



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 10:23 AM EDT

PDB ID : 3PU0 / pdb_00003pu0
Title : Crystal Structure of a vesicular stomatitis virus nucleocapsid-polyC complex
Authors : Luo, M.; Green, T.J.; Rowse, M.
Deposited on : 2010-12-03
Resolution : 3.09 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

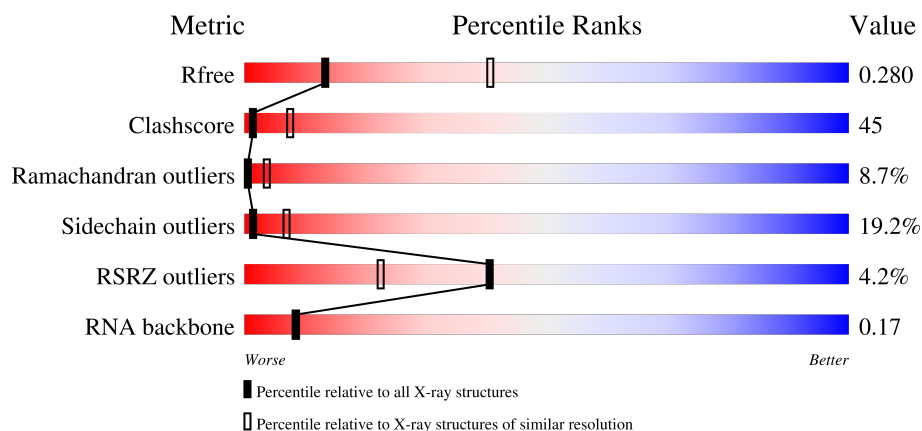
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)
RNA backbone	3983	1022 (3.32-2.88)

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	4% 39% 43% 16% .
1	B	421	4% 39% 41% 16% . .
1	C	421	4% 39% 42% 15% . .
1	D	421	6% 39% 43% 14% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	421	3% 40% 41% 16%
2	R	45	7% 33% 44% 16%

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.

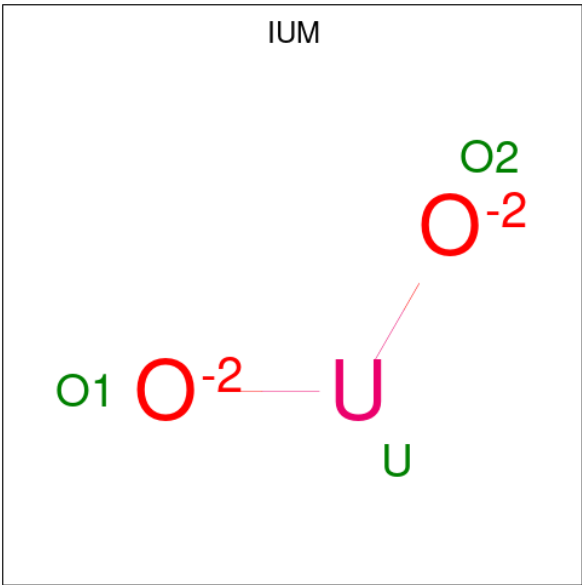
- Molecule 1 is a protein called Nucleoprotein.

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	135	315	45			

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



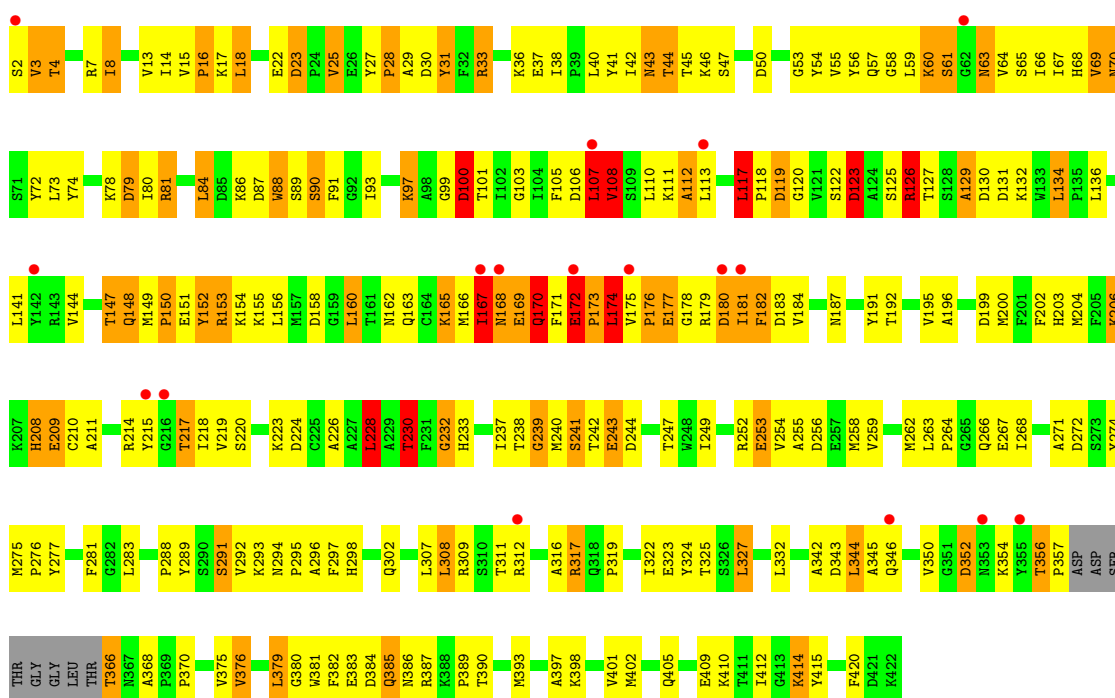
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	A	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	B	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	C	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	D	1	Total U 1 1	0	0
3	D	1	Total U 1 1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

Continued on next page...

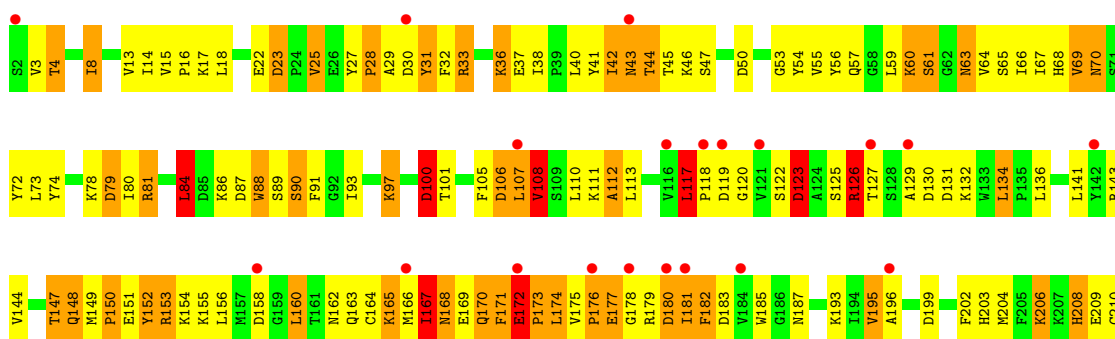
Continued from previous page...

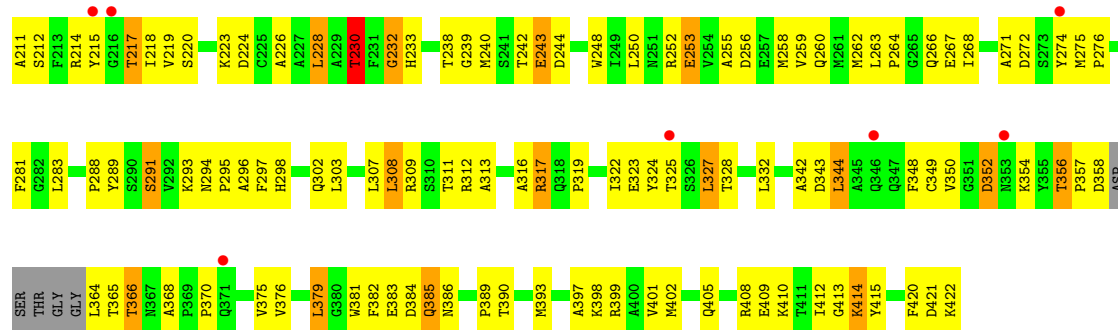
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0
3	R	1	Total 1	U 1	0	0

- Molecule 1: Nucleoprotein

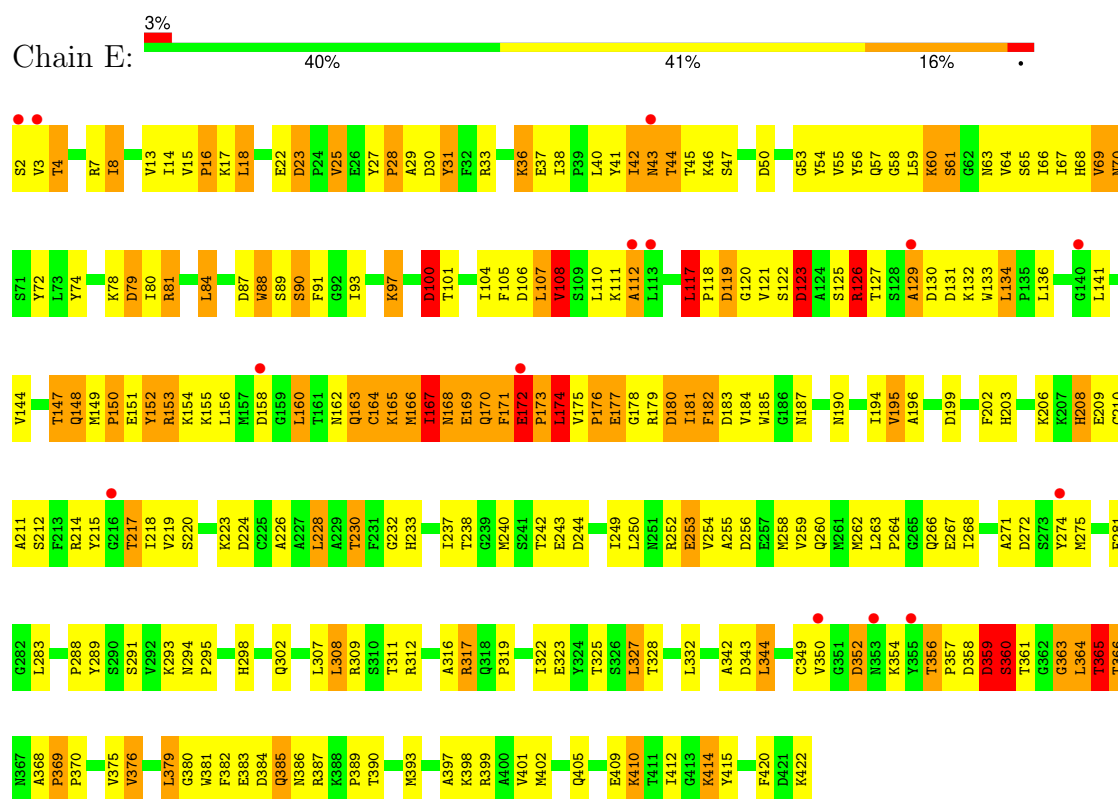


- Molecule 1: Nucleoprotein

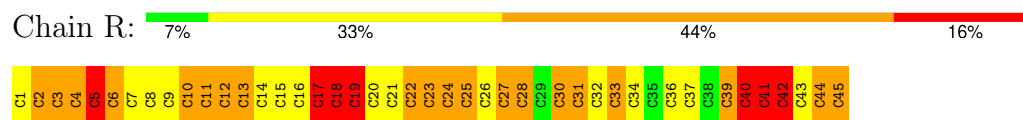




• Molecule 1: Nucleoprotein



• 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	164.65Å 235.55Å 75.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 3.09 49.75 – 3.09	Depositor EDS
% Data completeness (in resolution range)	78.5 (49.75-3.09) 78.5 (49.75-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.16 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.6_289	Depositor
R, R_{free}	0.250 , 0.290 0.239 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.879	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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	0.66	1/3403 (0.0%)	1.00	15/4607 (0.3%)
1	B	0.66	0/3365	0.97	13/4554 (0.3%)
1	C	0.65	0/3350	0.98	11/4533 (0.2%)
1	D	0.68	0/3373	0.99	12/4565 (0.3%)
1	E	0.65	0/3403	0.98	14/4607 (0.3%)
2	R	0.53	0/989	1.45	24/1526 (1.6%)
All	All	0.65	1/17883 (0.0%)	1.02	89/24392 (0.4%)

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	2
1	B	0	4
1	C	0	1
1	D	0	1
1	E	0	3
All	All	0	11

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	358	ASP	CA-C	5.74	1.55	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	15	C	N1-C1'-C2'	9.66	126.49	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	362	GLY	N-CA-C	9.56	124.56	110.60
1	D	168	ASN	N-CA-C	8.98	123.47	110.10
2	R	18	C	N1-C1'-C2'	-8.57	99.14	112.00
2	R	6	C	N1-C1'-C2'	7.06	122.60	112.00
2	R	27	C	O3'-P-O5'	-6.87	93.70	104.00
1	A	61	SER	CB-CA-C	6.73	123.81	110.42
1	B	232	GLY	N-CA-C	-6.64	107.37	114.67
1	A	108	VAL	N-CA-C	6.62	123.10	109.34
2	R	17	C	N1-C1'-C2'	6.52	121.78	112.00
1	A	360	SER	N-CA-C	6.47	120.14	108.17
1	C	230	THR	N-CA-C	-6.34	105.52	113.20
2	R	11	C	P-O5'-C5'	6.29	130.34	120.90
1	D	167	ILE	N-CA-C	6.28	122.40	109.34
1	C	232	GLY	N-CA-C	-6.26	107.79	114.67
1	A	232	GLY	N-CA-C	-6.25	107.79	114.67
1	A	182	PHE	N-CA-C	-6.20	104.88	112.88
2	R	2	C	P-O3'-C3'	-6.17	110.94	120.20
1	B	33	ARG	N-CA-C	-6.16	105.59	113.23
2	R	5	C	N1-C1'-C2'	6.16	121.24	112.00
2	R	27	C	O4'-C1'-N1	6.16	117.74	108.50
1	E	108	VAL	N-CA-C	6.09	122.01	109.34
2	R	4	C	P-O3'-C3'	-6.05	111.12	120.20
2	R	33	C	N1-C1'-C2'	6.04	121.06	112.00
1	D	324	TYR	N-CA-C	6.03	117.52	111.07
1	C	108	VAL	N-CA-C	6.02	121.86	109.34
1	D	108	VAL	N-CA-C	6.01	121.84	109.34
1	B	108	VAL	N-CA-C	5.96	121.73	109.34
1	D	33	ARG	N-CA-C	-5.95	105.86	113.23
1	C	182	PHE	N-CA-C	-5.93	105.23	112.88
1	D	170	GLN	N-CA-C	5.92	119.11	107.98
1	D	349	CYS	N-CA-C	5.92	116.05	108.24
2	R	4	C	N1-C1'-C2'	5.90	120.85	112.00
2	R	42	C	N1-C1'-C2'	5.89	120.84	112.00
1	B	61	SER	CB-CA-C	5.88	122.11	110.42
1	E	232	GLY	N-CA-C	-5.83	108.26	114.67
1	D	182	PHE	N-CA-C	-5.76	105.44	112.88
2	R	30	C	N1-C1'-C2'	5.75	120.63	112.00
2	R	12	C	N1-C1'-C2'	5.74	120.61	112.00
1	C	324	TYR	N-CA-C	5.71	117.18	111.07
1	A	349	CYS	N-CA-C	5.69	115.75	108.24
2	R	41	C	N1-C1'-C2'	-5.69	103.47	112.00
2	R	40	C	N1-C1'-C2'	5.67	120.50	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ARG	N-CA-C	-5.65	106.22	113.23
1	A	18	LEU	CA-C-N	5.62	126.86	119.84
1	A	18	LEU	C-N-CA	5.62	126.86	119.84
1	B	147	THR	N-CA-C	5.56	117.25	110.41
1	D	230	THR	N-CA-C	-5.54	106.50	113.20
1	B	109	SER	N-CA-C	5.53	118.54	109.76
1	A	230	THR	N-CA-C	-5.51	106.59	113.15
2	R	24	C	N1-C1'-C2'	5.51	120.27	112.00
2	R	43	C	N1-C1'-C2'	5.50	120.26	112.00
1	A	147	THR	N-CA-C	5.50	117.18	110.41
1	B	324	TYR	N-CA-C	5.48	116.93	111.07
1	B	182	PHE	N-CA-C	-5.42	105.89	112.88
2	R	20	C	P-O3'-C3'	-5.41	112.08	120.20
1	E	369	PRO	CA-C-N	5.40	126.59	119.84
1	E	369	PRO	C-N-CA	5.40	126.59	119.84
1	E	349	CYS	N-CA-C	5.39	115.35	108.24
1	B	121	VAL	N-CA-C	5.38	115.01	107.37
1	D	232	GLY	N-CA-C	-5.36	108.45	114.40
1	B	349	CYS	N-CA-C	5.36	115.31	108.24
2	R	19	C	N1-C1'-C2'	5.34	120.00	112.00
1	E	360	SER	N-CA-C	5.33	122.14	110.80
1	B	126	ARG	N-CA-C	5.32	117.42	109.59
1	E	359	ASP	N-CA-C	-5.32	104.51	112.54
2	R	43	C	P-O3'-C3'	5.31	128.17	120.20
1	C	170	GLN	N-CA-C	5.31	122.10	110.80
1	C	147	THR	N-CA-C	5.30	116.93	110.41
1	A	33	ARG	N-CA-C	-5.28	106.69	113.23
1	E	147	THR	N-CA-C	5.28	116.90	110.41
1	E	182	PHE	N-CA-C	-5.19	106.18	112.88
2	R	39	C	N1-C1'-C2'	5.19	119.78	112.00
1	E	163	GLN	N-CA-C	-5.18	105.25	112.45
1	A	121	VAL	N-CA-C	5.17	114.71	107.37
1	A	8	ILE	CA-C-N	-5.16	117.66	122.66
1	A	8	ILE	C-N-CA	-5.16	117.66	122.66
1	C	126	ARG	N-CA-C	5.15	117.16	109.59
2	R	41	C	C3'-C2'-C1'	5.15	106.45	101.30
1	E	121	VAL	N-CA-C	5.11	114.63	107.37
1	E	126	ARG	N-CA-C	5.07	117.04	109.59
1	E	18	LEU	CA-C-N	5.04	126.15	119.84
1	E	18	LEU	C-N-CA	5.04	126.15	119.84
1	D	126	ARG	N-CA-C	5.04	117.52	109.96
1	B	368	ALA	CA-C-N	5.03	125.56	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	368	ALA	C-N-CA	5.03	125.56	120.38
1	C	18	LEU	CA-C-N	5.03	126.13	119.84
1	C	18	LEU	C-N-CA	5.03	126.13	119.84
1	D	147	THR	N-CA-C	5.01	116.57	110.41

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	GLU	Peptide
1	A	78	LYS	Peptide
1	B	107	LEU	Peptide
1	B	167	ILE	Peptide
1	B	169	GLU	Peptide
1	B	170	GLN	Peptide
1	C	107	LEU	Peptide
1	D	107	LEU	Peptide
1	E	166	MET	Peptide
1	E	167	ILE	Peptide
1	E	169	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3327	0	3287	313	0
1	B	3290	0	3253	332	0
1	C	3275	0	3242	338	0
1	D	3298	0	3264	309	0
1	E	3327	0	3287	304	0
2	R	900	0	496	84	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	R	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17437	0	16829	1542	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 45.

