



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:52 PM UTC

PDB ID : 3GUT / pdb_00003gut
Title : Crystal structure of a higher-order complex of p50:RelA bound to the HIV-1 LTR
Authors : Stroud, J.C.; Oltman, A.J.; Han, A.; Bates, D.L.; Chen, L.
Deposited on : 2009-03-30
Resolution : 3.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

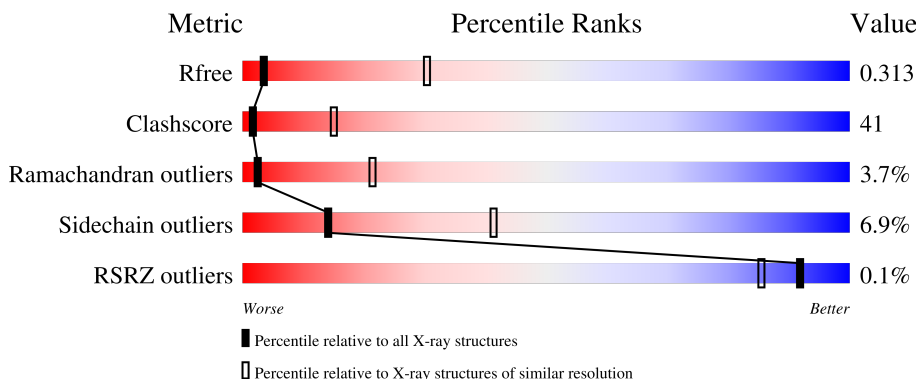
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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.



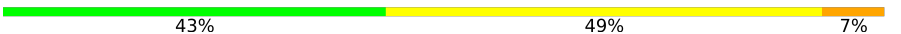
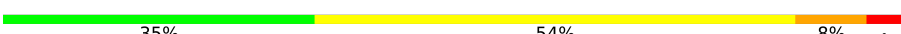
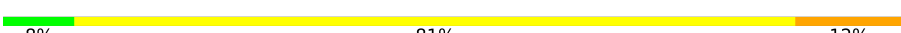
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	273	41% 50% 8%
1	C	273	40% 48% 11% .
1	E	273	38% 51% 11%
1	G	273	40% 48% 11% .
2	B	312	45% 46% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	312	 42%48%9% •
2	F	312	 43%49%7% •
2	H	312	 42%47%10% •
3	I	26	 38%54%8% •
3	X	26	 35%54%8% •
4	J	26	 8%81%12% •
4	Y	26	 12%81%8% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20640 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 Transcription factor p65.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			
1	C	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			
1	E	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			
1	G	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	-	expression tag	UNP Q04206
A	99	TYR	PHE	SEE REMARK 999	UNP Q04206
A	103	ASP	GLU	SEE REMARK 999	UNP Q04206
A	109	SER	CYS	SEE REMARK 999	UNP Q04206
A	142	HIS	GLN	SEE REMARK 999	UNP Q04206
A	169	ALA	SER	SEE REMARK 999	UNP Q04206
A	174	LEU	ARG	SEE REMARK 999	UNP Q04206
A	176	THR	PRO	SEE REMARK 999	UNP Q04206
C	19	ALA	-	expression tag	UNP Q04206
C	99	TYR	PHE	SEE REMARK 999	UNP Q04206
C	103	ASP	GLU	SEE REMARK 999	UNP Q04206
C	109	SER	CYS	SEE REMARK 999	UNP Q04206
C	142	HIS	GLN	SEE REMARK 999	UNP Q04206
C	169	ALA	SER	SEE REMARK 999	UNP Q04206
C	174	LEU	ARG	SEE REMARK 999	UNP Q04206
C	176	THR	PRO	SEE REMARK 999	UNP Q04206
E	19	ALA	-	expression tag	UNP Q04206
E	99	TYR	PHE	SEE REMARK 999	UNP Q04206
E	103	ASP	GLU	SEE REMARK 999	UNP Q04206
E	109	SER	CYS	SEE REMARK 999	UNP Q04206
E	142	HIS	GLN	SEE REMARK 999	UNP Q04206

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	169	ALA	SER	SEE REMARK 999	UNP Q04206
E	174	LEU	ARG	SEE REMARK 999	UNP Q04206
E	176	THR	PRO	SEE REMARK 999	UNP Q04206
G	19	ALA	-	expression tag	UNP Q04206
G	99	TYR	PHE	SEE REMARK 999	UNP Q04206
G	103	ASP	GLU	SEE REMARK 999	UNP Q04206
G	109	SER	CYS	SEE REMARK 999	UNP Q04206
G	142	HIS	GLN	SEE REMARK 999	UNP Q04206
G	169	ALA	SER	SEE REMARK 999	UNP Q04206
G	174	LEU	ARG	SEE REMARK 999	UNP Q04206
G	176	THR	PRO	SEE REMARK 999	UNP Q04206

- Molecule 2 is a protein called Nuclear factor NF-kappa-B p105 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			
2	D	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			
2	F	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			
2	H	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	420	VAL	ILE	SEE REMARK 999	UNP P19838
B	471	SER	PRO	SEE REMARK 999	UNP P19838
B	487	THR	GLY	SEE REMARK 999	UNP P19838
B	493	ILE	LEU	SEE REMARK 999	UNP P19838
B	499	VAL	LEU	SEE REMARK 999	UNP P19838
B	619	VAL	ILE	SEE REMARK 999	UNP P19838
D	420	VAL	ILE	SEE REMARK 999	UNP P19838
D	471	SER	PRO	SEE REMARK 999	UNP P19838
D	487	THR	GLY	SEE REMARK 999	UNP P19838
D	493	ILE	LEU	SEE REMARK 999	UNP P19838
D	499	VAL	LEU	SEE REMARK 999	UNP P19838
D	619	VAL	ILE	SEE REMARK 999	UNP P19838
F	420	VAL	ILE	SEE REMARK 999	UNP P19838
F	471	SER	PRO	SEE REMARK 999	UNP P19838
F	487	THR	GLY	SEE REMARK 999	UNP P19838

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	493	ILE	LEU	SEE REMARK 999	UNP P19838
F	499	VAL	LEU	SEE REMARK 999	UNP P19838
F	619	VAL	ILE	SEE REMARK 999	UNP P19838
H	420	VAL	ILE	SEE REMARK 999	UNP P19838
H	471	SER	PRO	SEE REMARK 999	UNP P19838
H	487	THR	GLY	SEE REMARK 999	UNP P19838
H	493	ILE	LEU	SEE REMARK 999	UNP P19838
H	499	VAL	LEU	SEE REMARK 999	UNP P19838
H	619	VAL	ILE	SEE REMARK 999	UNP P19838

- Molecule 3 is a DNA chain called HIV-LTR Core Forward Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	26	Total	C	N	O	P	0	0	0
			530	253	95	157	25			
3	I	26	Total	C	N	O	P	0	0	0
			530	253	95	157	25			

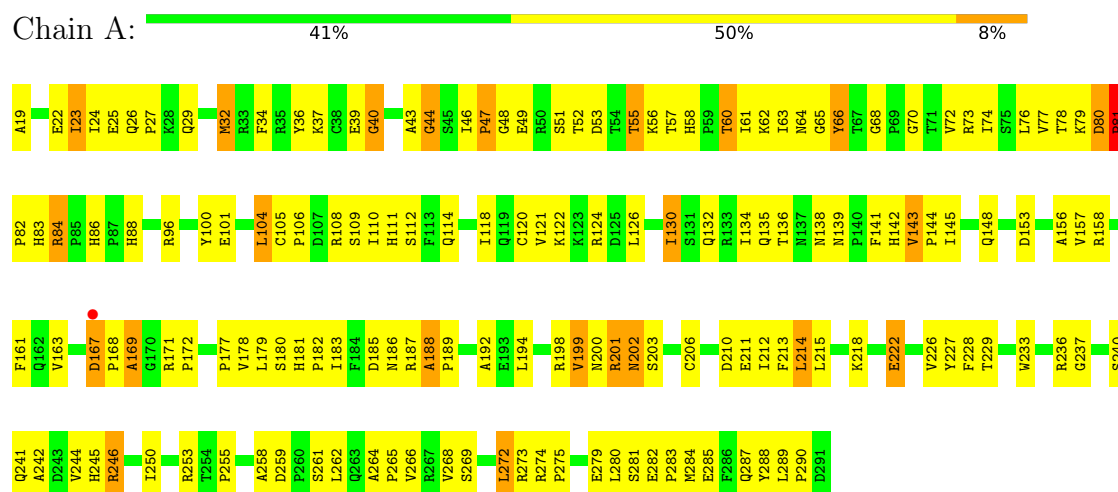
- Molecule 4 is a DNA chain called HIV-LTR Core Reverse Strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Y	26	Total	C	N	O	P	0	0	0
			530	252	102	151	25			
4	J	26	Total	C	N	O	P	0	0	0
			530	252	102	151	25			

