



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:38 PM UTC

PDB ID : 3PU4 / pdb_00003pu4
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyU complex
Authors : Luo, M.; Green, T.J.; Rowse, M.
Deposited on : 2010-12-03
Resolution : 3.00 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

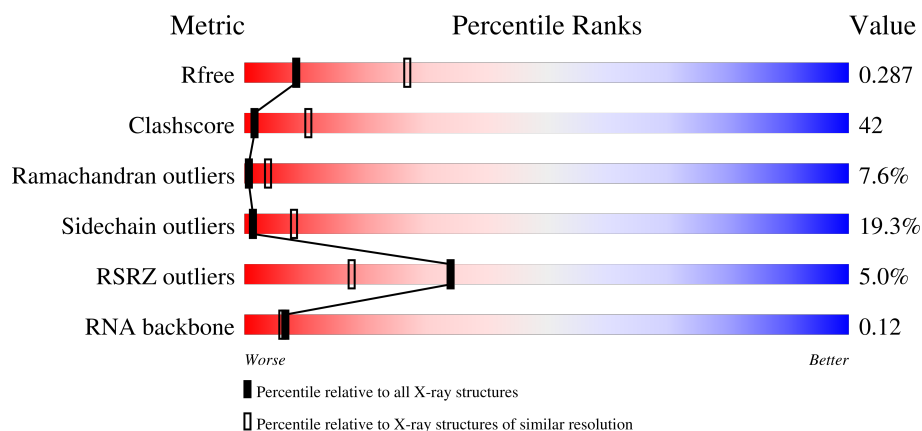
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	421	5% 43% 39% 14% .
1	B	421	4% 42% 40% 13% ..
1	C	421	6% 43% 39% 14% ..
1	D	421	7% 43% 40% 13% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	421	3% 43% 41% 14%
2	R	45	36% 33% 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

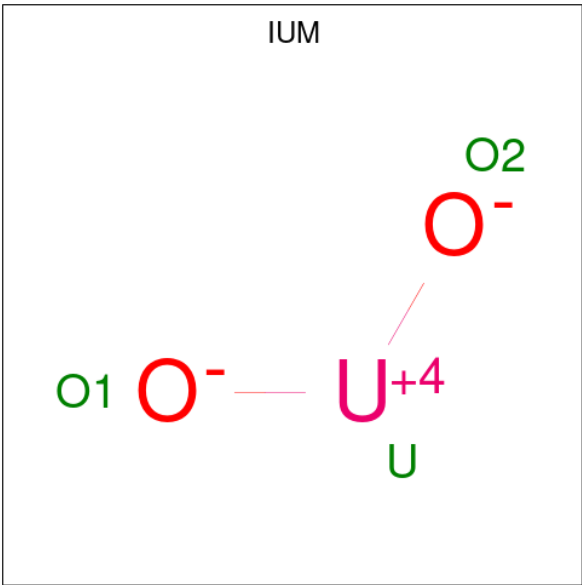
- Molecule 1 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			
1	B	415	Total	C	N	O	S	0	0	0
			3290	2097	552	623	18			
1	C	413	Total	C	N	O	S	0	0	0
			3275	2089	550	618	18			
1	D	416	Total	C	N	O	S	0	0	0
			3298	2103	553	624	18			
1	E	421	Total	C	N	O	S	0	0	0
			3327	2118	558	633	18			

- Molecule 2 is a RNA chain called RNA (45-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	45	Total	C	N	O	P	0	0	0
			900	405	90	360	45			

- Molecule 3 is URANYL (VI) ION (CCD ID: IUM) (formula: O₂U).

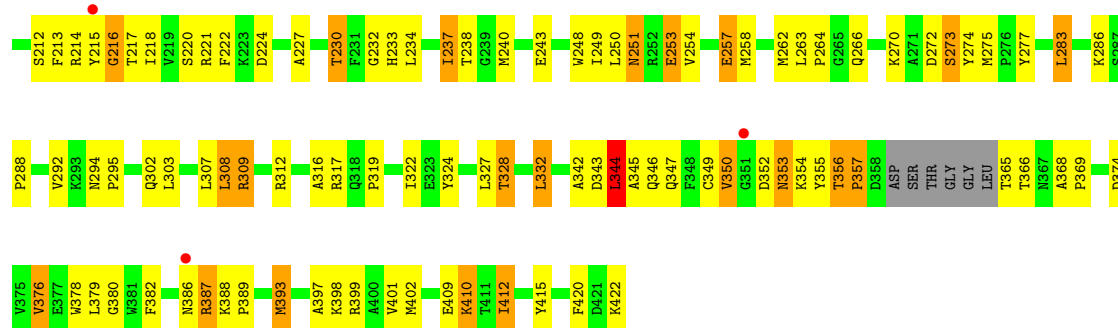


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		
3	A	1	Total	U	0	0
			1	1		
3	B	1	Total	U	0	0
			1	1		
3	B	1	Total	U	0	0
			1	1		
3	B	1	Total	U	0	0
			1	1		
3	C	1	Total	U	0	0
			1	1		
3	C	1	Total	U	0	0
			1	1		
3	C	1	Total	U	0	0
			1	1		
3	D	1	Total	U	0	0
			1	1		
3	D	1	Total	U	0	0
			1	1		
3	E	1	Total	U	0	0
			1	1		
3	E	1	Total	U	0	0
			1	1		

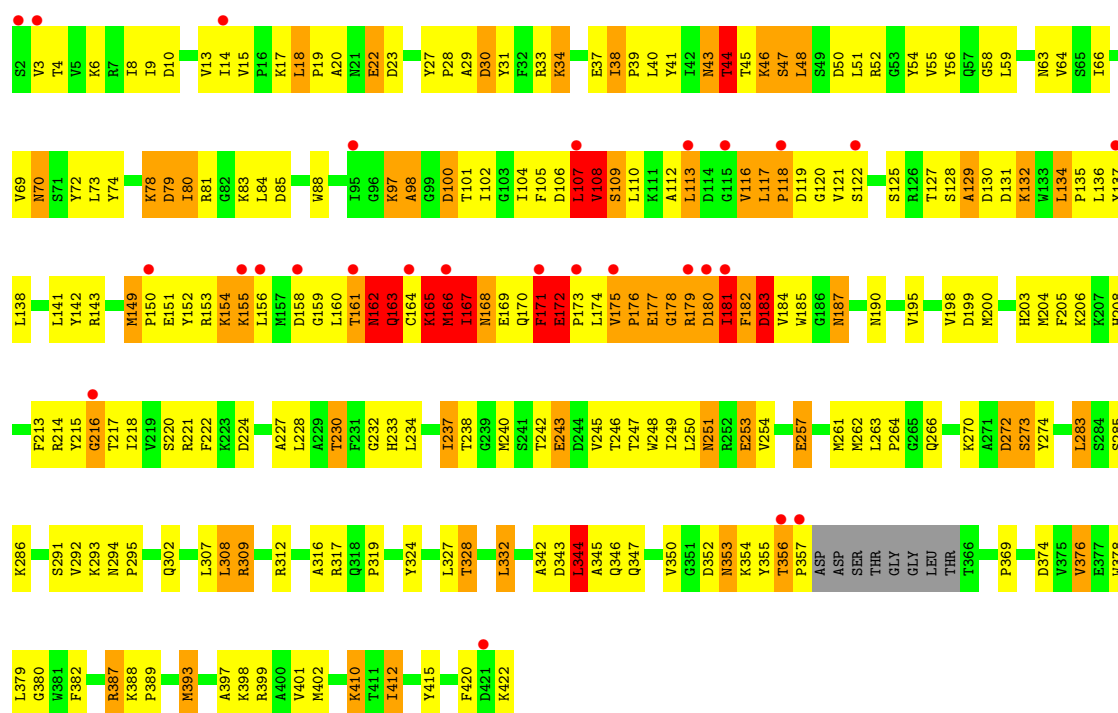
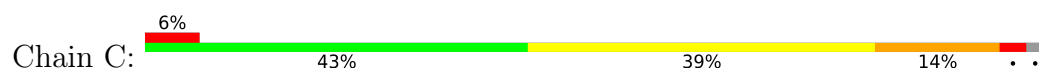
Continued on next page...

Continued from previous page...

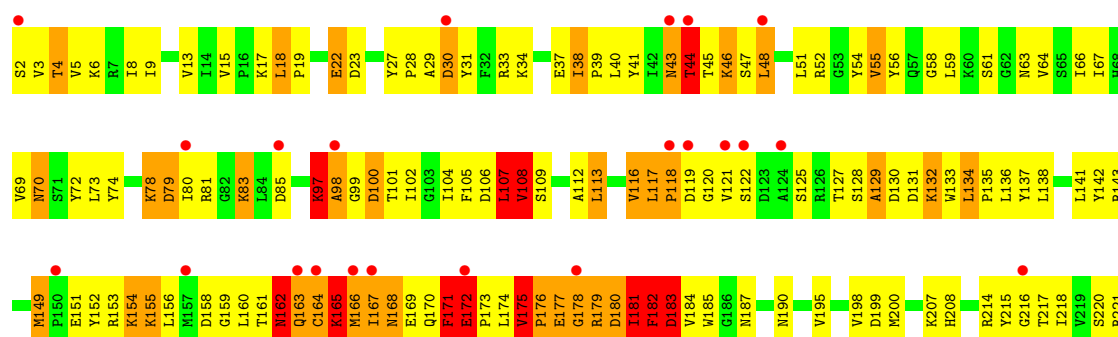
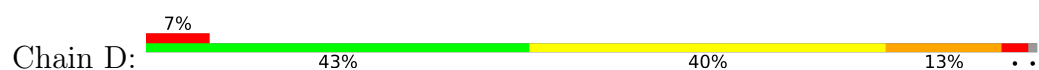
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0

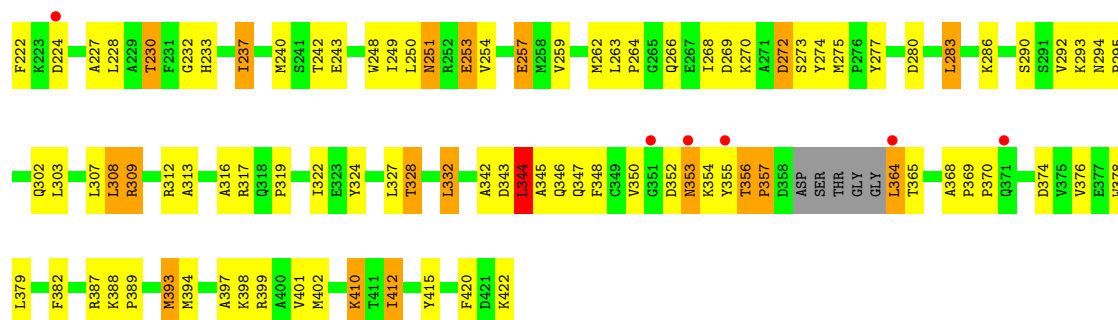


- Molecule 1: Nucleoprotein

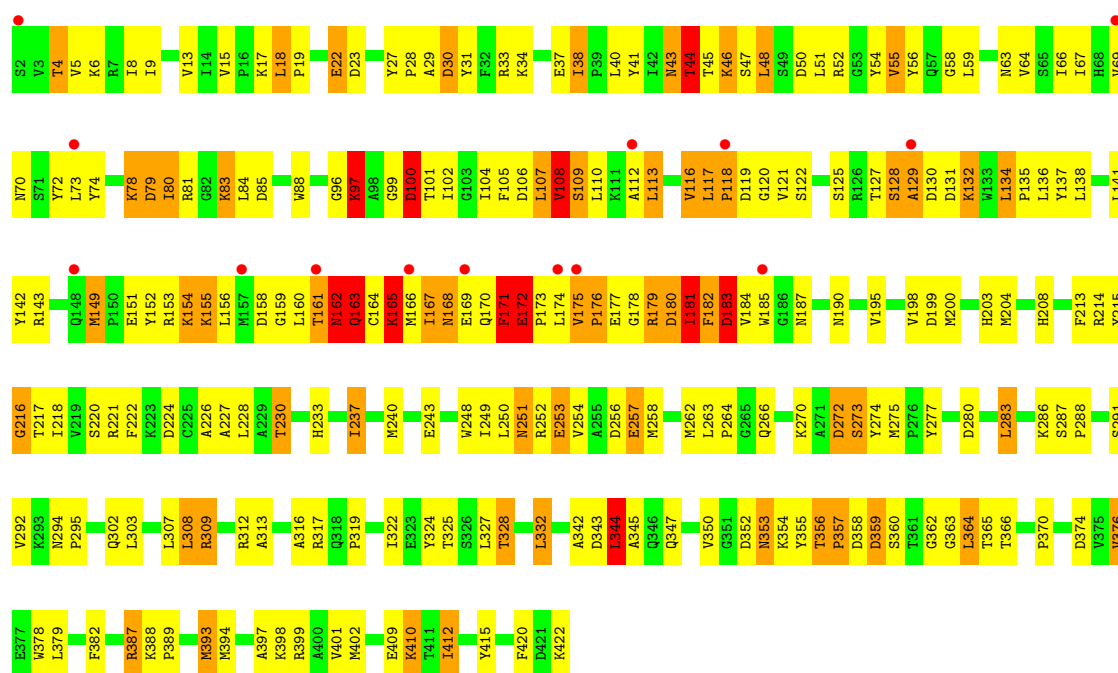
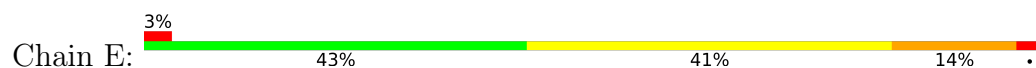


- Molecule 1: Nucleoprotein





• Molecule 1: Nucleoprotein



• Molecule 2: RNA (45-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.48Å 235.06Å 75.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 3.00 34.77 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.0 (34.77-3.00) 83.0 (34.77-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.251 , 0.288 0.246 , 0.287	Depositor DCC
R_{free} test set	2000 reflections (3.69%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IUM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.68	0/3403	0.98	12/4607 (0.3%)
1	B	0.68	1/3365 (0.0%)	0.97	10/4554 (0.2%)
1	C	0.69	0/3350	0.99	14/4533 (0.3%)
1	D	0.66	0/3373	0.97	10/4565 (0.2%)
1	E	0.64	0/3403	0.94	7/4607 (0.2%)
2	R	0.49	0/989	1.24	16/1526 (1.0%)
All	All	0.66	1/17883 (0.0%)	0.99	69/24392 (0.3%)

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	A	0	3
1	B	0	4
1	C	0	3
1	D	0	3
1	E	0	4
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	179	ARG	C-N	9.16	1.46	1.33

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	MET	CB-CA-C	12.06	129.46	109.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	GLY	N-CA-C	-8.80	102.78	115.64
1	C	166	MET	CB-CA-C	8.62	123.78	109.56
1	D	178	GLY	N-CA-C	-8.59	102.74	115.72
1	A	178	GLY	N-CA-C	-8.59	102.75	115.72
1	D	175	VAL	CA-C-N	7.92	129.74	119.84
1	D	175	VAL	C-N-CA	7.92	129.74	119.84
1	C	175	VAL	CA-C-N	7.73	129.50	119.84
1	C	175	VAL	C-N-CA	7.73	129.50	119.84
1	A	175	VAL	CA-C-N	7.33	129.00	119.84
1	A	175	VAL	C-N-CA	7.33	129.00	119.84
1	C	167	ILE	N-CA-CB	-7.28	100.37	111.57
1	B	178	GLY	N-CA-C	-7.12	105.25	115.64
1	A	129	ALA	N-CA-C	-7.11	99.68	110.70
2	R	39	U	N1-C1'-C2'	7.10	122.66	112.00
1	C	129	ALA	N-CA-C	-6.75	100.24	110.70
2	R	13	U	O4'-C1'-N1	6.65	118.17	108.20
1	B	108	VAL	N-CA-C	6.58	123.02	109.34
1	A	108	VAL	N-CA-C	6.54	122.95	109.34
1	E	108	VAL	N-CA-C	6.45	122.75	109.34
1	C	108	VAL	N-CA-C	6.36	122.58	109.34
1	C	112	ALA	N-CA-C	6.30	116.76	107.88
1	A	109	SER	N-CA-C	6.26	118.92	108.96
1	D	112	ALA	N-CA-C	6.24	116.68	107.88
2	R	28	U	N1-C1'-C2'	6.22	121.34	112.00
1	D	109	SER	N-CA-C	6.22	118.84	108.96
1	E	109	SER	N-CA-C	6.20	118.81	108.96
2	R	22	U	O3'-P-O5'	-6.16	94.76	104.00
2	R	39	U	O4'-C1'-N1	-6.10	99.36	108.50
2	R	9	U	O4'-C1'-N1	6.04	117.56	108.50
1	D	108	VAL	N-CA-C	6.02	121.87	109.34
1	B	112	ALA	N-CA-C	5.96	116.28	107.88
1	A	112	ALA	N-CA-C	5.95	116.27	107.88
1	B	129	ALA	N-CA-C	-5.93	99.96	109.39
2	R	27	U	O4'-C1'-N1	5.87	117.30	108.50
1	E	112	ALA	N-CA-C	5.86	116.14	107.88
2	R	25	U	P-O3'-C3'	5.84	128.97	120.20
1	B	109	SER	N-CA-C	5.84	119.15	109.46
2	R	12	U	O3'-P-O5'	-5.82	95.27	104.00
1	D	129	ALA	N-CA-C	-5.80	100.17	109.39
1	B	166	MET	N-CA-C	-5.74	105.95	113.12
2	R	10	U	P-O3'-C3'	5.72	128.77	120.20
1	C	369	PRO	CA-C-N	5.64	126.89	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	PRO	C-N-CA	5.64	126.89	119.84
1	A	33	ARG	N-CA-C	-5.62	103.98	111.24
1	B	349	CYS	N-CA-C	5.61	115.95	108.38
1	B	174	LEU	N-CA-C	-5.54	105.81	113.18
1	C	109	SER	N-CA-C	5.51	117.73	108.96
2	R	26	U	P-O3'-C3'	-5.46	112.00	120.20
2	R	24	U	P-O3'-C3'	5.46	128.40	120.20
1	A	163	GLN	N-CA-C	5.38	122.27	110.80
1	E	161	THR	N-CA-C	-5.38	106.41	112.87
1	A	174	LEU	N-CA-C	-5.38	106.03	113.18
1	E	129	ALA	N-CA-C	-5.37	100.85	109.39
1	B	4	THR	N-CA-C	5.35	117.11	108.34
1	D	4	THR	N-CA-C	5.28	117.00	108.34
1	A	182	PHE	N-CA-C	-5.23	106.92	113.72
1	C	161	THR	N-CA-C	-5.22	106.60	112.87
1	D	182	PHE	N-CA-C	-5.22	106.93	113.72
2	R	19	U	P-O3'-C3'	5.22	128.03	120.20
1	A	161	THR	N-CA-C	-5.22	106.61	112.87
1	D	5	VAL	CB-CA-C	-5.20	103.39	110.77
1	E	4	THR	N-CA-C	5.18	116.83	108.34
2	R	23	U	N1-C1'-C2'	5.14	119.71	112.00
1	C	245	VAL	CB-CA-C	-5.13	105.32	112.04
1	E	5	VAL	CB-CA-C	-5.07	103.57	110.77
2	R	43	U	O3'-P-O5'	-5.04	96.44	104.00
2	R	18	U	O4'-C1'-N1	5.03	116.05	108.50
1	C	4	THR	N-CA-C	5.01	116.56	108.34

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	LEU	Peptide
1	A	98	ALA	Peptide
1	A	99	GLY	Peptide
1	B	107	LEU	Peptide
1	B	163	GLN	Peptide
1	B	165	LYS	Peptide
1	B	97	LYS	Peptide
1	C	107	LEU	Peptide
1	C	163	GLN	Peptide
1	C	165	LYS	Peptide
1	D	107	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	167	ILE	Peptide
1	D	97	LYS	Peptide
1	E	107	LEU	Peptide
1	E	128	SER	Peptide
1	E	165	LYS	Peptide
1	E	97	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3327	0	3287	286	0
1	B	3290	0	3253	282	0
1	C	3275	0	3242	302	0
1	D	3298	0	3264	288	0
1	E	3327	0	3287	276	0
2	R	900	0	451	86	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
3	E	3	0	0	0	0
3	R	5	0	0	0	0
All	All	17437	0	16784	1425	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 42.