All (1542) 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:E:163:GLN:O	1:E:167:ILE:HB	1.36	1.25
1:B:317:ARG:HD3	2:R:22:C:O2'	1.41	1.18
1:E:177:GLU:HA	1:E:181:ILE:HD11	1.31	1.12
1:C:317:ARG:NH2	2:R:14:C:H5'	1.64	1.11
1:A:317:ARG:NH2	2:R:32:C:H5'	1.64	1.11
1:D:177:GLU:HA	1:D:181:ILE:HD11	1.32	1.10
1:C:177:GLU:HA	1:C:181:ILE:HD11	1.33	1.09
1:A:177:GLU:HA	1:A:181:ILE:HD11	1.33	1.09
1:B:60:LYS:O	1:B:61:SER:HB3	1.53	1.09
1:B:317:ARG:NH2	2:R:23:C:H5'	1.66	1.09
1:D:364:LEU:HD23	1:D:365:THR:H	1.16	1.09
1:E:169:GLU:HG2	1:E:170:GLN:H	1.15	1.06
1:B:168:ASN:O	1:B:169:GLU:HG2	1.53	1.05
1:B:177:GLU:HA	1:B:181:ILE:HD11	1.33	1.05
1:D:72:TYR:HE1	1:D:134:LEU:HD12	1.22	1.05
1:B:72:TYR:HE1	1:B:134:LEU:HD12	1.22	1.04
1:E:72:TYR:HE1	1:E:134:LEU:HD12	1.21	1.04
1:A:389:PRO:HA	1:A:393:MET:HE2	1.39	1.02
1:E:317:ARG:NH2	2:R:41:C:H5'	1.72	1.02
1:D:263:LEU:HD12	1:D:264:PRO:HD2	1.42	1.02
1:C:389:PRO:HA	1:C:393:MET:HE2	1.41	1.02
1:E:263:LEU:HD12	1:E:264:PRO:HD2	1.41	1.01
1:A:263:LEU:HD12	1:A:264:PRO:HD2	1.40	1.01
1:E:389:PRO:HA	1:E:393:MET:HE2	1.43	1.01
1:D:389:PRO:HA	1:D:393:MET:HE2	1.44	1.00
1:B:389:PRO:HA	1:B:393:MET:HE2	1.42	1.00
1:B:263:LEU:HD12	1:B:264:PRO:HD2	1.45	0.98
1:C:263:LEU:HD12	1:C:264:PRO:HD2	1.46	0.98
1:A:72:TYR:HE1	1:A:134:LEU:HD12	1.28	0.97
1:B:117:LEU:HB2	1:B:118:PRO:HD3	1.44	0.97
1:B:317:ARG:HD3	2:R:22:C:HO2'	1.22	0.96
1:A:165:LYS:O	1:A:167:ILE:HD12	1.65	0.96
1:B:356:THR:HG23	1:B:357:PRO:HD3	1.46	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:THR:HG23	1:C:357:PRO:HD3	1.45	0.95
1:A:117:LEU:HB2	1:A:118:PRO:HD3	1.48	0.95
1:C:72:TYR:HE1	1:C:134:LEU:HD12	1.28	0.94
1:D:356:THR:HG23	1:D:357:PRO:HD3	1.50	0.94
1:A:60:LYS:O	1:A:61:SER:HB3	1.68	0.93
1:A:356:THR:HG23	1:A:357:PRO:HD3	1.51	0.93
1:E:117:LEU:HB2	1:E:118:PRO:HD3	1.51	0.92
1:D:43:ASN:HA	1:D:111:LYS:HG3	1.48	0.92
1:B:43:ASN:HA	1:B:111:LYS:HG3	1.50	0.92
1:A:65:SER:HB2	1:A:117:LEU:HD11	1.50	0.91
1:C:317:ARG:HD3	2:R:13:C:O2'	1.68	0.91
1:D:65:SER:HB2	1:D:117:LEU:HD11	1.51	0.91
1:E:43:ASN:HA	1:E:111:LYS:HG3	1.51	0.91
1:E:356:THR:HG23	1:E:357:PRO:HD3	1.49	0.91
1:C:43:ASN:HA	1:C:111:LYS:HG3	1.49	0.91
1:C:117:LEU:HB2	1:C:118:PRO:HD3	1.50	0.91
1:B:168:ASN:C	1:B:169:GLU:HG2	1.93	0.90
1:E:60:LYS:O	1:E:61:SER:HB3	1.72	0.90
1:E:65:SER:HB2	1:E:117:LEU:HD11	1.50	0.90
1:B:150:PRO:HA	1:B:152:TYR:CE1	2.05	0.90
1:A:43:ASN:HA	1:A:111:LYS:HG3	1.51	0.90
1:B:398:LYS:HG2	1:B:402:MET:HE3	1.54	0.89
1:D:117:LEU:HB2	1:D:118:PRO:HD3	1.52	0.89
1:B:164:CYS:HA	1:B:168:ASN:HA	1.52	0.89
1:C:317:ARG:NE	1:C:317:ARG:H	1.70	0.89
1:D:354:LYS:HE3	1:D:356:THR:HA	1.55	0.89
1:A:150:PRO:HA	1:A:152:TYR:CE1	2.07	0.89
1:C:65:SER:HB2	1:C:117:LEU:HD11	1.51	0.89
1:C:150:PRO:HA	1:C:152:TYR:CE1	2.08	0.89
1:D:316:ALA:HA	1:D:317:ARG:NH2	1.88	0.89
1:E:354:LYS:HE3	1:E:356:THR:HA	1.55	0.89
1:B:317:ARG:CD	2:R:22:C:O2'	2.20	0.88
1:B:262:MET:HE2	1:B:262:MET:HA	1.53	0.88
1:E:262:MET:HE2	1:E:262:MET:HA	1.53	0.88
1:B:380:GLY:HA2	1:C:354:LYS:NZ	1.88	0.88
1:B:65:SER:HB2	1:B:117:LEU:HD11	1.52	0.88
1:E:317:ARG:HG3	2:R:40:C:N3	1.88	0.87
1:E:398:LYS:HG2	1:E:402:MET:HE3	1.54	0.87
1:D:262:MET:HE2	1:D:262:MET:HA	1.54	0.87
1:C:167:ILE:O	1:C:169:GLU:HG2	1.74	0.87
1:A:398:LYS:HG2	1:A:402:MET:HE3	1.53	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HG2	1:B:179:ARG:H	1.40	0.87
1:D:42:ILE:HD12	1:D:74:TYR:HB2	1.55	0.87
1:A:42:ILE:HD12	1:A:74:TYR:HB2	1.57	0.86
1:D:150:PRO:HA	1:D:152:TYR:CE1	2.11	0.86
1:C:177:GLU:HG2	1:C:179:ARG:H	1.40	0.85
1:C:354:LYS:HE3	1:C:356:THR:HA	1.57	0.85
1:D:60:LYS:O	1:D:61:SER:HB3	1.73	0.85
1:E:169:GLU:HG2	1:E:170:GLN:N	1.86	0.85
1:A:177:GLU:HG2	1:A:179:ARG:H	1.41	0.84
1:C:398:LYS:HG2	1:C:402:MET:HE3	1.58	0.84
1:B:354:LYS:HE3	1:B:356:THR:HA	1.59	0.84
1:C:376:VAL:HG13	1:D:354:LYS:HB2	1.57	0.84
1:E:165:LYS:O	1:E:167:ILE:HG13	1.76	0.84
1:B:42:ILE:HD12	1:B:74:TYR:HB2	1.57	0.84
1:D:72:TYR:CE1	1:D:134:LEU:HD12	2.12	0.84
1:E:150:PRO:HA	1:E:152:TYR:CE1	2.11	0.84
1:D:165:LYS:O	1:D:167:ILE:HD12	1.78	0.84
1:C:165:LYS:HG2	1:C:166:MET:HG3	1.58	0.84
1:E:163:GLN:O	1:E:167:ILE:CB	2.22	0.84
1:D:177:GLU:HG2	1:D:179:ARG:H	1.43	0.84
1:C:317:ARG:HH21	2:R:14:C:H5'	1.40	0.83
1:E:42:ILE:HD12	1:E:74:TYR:HB2	1.57	0.83
1:E:177:GLU:HG2	1:E:179:ARG:H	1.41	0.83
1:D:74:TYR:CE1	1:D:78:LYS:HD2	2.14	0.83
1:E:72:TYR:CE1	1:E:134:LEU:HD12	2.11	0.82
1:D:317:ARG:H	1:D:317:ARG:NE	1.77	0.82
1:E:37:GLU:HB2	1:E:108:VAL:HG11	1.61	0.82
1:B:317:ARG:H	1:B:317:ARG:NE	1.76	0.82
1:A:262:MET:HA	1:A:262:MET:HE2	1.60	0.82
1:A:354:LYS:HE3	1:A:356:THR:HA	1.62	0.81
1:D:398:LYS:HG2	1:D:402:MET:HE3	1.61	0.81
1:B:376:VAL:HG21	1:C:352:ASP:OD1	1.80	0.81
1:B:317:ARG:HH21	2:R:23:C:H5'	1.43	0.81
1:C:60:LYS:O	1:C:61:SER:HB3	1.78	0.81
1:B:2:SER:O	1:C:243:GLU:HG3	1.81	0.81
1:A:376:VAL:HG21	1:B:352:ASP:OD1	1.82	0.80
1:C:317:ARG:CD	2:R:13:C:O2'	2.29	0.80
1:A:316:ALA:HA	1:A:317:ARG:NH2	1.97	0.80
1:C:42:ILE:HD12	1:C:74:TYR:HB2	1.63	0.80
1:E:74:TYR:CE1	1:E:78:LYS:HD2	2.17	0.79
1:D:37:GLU:HB2	1:D:108:VAL:HG11	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:TYR:CE1	1:C:134:LEU:HD12	2.17	0.79
1:C:262:MET:HA	1:C:262:MET:HE2	1.64	0.79
1:A:37:GLU:HB2	1:A:108:VAL:HG11	1.64	0.79
1:A:166:MET:H	1:E:184:VAL:HG11	1.47	0.79
1:B:74:TYR:CE1	1:B:78:LYS:HD2	2.18	0.78
1:D:364:LEU:HD23	1:D:365:THR:N	1.98	0.78
1:E:136:LEU:HD22	1:E:163:GLN:HE21	1.48	0.78
1:E:169:GLU:CG	1:E:170:GLN:H	1.95	0.78
1:B:72:TYR:CE1	1:B:134:LEU:HD12	2.12	0.78
1:C:37:GLU:HB2	1:C:108:VAL:HG11	1.64	0.78
1:A:126:ARG:HA	1:A:126:ARG:HH11	1.48	0.78
1:A:317:ARG:NE	1:A:317:ARG:H	1.80	0.78
1:C:136:LEU:HD22	1:C:163:GLN:HE21	1.47	0.78
1:B:54:TYR:CE1	1:B:118:PRO:HB2	2.19	0.78
1:A:74:TYR:CE1	1:A:78:LYS:HD2	2.19	0.78
1:D:214:ARG:HA	1:D:217:THR:HG22	1.65	0.78
1:A:153:ARG:HH12	1:A:176:PRO:C	1.92	0.77
1:B:133:TRP:HB3	1:B:167:ILE:HD13	1.64	0.77
1:E:126:ARG:HA	1:E:126:ARG:HH11	1.49	0.77
1:E:45:THR:H	1:E:111:LYS:HZ1	1.31	0.77
1:B:47:SER:HB3	1:B:50:ASP:HB2	1.67	0.77
1:B:316:ALA:HA	1:B:317:ARG:NH2	1.99	0.77
1:D:208:HIS:HD1	1:D:210:CYS:H	1.32	0.77
1:D:44:THR:HG22	1:D:46:LYS:HG2	1.67	0.77
2:R:21:C:H5'	2:R:21:C:H6	1.49	0.77
1:A:45:THR:H	1:A:111:LYS:HZ1	1.32	0.76
1:B:380:GLY:HA2	1:C:354:LYS:HZ3	1.48	0.76
1:B:214:ARG:HA	1:B:217:THR:HG22	1.67	0.76
1:B:44:THR:HG22	1:B:46:LYS:HG2	1.68	0.76
1:C:74:TYR:CE1	1:C:78:LYS:HD2	2.20	0.76
1:B:349:CYS:SG	1:E:8:ILE:HG22	2.25	0.76
1:E:130:ASP:C	1:E:132:LYS:H	1.93	0.76
1:C:165:LYS:NZ	1:C:165:LYS:HB2	2.00	0.76
1:E:54:TYR:CE1	1:E:118:PRO:HB2	2.21	0.76
1:A:44:THR:HG23	1:A:46:LYS:HE2	1.68	0.75
1:D:45:THR:H	1:D:111:LYS:HZ1	1.33	0.75
1:D:317:ARG:H	1:D:317:ARG:CZ	1.98	0.75
1:A:130:ASP:C	1:A:132:LYS:H	1.94	0.75
1:A:317:ARG:HH21	2:R:32:C:H5'	1.48	0.75
1:A:105:PHE:C	1:A:107:LEU:H	1.95	0.75
1:A:214:ARG:HA	1:A:217:THR:HG22	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:TYR:CE1	1:D:118:PRO:HB2	2.21	0.75
1:E:214:ARG:HA	1:E:217:THR:HG22	1.68	0.75
1:D:130:ASP:C	1:D:132:LYS:H	1.93	0.75
1:A:54:TYR:CE1	1:A:118:PRO:HB2	2.22	0.75
1:B:37:GLU:HB2	1:B:108:VAL:HG11	1.67	0.75
1:A:47:SER:HB3	1:A:50:ASP:HB2	1.69	0.75
1:D:136:LEU:HD22	1:D:163:GLN:HE21	1.50	0.74
1:C:184:VAL:HG13	1:D:165:LYS:HG3	1.69	0.74
1:A:72:TYR:CE1	1:A:134:LEU:HD12	2.18	0.74
1:A:136:LEU:HD22	1:A:163:GLN:HE21	1.52	0.74
2:R:18:C:H2'	2:R:19:C:O4'	1.87	0.74
1:A:226:ALA:HB2	2:R:31:C:H5'	1.69	0.74
1:C:214:ARG:HA	1:C:217:THR:HG22	1.69	0.74
1:A:60:LYS:O	1:A:61:SER:CB	2.36	0.74
1:C:44:THR:HG22	1:C:46:LYS:HG2	1.69	0.74
1:B:130:ASP:C	1:B:132:LYS:H	1.95	0.74
1:B:136:LEU:HD22	1:B:163:GLN:HE21	1.52	0.74
1:B:253:GLU:H	1:B:253:GLU:CD	1.96	0.74
1:B:230:THR:HG21	1:B:298:HIS:CE1	2.23	0.73
1:B:383:GLU:HG3	1:C:354:LYS:HE2	1.71	0.73
1:D:126:ARG:HH11	1:D:126:ARG:HA	1.52	0.73
1:D:151:GLU:OE1	1:D:155:LYS:NZ	2.21	0.73
1:B:376:VAL:HG13	1:C:354:LYS:HB2	1.71	0.73
1:C:181:ILE:H	1:C:181:ILE:HD12	1.52	0.73
1:D:91:PHE:CZ	1:D:267:GLU:HG3	2.24	0.73
1:D:253:GLU:H	1:D:253:GLU:CD	1.96	0.73
1:E:133:TRP:HB3	1:E:167:ILE:HD13	1.69	0.73
1:A:2:SER:O	1:B:243:GLU:HG3	1.88	0.73
1:B:105:PHE:C	1:B:107:LEU:H	1.96	0.73
1:C:130:ASP:C	1:C:132:LYS:H	1.95	0.73
1:B:171:PHE:CZ	1:B:173:PRO:HG2	2.24	0.73
1:A:167:ILE:HG22	1:A:169:GLU:HG2	1.71	0.73
1:D:364:LEU:HD22	1:D:368:ALA:HB2	1.70	0.73
1:B:126:ARG:HH11	1:B:126:ARG:HA	1.52	0.73
1:A:380:GLY:HA2	1:B:354:LYS:NZ	2.04	0.73
1:B:173:PRO:C	1:B:174:LEU:HG	2.12	0.73
1:C:380:GLY:HA2	1:D:354:LYS:NZ	2.04	0.72
1:D:27:TYR:HB3	1:D:266:GLN:NE2	2.04	0.72
1:D:230:THR:HG21	1:D:298:HIS:CE1	2.24	0.72
1:E:253:GLU:CD	1:E:253:GLU:H	1.97	0.72
1:E:153:ARG:HH12	1:E:176:PRO:C	1.96	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ARG:H	1:E:317:ARG:NE	1.87	0.72
1:E:364:LEU:HB2	1:E:368:ALA:HB2	1.70	0.72
1:A:380:GLY:HA2	1:B:354:LYS:HZ3	1.54	0.72
1:C:317:ARG:O	1:C:319:PRO:HD3	1.90	0.72
1:D:74:TYR:CD1	1:D:78:LYS:HD2	2.24	0.72
1:E:288:PRO:HG2	1:E:289:TYR:CE2	2.24	0.72
2:R:36:C:H2'	2:R:37:C:O4'	1.90	0.72
1:B:44:THR:HG23	1:B:46:LYS:HE2	1.71	0.72
1:D:29:ALA:HB2	1:D:91:PHE:CE2	2.25	0.72
1:D:42:ILE:CD1	1:D:74:TYR:HB2	2.18	0.72
1:D:173:PRO:C	1:D:174:LEU:HG	2.12	0.72
1:E:44:THR:HG23	1:E:46:LYS:HE2	1.72	0.72
1:E:47:SER:HB3	1:E:50:ASP:HB2	1.71	0.72
1:E:60:LYS:O	1:E:61:SER:CB	2.37	0.72
1:C:126:ARG:HA	1:C:126:ARG:HH11	1.52	0.72
1:B:29:ALA:HB2	1:B:91:PHE:HE2	1.54	0.72
1:B:60:LYS:O	1:B:61:SER:CB	2.33	0.72
1:E:316:ALA:HA	1:E:317:ARG:NH2	2.04	0.72
1:B:184:VAL:HG11	1:C:166:MET:H	1.55	0.72
1:A:153:ARG:NH1	1:A:176:PRO:C	2.48	0.72
1:C:44:THR:HG23	1:C:46:LYS:HE2	1.72	0.72
1:D:29:ALA:HB2	1:D:91:PHE:HE2	1.54	0.72
1:D:44:THR:HG23	1:D:46:LYS:HE2	1.72	0.72
1:E:74:TYR:CD1	1:E:78:LYS:HD2	2.25	0.72
1:C:105:PHE:C	1:C:107:LEU:H	1.98	0.71
1:D:153:ARG:HH12	1:D:176:PRO:C	1.98	0.71
1:A:42:ILE:CD1	1:A:74:TYR:HB2	2.21	0.71
1:A:181:ILE:HD12	1:A:181:ILE:H	1.54	0.71
1:A:74:TYR:CD1	1:A:78:LYS:HD2	2.26	0.71
1:C:54:TYR:CE1	1:C:118:PRO:HB2	2.25	0.71
1:D:41:TYR:HE1	1:D:110:LEU:HD12	1.56	0.71
1:E:105:PHE:C	1:E:107:LEU:H	1.98	0.71
1:C:230:THR:HG21	1:C:298:HIS:CE1	2.26	0.71
1:D:47:SER:HB3	1:D:50:ASP:HB2	1.73	0.71
1:E:173:PRO:C	1:E:174:LEU:HG	2.14	0.71
1:B:317:ARG:O	1:B:319:PRO:HD3	1.91	0.71
1:A:44:THR:HG22	1:A:46:LYS:HG2	1.72	0.70
1:C:316:ALA:HA	1:C:317:ARG:NH2	2.06	0.70
1:D:288:PRO:HG2	1:D:289:TYR:CE2	2.26	0.70
1:E:165:LYS:O	1:E:167:ILE:CG1	2.39	0.70
1:B:74:TYR:CD1	1:B:78:LYS:HD2	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASN:O	1:B:169:GLU:CG	2.36	0.70
1:C:47:SER:HB3	1:C:50:ASP:HB2	1.73	0.70
1:B:42:ILE:CD1	1:B:74:TYR:HB2	2.21	0.70
1:C:149:MET:C	1:C:151:GLU:H	1.99	0.70
1:C:173:PRO:C	1:C:174:LEU:HG	2.15	0.70
1:A:253:GLU:CD	1:A:253:GLU:H	1.99	0.70
1:A:354:LYS:HB2	1:E:376:VAL:HG13	1.73	0.70
1:C:317:ARG:NE	2:R:13:C:O2'	2.24	0.70
1:A:168:ASN:O	1:A:169:GLU:OE2	2.09	0.70
1:E:44:THR:HG22	1:E:46:LYS:HG2	1.72	0.70
1:E:91:PHE:CZ	1:E:267:GLU:HG3	2.26	0.70
1:D:317:ARG:NH2	2:R:5:C:O5'	2.25	0.70
1:E:230:THR:HG21	1:E:298:HIS:CE1	2.26	0.70
1:A:376:VAL:HG13	1:B:354:LYS:HB2	1.74	0.69
1:B:106:ASP:C	1:B:107:LEU:HD12	2.16	0.69
1:C:380:GLY:HA2	1:D:354:LYS:HZ3	1.56	0.69
1:D:149:MET:C	1:D:151:GLU:H	2.00	0.69
1:A:173:PRO:C	1:A:174:LEU:HG	2.16	0.69
1:A:317:ARG:O	1:A:319:PRO:HD3	1.92	0.69
1:E:42:ILE:CD1	1:E:74:TYR:HB2	2.22	0.69
1:C:74:TYR:CD1	1:C:78:LYS:HD2	2.27	0.69
1:C:149:MET:O	1:C:151:GLU:N	2.26	0.69
1:D:199:ASP:OD1	1:D:214:ARG:HD2	1.93	0.69
1:A:167:ILE:HG22	1:A:169:GLU:CG	2.23	0.69
1:B:117:LEU:HB2	1:B:118:PRO:CD	2.22	0.69
1:C:153:ARG:HH12	1:C:176:PRO:C	2.00	0.69
1:C:376:VAL:HG21	1:D:352:ASP:OD1	1.92	0.69
1:A:44:THR:CG2	1:A:46:LYS:HE2	2.23	0.69
1:A:91:PHE:CZ	1:A:267:GLU:HG3	2.27	0.69
1:C:29:ALA:HB2	1:C:91:PHE:HE2	1.57	0.69
1:C:253:GLU:CD	1:C:253:GLU:H	2.01	0.69
1:E:164:CYS:O	1:E:168:ASN:OD1	2.11	0.69
1:D:149:MET:O	1:D:151:GLU:N	2.26	0.68
1:E:389:PRO:CA	1:E:393:MET:HE2	2.23	0.68
1:A:165:LYS:HB2	1:A:165:LYS:NZ	2.08	0.68
1:A:230:THR:HG21	1:A:298:HIS:CE1	2.28	0.68
1:B:29:ALA:HB2	1:B:91:PHE:CE2	2.28	0.68
1:E:153:ARG:NH1	1:E:176:PRO:C	2.52	0.68
2:R:7:C:H4'	2:R:7:C:OP2	1.94	0.68
1:A:43:ASN:O	1:A:44:THR:C	2.36	0.68
1:B:18:LEU:CD1	1:C:232:GLY:HA2	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:LYS:O	1:B:100:ASP:HB2	1.92	0.68
1:B:181:ILE:HD12	1:B:181:ILE:H	1.59	0.68
1:C:288:PRO:HG2	1:C:289:TYR:CE2	2.28	0.68
1:B:27:TYR:HB3	1:B:266:GLN:NE2	2.09	0.68
1:C:389:PRO:CA	1:C:393:MET:HE2	2.22	0.68
1:D:31:TYR:C	1:D:31:TYR:CD1	2.71	0.68
1:A:67:ILE:HD12	1:A:67:ILE:H	1.59	0.67
1:B:31:TYR:CD1	1:B:31:TYR:C	2.71	0.67
1:B:91:PHE:CZ	1:B:267:GLU:HG3	2.28	0.67
1:B:153:ARG:HH12	1:B:176:PRO:C	2.01	0.67
1:E:43:ASN:O	1:E:44:THR:C	2.37	0.67
1:C:317:ARG:H	1:C:317:ARG:CZ	2.06	0.67
1:D:105:PHE:C	1:D:107:LEU:H	2.02	0.67
1:B:168:ASN:C	1:B:169:GLU:CG	2.65	0.67
1:E:25:VAL:HG11	1:E:288:PRO:HA	1.77	0.67
1:E:149:MET:C	1:E:151:GLU:H	2.01	0.67
1:E:181:ILE:H	1:E:181:ILE:HD12	1.60	0.67
1:E:317:ARG:O	1:E:319:PRO:HD3	1.95	0.67
1:B:43:ASN:O	1:B:44:THR:C	2.38	0.67
1:C:29:ALA:HB2	1:C:91:PHE:CE2	2.30	0.67
1:C:31:TYR:CD1	1:C:31:TYR:C	2.72	0.67
1:C:148:GLN:HG2	1:C:179:ARG:NH1	2.09	0.67
1:B:149:MET:C	1:B:151:GLU:H	2.02	0.67
1:D:317:ARG:CZ	2:R:5:C:OP2	2.43	0.67
1:E:67:ILE:HD12	1:E:67:ILE:H	1.60	0.67
1:E:149:MET:O	1:E:151:GLU:N	2.28	0.67
1:A:97:LYS:O	1:A:100:ASP:HB2	1.95	0.67
1:E:41:TYR:HE1	1:E:110:LEU:HD12	1.59	0.67
1:A:7:ARG:NH1	1:B:259:VAL:HG21	2.09	0.66
1:A:199:ASP:OD1	1:A:214:ARG:HD2	1.95	0.66
1:B:352:ASP:OD1	1:B:352:ASP:C	2.38	0.66
1:D:153:ARG:NH1	1:D:176:PRO:C	2.54	0.66
1:C:2:SER:O	1:D:243:GLU:HG3	1.95	0.66
1:A:165:LYS:O	1:A:166:MET:HB2	1.95	0.66
1:B:117:LEU:CB	1:B:118:PRO:HD3	2.23	0.66
1:C:42:ILE:CD1	1:C:74:TYR:HB2	2.24	0.66
1:C:167:ILE:O	1:C:169:GLU:CG	2.42	0.66
1:A:151:GLU:OE1	1:A:155:LYS:NZ	2.29	0.66
1:B:107:LEU:HD12	1:B:107:LEU:N	2.10	0.66
1:B:199:ASP:OD1	1:B:214:ARG:HD2	1.95	0.66
1:B:224:ASP:CG	2:R:21:C:H4'	2.20	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ALA:O	1:E:230:THR:HG23	1.96	0.66
1:A:165:LYS:HB2	1:A:165:LYS:HZ2	1.60	0.66
1:C:27:TYR:HB3	1:C:266:GLN:NE2	2.10	0.66
1:C:352:ASP:OD1	1:C:352:ASP:C	2.38	0.66
1:E:164:CYS:HA	1:E:168:ASN:HA	1.77	0.66
1:E:302:GLN:HG2	1:E:316:ALA:CB	2.26	0.66
1:A:27:TYR:HB3	1:A:266:GLN:NE2	2.11	0.65
1:A:149:MET:C	1:A:151:GLU:H	2.04	0.65
1:A:31:TYR:CD1	1:A:31:TYR:C	2.73	0.65
1:D:43:ASN:O	1:D:44:THR:C	2.38	0.65
1:E:199:ASP:OD1	1:E:214:ARG:HD2	1.96	0.65
1:B:18:LEU:HD12	1:C:232:GLY:HA2	1.78	0.65
1:C:45:THR:C	1:C:46:LYS:HD3	2.22	0.65
1:A:302:GLN:HG2	1:A:316:ALA:CB	2.27	0.65
1:B:149:MET:O	1:B:151:GLU:N	2.30	0.65
1:C:151:GLU:OE1	1:C:155:LYS:NZ	2.29	0.65
1:C:376:VAL:HG13	1:D:354:LYS:CB	2.26	0.65
1:B:153:ARG:NH1	1:B:176:PRO:C	2.55	0.65
1:C:317:ARG:NE	2:R:13:C:HO2'	1.95	0.65
1:B:148:GLN:HG2	1:B:179:ARG:NH1	2.11	0.65
1:B:151:GLU:OE1	1:B:155:LYS:NZ	2.29	0.65
1:B:317:ARG:NE	1:B:317:ARG:N	2.44	0.65
1:C:153:ARG:NH1	1:C:176:PRO:C	2.54	0.65
1:D:181:ILE:HD12	1:D:181:ILE:H	1.62	0.65
1:A:117:LEU:HB2	1:A:118:PRO:CD	2.25	0.65
1:C:61:SER:O	1:C:63:ASN:N	2.30	0.65
1:D:97:LYS:O	1:D:100:ASP:HB2	1.97	0.65
1:E:357:PRO:HA	1:E:360:SER:OG	1.96	0.65
1:A:226:ALA:HB2	2:R:31:C:C5'	2.26	0.65
1:B:67:ILE:HD12	1:B:67:ILE:H	1.62	0.65
1:B:171:PHE:CG	1:B:172:GLU:N	2.60	0.65
1:C:41:TYR:HE1	1:C:110:LEU:HD12	1.61	0.65
1:B:317:ARG:H	1:B:317:ARG:CZ	2.10	0.64
1:D:61:SER:O	1:D:63:ASN:N	2.30	0.64
1:D:143:ARG:HH12	2:R:9:C:H5'	1.63	0.64
1:D:226:ALA:O	1:D:230:THR:HG23	1.98	0.64
1:E:31:TYR:CD1	1:E:31:TYR:C	2.75	0.64
1:E:44:THR:CG2	1:E:46:LYS:HE2	2.28	0.64
1:E:81:ARG:CB	1:E:208:HIS:HE2	2.11	0.64
1:A:29:ALA:HB2	1:A:91:PHE:HE2	1.62	0.64
1:A:263:LEU:CD1	1:A:264:PRO:HD2	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:ASP:OD1	1:D:352:ASP:C	2.40	0.64
1:B:81:ARG:CB	1:B:208:HIS:HE2	2.11	0.64
1:D:67:ILE:HD12	1:D:67:ILE:H	1.61	0.64
1:A:41:TYR:HE1	1:A:110:LEU:HD12	1.62	0.64
1:C:67:ILE:HD12	1:C:67:ILE:H	1.63	0.64
1:A:389:PRO:CA	1:A:393:MET:HE2	2.22	0.64
1:C:117:LEU:HB2	1:C:118:PRO:CD	2.27	0.64
1:D:364:LEU:CD2	1:D:365:THR:H	2.04	0.64
1:D:44:THR:CG2	1:D:46:LYS:HE2	2.27	0.64
1:E:214:ARG:HA	1:E:217:THR:CG2	2.28	0.64
1:B:44:THR:CG2	1:B:46:LYS:HE2	2.27	0.64
1:B:165:LYS:O	1:B:167:ILE:HD12	1.98	0.64
1:D:50:ASP:OD2	1:D:120:GLY:HA2	1.98	0.64
1:B:288:PRO:HG2	1:B:289:TYR:CE2	2.32	0.64
1:D:155:LYS:NZ	2:R:8:C:OP2	2.28	0.64
1:E:97:LYS:O	1:E:100:ASP:HB2	1.98	0.64
1:C:97:LYS:O	1:C:100:ASP:HB2	1.97	0.63
1:A:317:ARG:H	1:A:317:ARG:CZ	2.11	0.63
1:C:228:LEU:HB2	1:C:289:TYR:HB3	1.79	0.63
1:D:317:ARG:NH1	2:R:5:C:OP2	2.32	0.63
1:E:148:GLN:HG2	1:E:179:ARG:NH1	2.13	0.63
1:A:352:ASP:OD1	1:A:352:ASP:C	2.42	0.63
1:C:165:LYS:O	1:C:166:MET:HB2	1.97	0.63