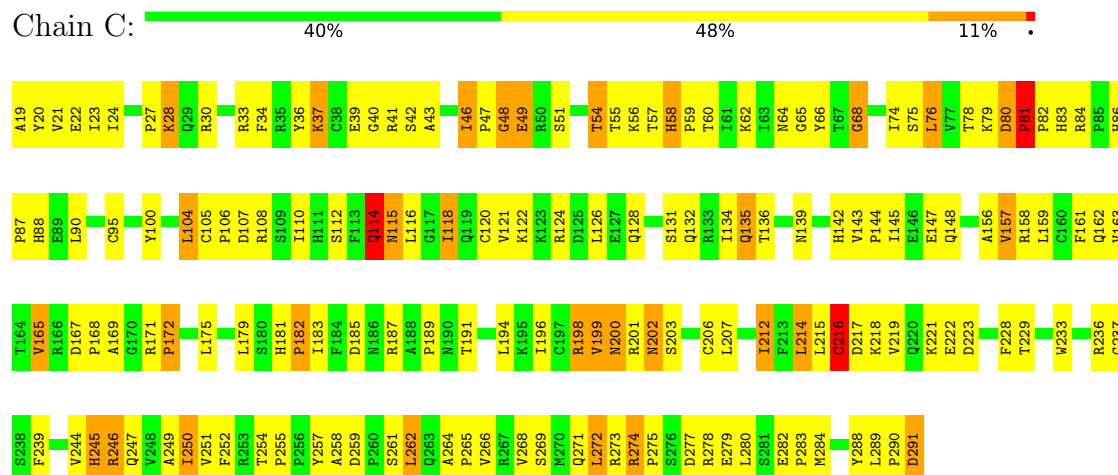
3 Residue-property plots

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

• Molecule 1: Transcription factor p65

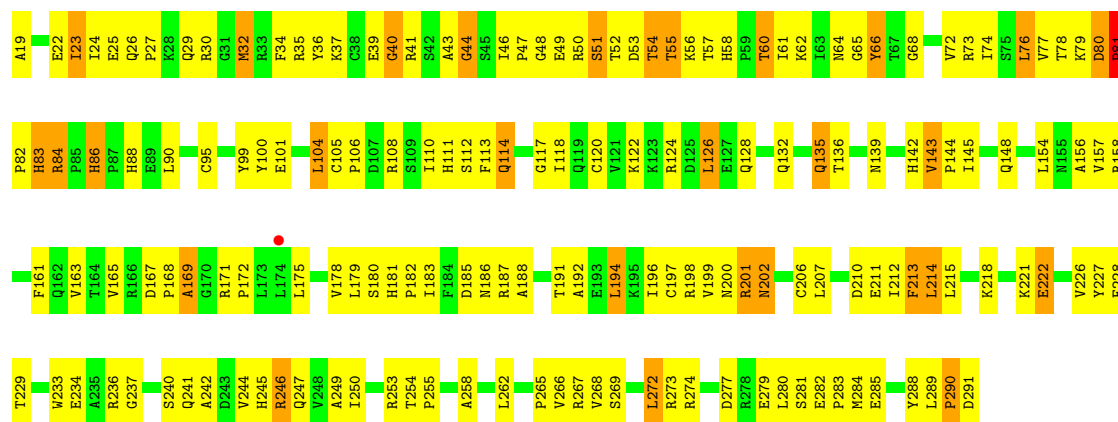


• Molecule 1: Transcription factor p65

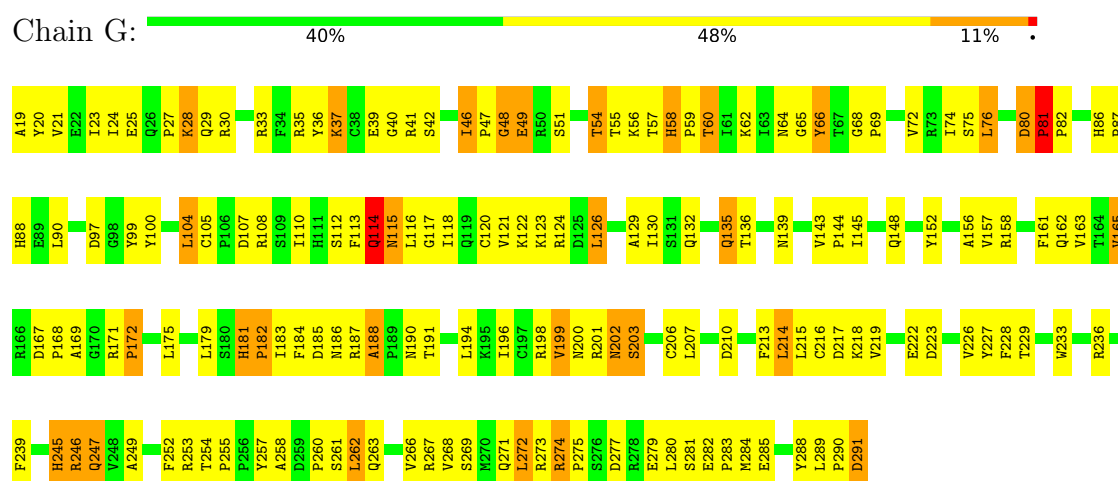


• Molecule 1: Transcription factor p65

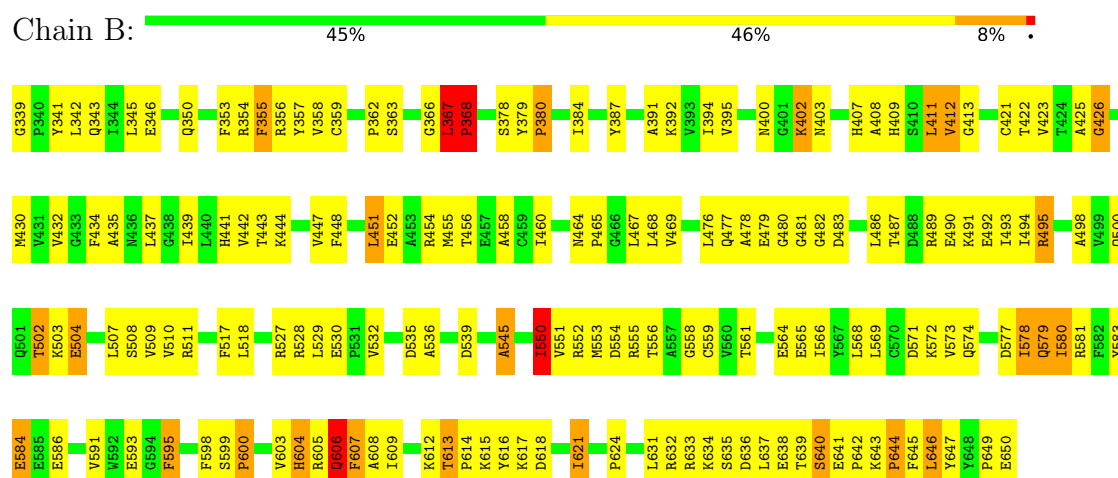




• Molecule 1: Transcription factor p65

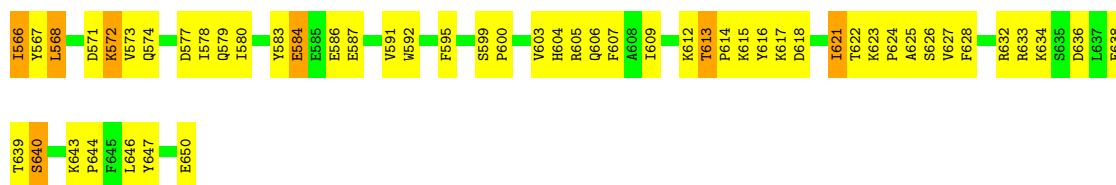


• Molecule 2: Nuclear factor NF-kappa-B p105 subunit



• Molecule 2: Nuclear factor NF-kappa-B p105 subunit





• Molecule 3: HIV-LTR Core Forward Strand

Chain X: 35% 54% 8%



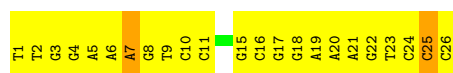
• Molecule 3: HIV-LTR Core Forward Strand

Chain I: 38% 54% 8%



• Molecule 4: HIV-LTR Core Reverse Strand

Chain Y: 12% 81% 8%



• Molecule 4: HIV-LTR Core Reverse Strand

Chain J: 8% 81% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	167.49Å 167.49Å 172.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.45 – 3.59 46.45 – 3.59	Depositor EDS
% Data completeness (in resolution range)	81.2 (46.45-3.59) 92.0 (46.45-3.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.301 0.259 , 0.313	Depositor DCC
R_{free} test set	5648 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	118.8	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 194.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k 0.005 for -h,l,k 0.006 for l,-k,h 0.012 for -l,-k,-h 0.438 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20640	wwPDB-VP
Average B, all atoms (Å ²)	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9062e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.67	0/2228	1.22	22/3021 (0.7%)
1	C	0.69	0/2228	1.26	25/3021 (0.8%)
1	E	0.66	0/2228	1.22	24/3021 (0.8%)
1	G	0.67	0/2228	1.24	32/3021 (1.1%)
2	B	0.83	9/2506 (0.4%)	1.44	29/3384 (0.9%)
2	D	0.83	6/2506 (0.2%)	1.37	42/3384 (1.2%)
2	F	0.66	0/2506	1.15	20/3384 (0.6%)
2	H	0.86	7/2506 (0.3%)	1.37	41/3384 (1.2%)
3	I	0.52	0/593	1.00	2/914 (0.2%)
3	X	0.54	0/593	1.03	2/914 (0.2%)
4	J	0.54	0/595	0.95	1/916 (0.1%)
4	Y	0.56	0/595	0.95	0/916
All	All	0.72	22/21312 (0.1%)	1.25	240/29280 (0.8%)

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	G	0	1
2	B	0	1
2	D	0	1
2	H	0	1
3	I	0	2
3	X	0	2
4	J	0	3
4	Y	0	2
All	All	0	13

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	370	ALA	CA-C	-13.01	1.35	1.52
2	H	370	ALA	CA-C	-12.40	1.36	1.52
2	B	367	LEU	CG-CD2	-11.82	1.13	1.52
2	H	370	ALA	C-O	9.96	1.36	1.23
2	B	367	LEU	CA-C	-9.13	1.41	1.52
2	D	370	ALA	C-O	8.89	1.34	1.23
2	B	368	PRO	CA-CB	-8.50	1.41	1.53
2	B	368	PRO	N-CD	8.21	1.59	1.47
2	B	367	LEU	CA-CB	7.29	1.65	1.53
2	H	379	TYR	CA-C	-6.34	1.45	1.52
2	D	379	TYR	CA-C	-6.06	1.45	1.52
2	D	365	GLY	C-O	-5.91	1.16	1.23
2	B	367	LEU	CB-CG	5.72	1.64	1.53
2	B	367	LEU	N-CA	-5.69	1.38	1.46
2	H	371	SER	CA-C	5.55	1.60	1.52
2	H	379	TYR	CA-CB	5.47	1.58	1.53
2	D	367	LEU	C-O	-5.45	1.17	1.24
2	H	379	TYR	C-O	-5.44	1.19	1.24
2	B	368	PRO	CA-C	5.40	1.60	1.52
2	H	376	LYS	C-O	-5.13	1.17	1.24
2	D	371	SER	CA-C	5.12	1.59	1.52
2	B	367	LEU	CG-CD1	5.02	1.69	1.52

