:HE2	39:B:9120:HOH:O	1.98	0.45
5:C:47:GLY:HA2	5:C:92:PRO:HB2	1.97	0.45
7:E:84:MET:HE2	7:E:133:VAL:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:134:ILE:HG22	11:I:135:GLU:N	2.31	0.45
14:L:57:VAL:O	14:L:57:VAL:HG12	2.17	0.45
20:R:119:VAL:O	20:R:119:VAL:HG12	2.16	0.45
1:O:1589:G:N2	1:O:1605:G:H1'	2.31	0.45
1:O:2781:U:H2'	1:O:2782:G:H5'	1.99	0.45
6:D:27:ILE:HD11	6:D:37:ALA:HB3	1.99	0.45
6:D:59:GLY:O	6:D:61:PHE:N	2.47	0.45
1:O:1205:U:H2'	1:O:1206:U:H5'	1.99	0.45
1:O:2112:A:H2'	1:O:2113:G:C8	2.52	0.45
2:9:28:U:H2'	2:9:29:C:C6	2.52	0.45
2:9:52:A:H2'	2:9:53:G:O4'	2.17	0.45
3:A:123:GLY:HA3	3:A:162:GLY:HA2	1.99	0.45
3:A:128:LEU:HG	39:A:9038:HOH:O	2.15	0.45
3:A:132:ASP:OD1	3:A:133:ARG:N	2.48	0.45
4:B:277:GLU:N	4:B:278:PRO:HD2	2.31	0.45
7:E:6:GLU:HA	7:E:46:THR:HG22	1.98	0.45
9:G:27:ILE:HD13	9:G:71:LEU:HD23	1.98	0.45
14:L:119:THR:HG23	14:L:139:SER:OG	2.17	0.45
15:M:81:ARG:HG3	15:M:85:ARG:HB2	1.98	0.45
16:N:37:ARG:CZ	39:N:8832:HOH:O	2.64	0.45
19:Q:11:ARG:NH1	39:Q:5620:HOH:O	2.49	0.45
24:V:12:THR:CG2	24:V:15:GLU:HG3	2.40	0.45
24:V:39:ALA:C	24:V:41:GLU:N	2.67	0.45
27:Y:174:VAL:O	27:Y:174:VAL:HG12	2.17	0.45
1:O:558:C:H5'	39:O:5710:HOH:O	2.16	0.45
1:O:820:G:C6	3:A:171:LYS:HB2	2.52	0.45
1:O:2032:U:H5'	39:O:4980:HOH:O	2.16	0.45
1:O:2064:U:H4'	1:O:2653:A:OP1	2.16	0.45
1:O:2421:G:H3'	1:O:2422:U:C5'	2.47	0.45
4:B:139:ASP:HB2	4:B:165:ARG:HE	1.82	0.45
4:B:304:PRO:HD2	4:B:307:ARG:NE	2.32	0.45
4:B:305:ASP:O	4:B:306:LYS:CB	2.62	0.45
6:D:63:ILE:HG13	6:D:64:ARG:N	2.32	0.45
10:H:50:ILE:HD12	10:H:149:VAL:CG1	2.47	0.45
15:M:99:ARG:HE	15:M:170:ASN:ND2	2.15	0.45
17:O:21:SER:OG	17:O:106:PRO:HB2	2.17	0.45
20:R:114:VAL:HA	20:R:144:GLU:O	2.16	0.45
22:T:45:GLY:C	39:T:3851:HOH:O	2.59	0.45
1:O:932:U:H2'	1:O:933:C:C6	2.52	0.45
1:O:1878:G:O2'	1:O:1879:U:P	2.75	0.45
1:O:1979:G:H2'	39:O:3782: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:O:2717:C:OP1	4:B:207:LYS:HG3	2.17	0.45
7:E:3:VAL:CG2	7:E:49:ILE:HB	2.42	0.45
14:L:10:SER:O	14:L:11:ARG:HB3	2.17	0.45
14:L:143:THR:CG2	14:L:144:ASP:N	2.77	0.45
16:N:72:GLU:H	16:N:171:HIS:HE1	1.65	0.45
18:P:16:VAL:CG1	18:P:20:ARG:HB2	2.46	0.45
1:O:1163:G:N2	39:O:5189:HOH:O	2.49	0.45
1:O:1406:A:H4'	1:O:1407:A:H5''	1.98	0.45
1:O:2649:A:H5'	1:O:2649:A:H8	1.81	0.45
1:O:2756:U:N3	1:O:2896:A:C2	2.75	0.45
2:9:24:U:H3'	2:9:25:G:H5'	1.98	0.45
5:C:107:ARG:NH2	39:C:8661:HOH:O	2.47	0.45
10:H:33:GLN:H	10:H:69:ARG:HH11	1.65	0.45
13:K:4:LEU:HD22	13:K:116:GLU:HB3	1.99	0.45
13:K:58:THR:HG22	13:K:59:LYS:HG3	1.99	0.45
14:L:67:ARG:HB2	14:L:112:GLY:HA3	1.98	0.45
16:N:61:ALA:CB	16:N:88:ALA:HB2	2.47	0.45
16:N:143:ARG:HA	16:N:172:PHE:CD2	2.52	0.45
20:R:29:LYS:HD3	39:R:8937:HOH:O	2.17	0.45
21:S:8:PRO:HD2	24:V:32:ALA:HA	1.99	0.45
1:O:951:A:O2'	1:O:952:G:H5'	2.17	0.45
1:O:1174:A:C5	1:O:1201:C:H4'	2.52	0.45
1:O:1943:C:H4'	3:A:211:LYS:O	2.16	0.45
1:O:1947:G:H2'	1:O:1948:G:C8	2.51	0.45
1:O:2852:A:H5''	39:O:5686:HOH:O	2.17	0.45
5:C:27:ARG:HG2	5:C:30:LEU:CD1	2.46	0.45
6:D:76:ARG:O	6:D:77:ASP:HB2	2.17	0.45
7:E:18:LEU:HD13	7:E:34:TRP:CG	2.52	0.45
9:G:67:LEU:O	9:G:71:LEU:HG	2.16	0.45
15:M:99:ARG:HH21	15:M:170:ASN:ND2	2.11	0.45
31:3:30:GLN:NE2	39:3:8980:HOH:O	2.45	0.45
31:3:42:ARG:HH11	31:3:42:ARG:HG3	1.81	0.45
1:O:1060:C:H6	1:O:1060:C:H5'	1.82	0.45
1:O:1592:G:O2'	1:O:1593:C:O4'	2.33	0.45
4:B:5:ARG:NH1	4:B:8:LYS:HE2	2.32	0.45
4:B:154:VAL:CG1	4:B:156:LYS:HG2	2.47	0.45
6:D:27:ILE:HD11	6:D:37:ALA:CB	2.47	0.45
7:E:126:ILE:HB	7:E:131:LEU:HD23	1.98	0.45
9:G:69:ARG:NH1	39:G:3513:HOH:O	2.50	0.45
10:H:149:VAL:HG13	39:H:9028:HOH:O	2.16	0.45
18:P:134:VAL:O	18:P:137:LEU:HB3	2.18	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:2:18:ASN:HD21	30:2:40:ARG:H	1.65	0.45
1:0:1007:A:H2'	10:H:22:TYR:CZ	2.52	0.44
1:0:1654:U:H2'	3:A:47:HIS:HD2	1.82	0.44
1:0:2361:A:H5''	39:0:9501:HOH:O	2.17	0.44
4:B:82:VAL:O	4:B:82:VAL:CG1	2.65	0.44
5:C:35:VAL:HG21	5:C:227:GLY:HA2	1.98	0.44
7:E:11:VAL:HG13	7:E:23:GLU:O	2.17	0.44
7:E:116:THR:CG2	7:E:151:LEU:HD22	2.45	0.44
8:F:48:VAL:HG23	8:F:74:PHE:CB	2.47	0.44
1:0:397:A:O2'	1:0:417:G:N3	2.49	0.44
1:0:969:G:H1	1:0:999:C:H42	1.65	0.44
1:0:2866:U:H4'	1:0:2867:G:H5'	1.98	0.44
3:A:192:VAL:HG12	3:A:207:GLN:CB	2.47	0.44
14:L:143:THR:HG21	39:L:8833:HOH:O	2.18	0.44
16:N:108:SER:HA	16:N:109:PRO:HD3	1.80	0.44
1:0:380:A:H2'	39:0:7660:HOH:O	2.16	0.44
1:0:634:G:O2'	1:0:1358:A:OP1	2.34	0.44
1:0:960:G:N3	1:0:960:G:C2'	2.80	0.44
1:0:1150:A:C2	9:G:20:VAL:HG21	2.52	0.44
1:0:1555:G:H4'	1:0:1630:A:H2	1.82	0.44
1:0:1755:A:H2'	1:0:1756:G:O4'	2.17	0.44
1:0:2256:G:C2'	1:0:2257:G:H5'	2.47	0.44
5:C:16:VAL:HG12	5:C:17:ASP:N	2.31	0.44
5:C:150:THR:HA	5:C:203:ALA:O	2.17	0.44
23:U:9:CYS:O	23:U:52:THR:HG23	2.16	0.44
25:W:52:VAL:HG22	25:W:53:ALA:H	1.82	0.44
1:0:204:A:C2'	1:0:205:U:H5'	2.48	0.44
1:0:524:A:C5'	20:R:29:LYS:HE2	2.47	0.44
1:0:2003:U:H4'	1:0:2004:U:H5	1.82	0.44
25:W:38:THR:HB	39:W:5390:HOH:O	2.17	0.44
1:0:308:U:C4	1:0:342:C:H1'	2.52	0.44
1:0:488:U:H2'	39:0:4480:HOH:O	2.17	0.44
1:0:2548:C:OP2	4:B:5:ARG:NH2	2.50	0.44
4:B:30:PRO:HB2	4:B:39:GLN:NE2	2.32	0.44
4:B:217:ARG:HG3	4:B:257:THR:CG2	2.48	0.44
5:C:236:THR:C	39:C:8653:HOH:O	2.60	0.44
1:0:2104:C:O2	1:0:2485:A:N1	2.51	0.44
1:0:2756:U:N3	1:0:2896:A:H2	2.13	0.44
2:9:50:G:H5''	16:N:159:TYR:HE1	1.83	0.44
4:B:232:TRP:CD1	4:B:235:ARG:HD2	2.53	0.44
5:C:46:TYR:CE2	5:C:98:ARG:NH1	2.86	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:74:ARG:HH12	12:J:76:ASP:CB	2.30	0.44
14:L:121:ILE:HG12	14:L:141:GLU:HB2	1.98	0.44
16:N:15:GLU:HB2	16:N:17:ARG:HG3	1.98	0.44
17:O:98:LEU:O	17:O:102:ILE:HG13	2.17	0.44
18:P:131:PHE:CD1	18:P:137:LEU:HD13	2.53	0.44
29:1:28:HIS:CD2	29:1:30:LYS:HB2	2.52	0.44
31:3:91:GLN:O	31:3:92:GLU:HB2	2.17	0.44
1:0:559:U:H2'	1:0:560:U:O4'	2.17	0.44
1:0:1131:G:C6	1:0:1230:A:C4	3.06	0.44
1:0:1137:G:H1'	39:0:4354:HOH:O	2.17	0.44
3:A:36:ASP:O	3:A:36:ASP:CG	2.61	0.44
3:A:153:ARG:HD3	39:A:8995:HOH:O	2.16	0.44
6:D:146:LYS:NZ	16:N:107:ASN:ND2	2.64	0.44
14:L:53:ARG:NH2	14:L:57:VAL:HG12	2.33	0.44
16:N:154:LEU:O	16:N:155:GLU:CB	2.66	0.44
20:R:39:THR:HB	20:R:42:GLU:CD	2.42	0.44
22:T:9:LYS:HE3	22:T:13:ARG:HH11	1.72	0.44
23:U:6:CYS:C	23:U:8:TYR:H	2.26	0.44
25:W:11:VAL:O	25:W:12:ASN:HB2	2.16	0.44
1:0:138:U:OP2	1:0:139:C:H5	2.00	0.44
1:0:1044:C:H3'	1:0:1045:G:H5''	1.99	0.44
1:0:2642:G:H2'	1:0:2643:G:O4'	2.18	0.44
1:0:2793:A:H2'	1:0:2794:G:H5'	1.99	0.44
2:9:57:A:C8	6:D:141:VAL:HG21	2.53	0.44
3:A:81:GLN:H	3:A:92:ASN:ND2	2.16	0.44
6:D:49:PRO:HA	6:D:73:VAL:HG22	1.98	0.44
8:F:46:GLU:N	39:F:3461:HOH:O	2.51	0.44
16:N:67:ALA:C	16:N:69:TYR:H	2.26	0.44
22:T:79:LEU:HG	22:T:89:ARG:HB2	1.98	0.44
1:0:1307:A:H2'	1:0:1308:A:C8	2.53	0.44
6:D:64:ARG:HG2	6:D:67:ASP:HB3	2.00	0.44
7:E:132:THR:HB	39:E:2227:HOH:O	2.17	0.44
11:I:76:ASP:C	11:I:78:ALA:H	2.26	0.44
12:J:90:LYS:HB2	36:J:8802:CL:CL	2.54	0.44
21:S:11:THR:H	21:S:14:ALA:HB3	1.81	0.44
26:X:25:ARG:CG	39:X:5356:HOH:O	2.65	0.44
31:3:75:GLY:C	39:3:9000:HOH:O	2.60	0.44
1:0:1119:G:C8	12:J:52:GLN:NE2	2.86	0.43
1:0:1181:A:N1	1:0:1192:A:O2'	2.50	0.43
1:0:1946:C:H2'	1:0:1971:G:C8	2.53	0.43
1:0:2524:G:H21	1:0:2526:C:N4	2.16	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:108:GLU:HB3	4:B:111:ARG:HD2	2.00	0.43
9:G:19:GLU:O	9:G:23:ILE:HG13	2.18	0.43
16:N:67:ALA:C	16:N:69:TYR:N	2.76	0.43
23:U:17:THR:HG21	39:U:3194:HOH:O	2.17	0.43
25:W:119:HIS:HD2	25:W:120:PRO:O	2.01	0.43
27:Y:95:THR:N	27:Y:236:VAL:O	2.51	0.43
1:0:392:U:C5'	15:M:193:LYS:HB3	2.49	0.43