1:D:389:PRO:CA	1:D:393:MET:HE2	2.26	0.63
1:E:375:VAL:O	1:E:379:LEU:HB2	1.99	0.63
1:A:288:PRO:HG2	1:A:289:TYR:CE2	2.34	0.63
1:A:383:GLU:HG3	1:B:354:LYS:HE2	1.80	0.63
1:B:184:VAL:HG11	1:C:166:MET:N	2.13	0.63
1:D:117:LEU:CB	1:D:118:PRO:HD3	2.27	0.63
1:D:148:GLN:HG2	1:D:179:ARG:NH1	2.13	0.63
1:C:81:ARG:CB	1:C:208:HIS:HE2	2.11	0.63
1:C:117:LEU:CB	1:C:118:PRO:HD3	2.27	0.63
1:D:148:GLN:O	1:D:152:TYR:HE2	1.82	0.63
1:A:106:ASP:C	1:A:107:LEU:HD12	2.23	0.63
1:B:18:LEU:HD12	1:C:232:GLY:CA	2.29	0.63
1:B:50:ASP:OD2	1:B:120:GLY:HA2	1.98	0.63
1:D:412:ILE:C	1:D:412:ILE:HD12	2.24	0.63
1:A:317:ARG:HD3	2:R:31:C:H2'	1.80	0.63
1:B:89:SER:O	1:B:90:SER:HB2	1.99	0.63
1:D:29:ALA:O	1:D:31:TYR:N	2.30	0.63
1:C:165:LYS:HB2	1:C:165:LYS:HZ2	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ALA:C	1:D:31:TYR:H	2.07	0.62
1:B:29:ALA:C	1:B:31:TYR:H	2.08	0.62
1:C:44:THR:CG2	1:C:46:LYS:HE2	2.28	0.62
1:C:59:LEU:O	1:C:61:SER:N	2.29	0.62
1:D:214:ARG:HA	1:D:217:THR:CG2	2.29	0.62
1:E:410:LYS:NZ	2:R:40:C:H42	1.98	0.62
1:A:89:SER:O	1:A:90:SER:HB2	1.99	0.62
1:C:42:ILE:HD12	1:C:74:TYR:HD2	1.62	0.62
1:C:302:GLN:HG2	1:C:316:ALA:CB	2.30	0.62
1:A:127:THR:HG23	1:A:129:ALA:H	1.64	0.62
1:B:25:VAL:HG11	1:B:288:PRO:HA	1.82	0.62
1:B:375:VAL:O	1:B:379:LEU:HB2	1.97	0.62
1:A:228:LEU:HB2	1:A:289:TYR:HB3	1.82	0.62
1:C:180:ASP:OD2	1:C:180:ASP:C	2.43	0.62
1:A:117:LEU:CB	1:A:118:PRO:HD3	2.26	0.62
1:D:127:THR:HG23	1:D:129:ALA:H	1.64	0.62
1:E:133:TRP:CB	1:E:167:ILE:HD13	2.29	0.62
1:C:91:PHE:CZ	1:C:267:GLU:HG3	2.34	0.62
1:D:302:GLN:HG2	1:D:316:ALA:CB	2.30	0.62
1:E:27:TYR:HB3	1:E:266:GLN:NE2	2.14	0.62
1:E:224:ASP:CG	2:R:39:C:H4'	2.25	0.62
1:B:263:LEU:CD1	1:B:264:PRO:HD2	2.27	0.62
1:E:117:LEU:HB2	1:E:118:PRO:CD	2.27	0.62
1:D:263:LEU:CD1	1:D:264:PRO:HD2	2.25	0.61
1:A:375:VAL:O	1:A:379:LEU:HB2	2.00	0.61
1:B:150:PRO:CA	1:B:152:TYR:CE1	2.79	0.61
1:E:317:ARG:NH2	2:R:41:C:C5'	2.58	0.61
1:D:375:VAL:O	1:D:379:LEU:HB2	2.00	0.61
1:A:226:ALA:O	1:A:230:THR:HG23	2.00	0.61
1:C:45:THR:H	1:C:111:LYS:HZ1	1.46	0.61
1:B:184:VAL:HG13	1:C:165:LYS:HG3	1.82	0.61
1:C:106:ASP:C	1:C:107:LEU:HD12	2.25	0.61
1:C:199:ASP:OD1	1:C:214:ARG:HD2	1.99	0.61
1:E:89:SER:O	1:E:90:SER:HB2	2.00	0.61
1:A:107:LEU:HD12	1:A:107:LEU:N	2.15	0.61
1:C:29:ALA:O	1:C:31:TYR:N	2.30	0.61
1:C:323:GLU:OE1	1:D:239:GLY:HA3	2.01	0.61
1:A:317:ARG:HH22	2:R:32:C:H5'	1.61	0.61
1:D:106:ASP:C	1:D:107:LEU:HD12	2.26	0.61
1:D:117:LEU:HB2	1:D:118:PRO:CD	2.28	0.61
1:D:228:LEU:HB2	1:D:289:TYR:HB3	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:VAL:HG11	1:A:288:PRO:HA	1.83	0.61
1:A:214:ARG:HA	1:A:217:THR:CG2	2.31	0.61
1:A:259:VAL:HG21	1:E:7:ARG:NH1	2.16	0.61
1:B:29:ALA:O	1:B:31:TYR:N	2.30	0.61
1:B:214:ARG:HA	1:B:217:THR:CG2	2.30	0.61
1:A:150:PRO:CA	1:A:152:TYR:CE1	2.81	0.60
1:B:41:TYR:HE1	1:B:110:LEU:HD12	1.66	0.60
1:B:66:ILE:O	1:B:69:VAL:HG13	2.00	0.60
1:C:29:ALA:C	1:C:31:TYR:H	2.08	0.60
1:C:43:ASN:O	1:C:44:THR:C	2.43	0.60
1:C:199:ASP:HB2	1:C:217:THR:HG23	1.83	0.60
1:E:263:LEU:CD1	1:E:264:PRO:HD2	2.23	0.60
1:C:107:LEU:HD12	1:C:107:LEU:N	2.16	0.60
1:A:81:ARG:CB	1:A:208:HIS:HE2	2.14	0.60
1:E:151:GLU:OE1	1:E:155:LYS:NZ	2.35	0.60
1:B:302:GLN:HG2	1:B:316:ALA:CB	2.31	0.60
1:C:25:VAL:HG11	1:C:288:PRO:HA	1.84	0.60
1:B:45:THR:C	1:B:46:LYS:HD3	2.26	0.60
1:A:149:MET:O	1:A:151:GLU:N	2.34	0.60
1:B:150:PRO:HA	1:B:152:TYR:CD1	2.36	0.60
1:E:317:ARG:H	1:E:317:ARG:CZ	2.14	0.60
1:D:45:THR:C	1:D:46:LYS:HD3	2.27	0.60
1:A:148:GLN:O	1:A:152:TYR:HE2	1.85	0.60
1:A:344:LEU:HD13	1:E:250:LEU:HB3	1.83	0.60
1:B:45:THR:H	1:B:111:LYS:HZ1	1.50	0.60
1:B:184:VAL:HG13	1:C:165:LYS:HA	1.84	0.60
1:B:317:ARG:CD	2:R:22:C:HO2'	2.02	0.60
1:C:167:ILE:O	1:C:168:ASN:C	2.44	0.60
1:C:180:ASP:OD2	1:D:164:CYS:HB3	2.00	0.60
1:C:317:ARG:NE	1:C:317:ARG:N	2.45	0.60
1:D:136:LEU:C	1:D:136:LEU:HD23	2.27	0.60
1:A:66:ILE:O	1:A:69:VAL:HG13	2.01	0.60
1:D:89:SER:O	1:D:90:SER:HB2	2.00	0.60
1:E:87:ASP:OD2	1:E:97:LYS:HG3	2.01	0.60
2:R:11:C:H2'	2:R:12:C:O4'	2.02	0.60
1:A:29:ALA:O	1:A:31:TYR:N	2.30	0.59
1:B:165:LYS:HB2	1:B:165:LYS:NZ	2.17	0.59
1:D:166:MET:C	1:D:167:ILE:HG13	2.25	0.59
1:D:224:ASP:CG	2:R:3:C:H4'	2.27	0.59
1:E:66:ILE:O	1:E:69:VAL:HG13	2.02	0.59
1:E:165:LYS:O	1:E:166:MET:HB2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:12:C:C2'	2:R:13:C:H5'	2.31	0.59
1:B:228:LEU:HB2	1:B:289:TYR:HB3	1.84	0.59
1:A:148:GLN:HG2	1:A:179:ARG:NH1	2.16	0.59
1:C:42:ILE:HD12	1:C:74:TYR:CD2	2.36	0.59
1:E:117:LEU:CB	1:E:118:PRO:HD3	2.27	0.59
1:E:127:THR:HG23	1:E:129:ALA:H	1.66	0.59
1:B:383:GLU:HG3	1:C:354:LYS:CE	2.31	0.59
1:A:87:ASP:OD2	1:A:97:LYS:HG3	2.03	0.59
1:E:412:ILE:C	1:E:412:ILE:HD12	2.27	0.59
1:A:180:ASP:OD2	1:A:180:ASP:C	2.44	0.59
1:D:317:ARG:O	1:D:319:PRO:HD3	2.02	0.59
1:C:167:ILE:O	1:C:169:GLU:CD	2.46	0.59
1:C:214:ARG:HA	1:C:217:THR:CG2	2.32	0.59
1:E:29:ALA:C	1:E:31:TYR:H	2.11	0.59
1:C:263:LEU:CD1	1:C:264:PRO:HD2	2.27	0.59
1:D:15:VAL:O	1:D:17:LYS:HG2	2.03	0.59
1:A:169:GLU:HA	1:A:170:GLN:NE2	2.17	0.59
1:B:226:ALA:O	1:B:230:THR:HG23	2.02	0.59
1:E:228:LEU:HB2	1:E:289:TYR:HB3	1.84	0.59
1:D:25:VAL:HG11	1:D:288:PRO:HA	1.85	0.58
1:D:66:ILE:O	1:D:69:VAL:HG13	2.03	0.58
1:E:106:ASP:C	1:E:107:LEU:HD12	2.28	0.58
1:A:382:PHE:HE1	1:A:393:MET:HE1	1.68	0.58
1:B:22:GLU:HB3	1:C:206:LYS:NZ	2.18	0.58
1:C:50:ASP:OD2	1:C:120:GLY:HA2	2.03	0.58
1:E:352:ASP:C	1:E:352:ASP:OD1	2.46	0.58
1:A:152:TYR:HD1	1:A:153:ARG:H	1.51	0.58
1:B:148:GLN:O	1:B:152:TYR:HE2	1.87	0.58
2:R:25:C:H2'	2:R:26:C:C6	2.38	0.58
1:C:375:VAL:O	1:C:379:LEU:HB2	2.03	0.58
1:D:152:TYR:HD1	1:D:153:ARG:H	1.52	0.58
1:B:68:HIS:HE1	1:B:117:LEU:HG	1.67	0.58
1:A:317:ARG:NE	1:A:317:ARG:N	2.50	0.58
1:B:136:LEU:C	1:B:136:LEU:HD23	2.28	0.58
1:B:81:ARG:HB2	1:B:208:HIS:HE2	1.68	0.58
1:C:226:ALA:O	1:C:230:THR:HG23	2.04	0.58
1:B:127:THR:HG23	1:B:129:ALA:H	1.69	0.58
1:A:150:PRO:HA	1:A:152:TYR:CD1	2.38	0.57
1:C:150:PRO:CA	1:C:152:TYR:CE1	2.83	0.57
1:D:107:LEU:HD12	1:D:107:LEU:N	2.19	0.57
1:A:130:ASP:O	1:A:132:LYS:N	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:OD2	1:B:97:LYS:HG3	2.05	0.57
1:C:66:ILE:O	1:C:69:VAL:HG13	2.04	0.57
1:C:152:TYR:HD1	1:C:153:ARG:H	1.52	0.57
1:E:130:ASP:O	1:E:132:LYS:N	2.36	0.57
1:A:14:ILE:HG23	1:A:16:PRO:HD3	1.87	0.57
1:A:165:LYS:NZ	1:A:165:LYS:CB	2.67	0.57
1:D:317:ARG:NE	1:D:317:ARG:N	2.48	0.57
1:C:165:LYS:O	1:C:166:MET:CB	2.53	0.57
1:D:87:ASP:OD2	1:D:97:LYS:HG3	2.05	0.57
1:E:45:THR:C	1:E:46:LYS:HD3	2.29	0.57
1:E:50:ASP:OD2	1:E:120:GLY:HA2	2.05	0.57
1:E:165:LYS:HB2	1:E:165:LYS:NZ	2.18	0.57
1:A:29:ALA:HB2	1:A:91:PHE:CE2	2.39	0.57
1:C:14:ILE:HD11	1:D:259:VAL:HA	1.86	0.57
1:C:294:ASN:N	1:C:295:PRO:HD3	2.20	0.57
1:A:29:ALA:C	1:A:31:TYR:H	2.13	0.57
1:C:14:ILE:HG23	1:C:16:PRO:HD3	1.87	0.57
1:C:342:ALA:HB1	1:C:344:LEU:HD23	1.87	0.57
1:C:383:GLU:HG3	1:D:354:LYS:HE2	1.86	0.57
1:E:149:MET:C	1:E:151:GLU:N	2.62	0.57
1:E:199:ASP:HB2	1:E:217:THR:HG23	1.86	0.57
2:R:21:C:C2'	2:R:22:C:H5'	2.35	0.57
1:A:70:ASN:N	1:A:70:ASN:HD22	2.03	0.57
1:A:117:LEU:HD23	1:A:117:LEU:N	2.20	0.57
1:B:152:TYR:HD1	1:B:153:ARG:H	1.53	0.57
1:C:136:LEU:C	1:C:136:LEU:HD23	2.29	0.57
1:C:292:VAL:HG12	2:R:13:C:H5	1.70	0.57
1:A:323:GLU:OE1	1:B:239:GLY:HA3	2.05	0.57
1:B:389:PRO:CA	1:B:393:MET:HE2	2.25	0.57
1:C:46:LYS:HD3	1:C:46:LYS:N	2.19	0.57
1:D:143:ARG:NH1	2:R:9:C:H5'	2.20	0.57
1:D:171:PHE:CG	1:D:172:GLU:N	2.73	0.57
1:D:27:TYR:HB3	1:D:266:GLN:HE22	1.68	0.56
1:B:31:TYR:C	1:B:33:ARG:H	2.12	0.56
1:D:215:TYR:HA	2:R:9:C:O4'	2.04	0.56
1:A:31:TYR:C	1:A:33:ARG:H	2.13	0.56
1:A:199:ASP:OD1	1:A:217:THR:HG23	2.05	0.56
1:C:150:PRO:HA	1:C:152:TYR:CD1	2.40	0.56
1:C:165:LYS:NZ	1:C:165:LYS:CB	2.67	0.56
1:D:70:ASN:N	1:D:70:ASN:HD22	2.04	0.56
1:E:152:TYR:HD1	1:E:153:ARG:H	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:CG	1:A:172:GLU:N	2.73	0.56
1:A:199:ASP:HB2	1:A:217:THR:HG23	1.87	0.56
1:B:133:TRP:CB	1:B:167:ILE:HD13	2.34	0.56
1:C:31:TYR:C	1:C:33:ARG:H	2.13	0.56
1:C:89:SER:O	1:C:90:SER:HB2	2.05	0.56
1:D:180:ASP:OD2	1:D:180:ASP:C	2.48	0.56
1:C:68:HIS:HE1	1:C:117:LEU:HG	1.70	0.56
1:C:117:LEU:N	1:C:117:LEU:HD23	2.21	0.56
1:D:214:ARG:CA	1:D:217:THR:HG22	2.35	0.56
1:C:199:ASP:CB	1:C:217:THR:HG23	2.36	0.56
1:E:58:GLY:O	1:E:63:ASN:O	2.24	0.56
1:B:149:MET:C	1:B:152:TYR:CE2	2.84	0.56
1:D:148:GLN:O	1:D:152:TYR:CE2	2.59	0.56
2:R:40:C:H2'	2:R:40:C:O2	2.04	0.56
1:B:42:ILE:HD12	1:B:74:TYR:HD2	1.70	0.55
1:D:143:ARG:HH12	2:R:9:C:C5'	2.19	0.55
1:E:107:LEU:HD12	1:E:107:LEU:N	2.21	0.55
1:A:42:ILE:HD12	1:A:74:TYR:HD2	1.72	0.55
1:A:136:LEU:HD23	1:A:136:LEU:C	2.32	0.55
1:D:72:TYR:C	1:D:72:TYR:CD2	2.82	0.55
1:D:149:MET:C	1:D:151:GLU:N	2.62	0.55
1:D:150:PRO:CA	1:D:152:TYR:CE1	2.86	0.55
1:D:178:GLY:O	1:D:179:ARG:HB2	2.05	0.55
1:A:45:THR:C	1:A:46:LYS:HD3	2.30	0.55
1:A:165:LYS:O	1:A:167:ILE:CD1	2.48	0.55
1:B:22:GLU:HB3	1:C:206:LYS:HZ3	1.71	0.55
1:B:149:MET:C	1:B:151:GLU:N	2.64	0.55
1:D:68:HIS:HE1	1:D:117:LEU:HG	1.71	0.55
1:A:68:HIS:HE1	1:A:117:LEU:HG	1.70	0.55
1:B:163:GLN:O	1:B:167:ILE:HD12	2.05	0.55
1:B:178:GLY:O	1:B:179:ARG:HB2	2.05	0.55
1:C:127:THR:HG23	1:C:129:ALA:H	1.70	0.55
1:E:29:ALA:O	1:E:31:TYR:N	2.33	0.55
1:E:180:ASP:OD2	1:E:180:ASP:C	2.49	0.55
1:E:150:PRO:CA	1:E:152:TYR:CE1	2.87	0.55
1:A:199:ASP:CB	1:A:217:THR:HG23	2.36	0.55
1:C:36:LYS:HG3	1:C:93:ILE:HD11	1.89	0.55
1:D:31:TYR:C	1:D:33:ARG:H	2.14	0.55
1:E:148:GLN:O	1:E:152:TYR:HE2	1.90	0.55
1:E:178:GLY:O	1:E:179:ARG:HB2	2.06	0.55
1:E:14:ILE:HG23	1:E:16:PRO:HD3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:ILE:HD12	1:C:412:ILE:C	2.32	0.55
1:D:165:LYS:HB2	1:D:165:LYS:NZ	2.22	0.55
1:E:68:HIS:HE1	1:E:117:LEU:HG	1.70	0.55
1:A:58:GLY:O	1:A:63:ASN:O	2.24	0.55
1:B:15:VAL:O	1:B:17:LYS:HG2	2.07	0.55
1:B:42:ILE:HD12	1:B:74:TYR:CD2	2.42	0.55
1:B:130:ASP:C	1:B:132:LYS:N	2.65	0.55
1:B:171:PHE:HZ	1:B:173:PRO:HG2	1.72	0.55
1:B:117:LEU:N	1:B:117:LEU:HD23	2.21	0.54
1:B:350:VAL:HG13	1:E:4:THR:O	2.07	0.54
2:R:16:C:H2'	2:R:17:C:C6	2.42	0.54
1:A:166:MET:H	1:E:184:VAL:CG1	2.18	0.54
1:A:167:ILE:HG22	1:A:169:GLU:OE1	2.07	0.54
1:A:214:ARG:CA	1:A:217:THR:HG22	2.37	0.54
1:B:72:TYR:C	1:B:72:TYR:CD2	2.82	0.54
1:B:105:PHE:C	1:B:107:LEU:N	2.66	0.54
1:B:365:THR:HG23	1:B:366:THR:H	1.72	0.54
1:E:136:LEU:C	1:E:136:LEU:HD23	2.32	0.54
1:A:385:GLN:HG2	1:A:390:THR:HG22	1.89	0.54
1:B:203:HIS:O	1:B:206:LYS:HG3	2.07	0.54
1:B:385:GLN:HG2	1:B:390:THR:HG22	1.89	0.54
1:C:70:ASN:N	1:C:70:ASN:HD22	2.05	0.54
1:C:385:GLN:HG2	1:C:390:THR:HG22	1.90	0.54
1:E:294:ASN:N	1:E:295:PRO:HD3	2.22	0.54
1:B:43:ASN:OD1	1:B:112:ALA:N	2.41	0.54
1:B:81:ARG:HD2	1:B:208:HIS:HE2	1.73	0.54
1:C:72:TYR:C	1:C:72:TYR:CD2	2.83	0.54
1:D:42:ILE:HD12	1:D:74:TYR:HD2	1.73	0.54
1:D:70:ASN:HD22	1:D:70:ASN:H	1.55	0.54
1:E:214:ARG:CA	1:E:217:THR:HG22	2.37	0.54
1:A:149:MET:C	1:A:152:TYR:CE2	2.85	0.54
1:A:153:ARG:NH1	1:A:176:PRO:O	2.39	0.54
1:D:42:ILE:HD12	1:D:74:TYR:CD2	2.43	0.54
1:D:130:ASP:O	1:D:132:LYS:N	2.36	0.54
1:D:385:GLN:HG2	1:D:390:THR:HG22	1.90	0.54
2:R:12:C:H2'	2:R:13:C:H5'	1.89	0.54
1:A:218:ILE:C	1:A:220:SER:H	2.15	0.54
1:C:43:ASN:OD1	1:C:112:ALA:N	2.41	0.54
1:C:149:MET:C	1:C:151:GLU:N	2.63	0.54
1:C:203:HIS:O	1:C:206:LYS:HG3	2.08	0.54
1:C:293:LYS:C	1:C:295:PRO:HD3	2.32	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:PRO:HA	1:D:152:TYR:CD1	2.41	0.54
1:D:203:HIS:O	1:D:206:LYS:HG3	2.07	0.54
1:E:70:ASN:HD22	1:E:70:ASN:N	2.05	0.54
1:A:42:ILE:HD12	1:A:74:TYR:CD2	2.43	0.54
1:B:130:ASP:O	1:B:132:LYS:N	2.39	0.54
1:B:295:PRO:HB2	1:B:322:ILE:CG2	2.38	0.54
1:C:130:ASP:C	1:C:132:LYS:N	2.65	0.54
1:E:42:ILE:HD12	1:E:74:TYR:HD2	1.73	0.54
1:E:171:PHE:CG	1:E:172:GLU:N	2.74	0.54
1:A:149:MET:C	1:A:151:GLU:N	2.66	0.54
1:A:364:LEU:O	1:A:365:THR:C	2.50	0.54
1:B:150:PRO:HD3	1:B:152:TYR:OH	2.08	0.54
1:C:130:ASP:O	1:C:132:LYS:N	2.38	0.54
1:C:203:HIS:HD2	1:C:272:ASP:OD1	1.89	0.54
1:A:243:GLU:HG3	1:E:2:SER:O	2.08	0.54
1:B:214:ARG:CA	1:B:217:THR:HG22	2.38	0.54
1:C:309:ARG:N	1:C:309:ARG:HD2	2.23	0.54
1:E:130:ASP:C	1:E:132:LYS:N	2.62	0.54
1:E:167:ILE:HG22	1:E:168:ASN:N	2.22	0.54
1:E:359:ASP:O	1:E:361:THR:HG23	2.07	0.54
1:B:5:VAL:CG1	1:D:348:PHE:HB3	2.38	0.54
1:C:87:ASP:OD2	1:C:97:LYS:HG3	2.08	0.54
1:C:308:LEU:O	1:C:309:ARG:HB2	2.08	0.54
1:A:50:ASP:OD2	1:A:120:GLY:HA2	2.08	0.53
1:B:46:LYS:HD3	1:B:46:LYS:N	2.21	0.53
1:C:385:GLN:O	1:C:386:ASN:HB2	2.08	0.53
1:E:81:ARG:HB2	1:E:208:HIS:HE2	1.72	0.53
1:A:323:GLU:O	1:A:327:LEU:HD22	2.08	0.53
1:D:147:THR:HG21	1:D:152:TYR:HB3	1.89	0.53
1:D:130:ASP:C	1:D:132:LYS:N	2.62	0.53
1:A:294:ASN:N	1:A:295:PRO:HD3	2.23	0.53
1:C:148:GLN:O	1:C:152:TYR:HE2	1.91	0.53
1:D:60:LYS:O	1:D:61:SER:CB	2.46	0.53
1:E:308:LEU:O	1:E:309:ARG:HB2	2.09	0.53
1:B:70:ASN:N	1:B:70:ASN:HD22	2.07	0.53
1:C:38:ILE:HD11	1:C:107:LEU:O	2.09	0.53
1:E:385:GLN:HG2	1:E:390:THR:HG22	1.89	0.53
1:D:309:ARG:HD2	1:D:309:ARG:N	2.24	0.53
1:E:323:GLU:O	1:E:327:LEU:HD22	2.09	0.53
1:B:380:GLY:CA	1:C:354:LYS:HZ3	2.18	0.53
1:C:172:GLU:HB3	1:C:173:PRO:CD	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:GLY:O	1:C:179:ARG:HB2	2.08	0.53
1:E:166:MET:HB2	1:E:167:ILE:HG13	1.89	0.53
1:E:382:PHE:HE1	1:E:393:MET:HE1	1.72	0.53
1:A:370:PRO:HD3	1:A:381:TRP:CG	2.44	0.53
1:A:412:ILE:HD12	1:A:412:ILE:C	2.34	0.53
1:E:150:PRO:HA	1:E:152:TYR:CD1	2.43	0.53
1:A:130:ASP:C	1:A:132:LYS:N	2.63	0.53
1:A:203:HIS:HD2	1:A:272:ASP:OD1	1.91	0.53
1:B:27:TYR:HB3	1:B:266:GLN:HE22	1.73	0.53
1:B:294:ASN:N	1:B:295:PRO:HD3	2.24	0.53
1:D:117:LEU:HD23	1:D:117:LEU:N	2.24	0.53
1:B:180:ASP:OD2	1:B:180:ASP:C	2.50	0.53
1:B:230:THR:HG21	1:B:298:HIS:ND1	2.22	0.53
1:D:382:PHE:HE1	1:D:393:MET:HE1	1.74	0.53
1:E:199:ASP:CB	1:E:217:THR:HG23	2.38	0.53
1:A:203:HIS:O	1:A:206:LYS:HG3	2.09	0.52
1:A:293:LYS:C	1:A:295:PRO:HD3	2.35	0.52
1:B:45:THR:H	1:B:111:LYS:NZ	2.06	0.52
1:B:240:MET:HE3	1:B:244:ASP:HB3	1.92	0.52
1:B:412:ILE:C	1:B:412:ILE:HD12	2.34	0.52
1:E:104:ILE:O	1:E:107:LEU:HD13	2.10	0.52
1:D:230:THR:HG21	1:D:298:HIS:ND1	2.24	0.52
1:D:203:HIS:HD2	1:D:272:ASP:OD1	1.92	0.52
1:E:203:HIS:O	1:E:206:LYS:HG3	2.09	0.52
1:E:230:THR:HG21	1:E:298:HIS:ND1	2.24	0.52
1:A:402:MET:SD	1:E:422:LYS:HD2	2.49	0.52
1:B:54:TYR:CD1	1:B:122:SER:HB2	2.45	0.52
1:B:308:LEU:O	1:B:309:ARG:HB2	2.08	0.52
1:C:105:PHE:C	1:C:107:LEU:N	2.67	0.52
1:C:165:LYS:O	1:C:167:ILE:HG12	2.08	0.52
1:D:308:LEU:O	1:D:309:ARG:HB2	2.10	0.52
1:B:223:LYS:O	1:B:224:ASP:HB2	2.09	0.52
1:C:238:THR:C	1:C:240:MET:H	2.16	0.52
1:D:253:GLU:OE2	1:D:253:GLU:N	2.41	0.52
1:E:169:GLU:CG	1:E:170:GLN:N	2.60	0.52
2:R:27:C:C2'	2:R:28:C:O5'	2.58	0.52
1:A:43:ASN:OD1	1:A:112:ALA:N	2.42	0.52
1:A:149:MET:C	1:A:152:TYR:CZ	2.88	0.52
1:A:298:HIS:NE2	1:A:317:ARG:NH1	2.58	0.52
1:A:309:ARG:N	1:A:309:ARG:HD2	2.25	0.52
1:C:151:GLU:O	1:C:155:LYS:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:ASN:N	1:D:295:PRO:HD3	2.25	0.52
1:E:163:GLN:O	1:E:167:ILE:HD12	2.10	0.52
1:A:178:GLY:O	1:A:179:ARG:HB2	2.08	0.51
1:B:253:GLU:OE2	1:B:253:GLU:N	2.39	0.51
1:B:370:PRO:HD3	1:B:381:TRP:CG	2.45	0.51
1:D:208:HIS:HD1	1:D:210:CYS:N	2.05	0.51
1:D:370:PRO:HD3	1:D:381:TRP:CG	2.45	0.51
1:E:215:TYR:C	1:E:215:TYR:CD2	2.87	0.51
1:B:309:ARG:HD2	1:B:309:ARG:N	2.25	0.51
1:C:45:THR:H	1:C:111:LYS:NZ	2.07	0.51
1:C:342:ALA:CB	1:C:344:LEU:HD23	2.39	0.51
1:D:59:LEU:O	1:D:61:SER:N	2.42	0.51
1:E:36:LYS:HG3	1:E:93:ILE:HD11	1.92	0.51
1:E:54:TYR:CD1	1:E:122:SER:HB2	2.46	0.51
1:E:317:ARG:NE	1:E:317:ARG:N	2.56	0.51
1:C:81:ARG:HD2	1:C:208:HIS:HE2	1.74	0.51
1:A:149:MET:O	1:A:152:TYR:CD2	2.64	0.51
1:B:298:HIS:NE2	1:B:317:ARG:NH1	2.59	0.51
1:C:370:PRO:HD3	1:C:381:TRP:CG	2.45	0.51
1:D:54:TYR:CD1	1:D:122:SER:HB2	2.46	0.51
1:D:293:LYS:C	1:D:295:PRO:HD3	2.35	0.51
1:E:59:LEU:HB3	1:E:172:GLU:HG2	1.93	0.51
1:E:61:SER:O	1:E:63:ASN:N	2.38	0.51
1:E:293:LYS:C	1:E:295:PRO:HD3	2.36	0.51
1:A:81:ARG:HD2	1:A:208:HIS:HE2	1.76	0.51
1:A:148:GLN:O	1:A:152:TYR:CE2	2.62	0.51
1:B:72:TYR:CD2	1:B:72:TYR:O	2.63	0.51
1:B:258:MET:HE3	1:B:262:MET:HG3	1.92	0.51
1:B:293:LYS:C	1:B:295:PRO:HD3	2.36	0.51
1:C:72:TYR:CD2	1:C:72:TYR:O	2.63	0.51
1:C:81:ARG:HB2	1:C:208:HIS:HE2	1.72	0.51
1:E:295:PRO:HB2	1:E:322:ILE:CG2	2.40	0.51
2:R:27:C:H2'	2:R:28:C:O5'	2.11	0.51
1:B:14:ILE:HG23	1:B:16:PRO:HD3	1.93	0.51
1:C:27:TYR:HB3	1:C:266:GLN:HE22	1.74	0.51
1:C:54:TYR:CD1	1:C:122:SER:HB2	2.45	0.51
1:C:184:VAL:HG13	1:D:165:LYS:CG	2.40	0.51
1:E:81:ARG:HD2	1:E:208:HIS:HE2	1.74	0.51
1:E:298:HIS:NE2	1:E:317:ARG:NH1	2.59	0.51
1:A:308:LEU:O	1:A:309:ARG:HB2	2.10	0.51
1:B:171:PHE:HE2	1:B:173:PRO:O	1.94	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:MET:HB3	1:C:150:PRO:HD2	1.92	0.51