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	367	LEU	CA-C-N	31.06	158.66	119.84
2	B	367	LEU	C-N-CA	31.06	158.66	119.84
2	H	371	SER	N-CA-CB	15.12	136.04	110.49
2	D	371	SER	N-CA-CB	15.10	136.00	110.49
2	B	367	LEU	C-N-CD	-14.86	64.09	125.00
2	H	370	ALA	O-C-N	12.98	138.22	123.16
2	D	370	ALA	O-C-N	12.70	138.00	123.01
2	B	368	PRO	CA-N-CD	-12.36	94.69	112.00
2	F	367	LEU	CA-C-N	10.79	130.90	119.78
2	F	367	LEU	C-N-CA	10.79	130.90	119.78
1	A	81	PRO	N-CA-C	10.69	123.74	110.70
2	D	371	SER	CA-C-O	10.57	135.63	120.51
2	H	371	SER	CA-C-O	10.50	135.53	120.51
1	E	81	PRO	N-CA-C	10.08	123.00	110.70
1	A	80	ASP	CA-C-N	9.90	130.58	120.38
1	A	80	ASP	C-N-CA	9.90	130.58	120.38
1	G	81	PRO	N-CA-C	9.75	122.60	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ASP	CA-C-N	9.57	130.24	120.38
1	C	80	ASP	C-N-CA	9.57	130.24	120.38
1	C	81	PRO	N-CA-C	9.31	122.06	110.70
1	C	139	ASN	CA-C-N	9.26	129.00	119.56
1	C	139	ASN	C-N-CA	9.26	129.00	119.56
1	G	80	ASP	CA-C-N	9.10	129.75	120.38
1	G	80	ASP	C-N-CA	9.10	129.75	120.38
2	H	370	ALA	CA-C-O	9.04	131.31	120.92
2	H	371	SER	CA-CB-OG	-9.01	93.08	111.10
2	D	371	SER	CA-CB-OG	-8.99	93.13	111.10
2	B	367	LEU	N-CA-CB	8.74	125.93	110.37
1	A	55	THR	N-CA-C	8.73	123.06	109.52
2	B	350	GLN	N-CA-C	8.69	120.37	111.07
1	E	274	ARG	CA-C-N	8.69	128.00	118.97
1	E	274	ARG	C-N-CA	8.69	128.00	118.97
2	F	578	ILE	N-CA-C	8.62	119.72	108.35
1	E	188	ALA	CA-C-N	8.54	130.51	119.84
1	E	188	ALA	C-N-CA	8.54	130.51	119.84
1	A	188	ALA	CA-C-N	8.53	130.50	119.84
1	A	188	ALA	C-N-CA	8.53	130.50	119.84
2	D	370	ALA	CA-C-O	8.31	130.52	121.05
2	B	599	SER	CA-C-N	8.31	130.23	119.84
2	B	599	SER	C-N-CA	8.31	130.23	119.84
2	F	604	HIS	N-CA-C	8.30	121.54	108.67
1	E	55	THR	N-CA-C	8.22	121.65	109.24
2	B	607	PHE	N-CA-C	8.13	124.19	113.30
1	G	29	GLN	N-CA-C	8.09	119.87	111.14
2	D	370	ALA	N-CA-CB	7.84	121.89	110.06
2	F	350	GLN	N-CA-C	7.75	119.36	111.07
2	D	377	LYS	N-CA-C	7.74	127.29	110.80
2	H	377	LYS	N-CA-C	7.72	127.25	110.80
2	D	634	LYS	N-CA-C	-7.63	102.56	111.03
2	D	551	VAL	N-CA-C	7.59	118.36	110.62
2	D	370	ALA	N-CA-C	7.57	122.16	110.20
2	D	349	LYS	N-CA-C	-7.54	99.86	110.50
1	G	143	VAL	CA-C-N	7.43	127.47	119.89
1	G	143	VAL	C-N-CA	7.43	127.47	119.89
2	H	634	LYS	N-CA-C	-7.43	102.34	111.40
2	H	551	VAL	N-CA-C	7.42	117.55	110.42
1	A	274	ARG	CA-C-N	7.42	126.96	119.24
1	A	274	ARG	C-N-CA	7.42	126.96	119.24
2	H	607	PHE	N-CA-C	7.42	122.50	113.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	643	LYS	CA-C-N	7.42	127.86	119.93
2	B	643	LYS	C-N-CA	7.42	127.86	119.93
1	E	80	ASP	CA-C-N	7.39	128.00	120.38
1	E	80	ASP	C-N-CA	7.39	128.00	120.38
1	G	46	ILE	N-CA-C	7.39	117.01	108.96
1	C	46	ILE	CA-C-N	7.30	127.46	120.31
1	C	46	ILE	C-N-CA	7.30	127.46	120.31
2	B	412	VAL	N-CA-C	7.27	119.94	108.89
1	E	41	ARG	N-CA-C	-7.18	104.51	113.55
2	H	370	ALA	N-CA-C	7.08	121.85	109.96
2	H	370	ALA	N-CA-CB	7.08	121.69	110.23
2	D	480	GLY	N-CA-C	-7.07	104.01	114.90
1	A	143	VAL	CA-C-N	7.02	127.05	119.89
1	A	143	VAL	C-N-CA	7.02	127.05	119.89
1	C	274	ARG	CA-C-N	6.98	128.56	119.84
1	C	274	ARG	C-N-CA	6.98	128.56	119.84
2	D	363	SER	N-CA-C	6.95	119.71	111.02
1	E	143	VAL	CA-C-N	6.94	126.93	119.78
1	E	143	VAL	C-N-CA	6.94	126.93	119.78
2	D	542	ALA	N-CA-C	-6.92	101.35	110.07
1	G	139	ASN	CA-C-N	6.82	127.39	119.47
1	G	139	ASN	C-N-CA	6.82	127.39	119.47
2	D	371	SER	CA-C-N	6.70	133.56	123.24
2	D	371	SER	C-N-CA	6.70	133.56	123.24
2	F	643	LYS	CA-C-N	6.70	128.22	119.84
2	F	643	LYS	C-N-CA	6.70	128.22	119.84
1	C	271	GLN	N-CA-C	6.64	118.95	108.79
2	H	371	SER	CA-C-N	6.61	133.42	123.24
2	H	371	SER	C-N-CA	6.61	133.42	123.24
2	H	363	SER	N-CA-C	6.55	119.21	111.02
1	G	181	HIS	CA-C-N	6.41	126.44	119.90
1	G	181	HIS	C-N-CA	6.41	126.44	119.90
1	E	105	CYS	N-CA-C	-6.37	99.99	109.42
2	D	447	VAL	N-CA-C	6.36	117.14	110.72
1	E	197	CYS	N-CA-C	6.32	119.11	111.40
2	B	604	HIS	N-CA-C	6.30	118.89	109.25
2	B	640	SER	N-CA-C	-6.24	102.48	110.53
1	A	139	ASN	CA-C-N	6.20	125.94	119.05
1	A	139	ASN	C-N-CA	6.20	125.94	119.05
1	G	188	ALA	CA-C-N	6.20	125.89	119.82
1	G	188	ALA	C-N-CA	6.20	125.89	119.82
1	A	32	MET	N-CA-C	6.17	118.77	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	356	ARG	N-CA-C	6.17	118.95	108.90
2	H	375	ASN	N-CA-C	6.13	120.62	113.20
2	D	599	SER	CA-C-N	6.13	127.50	119.84
2	D	599	SER	C-N-CA	6.13	127.50	119.84
1	G	263	GLN	N-CA-C	-6.12	105.84	113.55
1	C	143	VAL	CA-C-N	6.11	126.12	119.89
1	C	143	VAL	C-N-CA	6.11	126.12	119.89
1	E	139	ASN	CA-C-N	6.11	126.00	119.28
1	E	139	ASN	C-N-CA	6.11	126.00	119.28
2	H	368	PRO	N-CA-CB	-6.10	96.85	103.25
1	A	84	ARG	N-CA-C	-6.09	101.68	110.08
2	D	368	PRO	N-CA-CB	-6.09	96.86	103.25
1	G	274	ARG	CA-C-N	6.07	127.43	119.84
1	G	274	ARG	C-N-CA	6.07	127.43	119.84
2	D	375	ASN	N-CA-C	6.04	120.51	113.20
2	H	471	SER	N-CA-C	6.04	118.35	111.11
2	B	595	PHE	N-CA-C	6.03	119.30	109.59
2	H	640	SER	N-CA-C	-6.03	102.03	110.35
1	E	60	THR	N-CA-C	6.02	119.32	110.59
2	D	367	LEU	CA-C-N	-5.96	112.39	119.84
2	D	367	LEU	C-N-CA	-5.96	112.39	119.84
1	C	212	ILE	N-CA-C	5.95	116.57	107.77
1	E	84	ARG	N-CA-C	-5.95	101.87	110.08
1	G	60	THR	N-CA-C	5.92	118.56	108.02
3	I	11	DC	C2'-C3'-O3'	5.89	120.34	111.50
1	G	115	ASN	N-CA-C	5.86	117.57	109.54
2	D	471	SER	N-CA-C	5.83	118.11	111.11
1	E	227	TYR	N-CA-C	5.83	118.25	108.23
2	D	468	LEU	N-CA-C	5.82	120.51	113.41
1	G	290	PRO	N-CA-C	-5.82	101.96	111.21
2	H	381	GLN	N-CA-C	5.80	118.34	108.02
1	C	68	GLY	CA-C-N	5.79	125.81	119.90
1	C	68	GLY	C-N-CA	5.79	125.81	119.90
2	F	613	THR	N-CA-C	5.79	117.89	109.84
2	H	378	SER	CA-C-N	5.79	129.24	122.52
2	H	378	SER	C-N-CA	5.79	129.24	122.52
2	D	381	GLN	N-CA-C	5.79	118.32	108.02
2	B	550	ILE	N-CA-C	-5.77	99.56	107.99
2	F	480	GLY	N-CA-C	-5.77	106.02	114.90
2	H	480	GLY	N-CA-C	-5.76	106.03	114.61
1	G	271	GLN	N-CA-C	5.76	117.60	108.79
1	C	245	HIS	N-CA-C	5.75	117.83	108.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	607	PHE	N-CA-C	5.70	121.13	113.72
2	B	578	ILE	N-CA-C	5.67	118.00	108.81
3	X	17	DG	N9-C1'-C2'	-5.63	105.05	113.50
1	E	194	LEU	N-CA-C	5.63	117.47	108.41
2	H	368	PRO	N-CA-C	5.63	124.06	112.47
1	G	245	HIS	N-CA-C	5.62	117.62	108.63
2	F	493	ILE	N-CA-C	-5.61	105.06	110.72
2	H	371	SER	N-CA-C	-5.59	98.88	110.80
2	H	447	VAL	N-CA-C	5.58	116.36	110.72
2	D	371	SER	N-CA-C	-5.57	98.93	110.80
2	D	607	PHE	N-CA-C	5.57	120.96	113.72
1	A	105	CYS	N-CA-C	-5.56	101.19	109.42
2	H	366	GLY	N-CA-C	-5.55	102.98	112.64
2	B	368	PRO	N-CA-C	5.54	123.88	112.47
2	D	339	GLY	CA-C-N	5.53	126.75	119.84
2	D	339	GLY	C-N-CA	5.53	126.75	119.84
2	D	413	GLY	N-CA-C	5.53	116.96	111.21
2	F	369	GLY	N-CA-C	-5.52	104.24	113.02
2	H	341	TYR	N-CA-C	5.52	117.37	109.14
2	B	480	GLY	N-CA-C	-5.52	106.39	114.61
2	D	379	TYR	N-CA-C	-5.50	97.64	109.81
2	B	339	GLY	CA-C-N	5.50	127.94	120.79
2	B	339	GLY	C-N-CA	5.50	127.94	120.79
1	E	86	HIS	N-CA-C	5.50	116.75	109.93
2	B	535	ASP	N-CA-C	-5.49	103.29	110.53
2	D	341	TYR	N-CA-C	5.49	117.31	109.14
1	E	213	PHE	N-CA-C	-5.49	100.75	109.96
2	H	367	LEU	CA-C-N	-5.48	112.99	119.84
2	H	367	LEU	C-N-CA	-5.48	112.99	119.84
2	D	631	LEU	N-CA-C	-5.48	101.89	110.17
2	B	646	LEU	N-CA-C	5.47	117.44	108.52
1	A	241	GLN	N-CA-C	-5.42	105.76	112.38
2	F	447	VAL	N-CA-C	5.42	115.62	110.42
1	C	182	PRO	N-CA-C	5.41	119.58	111.14
2	F	595	PHE	N-CA-C	5.40	118.28	109.59
2	D	367	LEU	C-N-CD	-5.40	102.87	125.00
1	A	227	TYR	N-CA-C	5.39	117.47	107.99
2	F	599	SER	CA-C-N	5.38	126.57	119.84
2	F	599	SER	C-N-CA	5.38	126.57	119.84
1	A	169	ALA	N-CA-C	5.38	116.84	110.97
2	H	468	LEU	N-CA-C	5.38	119.97	113.41
2	B	367	LEU	O-C-N	-5.37	115.14	121.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	68	GLY	CA-C-N	5.37	125.29	119.76
1	G	68	GLY	C-N-CA	5.37	125.29	119.76
2	B	644	PRO	N-CA-C	5.36	120.00	111.26
1	G	80	ASP	N-CA-C	5.35	117.67	110.29
1	C	58	HIS	N-CA-C	5.33	114.27	108.14
3	I	7	DT	N1-C1'-C2'	5.33	121.49	113.50
1	G	49	GLU	N-CA-C	-5.32	106.28	114.16
2	B	355	PHE	N-CA-C	-5.32	102.61	110.48
1	E	169	ALA	N-CA-C	5.30	116.75	110.97
1	C	80	ASP	N-CA-C	5.30	117.98	110.24
2	H	367	LEU	C-N-CD	-5.29	103.30	125.00
1	G	182	PRO	N-CA-C	5.27	119.48	111.15
1	C	290	PRO	N-CA-C	-5.26	102.84	111.21
2	F	473	LEU	N-CA-C	-5.24	105.61	113.89
2	F	412	VAL	N-CA-C	5.23	117.15	108.99
1	E	54	THR	N-CA-C	5.22	119.63	113.16
2	D	379	TYR	CA-CB-CG	5.21	123.28	113.90
2	H	580	ILE	N-CA-C	-5.21	100.38	107.99
3	X	7	DT	N1-C1'-C2'	5.21	121.31	113.50
2	D	368	PRO	N-CA-C	5.20	123.19	112.47
2	H	349	LYS	N-CA-C	-5.20	102.05	110.32
2	H	546	SER	N-CA-C	-5.19	102.07	110.32
2	H	347	GLN	N-CA-C	5.17	116.33	109.93
2	D	546	SER	N-CA-C	-5.16	102.84	110.48
1	G	184	PHE	N-CA-C	5.16	117.47	108.76
2	B	468	LEU	N-CA-C	5.15	119.55	113.12
1	G	216	CYS	N-CA-C	5.14	114.82	108.19
1	E	49	GLU	N-CA-C	5.13	116.56	111.07
1	A	60	THR	N-CA-C	5.13	118.03	110.59
1	C	114	GLN	CA-C-N	-5.13	115.48	122.87
1	C	114	GLN	C-N-CA	-5.13	115.48	122.87
1	G	285	GLU	N-CA-C	5.13	117.78	110.24
1	C	251	VAL	N-CA-C	-5.11	100.95	108.11
2	H	566	ILE	N-CA-C	5.11	115.84	108.48
1	G	114	GLN	CA-C-N	-5.11	115.52	122.87
1	G	114	GLN	C-N-CA	-5.11	115.52	122.87
1	A	47	PRO	N-CA-C	-5.10	103.54	111.13
2	F	468	LEU	N-CA-C	5.10	119.58	112.90
1	C	216	CYS	N-CA-C	5.09	114.76	108.19
2	D	447	VAL	CB-CA-C	-5.07	105.22	112.22
1	C	159	LEU	N-CA-C	-5.07	101.45	109.76
2	H	599	SER	CA-C-N	5.06	126.17	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	599	SER	C-N-CA	5.06	126.17	119.84
2	H	622	THR	N-CA-C	-5.06	107.49	113.97
2	H	356	ARG	N-CA-C	5.05	117.13	108.90
4	J	13	DC	C4'-C3'-O3'	5.05	117.58	110.00
2	H	379	TYR	CA-CB-CG	5.04	122.98	113.90
2	D	581	ARG	N-CA-C	5.04	116.91	107.99
2	D	376	LYS	CB-CA-C	-5.03	102.45	110.04
2	B	613	THR	N-CA-C	5.02	116.82	109.84
1	G	58	HIS	N-CA-C	5.02	113.92	108.14
2	F	352	GLY	N-CA-C	5.02	120.66	114.69
2	B	493	ILE	N-CA-C	-5.01	105.51	110.62
1	A	264	ALA	CA-C-N	5.01	125.01	119.90
1	A	264	ALA	C-N-CA	5.01	125.01	119.90