All (1425) 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:B:165:LYS:HB3	1:B:166:MET:SD	1.48	1.53
1:C:165:LYS:HB3	1:C:166:MET:SD	1.47	1.51
1:B:167:ILE:HD13	1:B:168:ASN:N	1.30	1.37
1:A:165:LYS:HB3	1:A:166:MET:SD	1.67	1.33
1:B:165:LYS:CB	1:B:166:MET:SD	2.28	1.22

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:LYS:CB	1:C:166:MET:SD	2.27	1.21
1:E:160:LEU:O	1:E:163:GLN:HB2	1.41	1.20
1:C:160:LEU:O	1:C:163:GLN:HB2	1.39	1.20
1:E:163:GLN:OE1	1:E:163:GLN:HA	1.43	1.19
1:A:87:ASP:OD2	1:A:97:LYS:HG3	1.38	1.17
1:C:163:GLN:OE1	1:C:163:GLN:HA	1.43	1.17
1:B:160:LEU:O	1:B:163:GLN:HB2	1.42	1.15
1:B:163:GLN:HA	1:B:163:GLN:OE1	1.43	1.10
1:D:165:LYS:C	1:D:166:MET:SD	2.41	1.04
1:E:117:LEU:HB3	1:E:118:PRO:CD	1.88	1.03
1:B:117:LEU:HB3	1:B:118:PRO:CD	1.89	1.01
1:D:117:LEU:HB3	1:D:118:PRO:CD	1.90	1.01
1:A:364:LEU:HB2	1:A:368:ALA:HB2	1.36	1.01
1:C:117:LEU:HB3	1:C:118:PRO:CD	1.89	1.01
1:A:117:LEU:HB3	1:A:118:PRO:CD	1.90	1.00
1:C:184:VAL:HB	1:D:166:MET:HE1	1.41	1.00
1:A:165:LYS:CB	1:A:166:MET:SD	2.49	0.99
1:E:117:LEU:HB3	1:E:118:PRO:HD2	1.45	0.99
1:B:167:ILE:CD1	1:B:168:ASN:N	2.25	0.98
1:C:137:TYR:HD1	1:C:163:GLN:HE21	1.12	0.97
1:C:48:LEU:HD22	1:C:48:LEU:H	1.30	0.96
1:A:117:LEU:HB3	1:A:118:PRO:HD2	1.49	0.95
1:A:48:LEU:H	1:A:48:LEU:HD22	1.32	0.94
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.49	0.94
1:C:180:ASP:H	1:C:183:ASP:CG	1.76	0.94
1:E:137:TYR:HD1	1:E:163:GLN:HE21	1.07	0.94
1:C:117:LEU:HB3	1:C:118:PRO:HD2	1.48	0.94
1:D:117:LEU:HB3	1:D:118:PRO:HD2	1.49	0.93
1:E:167:ILE:HD13	1:E:168:ASN:H	1.33	0.93
1:E:302:GLN:HB3	1:E:412:ILE:CD1	1.99	0.93
1:B:48:LEU:H	1:B:48:LEU:HD22	1.34	0.92
1:B:117:LEU:HB3	1:B:118:PRO:HD2	1.50	0.92
1:D:48:LEU:H	1:D:48:LEU:HD22	1.36	0.91
1:C:160:LEU:HA	1:C:163:GLN:HG2	1.54	0.90
1:E:149:MET:HG3	2:R:42:U:O4'	1.71	0.90
1:B:302:GLN:HB3	1:B:412:ILE:CD1	2.02	0.90
1:D:177:GLU:HA	1:D:181:ILE:HD13	1.53	0.89
1:E:160:LEU:C	1:E:163:GLN:HB2	1.98	0.89
1:D:302:GLN:HB3	1:D:412:ILE:CD1	2.03	0.89
1:E:180:ASP:H	1:E:183:ASP:CG	1.80	0.89
2:R:10:U:H2'	2:R:11:U:C6	2.08	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.55	0.88
1:C:302:GLN:HB3	1:C:412:ILE:CD1	2.03	0.88
1:E:48:LEU:HD22	1:E:48:LEU:H	1.37	0.88
1:A:167:ILE:HD13	1:A:168:ASN:H	1.37	0.88
1:C:376:VAL:HG13	1:D:354:LYS:HB2	1.55	0.88
1:E:160:LEU:HA	1:E:163:GLN:HG2	1.55	0.87
1:B:137:TYR:HD1	1:B:163:GLN:HE21	1.16	0.87
1:D:167:ILE:HG22	1:D:167:ILE:O	1.73	0.87
1:D:97:LYS:O	1:D:100:ASP:HB2	1.74	0.86
1:A:177:GLU:HA	1:A:181:ILE:HD13	1.57	0.86
1:E:365:THR:HG23	1:E:366:THR:N	1.91	0.86
1:D:74:TYR:CE1	1:D:78:LYS:HD3	2.10	0.86
1:A:180:ASP:H	1:A:183:ASP:CG	1.84	0.86
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.56	0.86
1:B:160:LEU:HA	1:B:163:GLN:HG2	1.58	0.86
2:R:25:U:H2'	2:R:26:U:C6	2.11	0.85
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.57	0.85
1:D:180:ASP:H	1:D:183:ASP:CG	1.85	0.85
1:E:160:LEU:O	1:E:163:GLN:CB	2.24	0.85
1:A:97:LYS:HG2	1:A:98:ALA:H	1.40	0.85
1:C:354:LYS:HE3	1:C:356:THR:HA	1.58	0.85
1:A:302:GLN:HB3	1:A:412:ILE:CD1	2.06	0.85
1:C:177:GLU:HA	1:C:181:ILE:HD13	1.58	0.85
1:B:167:ILE:HD13	1:B:167:ILE:C	2.01	0.85
1:D:137:TYR:HD1	1:D:163:GLN:HE21	1.22	0.85
1:A:167:ILE:H	1:A:167:ILE:CD1	1.89	0.84
1:B:97:LYS:O	1:B:100:ASP:HB2	1.76	0.84
1:C:160:LEU:C	1:C:163:GLN:HB2	2.02	0.84
1:A:137:TYR:HD1	1:A:163:GLN:HE21	1.22	0.84
1:B:18:LEU:HD12	1:C:232:GLY:HA2	1.59	0.84
1:D:165:LYS:CA	1:D:166:MET:SD	2.66	0.84
1:C:182:PHE:HD2	1:C:183:ASP:N	1.74	0.83
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.58	0.83
1:D:354:LYS:HE3	1:D:356:THR:HA	1.60	0.83
1:A:182:PHE:HD2	1:A:183:ASP:N	1.75	0.83
1:A:214:ARG:HA	1:A:217:THR:HG22	1.59	0.83
1:E:74:TYR:CE1	1:E:78:LYS:HD3	2.13	0.83
1:A:97:LYS:CG	1:A:98:ALA:H	1.90	0.83
1:B:167:ILE:HD13	1:B:168:ASN:H	1.04	0.83
1:A:74:TYR:CE1	1:A:78:LYS:HD3	2.14	0.83
1:E:364:LEU:H	1:E:364:LEU:HD12	1.44	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:THR:HG21	1:D:415:TYR:OH	1.79	0.82
1:D:182:PHE:HD2	1:D:183:ASP:N	1.77	0.82
1:B:153:ARG:NH2	1:B:176:PRO:HA	1.94	0.82
1:B:354:LYS:HE3	1:B:356:THR:HA	1.60	0.82
1:E:182:PHE:HD2	1:E:183:ASP:N	1.76	0.82
1:C:214:ARG:HA	1:C:217:THR:HG22	1.62	0.82
1:B:182:PHE:HD2	1:B:183:ASP:N	1.77	0.81
1:C:160:LEU:O	1:C:163:GLN:CB	2.25	0.81
1:E:215:TYR:CD1	2:R:45:U:H5''	2.15	0.81
1:A:97:LYS:HG2	1:A:98:ALA:N	1.96	0.81
1:A:199:ASP:OD1	1:A:217:THR:HG23	1.80	0.81
1:D:133:TRP:HB3	1:D:167:ILE:CD1	2.10	0.81
1:D:166:MET:SD	1:D:166:MET:N	2.54	0.81
1:B:214:ARG:HA	1:B:217:THR:HG22	1.63	0.81
1:C:181:ILE:HD12	1:C:181:ILE:N	1.96	0.80
1:E:354:LYS:HE3	1:E:356:THR:HA	1.61	0.80
1:A:364:LEU:HB2	1:A:368:ALA:CB	2.12	0.80
1:B:342:ALA:HB1	1:B:344:LEU:HD23	1.63	0.80
1:A:354:LYS:HE3	1:A:356:THR:HA	1.62	0.80
1:B:160:LEU:C	1:B:163:GLN:HB2	2.05	0.80
1:A:87:ASP:OD2	1:A:97:LYS:CG	2.25	0.80
1:C:199:ASP:OD1	1:C:217:THR:HG23	1.82	0.80
1:E:214:ARG:HA	1:E:217:THR:HG22	1.63	0.80
1:E:199:ASP:OD1	1:E:217:THR:HG23	1.81	0.80
1:A:167:ILE:HD13	1:A:167:ILE:H	1.44	0.79
1:B:74:TYR:CE1	1:B:78:LYS:HD3	2.17	0.79
1:C:167:ILE:HD13	1:C:168:ASN:H	1.47	0.79
1:C:66:ILE:HG13	1:C:70:ASN:HD21	1.47	0.79
1:B:180:ASP:H	1:B:183:ASP:CG	1.91	0.79
1:B:199:ASP:OD1	1:B:217:THR:HG23	1.82	0.79
1:A:181:ILE:HD12	1:A:181:ILE:N	1.98	0.79
1:B:160:LEU:O	1:B:163:GLN:CB	2.29	0.79
1:D:141:LEU:HD13	1:D:182:PHE:HD1	1.48	0.79
1:B:152:TYR:OH	1:B:176:PRO:HB3	1.83	0.78
1:D:214:ARG:HA	1:D:217:THR:HG22	1.66	0.78
1:C:74:TYR:CE1	1:C:78:LYS:HD3	2.17	0.78
1:A:167:ILE:HD13	1:A:168:ASN:N	1.97	0.78
1:A:54:TYR:HE1	1:A:118:PRO:HB2	1.49	0.78
1:C:308:LEU:O	1:C:309:ARG:HB2	1.83	0.78
1:D:133:TRP:CD1	1:D:167:ILE:HD13	2.19	0.78
1:E:167:ILE:HD13	1:E:168:ASN:N	1.97	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HD12	1:A:97:LYS:H	1.47	0.77
1:B:224:ASP:CG	2:R:21:U:H4'	2.10	0.77
1:D:66:ILE:HG13	1:D:70:ASN:HD21	1.49	0.77
1:D:364:LEU:HB2	1:D:368:ALA:HB2	1.66	0.77
1:B:106:ASP:O	1:B:107:LEU:HG	1.85	0.77
1:C:48:LEU:H	1:C:48:LEU:CD2	1.97	0.77
1:B:141:LEU:HD13	1:B:182:PHE:HD1	1.50	0.76
1:C:342:ALA:HB1	1:C:344:LEU:HD23	1.67	0.76
1:D:302:GLN:HB3	1:D:412:ILE:HD11	1.67	0.76
1:A:342:ALA:HB1	1:A:344:LEU:HD23	1.67	0.76
1:B:328:THR:HG21	1:B:415:TYR:OH	1.85	0.76
1:C:48:LEU:HD22	1:C:48:LEU:N	1.99	0.76
1:A:181:ILE:HD12	1:A:181:ILE:H	1.50	0.76
1:B:28:PRO:HD2	1:B:266:GLN:HE21	1.50	0.76
1:C:54:TYR:HE1	1:C:118:PRO:HB2	1.51	0.76
1:D:199:ASP:OD1	1:D:217:THR:HG23	1.84	0.76
1:E:66:ILE:HG13	1:E:70:ASN:HD21	1.49	0.76
1:A:66:ILE:HG13	1:A:70:ASN:HD21	1.49	0.76
1:B:178:GLY:O	1:B:179:ARG:HB2	1.84	0.76
1:D:141:LEU:HD22	1:D:182:PHE:CE1	2.21	0.76
1:A:28:PRO:HD2	1:A:266:GLN:HE21	1.51	0.75
1:B:54:TYR:HE1	1:B:118:PRO:HB2	1.51	0.75
1:C:181:ILE:HD12	1:C:181:ILE:H	1.51	0.75
1:E:28:PRO:HD2	1:E:266:GLN:HE21	1.51	0.75
1:A:364:LEU:HD12	1:A:364:LEU:H	1.51	0.75
1:B:81:ARG:HB3	1:B:208:HIS:HE2	1.51	0.75
2:R:17:U:H2'	2:R:18:U:H5''	1.67	0.75
1:A:48:LEU:HD22	1:A:48:LEU:N	2.01	0.75
1:D:286:LYS:HD2	2:R:2:U:H5''	1.67	0.75
1:E:181:ILE:H	1:E:181:ILE:HD12	1.52	0.75
1:D:106:ASP:O	1:D:107:LEU:HG	1.87	0.75
1:A:48:LEU:H	1:A:48:LEU:CD2	1.98	0.75
1:A:308:LEU:O	1:A:309:ARG:HB2	1.86	0.75
1:D:81:ARG:HB3	1:D:208:HIS:HE2	1.50	0.75
1:E:181:ILE:HD12	1:E:181:ILE:N	2.02	0.75
1:E:175:VAL:O	1:E:176:PRO:O	2.04	0.74
1:E:54:TYR:HE1	1:E:118:PRO:HB2	1.50	0.74
1:C:81:ARG:HB3	1:C:208:HIS:HE2	1.51	0.74
1:D:28:PRO:HD2	1:D:266:GLN:HE21	1.53	0.74
1:D:181:ILE:HD12	1:D:181:ILE:H	1.51	0.74
1:B:380:GLY:HA2	1:C:354:LYS:NZ	2.03	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LEU:HD23	1:B:274:TYR:OH	1.88	0.74
1:D:54:TYR:HE1	1:D:118:PRO:HB2	1.53	0.74
1:E:117:LEU:CB	1:E:118:PRO:HD2	2.17	0.73
1:E:160:LEU:HA	1:E:163:GLN:CG	2.17	0.73
1:C:117:LEU:CB	1:C:118:PRO:HD2	2.19	0.73
1:A:167:ILE:CD1	1:A:167:ILE:N	2.49	0.73
1:B:181:ILE:N	1:B:181:ILE:HD12	2.03	0.73
1:B:141:LEU:HD22	1:B:182:PHE:CE1	2.23	0.73
1:D:342:ALA:HB1	1:D:344:LEU:HD23	1.70	0.73
1:B:48:LEU:H	1:B:48:LEU:CD2	2.01	0.73
1:C:141:LEU:HD13	1:C:182:PHE:HD1	1.52	0.73
1:D:181:ILE:HD12	1:D:181:ILE:N	2.02	0.73
1:E:177:GLU:HG2	1:E:183:ASP:OD1	1.88	0.73
1:E:302:GLN:HB3	1:E:412:ILE:HD11	1.68	0.73
1:D:141:LEU:HD22	1:D:182:PHE:HE1	1.54	0.73
1:E:28:PRO:HD2	1:E:266:GLN:NE2	2.04	0.73
1:E:81:ARG:HB3	1:E:208:HIS:HE2	1.52	0.73
1:A:117:LEU:CB	1:A:118:PRO:HD2	2.19	0.73
1:B:66:ILE:HG13	1:B:70:ASN:HD21	1.53	0.73
1:E:69:VAL:HG23	1:E:138:LEU:HD13	1.70	0.73
1:E:237:ILE:HD13	1:E:237:ILE:O	1.88	0.72
1:A:81:ARG:HB3	1:A:208:HIS:HE2	1.53	0.72
1:A:143:ARG:HD2	1:A:216:GLY:HA2	1.71	0.72
1:E:160:LEU:CA	1:E:163:GLN:HB2	2.19	0.72
1:E:342:ALA:HB1	1:E:344:LEU:HD23	1.71	0.72
1:E:358:ASP:CG	1:E:359:ASP:H	1.97	0.72
1:B:177:GLU:CD	1:B:178:GLY:H	1.97	0.72
1:D:48:LEU:H	1:D:48:LEU:CD2	2.02	0.72
1:E:141:LEU:HD13	1:E:182:PHE:HD1	1.52	0.72
1:A:354:LYS:HB2	1:E:376:VAL:HG13	1.71	0.72
1:D:117:LEU:CB	1:D:118:PRO:HD2	2.20	0.72
1:A:87:ASP:CG	1:A:97:LYS:HG3	2.14	0.72
1:A:143:ARG:HH12	2:R:36:U:H5'	1.53	0.72
1:B:181:ILE:HD12	1:B:181:ILE:H	1.53	0.72
1:C:167:ILE:HD13	1:C:168:ASN:N	2.03	0.72
1:B:79:ASP:O	1:B:79:ASP:OD2	2.08	0.72
1:E:160:LEU:HA	1:E:163:GLN:HB2	1.72	0.72
1:B:308:LEU:O	1:B:309:ARG:HB2	1.87	0.72
1:C:107:LEU:HD23	1:C:274:TYR:OH	1.90	0.72
1:E:163:GLN:OE1	1:E:163:GLN:CA	2.30	0.72
1:A:106:ASP:O	1:A:107:LEU:HG	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:OE1	1:B:163:GLN:CA	2.30	0.72
1:B:365:THR:HG23	1:B:366:THR:N	2.05	0.72
1:C:162:ASN:O	1:C:164:CYS:N	2.22	0.71
1:D:308:LEU:O	1:D:309:ARG:HB2	1.90	0.71
1:B:162:ASN:O	1:B:164:CYS:N	2.22	0.71
1:E:29:ALA:O	1:E:31:TYR:N	2.22	0.71
1:E:137:TYR:HD1	1:E:163:GLN:NE2	1.87	0.71
1:B:28:PRO:HD2	1:B:266:GLN:NE2	2.05	0.71
1:C:141:LEU:HD22	1:C:182:PHE:CE1	2.26	0.71
1:A:143:ARG:HE	1:A:155:LYS:NZ	1.89	0.71
1:B:376:VAL:HG13	1:C:354:LYS:HB2	1.73	0.71
1:C:143:ARG:HD2	1:C:216:GLY:HA2	1.71	0.71
2:R:19:U:HO2'	2:R:20:U:H6	1.37	0.71
1:D:160:LEU:O	1:D:163:GLN:HB2	1.91	0.71
1:B:117:LEU:CB	1:B:118:PRO:HD2	2.20	0.71
1:B:302:GLN:HB3	1:B:412:ILE:HD11	1.71	0.71
1:D:48:LEU:HD22	1:D:48:LEU:N	2.06	0.71
1:E:97:LYS:O	1:E:100:ASP:HB2	1.91	0.71
1:E:117:LEU:CB	1:E:118:PRO:CD	2.69	0.71
1:A:141:LEU:HD22	1:A:182:PHE:CE1	2.25	0.71
1:B:141:LEU:HD22	1:B:182:PHE:HE1	1.56	0.71
1:A:163:GLN:O	1:A:165:LYS:N	2.23	0.70
1:A:376:VAL:HG13	1:B:354:LYS:HB2	1.72	0.70
1:B:18:LEU:CD1	1:C:232:GLY:HA2	2.21	0.70
1:B:143:ARG:HD2	1:B:216:GLY:HA2	1.72	0.70
1:C:160:LEU:HA	1:C:163:GLN:CG	2.22	0.70
1:E:141:LEU:HD22	1:E:182:PHE:CE1	2.25	0.70
1:C:117:LEU:CB	1:C:118:PRO:CD	2.69	0.70
1:C:165:LYS:HB2	1:C:166:MET:SD	2.31	0.70
1:E:308:LEU:O	1:E:309:ARG:HB2	1.90	0.70
1:E:328:THR:HG21	1:E:415:TYR:OH	1.91	0.70
1:D:69:VAL:HG23	1:D:138:LEU:HD13	1.74	0.70
1:E:143:ARG:HD2	1:E:216:GLY:HA2	1.72	0.70
1:A:141:LEU:HD13	1:A:182:PHE:HD1	1.54	0.70
1:B:130:ASP:CG	1:B:131:ASP:H	1.97	0.70
1:E:107:LEU:HD23	1:E:274:TYR:OH	1.92	0.70
1:A:160:LEU:O	1:A:163:GLN:HB2	1.92	0.70
1:B:106:ASP:C	1:B:107:LEU:HG	2.14	0.70
1:D:177:GLU:CD	1:D:178:GLY:H	2.00	0.70
1:D:253:GLU:H	1:D:253:GLU:CD	1.99	0.70
1:C:28:PRO:HD2	1:C:266:GLN:HE21	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:LEU:HD23	1:D:274:TYR:OH	1.90	0.70
1:E:130:ASP:CG	1:E:131:ASP:H	1.99	0.70
1:E:152:TYR:OH	1:E:176:PRO:HB3	1.91	0.70
2:R:36:U:H2'	2:R:37:U:O4'	1.92	0.70
1:B:48:LEU:HD22	1:B:48:LEU:N	2.07	0.69
1:A:177:GLU:CD	1:A:178:GLY:H	2.00	0.69
1:C:28:PRO:HD2	1:C:266:GLN:NE2	2.07	0.69
1:B:117:LEU:CB	1:B:118:PRO:CD	2.69	0.69
1:B:179:ARG:O	1:C:161:THR:HG22	1.92	0.69
1:C:97:LYS:O	1:C:98:ALA:C	2.35	0.69
1:A:69:VAL:HG23	1:A:138:LEU:HD13	1.74	0.69
1:A:214:ARG:HA	1:A:217:THR:CG2	2.22	0.69
1:E:48:LEU:HD22	1:E:48:LEU:N	2.05	0.69
1:E:48:LEU:H	1:E:48:LEU:CD2	2.04	0.69
1:E:153:ARG:NH2	1:E:176:PRO:HA	2.07	0.69
1:A:141:LEU:HD22	1:A:182:PHE:HE1	1.58	0.69
1:A:328:THR:HG21	1:A:415:TYR:OH	1.92	0.69
1:E:106:ASP:O	1:E:107:LEU:HG	1.91	0.69
1:A:54:TYR:CE1	1:A:118:PRO:HB2	2.27	0.69
1:C:163:GLN:OE1	1:C:163:GLN:CA	2.30	0.69
1:C:177:GLU:CD	1:C:178:GLY:H	2.00	0.69
1:D:28:PRO:HD2	1:D:266:GLN:NE2	2.07	0.69
1:D:257:GLU:HG2	1:D:294:ASN:HA	1.72	0.69
1:B:214:ARG:HA	1:B:217:THR:CG2	2.22	0.69
1:B:356:THR:N	1:B:357:PRO:HD2	2.07	0.69
1:D:51:LEU:O	1:D:55:VAL:HG22	1.93	0.68
1:D:141:LEU:HD13	1:D:182:PHE:CD1	2.28	0.68
1:B:130:ASP:CG	1:B:131:ASP:N	2.49	0.68
1:B:167:ILE:CD1	1:B:168:ASN:H	1.94	0.68
1:A:161:THR:HB	1:E:179:ARG:HB2	1.75	0.68
1:B:69:VAL:HG23	1:B:138:LEU:HD13	1.74	0.68
1:C:328:THR:HG21	1:C:415:TYR:OH	1.94	0.68
1:C:141:LEU:HD22	1:C:182:PHE:HE1	1.58	0.68
1:D:29:ALA:O	1:D:31:TYR:N	2.22	0.68
1:E:141:LEU:HD22	1:E:182:PHE:HE1	1.57	0.68
1:A:28:PRO:HD2	1:A:266:GLN:NE2	2.08	0.68
1:A:130:ASP:CG	1:A:131:ASP:H	2.01	0.68
1:A:290:SER:HB2	2:R:30:U:H5'	1.73	0.68
1:A:29:ALA:O	1:A:31:TYR:N	2.26	0.68
1:B:29:ALA:O	1:B:31:TYR:N	2.23	0.68
1:D:133:TRP:HB3	1:D:167:ILE:HD12	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:ARG:HA	1:E:217:THR:CG2	2.24	0.67
1:E:365:THR:HG23	1:E:366:THR:H	1.57	0.67
1:B:58:GLY:HA3	1:B:64:VAL:HB	1.76	0.67
1:C:29:ALA:O	1:C:31:TYR:N	2.24	0.67
1:C:54:TYR:CE1	1:C:118:PRO:HB2	2.29	0.67
1:C:172:GLU:HB3	1:C:173:PRO:HD3	1.77	0.67
1:C:58:GLY:HA3	1:C:64:VAL:HB	1.77	0.67
1:C:69:VAL:HG23	1:C:138:LEU:HD13	1.76	0.67
1:C:214:ARG:HA	1:C:217:THR:CG2	2.24	0.67
1:D:165:LYS:HA	1:D:166:MET:SD	2.33	0.67
1:A:163:GLN:C	1:A:165:LYS:H	2.02	0.67
1:B:141:LEU:HD13	1:B:182:PHE:CD1	2.30	0.67
1:C:79:ASP:O	1:C:79:ASP:OD2	2.13	0.67
1:E:54:TYR:CE1	1:E:118:PRO:HB2	2.29	0.67
1:B:237:ILE:HD13	1:B:237:ILE:O	1.95	0.67
1:B:160:LEU:HA	1:B:163:GLN:CG	2.25	0.67
1:E:224:ASP:CG	2:R:39:U:H4'	2.20	0.67
1:B:54:TYR:CE1	1:B:118:PRO:HB2	2.29	0.66
1:C:130:ASP:CG	1:C:131:ASP:N	2.53	0.66
1:E:106:ASP:C	1:E:107:LEU:HG	2.20	0.66
2:R:39:U:H5''	2:R:39:U:H6	1.61	0.66
1:B:70:ASN:H	1:B:70:ASN:HD22	1.43	0.66
1:C:97:LYS:O	1:C:100:ASP:HB2	1.96	0.66
1:D:356:THR:N	1:D:357:PRO:HD2	2.10	0.66
1:E:58:GLY:HA3	1:E:64:VAL:HB	1.77	0.66
1:B:179:ARG:HB3	1:C:161:THR:HB	1.77	0.66
1:C:184:VAL:CB	1:D:166:MET:HE1	2.24	0.66
1:B:165:LYS:HB2	1:B:166:MET:SD	2.31	0.66
1:D:169:GLU:C	1:D:170:GLN:HG2	2.21	0.66
1:B:22:GLU:OE2	1:B:22:GLU:HA	1.94	0.66
1:B:129:ALA:HA	1:B:132:LYS:CE	2.26	0.66
1:C:141:LEU:HD13	1:C:182:PHE:CD1	2.30	0.66
1:C:257:GLU:HG2	1:C:294:ASN:HA	1.77	0.66
1:A:106:ASP:C	1:A:107:LEU:HG	2.19	0.66
1:A:356:THR:N	1:A:357:PRO:HD2	2.11	0.66
1:C:70:ASN:HD22	1:C:70:ASN:H	1.44	0.66
1:E:257:GLU:HG2	1:E:294:ASN:HA	1.78	0.66
1:D:143:ARG:HH21	2:R:8:U:H5''	1.59	0.66
1:D:117:LEU:CB	1:D:118:PRO:CD	2.70	0.65
1:E:162:ASN:O	1:E:164:CYS:N	2.28	0.65
1:A:98:ALA:O	1:A:100:ASP:N	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLY:HA2	1:C:354:LYS:HZ3	1.59	0.65
1:C:302:GLN:HB3	1:C:412:ILE:HD11	1.77	0.65
1:A:117:LEU:CB	1:A:118:PRO:CD	2.69	0.65
1:D:130:ASP:CG	1:D:131:ASP:H	2.03	0.65
1:B:253:GLU:H	1:B:253:GLU:CD	2.03	0.65
1:D:54:TYR:CE1	1:D:118:PRO:HB2	2.31	0.65
1:D:58:GLY:HA3	1:D:64:VAL:HB	1.79	0.65
1:A:130:ASP:CG	1:A:131:ASP:N	2.54	0.65
1:C:130:ASP:CG	1:C:131:ASP:H	2.01	0.65
1:D:133:TRP:CG	1:D:167:ILE:HD13	2.30	0.65
1:D:70:ASN:H	1:D:70:ASN:HD22	1.44	0.65
1:D:143:ARG:HD2	1:D:216:GLY:HA2	1.77	0.65
1:A:58:GLY:HA3	1:A:64:VAL:HB	1.78	0.65
1:E:177:GLU:HA	1:E:181:ILE:HD13	1.79	0.65
1:E:253:GLU:CD	1:E:253:GLU:H	2.02	0.65
1:A:107:LEU:HD23	1:A:274:TYR:OH	1.97	0.65
1:D:214:ARG:HA	1:D:217:THR:CG2	2.26	0.65
1:D:74:TYR:O	1:D:78:LYS:HG3	1.96	0.65
1:E:104:ILE:O	1:E:107:LEU:HD12	1.97	0.65
1:E:130:ASP:CG	1:E:131:ASP:N	2.51	0.65