1:D:147:THR:CG2	1:D:152:TYR:HB3	2.41	0.51
1:D:408:ARG:NH2	2:R:6:C:H2'	2.26	0.51
1:E:309:ARG:HD2	1:E:309:ARG:N	2.26	0.51
1:A:342:ALA:HB1	1:A:344:LEU:HD23	1.93	0.51
1:C:147:THR:HG21	1:C:152:TYR:HB3	1.92	0.51
1:C:199:ASP:OD1	1:C:217:THR:HG23	2.10	0.51
1:C:214:ARG:CA	1:C:217:THR:HG22	2.40	0.51
1:A:72:TYR:C	1:A:72:TYR:CD2	2.85	0.51
1:B:171:PHE:CE2	1:B:173:PRO:O	2.64	0.51
1:B:382:PHE:HE1	1:B:393:MET:HE1	1.74	0.51
1:C:323:GLU:O	1:C:327:LEU:HD22	2.10	0.51
1:D:199:ASP:HB2	1:D:217:THR:HG23	1.91	0.51
1:E:15:VAL:O	1:E:17:LYS:HG2	2.11	0.51
1:E:151:GLU:O	1:E:155:LYS:HB2	2.10	0.51
1:A:54:TYR:CD1	1:A:122:SER:HB2	2.46	0.51
1:A:383:GLU:HG3	1:B:354:LYS:CE	2.41	0.51
1:D:401:VAL:HG21	1:D:420:PHE:HB2	1.92	0.51
1:E:42:ILE:HD12	1:E:74:TYR:CD2	2.45	0.51
1:E:147:THR:HG21	1:E:152:TYR:HB3	1.93	0.51
1:A:41:TYR:CE1	1:A:110:LEU:HD12	2.45	0.50
1:A:147:THR:HG21	1:A:152:TYR:HB3	1.91	0.50
1:A:149:MET:HB3	1:A:150:PRO:HD2	1.93	0.50
1:A:167:ILE:HG22	1:A:169:GLU:CD	2.36	0.50
1:D:72:TYR:CD2	1:D:72:TYR:O	2.63	0.50
1:E:233:HIS:HB2	1:E:312:ARG:NH1	2.26	0.50
2:R:18:C:O2'	2:R:19:C:H5'	2.11	0.50
1:B:149:MET:C	1:B:152:TYR:CZ	2.89	0.50
1:C:155:LYS:NZ	2:R:17:C:OP2	2.39	0.50
1:C:184:VAL:HG11	1:D:166:MET:H	1.76	0.50
1:D:316:ALA:HA	1:D:317:ARG:CZ	2.41	0.50
1:E:70:ASN:HD22	1:E:70:ASN:H	1.58	0.50
1:B:323:GLU:OE1	1:C:239:GLY:HA3	2.11	0.50
1:C:258:MET:HE3	1:C:262:MET:HG3	1.93	0.50
1:E:72:TYR:C	1:E:72:TYR:CD2	2.86	0.50
1:B:255:ALA:O	1:B:256:ASP:C	2.53	0.50
1:E:172:GLU:HB3	1:E:173:PRO:CD	2.41	0.50
1:E:177:GLU:HG2	1:E:178:GLY:N	2.26	0.50
1:E:253:GLU:OE2	1:E:253:GLU:N	2.41	0.50
1:B:323:GLU:O	1:B:327:LEU:HD22	2.11	0.50
2:R:10:C:H5''	2:R:11:C:OP2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:34:C:O2	2:R:34:C:O4'	2.28	0.50
1:B:199:ASP:HB2	1:B:217:THR:HG23	1.93	0.50
1:E:354:LYS:CE	1:E:356:THR:HA	2.33	0.50
1:C:295:PRO:HB2	1:C:322:ILE:CG2	2.41	0.50
1:D:238:THR:C	1:D:240:MET:H	2.20	0.50
1:D:328:THR:HG21	1:D:415:TYR:OH	2.11	0.50
1:E:55:VAL:O	1:E:56:TYR:C	2.55	0.50
1:A:172:GLU:HB3	1:A:173:PRO:CD	2.42	0.50
1:B:151:GLU:O	1:B:155:LYS:HB2	2.12	0.50
1:C:60:LYS:O	1:C:61:SER:CB	2.52	0.50
1:C:181:ILE:H	1:C:181:ILE:CD1	2.17	0.50
1:A:230:THR:HG21	1:A:298:HIS:ND1	2.27	0.49
1:A:314:ARG:O	1:A:413:GLY:HA3	2.12	0.49
1:B:184:VAL:CG1	1:C:165:LYS:HA	2.41	0.49
1:C:230:THR:HG21	1:C:298:HIS:ND1	2.26	0.49
1:A:81:ARG:HB2	1:A:208:HIS:HE2	1.75	0.49
1:E:91:PHE:CE2	1:E:267:GLU:HG3	2.47	0.49
1:A:177:GLU:HG2	1:A:178:GLY:N	2.27	0.49
1:B:14:ILE:HD11	1:C:259:VAL:HA	1.94	0.49
1:B:68:HIS:CE1	1:B:117:LEU:HG	2.46	0.49
1:B:199:ASP:CB	1:B:217:THR:HG23	2.41	0.49
1:D:170:GLN:O	1:D:171:PHE:HB3	2.13	0.49
1:D:179:ARG:HA	1:D:183:ASP:OD1	2.12	0.49
1:D:240:MET:HE3	1:D:244:ASP:HB3	1.95	0.49
1:E:31:TYR:C	1:E:33:ARG:H	2.20	0.49
1:E:65:SER:HB3	1:E:68:HIS:ND1	2.27	0.49
1:E:153:ARG:NH1	1:E:176:PRO:O	2.45	0.49
1:E:203:HIS:HD2	1:E:272:ASP:OD1	1.94	0.49
1:B:37:GLU:HB2	1:B:108:VAL:HG21	1.95	0.49
1:D:38:ILE:HD11	1:D:107:LEU:O	2.11	0.49
1:E:38:ILE:HD11	1:E:107:LEU:O	2.12	0.49
1:E:149:MET:HB3	1:E:150:PRO:HD2	1.95	0.49
1:E:163:GLN:C	1:E:165:LYS:N	2.67	0.49
1:E:370:PRO:HD3	1:E:381:TRP:CG	2.47	0.49
1:A:28:PRO:O	1:A:29:ALA:C	2.55	0.49
1:A:165:LYS:HG3	1:E:184:VAL:HG13	1.94	0.49
1:A:238:THR:C	1:A:240:MET:H	2.20	0.49
1:B:177:GLU:HG2	1:B:178:GLY:N	2.28	0.49
1:B:379:LEU:CD1	1:C:346:GLN:HB2	2.42	0.49
1:C:233:HIS:HB2	1:C:312:ARG:NH1	2.27	0.49
1:D:8:ILE:HG13	1:D:8:ILE:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:TYR:CE1	1:D:110:LEU:HD12	2.43	0.49
1:D:43:ASN:OD1	1:D:112:ALA:N	2.46	0.49
1:D:141:LEU:HD22	1:D:182:PHE:CE1	2.47	0.49
1:D:215:TYR:C	1:D:215:TYR:CD2	2.90	0.49
1:D:298:HIS:NE2	1:D:317:ARG:NH1	2.59	0.49
1:A:151:GLU:O	1:A:155:LYS:HB2	2.12	0.49
1:D:122:SER:O	1:D:123:ASP:HB2	2.10	0.49
1:D:230:THR:HB	1:D:302:GLN:OE1	2.12	0.49
1:E:8:ILE:O	1:E:8:ILE:HG13	2.11	0.49
1:E:259:VAL:O	1:E:260:GLN:C	2.54	0.49
1:E:366:THR:C	1:E:368:ALA:H	2.21	0.49
1:A:72:TYR:CD2	1:A:72:TYR:O	2.65	0.49
1:A:385:GLN:O	1:A:386:ASN:HB2	2.13	0.49
1:B:149:MET:O	1:B:152:TYR:CD2	2.65	0.49
1:B:218:ILE:C	1:B:220:SER:H	2.21	0.49
1:B:240:MET:HE3	1:B:244:ASP:CB	2.41	0.49
1:C:240:MET:HE3	1:C:244:ASP:HB3	1.95	0.49
1:D:172:GLU:HB3	1:D:173:PRO:CD	2.42	0.49
1:E:117:LEU:N	1:E:117:LEU:HD23	2.28	0.49
1:C:177:GLU:HG2	1:C:178:GLY:N	2.28	0.49
1:E:364:LEU:O	1:E:365:THR:C	2.56	0.49
1:A:122:SER:O	1:A:123:ASP:HB2	2.12	0.49
1:A:150:PRO:HD3	1:A:152:TYR:OH	2.12	0.49
1:A:239:GLY:HA3	1:E:323:GLU:OE1	2.12	0.49
1:B:262:MET:HA	1:B:262:MET:CE	2.35	0.49
1:C:218:ILE:C	1:C:220:SER:H	2.20	0.49
1:E:46:LYS:HD3	1:E:46:LYS:N	2.26	0.49
1:A:27:TYR:HB3	1:A:266:GLN:HE22	1.78	0.49
1:A:38:ILE:HD11	1:A:107:LEU:O	2.13	0.49
1:B:54:TYR:CD1	1:B:118:PRO:HB2	2.48	0.49
1:C:223:LYS:O	1:C:224:ASP:HB2	2.13	0.49
1:D:212:SER:HA	2:R:9:C:O2	2.12	0.49
1:E:72:TYR:CD2	1:E:72:TYR:O	2.66	0.49
1:A:15:VAL:O	1:A:17:LYS:HG2	2.12	0.48
1:A:163:GLN:N	1:A:163:GLN:CD	2.71	0.48
1:B:122:SER:O	1:B:123:ASP:HB2	2.12	0.48
1:B:354:LYS:CE	1:B:356:THR:HA	2.37	0.48
1:B:376:VAL:HG13	1:C:354:LYS:CB	2.39	0.48
1:D:165:LYS:O	1:D:167:ILE:CD1	2.58	0.48
1:D:295:PRO:HB2	1:D:322:ILE:CG2	2.43	0.48
1:E:37:GLU:HB2	1:E:108:VAL:HG21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:218:ILE:C	1:E:220:SER:H	2.20	0.48
1:B:317:ARG:CD	1:B:317:ARG:H	2.25	0.48
1:C:141:LEU:HD22	1:C:182:PHE:CE1	2.47	0.48
1:D:199:ASP:CB	1:D:217:THR:HG23	2.43	0.48
1:E:43:ASN:OD1	1:E:112:ALA:N	2.46	0.48
1:E:275:MET:SD	1:E:275:MET:C	2.96	0.48
2:R:18:C:H5'	2:R:18:C:C6	2.48	0.48
1:A:241:SER:OG	1:A:243:GLU:HG2	2.14	0.48
1:A:295:PRO:HB2	1:A:322:ILE:CG2	2.42	0.48
1:B:238:THR:C	1:B:240:MET:H	2.21	0.48
1:C:166:MET:HB2	1:C:167:ILE:CD1	2.43	0.48
1:C:180:ASP:OD2	1:C:180:ASP:O	2.31	0.48
1:C:401:VAL:HG21	1:C:420:PHE:HB2	1.94	0.48
1:E:262:MET:HA	1:E:262:MET:CE	2.35	0.48
1:B:179:ARG:HA	1:B:183:ASP:OD1	2.12	0.48
1:C:37:GLU:HB2	1:C:108:VAL:HG21	1.95	0.48
1:C:356:THR:CG2	1:C:357:PRO:HD3	2.29	0.48
1:D:151:GLU:O	1:D:155:LYS:HB2	2.13	0.48
1:E:238:THR:C	1:E:240:MET:H	2.21	0.48
1:A:18:LEU:HD12	1:B:232:GLY:HA2	1.95	0.48
1:B:36:LYS:HG3	1:B:93:ILE:HD11	1.95	0.48
1:B:148:GLN:O	1:B:152:TYR:CE2	2.65	0.48
1:B:149:MET:HB3	1:B:150:PRO:HD2	1.95	0.48
1:B:165:LYS:HB2	1:B:165:LYS:HZ2	1.78	0.48
1:C:68:HIS:CE1	1:C:117:LEU:HG	2.48	0.48
1:C:171:PHE:CG	1:C:172:GLU:N	2.72	0.48
1:C:380:GLY:CA	1:D:354:LYS:HZ3	2.25	0.48
1:E:122:SER:O	1:E:123:ASP:HB2	2.12	0.48
2:R:44:C:H5''	2:R:45:C:OP2	2.12	0.48
1:B:29:ALA:C	1:B:31:TYR:N	2.72	0.48
1:B:253:GLU:HA	1:B:256:ASP:HB2	1.95	0.48
1:B:385:GLN:O	1:B:386:ASN:HB2	2.14	0.48
1:C:215:TYR:CD2	1:C:215:TYR:C	2.91	0.48
1:D:68:HIS:CE1	1:D:118:PRO:HD2	2.49	0.48
1:B:147:THR:HG21	1:B:152:TYR:HB3	1.94	0.48
1:D:149:MET:HB3	1:D:150:PRO:HD2	1.95	0.48
1:A:168:ASN:C	1:A:169:GLU:OE2	2.57	0.48
1:A:253:GLU:HA	1:A:256:ASP:HB2	1.95	0.48
1:C:29:ALA:C	1:C:31:TYR:N	2.72	0.48
1:A:240:MET:HE3	1:A:244:ASP:HB3	1.96	0.48
1:C:59:LEU:HB3	1:C:172:GLU:HG2	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:MET:C	1:C:152:TYR:CE2	2.91	0.48
1:C:382:PHE:HE1	1:C:393:MET:HE1	1.78	0.48
1:E:147:THR:CG2	1:E:152:TYR:HB3	2.44	0.48
1:E:255:ALA:O	1:E:259:VAL:HG23	2.14	0.48
1:B:199:ASP:OD1	1:B:217:THR:HG23	2.13	0.48
1:B:317:ARG:NE	2:R:22:C:O2'	2.47	0.48
1:C:136:LEU:HD23	1:C:136:LEU:O	2.14	0.48
1:C:283:LEU:HD23	1:C:283:LEU:N	2.29	0.48
1:D:68:HIS:CE1	1:D:117:LEU:HG	2.49	0.48
1:A:230:THR:HB	1:A:302:GLN:OE1	2.14	0.47
1:C:172:GLU:HB3	1:C:173:PRO:HD3	1.96	0.47
1:C:179:ARG:HA	1:C:183:ASP:OD1	2.13	0.47
1:D:59:LEU:HB3	1:D:172:GLU:HG2	1.96	0.47
1:D:78:LYS:O	1:D:80:ILE:HD12	2.14	0.47
1:D:149:MET:C	1:D:152:TYR:CE2	2.92	0.47
1:D:253:GLU:HA	1:D:256:ASP:HB2	1.95	0.47
1:E:149:MET:C	1:E:152:TYR:CE2	2.91	0.47
1:E:409:GLU:HG3	1:E:414:LYS:HD3	1.96	0.47
2:R:27:C:H2'	2:R:28:C:O4'	2.13	0.47
1:A:46:LYS:HD3	1:A:46:LYS:N	2.27	0.47
1:A:147:THR:CG2	1:A:152:TYR:HB3	2.44	0.47
1:B:43:ASN:OD1	1:B:112:ALA:HB3	2.15	0.47
1:B:295:PRO:HB2	1:B:322:ILE:HG21	1.96	0.47
1:C:141:LEU:HD22	1:C:182:PHE:CD1	2.49	0.47
1:D:36:LYS:HG3	1:D:93:ILE:HD11	1.96	0.47
1:E:141:LEU:HD22	1:E:182:PHE:CE1	2.49	0.47
1:A:59:LEU:HB3	1:A:172:GLU:HG2	1.97	0.47
1:A:70:ASN:HD22	1:A:70:ASN:H	1.60	0.47
1:A:136:LEU:HD23	1:A:136:LEU:O	2.15	0.47
1:C:317:ARG:CZ	2:R:13:C:O2'	2.62	0.47
1:D:153:ARG:CZ	1:D:176:PRO:HA	2.44	0.47
1:E:144:VAL:O	1:E:147:THR:HG22	2.14	0.47
1:A:180:ASP:OD2	1:A:180:ASP:O	2.32	0.47
1:A:409:GLU:HG3	1:A:414:LYS:HD3	1.96	0.47
1:D:385:GLN:O	1:D:386:ASN:HB2	2.14	0.47
1:A:36:LYS:HG3	1:A:93:ILE:HD11	1.97	0.47
1:A:59:LEU:O	1:A:61:SER:N	2.47	0.47
1:A:141:LEU:HD22	1:A:182:PHE:CE1	2.50	0.47
1:D:218:ILE:C	1:D:220:SER:H	2.23	0.47
1:D:354:LYS:CE	1:D:356:THR:HA	2.34	0.47
1:E:54:TYR:OH	1:E:120:GLY:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:212:SER:HA	2:R:45:C:C6	2.50	0.47
1:A:8:ILE:HG13	1:A:8:ILE:O	2.15	0.47
1:B:150:PRO:N	1:B:152:TYR:CZ	2.83	0.47
1:B:171:PHE:CD2	1:B:172:GLU:N	2.82	0.47
1:B:214:ARG:O	1:B:215:TYR:C	2.55	0.47
1:B:380:GLY:HA2	1:C:354:LYS:HZ1	1.71	0.47
1:C:409:GLU:HG3	1:C:414:LYS:HD3	1.95	0.47
1:D:223:LYS:O	1:D:224:ASP:HB2	2.15	0.47
1:D:366:THR:C	1:D:368:ALA:H	2.22	0.47
1:A:68:HIS:CE1	1:A:117:LEU:HG	2.48	0.47
1:A:149:MET:O	1:A:152:TYR:CG	2.68	0.47
1:A:151:GLU:CD	1:A:155:LYS:HZ2	2.23	0.47
1:A:328:THR:HG21	1:A:415:TYR:OH	2.15	0.47
1:B:163:GLN:N	1:B:163:GLN:CD	2.73	0.47
1:C:43:ASN:OD1	1:C:112:ALA:HB3	2.15	0.47
1:C:78:LYS:O	1:C:80:ILE:HD12	2.14	0.47
1:C:78:LYS:O	1:C:80:ILE:N	2.47	0.47
1:C:122:SER:O	1:C:123:ASP:HB2	2.14	0.47
1:C:240:MET:HE3	1:C:244:ASP:CB	2.45	0.47
1:C:255:ALA:O	1:C:256:ASP:C	2.56	0.47
1:C:376:VAL:HG13	1:D:354:LYS:CA	2.43	0.47
1:D:136:LEU:HD23	1:D:136:LEU:O	2.15	0.47
1:D:177:GLU:HG2	1:D:178:GLY:N	2.30	0.47
1:E:177:GLU:HG2	1:E:178:GLY:H	1.80	0.47
1:E:181:ILE:HB	1:E:182:PHE:CD2	2.50	0.47
1:A:79:ASP:HB2	1:A:81:ARG:NE	2.30	0.47
1:A:89:SER:O	1:A:90:SER:CB	2.63	0.47
1:D:29:ALA:C	1:D:31:TYR:N	2.71	0.47
1:D:240:MET:HE3	1:D:244:ASP:CB	2.45	0.47
1:E:55:VAL:HG12	1:E:64:VAL:HG21	1.96	0.47
1:D:55:VAL:HG12	1:D:64:VAL:HG21	1.97	0.47
1:E:163:GLN:O	1:E:165:LYS:N	2.48	0.47
2:R:21:C:H5"	2:R:21:C:C6	2.39	0.47
1:A:105:PHE:C	1:A:107:LEU:N	2.64	0.47
1:A:223:LYS:O	1:A:224:ASP:HB2	2.14	0.47
1:B:38:ILE:HD11	1:B:107:LEU:O	2.14	0.47
1:C:148:GLN:O	1:C:152:TYR:CE2	2.68	0.47
1:C:163:GLN:CD	1:C:163:GLN:N	2.73	0.47
1:C:253:GLU:HA	1:C:256:ASP:HB2	1.97	0.47
1:D:147:THR:HG21	1:D:152:TYR:HA	1.96	0.47
1:D:364:LEU:HB3	1:D:368:ALA:CB	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:TYR:CE1	1:E:110:LEU:HD12	2.44	0.47
1:E:68:HIS:CE1	1:E:117:LEU:HG	2.49	0.47
1:E:163:GLN:CD	1:E:163:GLN:N	2.73	0.47
1:B:81:ARG:HB2	1:B:208:HIS:NE2	2.29	0.46
1:B:86:LYS:HB3	1:B:87:ASP:H	1.56	0.46
1:B:208:HIS:CE1	1:B:210:CYS:HB2	2.50	0.46
1:C:196:ALA:HB3	1:C:281:PHE:CE1	2.51	0.46
1:D:123:ASP:C	1:D:125:SER:H	2.22	0.46
1:E:28:PRO:O	1:E:31:TYR:HB3	2.15	0.46
1:E:385:GLN:O	1:E:386:ASN:HB2	2.15	0.46
1:A:18:LEU:HD12	1:B:232:GLY:CA	2.45	0.46
1:B:283:LEU:N	1:B:283:LEU:HD23	2.29	0.46
1:E:136:LEU:HD23	1:E:136:LEU:O	2.16	0.46
1:E:179:ARG:HA	1:E:183:ASP:OD1	2.15	0.46
1:B:59:LEU:HB3	1:B:172:GLU:HG2	1.97	0.46
1:B:70:ASN:HD22	1:B:70:ASN:H	1.60	0.46
1:B:172:GLU:HB3	1:B:173:PRO:CD	2.45	0.46
1:B:356:THR:CG2	1:B:357:PRO:HD3	2.31	0.46
1:C:153:ARG:NH1	1:C:176:PRO:O	2.44	0.46
1:E:107:LEU:HD23	1:E:274:TYR:HE2	1.81	0.46
1:A:81:ARG:CD	1:A:208:HIS:HE2	2.28	0.46
1:A:167:ILE:O	1:A:168:ASN:HB2	2.16	0.46
1:A:179:ARG:HA	1:A:183:ASP:OD1	2.15	0.46
1:C:14:ILE:CD1	1:D:259:VAL:HA	2.44	0.46
1:D:151:GLU:HG2	1:D:155:LYS:HD3	1.98	0.46
1:D:255:ALA:O	1:D:256:ASP:C	2.56	0.46
1:E:283:LEU:HD23	1:E:283:LEU:N	2.30	0.46
1:E:317:ARG:HG3	2:R:40:C:C2	2.49	0.46
1:E:363:GLY:C	1:E:365:THR:H	2.23	0.46
1:A:73:LEU:O	1:A:74:TYR:C	2.59	0.46
1:A:200:MET:HB2	1:A:277:TYR:CE2	2.51	0.46
1:A:237:ILE:CD1	1:A:310:SER:HB2	2.45	0.46
1:B:54:TYR:OH	1:B:120:GLY:N	2.48	0.46
1:B:58:GLY:O	1:B:63:ASN:O	2.34	0.46
1:B:81:ARG:CD	1:B:208:HIS:HE2	2.29	0.46
1:B:366:THR:C	1:B:368:ALA:H	2.21	0.46
1:C:147:THR:CG2	1:C:152:TYR:HB3	2.45	0.46
1:D:78:LYS:O	1:D:80:ILE:N	2.48	0.46
1:E:74:TYR:O	1:E:78:LYS:HD3	2.16	0.46
1:E:151:GLU:HA	1:E:154:LYS:HB3	1.98	0.46
1:E:255:ALA:O	1:E:256:ASP:C	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:GLU:HG2	1:A:178:GLY:H	1.80	0.46
1:B:158:ASP:C	1:B:160:LEU:H	2.24	0.46
1:B:230:THR:HB	1:B:302:GLN:OE1	2.15	0.46
1:C:55:VAL:O	1:C:56:TYR:C	2.58	0.46
1:C:181:ILE:HB	1:C:182:PHE:CD2	2.51	0.46
1:C:366:THR:C	1:C:368:ALA:H	2.23	0.46
1:A:37:GLU:HB2	1:A:108:VAL:HG21	1.98	0.46
1:A:78:LYS:HE2	1:A:78:LYS:HB2	1.76	0.46
1:B:55:VAL:O	1:B:56:TYR:C	2.57	0.46
1:C:14:ILE:HD12	1:D:259:VAL:HG22	1.98	0.46
1:C:45:THR:O	1:C:46:LYS:HD3	2.15	0.46
1:C:382:PHE:O	1:C:383:GLU:C	2.59	0.46
1:D:45:THR:O	1:D:46:LYS:HD3	2.15	0.46
1:D:365:THR:HG23	1:D:366:THR:H	1.81	0.46
1:E:37:GLU:CB	1:E:108:VAL:HG11	2.40	0.46
1:E:105:PHE:C	1:E:107:LEU:N	2.67	0.46
1:E:226:ALA:HB2	2:R:40:C:H5'	1.98	0.46
1:A:153:ARG:CZ	1:A:176:PRO:HA	2.46	0.46
1:A:253:GLU:OE2	1:A:253:GLU:N	2.44	0.46
1:B:68:HIS:CE1	1:B:118:PRO:HD2	2.51	0.46
1:B:147:THR:CG2	1:B:152:TYR:HB3	2.46	0.46
1:C:41:TYR:CE1	1:C:110:LEU:HD12	2.47	0.46
1:C:107:LEU:HD23	1:C:274:TYR:HE2	1.80	0.46
1:D:262:MET:HA	1:D:262:MET:CE	2.36	0.46
1:E:258:MET:HE3	1:E:262:MET:HG3	1.96	0.46
1:C:226:ALA:HB3	1:C:291:SER:HB3	1.98	0.46
1:D:81:ARG:HB2	1:D:208:HIS:NE2	2.31	0.46
1:D:158:ASP:C	1:D:160:LEU:H	2.24	0.46
1:A:55:VAL:HG12	1:A:64:VAL:HG21	1.97	0.46
1:A:65:SER:HB3	1:A:68:HIS:ND1	2.31	0.46
1:A:107:LEU:HD23	1:A:274:TYR:HE2	1.81	0.46
1:A:401:VAL:HG21	1:A:420:PHE:HB2	1.96	0.46
1:B:31:TYR:C	1:B:33:ARG:N	2.74	0.46
1:B:408:ARG:HD3	2:R:24:C:C4	2.51	0.46
1:C:149:MET:C	1:C:152:TYR:CZ	2.94	0.46
1:D:144:VAL:O	1:D:147:THR:HG22	2.15	0.46
1:D:258:MET:HE3	1:D:262:MET:HG3	1.98	0.46
1:E:148:GLN:O	1:E:152:TYR:CE2	2.68	0.46
1:E:382:PHE:CD2	1:E:387:ARG:HA	2.50	0.46
2:R:9:C:C6	2:R:10:C:C5	3.04	0.46
1:A:151:GLU:CD	2:R:33:C:H4'	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:CE1	1:B:122:SER:HB2	2.51	0.45
1:B:203:HIS:HD2	1:B:272:ASP:OD1	1.98	0.45
1:B:401:VAL:HG21	1:B:420:PHE:HB2	1.96	0.45
1:D:37:GLU:HB2	1:D:108:VAL:HG21	1.98	0.45
1:D:181:ILE:HB	1:D:182:PHE:CD2	2.51	0.45
1:D:283:LEU:N	1:D:283:LEU:HD23	2.30	0.45
1:E:147:THR:HG21	1:E:152:TYR:HA	1.97	0.45
1:A:54:TYR:CD1	1:A:118:PRO:HB2	2.50	0.45
1:B:107:LEU:HD23	1:B:274:TYR:HE2	1.80	0.45
1:C:73:LEU:O	1:C:74:TYR:C	2.59	0.45
1:C:119:ASP:OD1	1:C:119:ASP:N	2.50	0.45
1:C:177:GLU:HG2	1:C:178:GLY:H	1.81	0.45
1:D:149:MET:C	1:D:152:TYR:CZ	2.94	0.45
1:E:172:GLU:HB3	1:E:173:PRO:HD3	1.98	0.45
1:A:258:MET:HE3	1:A:262:MET:HG3	1.99	0.45
1:B:151:GLU:HA	1:B:154:LYS:HB3	1.99	0.45
1:B:215:TYR:C	1:B:215:TYR:CD2	2.94	0.45
1:C:317:ARG:H	1:C:317:ARG:CD	2.30	0.45
1:D:42:ILE:HD12	1:D:74:TYR:CB	2.38	0.45
1:D:226:ALA:HB2	2:R:4:C:O5'	2.17	0.45
1:D:317:ARG:CZ	1:D:317:ARG:N	2.74	0.45
1:E:167:ILE:HG22	1:E:168:ASN:H	1.80	0.45
1:E:409:GLU:HA	1:E:414:LYS:HD2	1.99	0.45
1:A:55:VAL:O	1:A:56:TYR:C	2.57	0.45
1:B:153:ARG:NH1	1:B:176:PRO:O	2.47	0.45
1:B:317:ARG:NH2	2:R:23:C:C5'	2.59	0.45
1:C:70:ASN:HD22	1:C:70:ASN:H	1.65	0.45
1:C:81:ARG:CD	1:C:208:HIS:HE2	2.29	0.45
1:D:89:SER:O	1:D:90:SER:CB	2.64	0.45
1:D:409:GLU:HG3	1:D:414:LYS:HD3	1.97	0.45
1:E:328:THR:HG21	1:E:415:TYR:OH	2.16	0.45
1:A:283:LEU:N	1:A:283:LEU:HD23	2.32	0.45
1:B:385:GLN:HG2	1:B:390:THR:CG2	2.47	0.45
1:C:15:VAL:O	1:C:17:LYS:HG2	2.17	0.45
1:C:415:TYR:CD1	1:C:415:TYR:C	2.95	0.45
1:D:74:TYR:O	1:D:78:LYS:HD3	2.16	0.45
2:R:32:C:N4	2:R:34:C:C5	2.84	0.45
1:A:59:LEU:O	1:A:61:SER:O	2.34	0.45
1:C:3:VAL:O	1:C:4:THR:HB	2.15	0.45
1:D:141:LEU:HD22	1:D:182:PHE:CD1	2.52	0.45
1:D:172:GLU:HB3	1:D:173:PRO:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:TYR:HB3	1:E:266:GLN:HE22	1.82	0.45
1:E:29:ALA:C	1:E:31:TYR:N	2.75	0.45
1:A:31:TYR:C	1:A:33:ARG:N	2.74	0.45
1:B:41:TYR:CE1	1:B:110:LEU:HD12	2.50	0.45
1:C:150:PRO:HD3	1:C:152:TYR:OH	2.17	0.45
1:D:151:GLU:CD	1:D:155:LYS:HZ2	2.25	0.45
1:E:253:GLU:HA	1:E:256:ASP:HB2	1.98	0.45
1:A:313:ALA:O	1:A:412:ILE:HD11	2.17	0.45
1:B:8:ILE:HG13	1:B:8:ILE:O	2.17	0.45
1:B:79:ASP:HB2	1:B:81:ARG:NE	2.32	0.45
1:C:38:ILE:O	1:C:108:VAL:HB	2.16	0.45
1:D:54:TYR:CD1	1:D:118:PRO:HB2	2.52	0.45
1:D:196:ALA:HB3	1:D:281:PHE:CE1	2.52	0.45
1:E:79:ASP:CG	1:E:79:ASP:O	2.60	0.45
1:E:81:ARG:CD	1:E:208:HIS:HE2	2.29	0.45
1:A:22:GLU:HB3	1:B:206:LYS:NZ	2.32	0.45
1:A:382:PHE:CD2	1:A:387:ARG:HA	2.52	0.45
1:B:91:PHE:CE2	1:B:267:GLU:HG3	2.52	0.45
1:C:184:VAL:HG11	1:D:166:MET:N	2.32	0.45
1:C:275:MET:HB3	1:C:276:PRO:HD3	1.99	0.45