1:0:432:G:O2'	1:0:433:C:H5'	2.18	0.43
1:0:559:U:H5'	1:0:559:U:C6	2.41	0.43
1:0:1252:A:H2'	1:0:1253:C:O4'	2.19	0.43
1:0:1393:A:H2'	1:0:1394:C:C6	2.53	0.43
3:A:223:ARG:NE	39:A:9037:HOH:O	2.51	0.43
4:B:51:VAL:HG23	4:B:327:VAL:HG13	1.98	0.43
15:M:59:GLY:C	15:M:141:ILE:HD11	2.43	0.43
27:Y:115:ARG:HB3	27:Y:115:ARG:HH11	1.83	0.43
1:0:1119:G:C6	1:0:1244:U:C5	3.06	0.43
1:0:1730:G:H5'	1:0:1731:C:H5	1.81	0.43
1:0:1733:A:H4'	4:B:212:GLN:HA	1.99	0.43
1:0:2864:U:O2'	1:0:2865:G:H5'	2.18	0.43
10:H:168:VAL:HG13	39:H:9009:HOH:O	2.17	0.43
12:J:107:ASN:HD22	12:J:108:PRO:N	2.16	0.43
14:L:145:LEU:HD23	14:L:145:LEU:C	2.43	0.43
25:W:13:MET:HE2	25:W:18:GLN:N	2.33	0.43
26:X:73:ARG:HB2	26:X:88:GLU:OE2	2.19	0.43
28:Z:19:GLY:O	28:Z:23:ARG:HG2	2.18	0.43
1:0:517:U:H1'	39:0:7997:HOH:O	2.18	0.43
1:0:542:A:H2'	1:0:543:G:O4'	2.18	0.43
1:0:2115:U:H2'	1:0:2116:U:C6	2.53	0.43
1:0:2526:C:C6	1:0:2526:C:H5'	2.53	0.43
3:A:70:ALA:HA	3:A:71:PRO:HD3	1.81	0.43
10:H:57:THR:O	10:H:58:VAL:HG13	2.19	0.43
11:I:67:VAL:CG1	11:I:68:PRO:HD2	2.48	0.43
13:K:113:ILE:CG2	13:K:114:ALA:N	2.81	0.43
15:M:59:GLY:HA3	15:M:141:ILE:CD1	2.49	0.43
21:S:20:PHE:N	21:S:20:PHE:CD2	2.85	0.43
1:0:284:C:H4'	1:0:285:A:H8	1.83	0.43
1:0:790:A:H2'	1:0:791:A:O4'	2.18	0.43
1:0:920:C:H5'	1:0:921:G:C4	2.53	0.43
1:0:2090:G:H2'	1:0:2091:G:C8	2.53	0.43
1:0:2326:C:H4'	1:0:2412:G:C4'	2.49	0.43
1:0:2649:A:H5'	1:0:2649:A:C8	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:45:VAL:HG22	12:J:46:ILE:N	2.33	0.43
14:L:122:ALA:HB3	14:L:125:PHE:CZ	2.54	0.43
16:N:73:ALA:N	39:N:8863:HOH:O	2.48	0.43
31:3:70:ARG:CG	31:3:77:ALA:HB2	2.47	0.43
1:0:130:C:H5'	39:0:5666:HOH:O	2.18	0.43
1:0:1484:G:H2'	39:0:9594:HOH:O	2.17	0.43
1:0:2121:G:O2'	1:0:2122:C:H5'	2.19	0.43
1:0:2819:C:H2'	1:0:2820:A:C8	2.53	0.43
1:0:2831:C:O3'	20:R:71:LYS:HE2	2.18	0.43
1:0:2868:C:H2'	1:0:2869:G:O4'	2.19	0.43
3:A:39:ALA:O	3:A:61:GLU:HG3	2.18	0.43
4:B:175:LEU:O	4:B:175:LEU:HD23	2.19	0.43
7:E:77:THR:OG1	7:E:78:GLU:N	2.51	0.43
13:K:28:GLU:HG2	13:K:58:THR:HB	2.00	0.43
16:N:77:ASN:OD1	16:N:80:SER:HB2	2.18	0.43
22:T:71:VAL:CG1	22:T:72:ILE:N	2.81	0.43
22:T:75:GLU:O	22:T:76:ASP:HB2	2.18	0.43
25:W:29:VAL:O	25:W:30:ASN:HB2	2.18	0.43
27:Y:107:PRO:HB3	27:Y:182:PHE:CD2	2.54	0.43
1:0:189:A:OP1	15:M:171:ARG:NH2	2.51	0.43
1:0:622:G:P	27:Y:148:GLY:HA3	2.58	0.43
1:0:920:C:H4'	1:0:921:G:C2	2.54	0.43
3:A:211:LYS:NZ	39:A:9082:HOH:O	2.49	0.43
5:C:235:PHE:HE2	5:C:243:VAL:HG21	1.84	0.43
7:E:93:MET:HE1	7:E:165:GLY:H	1.84	0.43
13:K:75:ARG:HD3	13:K:112:PRO:O	2.19	0.43
16:N:71:TRP:CE3	16:N:175:LEU:HD22	2.53	0.43
16:N:82:TYR:CD2	16:N:82:TYR:C	2.97	0.43
20:R:119:VAL:O	20:R:119:VAL:CG1	2.65	0.43
22:T:92:ASP:OD1	22:T:94:SER:HB3	2.19	0.43
1:0:137:U:OP1	1:0:259:G:O2'	2.35	0.43
1:0:512:G:O3'	1:0:513:A:H8	2.02	0.43
1:0:2031:C:H2'	1:0:2032:U:O4'	2.19	0.43
1:0:2256:G:O2'	1:0:2257:G:H5'	2.19	0.43
1:0:2372:A:H2'	1:0:2373:U:C6	2.54	0.43
3:A:125:ASN:CB	3:A:158:VAL:HG12	2.49	0.43
6:D:149:ARG:HH12	16:N:15:GLU:HA	1.84	0.43
15:M:164:THR:CG2	15:M:165:GLY:N	2.82	0.43
20:R:15:LYS:HE3	39:R:8984:HOH:O	2.18	0.43
1:0:1335:C:OP2	27:Y:207:SER:HB3	2.18	0.43
1:0:1853:C:O2'	3:A:217:ARG:NH2	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:2133:U:H4'	1:0:2134:G:C5'	2.48	0.43
1:0:2326:C:H4'	1:0:2412:G:H4'	2.01	0.43
1:0:2403:C:OP1	19:Q:49:ASN:HB3	2.19	0.43
4:B:40:GLY:HA3	39:B:9118:HOH:O	2.19	0.43
4:B:41:PHE:CZ	4:B:79:MET:HG3	2.54	0.43
4:B:53:LEU:HD11	4:B:327:VAL:HG22	2.01	0.43
5:C:166:ILE:HD11	5:C:207:LEU:HD13	2.01	0.43
7:E:86:VAL:CG1	7:E:129:GLU:HA	2.49	0.43
13:K:66:ARG:HG2	13:K:66:ARG:HH11	1.84	0.43
16:N:89:GLY:O	16:N:92:ALA:HB3	2.18	0.43
1:0:944:G:C8	25:W:23:MET:HE1	2.54	0.43
1:0:1158:G:O2'	1:0:1159:G:H5'	2.19	0.43
1:0:1185:U:H5'	39:0:7891:HOH:O	2.18	0.43
1:0:2103:A:O2'	1:0:2104:C:H5'	2.19	0.43
3:A:186:TRP:CG	3:A:187:PRO:HA	2.54	0.43
4:B:79:MET:HE1	39:B:9094:HOH:O	2.18	0.43
4:B:314:ALA:CB	4:B:317:PRO:HG3	2.49	0.43
6:D:20:LYS:HA	6:D:75:LEU:O	2.19	0.43
8:F:60:VAL:O	8:F:60:VAL:HG12	2.19	0.43
10:H:157:TYR:CD1	10:H:157:TYR:C	2.97	0.43
15:M:99:ARG:CD	15:M:167:GLY:HA2	2.49	0.43
19:Q:55:ARG:HD2	39:Q:2875:HOH:O	2.19	0.43
21:S:57:THR:HG22	21:S:59:ASP:HB2	2.01	0.43
22:T:18:GLU:O	22:T:21:LYS:HG2	2.19	0.43
1:0:56:G:H5''	24:V:50:ARG:NH1	2.33	0.42
1:0:263:U:C2	8:F:59:ILE:CD1	3.02	0.42
1:0:451:C:O2'	1:0:452:G:H5'	2.19	0.42
1:0:524:A:H5'	20:R:29:LYS:HE2	2.01	0.42
1:0:1218:U:H2'	1:0:1219:U:C6	2.53	0.42
1:0:1768:C:H2'	1:0:1769:C:O4'	2.19	0.42
1:0:2316:G:H4'	39:0:6539:HOH:O	2.18	0.42
1:0:2768:A:O2'	1:0:2769:C:H5'	2.19	0.42
2:9:56:A:C3'	2:9:57:A:H5''	2.48	0.42
7:E:15:GLN:HG3	7:E:20:ILE:HG12	2.00	0.42
7:E:22:VAL:O	7:E:28:SER:HA	2.19	0.42
8:F:111:ILE:O	8:F:115:VAL:HG23	2.18	0.42
11:I:88:GLN:HA	11:I:91:PHE:HE2	1.84	0.42
16:N:143:ARG:HH12	16:N:173:ASP:CG	2.27	0.42
1:0:241:A:C2	1:0:378:A:H4'	2.54	0.42
1:0:567:U:H5''	39:0:5740:HOH:O	2.19	0.42
1:0:1165:G:H4'	1:0:1174:A:HO2'	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1202:A:H2'	1:0:1203:G:O4'	2.19	0.42
1:0:2630:G:O6	3:A:206:ARG:NH2	2.49	0.42
3:A:37:VAL:HG22	39:A:9059:HOH:O	2.19	0.42
3:A:107:ASN:OD1	3:A:120:ARG:HD2	2.19	0.42
3:A:135:VAL:N	39:A:9058:HOH:O	2.51	0.42
6:D:37:ALA:HA	39:D:5583:HOH:O	2.19	0.42
8:F:32:GLY:N	39:F:3111:HOH:O	2.52	0.42
17:O:32:ARG:HH21	17:O:35:LYS:HD2	1.84	0.42
18:P:59:ARG:HD3	39:P:191:HOH:O	2.19	0.42
18:P:64:GLU:HG2	39:P:167:HOH:O	2.18	0.42
22:T:112:LEU:CD2	22:T:119:ALA:HB3	2.49	0.42
28:Z:22:SER:O	28:Z:26:VAL:HG23	2.19	0.42
1:0:1287:A:O4'	25:W:117:ARG:HD3	2.20	0.42
1:0:1439:C:OP1	30:2:41:HIS:HE1	2.03	0.42
1:0:1573:A:H2'	1:0:1574:C:O4'	2.19	0.42
1:0:1846:U:O2'	3:A:172:ALA:HB2	2.19	0.42
1:0:2718:C:H5'	1:0:2718:C:C6	2.51	0.42
7:E:88:TYR:CD1	7:E:88:TYR:C	2.96	0.42
15:M:15:PRO:HA	15:M:20:LEU:HD23	2.01	0.42
16:N:37:ARG:NH2	39:N:8832:HOH:O	2.52	0.42
20:R:61:GLN:NE2	39:R:8944:HOH:O	2.53	0.42
25:W:3:ALA:O	25:W:54:PHE:HA	2.19	0.42
25:W:35:VAL:HG23	25:W:41:TYR:CD2	2.54	0.42
26:X:43:VAL:HG12	26:X:44:ASP:H	1.84	0.42
27:Y:184:GLU:CD	27:Y:204:ARG:HH11	2.27	0.42
1:0:903:U:OP2	14:L:11:ARG:NH1	2.50	0.42
1:0:926:A:O2'	14:L:41:HIS:HD2	2.01	0.42
1:0:1029:U:H5'	1:0:1031:G:N7	2.34	0.42
1:0:1066:U:H2'	1:0:1067:A:C8	2.54	0.42
1:0:1562:C:N4	39:0:6317:HOH:O	2.34	0.42
1:0:1948:G:H2'	1:0:1949:G:O4'	2.20	0.42
1:0:2353:A:H4'	1:0:2354:A:O5'	2.18	0.42
39:0:6168:HOH:O	13:K:87:ARG:NE	2.52	0.42
3:A:175:LYS:HE2	39:A:9040:HOH:O	2.19	0.42
5:C:246:ARG:NH2	39:C:8630:HOH:O	2.46	0.42
7:E:107:PHE:CZ	7:E:108:LEU:HD13	2.54	0.42
8:F:38:LYS:HZ1	15:M:3:SER:HA	1.84	0.42
22:T:48:VAL:HG22	22:T:97:ARG:C	2.44	0.42
1:0:392:U:H5''	15:M:193:LYS:HB3	2.01	0.42
1:0:646:G:H2'	1:0:647:U:C6	2.54	0.42
1:0:669:G:O2'	1:0:670:G:H5'	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:0:1845:A:O3'	3:A:187:PRO:HB2	2.19	0.42
1:0:1940:C:H4'	39:0:7777:HOH:O	2.18	0.42
1:0:2478:U:O2'	1:0:2479:A:H5'	2.19	0.42
1:0:2676:C:H4'	12:J:70:PHE:CD1	2.54	0.42
3:A:217:ARG:HH11	3:A:217:ARG:CG	2.33	0.42
4:B:36:PRO:CA	4:B:168:GLY:HA3	2.43	0.42
4:B:139:ASP:HB2	39:B:8998:HOH:O	2.18	0.42
4:B:162:MET:HG3	4:B:310:ARG:HD3	2.01	0.42
5:C:133:ARG:NE	5:C:138:VAL:HG22	2.34	0.42
5:C:236:THR:O	5:C:237:GLU:C	2.63	0.42
10:H:66:GLU:O	10:H:70:LEU:HB2	2.20	0.42
15:M:152:ALA:HB1	39:M:8934:HOH:O	2.20	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CE2	2.55	0.42
1:0:1406:A:H4'	1:0:1407:A:C5'	2.50	0.42
1:0:1500:U:OP2	18:P:41:ARG:NH2	2.53	0.42
1:0:1626:A:H2'	1:0:1627:G:O4'	2.19	0.42