1:A:84:LEU:HD12	1:A:97:LYS:N	2.12	0.65
1:B:152:TYR:CE1	1:B:177:GLU:HB2	2.32	0.65
1:C:163:GLN:O	1:C:165:LYS:N	2.30	0.65
1:E:164:CYS:O	1:E:165:LYS:C	2.40	0.65
1:A:141:LEU:HD13	1:A:182:PHE:CD1	2.32	0.64
1:B:163:GLN:O	1:B:165:LYS:N	2.30	0.64
1:E:163:GLN:O	1:E:165:LYS:N	2.30	0.64
1:B:136:LEU:HD23	1:B:136:LEU:O	1.97	0.64
1:E:141:LEU:HD13	1:E:182:PHE:CD1	2.31	0.64
1:A:151:GLU:O	1:A:154:LYS:HB2	1.97	0.64
1:E:70:ASN:HD22	1:E:70:ASN:H	1.44	0.64
1:B:257:GLU:HG2	1:B:294:ASN:HA	1.80	0.64
1:C:160:LEU:CA	1:C:163:GLN:HB2	2.27	0.64
1:C:399:ARG:HA	1:C:402:MET:HE3	1.79	0.64
1:D:131:ASP:O	1:D:135:PRO:HD2	1.98	0.64
1:A:129:ALA:HA	1:A:132:LYS:CE	2.28	0.64
1:B:51:LEU:O	1:B:55:VAL:HG22	1.98	0.64
1:B:151:GLU:O	1:B:154:LYS:HB2	1.98	0.64
1:D:167:ILE:O	1:D:167:ILE:CG2	2.45	0.64
1:A:23:ASP:HB2	1:A:286:LYS:HD3	1.80	0.64
1:A:116:VAL:C	1:A:117:LEU:HD12	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ASP:CG	1:D:131:ASP:N	2.53	0.64
1:C:131:ASP:O	1:C:132:LYS:C	2.41	0.64
1:D:398:LYS:HG2	1:D:402:MET:HE2	1.79	0.64
1:A:253:GLU:CD	1:A:253:GLU:H	2.03	0.63
1:C:356:THR:N	1:C:357:PRO:HD2	2.12	0.63
1:D:106:ASP:C	1:D:107:LEU:HG	2.21	0.63
1:D:129:ALA:HA	1:D:132:LYS:CE	2.28	0.63
1:D:133:TRP:HB3	1:D:167:ILE:HD13	1.79	0.63
1:D:364:LEU:CB	1:D:368:ALA:HB2	2.28	0.63
1:A:74:TYR:O	1:A:78:LYS:HG3	1.98	0.63
1:B:169:GLU:C	1:B:170:GLN:HG2	2.23	0.63
1:C:106:ASP:O	1:C:107:LEU:HG	1.98	0.63
1:C:180:ASP:CG	1:D:164:CYS:SG	2.81	0.63
1:D:30:ASP:HA	1:D:33:ARG:HE	1.62	0.63
1:B:398:LYS:HG2	1:B:402:MET:HE2	1.80	0.63
1:C:43:ASN:O	1:C:44:THR:C	2.42	0.63
1:E:151:GLU:O	1:E:154:LYS:HB2	1.98	0.63
1:A:302:GLN:HB3	1:A:412:ILE:HD11	1.79	0.63
1:B:399:ARG:HA	1:B:402:MET:HE3	1.80	0.63
1:E:398:LYS:HG2	1:E:402:MET:HE2	1.80	0.63
1:A:131:ASP:O	1:A:132:LYS:C	2.42	0.63
1:C:105:PHE:C	1:C:107:LEU:H	2.07	0.63
1:E:354:LYS:CE	1:E:356:THR:HA	2.28	0.63
1:D:136:LEU:HD23	1:D:136:LEU:O	1.99	0.63
1:E:74:TYR:O	1:E:78:LYS:HG3	1.99	0.63
1:C:151:GLU:O	1:C:154:LYS:HB2	1.98	0.63
1:D:237:ILE:HD13	1:D:237:ILE:O	1.99	0.63
1:A:131:ASP:O	1:A:135:PRO:HD2	1.98	0.63
1:E:23:ASP:HB2	1:E:286:LYS:HD3	1.81	0.63
1:E:131:ASP:O	1:E:132:LYS:C	2.41	0.63
1:A:181:ILE:H	1:A:181:ILE:CD1	2.12	0.63
1:A:22:GLU:OE2	1:A:22:GLU:HA	1.98	0.62
1:D:22:GLU:HA	1:D:22:GLU:OE2	1.98	0.62
1:A:143:ARG:HG2	1:A:155:LYS:HE3	1.79	0.62
1:D:163:GLN:HA	1:D:163:GLN:OE1	1.99	0.62
1:A:398:LYS:HG2	1:A:402:MET:HE2	1.81	0.62
1:A:399:ARG:HA	1:A:402:MET:HE3	1.82	0.62
1:B:131:ASP:O	1:B:132:LYS:C	2.42	0.62
1:C:28:PRO:O	1:C:31:TYR:HB3	1.99	0.62
1:C:137:TYR:HD1	1:C:163:GLN:NE2	1.91	0.62
1:D:28:PRO:O	1:D:31:TYR:HB3	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:PRO:O	1:E:31:TYR:HB3	1.98	0.62
1:D:143:ARG:NH2	2:R:9:U:OP2	2.31	0.62
1:D:151:GLU:O	1:D:154:LYS:HB2	1.99	0.62
1:A:136:LEU:HD23	1:A:136:LEU:O	1.99	0.62
1:A:169:GLU:C	1:A:170:GLN:HG2	2.25	0.62
1:A:176:PRO:O	1:A:177:GLU:HB2	2.00	0.62
1:A:257:GLU:HG2	1:A:294:ASN:HA	1.82	0.62
1:E:160:LEU:HA	1:E:163:GLN:CB	2.29	0.62
1:E:356:THR:N	1:E:357:PRO:HD2	2.14	0.62
2:R:18:U:H4'	2:R:18:U:OP1	1.98	0.62
1:A:224:ASP:CG	2:R:30:U:H4'	2.24	0.62
1:B:179:ARG:O	1:C:161:THR:CG2	2.47	0.62
1:B:355:TYR:C	1:B:357:PRO:HD2	2.25	0.62
1:A:143:ARG:HE	1:A:155:LYS:HZ1	1.47	0.62
1:B:59:LEU:HB3	1:B:172:GLU:HG2	1.80	0.62
1:A:70:ASN:HD22	1:A:70:ASN:H	1.45	0.62
1:C:181:ILE:H	1:C:181:ILE:CD1	2.12	0.62
2:R:19:U:O2'	2:R:20:U:H6	1.82	0.62
1:C:81:ARG:CB	1:C:208:HIS:HE2	2.13	0.61
2:R:6:U:O5'	2:R:6:U:H6	1.83	0.61
1:A:51:LEU:O	1:A:55:VAL:HG22	1.99	0.61
1:B:177:GLU:HA	1:B:181:ILE:HD13	1.81	0.61
1:E:79:ASP:O	1:E:79:ASP:OD2	2.18	0.61
1:E:81:ARG:CB	1:E:208:HIS:HE2	2.13	0.61
1:A:172:GLU:HB3	1:A:173:PRO:HD3	1.82	0.61
1:B:81:ARG:CB	1:B:208:HIS:HE2	2.12	0.61
1:D:172:GLU:HB3	1:D:173:PRO:HD3	1.82	0.61
1:D:182:PHE:CD2	1:D:183:ASP:N	2.66	0.61
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.82	0.61
1:E:104:ILE:HD13	1:E:198:VAL:HG22	1.82	0.61
1:B:30:ASP:HA	1:B:33:ARG:HE	1.64	0.61
1:E:169:GLU:C	1:E:170:GLN:HG2	2.25	0.61
1:E:353:ASN:OD1	1:E:353:ASN:N	2.33	0.61
1:D:164:CYS:O	1:D:166:MET:N	2.33	0.61
1:E:129:ALA:HA	1:E:132:LYS:CE	2.30	0.61
1:C:398:LYS:HG2	1:C:402:MET:HE2	1.81	0.61
1:D:38:ILE:O	1:D:38:ILE:HG13	1.99	0.61
1:D:104:ILE:O	1:D:107:LEU:HD12	2.00	0.61
1:E:136:LEU:O	1:E:136:LEU:HD23	2.00	0.61
1:B:28:PRO:O	1:B:31:TYR:HB3	2.01	0.61
1:B:43:ASN:O	1:B:44:THR:C	2.44	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASP:HB2	1:C:286:LYS:HD3	1.82	0.61
1:C:129:ALA:HA	1:C:132:LYS:CE	2.30	0.61
1:C:176:PRO:O	1:C:177:GLU:HB2	2.00	0.61
1:B:160:LEU:HA	1:B:163:GLN:HB2	1.81	0.61
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.31	0.61
1:D:354:LYS:CE	1:D:356:THR:HA	2.30	0.61
1:E:399:ARG:HA	1:E:402:MET:HE3	1.83	0.61
1:A:43:ASN:O	1:A:44:THR:C	2.44	0.60
1:A:219:VAL:HG12	2:R:35:U:O4	2.01	0.60
1:A:237:ILE:HD13	1:A:237:ILE:O	2.01	0.60
1:C:160:LEU:HA	1:C:163:GLN:HB2	1.81	0.60
1:C:182:PHE:CD2	1:C:183:ASP:N	2.65	0.60
1:E:178:GLY:O	1:E:179:ARG:HB2	2.01	0.60
1:E:355:TYR:C	1:E:357:PRO:HD2	2.26	0.60
1:B:160:LEU:CA	1:B:163:GLN:HB2	2.29	0.60
1:E:182:PHE:CD2	1:E:183:ASP:N	2.66	0.60
1:B:38:ILE:HG13	1:B:38:ILE:O	2.01	0.60
1:C:51:LEU:O	1:C:55:VAL:HG22	2.01	0.60
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.83	0.60
1:A:79:ASP:O	1:A:79:ASP:OD2	2.19	0.60
1:A:354:LYS:CE	1:A:356:THR:HA	2.31	0.60
1:C:106:ASP:C	1:C:107:LEU:HG	2.25	0.60
1:D:176:PRO:O	1:D:177:GLU:HB2	2.00	0.60
1:B:365:THR:HG22	1:B:368:ALA:CB	2.32	0.60
1:C:22:GLU:OE2	1:C:22:GLU:HA	2.01	0.60
1:D:116:VAL:C	1:D:117:LEU:HD12	2.27	0.60
1:E:131:ASP:O	1:E:135:PRO:HD2	2.02	0.60
1:E:283:LEU:HD23	1:E:283:LEU:N	2.16	0.60
1:A:28:PRO:O	1:A:31:TYR:HB3	2.02	0.60
1:C:169:GLU:C	1:C:170:GLN:HG2	2.26	0.60
1:E:22:GLU:OE2	1:E:22:GLU:HA	2.01	0.60
1:A:232:GLY:HA2	1:E:18:LEU:HD12	1.84	0.60
1:A:283:LEU:N	1:A:283:LEU:HD23	2.17	0.60
1:C:136:LEU:O	1:C:136:LEU:HD23	2.01	0.60
1:C:355:TYR:C	1:C:357:PRO:HD2	2.27	0.60
1:E:43:ASN:O	1:E:44:THR:C	2.45	0.60
1:E:105:PHE:C	1:E:107:LEU:H	2.09	0.60
1:E:172:GLU:HB3	1:E:173:PRO:HD3	1.83	0.60
1:C:116:VAL:C	1:C:117:LEU:HD12	2.27	0.60
1:D:59:LEU:HB3	1:D:172:GLU:HG2	1.82	0.60
1:E:59:LEU:HB3	1:E:172:GLU:HG2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:GLU:CD	1:C:253:GLU:H	2.08	0.60
1:D:131:ASP:O	1:D:132:LYS:C	2.45	0.60
1:A:81:ARG:CB	1:A:208:HIS:HE2	2.15	0.59
1:B:72:TYR:CZ	1:B:134:LEU:HD12	2.37	0.59
1:A:163:GLN:OE1	1:A:163:GLN:HA	2.03	0.59
1:B:172:GLU:HB3	1:B:173:PRO:HD3	1.85	0.59
1:E:30:ASP:HA	1:E:33:ARG:HE	1.67	0.59
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.83	0.59
1:A:312:ARG:HG2	2:R:32:U:C2	2.37	0.59
1:C:59:LEU:HB3	1:C:172:GLU:HG2	1.83	0.59
1:C:72:TYR:CZ	1:C:134:LEU:HD12	2.37	0.59
1:B:74:TYR:O	1:B:78:LYS:HG3	2.01	0.59
1:C:162:ASN:O	1:C:163:GLN:C	2.44	0.59
1:C:237:ILE:HD13	1:C:237:ILE:O	2.02	0.59
2:R:9:U:O3'	2:R:10:U:H6	1.85	0.59
1:B:104:ILE:O	1:B:107:LEU:HD12	2.03	0.59
1:C:354:LYS:CE	1:C:356:THR:HA	2.29	0.59
1:E:151:GLU:HA	1:E:154:LYS:NZ	2.17	0.59
1:A:59:LEU:HB3	1:A:172:GLU:HG2	1.83	0.59
1:A:355:TYR:C	1:A:357:PRO:HD2	2.28	0.59
1:D:179:ARG:HA	1:D:183:ASP:CG	2.27	0.59
1:D:355:TYR:C	1:D:357:PRO:HD2	2.28	0.59
1:E:181:ILE:H	1:E:181:ILE:CD1	2.14	0.59
1:C:74:TYR:O	1:C:78:LYS:HG3	2.02	0.59
1:D:23:ASP:HB2	1:D:286:LYS:HD3	1.83	0.59
1:A:182:PHE:CD2	1:A:183:ASP:N	2.65	0.59
1:B:117:LEU:HB3	1:B:118:PRO:HD3	1.83	0.59
1:B:178:GLY:O	1:B:179:ARG:CB	2.50	0.59
1:D:81:ARG:CB	1:D:208:HIS:HE2	2.15	0.59
1:B:162:ASN:O	1:B:163:GLN:C	2.46	0.59
1:B:365:THR:HG23	1:B:366:THR:H	1.68	0.59
1:C:131:ASP:O	1:C:135:PRO:HD2	2.02	0.59
1:E:72:TYR:CZ	1:E:134:LEU:HD12	2.38	0.59
1:B:104:ILE:HD13	1:B:198:VAL:HG22	1.85	0.58
1:C:181:ILE:N	1:C:183:ASP:OD2	2.35	0.58
1:D:79:ASP:O	1:D:79:ASP:OD2	2.21	0.58
1:A:380:GLY:HA2	1:B:354:LYS:NZ	2.18	0.58
1:D:181:ILE:H	1:D:181:ILE:CD1	2.14	0.58
1:B:136:LEU:HD23	1:B:136:LEU:C	2.28	0.58
1:C:246:THR:HG22	1:D:348:PHE:CG	2.38	0.58
1:E:162:ASN:O	1:E:163:GLN:C	2.45	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:39:U:H2'	2:R:40:U:O4'	2.03	0.58
1:A:152:TYR:HE1	1:A:176:PRO:O	1.87	0.58
1:B:181:ILE:H	1:B:181:ILE:CD1	2.16	0.58
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.85	0.58
1:A:214:ARG:HH21	1:A:218:ILE:HG13	1.68	0.58
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.33	0.58
1:B:18:LEU:HD12	1:C:232:GLY:CA	2.31	0.58
1:C:180:ASP:N	1:C:183:ASP:CG	2.55	0.58
1:B:131:ASP:O	1:B:135:PRO:HD2	2.03	0.58
1:D:105:PHE:C	1:D:107:LEU:H	2.12	0.58
1:D:152:TYR:CE2	1:D:153:ARG:HG2	2.39	0.58
1:A:165:LYS:C	1:A:166:MET:SD	2.87	0.58
1:E:38:ILE:O	1:E:108:VAL:HB	2.04	0.58
1:E:116:VAL:C	1:E:117:LEU:HD12	2.29	0.58
1:C:181:ILE:N	1:C:181:ILE:CD1	2.66	0.57
1:E:136:LEU:HD23	1:E:136:LEU:C	2.29	0.57
1:A:152:TYR:CE2	1:A:153:ARG:HG2	2.40	0.57
1:B:116:VAL:C	1:B:117:LEU:HD12	2.30	0.57
1:B:365:THR:HG22	1:B:368:ALA:HB3	1.85	0.57
1:C:43:ASN:O	1:C:44:THR:O	2.23	0.57
1:D:286:LYS:NZ	2:R:2:U:OP1	2.35	0.57
1:D:399:ARG:HA	1:D:402:MET:HE3	1.86	0.57
1:D:286:LYS:NZ	2:R:2:U:P	2.77	0.57
1:A:104:ILE:O	1:A:107:LEU:HD12	2.04	0.57
1:E:177:GLU:CD	1:E:178:GLY:H	2.12	0.57
1:A:105:PHE:C	1:A:107:LEU:H	2.12	0.57
1:D:81:ARG:O	1:D:102:ILE:O	2.23	0.57
1:A:104:ILE:HD13	1:A:198:VAL:HG22	1.87	0.57
1:A:178:GLY:O	1:A:179:ARG:HB2	2.05	0.57
1:C:104:ILE:HD13	1:C:198:VAL:HG22	1.87	0.57
1:A:179:ARG:O	1:A:180:ASP:HB2	2.04	0.57
1:D:104:ILE:HD13	1:D:198:VAL:HG22	1.87	0.57
1:E:397:ALA:O	1:E:401:VAL:HG22	2.05	0.57
1:A:30:ASP:HA	1:A:33:ARG:HE	1.70	0.56
1:A:38:ILE:O	1:A:108:VAL:HB	2.04	0.56
1:C:38:ILE:O	1:C:108:VAL:HB	2.05	0.56
1:D:129:ALA:HA	1:D:132:LYS:NZ	2.20	0.56
1:A:72:TYR:CZ	1:A:134:LEU:HD12	2.40	0.56
1:A:151:GLU:HA	1:A:154:LYS:NZ	2.19	0.56
1:C:214:ARG:CA	1:C:217:THR:HG22	2.33	0.56
1:D:136:LEU:HD23	1:D:136:LEU:C	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:ARG:HH21	1:D:218:ILE:HG13	1.70	0.56
1:D:218:ILE:HD12	2:R:10:U:OP2	2.05	0.56
1:A:66:ILE:HG13	1:A:70:ASN:ND2	2.19	0.56
1:B:105:PHE:C	1:B:107:LEU:H	2.13	0.56
1:B:152:TYR:CE2	1:B:153:ARG:HG2	2.40	0.56
1:C:149:MET:HG3	2:R:15:U:O4'	2.05	0.56
1:C:179:ARG:HA	1:C:183:ASP:CG	2.29	0.56
1:E:152:TYR:CE1	1:E:153:ARG:NH1	2.73	0.56
1:A:66:ILE:HD12	1:A:69:VAL:CG1	2.35	0.56
1:A:179:ARG:HA	1:A:183:ASP:CG	2.31	0.56
1:B:44:THR:HG22	1:B:46:LYS:HZ2	1.70	0.56
1:B:151:GLU:HA	1:B:154:LYS:NZ	2.20	0.56
1:C:152:TYR:HE1	1:C:176:PRO:O	1.87	0.56
1:C:283:LEU:HD23	1:C:283:LEU:N	2.20	0.56
1:C:380:GLY:HA2	1:D:354:LYS:NZ	2.21	0.56
1:D:31:TYR:C	1:D:31:TYR:CD1	2.84	0.56
1:D:38:ILE:O	1:D:108:VAL:HB	2.05	0.56
1:A:317:ARG:O	1:A:319:PRO:HD3	2.06	0.56
1:D:151:GLU:HA	1:D:154:LYS:NZ	2.20	0.56
1:A:344:LEU:HD13	1:E:250:LEU:HB3	1.87	0.56
1:A:389:PRO:HB3	1:A:393:MET:HE2	1.87	0.56
1:D:214:ARG:CA	1:D:217:THR:HG22	2.35	0.56
1:E:66:ILE:HG13	1:E:70:ASN:ND2	2.19	0.56
1:B:152:TYR:CE1	1:B:153:ARG:NH1	2.74	0.56
1:C:66:ILE:HD12	1:C:69:VAL:CG1	2.36	0.56
1:C:302:GLN:HB3	1:C:412:ILE:HD13	1.88	0.56
1:C:389:PRO:HB3	1:C:393:MET:HE2	1.87	0.56
1:D:152:TYR:HE1	1:D:176:PRO:O	1.88	0.56
1:A:43:ASN:O	1:A:44:THR:O	2.24	0.56
1:C:179:ARG:O	1:C:180:ASP:HB2	2.05	0.56
1:C:136:LEU:HD23	1:C:136:LEU:C	2.31	0.56
1:D:55:VAL:HG23	1:D:56:TYR:H	1.70	0.56
1:A:22:GLU:O	1:A:23:ASP:C	2.49	0.55
1:A:345:ALA:O	1:A:347:GLN:HG2	2.06	0.55
1:C:104:ILE:O	1:C:107:LEU:HD12	2.06	0.55
1:D:72:TYR:CZ	1:D:134:LEU:HD12	2.42	0.55
1:E:143:ARG:HH22	2:R:44:U:H3'	1.70	0.55
1:B:45:THR:C	1:B:46:LYS:HE3	2.31	0.55
1:C:151:GLU:HA	1:C:154:LYS:NZ	2.21	0.55
1:D:356:THR:O	1:D:357:PRO:C	2.49	0.55
1:E:66:ILE:HD12	1:E:69:VAL:CG1	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:CB	1:A:368:ALA:HB2	2.24	0.55
1:C:15:VAL:O	1:C:17:LYS:HG2	2.06	0.55
1:C:66:ILE:HG13	1:C:70:ASN:ND2	2.19	0.55
1:A:180:ASP:N	1:A:183:ASP:CG	2.62	0.55
1:A:312:ARG:HG2	2:R:32:U:O2	2.06	0.55
1:B:31:TYR:CD1	1:B:31:TYR:C	2.82	0.55
1:C:180:ASP:HB3	1:C:181:ILE:HD12	1.89	0.55
1:C:324:TYR:O	1:C:328:THR:CG2	2.55	0.55
1:D:178:GLY:O	1:D:179:ARG:HB2	2.07	0.55
1:A:136:LEU:HD23	1:A:136:LEU:C	2.31	0.55
1:B:23:ASP:HB2	1:B:286:LYS:HD3	1.87	0.55
1:C:30:ASP:HA	1:C:33:ARG:HE	1.70	0.55
1:C:353:ASN:OD1	1:C:353:ASN:N	2.38	0.55
1:D:353:ASN:N	1:D:353:ASN:OD1	2.38	0.55
1:B:389:PRO:HB3	1:B:393:MET:HE2	1.89	0.55
1:A:214:ARG:CA	1:A:217:THR:HG22	2.33	0.55
1:B:38:ILE:O	1:B:108:VAL:HB	2.07	0.55
1:B:379:LEU:CD1	1:C:346:GLN:HB2	2.37	0.55
1:C:151:GLU:OE1	2:R:17:U:OP1	2.24	0.55
1:D:182:PHE:HD2	1:D:183:ASP:H	1.54	0.55
1:E:51:LEU:O	1:E:55:VAL:HG22	2.06	0.55
1:B:22:GLU:O	1:B:23:ASP:C	2.49	0.55
1:B:214:ARG:CA	1:B:217:THR:HG22	2.34	0.55
1:D:169:GLU:O	1:D:170:GLN:HG2	2.07	0.55
1:D:364:LEU:O	1:D:368:ALA:HB3	2.07	0.55
1:E:81:ARG:O	1:E:102:ILE:O	2.24	0.55
1:E:214:ARG:HH21	1:E:218:ILE:HG13	1.71	0.55
1:E:262:MET:HE2	1:E:262:MET:HA	1.88	0.55
1:A:15:VAL:O	1:A:17:LYS:HG2	2.07	0.54
1:A:401:VAL:HG21	1:A:420:PHE:HB2	1.88	0.54
1:B:283:LEU:N	1:B:283:LEU:HD23	2.20	0.54
1:B:354:LYS:CE	1:B:356:THR:HA	2.32	0.54
1:E:275:MET:SD	1:E:275:MET:C	2.90	0.54
1:D:43:ASN:O	1:D:44:THR:C	2.51	0.54
1:E:38:ILE:O	1:E:38:ILE:HG13	2.05	0.54
1:B:129:ALA:HA	1:B:132:LYS:NZ	2.21	0.54
1:C:214:ARG:HH21	1:C:218:ILE:HG13	1.71	0.54
1:D:117:LEU:HB3	1:D:118:PRO:HD3	1.86	0.54
1:D:214:ARG:O	1:D:217:THR:HG22	2.06	0.54
1:E:41:TYR:HB2	1:E:190:ASN:HD21	1.71	0.54
2:R:31:U:H3'	2:R:31:U:H6	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:H	1:A:46:LYS:NZ	2.06	0.54
1:A:182:PHE:CD2	1:A:182:PHE:C	2.85	0.54
1:A:353:ASN:OD1	1:A:353:ASN:N	2.39	0.54
1:D:155:LYS:O	1:D:159:GLY:N	2.38	0.54
1:D:374:ASP:O	1:D:378:TRP:HD1	1.90	0.54
1:A:128:SER:HA	1:A:130:ASP:HB2	1.89	0.54
1:A:302:GLN:HB3	1:A:412:ILE:HD13	1.89	0.54
1:B:43:ASN:O	1:B:44:THR:O	2.26	0.54
1:C:152:TYR:CE2	1:C:153:ARG:HG2	2.42	0.54
1:E:45:THR:C	1:E:46:LYS:HE3	2.32	0.54
1:C:31:TYR:CD1	1:C:31:TYR:C	2.86	0.54
1:C:160:LEU:HA	1:C:163:GLN:CB	2.38	0.54
1:C:221:ARG:O	1:C:222:PHE:HB2	2.08	0.54
1:D:165:LYS:HB3	1:D:166:MET:SD	2.47	0.54
1:E:227:ALA:HA	1:E:230:THR:HG23	1.90	0.54
2:R:28:U:H2'	2:R:29:U:O4'	2.08	0.54
1:A:27:TYR:HB3	1:A:266:GLN:NE2	2.22	0.54
1:B:137:TYR:HD1	1:B:163:GLN:NE2	1.95	0.54
1:C:397:ALA:O	1:C:401:VAL:HG22	2.07	0.54
1:D:181:ILE:N	1:D:181:ILE:CD1	2.71	0.54
1:D:262:MET:HE2	1:D:262:MET:HA	1.88	0.54
1:E:152:TYR:CE2	1:E:153:ARG:HG2	2.43	0.54
2:R:39:U:H5''	2:R:39:U:C6	2.41	0.54
1:A:41:TYR:HB2	1:A:190:ASN:HD21	1.73	0.54
1:B:182:PHE:C	1:B:184:VAL:H	2.15	0.54
1:C:38:ILE:O	1:C:38:ILE:HG13	2.06	0.54
1:B:214:ARG:HH21	1:B:218:ILE:HG13	1.73	0.54
1:C:155:LYS:O	1:C:159:GLY:N	2.39	0.54
1:C:214:ARG:O	1:C:217:THR:HG22	2.07	0.54
1:D:22:GLU:O	1:D:23:ASP:C	2.51	0.54
1:A:38:ILE:O	1:A:38:ILE:HG13	2.07	0.53
1:C:143:ARG:NH2	2:R:17:U:H5''	2.23	0.53
1:C:178:GLY:O	1:C:179:ARG:HB2	2.08	0.53
1:B:128:SER:HA	1:B:130:ASP:HB2	1.91	0.53
1:B:214:ARG:O	1:B:217:THR:HG22	2.08	0.53
1:C:66:ILE:O	1:C:70:ASN:ND2	2.41	0.53
1:D:152:TYR:CE1	1:D:153:ARG:NH1	2.76	0.53
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.37	0.53
1:E:182:PHE:HD2	1:E:183:ASP:H	1.55	0.53
1:A:160:LEU:C	1:A:162:ASN:N	2.66	0.53
1:C:172:GLU:CB	1:C:173:PRO:HD3	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:O	1:B:222:PHE:HB2	2.06	0.53
1:B:182:PHE:HD2	1:B:183:ASP:H	1.54	0.53
1:C:143:ARG:HH22	2:R:17:U:H3'	1.74	0.53
1:C:379:LEU:CD1	1:D:346:GLN:HB2	2.38	0.53
1:E:31:TYR:CD1	1:E:31:TYR:C	2.87	0.53
1:B:342:ALA:CB	1:B:344:LEU:HD23	2.38	0.53
1:B:422:LYS:HE3	1:C:399:ARG:HB3	1.91	0.53
1:C:45:THR:C	1:C:46:LYS:HE3	2.34	0.53
1:D:74:TYR:CD1	1:D:78:LYS:HD3	2.44	0.53