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	367	LEU	Mainchain
2	D	371	SER	Mainchain
1	G	227	TYR	Sidechain
2	H	371	SER	Mainchain
3	I	17	DG	Sidechain
3	I	25	DC	Sidechain
4	J	16	DC	Sidechain
4	J	7	DA	Sidechain
4	J	9	DT	Sidechain
3	X	16	DG	Sidechain
3	X	17	DG	Sidechain
4	Y	25	DC	Sidechain
4	Y	7	DA	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2176	0	2137	200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2176	0	2137	187	0
1	E	2176	0	2137	231	0
1	G	2176	0	2137	189	0
2	B	2454	0	2451	175	0
2	D	2454	0	2451	177	0
2	F	2454	0	2451	182	0
2	H	2454	0	2451	176	0
3	I	530	0	295	28	0
3	X	530	0	295	39	0
4	J	530	0	290	74	0
4	Y	530	0	288	72	0
All	All	20640	0	19520	1652	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 41.

All (1652) 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)
2:B:572:LYS:NZ	2:B:606:GLN:HG2	1.45	1.32
2:F:572:LYS:NZ	2:F:606:GLN:HG2	1.53	1.23
2:H:572:LYS:NZ	2:H:606:GLN:HG2	1.59	1.18
3:I:15:DG:H2''	3:I:16:DG:H5''	1.17	1.15
4:Y:9:DT:H2''	4:Y:10:DC:H5''	1.14	1.13
4:J:9:DT:H2''	4:J:10:DC:H5''	1.27	1.12
3:X:15:DG:H2''	3:X:16:DG:H5''	1.17	1.10
2:D:572:LYS:NZ	2:D:606:GLN:HG2	1.67	1.10
1:A:51:SER:HB2	1:A:57:THR:CG2	1.82	1.09
4:Y:18:DG:H2''	4:Y:19:DA:H5''	1.30	1.08
4:Y:9:DT:H2''	4:Y:10:DC:C5'	1.84	1.07
2:B:572:LYS:HZ3	2:B:606:GLN:HG2	0.94	1.06
4:Y:15:DG:H2''	4:Y:16:DC:H5''	1.33	1.06
4:J:18:DG:H2''	4:J:19:DA:H5''	1.33	1.06
2:F:572:LYS:HZ1	2:F:606:GLN:HG2	1.06	1.05
1:A:52:THR:HG22	1:A:53:ASP:H	1.20	1.05
3:X:15:DG:C2'	3:X:16:DG:H5''	1.86	1.04
1:C:24:ILE:HD11	1:C:62:LYS:HB2	1.38	1.04
1:G:282:GLU:HG2	1:G:283:PRO:HD2	1.34	1.04
1:G:24:ILE:HD11	1:G:62:LYS:HB2	1.35	1.03
3:I:15:DG:C2'	3:I:16:DG:H5''	1.88	1.03
4:Y:9:DT:C2'	4:Y:10:DC:H5''	1.88	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:SER:HB2	1:E:57:THR:CG2	1.90	1.02
1:E:262:LEU:HD21	1:E:266:VAL:HG12	1.43	1.00
1:A:46:ILE:HD11	1:A:118:ILE:HD11	1.43	0.98
4:J:15:DG:H2''	4:J:16:DC:H5''	1.43	0.97
1:A:211:GLU:O	1:A:212:ILE:HD13	1.66	0.96
2:H:367:LEU:HD11	2:H:439:ILE:HD11	1.48	0.95
2:D:367:LEU:HD11	2:D:439:ILE:HD11	1.46	0.94
1:E:211:GLU:O	1:E:212:ILE:HD13	1.68	0.94
2:D:489:ARG:O	2:D:489:ARG:HD3	1.69	0.93
4:J:16:DC:H2''	4:J:17:DG:H5''	1.51	0.92
1:E:52:THR:HG22	1:E:53:ASP:H	1.34	0.92
1:G:74:ILE:HD12	1:G:161:PHE:CD2	2.04	0.92
4:Y:18:DG:H2''	4:Y:19:DA:C5'	1.99	0.92
4:J:9:DT:H2''	4:J:10:DC:C5'	2.01	0.91
1:A:262:LEU:HD21	1:A:266:VAL:HG12	1.52	0.91
2:D:487:THR:OG1	2:D:490:GLU:HG3	1.70	0.91
4:J:9:DT:C2'	4:J:10:DC:H5''	1.98	0.91
3:X:15:DG:H2''	3:X:16:DG:C5'	2.01	0.91
1:C:74:ILE:HD12	1:C:161:PHE:CD2	2.06	0.91
3:I:15:DG:H2''	3:I:16:DG:C5'	2.01	0.91
2:F:402:LYS:N	2:F:402:LYS:HE3	1.86	0.90
2:H:572:LYS:HZ1	2:H:606:GLN:HG2	1.21	0.90
1:A:51:SER:HB2	1:A:57:THR:CB	2.02	0.89
1:G:88:HIS:CE1	1:G:120:CYS:HB2	2.06	0.89
3:X:7:DT:O2	4:Y:22:DG:N2	2.06	0.89
4:Y:18:DG:C2'	4:Y:19:DA:H5''	2.02	0.89
1:E:46:ILE:HD11	1:E:118:ILE:HD11	1.51	0.89
1:E:48:GLY:H	1:E:57:THR:HG21	1.37	0.89
1:A:48:GLY:H	1:A:57:THR:CG2	1.86	0.89
1:E:51:SER:HB2	1:E:57:THR:HB	1.53	0.89
1:E:51:SER:HB2	1:E:57:THR:CB	2.01	0.89
2:D:572:LYS:HZ1	2:D:606:GLN:HG2	1.35	0.89
4:Y:15:DG:C2'	4:Y:16:DC:H5''	2.03	0.89
1:C:282:GLU:HG2	1:C:283:PRO:HD2	1.55	0.88
2:D:397:LEU:HD21	2:D:411:LEU:HD13	1.57	0.87
1:E:48:GLY:H	1:E:57:THR:CG2	1.87	0.87
1:G:236:ARG:HH11	1:G:236:ARG:HG3	1.40	0.87
1:A:167:ASP:HB2	1:A:168:PRO:HD2	1.54	0.86
2:B:367:LEU:HD12	2:B:367:LEU:O	1.74	0.86
2:B:402:LYS:HE3	2:B:402:LYS:N	1.90	0.86
2:F:402:LYS:HE3	2:F:402:LYS:H	1.38	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:621:ILE:HD13	2:F:649:PRO:HB3	1.57	0.86
1:C:21:VAL:HG21	1:C:163:VAL:HG21	1.58	0.86
4:Y:24:DC:H2''	4:Y:25:DC:H5'	1.54	0.86
2:B:621:ILE:HD13	2:B:649:PRO:HB3	1.54	0.86
1:E:167:ASP:OD1	1:E:169:ALA:HB3	1.75	0.86
2:D:382:VAL:HG12	2:D:383:LYS:H	1.39	0.86
2:F:423:VAL:HG21	2:F:432:VAL:HG11	1.58	0.85
2:D:345:LEU:HB2	2:D:381:GLN:O	1.76	0.85
4:J:18:DG:C2'	4:J:19:DA:H5''	2.06	0.85
1:A:167:ASP:OD1	1:A:169:ALA:HB3	1.76	0.85
2:F:366:GLY:O	2:F:368:PRO:HD3	1.76	0.85
2:F:489:ARG:O	2:F:489:ARG:HD3	1.76	0.85
3:I:22:DT:O2	4:J:7:DA:H2	1.59	0.85
2:F:487:THR:OG1	2:F:490:GLU:HG3	1.76	0.84
4:J:18:DG:H2''	4:J:19:DA:C5'	2.06	0.84
1:E:77:VAL:HG23	1:E:158:ARG:HB2	1.60	0.84
2:F:561:THR:O	2:F:615:LYS:HG3	1.77	0.84
2:H:382:VAL:HG12	2:H:383:LYS:H	1.43	0.84
2:H:487:THR:OG1	2:H:490:GLU:HG3	1.77	0.84
4:J:16:DC:C2'	4:J:17:DG:H5''	2.07	0.83
1:A:51:SER:HB2	1:A:57:THR:HB	1.58	0.83
2:H:489:ARG:O	2:H:489:ARG:HD3	1.78	0.83
2:F:391:ALA:HB3	2:F:425:ALA:HB3	1.59	0.83
2:H:409:HIS:HD2	2:H:442:VAL:HG22	1.44	0.83
2:B:489:ARG:O	2:B:489:ARG:HD3	1.79	0.82
1:C:196:ILE:HG13	1:C:272:LEU:HD22	1.61	0.82
1:G:229:THR:HG23	1:G:269:SER:HB3	1.60	0.82
1:A:236:ARG:HG3	1:A:236:ARG:HH11	1.44	0.82
2:B:395:VAL:HB	2:B:421:CYS:HB3	1.60	0.82
2:B:572:LYS:HZ3	2:B:606:GLN:CG	1.86	0.82
2:B:460:ILE:HG12	2:B:486:LEU:HD13	1.62	0.82
2:H:565:GLU:C	2:H:566:ILE:HD12	2.04	0.82
2:F:550:ILE:HD12	2:F:550:ILE:N	1.94	0.82
2:H:407:HIS:ND1	2:H:510:VAL:HG23	1.93	0.82
1:A:19:ALA:HA	1:A:64:ASN:O	1.80	0.82
1:E:167:ASP:HB2	1:E:168:PRO:HD2	1.60	0.82
2:D:387:TYR:CE1	2:D:518:LEU:HD13	2.15	0.81
2:H:409:HIS:CD2	2:H:442:VAL:HG22	2.15	0.81
4:J:15:DG:C2'	4:J:16:DC:H5''	2.10	0.81
1:C:86:HIS:ND1	1:C:87:PRO:HD2	1.96	0.81