1:0:1925:G:O2'	1:0:1926:G:H5'	2.20	0.42
1:0:2781:U:C2'	1:0:2782:G:H5'	2.49	0.42
2:9:59:C:O5'	2:9:59:C:H6	2.02	0.42
7:E:43:ASP:HA	39:E:5864:HOH:O	2.18	0.42
8:F:99:THR:HG23	8:F:99:THR:O	2.20	0.42
9:G:64:ASN:N	9:G:64:ASN:ND2	2.68	0.42
12:J:26:VAL:HG13	12:J:36:VAL:HG11	2.01	0.42
14:L:92:ASP:HB3	14:L:95:ASP:OD2	2.19	0.42
21:S:57:THR:CG2	21:S:59:ASP:HB2	2.50	0.42
23:U:13:ILE:HG12	23:U:32:CYS:HB3	2.00	0.42
26:X:41:PHE:O	26:X:43:VAL:HG23	2.19	0.42
27:Y:189:ASN:C	27:Y:189:ASN:ND2	2.77	0.42
31:3:20:HIS:HA	31:3:70:ARG:O	2.19	0.42
1:0:2442:G:H3'	39:0:7065:HOH:O	2.19	0.42
1:0:2754:G:H2'	1:0:2755:G:O4'	2.19	0.42
4:B:41:PHE:HB3	4:B:190:MET:HE1	2.01	0.42
12:J:71:TYR:CD1	12:J:72:PRO:HD2	2.54	0.42
21:S:56:ASN:O	30:2:8:LYS:NZ	2.47	0.42
22:T:47:THR:HB	22:T:100:ASP:HB3	2.02	0.42
25:W:107:LEU:O	25:W:112:LEU:HB2	2.18	0.42
31:3:11:CYS:HB2	31:3:20:HIS:CE1	2.55	0.42
1:0:926:A:O2'	14:L:41:HIS:CD2	2.73	0.42
1:0:962:C:H1'	16:N:5:ARG:HH12	1.79	0.42
1:0:1902:G:H2'	1:0:1903:U:O4'	2.20	0.42
1:0:2401:A:H2'	1:0:2402:A:C8	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:23:ASN:HD21	13:K:107:THR:HB	1.83	0.42
14:L:6:ARG:NH2	39:L:8842:HOH:O	2.47	0.42
17:O:41:ALA:HA	39:O:5104:HOH:O	2.19	0.42
23:U:45:GLU:HB2	23:U:48:ASN:ND2	2.35	0.42
24:V:60:GLN:O	24:V:65:ASP:N	2.52	0.42
25:W:19:ASP:O	25:W:23:MET:HG3	2.20	0.42
27:Y:99:ALA:HB2	27:Y:233:TYR:CZ	2.54	0.42
1:0:441:A:H1'	1:0:442:A:N7	2.35	0.42
1:0:635:A:H2'	1:0:636:G:H5''	2.01	0.42
1:0:1162:G:H1'	11:I:112:LEU:CD1	2.49	0.42
1:0:2072:G:H3'	1:0:2073:G:C5'	2.50	0.42
1:0:2578:G:H5'	1:0:2578:G:C8	2.51	0.42
2:9:42:C:O2	6:D:76:ARG:NH1	2.53	0.42
3:A:135:VAL:HG11	3:A:147:ARG:NH1	2.35	0.42
5:C:78:ARG:NH1	5:C:78:ARG:CG	2.74	0.42
5:C:219:ASN:N	5:C:222:ASP:OD1	2.52	0.42
5:C:219:ASN:O	5:C:222:ASP:OD1	2.37	0.42
6:D:25:MET:HE1	6:D:37:ALA:O	2.19	0.42
16:N:140:GLN:O	16:N:143:ARG:HB2	2.19	0.42
22:T:96:VAL:HG13	22:T:97:ARG:N	2.35	0.42
27:Y:117:LEU:HD12	27:Y:174:VAL:HG11	2.02	0.42
31:3:31:THR:HB	31:3:33:MET:HE3	2.02	0.42
1:0:214:U:H5'	39:0:6586:HOH:O	2.19	0.42
1:0:1209:C:H2'	1:0:1210:G:C8	2.51	0.42
1:0:1684:A:O2'	1:0:1685:A:H5''	2.19	0.42
4:B:248:ARG:NH2	39:B:8993:HOH:O	2.50	0.42
7:E:24:GLY:HA3	7:E:76:VAL:HB	2.02	0.42
8:F:24:ARG:NH2	39:F:6800:HOH:O	2.48	0.42
11:I:127:CYS:C	11:I:129:SER:N	2.77	0.42
12:J:46:ILE:HD11	12:J:53:ILE:HG23	2.01	0.42
15:M:5:TYR:HE2	15:M:46:LEU:HD13	1.84	0.42
15:M:145:ASP:HA	39:M:8909:HOH:O	2.19	0.42
18:P:10:ALA:CA	18:P:13:VAL:HG12	2.46	0.42
1:0:304:G:H1'	1:0:347:A:H61	1.85	0.41
1:0:482:G:H4'	1:0:508:A:N1	2.35	0.41
1:0:776:A:H1'	1:0:779:U:O4	2.20	0.41
1:0:1754:A:H2'	1:0:1755:A:O4'	2.20	0.41
3:A:105:VAL:CG1	3:A:106:CYS:N	2.82	0.41
3:A:206:ARG:NH1	39:A:8979:HOH:O	2.53	0.41
4:B:132:HIS:CE1	4:B:171:VAL:HG21	2.55	0.41
5:C:138:VAL:O	5:C:234:VAL:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:G:24:VAL:O	9:G:28:GLU:HB2	2.19	0.41
11:I:109:PRO:HG2	11:I:110:ASP:H	1.84	0.41
11:I:127:CYS:C	11:I:129:SER:H	2.28	0.41
21:S:42:GLU:HG2	21:S:49:VAL:HG23	2.01	0.41
30:2:36:ASN:HB3	30:2:39:ARG:HG3	2.00	0.41
1:0:383:A:H2'	1:0:384:G:O4'	2.20	0.41
1:0:1197:G:N2	39:0:6679:HOH:O	2.52	0.41
1:0:1236:A:C8	12:J:63:ILE:HD11	2.55	0.41
1:0:1762:C:H4'	39:0:5120:HOH:O	2.21	0.41
1:0:2252:A:C5	1:0:2253:G:H1'	2.54	0.41
1:0:2336:G:H1'	39:D:5675:HOH:O	2.19	0.41
1:0:2503:A:OP1	10:H:154:ARG:NH2	2.47	0.41
1:0:2756:U:C2	1:0:2896:A:H2	2.37	0.41
5:C:127:ARG:HG2	5:C:127:ARG:HH11	1.84	0.41
5:C:246:ARG:NH1	5:C:246:ARG:HB3	2.35	0.41
10:H:72:ALA:HB2	10:H:156:ALA:HB2	2.02	0.41
10:H:154:ARG:HA	10:H:157:TYR:CE2	2.55	0.41
15:M:99:ARG:NH2	15:M:170:ASN:HD22	2.15	0.41
18:P:63:ARG:NH2	39:P:191:HOH:O	2.51	0.41
20:R:114:VAL:HG13	20:R:114:VAL:O	2.20	0.41
25:W:146:ILE:HD13	25:W:146:ILE:HA	1.89	0.41
1:0:1657:A:H2'	1:0:1658:A:C8	2.55	0.41
1:0:1730:G:H5''	1:0:1731:C:C6	2.54	0.41
1:0:1980:U:O2	1:0:2008:U:H4'	2.20	0.41
1:0:2726:U:O2	1:0:2749:U:O5'	2.38	0.41
3:A:129:LEU:C	39:A:9038:HOH:O	2.63	0.41
3:A:211:LYS:HD2	39:A:9081:HOH:O	2.21	0.41
4:B:189:ALA:HB1	39:B:9033:HOH:O	2.19	0.41
10:H:24:THR:O	10:H:123:ILE:HD12	2.20	0.41
10:H:146:ALA:O	10:H:149:VAL:HG12	2.20	0.41
11:I:129:SER:N	39:I:7330:HOH:O	2.47	0.41
12:J:42:GLU:O	12:J:131:THR:HG23	2.19	0.41
16:N:154:LEU:HG	16:N:155:GLU:N	2.35	0.41
1:0:827:A:H2'	1:0:828:G:O4'	2.19	0.41
1:0:1118:A:C8	1:0:1119:G:H5''	2.54	0.41
1:0:1181:A:H2'	1:0:1182:C:C5'	2.50	0.41
1:0:2415:A:N3	16:N:26:LEU:HD13	2.36	0.41
1:0:2547:C:OP2	4:B:5:ARG:NH1	2.53	0.41
4:B:54:VAL:O	4:B:55:ASN:C	2.63	0.41
5:C:118:THR:HG22	5:C:137:PRO:HB3	2.03	0.41
7:E:81:GLU:HA	7:E:133:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:K:78:LYS:HA	13:K:79:PRO:HD3	1.90	0.41
26:X:66:THR:CG2	26:X:67:PRO:HD2	2.48	0.41
1:0:1654:U:H2'	3:A:47:HIS:CD2	2.56	0.41
1:0:1739:G:O2'	1:0:1740:U:H5'	2.20	0.41
1:0:2241:C:O2'	1:0:2242:U:H5'	2.20	0.41
1:0:2416:G:O2'	16:N:25:ARG:HG2	2.19	0.41
6:D:10:PHE:N	39:D:7345:HOH:O	2.53	0.41
8:F:28:ALA:CB	8:F:99:THR:HG23	2.50	0.41
11:I:111:LEU:HD22	11:I:122:GLU:OE1	2.21	0.41
15:M:49:ALA:C	15:M:54:TYR:HB3	2.45	0.41
15:M:169:ARG:NH2	39:M:8852:HOH:O	2.47	0.41
16:N:39:SER:HB3	16:N:42:HIS:H	1.86	0.41
20:R:18:LEU:HG	20:R:91:LEU:HD13	2.03	0.41
21:S:51:GLN:NE2	21:S:53:ASN:HD21	2.13	0.41
1:0:88:G:H2'	1:0:89:G:C8	2.55	0.41
1:0:249:G:O2'	1:0:250:C:H5'	2.21	0.41
1:0:329:A:OP2	5:C:206:ASN:HB2	2.20	0.41
1:0:660:A:H4'	1:0:661:G:O5'	2.20	0.41
1:0:702:G:O2'	1:0:703:G:H5'	2.21	0.41
1:0:2543:G:H2'	1:0:2544:G:O4'	2.20	0.41
3:A:114:ASP:C	3:A:114:ASP:OD1	2.63	0.41
4:B:57:GLU:HA	4:B:58:PRO:HD2	1.96	0.41
5:C:154:VAL:O	5:C:158:GLU:HG3	2.21	0.41
7:E:16:ASP:O	7:E:17:HIS:HB2	2.19	0.41
10:H:151:GLU:OE1	10:H:151:GLU:HA	2.21	0.41
24:V:12:THR:CG2	24:V:15:GLU:H	2.34	0.41
30:2:19:SER:O	30:2:36:ASN:ND2	2.54	0.41
1:0:256:C:H2'	1:0:257:G:O4'	2.21	0.41
1:0:1352:A:H4'	1:0:1353:C:OP2	2.20	0.41
1:0:1596:U:H2'	1:0:1598:A:OP2	2.20	0.41
1:0:2054:A:H2	20:R:128:ARG:HH22	1.56	0.41
1:0:2498:C:O2'	1:0:2499:U:H5'	2.20	0.41
1:0:2724:U:H2'	1:0:2725:G:O4'	2.20	0.41
4:B:14:GLY:HA3	39:B:9076:HOH:O	2.21	0.41
5:C:57:PRO:HG2	5:C:73:LEU:HD13	2.02	0.41
5:C:136:VAL:HA	5:C:137:PRO:C	2.45	0.41
7:E:137:ASP:OD1	7:E:137:ASP:C	2.64	0.41
10:H:49:GLN:OE1	10:H:169:GLU:HB3	2.21	0.41
11:I:103:ILE:O	11:I:103:ILE:HG22	2.20	0.41
12:J:64:GLY:HA3	36:J:8821:CL:CL	2.58	0.41
14:L:38:HIS:CD2	14:L:39:GLU:HG3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:134:ILE:O	15:M:136:PRO:HD3	2.21	0.41
22:T:3:GLN:HA	22:T:4:PRO:HD3	1.82	0.41
22:T:41:ARG:NH1	22:T:42:VAL:O	2.53	0.41
30:2:36:ASN:C	30:2:38:LYS:H	2.27	0.41
1:0:23:G:C6	1:0:24:G:N1	2.89	0.41
1:0:95:A:H5''	1:0:97:G:O4'	2.21	0.41
1:0:1165:G:H1'	1:0:1174:A:H1'	2.03	0.41
1:0:2906:A:H5'	1:0:2907:C:O4'	2.21	0.41
8:F:5:ASP:O	8:F:119:ARG:NH1	2.53	0.41
8:F:117:GLU:C	8:F:119:ARG:N	2.78	0.41
15:M:184:ARG:HG3	15:M:185:PRO:HA	2.03	0.41
22:T:71:VAL:CG1	22:T:90:PRO:HB3	2.30	0.41
22:T:106:GLU:HG3	39:T:4913:HOH:O	2.21	0.41
1:0:64:G:H2'	1:0:65:C:O4'	2.21	0.41
1:0:222:A:H2'	1:0:223:G:O4'	2.20	0.41
1:0:366:U:H2'	1:0:367:G:O4'	2.20	0.41
1:0:522:U:O2'	1:0:1366:C:H5'	2.20	0.41
1:0:553:G:O2'	27:Y:179:PRO:HG3	2.21	0.41
1:0:958:G:H2'	1:0:959:C:C6	2.55	0.41
1:0:1098:A:H2'	1:0:1099:G:O4'	2.21	0.41
1:0:1976:G:O2'	1:0:1977:U:H5'	2.21	0.41
1:0:2089:A:C2'	1:0:2090:G:H5'	2.51	0.41
1:0:2515:C:H2'	1:0:2516:G:O4'	2.20	0.41
1:0:2559:C:H4'	39:0:7688:HOH:O	2.20	0.41
1:0:2740:G:H2'	1:0:2741:A:O4'	2.21	0.41
1:0:2883:A:H2'	1:0:2884:G:O4'	2.21	0.41