1:E:365:THR:CG2	1:E:366:THR:N	2.61	0.53
1:B:41:TYR:HB2	1:B:190:ASN:HD21	1.74	0.53
1:C:291:SER:HB3	2:R:13:U:OP2	2.08	0.53
1:D:130:ASP:O	1:D:131:ASP:C	2.52	0.53
1:D:397:ALA:O	1:D:401:VAL:HG22	2.09	0.53
1:E:43:ASN:O	1:E:44:THR:O	2.27	0.53
1:A:291:SER:HB3	2:R:31:U:OP2	2.09	0.53
1:B:55:VAL:HG23	1:B:56:TYR:H	1.73	0.53
1:B:66:ILE:HG13	1:B:70:ASN:ND2	2.22	0.53
1:A:129:ALA:HA	1:A:132:LYS:NZ	2.24	0.53
1:A:152:TYR:CE1	1:A:153:ARG:NH1	2.76	0.53
1:A:374:ASP:O	1:A:378:TRP:HD1	1.91	0.53
1:B:353:ASN:N	1:B:353:ASN:OD1	2.41	0.53
1:E:22:GLU:O	1:E:23:ASP:C	2.51	0.53
1:A:248:TRP:O	1:A:250:LEU:HG	2.09	0.53
1:B:155:LYS:O	1:B:159:GLY:N	2.38	0.53
1:C:151:GLU:OE1	1:C:155:LYS:HE2	2.09	0.53
1:D:15:VAL:O	1:D:17:LYS:HG2	2.09	0.53
1:E:15:VAL:O	1:E:17:LYS:HG2	2.08	0.53
2:R:8:U:C3'	2:R:9:U:H5''	2.38	0.53
1:A:155:LYS:O	1:A:159:GLY:N	2.39	0.52
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.38	0.52
1:A:181:ILE:N	1:A:183:ASP:OD2	2.43	0.52
1:B:227:ALA:HA	1:B:230:THR:HG23	1.91	0.52
1:C:152:TYR:CE1	1:C:153:ARG:NH1	2.77	0.52
1:C:342:ALA:CB	1:C:344:LEU:HD23	2.37	0.52
1:A:81:ARG:O	1:A:102:ILE:O	2.26	0.52
1:C:88:TRP:CE3	1:C:204:MET:HE3	2.44	0.52
1:C:163:GLN:C	1:C:165:LYS:H	2.17	0.52
1:C:182:PHE:C	1:C:184:VAL:H	2.16	0.52
1:D:79:ASP:OD2	1:D:81:ARG:HB2	2.09	0.52
1:D:257:GLU:CG	1:D:294:ASN:HA	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:ARG:CD	1:C:216:GLY:HA2	2.37	0.52
1:A:28:PRO:O	1:A:29:ALA:C	2.53	0.52
1:C:182:PHE:HD2	1:C:183:ASP:H	1.53	0.52
1:D:66:ILE:HG13	1:D:70:ASN:ND2	2.21	0.52
1:D:133:TRP:CB	1:D:167:ILE:HD13	2.39	0.52
1:E:182:PHE:CD2	1:E:182:PHE:C	2.87	0.52
1:A:163:GLN:C	1:A:165:LYS:N	2.64	0.52
1:B:169:GLU:O	1:B:170:GLN:HG2	2.10	0.52
1:B:182:PHE:CD2	1:B:183:ASP:N	2.66	0.52
1:C:55:VAL:O	1:C:56:TYR:C	2.53	0.52
1:C:81:ARG:O	1:C:102:ILE:O	2.28	0.52
1:D:133:TRP:CG	1:D:167:ILE:HG21	2.44	0.52
1:E:214:ARG:O	1:E:217:THR:HG22	2.09	0.52
1:A:84:LEU:CD1	1:A:97:LYS:N	2.73	0.52
1:D:227:ALA:HA	1:D:230:THR:HG23	1.92	0.52
1:E:365:THR:HG23	1:E:366:THR:O	2.10	0.52
1:A:84:LEU:HD12	1:A:97:LYS:O	2.10	0.52
1:A:160:LEU:HA	1:A:163:GLN:HB2	1.92	0.52
1:B:15:VAL:O	1:B:17:LYS:HG2	2.09	0.52
1:B:79:ASP:O	1:B:79:ASP:CG	2.52	0.52
1:B:160:LEU:HA	1:B:163:GLN:CB	2.40	0.52
1:E:155:LYS:O	1:E:159:GLY:N	2.39	0.52
1:E:182:PHE:C	1:E:184:VAL:H	2.16	0.52
1:E:214:ARG:CA	1:E:217:THR:HG22	2.35	0.52
1:E:345:ALA:O	1:E:347:GLN:HG2	2.10	0.52
1:B:81:ARG:O	1:B:102:ILE:O	2.27	0.51
1:B:200:MET:HB2	1:B:277:TYR:CE2	2.46	0.51
1:D:388:LYS:HE2	1:D:389:PRO:HD2	1.92	0.51
1:A:167:ILE:H	1:A:167:ILE:HD12	1.74	0.51
1:B:44:THR:HG22	1:B:46:LYS:NZ	2.25	0.51
1:D:149:MET:HG3	2:R:6:U:C1'	2.41	0.51
1:E:388:LYS:HE2	1:E:389:PRO:HD2	1.92	0.51
1:A:397:ALA:O	1:A:401:VAL:HG22	2.11	0.51
1:B:66:ILE:HD13	1:B:185:TRP:CD1	2.46	0.51
1:B:79:ASP:OD2	1:B:79:ASP:C	2.54	0.51
1:D:41:TYR:HB2	1:D:190:ASN:HD21	1.75	0.51
1:D:179:ARG:O	1:D:180:ASP:HB2	2.10	0.51
1:D:389:PRO:HB3	1:D:393:MET:HE2	1.92	0.51
1:E:167:ILE:CD1	1:E:168:ASN:N	2.72	0.51
1:B:374:ASP:O	1:B:378:TRP:HD1	1.94	0.51
1:D:332:LEU:HD13	1:D:393:MET:HE3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ARG:O	1:E:222:PHE:HB2	2.08	0.51
2:R:21:U:O4	2:R:22:U:O4	2.28	0.51
1:B:119:ASP:O	1:B:121:VAL:N	2.44	0.51
1:C:153:ARG:NH2	1:C:176:PRO:HA	2.25	0.51
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.40	0.51
1:E:389:PRO:HB3	1:E:393:MET:HE2	1.91	0.51
1:A:117:LEU:HB3	1:A:118:PRO:HD3	1.85	0.51
1:A:137:TYR:HB2	1:A:163:GLN:HE22	1.75	0.51
1:C:88:TRP:CD2	1:C:204:MET:HE3	2.46	0.51
1:A:153:ARG:NH2	1:A:176:PRO:HA	2.25	0.51
1:B:248:TRP:O	1:B:250:LEU:HG	2.11	0.51
1:C:79:ASP:O	1:C:79:ASP:CG	2.53	0.51
1:A:169:GLU:O	1:A:170:GLN:HG2	2.11	0.51
1:A:200:MET:HB2	1:A:277:TYR:CE2	2.46	0.51
1:C:46:LYS:N	1:C:46:LYS:HD2	2.25	0.51
1:C:180:ASP:N	1:C:183:ASP:OD2	2.31	0.51
1:D:45:THR:H	1:D:46:LYS:HZ2	1.58	0.51
1:D:45:THR:C	1:D:46:LYS:HE3	2.36	0.51
1:E:74:TYR:CD1	1:E:78:LYS:HD3	2.44	0.51
1:E:88:TRP:CD2	1:E:204:MET:HE3	2.46	0.51
1:E:128:SER:HA	1:E:130:ASP:HB2	1.92	0.51
1:A:227:ALA:HA	1:A:230:THR:HG23	1.93	0.51
1:C:22:GLU:O	1:C:23:ASP:C	2.54	0.51
1:C:182:PHE:CD2	1:C:182:PHE:C	2.86	0.51
1:D:128:SER:HA	1:D:130:ASP:HB2	1.92	0.51
1:A:143:ARG:CD	1:A:216:GLY:HA2	2.40	0.50
1:A:182:PHE:C	1:A:184:VAL:H	2.19	0.50
1:B:182:PHE:C	1:B:182:PHE:CD2	2.89	0.50
1:B:397:ALA:O	1:B:401:VAL:HG22	2.11	0.50
1:D:286:LYS:HZ2	2:R:2:U:P	2.33	0.50
1:E:119:ASP:O	1:E:121:VAL:N	2.44	0.50
1:E:374:ASP:O	1:E:378:TRP:HD1	1.94	0.50
2:R:21:U:H5''	2:R:21:U:H6	1.76	0.50
1:A:130:ASP:O	1:A:131:ASP:C	2.54	0.50
1:A:380:GLY:HA2	1:B:354:LYS:HZ3	1.75	0.50
1:B:214:ARG:O	1:B:215:TYR:C	2.54	0.50
1:D:182:PHE:C	1:D:184:VAL:H	2.19	0.50
1:C:27:TYR:HB3	1:C:266:GLN:NE2	2.26	0.50
1:D:160:LEU:C	1:D:162:ASN:N	2.68	0.50
1:D:290:SER:HB2	2:R:3:U:H5'	1.93	0.50
1:E:302:GLN:HB3	1:E:412:ILE:HD13	1.88	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLN:C	1:B:165:LYS:H	2.16	0.50
1:C:169:GLU:O	1:C:170:GLN:HG2	2.12	0.50
1:E:143:ARG:CD	1:E:216:GLY:HA2	2.40	0.50
1:B:66:ILE:HD12	1:B:69:VAL:CG1	2.42	0.50
1:C:380:GLY:HA2	1:D:354:LYS:HZ3	1.76	0.50
1:D:143:ARG:NH2	2:R:8:U:C5'	2.75	0.50
1:A:18:LEU:HD12	1:B:232:GLY:HA2	1.93	0.50
1:B:27:TYR:HB3	1:B:266:GLN:NE2	2.26	0.50
1:C:117:LEU:HB3	1:C:118:PRO:HD3	1.84	0.50
1:D:66:ILE:HD13	1:D:185:TRP:CD1	2.46	0.50
1:D:171:PHE:O	1:D:172:GLU:OE2	2.29	0.50
1:E:248:TRP:O	1:E:250:LEU:HG	2.12	0.50
1:A:45:THR:C	1:A:46:LYS:HE3	2.36	0.50
1:D:345:ALA:O	1:D:347:GLN:HG2	2.12	0.50
1:E:129:ALA:HA	1:E:132:LYS:NZ	2.27	0.50
1:E:172:GLU:CB	1:E:173:PRO:HD3	2.42	0.50
1:A:180:ASP:HB3	1:A:181:ILE:HD12	1.94	0.50
1:A:182:PHE:HD2	1:A:183:ASP:H	1.56	0.50
1:B:45:THR:H	1:B:46:LYS:NZ	2.09	0.50
1:A:31:TYR:CD1	1:A:31:TYR:C	2.89	0.50
1:A:273:SER:OG	1:A:274:TYR:N	2.43	0.50
1:A:214:ARG:O	1:A:215:TYR:C	2.54	0.49
1:D:97:LYS:O	1:D:98:ALA:C	2.55	0.49
1:E:169:GLU:O	1:E:170:GLN:HG2	2.10	0.49
1:C:41:TYR:HB2	1:C:190:ASN:HD21	1.76	0.49
1:C:143:ARG:HB2	1:C:216:GLY:HA2	1.94	0.49
1:C:247:THR:HA	1:D:348:PHE:HB2	1.95	0.49
1:D:137:TYR:HB2	1:D:163:GLN:HE22	1.77	0.49
1:A:172:GLU:CB	1:A:173:PRO:HD3	2.43	0.49
1:B:52:ARG:HD3	1:B:127:THR:O	2.12	0.49
1:B:388:LYS:HE2	1:B:389:PRO:HD2	1.93	0.49
1:C:167:ILE:HD13	1:C:167:ILE:H	1.76	0.49
1:E:55:VAL:O	1:E:56:TYR:C	2.55	0.49
2:R:25:U:H2'	2:R:26:U:C5	2.47	0.49
1:A:88:TRP:CE3	1:A:204:MET:HE3	2.48	0.49
1:E:171:PHE:O	1:E:172:GLU:OE2	2.31	0.49
1:C:14:ILE:HD12	1:D:259:VAL:HG22	1.94	0.49
1:C:374:ASP:O	1:C:378:TRP:HD1	1.94	0.49
2:R:34:U:H2'	2:R:35:U:O4'	2.12	0.49
1:B:143:ARG:CD	1:B:216:GLY:HA2	2.40	0.49
1:C:128:SER:HA	1:C:130:ASP:HB2	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:389:PRO:CB	1:C:393:MET:HE2	2.42	0.49
1:B:317:ARG:O	1:B:319:PRO:HD3	2.13	0.49
1:C:160:LEU:C	1:C:162:ASN:N	2.68	0.49
1:C:227:ALA:HA	1:C:230:THR:HG23	1.95	0.49
1:E:240:MET:HE1	1:E:248:TRP:CD1	2.47	0.49
1:B:180:ASP:N	1:B:183:ASP:CG	2.66	0.49
1:D:143:ARG:HH21	2:R:8:U:C5'	2.24	0.49
1:D:283:LEU:N	1:D:283:LEU:HD23	2.27	0.49
1:A:262:MET:HA	1:A:262:MET:HE2	1.95	0.49
1:B:240:MET:HE1	1:B:248:TRP:CD1	2.48	0.49
1:C:129:ALA:HA	1:C:132:LYS:NZ	2.28	0.49
1:D:172:GLU:CB	1:D:173:PRO:HD3	2.42	0.49
1:E:45:THR:H	1:E:46:LYS:NZ	2.11	0.49
1:E:52:ARG:HD3	1:E:127:THR:O	2.13	0.49
1:E:130:ASP:O	1:E:131:ASP:C	2.56	0.49
1:A:342:ALA:CB	1:A:344:LEU:HD23	2.41	0.48
1:E:117:LEU:HB3	1:E:118:PRO:HD3	1.86	0.48
1:B:172:GLU:CB	1:B:173:PRO:HD3	2.43	0.48
1:B:177:GLU:CG	1:B:178:GLY:H	2.26	0.48
1:C:119:ASP:O	1:C:121:VAL:N	2.46	0.48
1:C:143:ARG:HH21	2:R:17:U:H5''	1.77	0.48
1:E:88:TRP:CE3	1:E:204:MET:HE3	2.48	0.48
1:A:171:PHE:O	1:A:172:GLU:OE2	2.30	0.48
1:A:214:ARG:O	1:A:217:THR:HG22	2.12	0.48
1:A:324:TYR:O	1:A:328:THR:CG2	2.61	0.48
1:E:160:LEU:C	1:E:162:ASN:N	2.68	0.48
1:E:358:ASP:CG	1:E:359:ASP:N	2.69	0.48
1:A:128:SER:C	1:A:130:ASP:N	2.70	0.48
1:B:316:ALA:HA	2:R:23:U:H5'	1.95	0.48
1:B:356:THR:N	1:B:357:PRO:CD	2.76	0.48
1:C:158:ASP:HA	1:C:161:THR:OG1	2.13	0.48
1:C:214:ARG:O	1:C:215:TYR:C	2.53	0.48
1:D:143:ARG:CD	1:D:216:GLY:HA2	2.43	0.48
1:D:153:ARG:NH2	1:D:176:PRO:HA	2.28	0.48
1:E:79:ASP:O	1:E:79:ASP:CG	2.56	0.48
2:R:29:U:H2'	2:R:29:U:O2	2.12	0.48
1:A:88:TRP:CD2	1:A:204:MET:HE3	2.49	0.48
1:E:342:ALA:CB	1:E:344:LEU:HD23	2.40	0.48
1:A:221:ARG:O	1:A:222:PHE:HB2	2.14	0.48
1:B:317:ARG:HH21	1:B:410:LYS:HE2	1.79	0.48
1:D:66:ILE:HD12	1:D:69:VAL:CG1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:LEU:C	1:E:108:VAL:HG23	2.38	0.48
1:E:158:ASP:HA	1:E:161:THR:OG1	2.13	0.48
1:E:257:GLU:CG	1:E:294:ASN:HA	2.43	0.48
1:A:177:GLU:HA	1:A:181:ILE:CD1	2.37	0.48
1:A:240:MET:HE1	1:A:248:TRP:CD1	2.48	0.48
1:C:55:VAL:HG23	1:C:56:TYR:H	1.77	0.48
1:E:295:PRO:HB2	1:E:322:ILE:CG2	2.43	0.48
1:B:88:TRP:CE3	1:B:204:MET:HE3	2.49	0.48
1:B:171:PHE:O	1:B:172:GLU:OE2	2.31	0.48
1:C:324:TYR:O	1:C:328:THR:HG22	2.13	0.48
1:D:248:TRP:O	1:D:250:LEU:HG	2.13	0.48
1:E:180:ASP:N	1:E:183:ASP:OD2	2.40	0.48
1:C:273:SER:OG	1:C:274:TYR:N	2.47	0.48
1:D:158:ASP:HA	1:D:161:THR:OG1	2.14	0.48
1:D:180:ASP:N	1:D:183:ASP:CG	2.62	0.48
1:A:382:PHE:CE2	1:A:387:ARG:HA	2.48	0.48
1:A:388:LYS:HE2	1:A:389:PRO:HD2	1.94	0.48
1:B:151:GLU:HA	1:B:154:LYS:HZ2	1.79	0.48
1:C:317:ARG:HD3	2:R:13:U:C2	2.49	0.48
1:D:55:VAL:O	1:D:56:TYR:C	2.55	0.48
1:D:182:PHE:CD2	1:D:182:PHE:C	2.88	0.48
1:E:317:ARG:O	1:E:319:PRO:HD3	2.14	0.48
1:A:44:THR:HG22	1:A:46:LYS:NZ	2.28	0.47
1:A:55:VAL:HG23	1:A:56:TYR:H	1.78	0.47
1:A:79:ASP:OD2	1:A:81:ARG:HB2	2.14	0.47
1:A:119:ASP:O	1:A:121:VAL:N	2.46	0.47
1:C:130:ASP:O	1:C:131:ASP:C	2.57	0.47
1:D:303:LEU:HD22	1:D:328:THR:HB	1.96	0.47
1:A:137:TYR:HB2	1:A:163:GLN:NE2	2.29	0.47
2:R:37:U:C5	2:R:38:U:C5	3.02	0.47
1:B:160:LEU:C	1:B:162:ASN:N	2.68	0.47
1:B:257:GLU:CG	1:B:294:ASN:HA	2.44	0.47
1:C:180:ASP:N	1:C:183:ASP:OD1	2.47	0.47
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.69	0.47
1:A:379:LEU:CD1	1:B:346:GLN:HB2	2.44	0.47
1:B:251:ASN:OD1	1:B:251:ASN:N	2.48	0.47
1:B:345:ALA:O	1:B:347:GLN:HG2	2.13	0.47
1:C:182:PHE:HD2	1:C:182:PHE:C	2.19	0.47
1:D:132:LYS:HB3	1:D:167:ILE:HD11	1.97	0.47
1:B:149:MET:HG3	2:R:24:U:O4'	2.15	0.47
1:D:149:MET:HG3	2:R:6:U:N1	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:PHE:HD2	1:E:182:PHE:C	2.22	0.47
1:A:44:THR:HG22	1:A:46:LYS:HZ2	1.80	0.47
1:C:167:ILE:H	1:C:167:ILE:CD1	2.28	0.47
1:D:43:ASN:O	1:D:44:THR:O	2.33	0.47
1:A:158:ASP:HA	1:A:161:THR:OG1	2.15	0.47
1:B:88:TRP:CD2	1:B:204:MET:HE3	2.50	0.47
1:B:167:ILE:HD13	1:B:168:ASN:CA	2.33	0.47
1:B:179:ARG:O	1:B:180:ASP:HB2	2.15	0.47
1:C:18:LEU:HB2	1:C:19:PRO:HD2	1.97	0.47
1:C:240:MET:HE1	1:C:248:TRP:CD1	2.50	0.47
1:C:317:ARG:HH21	1:C:410:LYS:HE2	1.80	0.47
1:D:27:TYR:HB3	1:D:266:GLN:NE2	2.29	0.47
1:D:165:LYS:CB	1:D:166:MET:SD	3.02	0.47
1:D:342:ALA:CB	1:D:344:LEU:HD23	2.42	0.47
1:E:143:ARG:HB2	1:E:216:GLY:HA2	1.95	0.47
1:A:31:TYR:C	1:A:33:ARG:H	2.23	0.47
1:A:182:PHE:HD2	1:A:182:PHE:C	2.19	0.47
1:B:142:TYR:CD1	1:B:195:VAL:HG11	2.50	0.47
1:B:167:ILE:CD1	1:B:167:ILE:C	2.71	0.47
1:E:220:SER:HB2	1:E:280:ASP:OD2	2.15	0.47
2:R:17:U:H2'	2:R:18:U:C5'	2.42	0.47
1:A:46:LYS:HD2	1:A:46:LYS:N	2.30	0.47
1:A:324:TYR:O	1:A:328:THR:HG22	2.15	0.47
1:B:350:VAL:HG13	1:E:4:THR:O	2.15	0.47
1:A:162:ASN:O	1:A:164:CYS:N	2.48	0.47
1:A:167:ILE:N	1:A:167:ILE:HD12	2.27	0.47
1:A:178:GLY:O	1:A:179:ARG:CB	2.63	0.47
1:C:44:THR:HG22	1:C:46:LYS:HZ2	1.80	0.47
1:C:262:MET:HA	1:C:262:MET:HE2	1.96	0.47
1:E:48:LEU:N	1:E:48:LEU:CD2	2.74	0.47
1:A:344:LEU:CD1	1:E:250:LEU:HD13	2.45	0.46
1:B:234:LEU:O	1:B:238:THR:HG23	2.15	0.46
1:A:87:ASP:OD2	1:A:98:ALA:N	2.48	0.46
1:B:250:LEU:HB3	1:C:344:LEU:HD13	1.96	0.46
1:C:79:ASP:OD2	1:C:79:ASP:C	2.58	0.46
1:D:45:THR:H	1:D:46:LYS:NZ	2.12	0.46
1:D:52:ARG:HD3	1:D:127:THR:O	2.14	0.46
1:D:263:LEU:HA	1:D:264:PRO:HD3	1.75	0.46
1:D:317:ARG:HH21	1:D:410:LYS:HE2	1.79	0.46
1:E:409:GLU:O	1:E:410:LYS:HB2	2.16	0.46
1:A:275:MET:SD	1:A:275:MET:C	2.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:ASN:OD1	1:D:251:ASN:N	2.49	0.46
1:E:55:VAL:HG23	1:E:56:TYR:H	1.79	0.46
2:R:7:U:H2'	2:R:8:U:O4'	2.16	0.46
2:R:21:U:C4	2:R:22:U:C4	3.04	0.46
1:A:79:ASP:O	1:A:79:ASP:CG	2.57	0.46
1:A:167:ILE:HD13	1:A:167:ILE:N	2.13	0.46
1:B:181:ILE:N	1:B:183:ASP:OD2	2.48	0.46
1:B:182:PHE:C	1:B:184:VAL:N	2.73	0.46
1:B:379:LEU:HB3	1:C:354:LYS:HD2	1.98	0.46
1:C:44:THR:HG22	1:C:46:LYS:NZ	2.31	0.46
1:D:177:GLU:CG	1:D:178:GLY:H	2.28	0.46
1:E:142:TYR:CD1	1:E:195:VAL:HG11	2.51	0.46
1:A:344:LEU:HD11	1:E:250:LEU:HD13	1.98	0.46
1:E:181:ILE:N	1:E:183:ASP:OD2	2.48	0.46
1:D:44:THR:HG22	1:D:46:LYS:NZ	2.31	0.46
1:E:182:PHE:C	1:E:184:VAL:N	2.74	0.46
2:R:17:U:H2'	2:R:18:U:O4'	2.16	0.46
1:A:52:ARG:HD3	1:A:127:THR:O	2.16	0.46
1:A:137:TYR:O	1:A:141:LEU:HG	2.16	0.46
1:B:55:VAL:O	1:B:56:TYR:C	2.58	0.46
1:C:332:LEU:HD13	1:C:393:MET:HE3	1.97	0.46
1:C:388:LYS:HE2	1:C:389:PRO:HD2	1.97	0.46
1:D:275:MET:SD	1:D:275:MET:C	2.98	0.46
2:R:31:U:H3'	2:R:31:U:C6	2.51	0.46
1:A:389:PRO:CB	1:A:393:MET:HE2	2.46	0.46
1:B:143:ARG:HB2	1:B:216:GLY:HA2	1.98	0.46
1:C:128:SER:C	1:C:130:ASP:N	2.73	0.46
1:C:249:ILE:HD13	1:C:254:VAL:HG12	1.98	0.46
1:D:214:ARG:O	1:D:215:TYR:C	2.58	0.46
1:E:291:SER:HB3	2:R:40:U:O5'	2.15	0.46
1:A:31:TYR:C	1:A:33:ARG:N	2.73	0.46
1:C:182:PHE:C	1:C:184:VAL:N	2.73	0.46
1:C:224:ASP:CG	2:R:12:U:H4'	2.41	0.46
1:D:143:ARG:HB2	1:D:216:GLY:HA2	1.98	0.46
1:E:66:ILE:O	1:E:70:ASN:ND2	2.47	0.46
1:A:74:TYR:CD1	1:A:78:LYS:HD3	2.49	0.46
1:A:422:LYS:HA	1:A:422:LYS:HD3	1.63	0.46
1:B:233:HIS:NE2	1:B:312:ARG:NH1	2.63	0.46
1:C:152:TYR:CE1	1:C:153:ARG:CZ	2.99	0.46
1:C:175:VAL:HG13	1:C:181:ILE:CG1	2.46	0.46
1:D:324:TYR:O	1:D:328:THR:CG2	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:VAL:HG21	1:E:138:LEU:HD22	1.98	0.46
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.30	0.45
1:B:389:PRO:CB	1:B:393:MET:HE2	2.46	0.45
1:D:128:SER:C	1:D:130:ASP:N	2.73	0.45
1:E:152:TYR:HE1	1:E:153:ARG:NH1	2.12	0.45
1:D:178:GLY:O	1:D:179:ARG:CB	2.64	0.45
1:D:368:ALA:HA	1:D:369:PRO:HD3	1.79	0.45
1:A:364:LEU:H	1:A:364:LEU:CD1	2.27	0.45
1:C:228:LEU:HD23	1:C:228:LEU:HA	1.74	0.45
1:D:79:ASP:O	1:D:79:ASP:CG	2.58	0.45
1:A:177:GLU:CG	1:A:178:GLY:H	2.28	0.45
1:B:143:ARG:NH2	2:R:26:U:H2'	2.32	0.45
1:B:262:MET:HE2	1:B:262:MET:HA	1.98	0.45
1:B:303:LEU:HD22	1:B:328:THR:HB	1.99	0.45
1:B:342:ALA:O	1:B:343:ASP:C	2.58	0.45
1:C:171:PHE:O	1:C:172:GLU:OE2	2.34	0.45
1:C:324:TYR:O	1:C:328:THR:HG23	2.15	0.45
1:E:152:TYR:CE1	1:E:153:ARG:CZ	3.00	0.45
1:E:302:GLN:HG3	1:E:313:ALA:HB1	1.98	0.45
1:A:162:ASN:HB3	1:A:163:GLN:H	1.59	0.45
1:B:212:SER:HA	2:R:27:U:C5	2.51	0.45
1:C:167:ILE:CD1	1:C:168:ASN:N	2.78	0.45
1:D:18:LEU:HB2	1:D:19:PRO:HD2	1.98	0.45
1:C:142:TYR:CD1	1:C:195:VAL:HG11	2.52	0.45
1:C:175:VAL:HA	1:C:176:PRO:HD2	1.69	0.45
1:E:83:LYS:HD2	1:E:99:GLY:O	2.16	0.45
1:E:143:ARG:NH2	2:R:44:U:H5''	2.32	0.45
1:E:178:GLY:O	1:E:179:ARG:CB	2.62	0.45
1:E:233:HIS:NE2	1:E:312:ARG:NH1	2.64	0.45
1:E:332:LEU:HD13	1:E:393:MET:HE3	1.97	0.45
1:B:422:LYS:HA	1:B:422:LYS:HD3	1.63	0.45
1:C:178:GLY:O	1:C:179:ARG:CB	2.65	0.45
1:C:302:GLN:HG2	1:C:316:ALA:HB2	1.98	0.45
1:D:240:MET:HE1	1:D:248:TRP:CD1	2.52	0.45
1:E:70:ASN:H	1:E:70:ASN:ND2	2.14	0.45
1:E:72:TYR:CE1	1:E:134:LEU:HD13	2.51	0.45
1:B:130:ASP:O	1:B:131:ASP:C	2.60	0.45
1:C:233:HIS:NE2	1:C:312:ARG:NH1	2.65	0.45
1:C:285:SER:OG	1:D:207:LYS:HE3	2.17	0.45
1:C:317:ARG:O	1:C:319:PRO:HD3	2.17	0.45
1:C:345:ALA:O	1:C:347:GLN:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:LEU:HB2	1:E:19:PRO:HD2	1.99	0.45