1:E:153:ARG:CZ	1:E:176:PRO:HA	2.47	0.45
1:E:240:MET:HE3	1:E:244:ASP:HB3	1.99	0.45
1:A:167:ILE:CG2	1:A:169:GLU:HG2	2.43	0.45
1:A:181:ILE:HB	1:A:182:PHE:CD2	2.52	0.45
1:A:241:SER:O	1:A:245:VAL:HG23	2.17	0.45
1:A:275:MET:HB3	1:A:276:PRO:HD3	1.98	0.45
1:C:31:TYR:C	1:C:33:ARG:N	2.74	0.45
1:E:150:PRO:HD3	1:E:152:TYR:OH	2.17	0.45
1:A:88:TRP:CD2	1:A:204:MET:HE3	2.52	0.44
1:A:144:VAL:O	1:A:147:THR:HG22	2.17	0.44
1:B:165:LYS:O	1:B:167:ILE:CD1	2.65	0.44
1:D:55:VAL:O	1:D:56:TYR:C	2.60	0.44
1:E:401:VAL:HG21	1:E:420:PHE:HB2	1.98	0.44
1:A:215:TYR:C	1:A:215:TYR:CD2	2.94	0.44
1:C:144:VAL:O	1:C:147:THR:HG22	2.17	0.44
1:D:73:LEU:O	1:D:74:TYR:C	2.60	0.44
1:D:397:ALA:O	1:D:401:VAL:HG22	2.17	0.44
1:E:22:GLU:O	1:E:23:ASP:C	2.59	0.44
1:E:168:ASN:O	1:E:169:GLU:HB2	2.17	0.44
1:E:223:LYS:O	1:E:224:ASP:HB2	2.16	0.44
1:A:184:VAL:HG13	1:B:165:LYS:HG3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ALA:HB2	1:E:91:PHE:HE2	1.81	0.44
1:A:45:THR:O	1:A:46:LYS:HD3	2.18	0.44
1:B:73:LEU:O	1:B:74:TYR:C	2.61	0.44
1:B:147:THR:HG21	1:B:152:TYR:HA	1.98	0.44
1:B:275:MET:HB3	1:B:276:PRO:HD3	1.99	0.44
1:C:81:ARG:HB2	1:C:208:HIS:NE2	2.32	0.44
1:C:208:HIS:CE1	1:C:210:CYS:HB2	2.52	0.44
1:E:45:THR:H	1:E:111:LYS:NZ	2.07	0.44
1:E:149:MET:HG3	2:R:42:C:C6	2.53	0.44
1:E:317:ARG:HH21	2:R:41:C:H5'	1.73	0.44
1:A:208:HIS:CE1	1:A:210:CYS:HB2	2.52	0.44
1:A:364:LEU:HD22	1:A:368:ALA:HB2	2.00	0.44
1:B:409:GLU:HG3	1:B:414:LYS:HD3	1.99	0.44
1:C:397:ALA:O	1:C:401:VAL:HG22	2.17	0.44
1:E:46:LYS:HD3	1:E:46:LYS:HA	1.70	0.44
1:E:158:ASP:C	1:E:160:LEU:H	2.23	0.44
1:A:147:THR:HG21	1:A:152:TYR:HA	1.99	0.44
1:A:172:GLU:HB3	1:A:173:PRO:HD3	1.99	0.44
1:A:376:VAL:HG13	1:B:354:LYS:CB	2.45	0.44
1:B:103:GLY:N	1:B:106:ASP:OD2	2.48	0.44
1:B:328:THR:HG21	1:B:415:TYR:OH	2.17	0.44
1:C:54:TYR:OH	1:C:120:GLY:N	2.50	0.44
1:C:123:ASP:C	1:C:125:SER:H	2.25	0.44
1:C:354:LYS:CE	1:C:356:THR:HA	2.38	0.44
1:D:14:ILE:HG23	1:D:16:PRO:HD3	1.99	0.44
1:D:91:PHE:CE2	1:D:267:GLU:HG3	2.51	0.44
1:E:45:THR:O	1:E:46:LYS:HD3	2.18	0.44
1:E:53:GLY:O	1:E:54:TYR:C	2.59	0.44
1:E:123:ASP:C	1:E:125:SER:H	2.25	0.44
1:A:18:LEU:CD1	1:B:232:GLY:HA2	2.48	0.44
1:A:259:VAL:O	1:A:260:GLN:C	2.60	0.44
1:B:177:GLU:HG2	1:B:178:GLY:H	1.81	0.44
1:C:55:VAL:HG12	1:C:64:VAL:HG21	1.99	0.44
1:C:249:ILE:HD13	1:C:254:VAL:HG12	1.99	0.44
1:D:136:LEU:C	1:D:136:LEU:CD2	2.91	0.44
1:E:365:THR:HG23	1:E:366:THR:H	1.83	0.44
1:A:150:PRO:N	1:A:152:TYR:CZ	2.86	0.44
1:B:153:ARG:HH12	1:B:177:GLU:HB2	1.83	0.44
1:C:90:SER:O	1:C:91:PHE:HB2	2.18	0.44
1:C:253:GLU:OE2	1:C:253:GLU:N	2.44	0.44
1:D:113:LEU:N	1:D:113:LEU:HD23	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:ILE:H	1:D:181:ILE:CD1	2.26	0.44
1:E:196:ALA:HB3	1:E:281:PHE:CE1	2.53	0.44
1:A:151:GLU:HA	1:A:154:LYS:HB3	2.00	0.44
1:A:255:ALA:O	1:A:256:ASP:C	2.60	0.44
1:B:144:VAL:O	1:B:147:THR:HG22	2.17	0.44
1:B:181:ILE:HB	1:B:182:PHE:CD2	2.53	0.44
1:C:7:ARG:NH2	1:D:256:ASP:OD2	2.51	0.44
1:C:151:GLU:HA	1:C:154:LYS:HB3	2.00	0.44
1:D:107:LEU:HD23	1:D:274:TYR:HE2	1.83	0.44
1:D:163:GLN:N	1:D:163:GLN:CD	2.76	0.44
1:E:79:ASP:HB2	1:E:81:ARG:NE	2.32	0.44
1:E:81:ARG:HB2	1:E:208:HIS:NE2	2.33	0.44
2:R:9:C:H2'	2:R:10:C:O4'	2.17	0.44
1:A:78:LYS:O	1:A:80:ILE:HD12	2.18	0.43
1:B:141:LEU:HD22	1:B:182:PHE:CE1	2.53	0.43
1:B:342:ALA:HB1	1:B:344:LEU:HD23	1.99	0.43
1:D:22:GLU:O	1:D:23:ASP:C	2.61	0.43
1:D:54:TYR:CE1	1:D:122:SER:HB2	2.53	0.43
1:D:54:TYR:OH	1:D:120:GLY:N	2.50	0.43
1:E:68:HIS:CE1	1:E:118:PRO:HD2	2.53	0.43
1:A:409:GLU:HA	1:A:414:LYS:HD2	2.00	0.43
1:B:349:CYS:SG	1:E:8:ILE:CG2	3.02	0.43
1:E:141:LEU:HD22	1:E:182:PHE:CD1	2.53	0.43
1:E:149:MET:C	1:E:152:TYR:CZ	2.96	0.43
1:E:151:GLU:HG2	1:E:155:LYS:HD3	1.99	0.43
1:B:65:SER:HB3	1:B:68:HIS:ND1	2.33	0.43
1:C:18:LEU:CD1	1:D:232:GLY:HA2	2.49	0.43
1:C:79:ASP:CG	1:C:79:ASP:O	2.60	0.43
1:C:228:LEU:HD22	1:C:228:LEU:O	2.18	0.43
1:D:43:ASN:OD1	1:D:112:ALA:HB3	2.18	0.43
1:D:323:GLU:O	1:D:327:LEU:HD22	2.18	0.43
1:E:149:MET:O	1:E:152:TYR:CD2	2.71	0.43
1:E:410:LYS:HZ1	2:R:40:C:H42	1.65	0.43
2:R:39:C:H5'	2:R:40:C:OP2	2.19	0.43
1:B:170:GLN:HE21	1:B:170:GLN:HB3	1.59	0.43
1:B:303:LEU:CD2	1:B:328:THR:HA	2.48	0.43
1:C:28:PRO:O	1:C:29:ALA:C	2.62	0.43
1:D:153:ARG:NH2	1:D:176:PRO:HA	2.33	0.43
1:E:199:ASP:OD1	1:E:217:THR:HG23	2.18	0.43
1:E:342:ALA:HB1	1:E:344:LEU:HD23	2.00	0.43
2:R:40:C:O2	2:R:40:C:C2'	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:THR:O	1:B:46:LYS:HD3	2.18	0.43
1:B:376:VAL:HG13	1:C:354:LYS:CA	2.48	0.43
1:B:383:GLU:CG	1:C:354:LYS:HE2	2.46	0.43
1:A:158:ASP:C	1:A:160:LEU:H	2.27	0.43
1:A:343:ASP:HB2	1:A:344:LEU:H	1.68	0.43
1:B:78:LYS:O	1:B:80:ILE:N	2.52	0.43
1:B:134:LEU:N	1:B:135:PRO:CD	2.82	0.43
1:B:316:ALA:HA	1:B:317:ARG:CZ	2.47	0.43
1:C:247:THR:HA	1:D:348:PHE:HB2	2.01	0.43
1:D:4:THR:HG23	1:D:4:THR:O	2.18	0.43
1:D:149:MET:O	1:D:152:TYR:CD2	2.72	0.43
1:D:151:GLU:HA	1:D:154:LYS:HB3	2.01	0.43
2:R:9:C:C5	2:R:10:C:C5	3.06	0.43
1:A:79:ASP:C	1:A:81:ARG:N	2.77	0.43
1:A:167:ILE:O	1:A:169:GLU:OE1	2.37	0.43
1:A:364:LEU:O	1:A:366:THR:N	2.52	0.43
1:B:149:MET:O	1:B:152:TYR:CG	2.71	0.43
1:B:171:PHE:CZ	1:B:173:PRO:CG	3.00	0.43
1:C:136:LEU:CD2	1:C:163:GLN:HE21	2.25	0.43
1:C:230:THR:HB	1:C:302:GLN:OE1	2.19	0.43
1:D:164:CYS:HA	1:D:168:ASN:HA	2.00	0.43
1:B:19:PRO:CG	1:C:228:LEU:CD1	2.96	0.43
1:B:88:TRP:CD2	1:B:204:MET:HE3	2.54	0.43
1:B:259:VAL:O	1:B:260:GLN:C	2.61	0.43
1:C:214:ARG:O	1:C:215:TYR:C	2.62	0.43
1:C:238:THR:C	1:C:240:MET:N	2.76	0.43
1:D:233:HIS:HB2	1:D:312:ARG:NH1	2.33	0.43
1:D:238:THR:C	1:D:240:MET:N	2.76	0.43
1:E:230:THR:HB	1:E:302:GLN:OE1	2.18	0.43
1:A:54:TYR:OH	1:A:120:GLY:N	2.52	0.43
1:B:136:LEU:HD23	1:B:136:LEU:O	2.19	0.43
1:B:228:LEU:O	1:B:228:LEU:HD22	2.19	0.43
1:C:54:TYR:CE1	1:C:122:SER:HB2	2.53	0.43
1:C:79:ASP:HB2	1:C:81:ARG:NE	2.34	0.43
1:D:342:ALA:HB1	1:D:344:LEU:HD23	2.00	0.43
1:A:112:ALA:HB1	1:A:113:LEU:HD23	1.99	0.43
1:B:172:GLU:HB3	1:B:173:PRO:HD3	2.00	0.43
1:D:150:PRO:HD3	1:D:152:TYR:OH	2.19	0.43
1:E:382:PHE:O	1:E:383:GLU:C	2.62	0.43
2:R:10:C:C5'	2:R:11:C:OP2	2.67	0.43
1:A:385:GLN:HG2	1:A:390:THR:CG2	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ARG:HD2	1:D:208:HIS:NE2	2.34	0.42
1:D:409:GLU:HA	1:D:414:LYS:HD2	2.01	0.42
1:D:421:ASP:O	1:D:422:LYS:HB3	2.19	0.42
1:E:87:ASP:O	1:E:88:TRP:HB2	2.18	0.42
1:E:164:CYS:O	1:E:168:ASN:CG	2.62	0.42
1:E:165:LYS:HB2	1:E:165:LYS:HZ3	1.83	0.42
1:A:79:ASP:O	1:A:79:ASP:CG	2.61	0.42
1:A:91:PHE:CE2	1:A:267:GLU:HG3	2.54	0.42
1:C:22:GLU:O	1:C:23:ASP:C	2.62	0.42
1:D:255:ALA:O	1:D:259:VAL:HG23	2.20	0.42
1:D:259:VAL:O	1:D:260:GLN:C	2.61	0.42
1:E:90:SER:O	1:E:91:PHE:HB2	2.18	0.42
1:A:55:VAL:HG12	1:A:64:VAL:CG2	2.49	0.42
1:A:214:ARG:O	1:A:215:TYR:C	2.60	0.42
1:B:4:THR:HG23	1:B:4:THR:O	2.20	0.42
1:B:55:VAL:HG12	1:B:64:VAL:HG21	2.00	0.42
1:C:38:ILE:CD1	1:C:107:LEU:O	2.67	0.42
1:C:165:LYS:CB	1:C:165:LYS:HZ3	2.31	0.42
1:C:241:SER:OG	1:C:243:GLU:HG2	2.19	0.42
1:D:202:PHE:CG	1:D:211:ALA:HA	2.54	0.42
1:D:356:THR:CG2	1:D:357:PRO:HD3	2.35	0.42
1:D:382:PHE:O	1:D:383:GLU:C	2.61	0.42
1:D:412:ILE:HD12	1:D:413:GLY:N	2.34	0.42
1:E:89:SER:O	1:E:90:SER:CB	2.64	0.42
1:A:54:TYR:CE1	1:A:122:SER:HB2	2.54	0.42
1:A:68:HIS:CE1	1:A:118:PRO:HD2	2.55	0.42
1:A:123:ASP:C	1:A:125:SER:H	2.26	0.42
1:A:366:THR:C	1:A:368:ALA:H	2.27	0.42
1:B:57:GLN:HE21	1:B:60:LYS:NZ	2.18	0.42
1:C:147:THR:HG21	1:C:152:TYR:HA	2.00	0.42
1:D:79:ASP:CG	1:D:79:ASP:O	2.62	0.42
1:D:79:ASP:HB2	1:D:81:ARG:NE	2.34	0.42
1:E:356:THR:CG2	1:E:357:PRO:HD3	2.34	0.42
1:A:78:LYS:O	1:A:80:ILE:N	2.53	0.42
1:A:103:GLY:N	1:A:106:ASP:OD2	2.49	0.42
1:A:415:TYR:CD1	1:A:415:TYR:C	2.97	0.42
1:B:382:PHE:O	1:B:383:GLU:C	2.63	0.42
1:C:8:ILE:O	1:C:8:ILE:HG13	2.19	0.42
1:C:105:PHE:O	1:C:107:LEU:N	2.52	0.42
1:C:112:ALA:HB1	1:C:113:LEU:HD23	2.01	0.42
1:E:363:GLY:C	1:E:365:THR:N	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:ALA:HB3	1:B:281:PHE:CE1	2.55	0.42
1:C:170:GLN:HB3	1:C:171:PHE:H	1.42	0.42
1:D:55:VAL:HG12	1:D:64:VAL:CG2	2.50	0.42
1:D:224:ASP:HA	2:R:4:C:OP1	2.19	0.42
1:D:226:ALA:HB3	1:D:291:SER:HB3	2.02	0.42
1:E:54:TYR:CE1	1:E:122:SER:HB2	2.54	0.42
1:A:31:TYR:CD1	1:A:32:PHE:N	2.88	0.42
1:A:295:PRO:HB2	1:A:322:ILE:HG21	2.02	0.42
1:B:79:ASP:CG	1:B:79:ASP:O	2.62	0.42
1:C:409:GLU:HA	1:C:414:LYS:HD2	2.02	0.42
1:D:90:SER:O	1:D:91:PHE:HB2	2.20	0.42
1:D:208:HIS:CE1	1:D:210:CYS:HB2	2.54	0.42
1:D:228:LEU:O	1:D:228:LEU:HD22	2.19	0.42
1:A:74:TYR:O	1:A:78:LYS:HD3	2.19	0.42
1:A:81:ARG:HB2	1:A:208:HIS:NE2	2.34	0.42
1:B:66:ILE:HD13	1:B:185:TRP:CD1	2.54	0.42
1:B:369:PRO:HB3	1:B:381:TRP:CZ2	2.55	0.42
1:C:255:ALA:O	1:C:259:VAL:HG23	2.20	0.42
1:D:263:LEU:HD12	1:D:263:LEU:HA	1.91	0.42
1:D:399:ARG:HB3	1:D:399:ARG:NH1	2.35	0.42
1:E:54:TYR:CD1	1:E:118:PRO:HB2	2.52	0.42
1:E:119:ASP:OD1	1:E:119:ASP:N	2.53	0.42
1:B:231:PHE:HB2	1:B:297:PHE:CZ	2.54	0.42
1:B:382:PHE:CD2	1:B:387:ARG:HA	2.55	0.42
1:C:103:GLY:N	1:C:106:ASP:OD2	2.47	0.42
1:D:65:SER:HB3	1:D:68:HIS:ND1	2.34	0.42
1:D:180:ASP:OD2	1:D:180:ASP:O	2.38	0.42
1:E:399:ARG:NH1	1:E:399:ARG:HB3	2.35	0.42
1:E:415:TYR:CD1	1:E:415:TYR:C	2.98	0.42
1:B:18:LEU:HD11	1:C:232:GLY:HA2	2.01	0.42
1:B:151:GLU:CD	2:R:24:C:H4'	2.45	0.42
1:B:153:ARG:CZ	1:B:176:PRO:HA	2.50	0.42
1:B:237:ILE:CD1	1:B:310:SER:HB2	2.50	0.42
1:C:158:ASP:C	1:C:160:LEU:H	2.27	0.42
1:D:31:TYR:C	1:D:33:ARG:N	2.75	0.42
1:D:53:GLY:O	1:D:54:TYR:C	2.62	0.42
1:E:167:ILE:O	1:E:168:ASN:HB2	2.18	0.42
1:A:317:ARG:CD	2:R:31:C:H2'	2.48	0.41
1:C:65:SER:HB3	1:C:68:HIS:ND1	2.34	0.41
1:C:136:LEU:C	1:C:136:LEU:CD2	2.92	0.41
1:D:151:GLU:CD	1:D:155:LYS:NZ	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:313:ALA:O	1:D:412:ILE:HD11	2.20	0.41
1:E:249:ILE:HD13	1:E:254:VAL:HG12	2.02	0.41
1:E:397:ALA:O	1:E:401:VAL:HG22	2.20	0.41
1:A:37:GLU:CB	1:A:108:VAL:HG11	2.44	0.41
1:B:74:TYR:O	1:B:78:LYS:HD3	2.20	0.41
1:B:123:ASP:C	1:B:125:SER:H	2.27	0.41
1:C:42:ILE:O	1:C:43:ASN:O	2.38	0.41
1:C:238:THR:O	1:C:240:MET:N	2.53	0.41
1:C:298:HIS:NE2	1:C:317:ARG:NH1	2.66	0.41
1:D:195:VAL:CG2	1:D:196:ALA:N	2.82	0.41
1:D:397:ALA:HB1	1:D:420:PHE:CG	2.55	0.41
1:E:190:ASN:O	1:E:194:ILE:HG13	2.20	0.41
1:E:385:GLN:HG2	1:E:390:THR:CG2	2.51	0.41
1:A:43:ASN:OD1	1:A:112:ALA:HB3	2.20	0.41
1:B:79:ASP:C	1:B:81:ARG:N	2.78	0.41
1:B:171:PHE:CE2	1:B:173:PRO:C	2.98	0.41
1:C:18:LEU:HD12	1:D:232:GLY:CA	2.50	0.41
1:D:84:LEU:C	1:D:86:LYS:H	2.29	0.41
1:E:93:ILE:N	1:E:93:ILE:HD12	2.35	0.41
1:E:160:LEU:HA	1:E:163:GLN:OE1	2.20	0.41
1:E:369:PRO:HA	1:E:370:PRO:HD3	1.81	0.41
2:R:25:C:H2'	2:R:26:C:H6	1.82	0.41
1:A:22:GLU:O	1:A:23:ASP:C	2.63	0.41
1:A:240:MET:HE3	1:A:244:ASP:CB	2.50	0.41
1:A:296:ALA:O	1:A:297:PHE:C	2.60	0.41
1:A:356:THR:CG2	1:A:357:PRO:HD3	2.36	0.41
1:B:38:ILE:O	1:B:108:VAL:HB	2.21	0.41
1:B:90:SER:O	1:B:91:PHE:HB2	2.20	0.41
1:B:105:PHE:O	1:B:107:LEU:N	2.51	0.41
1:C:88:TRP:CD2	1:C:204:MET:HE3	2.56	0.41
1:C:99:GLY:O	1:C:100:ASP:C	2.63	0.41
1:C:149:MET:O	1:C:152:TYR:CD2	2.74	0.41
1:C:249:ILE:HD12	1:D:348:PHE:HE1	1.85	0.41
1:D:275:MET:HB3	1:D:276:PRO:HD3	2.03	0.41
1:D:317:ARG:H	1:D:317:ARG:CD	2.34	0.41
1:E:4:THR:O	1:E:4:THR:HG23	2.21	0.41
2:R:1:C:H2'	2:R:2:C:O4'	2.20	0.41
1:A:251:ASN:O	1:A:252:ARG:C	2.64	0.41
1:A:369:PRO:HA	1:A:370:PRO:HD3	1.80	0.41
1:B:81:ARG:HD2	1:B:208:HIS:NE2	2.33	0.41
1:B:136:LEU:C	1:B:136:LEU:CD2	2.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLU:CD	1:B:155:LYS:HZ2	2.28	0.41
1:B:160:LEU:HA	1:B:163:GLN:OE1	2.21	0.41
1:B:181:ILE:H	1:B:181:ILE:CD1	2.24	0.41
1:B:263:LEU:HD12	1:B:263:LEU:HA	1.88	0.41
1:C:107:LEU:C	1:C:108:VAL:HG23	2.46	0.41
1:C:200:MET:HB2	1:C:277:TYR:CE2	2.56	0.41
1:D:88:TRP:CD2	1:D:204:MET:HE3	2.56	0.41
1:E:38:ILE:CD1	1:E:107:LEU:O	2.69	0.41
1:A:151:GLU:HG2	1:A:155:LYS:HD3	2.02	0.41
1:A:160:LEU:HA	1:A:163:GLN:OE1	2.20	0.41
1:B:195:VAL:CG2	1:B:196:ALA:N	2.83	0.41
1:B:253:GLU:CD	1:B:253:GLU:N	2.71	0.41
1:B:397:ALA:HB1	1:B:420:PHE:CG	2.55	0.41
1:C:296:ALA:O	1:C:297:PHE:C	2.61	0.41
1:D:153:ARG:HH12	1:D:177:GLU:HB2	1.86	0.41
1:D:248:TRP:O	1:D:250:LEU:HG	2.20	0.41
1:D:253:GLU:CD	1:D:253:GLU:N	2.71	0.41
1:D:398:LYS:O	1:D:402:MET:HG2	2.20	0.41
1:E:31:TYR:C	1:E:33:ARG:N	2.78	0.41
1:E:240:MET:HE3	1:E:244:ASP:CB	2.50	0.41
1:A:380:GLY:CA	1:B:354:LYS:HZ3	2.28	0.41
1:B:233:HIS:HB2	1:B:312:ARG:NH1	2.35	0.41
1:C:68:HIS:CE1	1:C:118:PRO:HD2	2.56	0.41
1:C:79:ASP:C	1:C:81:ARG:N	2.79	0.41
1:C:160:LEU:HA	1:C:163:GLN:OE1	2.21	0.41
1:D:151:GLU:CD	2:R:6:C:H4'	2.45	0.41
1:D:177:GLU:HG2	1:D:178:GLY:H	1.84	0.41
1:E:78:LYS:HB2	1:E:78:LYS:HE2	1.73	0.41
1:E:195:VAL:CG2	1:E:196:ALA:N	2.84	0.41
1:B:150:PRO:N	1:B:152:TYR:CE1	2.89	0.41
1:C:18:LEU:HD12	1:D:232:GLY:HA2	2.02	0.41
1:C:54:TYR:CD1	1:C:118:PRO:HB2	2.55	0.41
1:C:81:ARG:HD2	1:C:208:HIS:NE2	2.34	0.41
1:C:91:PHE:CE2	1:C:267:GLU:HG3	2.56	0.41
1:D:149:MET:O	1:D:152:TYR:CG	2.74	0.41
1:D:303:LEU:CD2	1:D:328:THR:HA	2.51	0.41
1:E:81:ARG:HD2	1:E:208:HIS:NE2	2.34	0.41
1:E:397:ALA:HB1	1:E:420:PHE:CG	2.56	0.41
1:A:107:LEU:C	1:A:108:VAL:HG23	2.46	0.41
1:A:163:GLN:CD	1:A:163:GLN:H	2.29	0.41
1:A:163:GLN:C	1:A:165:LYS:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ILE:C	1:A:220:SER:N	2.78	0.41
1:A:255:ALA:O	1:A:259:VAL:HG23	2.20	0.41
1:A:354:LYS:CE	1:A:356:THR:HA	2.40	0.41
1:C:86:LYS:HB3	1:C:87:ASP:H	1.59	0.41
1:C:134:LEU:HD22	1:C:134:LEU:HA	1.95	0.41
1:C:153:ARG:CZ	1:C:176:PRO:HA	2.51	0.41
1:C:202:PHE:CG	1:C:211:ALA:HA	2.56	0.41
1:C:208:HIS:CE1	1:C:209:GLU:HG3	2.56	0.41
1:D:28:PRO:O	1:D:31:TYR:HB3	2.21	0.41
1:D:78:LYS:HE2	1:D:78:LYS:HB2	1.74	0.41
1:D:79:ASP:C	1:D:81:ARG:N	2.79	0.41
1:D:112:ALA:HB1	1:D:113:LEU:HD23	2.02	0.41
1:D:163:GLN:C	1:D:165:LYS:N	2.77	0.41
1:E:208:HIS:CE1	1:E:210:CYS:HB2	2.56	0.41
1:E:238:THR:C	1:E:240:MET:N	2.79	0.41
1:E:295:PRO:HB2	1:E:322:ILE:HG21	2.03	0.41
1:A:81:ARG:HD2	1:A:208:HIS:NE2	2.35	0.41
1:A:361:THR:HB	1:A:362:GLY:H	1.77	0.41
1:B:382:PHE:CE1	1:B:393:MET:HE1	2.55	0.41
1:D:134:LEU:HD22	1:D:134:LEU:HA	1.96	0.41
1:D:296:ALA:O	1:D:297:PHE:C	2.64	0.41
1:E:74:TYR:CD1	1:E:74:TYR:C	2.99	0.41
1:A:303:LEU:CD2	1:A:328:THR:HA	2.51	0.40
1:B:14:ILE:CD1	1:C:259:VAL:HA	2.51	0.40
1:C:150:PRO:N	1:C:152:TYR:CZ	2.89	0.40
1:D:31:TYR:CD1	1:D:32:PHE:N	2.88	0.40
1:E:38:ILE:O	1:E:108:VAL:HB	2.20	0.40
1:A:56:TYR:C	1:A:56:TYR:CD1	2.99	0.40
1:A:382:PHE:CE1	1:A:393:MET:HE1	2.51	0.40
1:A:397:ALA:HB1	1:A:420:PHE:CG	2.57	0.40
1:B:22:GLU:O	1:B:23:ASP:C	2.65	0.40
1:B:89:SER:O	1:B:90:SER:CB	2.65	0.40
1:C:58:GLY:O	1:C:63:ASN:O	2.39	0.40
1:C:163:GLN:C	1:C:165:LYS:N	2.79	0.40
1:C:382:PHE:CD2	1:C:387:ARG:HA	2.56	0.40
1:C:387:ARG:CZ	1:C:387:ARG:HB3	2.51	0.40
1:D:81:ARG:CB	1:D:208:HIS:NE2	2.84	0.40
1:D:214:ARG:O	1:D:215:TYR:C	2.63	0.40
1:A:38:ILE:O	1:A:108:VAL:HB	2.20	0.40
1:A:308:LEU:HD12	1:A:308:LEU:HA	1.86	0.40
1:B:14:ILE:HD12	1:C:259:VAL:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:TYR:CD1	1:B:32:PHE:N	2.89	0.40
1:B:249:ILE:HD13	1:B:254:VAL:HG12	2.02	0.40
1:C:151:GLU:HG2	1:C:155:LYS:HD3	2.03	0.40
1:D:66:ILE:HD13	1:D:185:TRP:CD1	2.56	0.40
1:E:182:PHE:CD2	1:E:182:PHE:N	2.90	0.40
1:E:202:PHE:CG	1:E:211:ALA:HA	2.56	0.40
1:A:86:LYS:HB3	1:A:87:ASP:H	1.58	0.40
1:A:170:GLN:CD	1:A:170:GLN:N	2.79	0.40
1:A:202:PHE:CG	1:A:211:ALA:HA	2.56	0.40
1:A:369:PRO:HB3	1:A:381:TRP:CZ2	2.56	0.40
1:A:421:ASP:O	1:A:422:LYS:HB3	2.20	0.40
1:C:88:TRP:CZ3	1:C:204:MET:HG2	2.57	0.40
1:C:93:ILE:N	1:C:93:ILE:HD12	2.37	0.40
1:E:66:ILE:HD13	1:E:185:TRP:CD1	2.57	0.40
1:E:153:ARG:HH12	1:E:177:GLU:HB2	1.87	0.40
1:E:215:TYR:CD1	2:R:45:C:H5"	2.56	0.40
1:E:382:PHE:CE1	1:E:393:MET:HE1	2.56	0.40
1:A:38:ILE:CD1	1:A:107:LEU:O	2.70	0.40
1:A:195:VAL:CG2	1:A:196:ALA:N	2.83	0.40
1:A:354:LYS:NZ	1:E:380:GLY:HA2	2.37	0.40
1:A:397:ALA:O	1:A:401:VAL:HG22	2.21	0.40
1:B:119:ASP:OD1	1:B:119:ASP:N	2.55	0.40
1:B:151:GLU:HG2	1:B:155:LYS:HD3	2.03	0.40
1:C:37:GLU:CB	1:C:108:VAL:HG11	2.43	0.40
1:C:53:GLY:O	1:C:54:TYR:C	2.63	0.40
1:C:56:TYR:C	1:C:56:TYR:CD1	2.99	0.40
1:C:74:TYR:O	1:C:78:LYS:HD3	2.20	0.40
1:C:191:TYR:O	1:C:192:THR:C	2.64	0.40
1:C:253:GLU:CD	1:C:253:GLU:N	2.77	0.40
1:D:309:ARG:HH11	1:D:309:ARG:HD3	1.78	0.40
1:E:79:ASP:C	1:E:81:ARG:N	2.78	0.40
1:E:263:LEU:HD12	1:E:263:LEU:HA	1.91	0.40
1:E:410:LYS:NZ	2:R:40:C:N4	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	306 (73%)	82 (20%)	31 (7%)	1	5
1	B	411/421 (98%)	302 (74%)	73 (18%)	36 (9%)	0	3
1	C	409/421 (97%)	296 (72%)	73 (18%)	40 (10%)	0	3
1	D	412/421 (98%)	303 (74%)	75 (18%)	34 (8%)	0	4
1	E	419/421 (100%)	303 (72%)	76 (18%)	40 (10%)	0	3
All	All	2070/2105 (98%)	1510 (73%)	379 (18%)	181 (9%)	0	4