1:0:2884:G:H5'	39:0:4600:HOH:O	2.20	0.41
39:0:4461:HOH:O	22:T:82:THR:HA	2.21	0.41
39:0:5740:HOH:O	25:W:122:ARG:CZ	2.68	0.41
2:9:4:G:H21	16:N:44:ARG:NH1	2.19	0.41
3:A:36:ASP:CB	3:A:85:SER:H	2.34	0.41
4:B:42:ALA:HB2	4:B:162:MET:HE2	2.03	0.41
6:D:170:TYR:CD1	6:D:170:TYR:N	2.89	0.41
6:D:173:GLU:HG3	6:D:174:VAL:N	2.35	0.41
8:F:33:THR:HG21	8:F:59:ILE:O	2.20	0.41
12:J:75:PRO:HB3	12:J:132:LEU:HB3	2.02	0.41
13:K:28:GLU:OE2	13:K:58:THR:HG21	2.20	0.41
13:K:109:LEU:CD1	13:K:113:ILE:HD11	2.48	0.41
14:L:12:THR:O	14:L:13:HIS:C	2.63	0.41
15:M:42:ARG:HA	15:M:43:PRO:HD3	1.91	0.41
15:M:46:LEU:HG	39:M:8917:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:M:61:ILE:HD12	15:M:61:ILE:N	2.35	0.41
15:M:69:LYS:HG3	15:M:126:GLN:CA	2.51	0.41
16:N:49:THR:HG22	16:N:56:ASP:CB	2.49	0.41
16:N:103:ASP:OD1	16:N:103:ASP:C	2.64	0.41
17:O:14:LEU:HG	17:O:102:ILE:HD11	2.03	0.41
20:R:33:ARG:NH1	39:R:8947:HOH:O	2.37	0.41
22:T:48:VAL:CG2	22:T:96:VAL:HG13	2.51	0.41
26:X:10:VAL:HG12	26:X:11:THR:N	2.35	0.41
26:X:23:HIS:CD2	26:X:24:LYS:HG3	2.56	0.41
26:X:30:MET:HE1	26:X:58:ALA:CB	2.40	0.41
26:X:74:ALA:HB1	26:X:85:VAL:HG22	2.03	0.41
29:1:28:HIS:O	29:1:32:LYS:N	2.47	0.41
1:0:155:C:OP2	15:M:188:ARG:HD3	2.20	0.41
1:0:612:U:H2'	1:0:613:C:C6	2.56	0.41
1:0:1249:U:H2'	1:0:1250:C:C6	2.56	0.41
1:0:1299:G:N2	39:0:5149:HOH:O	2.54	0.41
1:0:2015:A:H2'	1:0:2016:U:O4'	2.20	0.41
3:A:81:GLN:CB	3:A:92:ASN:ND2	2.84	0.41
4:B:26:PHE:CE1	4:B:310:ARG:HB3	2.56	0.41
6:D:49:PRO:HB3	39:D:5828:HOH:O	2.21	0.41
10:H:32:ALA:C	10:H:33:GLN:HG3	2.45	0.41
14:L:67:ARG:HG2	14:L:67:ARG:HH11	1.86	0.41
16:N:73:ALA:HB1	16:N:74:PRO:CD	2.50	0.41
20:R:96:VAL:HG13	20:R:106:GLY:HA3	2.03	0.41
24:V:51:LYS:O	24:V:55:ARG:HG3	2.21	0.41
26:X:43:VAL:HG12	26:X:47:ALA:HB3	2.02	0.41
1:0:447:A:O2'	1:0:448:G:H5'	2.22	0.40
1:0:1268:C:O2'	1:0:1269:G:H5'	2.20	0.40
1:0:1328:A:C8	27:Y:169:ARG:HD3	2.56	0.40
1:0:1773:G:C8	28:Z:16:ALA:HA	2.55	0.40
1:0:2382:A:H5'	39:3:8962:HOH:O	2.21	0.40
3:A:179:MET:HG2	3:A:186:TRP:HB2	2.01	0.40
6:D:99:ASP:N	6:D:103:ASN:O	2.30	0.40
10:H:61:ARG:NH1	10:H:61:ARG:HG3	2.36	0.40
11:I:66:GLY:O	11:I:67:VAL:C	2.63	0.40
11:I:95:LEU:HG	11:I:132:VAL:CG1	2.51	0.40
13:K:98:VAL:HG13	13:K:102:GLU:CA	2.46	0.40
18:P:40:VAL:O	18:P:44:VAL:HG23	2.21	0.40
22:T:48:VAL:HG23	22:T:98:VAL:HA	2.03	0.40
26:X:12:ILE:HD12	26:X:36:HIS:ND1	2.36	0.40
1:0:655:U:O2'	17:O:3:THR:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:254:GLN:NE2	39:B:9058:HOH:O	2.54	0.40
4:B:310:ARG:HD2	39:B:9057:HOH:O	2.20	0.40
6:D:88:LEU:C	6:D:90:LEU:H	2.28	0.40
7:E:32:ARG:O	7:E:33:LEU:HD23	2.21	0.40
8:F:8:VAL:HG13	8:F:12:LEU:HD13	2.02	0.40
9:G:12:ILE:N	9:G:13:PRO:CD	2.84	0.40
10:H:6:ALA:CB	10:H:61:ARG:HH12	2.33	0.40
12:J:46:ILE:HD11	12:J:53:ILE:CG2	2.51	0.40
22:T:49:GLU:OE2	22:T:51:LEU:HD21	2.21	0.40
29:1:37:CYS:SG	29:1:39:PHE:HB2	2.61	0.40
30:2:18:ASN:ND2	30:2:40:ARG:H	2.19	0.40
1:0:59:A:H5'	39:0:4798:HOH:O	2.20	0.40
1:0:1072:G:OP2	27:Y:154:ARG:NH2	2.54	0.40
1:0:1304:U:H2'	1:0:1305:C:C6	2.56	0.40
1:0:1398:G:H2'	1:0:1399:A:C8	2.56	0.40
8:F:52:GLU:HG3	8:F:77:VAL:O	2.21	0.40
16:N:51:GLY:HA2	16:N:52:PRO:HD3	1.94	0.40
16:N:129:ILE:HA	16:N:130:PRO:HD3	1.98	0.40
24:V:8:ILE:HG21	24:V:59:ILE:HG13	2.02	0.40
27:Y:108:ASP:OD1	27:Y:108:ASP:N	2.53	0.40
1:0:861:A:H4'	1:0:1697:G:H4'	2.03	0.40
1:0:1020:A:H1'	39:Q:6976:HOH:O	2.22	0.40
1:0:1186:C:H4'	11:I:114:TYR:HE1	1.87	0.40
1:0:2445:U:H2'	1:0:2446:G:C8	2.56	0.40
6:D:38:GLU:HB3	6:D:49:PRO:HG3	2.02	0.40
6:D:138:GLY:N	39:D:7597:HOH:O	2.29	0.40
7:E:139:GLU:CD	39:E:5919:HOH:O	2.64	0.40
8:F:107:ASP:O	8:F:111:ILE:HG13	2.21	0.40
13:K:99:ASP:OD1	13:K:101:ASN:N	2.53	0.40
16:N:72:GLU:H	16:N:171:HIS:CE1	2.39	0.40
16:N:86:LEU:HD12	16:N:125:ALA:HB2	2.04	0.40
21:S:57:THR:C	21:S:59:ASP:H	2.30	0.40
1:0:212:A:O4'	1:0:214:U:C6	2.75	0.40
1:0:278:A:H2'	1:0:279:C:O4'	2.21	0.40
1:0:820:G:C5	3:A:171:LYS:HB2	2.57	0.40
1:0:1039:G:H2'	1:0:1040:A:O4'	2.22	0.40
1:0:1829:A:H2'	1:0:1830:C:H5'	2.04	0.40
1:0:2435:U:OP1	31:3:28:GLY:HA3	2.20	0.40
1:0:2900:G:H2'	1:0:2901:C:O4'	2.22	0.40
39:0:4832:HOH:O	3:A:212:PRO:HB2	2.20	0.40
2:9:31:C:H2'	2:9:32:G:O4'	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:9:114:G:H2'	2:9:115:C:C6	2.57	0.40
5:C:6:TYR:HE1	5:C:133:ARG:HH22	1.68	0.40
10:H:33:GLN:H	10:H:69:ARG:NH1	2.19	0.40
16:N:38:LYS:HE3	16:N:38:LYS:HB2	1.80	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	
3	A	235/240 (98%)	218 (93%)	13 (6%)	4 (2%)	7	10
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	5	7
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/177 (76%)	103 (77%)	20 (15%)	11 (8%)	0	0
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	4	4
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	143 (92%)	13 (8%)	0	100	100
11	I	68/162 (42%)	49 (72%)	17 (25%)	2 (3%)	3	3
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	9	13
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	18	28
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	4	4
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	14	22
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	2	1
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	14
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	2	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	4	5
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	10	16

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
3	A	37	VAL
6	D	171	ASP
8	F	101	ALA
12	J	5	GLU
14	L	80	ASP
16	N	154	LEU
16	N	183	ASP
16	N	184	ILE
24	V	43	PRO
28	Z	81	ARG
4	B	139	ASP
6	D	27	ILE
6	D	56	ARG
6	D	65	GLU
6	D	173	GLU
12	J	143	LYS
22	T	53	GLY
25	W	77	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	Z	42	CYS
3	A	34	ASP
4	B	34	GLY
4	B	169	GLY
4	B	185	GLY
6	D	61	PHE
6	D	97	GLN
11	I	91	PHE
16	N	164	ASP
6	D	16	PRO
6	D	60	GLU
8	F	100	ASP
16	N	139	TRP
4	B	2	GLN
4	B	107	SER
4	B	184	ASP
6	D	28	GLY
25	W	49	ASN
28	Z	41	ASN
30	2	37	HIS
3	A	132	ASP
8	F	71	GLY
11	I	109	PRO
24	V	40	PRO
6	D	69	ILE
24	V	39	ALA

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	
3	A	179/182 (98%)	168 (94%)	11 (6%)	17	30
4	B	282/283 (100%)	267 (95%)	15 (5%)	20	36
5	C	193/193 (100%)	174 (90%)	19 (10%)	7	12
6	D	117/148 (79%)	113 (97%)	4 (3%)	32	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	E	152/156 (97%)	148 (97%)	4 (3%)	40	63
8	F	93/94 (99%)	91 (98%)	2 (2%)	45	67
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	30	51
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	111 (94%)	7 (6%)	18	31
13	K	106/106 (100%)	105 (99%)	1 (1%)	70	85
14	L	113/127 (89%)	109 (96%)	4 (4%)	32	53
15	M	158/158 (100%)	153 (97%)	5 (3%)	34	56
16	N	149/150 (99%)	144 (97%)	5 (3%)	32	54
17	O	93/94 (99%)	91 (98%)	2 (2%)	45	67
18	P	113/117 (97%)	110 (97%)	3 (3%)	39	62
19	Q	79/80 (99%)	76 (96%)	3 (4%)	29	49
20	R	117/122 (96%)	115 (98%)	2 (2%)	53	74
21	S	71/74 (96%)	70 (99%)	1 (1%)	59	79
22	T	105/106 (99%)	100 (95%)	5 (5%)	23	40
23	U	44/52 (85%)	43 (98%)	1 (2%)	44	66
24	V	51/57 (90%)	49 (96%)	2 (4%)	28	48
25	W	130/130 (100%)	124 (95%)	6 (5%)	24	41
26	X	66/74 (89%)	60 (91%)	6 (9%)	9	14
27	Y	120/196 (61%)	111 (92%)	9 (8%)	12	21
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	28	47

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	26	ASP
3	A	33	GLU
3	A	36	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	55	VAL
3	A	94	LEU
3	A	131	HIS
3	A	153	ARG
3	A	165	THR
3	A	175	LYS
3	A	179	MET
3	A	217	ARG
4	B	7	ARG
4	B	11	LEU