1:E:66:ILE:HD13	1:E:185:TRP:CD1	2.51	0.45
1:A:356:THR:N	1:A:357:PRO:CD	2.80	0.45
1:B:365:THR:CG2	1:B:366:THR:N	2.73	0.45
1:D:119:ASP:O	1:D:121:VAL:N	2.49	0.45
1:D:142:TYR:CD1	1:D:195:VAL:HG11	2.51	0.45
1:D:162:ASN:HB3	1:D:163:GLN:H	1.61	0.45
1:E:128:SER:C	1:E:130:ASP:N	2.75	0.45
1:A:55:VAL:O	1:A:56:TYR:C	2.56	0.45
1:A:160:LEU:HA	1:A:163:GLN:CG	2.46	0.45
1:C:10:ASP:C	1:C:10:ASP:OD2	2.58	0.45
1:C:151:GLU:CD	1:C:155:LYS:HE2	2.41	0.45
1:C:261:MET:O	1:C:262:MET:HE2	2.17	0.45
1:D:181:ILE:N	1:D:183:ASP:OD2	2.50	0.45
1:D:324:TYR:O	1:D:328:THR:HG23	2.16	0.45
1:B:46:LYS:HD2	1:B:46:LYS:N	2.32	0.44
1:B:73:LEU:O	1:B:74:TYR:C	2.60	0.44
1:B:158:ASP:HA	1:B:161:THR:OG1	2.17	0.44
1:C:137:TYR:O	1:C:141:LEU:HG	2.17	0.44
1:D:30:ASP:CG	1:D:33:ARG:HH21	2.25	0.44
1:E:180:ASP:HB3	1:E:181:ILE:HD12	1.99	0.44
1:E:342:ALA:O	1:E:343:ASP:C	2.60	0.44
1:A:66:ILE:HG23	1:A:67:ILE:N	2.33	0.44
1:B:2:SER:HB2	1:C:243:GLU:HG3	1.99	0.44
1:B:152:TYR:HE1	1:B:153:ARG:NH1	2.15	0.44
1:C:177:GLU:HA	1:C:181:ILE:CD1	2.39	0.44
1:C:203:HIS:HA	1:C:214:ARG:NH1	2.32	0.44
1:C:342:ALA:O	1:C:343:ASP:C	2.59	0.44
1:B:107:LEU:C	1:B:108:VAL:HG23	2.42	0.44
1:B:368:ALA:HA	1:B:369:PRO:HD3	1.82	0.44
1:C:177:GLU:CG	1:C:178:GLY:H	2.28	0.44
1:C:422:LYS:HA	1:C:422:LYS:HD3	1.63	0.44
1:A:218:ILE:C	1:A:220:SER:H	2.24	0.44
1:B:50:ASP:OD1	1:B:121:VAL:HG22	2.17	0.44
1:D:137:TYR:HD1	1:D:163:GLN:NE2	2.02	0.44
1:D:141:LEU:HD12	1:D:185:TRP:CZ3	2.52	0.44
1:D:180:ASP:HB3	1:D:181:ILE:HD12	1.99	0.44
1:B:72:TYR:CE1	1:B:134:LEU:HD13	2.52	0.44
1:C:45:THR:H	1:C:46:LYS:NZ	2.15	0.44
1:D:160:LEU:HA	1:D:163:GLN:HB2	1.98	0.44
1:D:214:ARG:C	1:D:217:THR:HG22	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:ASP:OD2	1:E:79:ASP:C	2.59	0.44
2:R:44:U:H5'	2:R:45:U:OP2	2.17	0.44
1:A:152:TYR:CE1	1:A:153:ARG:CZ	3.01	0.44
1:B:214:ARG:C	1:B:217:THR:HG22	2.43	0.44
1:C:72:TYR:CE1	1:C:134:LEU:HD13	2.53	0.44
1:C:224:ASP:OD1	2:R:12:U:H4'	2.18	0.44
1:C:352:ASP:O	1:C:352:ASP:CG	2.61	0.44
1:E:127:THR:OG1	1:E:128:SER:N	2.49	0.44
2:R:8:U:H5'	2:R:9:U:OP2	2.18	0.44
2:R:27:U:H2'	2:R:28:U:O4'	2.17	0.44
1:D:44:THR:HG21	1:D:116:VAL:HG11	1.99	0.44
1:D:175:VAL:HG13	1:D:181:ILE:HG12	1.99	0.44
1:A:143:ARG:HB2	1:A:216:GLY:HA2	1.98	0.44
1:B:128:SER:C	1:B:130:ASP:N	2.74	0.44
1:B:218:ILE:C	1:B:220:SER:H	2.25	0.44
1:B:379:LEU:HD23	1:B:379:LEU:HA	1.89	0.44
1:C:45:THR:O	1:C:46:LYS:HE3	2.18	0.44
1:C:376:VAL:HG13	1:D:354:LYS:CB	2.35	0.44
1:A:45:THR:H	1:A:46:LYS:HZ2	1.65	0.44
1:C:251:ASN:OD1	1:C:251:ASN:N	2.50	0.44
1:D:38:ILE:HA	1:D:39:PRO:HD2	1.90	0.44
1:A:161:THR:HB	1:E:179:ARG:CB	2.43	0.43
1:B:175:VAL:HG13	1:B:181:ILE:CG1	2.48	0.43
1:B:249:ILE:HD13	1:B:254:VAL:HG12	2.00	0.43
1:C:291:SER:HB3	2:R:13:U:P	2.58	0.43
1:D:117:LEU:O	1:D:118:PRO:C	2.60	0.43
1:E:303:LEU:HD22	1:E:328:THR:HB	2.00	0.43
1:B:352:ASP:O	1:B:352:ASP:CG	2.60	0.43
1:D:70:ASN:H	1:D:70:ASN:ND2	2.14	0.43
1:A:182:PHE:C	1:A:184:VAL:N	2.75	0.43
1:A:317:ARG:HH21	1:A:410:LYS:HE2	1.83	0.43
1:B:180:ASP:HB3	1:B:181:ILE:HD12	2.01	0.43
1:B:199:ASP:OD1	1:B:218:ILE:HA	2.18	0.43
1:C:38:ILE:HA	1:C:39:PRO:HD2	1.90	0.43
1:D:29:ALA:C	1:D:31:TYR:N	2.77	0.43
1:E:84:LEU:HD23	1:E:84:LEU:HA	1.78	0.43
1:E:175:VAL:HG13	1:E:181:ILE:CG1	2.48	0.43
1:E:251:ASN:OD1	1:E:251:ASN:N	2.51	0.43
1:A:199:ASP:OD1	1:A:218:ILE:HA	2.18	0.43
1:A:352:ASP:CG	1:A:352:ASP:O	2.62	0.43
1:B:45:THR:O	1:B:46:LYS:HE3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CE1	1:B:153:ARG:CZ	3.01	0.43
1:C:105:PHE:C	1:C:107:LEU:N	2.75	0.43
1:E:27:TYR:HB3	1:E:266:GLN:NE2	2.33	0.43
1:E:73:LEU:O	1:E:74:TYR:C	2.61	0.43
1:C:293:LYS:C	1:C:295:PRO:HD3	2.43	0.43
1:E:422:LYS:HA	1:E:422:LYS:HD3	1.62	0.43
2:R:17:U:C2'	2:R:18:U:H5''	2.42	0.43
1:A:240:MET:HE1	1:A:248:TRP:HD1	1.83	0.43
1:B:151:GLU:O	1:B:151:GLU:HG2	2.18	0.43
1:B:215:TYR:O	1:B:217:THR:N	2.51	0.43
1:B:275:MET:SD	1:B:275:MET:C	3.02	0.43
1:B:324:TYR:O	1:B:328:THR:CG2	2.66	0.43
1:C:127:THR:OG1	1:C:128:SER:N	2.49	0.43
1:D:220:SER:HB2	1:D:280:ASP:OD2	2.19	0.43
1:E:44:THR:HG21	1:E:116:VAL:HG11	2.00	0.43
1:E:79:ASP:OD2	1:E:81:ARG:HB2	2.19	0.43
1:E:149:MET:HG3	2:R:42:U:C6	2.54	0.43
1:E:162:ASN:ND2	1:E:165:LYS:NZ	2.67	0.43
2:R:21:U:C4	2:R:22:U:C5	3.07	0.43
2:R:36:U:O2'	2:R:37:U:H5''	2.18	0.43
1:B:84:LEU:HD11	1:B:96:GLY:HA3	2.01	0.43
1:C:28:PRO:O	1:C:29:ALA:C	2.60	0.43
1:D:72:TYR:CE1	1:D:134:LEU:HD13	2.53	0.43
1:D:164:CYS:O	1:D:165:LYS:C	2.61	0.43
1:E:199:ASP:OD1	1:E:218:ILE:HA	2.19	0.43
1:E:240:MET:HE1	1:E:248:TRP:HD1	1.83	0.43
1:A:69:VAL:HG21	1:A:138:LEU:HD22	2.01	0.43
1:C:29:ALA:C	1:C:31:TYR:N	2.76	0.43
1:C:152:TYR:HE1	1:C:153:ARG:NH1	2.17	0.43
1:D:162:ASN:O	1:D:164:CYS:N	2.51	0.43
1:E:29:ALA:C	1:E:31:TYR:N	2.76	0.43
1:E:136:LEU:C	1:E:136:LEU:CD2	2.92	0.43
1:E:214:ARG:O	1:E:215:TYR:C	2.58	0.43
1:A:45:THR:O	1:A:46:LYS:HE3	2.19	0.43
1:A:152:TYR:HE1	1:A:153:ARG:NH1	2.16	0.43
1:C:164:CYS:O	1:C:165:LYS:C	2.62	0.43
1:C:199:ASP:OD1	1:C:218:ILE:HA	2.18	0.43
1:C:257:GLU:CG	1:C:294:ASN:HA	2.45	0.43
1:D:160:LEU:HA	1:D:163:GLN:CG	2.48	0.43
1:D:233:HIS:NE2	1:D:312:ARG:NH1	2.67	0.43
1:D:352:ASP:CG	1:D:352:ASP:O	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:TRP:CZ2	1:E:200:MET:HE2	2.53	0.43
1:E:163:GLN:C	1:E:165:LYS:H	2.27	0.43
1:A:163:GLN:OE1	1:A:163:GLN:CA	2.67	0.43
1:B:162:ASN:HB3	1:B:163:GLN:H	1.63	0.43
1:C:151:GLU:O	1:C:151:GLU:HG2	2.18	0.43
1:C:175:VAL:HG13	1:C:181:ILE:HG12	2.00	0.43
1:D:137:TYR:HB2	1:D:163:GLN:NE2	2.33	0.43
1:D:182:PHE:C	1:D:184:VAL:N	2.76	0.43
1:E:46:LYS:HD2	1:E:46:LYS:N	2.34	0.43
1:A:66:ILE:HD12	1:A:69:VAL:HG11	2.01	0.42
1:A:79:ASP:OD2	1:A:79:ASP:C	2.62	0.42
1:B:38:ILE:HA	1:B:39:PRO:HD2	1.89	0.42
1:B:69:VAL:HG21	1:B:138:LEU:HD22	2.01	0.42
1:B:175:VAL:HG13	1:B:181:ILE:HG12	2.00	0.42
1:C:107:LEU:C	1:C:108:VAL:HG23	2.44	0.42
1:C:214:ARG:C	1:C:217:THR:HG22	2.43	0.42
1:E:249:ILE:HD13	1:E:254:VAL:HG12	2.01	0.42
1:E:317:ARG:HH21	1:E:410:LYS:HE2	1.84	0.42
1:B:295:PRO:HB2	1:B:322:ILE:CG2	2.49	0.42
1:B:382:PHE:CE2	1:B:387:ARG:HA	2.54	0.42
1:D:175:VAL:HA	1:D:176:PRO:HD2	1.67	0.42
1:D:382:PHE:CE2	1:D:387:ARG:HA	2.54	0.42
1:E:45:THR:O	1:E:46:LYS:HE3	2.19	0.42
1:E:200:MET:HB2	1:E:277:TYR:CE2	2.54	0.42
2:R:11:U:H2'	2:R:12:U:O4'	2.18	0.42
1:A:251:ASN:OD1	1:A:251:ASN:N	2.52	0.42
1:B:44:THR:HG21	1:B:116:VAL:HG11	2.01	0.42
1:B:175:VAL:O	1:B:176:PRO:C	2.61	0.42
1:C:20:ALA:HB2	1:D:269:ASP:O	2.20	0.42
1:C:52:ARG:HD3	1:C:127:THR:O	2.18	0.42
1:D:162:ASN:C	1:D:165:LYS:HD2	2.44	0.42
1:D:163:GLN:O	1:D:165:LYS:N	2.52	0.42
1:D:249:ILE:HD13	1:D:254:VAL:HG12	2.00	0.42
1:D:286:LYS:HZ1	2:R:2:U:P	2.42	0.42
1:B:386:ASN:O	1:B:387:ARG:C	2.62	0.42
1:C:47:SER:HB3	1:C:50:ASP:OD2	2.19	0.42
1:C:249:ILE:HD12	1:D:348:PHE:CE1	2.54	0.42
1:D:127:THR:OG1	1:D:128:SER:N	2.51	0.42
1:D:152:TYR:HE1	1:D:153:ARG:NH1	2.17	0.42
1:E:28:PRO:O	1:E:29:ALA:C	2.62	0.42
1:E:151:GLU:HA	1:E:154:LYS:HZ2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ALA:C	1:A:31:TYR:N	2.77	0.42
1:B:332:LEU:HD13	1:B:393:MET:HE3	2.01	0.42
1:B:347:GLN:HE21	1:B:347:GLN:HB3	1.71	0.42
1:C:73:LEU:O	1:C:74:TYR:C	2.62	0.42
1:C:136:LEU:HB2	1:C:213:PHE:CE2	2.55	0.42
1:E:80:ILE:HG12	1:E:80:ILE:O	2.19	0.42
1:E:252:ARG:NH2	1:E:256:ASP:OD1	2.52	0.42
1:E:356:THR:N	1:E:357:PRO:CD	2.81	0.42
1:E:389:PRO:CB	1:E:393:MET:HE2	2.50	0.42
1:A:50:ASP:OD1	1:A:121:VAL:HG22	2.20	0.42
1:A:342:ALA:O	1:A:343:ASP:C	2.62	0.42
1:C:285:SER:OG	1:D:207:LYS:CE	2.67	0.42
1:D:221:ARG:O	1:D:222:PHE:HB2	2.19	0.42
1:E:228:LEU:HA	1:E:228:LEU:HD23	1.76	0.42
1:E:272:ASP:OD2	1:E:272:ASP:N	2.53	0.42
1:E:382:PHE:CE2	1:E:387:ARG:HA	2.55	0.42
1:A:302:GLN:HG2	1:A:316:ALA:HB2	2.01	0.42
1:B:83:LYS:HD2	1:B:99:GLY:O	2.20	0.42
1:B:205:PHE:O	1:B:206:LYS:C	2.62	0.42
1:D:263:LEU:HA	1:D:263:LEU:HD12	1.89	0.42
1:E:29:ALA:H	1:E:266:GLN:HE22	1.67	0.42
1:E:44:THR:HG22	1:E:46:LYS:HZ2	1.84	0.42
1:E:214:ARG:C	1:E:217:THR:HG22	2.45	0.42
1:E:273:SER:OG	1:E:274:TYR:N	2.52	0.42
1:A:143:ARG:HE	1:A:155:LYS:HZ2	1.66	0.42
1:B:10:ASP:OD2	1:B:10:ASP:C	2.63	0.42
1:C:44:THR:HG21	1:C:116:VAL:HG11	2.02	0.42
1:C:97:LYS:O	1:C:98:ALA:O	2.37	0.42
1:C:205:PHE:O	1:C:206:LYS:C	2.62	0.42
1:C:294:ASN:N	1:C:295:PRO:HD3	2.34	0.42
1:C:382:PHE:CE2	1:C:387:ARG:HA	2.54	0.42
1:D:152:TYR:CE1	1:D:153:ARG:CZ	3.03	0.42
1:D:295:PRO:HB2	1:D:322:ILE:CG2	2.49	0.42
1:E:31:TYR:C	1:E:33:ARG:N	2.77	0.42
1:E:66:ILE:O	1:E:67:ILE:C	2.62	0.42
1:A:136:LEU:HB2	1:A:213:PHE:CE2	2.55	0.42
1:B:137:TYR:O	1:B:141:LEU:HG	2.20	0.42
1:C:162:ASN:HB3	1:C:163:GLN:H	1.61	0.42
1:D:73:LEU:O	1:D:74:TYR:C	2.62	0.42
1:D:83:LYS:HD2	1:D:99:GLY:O	2.20	0.42
1:D:177:GLU:HA	1:D:181:ILE:CD1	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ALA:O	1:D:346:GLN:C	2.63	0.42
1:E:136:LEU:HB2	1:E:213:PHE:CE2	2.54	0.42
1:E:302:GLN:CB	1:E:412:ILE:HD11	2.46	0.42
1:A:142:TYR:CD1	1:A:195:VAL:HG11	2.55	0.42
1:A:303:LEU:HD22	1:A:328:THR:HB	2.02	0.42
1:B:117:LEU:O	1:B:118:PRO:C	2.63	0.42
1:B:136:LEU:C	1:B:136:LEU:CD2	2.92	0.42
1:C:163:GLN:C	1:C:165:LYS:N	2.77	0.42
1:C:263:LEU:HD12	1:C:263:LEU:HA	1.92	0.42
1:E:141:LEU:HD12	1:E:185:TRP:CZ3	2.55	0.42
1:E:175:VAL:HG13	1:E:181:ILE:HG12	2.01	0.42
2:R:31:U:C6	2:R:31:U:C3'	3.03	0.42
1:A:317:ARG:HG3	2:R:32:U:OP2	2.19	0.41
1:B:25:VAL:HG11	1:B:288:PRO:HA	2.02	0.41
1:B:240:MET:HE1	1:B:248:TRP:HD1	1.84	0.41
1:C:69:VAL:HG21	1:C:138:LEU:HD22	2.02	0.41
1:C:234:LEU:O	1:C:238:THR:HG23	2.19	0.41
1:C:250:LEU:HD13	1:D:344:LEU:CD1	2.49	0.41
1:C:317:ARG:HD3	2:R:13:U:O2	2.20	0.41
1:D:38:ILE:O	1:D:38:ILE:CG1	2.68	0.41
1:D:55:VAL:HG23	1:D:56:TYR:N	2.33	0.41
1:D:107:LEU:CD2	1:D:274:TYR:OH	2.65	0.41
1:D:293:LYS:C	1:D:295:PRO:HD3	2.45	0.41
1:D:356:THR:N	1:D:357:PRO:CD	2.78	0.41
1:E:149:MET:CG	2:R:42:U:O4'	2.55	0.41
1:A:205:PHE:O	1:A:206:LYS:C	2.62	0.41
1:B:55:VAL:HG23	1:B:56:TYR:N	2.34	0.41
1:B:72:TYR:CE1	1:B:134:LEU:CD1	3.03	0.41
1:B:84:LEU:HA	1:B:84:LEU:HD23	1.76	0.41
1:B:302:GLN:CB	1:B:412:ILE:HD11	2.46	0.41
1:E:151:GLU:O	1:E:151:GLU:HG2	2.19	0.41
1:A:72:TYR:CE1	1:A:134:LEU:HD13	2.55	0.41
1:A:151:GLU:HA	1:A:154:LYS:HZ2	1.84	0.41
1:A:169:GLU:HB3	1:A:170:GLN:H	1.70	0.41
1:B:74:TYR:CD1	1:B:78:LYS:HD3	2.53	0.41
1:B:80:ILE:HG12	1:B:80:ILE:O	2.20	0.41
1:D:175:VAL:HG13	1:D:181:ILE:CG1	2.49	0.41
1:D:199:ASP:OD1	1:D:218:ILE:HA	2.20	0.41
1:D:272:ASP:OD2	1:D:272:ASP:N	2.53	0.41
1:E:66:ILE:HG23	1:E:67:ILE:N	2.35	0.41
2:R:4:U:O2'	2:R:5:U:H5'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:9:U:O3'	2:R:10:U:C6	2.70	0.41
1:A:97:LYS:HG3	1:A:98:ALA:H	1.80	0.41
1:A:175:VAL:HG13	1:A:181:ILE:CG1	2.50	0.41
1:A:364:LEU:HD12	1:A:364:LEU:N	2.28	0.41
1:C:18:LEU:HD12	1:D:232:GLY:HA2	2.03	0.41
1:C:19:PRO:HA	1:D:268:ILE:O	2.21	0.41
1:C:263:LEU:HA	1:C:264:PRO:HD3	1.78	0.41
1:D:317:ARG:O	1:D:319:PRO:HD3	2.20	0.41
1:D:379:LEU:HD23	1:D:379:LEU:HA	1.87	0.41
1:E:203:HIS:HA	1:E:214:ARG:NH1	2.36	0.41
1:B:141:LEU:HD12	1:B:185:TRP:CZ3	2.56	0.41
1:C:109:SER:O	1:C:110:LEU:HD23	2.20	0.41
1:D:302:GLN:HG3	1:D:313:ALA:HB1	2.01	0.41
1:E:84:LEU:HD11	1:E:96:GLY:HA3	2.02	0.41
1:E:180:ASP:N	1:E:183:ASP:CG	2.64	0.41
2:R:5:U:O2	2:R:5:U:H2'	2.20	0.41
1:A:2:SER:C	1:A:4:THR:N	2.77	0.41
1:A:105:PHE:C	1:A:107:LEU:N	2.78	0.41
1:A:175:VAL:HA	1:A:176:PRO:HD2	1.70	0.41
1:B:79:ASP:OD2	1:B:81:ARG:HB2	2.20	0.41
1:B:149:MET:HG3	2:R:24:U:C6	2.55	0.41
1:C:181:ILE:HD13	1:C:183:ASP:OD1	2.20	0.41
1:C:182:PHE:O	1:C:184:VAL:N	2.54	0.41
1:D:66:ILE:O	1:D:67:ILE:C	2.62	0.41
1:D:116:VAL:HB	1:D:117:LEU:H	1.68	0.41
1:D:422:LYS:HA	1:D:422:LYS:HD3	1.63	0.41
1:E:379:LEU:HD23	1:E:379:LEU:HA	1.95	0.41
1:A:66:ILE:HD13	1:A:185:TRP:CD1	2.56	0.41
1:A:295:PRO:HB2	1:A:322:ILE:CG2	2.51	0.41
1:B:263:LEU:HA	1:B:264:PRO:HD3	1.78	0.41
1:C:88:TRP:CZ2	1:C:200:MET:HE2	2.56	0.41
1:D:28:PRO:O	1:D:29:ALA:C	2.62	0.41
1:E:182:PHE:CD2	1:E:182:PHE:N	2.84	0.41
1:A:47:SER:HB3	1:A:50:ASP:OD2	2.20	0.41
1:B:409:GLU:O	1:B:410:LYS:HB2	2.21	0.41
1:C:66:ILE:HD12	1:C:69:VAL:HG11	2.03	0.41
1:C:218:ILE:C	1:C:220:SER:H	2.28	0.41
1:C:250:LEU:HB3	1:D:344:LEU:HD13	2.02	0.41
1:D:133:TRP:CD1	1:D:167:ILE:HG21	2.55	0.41
1:D:136:LEU:C	1:D:136:LEU:CD2	2.93	0.41
1:D:228:LEU:HD23	1:D:228:LEU:HA	1.69	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:ASP:OD1	1:E:121:VAL:HG22	2.21	0.41
1:A:10:ASP:OD2	1:A:12:THR:HG23	2.21	0.41
1:A:70:ASN:H	1:A:70:ASN:ND2	2.15	0.41
1:A:116:VAL:HB	1:A:117:LEU:H	1.66	0.41
1:A:263:LEU:HA	1:A:264:PRO:HD3	1.80	0.41
1:B:18:LEU:HB2	1:B:19:PRO:HD2	2.02	0.41
1:B:136:LEU:HB2	1:B:213:PHE:CE2	2.56	0.41
1:B:175:VAL:O	1:B:176:PRO:O	2.39	0.41
1:B:273:SER:OG	1:B:274:TYR:N	2.54	0.41
1:C:136:LEU:C	1:C:136:LEU:CD2	2.94	0.41
1:D:2:SER:C	1:D:4:THR:N	2.79	0.41
1:D:137:TYR:O	1:D:141:LEU:HG	2.21	0.41
1:D:176:PRO:HB2	1:D:177:GLU:H	1.69	0.41
1:D:294:ASN:N	1:D:295:PRO:HD3	2.36	0.41
1:E:324:TYR:O	1:E:325:THR:C	2.63	0.41
1:E:324:TYR:O	1:E:328:THR:CG2	2.69	0.41
1:B:66:ILE:O	1:B:67:ILE:C	2.63	0.41
1:B:150:PRO:O	1:B:154:LYS:HE3	2.21	0.41
1:B:152:TYR:OH	1:B:176:PRO:CB	2.63	0.41
1:C:50:ASP:OD1	1:C:121:VAL:HG22	2.20	0.41
1:C:150:PRO:O	1:C:154:LYS:HE3	2.21	0.41
1:C:187:ASN:HD22	1:C:187:ASN:HA	1.63	0.41
1:C:356:THR:O	1:C:357:PRO:C	2.63	0.41
1:D:45:THR:O	1:D:46:LYS:HE3	2.21	0.41
1:D:200:MET:HB2	1:D:277:TYR:CE2	2.55	0.41
1:D:224:ASP:CG	2:R:3:U:H4'	2.46	0.41
1:E:287:SER:HA	1:E:288:PRO:HD3	1.83	0.41
1:A:127:THR:OG1	1:A:128:SER:N	2.54	0.40
1:A:233:HIS:NE2	1:A:312:ARG:NH1	2.68	0.40
1:C:66:ILE:HD13	1:C:185:TRP:CD1	2.56	0.40
1:D:98:ALA:C	1:D:100:ASP:H	2.29	0.40
1:D:342:ALA:O	1:D:343:ASP:C	2.63	0.40
1:E:218:ILE:C	1:E:220:SER:H	2.28	0.40
1:A:409:GLU:O	1:A:410:LYS:HB2	2.20	0.40
1:A:412:ILE:HD13	1:A:412:ILE:HG21	1.75	0.40
1:B:22:GLU:HG2	1:C:206:LYS:NZ	2.36	0.40
1:B:258:MET:HE3	1:B:262:MET:HG3	2.03	0.40
1:C:79:ASP:OD2	1:C:81:ARG:HB2	2.21	0.40
1:C:80:ILE:HG12	1:C:80:ILE:O	2.20	0.40
1:D:66:ILE:O	1:D:70:ASN:ND2	2.48	0.40
1:D:180:ASP:N	1:D:183:ASP:OD1	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ILE:HD13	1:D:412:ILE:HG21	1.62	0.40
1:E:177:GLU:CG	1:E:183:ASP:HB3	2.52	0.40
1:E:352:ASP:O	1:E:352:ASP:CG	2.64	0.40
2:R:8:U:H2'	2:R:9:U:H5''	2.03	0.40
1:A:18:LEU:HB2	1:A:19:PRO:HD2	2.02	0.40
1:A:117:LEU:O	1:A:118:PRO:C	2.63	0.40
1:A:136:LEU:C	1:A:136:LEU:CD2	2.93	0.40
1:A:358:ASP:O	1:A:359:ASP:HB2	2.21	0.40
1:C:84:LEU:HA	1:C:84:LEU:HD23	1.77	0.40
1:C:272:ASP:OD2	1:C:272:ASP:N	2.54	0.40
1:D:31:TYR:C	1:D:33:ARG:N	2.79	0.40
1:E:109:SER:O	1:E:110:LEU:HD23	2.22	0.40
1:A:214:ARG:C	1:A:217:THR:HG22	2.47	0.40
1:B:38:ILE:O	1:B:38:ILE:CG1	2.68	0.40
1:D:389:PRO:CB	1:D:393:MET:HE2	2.51	0.40
1:E:66:ILE:HD12	1:E:69:VAL:HG11	2.02	0.40
1:E:263:LEU:HA	1:E:264:PRO:HD3	1.80	0.40
1:A:25:VAL:HG11	1:A:288:PRO:HA	2.04	0.40
1:A:203:HIS:HA	1:A:214:ARG:NH1	2.37	0.40
1:A:368:ALA:HA	1:A:369:PRO:HD3	1.79	0.40
1:C:356:THR:N	1:C:357:PRO:CD	2.81	0.40
1:E:45:THR:H	1:E:46:LYS:HZ2	1.70	0.40
1:E:167:ILE:HD13	1:E:167:ILE:H	1.87	0.40
1:E:226:ALA:HB2	2:R:40:U:OP1	2.22	0.40
1:E:258:MET:HE3	1:E:262:MET:HG3	2.04	0.40
1:E:295:PRO:HB2	1:E:322:ILE:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	419/421 (100%)	316 (75%)	70 (17%)	33 (8%)	1	3
1	B	411/421 (98%)	315 (77%)	67 (16%)	29 (7%)	1	4
1	C	409/421 (97%)	318 (78%)	62 (15%)	29 (7%)	1	4
1	D	412/421 (98%)	319 (77%)	61 (15%)	32 (8%)	1	4
1	E	419/421 (100%)	317 (76%)	67 (16%)	35 (8%)	0	3
All	All	2070/2105 (98%)	1585 (77%)	327 (16%)	158 (8%)	1	4