1:C:88:HIS:CE1	1:C:120:CYS:HB2	2.15	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:HIS:HD2	2:B:409:HIS:H	1.25	0.81
2:H:603:VAL:HG22	2:H:609:ILE:HG12	1.63	0.81
4:J:23:DT:H2''	4:J:24:DC:H5''	1.63	0.81
1:G:30:ARG:HE	1:G:191:THR:HB	1.46	0.81
1:G:262:LEU:HD21	1:G:266:VAL:HG12	1.62	0.81
3:X:23:DT:O2	4:Y:6:DA:H2	1.64	0.80
1:A:202:ASN:HD22	1:A:202:ASN:H	1.29	0.80
2:D:624:PRO:HB2	2:D:646:LEU:HD11	1.63	0.80
2:B:342:LEU:HD13	2:B:343:GLN:N	1.96	0.80
2:F:572:LYS:HZ1	2:F:606:GLN:CG	1.91	0.80
2:H:636:ASP:OD2	2:H:638:GLU:HG2	1.82	0.80
2:D:545:ALA:HA	2:D:633:ARG:NH2	1.96	0.80
1:E:236:ARG:HG3	1:E:236:ARG:HH11	1.47	0.80
4:J:15:DG:H2''	4:J:16:DC:C5'	2.11	0.80
2:B:367:LEU:O	2:B:367:LEU:CD1	2.30	0.80
2:B:391:ALA:HB3	2:B:425:ALA:HB3	1.63	0.80
2:B:402:LYS:HE3	2:B:402:LYS:H	1.44	0.80
2:F:452:GLU:OE2	2:F:495:ARG:HG3	1.80	0.80
4:J:24:DC:H2''	4:J:25:DC:H5'	1.63	0.80
2:H:353:PHE:HE2	2:H:439:ILE:HG12	1.47	0.80
4:Y:15:DG:H2''	4:Y:16:DC:C5'	2.11	0.80
3:I:6:DC:H42	4:J:22:DG:H1	1.29	0.80
1:E:55:THR:HA	2:H:375:ASN:OD1	1.81	0.79
3:I:8:DT:H2''	3:I:9:DT:OP2	1.82	0.79
1:A:51:SER:HB2	1:A:57:THR:HG21	1.61	0.79
2:D:402:LYS:HE3	2:D:402:LYS:H	1.46	0.79
1:A:237:GLY:HA2	1:A:255:PRO:HD3	1.65	0.79
2:F:402:LYS:H	2:F:402:LYS:CE	1.94	0.79
2:F:477:GLN:O	2:F:479:GLU:HG2	1.83	0.79
2:F:550:ILE:HD12	2:F:550:ILE:H	1.46	0.79
2:F:572:LYS:NZ	2:F:606:GLN:CG	2.43	0.79
1:G:51:SER:CB	1:G:57:THR:H	1.95	0.79
2:B:477:GLN:O	2:B:479:GLU:HG2	1.81	0.79
1:C:236:ARG:HG3	1:C:236:ARG:HH11	1.46	0.79
1:C:262:LEU:HD21	1:C:266:VAL:HG12	1.63	0.79
1:E:27:PRO:O	1:E:181:HIS:HE1	1.66	0.79
4:Y:23:DT:H2''	4:Y:24:DC:H5''	1.63	0.78
1:C:19:ALA:O	1:C:175:LEU:HD22	1.84	0.78
2:H:595:PHE:O	2:H:614:PRO:HB3	1.82	0.78
1:A:74:ILE:HG12	1:A:100:TYR:CD1	2.19	0.78
2:D:387:TYR:CE2	2:D:518:LEU:HD22	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:ASN:HD22	1:E:202:ASN:H	1.31	0.77
2:H:345:LEU:HB2	2:H:381:GLN:O	1.84	0.77
1:A:27:PRO:O	1:A:181:HIS:HE1	1.67	0.77
1:E:51:SER:HB2	1:E:57:THR:HG21	1.64	0.77
1:E:82:PRO:O	1:E:84:ARG:HG3	1.85	0.77
1:C:30:ARG:HE	1:C:191:THR:HB	1.48	0.77
1:E:273:ARG:HD2	1:E:280:LEU:HD21	1.67	0.77
1:A:36:TYR:CE2	3:X:8:DT:H2'	2.19	0.77
1:C:81:PRO:HB2	1:C:82:PRO:HD3	1.65	0.77
1:C:229:THR:HG23	1:C:269:SER:HB3	1.67	0.77
2:B:572:LYS:NZ	2:B:606:GLN:CG	2.39	0.77
2:H:387:TYR:CE2	2:H:518:LEU:HD22	2.20	0.77
1:E:25:GLU:OE2	1:E:50:ARG:HG2	1.85	0.76
1:E:185:ASP:C	1:E:187:ARG:H	1.93	0.76
3:X:8:DT:H2''	3:X:9:DT:OP2	1.83	0.76
1:G:196:ILE:HG12	1:G:272:LEU:HD22	1.65	0.76
2:D:565:GLU:C	2:D:566:ILE:HD12	2.11	0.76
4:J:16:DC:H2''	4:J:17:DG:C5'	2.15	0.76
4:Y:4:DG:H2''	4:Y:5:DA:H5''	1.67	0.76
2:B:423:VAL:HG21	2:B:432:VAL:HG11	1.67	0.76
2:D:402:LYS:HE3	2:D:402:LYS:N	2.01	0.76
2:D:409:HIS:HD2	2:D:442:VAL:HG22	1.50	0.76
1:E:48:GLY:HA3	1:E:57:THR:OG1	1.86	0.76
3:X:7:DT:C2	4:Y:22:DG:N2	2.53	0.76
2:F:460:ILE:HG12	2:F:486:LEU:HD13	1.68	0.76
1:G:185:ASP:C	1:G:187:ARG:H	1.92	0.76
2:H:542:ALA:HB3	2:H:545:ALA:HB3	1.68	0.76
1:A:82:PRO:O	1:A:84:ARG:HG3	1.86	0.76
2:B:487:THR:OG1	2:B:490:GLU:HG3	1.85	0.76
2:D:409:HIS:CD2	2:D:442:VAL:HG22	2.21	0.76
1:A:185:ASP:C	1:A:187:ARG:H	1.93	0.75
2:D:595:PHE:O	2:D:614:PRO:HB3	1.85	0.75
1:E:229:THR:HG23	1:E:269:SER:HB3	1.67	0.75
1:G:202:ASN:H	1:G:202:ASN:HD22	1.34	0.75
3:I:21:DT:C2	4:J:8:DG:N2	2.54	0.75
1:A:77:VAL:HG23	1:A:158:ARG:HB2	1.66	0.75
1:A:222:GLU:CD	1:A:222:GLU:H	1.94	0.75
2:F:409:HIS:CD2	2:F:441:HIS:HA	2.22	0.75
2:F:603:VAL:HG22	2:F:609:ILE:HG12	1.67	0.75
2:B:572:LYS:HZ2	2:B:606:GLN:HG2	1.52	0.75
1:G:218:LYS:NZ	1:G:218:LYS:HB3	2.02	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:572:LYS:HD3	2:H:573:VAL:N	2.02	0.75
1:G:196:ILE:CG1	1:G:272:LEU:HD22	2.17	0.75
1:A:48:GLY:H	1:A:57:THR:HG21	1.50	0.75
1:E:210:ASP:O	1:E:253:ARG:HA	1.87	0.75
1:C:24:ILE:CD1	1:C:62:LYS:HB2	2.15	0.75
2:B:366:GLY:O	2:B:368:PRO:HD3	1.86	0.74
1:E:81:PRO:HB2	1:E:82:PRO:HD3	1.69	0.74
1:C:51:SER:HB3	1:C:57:THR:H	1.51	0.74
1:C:76:LEU:HD13	1:C:90:LEU:HD13	1.70	0.74
1:A:60:THR:OG1	1:A:112:SER:HB3	1.88	0.74
2:B:613:THR:HG22	2:B:614:PRO:O	1.87	0.74
1:A:56:LYS:HB3	2:D:375:ASN:HD21	1.52	0.74
2:H:559:CYS:SG	2:H:650:GLU:HB2	2.28	0.74
4:J:19:DA:H2''	4:J:20:DA:C8	2.23	0.74
2:F:613:THR:HG23	2:F:614:PRO:HD2	1.69	0.74
2:H:545:ALA:HA	2:H:633:ARG:NH2	2.02	0.74
2:F:621:ILE:HD11	2:F:649:PRO:HD3	1.70	0.73
2:H:624:PRO:HB2	2:H:646:LEU:HD11	1.70	0.73
1:G:81:PRO:HB2	1:G:82:PRO:HD3	1.70	0.73
1:A:229:THR:HG23	1:A:269:SER:HB3	1.68	0.73
4:Y:17:DG:H4'	4:Y:17:DG:OP1	1.88	0.73
1:E:158:ARG:HD3	1:E:179:LEU:HD23	1.71	0.73
4:Y:19:DA:C2	4:Y:20:DA:C2	2.77	0.73
1:E:104:LEU:HD21	1:E:163:VAL:HG13	1.71	0.73
1:G:30:ARG:HH21	1:G:191:THR:HB	1.52	0.73
1:G:185:ASP:OD2	1:G:187:ARG:HB3	1.89	0.73
1:A:27:PRO:HG2	1:A:183:ILE:HD11	1.71	0.73
1:C:198:ARG:O	1:C:199:VAL:HG23	1.89	0.73
1:E:27:PRO:HG2	1:E:183:ILE:HD11	1.71	0.73
1:E:36:TYR:CE2	3:I:8:DT:H2''	2.24	0.73
2:F:467:LEU:N	2:F:467:LEU:HD12	2.04	0.73
2:F:646:LEU:HD13	2:F:646:LEU:C	2.14	0.73
2:B:451:LEU:O	2:B:455:MET:HG3	1.87	0.73
1:C:114:GLN:HE21	1:E:241:GLN:HB2	1.53	0.73
1:G:167:ASP:OD1	1:G:169:ALA:HB3	1.89	0.73
2:B:394:ILE:HG22	2:B:422:THR:OG1	1.89	0.72
2:D:387:TYR:CZ	2:D:518:LEU:HD22	2.24	0.72
1:E:23:ILE:HD12	1:E:23:ILE:H	1.53	0.72
1:E:233:TRP:HZ3	1:E:268:VAL:HG11	1.54	0.72
2:D:572:LYS:CE	2:D:606:GLN:HG2	2.19	0.72
1:E:215:LEU:HB3	2:F:604:HIS:CD2	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:23:DT:H2''	4:J:24:DC:C5'	2.20	0.72