4	B	27	ASN
4	B	49	THR
4	B	53	LEU
4	B	71	VAL
4	B	98	THR
4	B	162	MET
4	B	174	ARG
4	B	175	LEU
4	B	195	ARG
4	B	254	GLN
4	B	256	GLN
4	B	264	GLU
4	B	312	ARG
5	C	2	GLN
5	C	16	VAL
5	C	27	ARG
5	C	67	GLN
5	C	76	ARG
5	C	78	ARG
5	C	91	PRO
5	C	94	THR
5	C	101	ASP
5	C	136	VAL
5	C	162	VAL
5	C	187	ARG
5	C	214	THR
5	C	222	ASP
5	C	223	LEU
5	C	234	VAL
5	C	236	THR
5	C	240	LEU
5	C	243	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	D	24	HIS
6	D	133	ASN
6	D	136	ARG
6	D	137	PRO
7	E	7	ILE
7	E	16	ASP
7	E	86	VAL
7	E	102	VAL
8	F	12	LEU
8	F	46	GLU
10	H	21	GLU
10	H	54	VAL
10	H	87	LYS
10	H	91	ARG
10	H	162	PRO
12	J	7	ASP
12	J	39	VAL
12	J	46	ILE
12	J	52	GLN
12	J	74	ARG
12	J	93	ARG
12	J	127	ILE
13	K	10	GLN
14	L	35	ARG
14	L	104	ASP
14	L	117	GLU
14	L	140	VAL
15	M	46	LEU
15	M	81	ARG
15	M	93	ARG
15	M	99	ARG
15	M	164	THR
16	N	12	ARG
16	N	17	ARG
16	N	26	LEU
16	N	127	LEU
16	N	139	TRP
17	O	3	THR
17	O	111	VAL
18	P	21	VAL
18	P	52	LYS
18	P	98	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	Q	11	ARG
19	Q	16	ASN
19	Q	95	GLU
20	R	13	THR
20	R	39	THR
21	S	12	GLU
22	T	39	ASN
22	T	48	VAL
22	T	89	ARG
22	T	96	VAL
22	T	115	GLU
23	U	4	ARG
24	V	43	PRO
24	V	65	ASP
25	W	35	VAL
25	W	52	VAL
25	W	73	LEU
25	W	122	ARG
25	W	146	ILE
25	W	151	GLU
26	X	15	ARG
26	X	46	ASP
26	X	49	ARG
26	X	72	VAL
26	X	79	GLU
26	X	82	GLU
27	Y	103	THR
27	Y	115	ARG
27	Y	141	THR
27	Y	172	THR
27	Y	187	VAL
27	Y	189	ASN
27	Y	200	THR
27	Y	203	VAL
27	Y	235	GLU
30	2	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (94) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	92	ASN
3	A	199	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	218	ASN
4	B	27	ASN
4	B	145	HIS
4	B	221	GLN
4	B	238	ASN
4	B	243	ASN
4	B	260	HIS
4	B	320	GLN
4	B	332	ASN
5	C	2	GLN
5	C	39	GLN
5	C	67	GLN
5	C	129	HIS
6	D	47	GLN
6	D	103	ASN
6	D	133	ASN
7	E	106	ASN
7	E	119	HIS
7	E	143	GLN
9	G	64	ASN
10	H	34	HIS
10	H	59	GLN
10	H	62	HIS
10	H	75	HIS
11	I	88	GLN
11	I	99	GLN
11	I	106	GLN
12	J	25	GLN
12	J	29	GLN
12	J	52	GLN
12	J	107	ASN
12	J	126	ASN
13	K	10	GLN
14	L	18	HIS
14	L	41	HIS
14	L	42	ASN
14	L	58	GLN
15	M	24	GLN
15	M	26	GLN
15	M	58	GLN
15	M	170	ASN
16	N	22	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	N	107	ASN
17	O	110	HIS
18	P	50	GLN
18	P	66	GLN
18	P	73	HIS
18	P	118	GLN
19	Q	40	HIS
19	Q	67	GLN
20	R	22	GLN
20	R	61	GLN
20	R	94	ASN
20	R	98	ASN
20	R	113	HIS
20	R	117	HIS
20	R	140	GLN
21	S	25	GLN
21	S	51	GLN
21	S	53	ASN
21	S	55	GLN
22	T	39	ASN
22	T	43	ASN
22	T	73	HIS
23	U	39	ASN
24	V	4	HIS
24	V	6	GLN
24	V	60	GLN
25	W	14	HIS
25	W	27	HIS
25	W	28	HIS
25	W	59	GLN
25	W	110	GLN
25	W	119	HIS
25	W	125	HIS
25	W	141	HIS
27	Y	133	HIS
27	Y	134	HIS
27	Y	149	GLN
27	Y	188	HIS
27	Y	189	ASN
29	1	8	GLN
29	1	16	HIS
29	1	28	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	2	16	ASN
30	2	18	ASN
30	2	37	HIS
30	2	41	HIS
30	2	45	ASN
31	3	2	GLN
31	3	30	GLN
31	3	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	242 (8%)	34 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	258 (9%)	35 (1%)

All (258) 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	169	A
1	0	170	U
1	0	186	A
1	0	191	A
1	0	192	A
1	0	200	C
1	0	219	G
1	0	237	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	U
1	0	336	G
1	0	337	A
1	0	358	G
1	0	381	G
1	0	397	A
1	0	417	G
1	0	457	U
1	0	461	C
1	0	473	A
1	0	487	G
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	645	U
1	0	660	A
1	0	688	A
1	0	698	A
1	0	701	U
1	0	759	C
1	0	777	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	809	G
1	0	821	U
1	0	835	U
1	0	840	U
1	0	846	A
1	0	857	A
1	0	858	U
1	0	868	G
1	0	869	G
1	0	871	G
1	0	872	U
1	0	875	A
1	0	877	G
1	0	878	G
1	0	884	C
1	0	885	G
1	0	898	G
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	1088	A
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1185	U
1	0	1192	A
1	0	1193	A
1	0	1206	U
1	0	1216	G
1	0	1237	U
1	0	1238	C
1	0	1239	G
1	0	1246	A
1	0	1247	A
1	0	1279	U
1	0	1289	C
1	0	1342	C
1	0	1353	C
1	0	1360	C
1	0	1377	C
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	1526	A
1	0	1528	A
1	0	1562	C
1	0	1564	C
1	0	1592	G
1	0	1625	U
1	0	1626	A
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	1693	A
1	0	1701	A
1	0	1722	U
1	0	1723	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1725	C
1	0	1731	C
1	0	1732	A
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	1857	A
1	0	1879	U
1	0	1919	A
1	0	1942	A
1	0	1943	C
1	0	1971	G
1	0	1973	A
1	0	1978	A
1	0	1979	G
1	0	1980	U
1	0	1996	U
1	0	2008	U
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	2104	C
1	0	2110	G
1	0	2243	C
1	0	2258	A
1	0	2271	G
1	0	2272	G
1	0	2317	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	2476	C
1	0	2483	A
1	0	2507	G
1	0	2509	A
1	0	2511	A
1	0	2526	C
1	0	2527	U
1	0	2533	C
1	0	2537	G
1	0	2538	A
1	0	2539	U
1	0	2541	U
1	0	2553	A
1	0	2564	G
1	0	2589	U
1	0	2601	A
1	0	2602	G
1	0	2608	C
1	0	2613	G
1	0	2649	A
1	0	2650	U
1	0	2664	A
1	0	2676	C
1	0	2681	A
1	0	2682	C
1	0	2718	C
1	0	2719	A
1	0	2726	U
1	0	2727	A
1	0	2747	C
1	0	2748	G
1	0	2749	U
1	0	2750	G
1	0	2762	C
1	0	2768	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	2792	A
1	0	2800	A
1	0	2811	A
1	0	2812	A
1	0	2825	C
1	0	2876	G
1	0	2890	A
1	0	2896	A
1	0	2903	C
1	0	2914	A
2	9	2	U
2	9	14	G
2	9	22	G
2	9	23	U
2	9	24	U
2	9	25	G
2	9	40	C
2	9	41	C
2	9	43	G
2	9	44	A
2	9	52	A
2	9	57	A
2	9	66	G
2	9	77	A
2	9	114	G
2	9	122	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	69	A
1	0	129	A
1	0	169	A
1	0	603	A
1	0	644	G
1	0	699	C
1	0	834	G
1	0	857	A
1	0	871	G
1	0	877	G
1	0	1080	C
1	0	1232	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	0	1237	U
1	0	1246	A
1	0	1352	A
1	0	1377	C
1	0	1684	A
1	0	1685	A
1	0	1692	C
1	0	1856	C
1	0	1942	A
1	0	1979	G
1	0	2011	A
1	0	2103	A
1	0	2313	C
1	0	2467	A
1	0	2526	C
1	0	2536	C
1	0	2538	A
1	0	2649	A
1	0	2718	C
1	0	2726	U
1	0	2761	A
1	0	2791	U
2	9	65	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	UR3	0	2619	1	19,22,23	0.46	0	26,32,35	0.74	1 (3%)
1	1MA	0	628	1	21,25,26	0.72	1 (4%)	30,37,40	0.80	1 (3%)
1	PSU	0	2621	1	18,21,22	1.51	2 (11%)	21,30,33	1.27	3 (14%)
1	OMU	0	2587	1	19,22,23	0.25	0	25,31,34	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	0	2588	1	23,26,27	0.29	0	32,38,41	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1	-	1/7/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.18	1.43	1.36
1	0	2621	PSU	C6-C5	2.81	1.38	1.35
1	0	628	1MA	C6-N6	2.47	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.14	120.30	118.17
1	0	2621	PSU	O2-C2-N1	2.93	125.80	122.79
1	0	2621	PSU	C6-N1-C2	-2.86	120.04	122.69
1	0	2619	UR3	C4-N3-C2	2.85	126.87	124.58
1	0	628	1MA	N1-C2-N3	2.83	129.35	126.00

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	ZIT	0	9500	-	54,54,54	1.43	6 (11%)	82,83,83	1.10	5 (6%)

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
32	ZIT	0	9500	-	-	3/72/107/107	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	C22-C11	3.37	1.58	1.52
32	0	9500	ZIT	C13-C14	3.30	1.60	1.55
32	0	9500	ZIT	O13-C13	2.74	1.48	1.44
32	0	9500	ZIT	C6-C5	2.64	1.60	1.55
32	0	9500	ZIT	C13-C12	2.45	1.61	1.55
32	0	9500	ZIT	O6-C6	2.24	1.48	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C9-N10-C11	-3.07	106.97	112.06
32	0	9500	ZIT	C7-C8-C9	2.86	116.14	112.10
32	0	9500	ZIT	O6-C6-C7	2.21	113.87	108.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C4A-C3A-C2A	-2.17	106.90	110.02
32	0	9500	ZIT	C23-C13-C14	2.09	114.08	111.26

There are no chirality outliers.