All (158) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	99	GLY
1	A	117	LEU
1	A	120	GLY
1	A	132	LYS
1	A	163	GLN
1	A	176	PRO
1	A	177	GLU
1	A	180	ASP
1	A	344	LEU
1	A	358	ASP
1	B	30	ASP
1	B	34	LYS
1	B	117	LEU
1	B	120	GLY
1	B	163	GLN
1	B	176	PRO
1	B	180	ASP
1	B	344	LEU
1	C	34	LYS
1	C	117	LEU
1	C	120	GLY
1	C	132	LYS
1	C	163	GLN
1	C	176	PRO
1	C	177	GLU
1	C	180	ASP
1	C	344	LEU
1	D	30	ASP
1	D	34	LYS
1	D	117	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	120	GLY
1	D	163	GLN
1	D	165	LYS
1	D	176	PRO
1	D	177	GLU
1	D	180	ASP
1	D	344	LEU
1	E	30	ASP
1	E	34	LYS
1	E	117	LEU
1	E	120	GLY
1	E	163	GLN
1	E	165	LYS
1	E	176	PRO
1	E	344	LEU
1	E	360	SER
1	E	362	GLY
1	A	30	ASP
1	A	44	THR
1	A	108	VAL
1	A	113	LEU
1	A	171	PHE
1	A	181	ILE
1	A	309	ARG
1	B	44	THR
1	B	108	VAL
1	B	113	LEU
1	B	132	LYS
1	B	171	PHE
1	B	177	GLU
1	B	181	ILE
1	B	309	ARG
1	C	30	ASP
1	C	44	THR
1	C	98	ALA
1	C	108	VAL
1	C	113	LEU
1	C	171	PHE
1	C	181	ILE
1	C	309	ARG
1	D	44	THR
1	D	108	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	113	LEU
1	D	132	LYS
1	D	164	CYS
1	D	171	PHE
1	D	181	ILE
1	D	309	ARG
1	E	44	THR
1	E	100	ASP
1	E	108	VAL
1	E	113	LEU
1	E	132	LYS
1	E	171	PHE
1	E	180	ASP
1	E	181	ILE
1	E	359	ASP
1	A	43	ASN
1	A	122	SER
1	A	164	CYS
1	A	172	GLU
1	A	179	ARG
1	A	183	ASP
1	B	122	SER
1	B	172	GLU
1	B	183	ASP
1	C	122	SER
1	C	125	SER
1	C	172	GLU
1	C	179	ARG
1	C	183	ASP
1	C	387	ARG
1	D	43	ASN
1	D	98	ALA
1	D	122	SER
1	D	168	ASN
1	D	172	GLU
1	D	183	ASP
1	E	43	ASN
1	E	122	SER
1	E	162	ASN
1	E	172	GLU
1	E	179	ARG
1	E	183	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	309	ARG
1	A	125	SER
1	A	162	ASN
1	A	357	PRO
1	A	362	GLY
1	A	387	ARG
1	B	43	ASN
1	B	118	PRO
1	B	125	SER
1	C	43	ASN
1	C	118	PRO
1	C	162	ASN
1	D	118	PRO
1	D	125	SER
1	D	162	ASN
1	D	179	ARG
1	D	357	PRO
1	E	118	PRO
1	E	125	SER
1	A	118	PRO
1	B	162	ASN
1	B	179	ARG
1	E	363	GLY
1	E	387	ARG
1	B	357	PRO
1	B	387	ARG
1	A	116	VAL
1	B	80	ILE
1	B	116	VAL
1	C	80	ILE
1	C	116	VAL
1	D	80	ILE
1	D	116	VAL
1	D	370	PRO
1	E	80	ILE
1	E	116	VAL
1	E	357	PRO
1	E	370	PRO
1	A	80	ILE
1	A	28	PRO
1	B	216	GLY
1	C	216	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	216	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/362 (100%)	290 (80%)	72 (20%)	1	7
1	B	358/362 (99%)	289 (81%)	69 (19%)	1	8
1	C	356/362 (98%)	288 (81%)	68 (19%)	1	8
1	D	359/362 (99%)	288 (80%)	71 (20%)	1	8
1	E	362/362 (100%)	295 (82%)	67 (18%)	1	9
All	All	1797/1810 (99%)	1450 (81%)	347 (19%)	1	8