All (181) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	44	THR
1	A	60	LYS
1	A	61	SER
1	A	79	ASP
1	A	90	SER
1	A	131	ASP
1	A	150	PRO
1	B	43	ASN
1	B	60	LYS
1	B	61	SER
1	B	79	ASP
1	B	90	SER
1	B	131	ASP
1	B	150	PRO
1	B	168	ASN
1	B	169	GLU
1	C	43	ASN
1	C	60	LYS
1	C	79	ASP
1	C	90	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	131	ASP
1	C	150	PRO
1	C	170	GLN
1	D	43	ASN
1	D	44	THR
1	D	60	LYS
1	D	61	SER
1	D	79	ASP
1	D	90	SER
1	D	131	ASP
1	D	271	ALA
1	E	43	ASN
1	E	60	LYS
1	E	61	SER
1	E	79	ASP
1	E	90	SER
1	E	131	ASP
1	E	150	PRO
1	E	271	ALA
1	E	360	SER
1	E	365	THR
1	A	4	THR
1	A	30	ASP
1	A	84	LEU
1	A	100	ASP
1	A	172	GLU
1	A	173	PRO
1	A	271	ALA
1	B	4	THR
1	B	30	ASP
1	B	44	THR
1	B	84	LEU
1	B	100	ASP
1	B	170	GLN
1	B	173	PRO
1	B	176	PRO
1	B	208	HIS
1	B	271	ALA
1	B	344	LEU
1	C	4	THR
1	C	30	ASP
1	C	44	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	61	SER
1	C	100	ASP
1	C	172	GLU
1	C	173	PRO
1	C	176	PRO
1	C	208	HIS
1	C	271	ALA
1	C	343	ASP
1	D	4	THR
1	D	30	ASP
1	D	84	LEU
1	D	100	ASP
1	D	150	PRO
1	D	171	PHE
1	D	172	GLU
1	D	173	PRO
1	D	176	PRO
1	D	208	HIS
1	E	4	THR
1	E	44	THR
1	E	84	LEU
1	E	100	ASP
1	E	164	CYS
1	E	168	ASN
1	E	172	GLU
1	E	173	PRO
1	E	208	HIS
1	A	28	PRO
1	A	81	ARG
1	A	112	ALA
1	A	117	LEU
1	A	129	ALA
1	A	176	PRO
1	A	177	GLU
1	A	208	HIS
1	A	343	ASP
1	A	344	LEU
1	B	63	ASN
1	B	81	ARG
1	B	112	ALA
1	B	117	LEU
1	B	172	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	177	GLU
1	C	28	PRO
1	C	81	ARG
1	C	84	LEU
1	C	112	ALA
1	C	117	LEU
1	C	168	ASN
1	C	177	GLU
1	C	345	ALA
1	D	81	ARG
1	D	112	ALA
1	D	117	LEU
1	D	177	GLU
1	D	344	LEU
1	E	28	PRO
1	E	30	ASP
1	E	81	ARG
1	E	88	TRP
1	E	112	ALA
1	E	117	LEU
1	E	129	ALA
1	E	171	PHE
1	E	176	PRO
1	E	177	GLU
1	E	343	ASP
1	E	344	LEU
1	B	343	ASP
1	C	108	VAL
1	C	167	ILE
1	C	344	LEU
1	D	28	PRO
1	D	108	VAL
1	D	206	LYS
1	D	343	ASP
1	A	23	ASP
1	A	88	TRP
1	A	108	VAL
1	A	123	ASP
1	B	23	ASP
1	B	28	PRO
1	B	88	TRP
1	B	108	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	123	ASP
1	C	23	ASP
1	C	88	TRP
1	C	129	ALA
1	C	206	LYS
1	C	228	LEU
1	D	23	ASP
1	D	63	ASN
1	D	88	TRP
1	D	123	ASP
1	D	167	ILE
1	E	23	ASP
1	E	108	VAL
1	E	123	ASP
1	E	363	GLY
1	E	364	LEU
1	A	206	LYS
1	B	239	GLY
1	C	63	ASN
1	C	123	ASP
1	C	174	LEU
1	D	106	ASP
1	E	174	LEU
1	C	239	GLY
1	B	219	VAL
1	B	16	PRO
1	C	16	PRO
1	C	219	VAL
1	D	219	VAL
1	A	16	PRO
1	B	19	PRO
1	E	167	ILE
1	E	219	VAL
1	E	16	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/362 (100%)	292 (81%)	70 (19%)	1	7
1	B	358/362 (99%)	287 (80%)	71 (20%)	1	6
1	C	356/362 (98%)	290 (82%)	66 (18%)	1	8
1	D	359/362 (99%)	291 (81%)	68 (19%)	1	7
1	E	362/362 (100%)	292 (81%)	70 (19%)	1	7
All	All	1797/1810 (99%)	1452 (81%)	345 (19%)	1	7