1:G:74:ILE:CD1	1:G:161:PHE:CD2	2.72	0.72
1:C:51:SER:CB	1:C:57:THR:H	2.03	0.72
3:X:8:DT:O2	4:Y:21:DA:H2	1.72	0.72
4:J:24:DC:H2''	4:J:25:DC:C5'	2.19	0.72
3:X:22:DT:O2	4:Y:7:DA:H2	1.72	0.72
2:H:377:LYS:O	2:H:377:LYS:HG3	1.90	0.72
1:A:74:ILE:HB	1:A:100:TYR:HB3	1.70	0.72
1:C:21:VAL:HG21	1:C:163:VAL:CG2	2.19	0.72
1:E:207:LEU:HD12	1:E:291:ASP:OD2	1.89	0.72
2:F:409:HIS:CD2	2:F:442:VAL:H	2.08	0.72
2:B:552:ARG:HG3	2:B:553:MET:H	1.55	0.72
1:C:196:ILE:CG1	1:C:272:LEU:HD22	2.20	0.72
1:E:211:GLU:C	1:E:212:ILE:HD13	2.15	0.72
1:G:80:ASP:HB3	1:G:81:PRO:HD2	1.72	0.72
2:B:455:MET:HE2	2:B:469:VAL:HG13	1.71	0.71
2:D:377:LYS:O	2:D:377:LYS:HG3	1.89	0.71
1:A:273:ARG:HD2	1:A:280:LEU:HD21	1.71	0.71
1:E:229:THR:CG2	1:E:269:SER:HB3	2.20	0.71
1:G:185:ASP:O	1:G:187:ARG:N	2.21	0.71
1:G:24:ILE:CD1	1:G:62:LYS:HB2	2.16	0.71
1:A:32:MET:HG3	1:A:47:PRO:CD	2.21	0.71
1:C:185:ASP:OD2	1:C:187:ARG:HB3	1.91	0.71
1:E:25:GLU:HG2	1:E:58:HIS:O	1.90	0.71
1:E:222:GLU:CD	1:E:222:GLU:H	1.99	0.71
2:F:451:LEU:O	2:F:455:MET:HG3	1.91	0.71
1:A:201:ARG:HB3	1:A:212:ILE:HD12	1.73	0.71
1:C:236:ARG:O	1:C:255:PRO:HB3	1.90	0.71
1:G:23:ILE:H	1:G:23:ILE:HD12	1.55	0.71
1:A:48:GLY:H	1:A:57:THR:HG23	1.54	0.71
1:G:223:ASP:OD2	1:G:274:ARG:HG3	1.91	0.71
1:C:80:ASP:HB3	1:C:81:PRO:HD2	1.70	0.71
2:D:452:GLU:OE2	2:D:495:ARG:HG3	1.90	0.71
2:F:363:SER:CB	3:X:26:DA:H3'	2.21	0.70
1:G:132:GLN:O	1:G:136:THR:HG22	1.91	0.70
2:F:402:LYS:H	2:F:402:LYS:CD	2.04	0.70
1:A:244:VAL:HG22	1:A:250:ILE:CD1	2.20	0.70
1:E:19:ALA:HA	1:E:64:ASN:O	1.90	0.70
4:Y:16:DC:C2'	4:Y:17:DG:H5''	2.21	0.70
1:G:51:SER:HB3	1:G:57:THR:H	1.54	0.70
2:H:477:GLN:O	2:H:479:GLU:HG2	1.90	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:509:VAL:HG22	2:H:538:TYR:CD1	2.26	0.70
2:H:544:ASN:OD1	2:H:544:ASN:N	2.25	0.70
2:D:402:LYS:H	2:D:402:LYS:CE	2.05	0.70
2:H:626:SER:OG	2:H:646:LEU:HD23	1.92	0.70
4:Y:16:DC:H2''	4:Y:17:DG:H5''	1.73	0.70
2:F:572:LYS:CE	2:F:606:GLN:HG2	2.20	0.70
1:A:114:GLN:O	1:A:114:GLN:HG2	1.92	0.69
1:A:23:ILE:HD12	1:A:23:ILE:H	1.58	0.69
1:A:200:ASN:O	1:A:201:ARG:HB2	1.91	0.69
4:Y:17:DG:H5''	4:Y:17:DG:H8	1.57	0.69
2:D:509:VAL:HG22	2:D:538:TYR:HD1	1.56	0.69
2:H:353:PHE:CE2	2:H:439:ILE:HG12	2.27	0.69
2:F:559:CYS:SG	2:F:561:THR:HG23	2.33	0.69
1:G:229:THR:CG2	1:G:269:SER:HB3	2.22	0.69
1:E:214:LEU:HD23	1:E:214:LEU:O	1.93	0.69
2:F:618:ASP:OD2	2:F:621:ILE:HG22	1.92	0.69
1:G:114:GLN:O	1:G:115:ASN:ND2	2.24	0.69
1:A:46:ILE:CD1	1:A:118:ILE:HD11	2.23	0.69
1:A:57:THR:HG23	1:A:57:THR:O	1.92	0.69
2:B:580:ILE:HD13	2:B:598:PHE:CE2	2.27	0.69
2:D:387:TYR:CD1	2:D:518:LEU:HD13	2.26	0.69
1:E:226:VAL:HG12	1:E:228:PHE:CE1	2.27	0.69
2:H:566:ILE:HD12	2:H:566:ILE:N	2.08	0.69
4:J:17:DG:H4'	4:J:17:DG:OP1	1.91	0.69
1:A:104:LEU:HD21	1:A:163:VAL:HG13	1.74	0.69
1:G:198:ARG:O	1:G:199:VAL:HG23	1.93	0.69
4:J:25:DC:H2''	4:J:26:DC:C5	2.28	0.69
2:B:561:THR:O	2:B:615:LYS:HG3	1.92	0.69
2:B:618:ASP:OD2	2:B:621:ILE:HG22	1.93	0.69
2:D:572:LYS:NZ	2:D:606:GLN:CG	2.53	0.69
1:A:52:THR:HG22	1:A:53:ASP:N	2.00	0.68
1:G:188:ALA:HB1	1:G:190:ASN:HD21	1.57	0.68
2:H:348:PRO:HA	2:H:368:PRO:O	1.94	0.68
3:X:21:DT:C2	4:Y:8:DG:N2	2.61	0.68
1:A:210:ASP:O	1:A:253:ARG:HA	1.94	0.68
2:B:452:GLU:OE2	2:B:495:ARG:HG3	1.94	0.68
2:B:621:ILE:HD11	2:B:649:PRO:HD3	1.74	0.68
1:C:114:GLN:NE2	1:E:241:GLN:HB2	2.09	0.68
2:H:572:LYS:HD3	2:H:573:VAL:H	1.58	0.68
2:D:348:PRO:HA	2:D:368:PRO:O	1.93	0.68
1:A:215:LEU:HB3	2:B:604:HIS:CD2	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HD12	1:C:23:ILE:H	1.58	0.68
1:C:76:LEU:CD1	1:C:90:LEU:HD13	2.24	0.68
2:F:407:HIS:HD2	2:F:409:HIS:H	1.39	0.68
1:G:187:ARG:O	1:G:187:ARG:HG2	1.94	0.68
2:B:451:LEU:C	2:B:451:LEU:HD13	2.19	0.67
2:D:548:LEU:HD11	2:D:633:ARG:HG3	1.76	0.67
1:G:74:ILE:CD1	1:G:161:PHE:HD2	2.07	0.67
1:G:202:ASN:H	1:G:202:ASN:ND2	1.91	0.67
1:C:114:GLN:HE22	1:E:241:GLN:H	1.40	0.67
1:A:202:ASN:HD22	1:A:202:ASN:N	1.91	0.67
1:C:229:THR:CG2	1:C:269:SER:HB3	2.25	0.67
1:C:40:GLY:C	1:C:42:SER:N	2.47	0.67
1:E:214:LEU:HD23	1:E:214:LEU:C	2.18	0.67
2:H:387:TYR:CZ	2:H:518:LEU:HD22	2.30	0.67
1:A:23:ILE:HD12	1:A:23:ILE:N	2.10	0.67
2:F:550:ILE:HG23	2:F:568:LEU:HD11	1.76	0.67
2:F:584:GLU:O	2:F:591:VAL:HG23	1.95	0.67
1:C:132:GLN:O	1:C:136:THR:HG22	1.95	0.67
1:E:60:THR:HG22	1:E:61:ILE:N	2.08	0.67
1:G:236:ARG:O	1:G:255:PRO:HB3	1.95	0.67
1:A:194:LEU:HD22	1:A:279:GLU:HG3	1.75	0.67
2:B:402:LYS:H	2:B:402:LYS:CE	2.08	0.67
1:C:86:HIS:CE1	1:C:87:PRO:HD2	2.30	0.67
1:A:233:TRP:CD1	1:A:258:ALA:HB2	2.29	0.66
1:A:171:ARG:HE	1:A:171:ARG:HA	1.59	0.66
1:A:262:LEU:HD21	1:A:266:VAL:CG1	2.24	0.66
2:B:504:GLU:HA	2:B:504:GLU:OE1	1.94	0.66
1:C:74:ILE:CD1	1:C:161:PHE:CD2	2.78	0.66
2:F:363:SER:HB2	3:X:26:DA:H3'	1.77	0.66
3:X:1:DA:H2''	3:X:2:DG:O5'	1.95	0.66
1:C:23:ILE:HD12	1:C:23:ILE:N	2.11	0.66
1:G:21:VAL:HG21	1:G:163:VAL:HG21	1.78	0.66
2:H:402:LYS:CD	2:H:402:LYS:H	2.09	0.66
2:H:572:LYS:HZ3	2:H:606:GLN:HG2	1.58	0.66
1:E:244:VAL:HG22	1:E:250:ILE:HD12	1.76	0.66
2:F:434:PHE:HB3	2:F:437:LEU:HD22	1.77	0.66
1:A:74:ILE:HG12	1:A:100:TYR:HD1	1.61	0.66
1:G:66:TYR:CE2	1:G:165:VAL:HB	2.31	0.66
3:I:14:DT:H2''	3:I:15:DG:H5'	1.78	0.66
3:I:23:DT:O2	4:J:6:DA:H2	1.79	0.66
1:A:80:ASP:HB3	1:A:81:PRO:HD2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:VAL:HG21	1:E:179:LEU:HD11	1.78	0.65