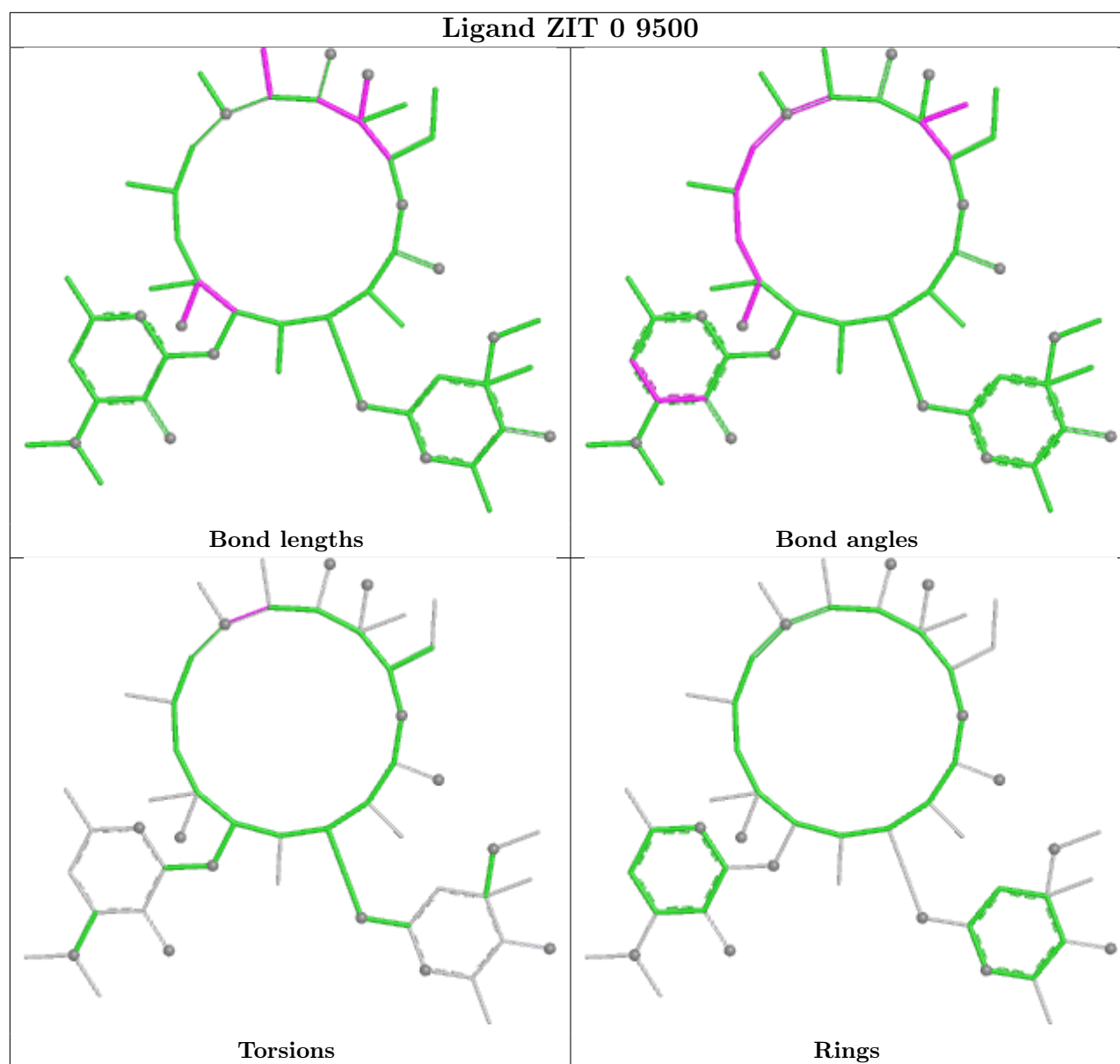
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	9500	ZIT	C12-C11-N10-C21
32	0	9500	ZIT	C22-C11-N10-C21
32	0	9500	ZIT	C12-C11-N10-C9

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.60	79 (2%) 53 50	15, 38, 82, 157	0
2	9	122/122 (100%)	0.15	4 (3%) 49 45	32, 58, 80, 139	0
3	A	237/240 (98%)	0.04	9 (3%) 44 40	19, 40, 75, 96	0
4	B	337/338 (99%)	0.16	5 (1%) 72 68	21, 46, 73, 84	0
5	C	246/246 (100%)	-0.07	2 (0%) 82 80	17, 36, 60, 69	0
6	D	140/177 (79%)	1.84	46 (32%) 1 1	51, 88, 114, 122	0
7	E	172/178 (96%)	0.59	11 (6%) 25 22	39, 61, 80, 84	0
8	F	119/120 (99%)	0.76	7 (5%) 28 24	38, 62, 88, 103	0
9	G	29/348 (8%)	1.46	8 (27%) 1 1	71, 87, 93, 95	0
10	H	160/177 (90%)	0.37	12 (7%) 20 17	31, 50, 83, 91	0
11	I	70/162 (43%)	3.11	53 (75%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.15	4 (2%) 55 51	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.02	2 (1%) 72 68	24, 43, 65, 77	0
14	L	145/165 (87%)	0.58	15 (10%) 12 9	18, 56, 101, 115	0
15	M	194/194 (100%)	-0.34	0 100 100	21, 33, 49, 56	0
16	N	186/187 (99%)	0.71	19 (10%) 12 9	34, 55, 102, 112	0
17	O	115/116 (99%)	0.19	4 (3%) 47 43	30, 45, 61, 69	0
18	P	143/149 (95%)	0.17	4 (2%) 55 51	30, 44, 57, 68	0
19	Q	95/96 (98%)	-0.13	1 (1%) 78 74	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.32	1 (0%) 84 81	25, 38, 58, 66	0
21	S	81/85 (95%)	0.14	2 (2%) 58 54	34, 50, 71, 80	0
22	T	119/120 (99%)	0.23	4 (3%) 48 44	29, 47, 76, 103	0
23	U	53/66 (80%)	0.25	1 (1%) 66 62	35, 48, 66, 78	0
24	V	65/71 (91%)	1.08	11 (16%) 4 3	43, 62, 107, 113	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.06	3 (1%) 66 62	29, 43, 58, 69	0
26	X	82/92 (89%)	0.48	6 (7%) 21 17	37, 50, 78, 94	0
27	Y	142/241 (58%)	-0.16	3 (2%) 63 59	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.51	4 (5%) 30 27	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.69	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.60	4 (8%) 16 13	26, 51, 75, 89	0
31	3	92/92 (100%)	0.12	1 (1%) 78 74	26, 48, 62, 77	0
All	All	6646/7480 (88%)	-0.07	325 (4%) 35 31	15, 43, 89, 157	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	V	1	THR	10.6
11	I	128	THR	8.3
6	D	10	PHE	8.0
2	9	1	U	7.8
11	I	74	ILE	6.4
11	I	71	ALA	6.4
26	X	88	GLU	5.9
11	I	112	LEU	5.8
6	D	174	VAL	5.5
6	D	107	GLY	5.4
3	A	37	VAL	5.4
6	D	63	ILE	5.3
16	N	166	ALA	5.2
6	D	55	LYS	5.1
6	D	172	VAL	5.0
1	0	1161	A	4.9
11	I	91	PHE	4.9
1	0	10	U	4.9
10	H	174	LEU	4.9
4	B	1	PRO	4.9
24	V	40	PRO	4.9
11	I	132	VAL	4.9
2	9	2	U	4.9
16	N	168	LEU	4.8
16	N	154	LEU	4.8
1	0	1176	C	4.8
28	Z	82	SER	4.8
11	I	83	GLY	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1175	G	4.7
11	I	134	ILE	4.7
24	V	39	ALA	4.6
7	E	10	ASP	4.5
24	V	2	VAL	4.5
14	L	77	ALA	4.4
1	0	1192	A	4.4
6	D	69	ILE	4.4
14	L	78	ALA	4.4
11	I	130	LEU	4.3
11	I	85	GLY	4.3
11	I	67	VAL	4.2
6	D	61	PHE	4.2
11	I	111	LEU	4.2
11	I	116	LEU	4.2
1	0	2345	A	4.2
11	I	133	THR	4.1
12	J	4	ALA	4.1
1	0	1165	G	4.1
11	I	88	GLN	4.1
11	I	129	SER	4.1
14	L	148	GLU	4.0
1	0	1173	A	4.0
11	I	80	PHE	4.0
6	D	11	HIS	4.0
30	2	49	GLU	3.9
1	0	138	U	3.9
1	0	1174	A	3.9
14	L	82	ALA	3.9
3	A	237	GLY	3.8
1	0	1160	G	3.8
3	A	36	ASP	3.8
11	I	73	LEU	3.8
14	L	99	GLU	3.8
11	I	124	VAL	3.8
11	I	114	TYR	3.8
7	E	154	ILE	3.8
6	D	26	GLY	3.7
24	V	43	PRO	3.7
11	I	120	ALA	3.7
1	0	1162	G	3.6
11	I	127	CYS	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	72	GLU	3.6
11	I	113	SER	3.6
10	H	171	GLY	3.6
11	I	100	VAL	3.5
6	D	59	GLY	3.5
11	I	119	ALA	3.5
1	0	1172	G	3.5
26	X	85	VAL	3.5
1	0	1169	U	3.5
11	I	70	THR	3.4
1	0	1524	U	3.4
1	0	1193	A	3.4
9	G	71	LEU	3.4
1	0	1167	G	3.4
14	L	149	ARG	3.4
11	I	84	SER	3.4
10	H	114	ASP	3.3
1	0	1166	A	3.3
1	0	1181	A	3.3
6	D	56	ARG	3.3
6	D	44	ILE	3.3
2	9	24	U	3.3
11	I	97	VAL	3.3
10	H	43	ALA	3.3
14	L	146	GLY	3.3
16	N	163	PHE	3.3
1	0	2769	C	3.3
11	I	82	THR	3.3
1	0	1191	A	3.2
11	I	123	VAL	3.2
13	K	119	GLN	3.2
14	L	150	GLN	3.2
10	H	172	GLU	3.2
11	I	95	LEU	3.2
11	I	109	PRO	3.2
11	I	92	VAL	3.2
6	D	106	PHE	3.2
1	0	1182	C	3.1
6	D	135	VAL	3.1
14	L	81	VAL	3.1
1	0	1164	U	3.1
28	Z	10	ARG	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
30	2	44	ARG	3.1
24	V	44	GLY	3.1
1	0	960	G	3.1
27	Y	216	ARG	3.1
1	0	1190	G	3.1
27	Y	235	GLU	3.1
7	E	45	ASP	3.1
4	B	57	GLU	3.0
8	F	90	GLU	3.0
6	D	75	LEU	3.0
16	N	158	LEU	3.0
12	J	70	PHE	3.0
6	D	74	THR	3.0
10	H	169	GLU	3.0
6	D	170	TYR	3.0
1	0	1199	A	3.0
11	I	69	PRO	3.0
1	0	1198	U	3.0
16	N	160	SER	3.0
21	S	81	ILE	2.9
1	0	1163	G	2.9
9	G	26	MET	2.9
16	N	169	PRO	2.9
6	D	62	ASP	2.9
6	D	171	ASP	2.9
1	0	1177	A	2.9
26	X	83	ALA	2.9
7	E	12	ASP	2.9
7	E	53	GLU	2.9
11	I	104	ALA	2.9
6	D	105	SER	2.9
1	0	999	C	2.9
6	D	57	THR	2.9
5	C	132	ASP	2.9
11	I	110	ASP	2.9
8	F	119	ARG	2.8
1	0	2506	A	2.8
1	0	1170	U	2.8
1	0	284	C	2.8
1	0	1168	C	2.8
6	D	104	PHE	2.8
11	I	66	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	I	108	HIS	2.8
28	Z	11	SER	2.8
6	D	17	ARG	2.8
9	G	73	ASP	2.8
26	X	87	ALA	2.7
2	9	23	U	2.7
7	E	11	VAL	2.7
16	N	159	TYR	2.7
22	T	118	SER	2.7
3	A	35	GLY	2.7
6	D	66	GLY	2.7
1	0	2508	C	2.7
30	2	35	ARG	2.7
8	F	102	GLY	2.7
11	I	87	PRO	2.7
1	0	128	A	2.7
1	0	1188	A	2.7
1	0	2909	G	2.7
6	D	54	ALA	2.7
1	0	1929	G	2.6
8	F	103	GLU	2.6
9	G	29	SER	2.6
11	I	89	GLU	2.6
6	D	35	ALA	2.6
8	F	101	ALA	2.6
30	2	37	HIS	2.6
14	L	145	LEU	2.6
19	Q	95	GLU	2.6
1	0	735	C	2.6
11	I	75	LYS	2.6
11	I	131	GLY	2.6
16	N	162	ASP	2.6
1	0	1279	U	2.6
9	G	12	ILE	2.6
11	I	106	GLN	2.6
16	N	165	ALA	2.6
16	N	150	TYR	2.6
22	T	53	GLY	2.6
6	D	18	ILE	2.6
1	0	2004	U	2.6
11	I	77	GLU	2.6
14	L	83	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	1171	A	2.6
1	0	1204	C	2.5
6	D	89	PRO	2.5
16	N	157	PRO	2.5
1	0	1951	G	2.5
6	D	101	THR	2.5
10	H	170	ARG	2.5
11	I	68	PRO	2.5
16	N	164	ASP	2.5
5	C	135	GLU	2.5
1	0	1525	G	2.5
3	A	32	VAL	2.5
13	K	118	ALA	2.5
10	H	173	GLU	2.5
26	X	7	GLU	2.5
1	0	970	U	2.5
1	0	1964	U	2.5
1	0	1203	G	2.5
17	O	22	GLY	2.5
6	D	53	LYS	2.5
16	N	186	LEU	2.5
4	B	56	ASP	2.4
6	D	154	LYS	2.4
7	E	126	ILE	2.4
1	0	1202	A	2.4
1	0	2344	G	2.4
10	H	39	LYS	2.4
17	O	23	GLY	2.4
7	E	87	PHE	2.4
11	I	93	ALA	2.4
1	0	1180	U	2.4
6	D	153	THR	2.4
14	L	60	GLU	2.4
18	P	116	SER	2.4
1	0	2914	A	2.4
1	0	87	C	2.4
11	I	103	ILE	2.4
7	E	156	ASP	2.4
16	N	167	ASP	2.4
1	0	2507	G	2.4
8	F	91	VAL	2.4
1	0	2637	A	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
6	D	60	GLU	2.4
1	0	1205	U	2.3
25	W	76	ASP	2.3
1	0	514	G	2.3
1	0	1948	G	2.3
18	P	143	ALA	2.3
17	O	1	SER	2.3
1	0	1183	C	2.3
1	0	1184	C	2.3
14	L	102	ASP	2.3
6	D	68	PRO	2.3
1	0	969	G	2.3
1	0	1197	G	2.3
1	0	1950	G	2.3
1	0	1189	A	2.3
24	V	46	ILE	2.3
1	0	1625	U	2.3
22	T	117	ASP	2.3
1	0	1178	G	2.3
16	N	147	ILE	2.3
11	I	101	LYS	2.3
14	L	147	GLU	2.3
3	A	211	LYS	2.2
6	D	93	LEU	2.2
1	0	1561	U	2.2
11	I	135	GLU	2.2
1	0	1157	C	2.2
11	I	118	ASN	2.2
17	O	24	ALA	2.2
6	D	12	GLU	2.2
16	N	152	GLU	2.2
11	I	78	ALA	2.2
6	D	131	THR	2.2
8	F	99	THR	2.2
4	B	138	GLY	2.2
9	G	27	ILE	2.2
16	N	184	ILE	2.2
4	B	183	GLU	2.2
6	D	165	PHE	2.2
6	D	58	VAL	2.2
6	D	52	THR	2.2
3	A	38	ILE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
18	P	110	ASP	2.2
23	U	47	ARG	2.2
1	0	283	U	2.2
18	P	18	LYS	2.2
1	0	2237	G	2.1
12	J	47	THR	2.1
7	E	32	ARG	2.1
28	Z	80	ARG	2.1
10	H	42	ASP	2.1
27	Y	236	VAL	2.1
1	0	2910	A	2.1
14	L	55	GLN	2.1
10	H	115	GLY	2.1
1	0	1523	G	2.1
31	3	41	GLU	2.1