All (345) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	ILE
1	A	13	VAL
1	A	25	VAL
1	A	31	TYR
1	A	36	LYS
1	A	40	LEU
1	A	42	ILE
1	A	57	GLN
1	A	69	VAL
1	A	70	ASN
1	A	84	LEU
1	A	97	LYS
1	A	100	ASP
1	A	101	THR
1	A	107	LEU
1	A	117	LEU
1	A	119	ASP
1	A	123	ASP
1	A	126	ARG
1	A	134	LEU
1	A	148	GLN
1	A	152	TYR
1	A	153	ARG
1	A	156	LEU
1	A	160	LEU
1	A	162	ASN
1	A	165	LYS
1	A	169	GLU
1	A	170	GLN
1	A	172	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	174	LEU
1	A	175	VAL
1	A	180	ASP
1	A	181	ILE
1	A	187	ASN
1	A	195	VAL
1	A	209	GLU
1	A	217	THR
1	A	228	LEU
1	A	230	THR
1	A	237	ILE
1	A	241	SER
1	A	242	THR
1	A	243	GLU
1	A	252	ARG
1	A	253	GLU
1	A	268	ILE
1	A	291	SER
1	A	307	LEU
1	A	308	LEU
1	A	311	THR
1	A	317	ARG
1	A	325	THR
1	A	327	LEU
1	A	332	LEU
1	A	350	VAL
1	A	352	ASP
1	A	356	THR
1	A	358	ASP
1	A	359	ASP
1	A	361	THR
1	A	364	LEU
1	A	365	THR
1	A	379	LEU
1	A	384	ASP
1	A	385	GLN
1	A	405	GLN
1	A	410	LYS
1	A	414	LYS
1	B	3	VAL
1	B	8	ILE
1	B	13	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	18	LEU
1	B	25	VAL
1	B	31	TYR
1	B	36	LYS
1	B	40	LEU
1	B	42	ILE
1	B	57	GLN
1	B	69	VAL
1	B	70	ASN
1	B	80	ILE
1	B	84	LEU
1	B	97	LYS
1	B	100	ASP
1	B	101	THR
1	B	107	LEU
1	B	117	LEU
1	B	119	ASP
1	B	123	ASP
1	B	126	ARG
1	B	134	LEU
1	B	148	GLN
1	B	152	TYR
1	B	153	ARG
1	B	156	LEU
1	B	160	LEU
1	B	162	ASN
1	B	165	LYS
1	B	167	ILE
1	B	169	GLU
1	B	170	GLN
1	B	172	GLU
1	B	174	LEU
1	B	175	VAL
1	B	180	ASP
1	B	181	ILE
1	B	187	ASN
1	B	195	VAL
1	B	209	GLU
1	B	217	THR
1	B	228	LEU
1	B	230	THR
1	B	237	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	242	THR
1	B	243	GLU
1	B	252	ARG
1	B	253	GLU
1	B	268	ILE
1	B	291	SER
1	B	307	LEU
1	B	308	LEU
1	B	311	THR
1	B	317	ARG
1	B	325	THR
1	B	327	LEU
1	B	332	LEU
1	B	350	VAL
1	B	352	ASP
1	B	356	THR
1	B	358	ASP
1	B	365	THR
1	B	366	THR
1	B	376	VAL
1	B	379	LEU
1	B	384	ASP
1	B	385	GLN
1	B	405	GLN
1	B	410	LYS
1	B	414	LYS
1	C	3	VAL
1	C	8	ILE
1	C	13	VAL
1	C	25	VAL
1	C	31	TYR
1	C	40	LEU
1	C	57	GLN
1	C	69	VAL
1	C	70	ASN
1	C	84	LEU
1	C	97	LYS
1	C	100	ASP
1	C	101	THR
1	C	107	LEU
1	C	117	LEU
1	C	119	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	123	ASP
1	C	126	ARG
1	C	134	LEU
1	C	148	GLN
1	C	152	TYR
1	C	153	ARG
1	C	156	LEU
1	C	160	LEU
1	C	162	ASN
1	C	165	LYS
1	C	167	ILE
1	C	169	GLU
1	C	170	GLN
1	C	172	GLU
1	C	174	LEU
1	C	175	VAL
1	C	180	ASP
1	C	181	ILE
1	C	187	ASN
1	C	195	VAL
1	C	209	GLU
1	C	217	THR
1	C	228	LEU
1	C	230	THR
1	C	237	ILE
1	C	241	SER
1	C	242	THR
1	C	243	GLU
1	C	252	ARG
1	C	253	GLU
1	C	268	ILE
1	C	291	SER
1	C	307	LEU
1	C	308	LEU
1	C	311	THR
1	C	317	ARG
1	C	325	THR
1	C	327	LEU
1	C	332	LEU
1	C	350	VAL
1	C	352	ASP
1	C	356	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	366	THR
1	C	376	VAL
1	C	379	LEU
1	C	384	ASP
1	C	385	GLN
1	C	405	GLN
1	C	410	LYS
1	C	414	LYS
1	D	3	VAL
1	D	8	ILE
1	D	13	VAL
1	D	18	LEU
1	D	25	VAL
1	D	31	TYR
1	D	36	LYS
1	D	40	LEU
1	D	42	ILE
1	D	57	GLN
1	D	69	VAL
1	D	70	ASN
1	D	84	LEU
1	D	97	LYS
1	D	100	ASP
1	D	101	THR
1	D	108	VAL
1	D	117	LEU
1	D	119	ASP
1	D	123	ASP
1	D	126	ARG
1	D	134	LEU
1	D	148	GLN
1	D	152	TYR
1	D	153	ARG
1	D	156	LEU
1	D	160	LEU
1	D	162	ASN
1	D	165	LYS
1	D	167	ILE
1	D	169	GLU
1	D	172	GLU
1	D	174	LEU
1	D	175	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	180	ASP
1	D	181	ILE
1	D	187	ASN
1	D	193	LYS
1	D	195	VAL
1	D	209	GLU
1	D	217	THR
1	D	228	LEU
1	D	230	THR
1	D	242	THR
1	D	243	GLU
1	D	252	ARG
1	D	253	GLU
1	D	268	ILE
1	D	291	SER
1	D	307	LEU
1	D	308	LEU
1	D	311	THR
1	D	317	ARG
1	D	325	THR
1	D	327	LEU
1	D	332	LEU
1	D	350	VAL
1	D	352	ASP
1	D	356	THR
1	D	358	ASP
1	D	366	THR
1	D	376	VAL
1	D	379	LEU
1	D	384	ASP
1	D	385	GLN
1	D	405	GLN
1	D	410	LYS
1	D	414	LYS
1	E	3	VAL
1	E	8	ILE
1	E	13	VAL
1	E	18	LEU
1	E	25	VAL
1	E	31	TYR
1	E	36	LYS
1	E	40	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	42	ILE
1	E	57	GLN
1	E	69	VAL
1	E	70	ASN
1	E	80	ILE
1	E	84	LEU
1	E	97	LYS
1	E	100	ASP
1	E	101	THR
1	E	107	LEU
1	E	117	LEU
1	E	119	ASP
1	E	123	ASP
1	E	126	ARG
1	E	134	LEU
1	E	148	GLN
1	E	152	TYR
1	E	153	ARG
1	E	156	LEU
1	E	160	LEU
1	E	162	ASN
1	E	165	LYS
1	E	170	GLN
1	E	172	GLU
1	E	174	LEU
1	E	175	VAL
1	E	180	ASP
1	E	181	ILE
1	E	187	ASN
1	E	195	VAL
1	E	209	GLU
1	E	217	THR
1	E	228	LEU
1	E	230	THR
1	E	237	ILE
1	E	242	THR
1	E	243	GLU
1	E	252	ARG
1	E	253	GLU
1	E	268	ILE
1	E	291	SER
1	E	307	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	308	LEU
1	E	311	THR
1	E	317	ARG
1	E	325	THR
1	E	327	LEU
1	E	332	LEU
1	E	350	VAL
1	E	352	ASP
1	E	356	THR
1	E	358	ASP
1	E	359	ASP
1	E	365	THR
1	E	366	THR
1	E	376	VAL
1	E	379	LEU
1	E	384	ASP
1	E	385	GLN
1	E	405	GLN
1	E	410	LYS
1	E	414	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	57	GLN
1	A	70	ASN
1	A	170	GLN
1	A	187	ASN
1	A	190	ASN
1	A	203	HIS
1	A	251	ASN
1	A	260	GLN
1	A	266	GLN
1	A	347	GLN
1	A	386	ASN
1	A	395	GLN
1	B	11	ASN
1	B	57	GLN
1	B	70	ASN
1	B	170	GLN
1	B	190	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	203	HIS
1	B	251	ASN
1	B	260	GLN
1	B	266	GLN
1	B	347	GLN
1	B	386	ASN
1	B	395	GLN
1	C	11	ASN
1	C	57	GLN
1	C	70	ASN
1	C	162	ASN
1	C	170	GLN
1	C	187	ASN
1	C	203	HIS
1	C	260	GLN
1	C	266	GLN
1	C	353	ASN
1	C	386	ASN
1	C	395	GLN
1	D	11	ASN
1	D	57	GLN
1	D	70	ASN
1	D	162	ASN
1	D	168	ASN
1	D	190	ASN
1	D	203	HIS
1	D	251	ASN
1	D	266	GLN
1	D	347	GLN
1	D	353	ASN
1	D	386	ASN
1	D	395	GLN
1	E	11	ASN
1	E	57	GLN
1	E	70	ASN
1	E	187	ASN
1	E	203	HIS
1	E	260	GLN
1	E	266	GLN
1	E	347	GLN
1	E	353	ASN
1	E	395	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	44/45 (97%)	18 (40%)	2 (4%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	5	C
2	R	10	C
2	R	13	C
2	R	17	C
2	R	18	C
2	R	19	C
2	R	22	C
2	R	23	C
2	R	25	C
2	R	28	C
2	R	30	C
2	R	31	C
2	R	40	C
2	R	41	C
2	R	42	C
2	R	44	C
2	R	45	C