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	8	ILE
1	A	9	ILE
1	A	13	VAL
1	A	18	LEU
1	A	22	GLU
1	A	34	LYS
1	A	38	ILE
1	A	40	LEU
1	A	44	THR
1	A	46	LYS
1	A	47	SER
1	A	48	LEU
1	A	55	VAL
1	A	61	SER
1	A	63	ASN
1	A	70	ASN
1	A	78	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	ASP
1	A	83	LYS
1	A	85	ASP
1	A	97	LYS
1	A	100	ASP
1	A	101	THR
1	A	107	LEU
1	A	113	LEU
1	A	134	LEU
1	A	149	MET
1	A	154	LYS
1	A	155	LYS
1	A	156	LEU
1	A	162	ASN
1	A	165	LYS
1	A	166	MET
1	A	167	ILE
1	A	168	ASN
1	A	171	PHE
1	A	172	GLU
1	A	174	LEU
1	A	175	VAL
1	A	181	ILE
1	A	182	PHE
1	A	183	ASP
1	A	187	ASN
1	A	230	THR
1	A	237	ILE
1	A	242	THR
1	A	243	GLU
1	A	251	ASN
1	A	253	GLU
1	A	257	GLU
1	A	270	LYS
1	A	272	ASP
1	A	273	SER
1	A	283	LEU
1	A	292	VAL
1	A	307	LEU
1	A	308	LEU
1	A	327	LEU
1	A	328	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	332	LEU
1	A	344	LEU
1	A	350	VAL
1	A	353	ASN
1	A	356	THR
1	A	364	LEU
1	A	365	THR
1	A	376	VAL
1	A	393	MET
1	A	394	MET
1	A	410	LYS
1	A	412	ILE
1	B	6	LYS
1	B	8	ILE
1	B	9	ILE
1	B	13	VAL
1	B	18	LEU
1	B	22	GLU
1	B	34	LYS
1	B	38	ILE
1	B	40	LEU
1	B	44	THR
1	B	46	LYS
1	B	47	SER
1	B	48	LEU
1	B	55	VAL
1	B	61	SER
1	B	63	ASN
1	B	70	ASN
1	B	78	LYS
1	B	79	ASP
1	B	83	LYS
1	B	85	ASP
1	B	97	LYS
1	B	100	ASP
1	B	101	THR
1	B	107	LEU
1	B	113	LEU
1	B	134	LEU
1	B	149	MET
1	B	154	LYS
1	B	155	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	156	LEU
1	B	162	ASN
1	B	163	GLN
1	B	165	LYS
1	B	166	MET
1	B	167	ILE
1	B	168	ASN
1	B	171	PHE
1	B	172	GLU
1	B	174	LEU
1	B	175	VAL
1	B	181	ILE
1	B	182	PHE
1	B	183	ASP
1	B	187	ASN
1	B	230	THR
1	B	237	ILE
1	B	243	GLU
1	B	251	ASN
1	B	253	GLU
1	B	257	GLU
1	B	270	LYS
1	B	272	ASP
1	B	273	SER
1	B	283	LEU
1	B	292	VAL
1	B	307	LEU
1	B	308	LEU
1	B	327	LEU
1	B	328	THR
1	B	332	LEU
1	B	344	LEU
1	B	350	VAL
1	B	353	ASN
1	B	356	THR
1	B	376	VAL
1	B	393	MET
1	B	410	LYS
1	B	412	ILE
1	C	3	VAL
1	C	6	LYS
1	C	8	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	9	ILE
1	C	13	VAL
1	C	18	LEU
1	C	22	GLU
1	C	34	LYS
1	C	38	ILE
1	C	40	LEU
1	C	44	THR
1	C	46	LYS
1	C	47	SER
1	C	48	LEU
1	C	63	ASN
1	C	70	ASN
1	C	78	LYS
1	C	79	ASP
1	C	83	LYS
1	C	85	ASP
1	C	97	LYS
1	C	100	ASP
1	C	101	THR
1	C	107	LEU
1	C	113	LEU
1	C	134	LEU
1	C	149	MET
1	C	154	LYS
1	C	155	LYS
1	C	156	LEU
1	C	162	ASN
1	C	163	GLN
1	C	165	LYS
1	C	166	MET
1	C	167	ILE
1	C	168	ASN
1	C	171	PHE
1	C	172	GLU
1	C	174	LEU
1	C	181	ILE
1	C	182	PHE
1	C	183	ASP
1	C	187	ASN
1	C	230	THR
1	C	237	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	242	THR
1	C	243	GLU
1	C	251	ASN
1	C	253	GLU
1	C	257	GLU
1	C	270	LYS
1	C	272	ASP
1	C	273	SER
1	C	283	LEU
1	C	292	VAL
1	C	307	LEU
1	C	308	LEU
1	C	327	LEU
1	C	328	THR
1	C	332	LEU
1	C	344	LEU
1	C	350	VAL
1	C	353	ASN
1	C	356	THR
1	C	376	VAL
1	C	393	MET
1	C	410	LYS
1	C	412	ILE
1	D	3	VAL
1	D	6	LYS
1	D	8	ILE
1	D	9	ILE
1	D	13	VAL
1	D	18	LEU
1	D	22	GLU
1	D	38	ILE
1	D	40	LEU
1	D	44	THR
1	D	46	LYS
1	D	47	SER
1	D	48	LEU
1	D	55	VAL
1	D	61	SER
1	D	63	ASN
1	D	70	ASN
1	D	78	LYS
1	D	79	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	83	LYS
1	D	85	ASP
1	D	97	LYS
1	D	100	ASP
1	D	101	THR
1	D	107	LEU
1	D	113	LEU
1	D	134	LEU
1	D	149	MET
1	D	154	LYS
1	D	155	LYS
1	D	156	LEU
1	D	162	ASN
1	D	165	LYS
1	D	166	MET
1	D	168	ASN
1	D	171	PHE
1	D	172	GLU
1	D	174	LEU
1	D	175	VAL
1	D	181	ILE
1	D	182	PHE
1	D	183	ASP
1	D	187	ASN
1	D	230	THR
1	D	237	ILE
1	D	242	THR
1	D	243	GLU
1	D	251	ASN
1	D	253	GLU
1	D	257	GLU
1	D	270	LYS
1	D	272	ASP
1	D	273	SER
1	D	283	LEU
1	D	292	VAL
1	D	307	LEU
1	D	308	LEU
1	D	327	LEU
1	D	328	THR
1	D	332	LEU
1	D	344	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	350	VAL
1	D	353	ASN
1	D	356	THR
1	D	364	LEU
1	D	365	THR
1	D	376	VAL
1	D	393	MET
1	D	394	MET
1	D	410	LYS
1	D	412	ILE
1	E	6	LYS
1	E	8	ILE
1	E	9	ILE
1	E	13	VAL
1	E	18	LEU
1	E	22	GLU
1	E	38	ILE
1	E	40	LEU
1	E	44	THR
1	E	46	LYS
1	E	47	SER
1	E	48	LEU
1	E	55	VAL
1	E	63	ASN
1	E	78	LYS
1	E	79	ASP
1	E	83	LYS
1	E	85	ASP
1	E	97	LYS
1	E	100	ASP
1	E	101	THR
1	E	113	LEU
1	E	134	LEU
1	E	149	MET
1	E	154	LYS
1	E	155	LYS
1	E	156	LEU
1	E	162	ASN
1	E	163	GLN
1	E	165	LYS
1	E	166	MET
1	E	167	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	168	ASN
1	E	171	PHE
1	E	172	GLU
1	E	174	LEU
1	E	175	VAL
1	E	181	ILE
1	E	182	PHE
1	E	183	ASP
1	E	187	ASN
1	E	230	THR
1	E	237	ILE
1	E	243	GLU
1	E	251	ASN
1	E	253	GLU
1	E	257	GLU
1	E	270	LYS
1	E	272	ASP
1	E	273	SER
1	E	283	LEU
1	E	292	VAL
1	E	307	LEU
1	E	308	LEU
1	E	327	LEU
1	E	328	THR
1	E	332	LEU
1	E	344	LEU
1	E	350	VAL
1	E	353	ASN
1	E	356	THR
1	E	364	LEU
1	E	376	VAL
1	E	393	MET
1	E	394	MET
1	E	410	LYS
1	E	412	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	70	ASN
1	A	162	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	187	ASN
1	A	203	HIS
1	A	260	GLN
1	A	266	GLN
1	A	347	GLN
1	A	385	GLN
1	A	395	GLN
1	A	405	GLN
1	B	68	HIS
1	B	70	ASN
1	B	162	ASN
1	B	187	ASN
1	B	203	HIS
1	B	260	GLN
1	B	266	GLN
1	B	347	GLN
1	B	385	GLN
1	B	395	GLN
1	C	57	GLN
1	C	70	ASN
1	C	162	ASN
1	C	187	ASN
1	C	203	HIS
1	C	260	GLN
1	C	266	GLN
1	C	347	GLN
1	C	385	GLN
1	C	395	GLN
1	C	405	GLN
1	D	57	GLN
1	D	68	HIS
1	D	70	ASN
1	D	187	ASN
1	D	203	HIS
1	D	260	GLN
1	D	266	GLN
1	D	347	GLN
1	D	385	GLN
1	D	395	GLN
1	E	57	GLN
1	E	68	HIS
1	E	70	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	162	ASN
1	E	187	ASN
1	E	203	HIS
1	E	260	GLN
1	E	266	GLN
1	E	347	GLN
1	E	385	GLN
1	E	395	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	44/45 (97%)	28 (63%)	1 (2%)