1	0	2911	C	2.1
24	V	42	ASN	2.1
1	0	1200	A	2.1
1	0	2768	A	2.1
3	A	236	GLY	2.1
6	D	90	LEU	2.1
6	D	169	THR	2.1
12	J	62	ASP	2.1
24	V	65	ASP	2.1
25	W	108	ARG	2.1
24	V	41	GLU	2.1
1	0	2664	A	2.1
3	A	64	ASP	2.1
7	E	121	ASP	2.1
21	S	1	SER	2.1
1	0	271	C	2.1
16	N	137	ALA	2.0
22	T	119	ALA	2.0
24	V	38	GLY	2.0
25	W	86	GLU	2.0
6	D	40	ILE	2.0
6	D	100	ASP	2.0
9	G	63	ARG	2.0
9	G	67	LEU	2.0
10	H	41	LYS	2.0
6	D	95	THR	2.0
26	X	66	THR	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	0	272	A	2.0
11	I	90	ASP	2.0
20	R	150	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	UR3	0	2619	21/22	0.97	0.06	29,33,35,41	0
1	OMU	0	2587	21/22	0.98	0.06	26,28,29,32	0
1	OMG	0	2588	24/25	0.98	0.06	23,27,29,30	0
1	1MA	0	628	23/24	0.98	0.05	22,24,25,28	0
1	PSU	0	2621	20/21	0.98	0.05	22,25,33,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	9006	1/1	0.60	0.19	200,200,200,200	0
33	MG	0	8085	1/1	0.70	0.21	90,90,90,90	0
35	NA	0	8571	1/1	0.71	0.27	79,79,79,79	0
37	SR	0	9000	1/1	0.75	0.19	150,150,150,150	0
35	NA	9	8543	1/1	0.76	0.25	41,41,41,41	0
37	SR	0	8991	1/1	0.77	0.18	167,167,167,167	0
37	SR	0	9004	1/1	0.78	0.26	176,176,176,176	0
37	SR	0	8996	1/1	0.79	0.31	185,185,185,185	0
37	SR	0	8997	1/1	0.81	0.21	171,171,171,171	0
37	SR	0	8976	1/1	0.81	0.21	159,159,159,159	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8947	1/1	0.82	0.19	148,148,148,148	0
37	SR	0	8951	1/1	0.82	0.13	137,137,137,137	0
35	NA	0	8561	1/1	0.82	0.36	62,62,62,62	0
35	NA	0	8562	1/1	0.82	0.29	59,59,59,59	0
35	NA	0	8564	1/1	0.82	0.12	55,55,55,55	0
33	MG	0	8038	1/1	0.82	0.12	65,65,65,65	0
35	NA	0	8548	1/1	0.82	0.20	50,50,50,50	0
35	NA	9	8572	1/1	0.82	0.21	59,59,59,59	0
37	SR	0	8938	1/1	0.82	0.13	147,147,147,147	0
37	SR	0	8957	1/1	0.83	0.23	176,176,176,176	0
33	MG	9	8074	1/1	0.83	0.20	64,64,64,64	0
37	SR	0	8986	1/1	0.84	0.34	169,169,169,169	0
37	SR	0	8989	1/1	0.84	0.19	148,148,148,148	0
33	MG	0	8039	1/1	0.84	0.11	60,60,60,60	0
33	MG	0	8073	1/1	0.84	0.20	76,76,76,76	0
37	SR	0	8955	1/1	0.84	0.21	169,169,169,169	0
35	NA	0	8525	1/1	0.84	0.23	65,65,65,65	0
35	NA	0	8536	1/1	0.84	0.12	46,46,46,46	0
37	SR	0	8979	1/1	0.84	0.17	184,184,184,184	0
33	MG	0	8071	1/1	0.85	0.21	54,54,54,54	0
37	SR	9	8980	1/1	0.85	0.14	162,162,162,162	0
37	SR	9	9003	1/1	0.85	0.10	141,141,141,141	0
37	SR	B	8987	1/1	0.85	0.51	189,189,189,189	0
37	SR	0	8971	1/1	0.86	0.19	158,158,158,158	0
37	SR	0	8974	1/1	0.86	0.17	159,159,159,159	0
35	NA	0	8520	1/1	0.86	0.19	50,50,50,50	0
37	SR	0	8944	1/1	0.86	0.18	146,146,146,146	0
33	MG	0	8063	1/1	0.86	0.24	71,71,71,71	0
37	SR	0	9001	1/1	0.87	0.12	160,160,160,160	0
37	SR	0	9002	1/1	0.87	0.18	162,162,162,162	0
37	SR	0	8919	1/1	0.87	0.19	169,169,169,169	0
33	MG	0	8040	1/1	0.87	0.13	78,78,78,78	0
35	NA	0	8573	1/1	0.87	0.13	55,55,55,55	0
37	SR	0	8983	1/1	0.87	0.14	149,149,149,149	0
37	SR	A	8929	1/1	0.87	0.23	123,123,123,123	0
35	NA	H	8518	1/1	0.87	0.29	66,66,66,66	0
33	MG	0	8037	1/1	0.88	0.16	77,77,77,77	0
35	NA	0	8544	1/1	0.89	0.12	49,49,49,49	0
35	NA	0	8565	1/1	0.89	0.15	46,46,46,46	0
35	NA	0	8555	1/1	0.89	0.21	43,43,43,43	0
35	NA	R	8575	1/1	0.90	0.14	73,73,73,73	0
33	MG	0	8079	1/1	0.90	0.06	40,40,40,40	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8924	1/1	0.90	0.09	123,123,123,123	0
37	SR	0	8927	1/1	0.90	0.12	133,133,133,133	0
37	SR	0	8959	1/1	0.90	0.11	132,132,132,132	0
37	SR	0	8990	1/1	0.90	0.09	106,106,106,106	0
37	SR	0	8968	1/1	0.90	0.12	142,142,142,142	0
35	NA	0	8563	1/1	0.90	0.19	56,56,56,56	0
37	SR	A	8977	1/1	0.90	0.09	143,143,143,143	0
35	NA	0	8542	1/1	0.90	0.19	51,51,51,51	0
35	NA	0	8521	1/1	0.91	0.16	55,55,55,55	0
33	MG	0	8080	1/1	0.91	0.06	53,53,53,53	0
37	SR	0	8981	1/1	0.91	0.13	141,141,141,141	0
37	SR	0	8982	1/1	0.91	0.41	152,152,152,152	0
35	NA	0	8574	1/1	0.91	0.26	48,48,48,48	0
33	MG	0	8053	1/1	0.91	0.09	58,58,58,58	0
35	NA	0	8569	1/1	0.91	0.14	61,61,61,61	0
35	NA	0	8554	1/1	0.92	0.18	52,52,52,52	0
33	MG	0	8036	1/1	0.92	0.06	36,36,36,36	0
35	NA	0	8557	1/1	0.92	0.12	54,54,54,54	0
33	MG	0	8082	1/1	0.92	0.08	44,44,44,44	0
37	SR	0	9007	1/1	0.92	0.42	154,154,154,154	0
35	NA	0	8506	1/1	0.92	0.11	50,50,50,50	0
37	SR	0	8993	1/1	0.92	0.13	143,143,143,143	0
37	SR	0	8922	1/1	0.92	0.22	161,161,161,161	0
37	SR	0	8956	1/1	0.92	0.09	127,127,127,127	0
35	NA	0	8535	1/1	0.92	0.07	40,40,40,40	0
37	SR	S	8961	1/1	0.92	0.08	113,113,113,113	0
33	MG	0	8081	1/1	0.93	0.09	55,55,55,55	0
37	SR	0	8973	1/1	0.93	0.08	113,113,113,113	0
35	NA	0	8567	1/1	0.93	0.17	53,53,53,53	0
35	NA	0	8560	1/1	0.93	0.15	54,54,54,54	0
35	NA	S	8510	1/1	0.93	0.07	24,24,24,24	0
35	NA	0	8511	1/1	0.93	0.08	59,59,59,59	0
33	MG	0	8092	1/1	0.93	0.05	47,47,47,47	0
33	MG	0	8030	1/1	0.93	0.12	48,48,48,48	0
35	NA	0	8556	1/1	0.93	0.27	37,37,37,37	0
37	SR	0	8960	1/1	0.93	0.10	128,128,128,128	0
37	SR	0	8962	1/1	0.93	0.25	139,139,139,139	0
37	SR	0	8928	1/1	0.93	0.12	112,112,112,112	0
37	SR	0	8970	1/1	0.93	0.12	109,109,109,109	0
37	SR	F	9005	1/1	0.93	0.08	106,106,106,106	0
37	SR	0	8994	1/1	0.93	0.34	168,168,168,168	0
35	NA	R	8532	1/1	0.94	0.04	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	T	8057	1/1	0.94	0.06	51,51,51,51	0
33	MG	0	8056	1/1	0.94	0.07	49,49,49,49	0
35	NA	0	8541	1/1	0.94	0.07	41,41,41,41	0
37	SR	0	8969	1/1	0.94	0.37	115,115,115,115	0
35	NA	0	8509	1/1	0.94	0.08	47,47,47,47	0
33	MG	0	8089	1/1	0.94	0.16	37,37,37,37	0
35	NA	0	8547	1/1	0.94	0.13	42,42,42,42	0
33	MG	0	8035	1/1	0.94	0.06	52,52,52,52	0
35	NA	0	8551	1/1	0.94	0.16	39,39,39,39	0
37	SR	0	8943	1/1	0.94	0.11	108,108,108,108	0
35	NA	0	8553	1/1	0.94	0.11	48,48,48,48	0
33	MG	0	8066	1/1	0.94	0.05	47,47,47,47	0
35	NA	0	8522	1/1	0.94	0.11	46,46,46,46	0
37	SR	0	8984	1/1	0.94	0.07	98,98,98,98	0
33	MG	A	8051	1/1	0.94	0.09	55,55,55,55	0
35	NA	0	8534	1/1	0.94	0.06	29,29,29,29	0
35	NA	0	8558	1/1	0.94	0.09	46,46,46,46	0
33	MG	0	8049	1/1	0.95	0.06	64,64,64,64	0
35	NA	0	8549	1/1	0.95	0.21	74,74,74,74	0
37	SR	0	8988	1/1	0.95	0.08	149,149,149,149	0
33	MG	0	8069	1/1	0.95	0.08	58,58,58,58	0
35	NA	0	8502	1/1	0.95	0.08	43,43,43,43	0
37	SR	0	8920	1/1	0.95	0.09	96,96,96,96	0
33	MG	0	8024	1/1	0.95	0.08	53,53,53,53	0
37	SR	0	8963	1/1	0.95	0.06	103,103,103,103	0
37	SR	0	8964	1/1	0.95	0.09	109,109,109,109	0
37	SR	0	8965	1/1	0.95	0.08	109,109,109,109	0
37	SR	0	8998	1/1	0.95	0.22	133,133,133,133	0
37	SR	0	8967	1/1	0.95	0.08	116,116,116,116	0
32	ZIT	0	9500	52/52	0.95	0.08	28,38,42,44	0
33	MG	0	8060	1/1	0.95	0.05	45,45,45,45	0
35	NA	0	8517	1/1	0.95	0.11	36,36,36,36	0
37	SR	0	8933	1/1	0.95	0.09	108,108,108,108	0
37	SR	0	8937	1/1	0.95	0.06	94,94,94,94	0
33	MG	0	8093	1/1	0.95	0.04	29,29,29,29	0
37	SR	0	8975	1/1	0.95	0.18	99,99,99,99	0
37	SR	0	8939	1/1	0.95	0.09	108,108,108,108	0
35	NA	0	8559	1/1	0.95	0.17	51,51,51,51	0
35	NA	0	8546	1/1	0.95	0.12	63,63,63,63	0
33	MG	0	8031	1/1	0.95	0.08	41,41,41,41	0
37	SR	H	8972	1/1	0.95	0.22	112,112,112,112	0
35	NA	J	8538	1/1	0.95	0.05	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
37	SR	0	8953	1/1	0.96	0.10	121,121,121,121	0
37	SR	0	8985	1/1	0.96	0.17	104,104,104,104	0
37	SR	0	8954	1/1	0.96	0.06	88,88,88,88	0
36	CL	0	8813	1/1	0.96	0.06	45,45,45,45	0
36	CL	J	8801	1/1	0.96	0.06	49,49,49,49	0
36	CL	J	8821	1/1	0.96	0.09	52,52,52,52	0
37	SR	0	8958	1/1	0.96	0.05	83,83,83,83	0