2:H:572:LYS:CE	2:H:606:GLN:HG2	2.24	0.65
1:A:81:PRO:HB2	1:A:82:PRO:HD3	1.78	0.65
2:F:580:ILE:HD13	2:F:598:PHE:CE2	2.31	0.65
1:C:54:THR:OG1	1:C:55:THR:HG23	1.97	0.65
1:E:199:VAL:CG1	1:E:201:ARG:O	2.45	0.65
1:C:239:PHE:HB3	1:C:252:PHE:CB	2.27	0.65
1:A:79:LYS:O	1:A:158:ARG:NE	2.30	0.65
2:B:366:GLY:O	2:B:367:LEU:C	2.36	0.65
4:Y:23:DT:H2''	4:Y:24:DC:C5'	2.27	0.65
3:I:7:DT:C2	4:J:22:DG:N2	2.65	0.65
1:G:86:HIS:ND1	1:G:87:PRO:HD2	2.11	0.65
2:F:395:VAL:HB	2:F:421:CYS:HB3	1.77	0.65
2:B:467:LEU:N	2:B:467:LEU:HD12	2.12	0.65
1:C:202:ASN:H	1:C:202:ASN:ND2	1.95	0.65
1:G:185:ASP:C	1:G:187:ARG:N	2.55	0.65
1:G:215:LEU:HB3	2:H:604:HIS:CD2	2.32	0.65
2:H:646:LEU:HD13	2:H:646:LEU:C	2.21	0.65
1:E:32:MET:SD	1:E:47:PRO:HD3	2.37	0.64
3:X:23:DT:O2	4:Y:6:DA:C2	2.50	0.64
1:E:171:ARG:HE	1:E:171:ARG:HA	1.60	0.64
2:D:636:ASP:OD2	2:D:638:GLU:HG2	1.96	0.64
1:C:202:ASN:H	1:C:202:ASN:HD22	1.42	0.64
1:E:108:ARG:HD2	1:E:110:ILE:O	1.98	0.64
2:D:554:ASP:OD2	2:D:567:TYR:HB2	1.98	0.64
2:F:550:ILE:HD11	2:F:640:SER:OG	1.97	0.64
1:A:68:GLY:HA2	1:A:106:PRO:O	1.98	0.64
2:D:592:TRP:CD1	2:D:617:LYS:HB3	2.33	0.64
1:E:118:ILE:N	1:E:118:ILE:HD12	2.13	0.64
1:A:199:VAL:CG1	1:A:201:ARG:O	2.45	0.64
2:B:621:ILE:CD1	2:B:649:PRO:HB3	2.28	0.64
2:D:407:HIS:ND1	2:D:510:VAL:HG23	2.13	0.64
1:C:27:PRO:CG	1:C:183:ILE:HD11	2.28	0.64
1:A:218:LYS:NZ	1:A:218:LYS:HB3	2.13	0.63
2:B:603:VAL:HG22	2:B:609:ILE:HG12	1.78	0.63
1:E:60:THR:OG1	1:E:112:SER:HB3	1.97	0.63
2:D:402:LYS:H	2:D:402:LYS:CD	2.11	0.63
2:F:451:LEU:CD1	2:F:498:ALA:HA	2.27	0.63
2:F:572:LYS:HD3	2:F:606:GLN:HB3	1.79	0.63
2:F:613:THR:HG22	2:F:614:PRO:O	1.99	0.63
4:J:2:DT:H1'	4:J:3:DG:H5''	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:THR:OG1	1:C:112:SER:HB3	1.99	0.63
2:F:580:ILE:N	2:F:580:ILE:HD12	2.14	0.63
1:G:21:VAL:HG21	1:G:163:VAL:CG2	2.28	0.63
1:A:77:VAL:HG21	1:A:179:LEU:HD11	1.80	0.63
2:B:646:LEU:C	2:B:646:LEU:HD13	2.23	0.63
2:H:543:PRO:HD2	2:H:544:ASN:OD1	1.98	0.63
2:H:572:LYS:NZ	2:H:606:GLN:CG	2.50	0.63
4:Y:20:DA:N1	4:Y:21:DA:C6	2.66	0.63
1:A:60:THR:HG22	1:A:61:ILE:N	2.14	0.63
1:E:68:GLY:HA2	1:E:106:PRO:O	1.99	0.63
1:E:185:ASP:OD2	1:E:187:ARG:HB2	1.98	0.63
1:E:244:VAL:HG22	1:E:250:ILE:CD1	2.29	0.63
4:Y:17:DG:H5''	4:Y:17:DG:C8	2.34	0.63
2:D:646:LEU:HD13	2:D:646:LEU:C	2.24	0.63
2:F:455:MET:HE2	2:F:469:VAL:HG13	1.81	0.63
2:H:633:ARG:NH1	2:H:638:GLU:HB2	2.14	0.63
4:Y:20:DA:C6	4:Y:21:DA:N6	2.66	0.63
2:D:566:ILE:HD12	2:D:566:ILE:N	2.13	0.63
4:Y:19:DA:H2''	4:Y:20:DA:C8	2.33	0.63
1:A:233:TRP:HZ3	1:A:268:VAL:HG11	1.64	0.63
1:E:199:VAL:HG12	1:E:201:ARG:H	1.64	0.63
1:G:30:ARG:NE	1:G:191:THR:HB	2.14	0.63
4:J:19:DA:C2	4:J:20:DA:C2	2.87	0.63
2:B:580:ILE:HD12	2:B:580:ILE:N	2.14	0.62
1:C:74:ILE:CD1	1:C:161:PHE:HD2	2.12	0.62
1:C:105:CYS:SG	1:C:107:ASP:OD1	2.57	0.62
1:A:214:LEU:C	1:A:214:LEU:HD23	2.23	0.62
1:C:233:TRP:HZ3	1:C:268:VAL:HG11	1.64	0.62
4:Y:23:DT:C2'	4:Y:24:DC:H5''	2.29	0.62
1:E:51:SER:CB	1:E:57:THR:HB	2.27	0.62
1:G:46:ILE:HD11	1:G:118:ILE:HD13	1.81	0.62
2:H:473:LEU:HD13	2:H:493:ILE:HG21	1.81	0.62
2:H:549:LYS:HB3	2:H:571:ASP:OD1	1.99	0.62
1:G:233:TRP:HZ3	1:G:268:VAL:HG11	1.65	0.62
2:B:454:ARG:HG2	2:B:454:ARG:HH11	1.64	0.62
2:B:559:CYS:SG	2:B:650:GLU:HB2	2.40	0.62
2:D:477:GLN:O	2:D:479:GLU:HG2	1.99	0.62
2:F:355:PHE:CD2	2:F:539:ASP:HB2	2.35	0.62
2:F:409:HIS:HD2	2:F:442:VAL:H	1.44	0.62
1:G:262:LEU:HD21	1:G:266:VAL:CG1	2.29	0.62
2:D:629:VAL:HG12	2:D:643:LYS:O	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ILE:CD1	1:E:118:ILE:HD11	2.26	0.62
2:F:555:ARG:HG2	2:F:555:ARG:HH11	1.64	0.62
1:G:19:ALA:O	1:G:175:LEU:HD22	1.99	0.62
4:J:23:DT:C2'	4:J:24:DC:H5''	2.29	0.62
2:B:552:ARG:HG3	2:B:553:MET:N	2.13	0.62
2:B:342:LEU:HD13	2:B:343:GLN:H	1.63	0.62
2:B:613:THR:HG23	2:B:614:PRO:HD2	1.82	0.62
2:H:561:THR:O	2:H:615:LYS:HG3	2.00	0.62
2:H:618:ASP:OD2	2:H:621:ILE:HG22	2.00	0.62
1:A:132:GLN:O	1:A:136:THR:HG22	1.99	0.61
1:A:185:ASP:C	1:A:187:ARG:N	2.57	0.61
2:B:555:ARG:HH11	2:B:555:ARG:HG2	1.65	0.61
2:D:572:LYS:HZ3	2:D:606:GLN:HG2	1.64	0.61
1:E:80:ASP:HB3	1:E:81:PRO:HD2	1.81	0.61
1:A:214:LEU:HD23	1:A:214:LEU:O	2.00	0.61
1:C:88:HIS:NE2	1:C:120:CYS:HB2	2.15	0.61
1:C:262:LEU:HD21	1:C:266:VAL:CG1	2.30	0.61
1:A:199:VAL:HG12	1:A:201:ARG:H	1.64	0.61
1:C:88:HIS:CE1	1:C:121:VAL:H	2.18	0.61
2:D:518:LEU:O	2:D:527:ARG:HG3	1.99	0.61
2:F:573:VAL:HG22	2:F:606:GLN:O	2.00	0.61
2:D:489:ARG:HD3	2:D:489:ARG:C	2.25	0.61
2:F:551:VAL:HG12	2:F:552:ARG:N	2.14	0.61
1:A:52:THR:CG2	1:A:53:ASP:H	2.01	0.61
2:B:451:LEU:O	2:B:451:LEU:HD13	2.00	0.61
2:D:348:PRO:HG3	2:D:512:LEU:HD12	1.82	0.61
1:E:27:PRO:CG	1:E:183:ILE:HD11	2.30	0.61
1:E:185:ASP:C	1:E:187:ARG:N	2.57	0.61
1:G:108:ARG:HD2	1:G:110:ILE:O	2.01	0.61
1:C:30:ARG:HH21	1:C:191:THR:HB	1.64	0.61
4:Y:25:DC:H2''	4:Y:26:DC:C5	2.36	0.61
2:D:382:VAL:HG12	2:D:383:LYS:N	2.13	0.61
1:E:194:LEU:HD22	1:E:279:GLU:HG3	1.82	0.61
2:F:444:LYS:O	2:F:447:VAL:HG23	2.00	0.61
1:G:236:ARG:HH11	1:G:236:ARG:CG	2.12	0.61
4:J:20:DA:N1	4:J:21:DA:C6	2.68	0.61
1:C:28:LYS:N	1:C:48:GLY:O	2.34	0.61
2:H:443:THR:O	2:H:447:VAL:HG23	2.01	0.61
2:D:583:TYR:CD1	2:D:583:TYR:C	2.78	0.61
1:G:218:LYS:HB3	1:G:218:LYS:HZ3	1.65	0.61
2:H:407:HIS:HD2	2:H:409:HIS:H	1.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG22	1:A:250:ILE:HD12	1.82	0.61
2:F:631:LEU:HB2	2:F:640:SER:HB3	1.83	0.61