All (28) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	2	U
2	R	3	U
2	R	5	U
2	R	9	U
2	R	10	U
2	R	12	U
2	R	13	U
2	R	14	U
2	R	17	U
2	R	18	U
2	R	19	U
2	R	20	U
2	R	23	U
2	R	24	U
2	R	25	U
2	R	26	U
2	R	27	U
2	R	29	U
2	R	31	U
2	R	32	U
2	R	33	U
2	R	38	U
2	R	39	U
2	R	40	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	41	U
2	R	42	U
2	R	44	U
2	R	45	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	26	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 20 are modelled with single atom - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	421/421 (100%)	0.33	21 (4%)	34	18	50, 81, 131, 148	0
1	B	415/421 (98%)	0.39	17 (4%)	41	23	50, 81, 130, 140	0
1	C	413/421 (98%)	0.43	27 (6%)	25	13	50, 81, 129, 141	0
1	D	416/421 (98%)	0.55	28 (6%)	24	12	50, 81, 129, 141	0
1	E	421/421 (100%)	0.32	14 (3%)	49	28	49, 82, 131, 145	0
2	R	45/45 (100%)	1.14	0	100	100	106, 124, 140, 151	0
All	All	2131/2150 (99%)	0.42	107 (5%)	34	18	49, 82, 131, 151	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	9.0
1	C	2	SER	7.3
1	B	2	SER	6.0
1	D	43	ASN	5.2
1	B	118	PRO	4.9
1	A	2	SER	4.9
1	D	98	ALA	4.1
1	D	172	GLU	4.0
1	D	118	PRO	4.0
1	C	158	ASP	3.8
1	D	124	ALA	3.8
1	E	118	PRO	3.5
1	C	171	PHE	3.5
1	D	121	VAL	3.4
1	C	118	PRO	3.4
1	D	2	SER	3.4
1	C	161	THR	3.3
1	B	80	ILE	3.2
1	D	351	GLY	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	171	PHE	3.1
1	C	356	THR	3.1
1	E	69	VAL	3.1
1	D	30	ASP	3.1
1	D	163	GLN	3.0
1	A	216	GLY	3.0
1	D	371	GLN	3.0
1	C	122	SER	2.9
1	D	166	MET	2.9
1	A	163	GLN	2.9
1	B	42	ILE	2.9
1	B	120	GLY	2.9
1	D	178	GLY	2.9
1	E	175	VAL	2.8
1	A	355	TYR	2.7
1	B	3	VAL	2.7
1	C	180	ASP	2.7
1	A	353	ASN	2.7
1	A	42	ILE	2.6
1	B	163	GLN	2.6
1	A	181	ILE	2.6
1	A	180	ASP	2.6
1	A	178	GLY	2.6
1	A	361	THR	2.6
1	E	185	TRP	2.6
1	C	164	CYS	2.6
1	C	216	GLY	2.6
1	E	73	LEU	2.6
1	A	118	PRO	2.5
1	C	3	VAL	2.5
1	A	356	THR	2.5
1	D	119	ASP	2.5
1	C	179	ARG	2.5
1	D	48	LEU	2.5
1	B	164	CYS	2.5
1	C	175	VAL	2.5
1	D	167	ILE	2.5
1	A	362	GLY	2.5
1	B	351	GLY	2.5
1	D	164	CYS	2.4
1	E	174	LEU	2.4
1	C	181	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	119	ASP	2.4
1	B	178	GLY	2.4
1	E	129	ALA	2.4
1	E	166	MET	2.4
1	E	169	GLU	2.4
1	B	137	TYR	2.3
1	A	175	VAL	2.3
1	B	122	SER	2.3
1	C	150	PRO	2.3
1	C	156	LEU	2.3
1	B	215	TYR	2.3
1	C	357	PRO	2.3
1	C	107	LEU	2.3
1	C	166	MET	2.2
1	B	386	ASN	2.2
1	D	150	PRO	2.2
1	A	57	GLN	2.2
1	D	80	ILE	2.2
1	C	113	LEU	2.2
1	D	364	LEU	2.2
1	A	174	LEU	2.2
1	E	157	MET	2.2
1	C	115	GLY	2.2
1	D	216	GLY	2.2
1	D	224	ASP	2.2
1	C	137	TYR	2.2
1	D	157	MET	2.2
1	E	112	ALA	2.1
1	B	185	TRP	2.1
1	A	142	TYR	2.1
1	D	355	TYR	2.1
1	D	353	ASN	2.1
1	B	55	VAL	2.1
1	D	44	THR	2.1
1	C	173	PRO	2.1
1	C	155	LYS	2.1
1	C	421	ASP	2.1
1	D	85	ASP	2.1
1	A	169	GLU	2.1
1	D	122	SER	2.0
1	C	14	ILE	2.0
1	A	68	HIS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	TYR	2.0
1	E	148	GLN	2.0
1	C	95	ILE	2.0
1	E	161	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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
3	IUM	R	538	1/3	0.74	0.19	272,272,272,272	0
3	IUM	R	539	1/3	0.77	0.29	265,265,265,265	0
3	IUM	R	536	1/3	0.87	0.11	245,245,245,245	0
3	IUM	R	537	1/3	0.87	0.21	258,258,258,258	0
3	IUM	R	540	1/3	0.87	0.16	257,257,257,257	0
3	IUM	B	525	1/3	0.90	0.14	187,187,187,187	0
3	IUM	D	531	1/3	0.92	0.13	188,188,188,188	0
3	IUM	B	527	1/3	0.93	0.16	199,199,199,199	0
3	IUM	E	535	1/3	0.96	0.16	186,186,186,186	0
3	IUM	A	521	1/3	0.96	0.12	162,162,162,162	0
3	IUM	E	533	1/3	0.96	0.11	173,173,173,173	0
3	IUM	A	523	1/3	0.97	0.08	174,174,174,174	0
3	IUM	C	530	1/3	0.98	0.04	151,151,151,151	0
3	IUM	A	524	1/3	0.98	0.05	158,158,158,158	0
3	IUM	C	528	1/3	0.98	0.07	138,138,138,138	0
3	IUM	C	529	1/3	0.99	0.02	105,105,105,105	0
3	IUM	E	534	1/3	0.99	0.04	105,105,105,105	0
3	IUM	A	522	1/3	0.99	0.03	109,109,109,109	0
3	IUM	B	526	1/3	0.99	0.02	104,104,104,104	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IUM	D	532	1/3	1.00	0.02	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.