36	CL	R	8806	1/1	0.96	0.05	40,40,40,40	0
37	SR	0	8910	1/1	0.96	0.10	80,80,80,80	0
37	SR	0	8995	1/1	0.96	0.08	112,112,112,112	0
37	SR	0	8916	1/1	0.96	0.10	95,95,95,95	0
37	SR	0	8917	1/1	0.96	0.07	90,90,90,90	0
35	NA	0	8512	1/1	0.96	0.08	36,36,36,36	0
35	NA	0	8514	1/1	0.96	0.09	41,41,41,41	0
35	NA	0	8570	1/1	0.96	0.06	35,35,35,35	0
33	MG	0	8067	1/1	0.96	0.04	29,29,29,29	0
33	MG	0	8083	1/1	0.96	0.04	41,41,41,41	0
35	NA	0	8504	1/1	0.96	0.05	26,26,26,26	0
33	MG	0	8022	1/1	0.96	0.06	30,30,30,30	0
37	SR	0	8934	1/1	0.96	0.15	116,116,116,116	0
35	NA	0	8523	1/1	0.96	0.05	31,31,31,31	0
33	MG	A	8050	1/1	0.96	0.05	33,33,33,33	0
35	NA	0	8526	1/1	0.96	0.06	36,36,36,36	0
35	NA	0	8550	1/1	0.96	0.13	41,41,41,41	0
35	NA	0	8533	1/1	0.96	0.04	50,50,50,50	0
33	MG	0	8075	1/1	0.96	0.09	31,31,31,31	0
36	CL	0	8811	1/1	0.96	0.08	45,45,45,45	0
35	NA	0	8529	1/1	0.97	0.08	32,32,32,32	0
35	NA	C	8503	1/1	0.97	0.05	29,29,29,29	0
35	NA	0	8530	1/1	0.97	0.07	37,37,37,37	0
35	NA	0	8531	1/1	0.97	0.04	29,29,29,29	0
35	NA	M	8539	1/1	0.97	0.05	28,28,28,28	0
37	SR	0	8941	1/1	0.97	0.10	90,90,90,90	0
37	SR	0	8942	1/1	0.97	0.06	110,110,110,110	0
35	NA	Q	8540	1/1	0.97	0.05	39,39,39,39	0
33	MG	0	8091	1/1	0.97	0.04	42,42,42,42	0
37	SR	0	8946	1/1	0.97	0.06	87,87,87,87	0
33	MG	0	8078	1/1	0.97	0.04	40,40,40,40	0
33	MG	0	8044	1/1	0.97	0.05	40,40,40,40	0
37	SR	0	8992	1/1	0.97	0.29	111,111,111,111	0
35	NA	0	8513	1/1	0.97	0.06	33,33,33,33	0
33	MG	0	8068	1/1	0.97	0.06	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	CL	0	8816	1/1	0.97	0.12	53,53,53,53	0
36	CL	A	8809	1/1	0.97	0.06	52,52,52,52	0
35	NA	0	8515	1/1	0.97	0.10	30,30,30,30	0
36	CL	J	8802	1/1	0.97	0.05	51,51,51,51	0
37	SR	0	8999	1/1	0.97	0.05	78,78,78,78	0
35	NA	0	8516	1/1	0.97	0.08	44,44,44,44	0
36	CL	L	8810	1/1	0.97	0.11	43,43,43,43	0
33	MG	0	8046	1/1	0.97	0.04	25,25,25,25	0
35	NA	0	8566	1/1	0.97	0.15	44,44,44,44	0
37	SR	0	8914	1/1	0.97	0.06	88,88,88,88	0
33	MG	0	8062	1/1	0.97	0.04	46,46,46,46	0
37	SR	0	9008	1/1	0.97	0.05	83,83,83,83	0
35	NA	0	8568	1/1	0.97	0.14	42,42,42,42	0
33	MG	0	8029	1/1	0.97	0.04	40,40,40,40	0
34	K	0	8401	1/1	0.97	0.16	58,58,58,58	0
37	SR	A	8930	1/1	0.97	0.05	82,82,82,82	0
33	MG	0	8033	1/1	0.97	0.06	32,32,32,32	0
37	SR	B	8950	1/1	0.97	0.07	90,90,90,90	0
33	MG	0	8076	1/1	0.97	0.11	28,28,28,28	0
37	SR	0	8926	1/1	0.97	0.06	95,95,95,95	0
33	MG	0	8090	1/1	0.97	0.10	49,49,49,49	0
37	SR	R	8912	1/1	0.97	0.05	77,77,77,77	0
35	NA	0	8527	1/1	0.97	0.09	31,31,31,31	0
36	CL	0	8815	1/1	0.98	0.07	47,47,47,47	0
35	NA	0	8552	1/1	0.98	0.12	48,48,48,48	0
36	CL	0	8817	1/1	0.98	0.05	46,46,46,46	0
36	CL	0	8822	1/1	0.98	0.22	48,48,48,48	0
33	MG	K	8054	1/1	0.98	0.03	34,34,34,34	0
36	CL	B	8819	1/1	0.98	0.09	46,46,46,46	0
33	MG	0	8052	1/1	0.98	0.10	23,23,23,23	0
33	MG	Y	8086	1/1	0.98	0.05	35,35,35,35	0
33	MG	0	8072	1/1	0.98	0.04	37,37,37,37	0
37	SR	0	8948	1/1	0.98	0.05	69,69,69,69	0
37	SR	0	8949	1/1	0.98	0.06	93,93,93,93	0
33	MG	0	8016	1/1	0.98	0.05	35,35,35,35	0
36	CL	N	8807	1/1	0.98	0.09	46,46,46,46	0
33	MG	0	8017	1/1	0.98	0.08	26,26,26,26	0
36	CL	Y	8820	1/1	0.98	0.05	35,35,35,35	0
37	SR	0	8908	1/1	0.98	0.05	71,71,71,71	0
35	NA	0	8537	1/1	0.98	0.05	32,32,32,32	0
35	NA	0	8505	1/1	0.98	0.10	33,33,33,33	0
37	SR	0	8915	1/1	0.98	0.06	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8047	1/1	0.98	0.05	46,46,46,46	0
35	NA	0	8507	1/1	0.98	0.03	27,27,27,27	0
35	NA	0	8524	1/1	0.98	0.10	31,31,31,31	0
35	NA	0	8508	1/1	0.98	0.08	40,40,40,40	0
37	SR	0	8921	1/1	0.98	0.04	66,66,66,66	0
37	SR	0	8966	1/1	0.98	0.04	89,89,89,89	0
33	MG	0	8077	1/1	0.98	0.06	26,26,26,26	0
37	SR	0	8923	1/1	0.98	0.04	78,78,78,78	0
33	MG	0	8034	1/1	0.98	0.08	35,35,35,35	0
37	SR	0	8925	1/1	0.98	0.06	75,75,75,75	0
36	CL	0	8803	1/1	0.98	0.06	41,41,41,41	0
36	CL	0	8805	1/1	0.98	0.08	45,45,45,45	0
35	NA	0	8528	1/1	0.98	0.10	32,32,32,32	0
37	SR	0	8931	1/1	0.98	0.04	86,86,86,86	0
33	MG	B	8042	1/1	0.98	0.04	52,52,52,52	0
37	SR	0	8978	1/1	0.98	0.06	82,82,82,82	0
36	CL	0	8814	1/1	0.98	0.08	40,40,40,40	0
37	SR	0	8935	1/1	0.99	0.02	60,60,60,60	0
37	SR	0	8936	1/1	0.99	0.03	67,67,67,67	0
33	MG	0	8010	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8088	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8027	1/1	0.99	0.06	32,32,32,32	0
37	SR	0	8940	1/1	0.99	0.06	66,66,66,66	0
35	NA	0	8545	1/1	0.99	0.07	29,29,29,29	0
33	MG	0	8064	1/1	0.99	0.03	34,34,34,34	0
36	CL	M	8818	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8065	1/1	0.99	0.06	45,45,45,45	0
37	SR	0	8945	1/1	0.99	0.06	92,92,92,92	0
36	CL	O	8808	1/1	0.99	0.05	54,54,54,54	0
33	MG	0	8013	1/1	0.99	0.02	24,24,24,24	0
33	MG	0	8043	1/1	0.99	0.02	46,46,46,46	0
36	CL	3	8804	1/1	0.99	0.04	47,47,47,47	0
37	SR	0	8901	1/1	0.99	0.03	71,71,71,71	0
37	SR	0	8905	1/1	0.99	0.12	48,48,48,48	0
35	NA	0	8519	1/1	0.99	0.04	36,36,36,36	0
33	MG	0	8003	1/1	0.99	0.04	23,23,23,23	0
37	SR	0	8911	1/1	0.99	0.04	65,65,65,65	0
33	MG	0	8045	1/1	0.99	0.03	29,29,29,29	0
33	MG	0	8070	1/1	0.99	0.07	36,36,36,36	0
33	MG	0	8004	1/1	0.99	0.03	22,22,22,22	0
33	MG	0	8032	1/1	0.99	0.06	36,36,36,36	0
37	SR	0	8918	1/1	0.99	0.03	66,66,66,66	0

Continued on next page...

Continued from previous page...

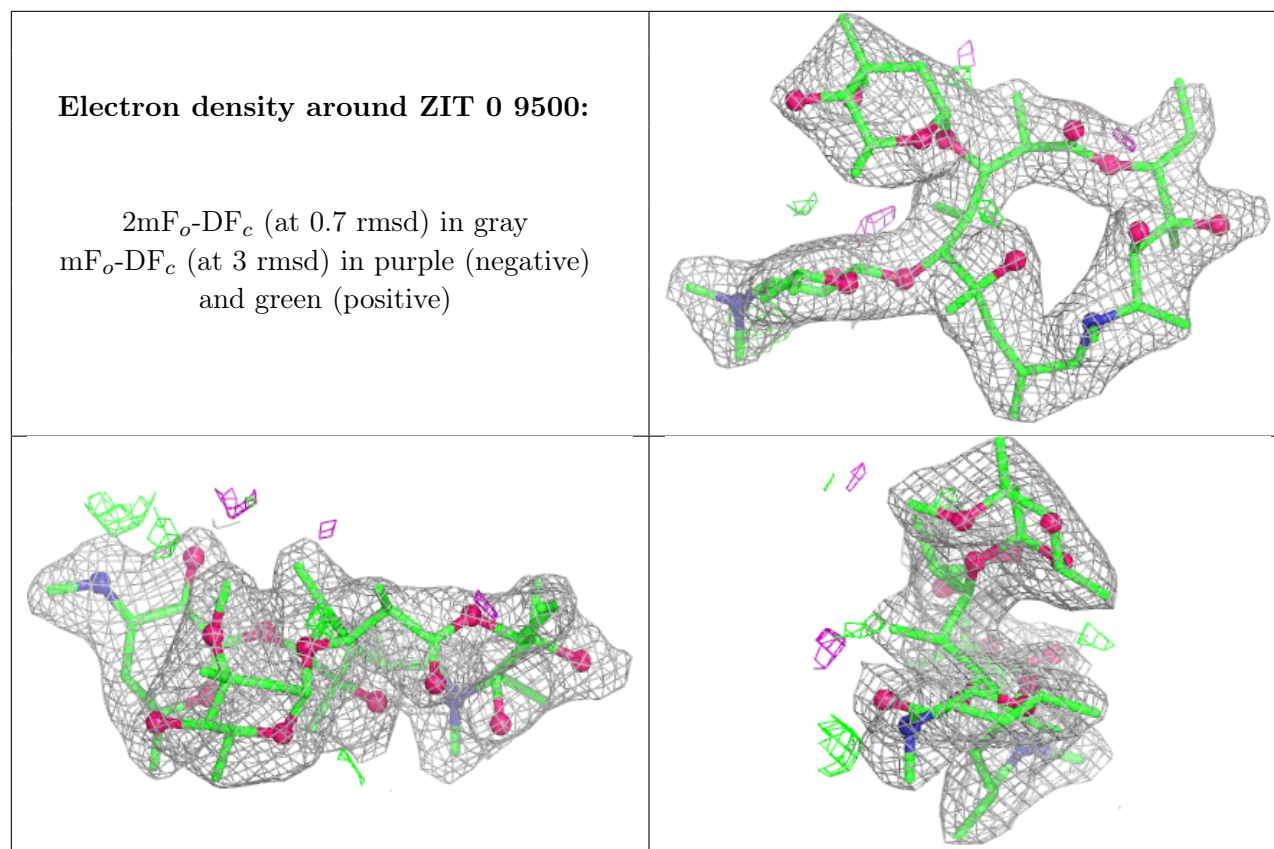
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8048	1/1	0.99	0.03	33,33,33,33	0
33	MG	0	8018	1/1	0.99	0.05	38,38,38,38	0
33	MG	0	8019	1/1	0.99	0.02	22,22,22,22	0
34	K	0	8402	1/1	0.99	0.16	46,46,46,46	0
35	NA	0	8501	1/1	0.99	0.06	26,26,26,26	0
36	CL	0	8812	1/1	0.99	0.03	39,39,39,39	0
33	MG	0	8020	1/1	0.99	0.05	37,37,37,37	0
33	MG	0	8055	1/1	0.99	0.02	29,29,29,29	0
33	MG	0	8021	1/1	0.99	0.02	28,28,28,28	0
33	MG	0	8058	1/1	0.99	0.03	26,26,26,26	0
33	MG	0	8059	1/1	0.99	0.06	27,27,27,27	0
33	MG	0	8008	1/1	0.99	0.02	26,26,26,26	0
33	MG	0	8061	1/1	0.99	0.02	23,23,23,23	0
37	SR	1	8913	1/1	0.99	0.05	70,70,70,70	0
37	SR	1	8952	1/1	0.99	0.04	62,62,62,62	0
37	SR	3	8932	1/1	0.99	0.03	58,58,58,58	0
38	CD	O	8705	1/1	0.99	0.05	58,58,58,58	0
38	CD	U	8701	1/1	0.99	0.02	55,55,55,55	0
38	CD	Z	8703	1/1	0.99	0.03	44,44,44,44	0
38	CD	1	8702	1/1	0.99	0.06	44,44,44,44	0
38	CD	3	8704	1/1	0.99	0.02	53,53,53,53	0
33	MG	0	8014	1/1	1.00	0.03	25,25,25,25	0
33	MG	0	8028	1/1	1.00	0.01	19,19,19,19	0
33	MG	0	8015	1/1	1.00	0.01	31,31,31,31	0
37	SR	0	8902	1/1	1.00	0.04	49,49,49,49	0
37	SR	0	8903	1/1	1.00	0.07	41,41,41,41	0
37	SR	0	8904	1/1	1.00	0.03	34,34,34,34	0
33	MG	0	8006	1/1	1.00	0.02	30,30,30,30	0
37	SR	0	8906	1/1	1.00	0.01	40,40,40,40	0
37	SR	0	8907	1/1	1.00	0.01	33,33,33,33	0
33	MG	0	8007	1/1	1.00	0.01	24,24,24,24	0
37	SR	0	8909	1/1	1.00	0.02	70,70,70,70	0
33	MG	0	8001	1/1	1.00	0.02	25,25,25,25	0
33	MG	0	8084	1/1	1.00	0.01	36,36,36,36	0
33	MG	0	8009	1/1	1.00	0.02	26,26,26,26	0
33	MG	0	8087	1/1	1.00	0.03	26,26,26,26	0
33	MG	0	8002	1/1	1.00	0.03	27,27,27,27	0
33	MG	0	8011	1/1	1.00	0.01	24,24,24,24	0
33	MG	0	8012	1/1	1.00	0.04	13,13,13,13	0
33	MG	0	8023	1/1	1.00	0.03	24,24,24,24	0
33	MG	0	8005	1/1	1.00	0.01	23,23,23,23	0
33	MG	0	8025	1/1	1.00	0.05	24,24,24,24	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8026	1/1	1.00	0.03	28,28,28,28	0
33	MG	0	8041	1/1	1.00	0.01	18,18,18,18	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.