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	R	18	C
2	R	41	C

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

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

5.5 Carbohydrates ⓘ

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	17 (4%) 42 23	70, 102, 138, 158	0
1	B	415/421 (98%)	0.34	15 (3%) 46 26	71, 101, 137, 157	0
1	C	413/421 (98%)	0.33	17 (4%) 41 23	71, 101, 137, 158	0
1	D	416/421 (98%)	0.42	27 (6%) 25 13	71, 102, 137, 158	0
1	E	421/421 (100%)	0.30	14 (3%) 49 29	70, 102, 140, 163	0
2	R	45/45 (100%)	-0.20	0 100 100	97, 110, 120, 121	0
All	All	2131/2150 (99%)	0.33	90 (4%) 40 22	70, 102, 138, 163	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	SER	9.2
1	A	2	SER	7.2
1	A	356	THR	6.2
1	B	2	SER	6.1
1	A	353	ASN	6.0
1	A	216	GLY	5.6
1	C	2	SER	5.2
1	B	274	TYR	5.1
1	D	129	ALA	4.9
1	C	216	GLY	4.2
1	A	361	THR	4.1
1	E	216	GLY	3.6
1	D	43	ASN	3.5
1	C	215	TYR	3.5
1	A	180	ASP	3.5
1	A	142	TYR	3.4
1	C	107	LEU	3.4
1	B	3	VAL	3.4
1	C	172	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	172	GLU	3.3
1	D	346	GLN	3.2
1	B	129	ALA	3.2
1	E	172	GLU	3.2
1	C	353	ASN	3.2
1	B	42	ILE	3.2
1	B	172	GLU	3.1
1	B	353	ASN	3.0
1	B	68	HIS	3.0
1	A	129	ALA	2.9
1	D	107	LEU	2.9
1	D	180	ASP	2.9
1	E	112	ALA	2.9
1	A	158	ASP	2.8
1	D	274	TYR	2.8
1	D	116	VAL	2.7
1	A	350	VAL	2.7
1	A	362	GLY	2.7
1	D	121	VAL	2.7
1	C	346	GLN	2.7
1	D	353	ASN	2.7
1	C	62	GLY	2.7
1	C	142	TYR	2.7
1	A	3	VAL	2.6
1	A	181	ILE	2.6
1	D	158	ASP	2.6
1	B	215	TYR	2.6
1	D	176	PRO	2.6
1	E	355	TYR	2.5
1	D	2	SER	2.5
1	B	325	THR	2.5
1	A	215	TYR	2.5
1	D	166	MET	2.5
1	B	158	ASP	2.4
1	D	325	THR	2.4
1	D	181	ILE	2.4
1	E	113	LEU	2.4
1	D	196	ALA	2.4
1	A	176	PRO	2.4
1	E	158	ASP	2.4
1	E	129	ALA	2.4
1	D	216	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	142	TYR	2.3
1	E	274	TYR	2.3
1	B	167	ILE	2.3
1	C	180	ASP	2.3
1	D	30	ASP	2.3
1	D	178	GLY	2.3
1	C	167	ILE	2.3
1	D	118	PRO	2.3
1	C	181	ILE	2.2
1	E	43	ASN	2.2
1	C	355	TYR	2.2
1	D	184	VAL	2.2
1	D	371	GLN	2.1
1	A	269	ASP	2.1
1	B	120	GLY	2.1
1	B	216	GLY	2.1
1	E	140	GLY	2.1
1	E	353	ASN	2.1
1	C	175	VAL	2.1
1	B	118	PRO	2.1
1	C	113	LEU	2.1
1	D	215	TYR	2.1
1	E	3	VAL	2.1
1	C	312	ARG	2.1
1	C	168	ASN	2.0
1	D	119	ASP	2.0
1	D	127	THR	2.0
1	A	146	ARG	2.0
1	E	350	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	IUM	B	527	1/3	0.92	0.07	156,156,156,156	1
3	IUM	E	535	1/3	0.94	0.05	160,160,160,160	1
3	IUM	A	521	1/3	0.96	0.05	132,132,132,132	1
3	IUM	D	531	1/3	0.96	0.05	156,156,156,156	1
3	IUM	B	524	1/3	0.96	0.04	165,165,165,165	1
3	IUM	A	523	1/3	0.97	0.04	175,175,175,175	1
3	IUM	B	525	1/3	0.98	0.04	134,134,134,134	1
3	IUM	D	530	1/3	0.98	0.04	166,166,166,166	1
3	IUM	B	526	1/3	0.99	0.04	125,125,125,125	0
3	IUM	C	528	1/3	0.99	0.02	136,136,136,136	1
3	IUM	E	533	1/3	0.99	0.04	132,132,132,132	1
3	IUM	E	534	1/3	0.99	0.05	132,132,132,132	0
3	IUM	C	529	1/3	0.99	0.03	136,136,136,136	0
3	IUM	R	536	1/3	0.99	0.04	130,130,130,130	0
3	IUM	R	537	1/3	0.99	0.03	122,122,122,122	1
3	IUM	R	538	1/3	0.99	0.02	126,126,126,126	0
3	IUM	R	539	1/3	0.99	0.02	112,112,112,112	1
3	IUM	D	532	1/3	1.00	0.03	125,125,125,125	0
3	IUM	A	522	1/3	1.00	0.03	129,129,129,129	0
3	IUM	R	540	1/3	1.00	0.03	126,126,126,126	1

6.5 Other polymers ⓘ

There are no such residues in this entry.