1:G:282:GLU:HG2	1:G:283:PRO:CD	2.21	0.61
1:E:25:GLU:OE2	1:E:50:ARG:CG	2.49	0.60
1:A:185:ASP:OD2	1:A:187:ARG:HB2	2.01	0.60
2:D:391:ALA:HB3	2:D:425:ALA:HB3	1.81	0.60
3:I:22:DT:O2	4:J:7:DA:C2	2.48	0.60
1:A:229:THR:CG2	1:A:269:SER:HB3	2.31	0.60
1:C:217:ASP:O	1:C:219:VAL:HG13	2.01	0.60
2:D:451:LEU:C	2:D:451:LEU:HD13	2.27	0.60
1:E:23:ILE:HD12	1:E:23:ILE:N	2.16	0.60
2:F:624:PRO:HB2	2:F:646:LEU:HD11	1.83	0.60
1:A:211:GLU:C	1:A:212:ILE:HD13	2.27	0.60
2:D:571:ASP:O	2:D:572:LYS:C	2.45	0.60
1:E:88:HIS:NE2	1:E:120:CYS:HB3	2.16	0.60
2:H:476:LEU:HD22	2:H:483:ASP:HB2	1.84	0.60
2:H:489:ARG:HD3	2:H:489:ARG:C	2.27	0.60
1:E:57:THR:HG23	1:E:57:THR:O	2.01	0.60
1:E:58:HIS:HE1	1:E:114:GLN:NE2	2.00	0.60
1:A:48:GLY:HA3	1:A:57:THR:OG1	2.01	0.60
1:C:273:ARG:O	1:C:275:PRO:HD3	2.02	0.60
1:E:54:THR:HG22	1:E:54:THR:O	2.02	0.60
2:F:443:THR:HA	4:J:22:DG:OP2	2.01	0.60
1:E:77:VAL:HG22	1:E:158:ARG:O	2.01	0.60
1:G:48:GLY:HA3	1:G:57:THR:OG1	2.00	0.60
4:Y:17:DG:H8	4:Y:17:DG:C5'	2.13	0.60
1:A:58:HIS:HB3	1:A:112:SER:HB2	1.82	0.60
1:E:95:CYS:SG	1:E:100:TYR:HB2	2.41	0.60
1:A:60:THR:HG23	1:A:111:HIS:C	2.27	0.59
2:B:636:ASP:OD2	2:B:638:GLU:HG2	2.02	0.59
1:E:158:ARG:NH1	1:E:182:PRO:HD3	2.16	0.59
2:H:509:VAL:HG22	2:H:538:TYR:HD1	1.66	0.59
1:A:55:THR:HG22	1:A:56:LYS:N	2.17	0.59
1:A:77:VAL:HG22	1:A:158:ARG:O	2.01	0.59
2:B:550:ILE:N	2:B:550:ILE:HD12	2.16	0.59
2:F:409:HIS:NE2	2:F:441:HIS:HA	2.17	0.59
1:G:88:HIS:CE1	1:G:120:CYS:CB	2.83	0.59
1:G:171:ARG:HE	1:G:172:PRO:CD	2.15	0.59
1:C:114:GLN:O	1:C:115:ASN:ND2	2.36	0.59
2:D:572:LYS:HD3	2:D:573:VAL:N	2.17	0.59
1:E:32:MET:HG3	1:E:47:PRO:CD	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:CYS:HA	1:E:288:TYR:CD1	2.38	0.59
2:H:571:ASP:O	2:H:573:VAL:HG13	2.02	0.59
2:D:380:PRO:O	2:D:433:GLY:HA2	2.03	0.59
2:F:646:LEU:HD13	2:F:647:TYR:N	2.16	0.59
3:X:5:DA:C2	3:X:6:DC:N3	2.70	0.59
1:C:40:GLY:O	1:C:41:ARG:C	2.43	0.59
1:G:20:TYR:CE1	1:G:64:ASN:HB2	2.38	0.59
4:Y:22:DG:H2''	4:Y:23:DT:OP2	2.03	0.59
1:A:88:HIS:CE1	1:A:120:CYS:HB2	2.38	0.59
2:D:458:ALA:O	2:D:465:PRO:HG3	2.01	0.59
3:X:8:DT:C2	4:Y:21:DA:H2	2.19	0.59
1:A:108:ARG:HD2	1:A:110:ILE:O	2.02	0.59
1:E:171:ARG:HE	1:E:172:PRO:CD	2.16	0.59
2:H:507:LEU:HD12	2:H:507:LEU:N	2.18	0.59
1:E:202:ASN:HD22	1:E:202:ASN:N	1.94	0.58
1:E:236:ARG:HH11	1:E:236:ARG:CG	2.16	0.58
1:G:88:HIS:ND1	1:G:120:CYS:HA	2.18	0.58
1:G:27:PRO:CG	1:G:183:ILE:HD11	2.33	0.58
1:A:32:MET:HG3	1:A:47:PRO:HD3	1.85	0.58
2:F:583:TYR:CD1	2:F:583:TYR:C	2.80	0.58
1:G:51:SER:HB2	1:G:56:LYS:HA	1.86	0.58
2:B:434:PHE:HB3	2:B:437:LEU:HD22	1.86	0.58
1:C:171:ARG:HE	1:C:172:PRO:CD	2.17	0.58
1:C:215:LEU:HB3	2:D:604:HIS:CD2	2.39	0.58
1:E:74:ILE:HD12	1:E:161:PHE:CD2	2.38	0.58
1:G:144:PRO:O	1:G:148:GLN:HG3	2.03	0.58
2:H:395:VAL:HB	2:H:421:CYS:HB3	1.85	0.58
2:F:444:LYS:HB2	4:J:22:DG:OP1	2.04	0.58
2:F:464:ASN:ND2	2:F:528:ARG:NH1	2.51	0.58
2:H:407:HIS:CE1	2:H:510:VAL:HG23	2.38	0.58
2:B:572:LYS:CE	2:B:606:GLN:HG2	2.32	0.58
1:C:206:CYS:HA	1:C:288:TYR:CD1	2.38	0.58
1:G:198:ARG:HD2	2:H:567:TYR:OH	2.04	0.58
2:H:380:PRO:O	2:H:433:GLY:HA2	2.03	0.58
3:I:1:DA:H2''	3:I:2:DG:O5'	2.03	0.58
2:H:632:ARG:HG3	2:H:639:THR:HG22	1.84	0.57
1:A:236:ARG:HH11	1:A:236:ARG:CG	2.12	0.57
1:E:84:ARG:HG2	1:E:143:VAL:HG11	1.85	0.57
1:G:30:ARG:NH2	1:G:191:THR:HB	2.17	0.57
1:G:88:HIS:NE2	1:G:120:CYS:HB2	2.19	0.57
2:H:625:ALA:O	2:H:646:LEU:HD22	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:6:DC:N4	4:J:22:DG:H1	2.01	0.57
1:A:84:ARG:HG2	1:A:143:VAL:HG11	1.86	0.57
1:E:185:ASP:O	1:E:187:ARG:N	2.35	0.57
2:H:382:VAL:HG12	2:H:383:LYS:N	2.16	0.57
3:X:22:DT:C2	4:Y:7:DA:H2	2.21	0.57
1:G:86:HIS:CE1	1:G:87:PRO:HD2	2.39	0.57
2:D:464:ASN:ND2	2:D:528:ARG:NH1	2.53	0.57
2:D:646:LEU:HD13	2:D:647:TYR:N	2.19	0.57
1:E:262:LEU:O	1:E:290:PRO:HB3	2.03	0.57
2:F:412:VAL:HG22	2:F:413:GLY:N	2.20	0.57
2:B:490:GLU:O	2:B:494:ILE:HG12	2.05	0.57
1:E:76:LEU:HD13	1:E:90:LEU:HD22	1.85	0.57
1:G:36:TYR:CD1	1:G:36:TYR:N	2.73	0.57
1:G:245:HIS:HB3	1:G:249:ALA:HB3	1.86	0.57
1:A:78:THR:O	1:A:158:ARG:HD2	2.04	0.57
2:B:454:ARG:HG2	2:B:454:ARG:NH1	2.18	0.57
2:F:504:GLU:OE1	2:F:504:GLU:HA	2.05	0.57
3:X:7:DT:N3	4:Y:22:DG:N2	2.53	0.57
1:C:156:ALA:O	1:C:157:VAL:HG13	2.05	0.57
2:F:500:GLN:O	2:F:503:LYS:HG2	2.05	0.57
1:G:219:VAL:O	1:G:247:GLN:HB3	2.05	0.57
2:D:353:PHE:HE2	2:D:439:ILE:HG12	1.68	0.57
1:E:26:GLN:HB3	1:E:181:HIS:NE2	2.19	0.57
2:H:354:ARG:HD2	2:H:356:ARG:HD3	1.87	0.57
1:A:55:THR:CG2	1:A:56:LYS:N	2.68	0.56
1:A:72:VAL:O	1:A:101:GLU:HA	2.05	0.56
1:C:58:HIS:HB3	1:C:59:PRO:HD2	1.86	0.56
1:E:52:THR:HG22	1:E:53:ASP:N	2.14	0.56
1:E:62:LYS:HE2	1:E:64:ASN:ND2	2.20	0.56
1:G:76:LEU:HD13	1:G:90:LEU:HD13	1.85	0.56
4:Y:5:DA:H2"	4:Y:6:DA:C8	2.39	0.56
4:J:19:DA:N3	4:J:20:DA:C5	2.73	0.56
2:B:384:ILE:HD12	2:B:430:MET:HE3	1.86	0.56
1:E:74:ILE:HG12	1:E:100:TYR:CD1	2.39	0.56
1:E:262:LEU:HD21	1:E:266:VAL:CG1	2.27	0.56
2:B:355:PHE:CD2	2:B:539:ASP:HB2	2.41	0.56
2:B:550:ILE:HD11	2:B:640:SER:OG	2.06	0.56
1:C:167:ASP:HB2	1:C:168:PRO:HD2	1.86	0.56
1:E:48:GLY:N	1:E:57:THR:HG21	2.17	0.56
1:E:132:GLN:O	1:E:136:THR:HG22	2.06	0.56
1:G:46:ILE:HD11	1:G:118:ILE:CD1	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:HIS:CG	1:G:87:PRO:HD2	2.40	0.56
2:H:504:GLU:OE1	2:H:504:GLU:HA	2.04	0.56
2:H:583:TYR:HA	2:H:592:TRP:O	2.04	0.56
2:B:559:CYS:SG	2:B:561:THR:HG23	2.46	0.56
2:D:460:ILE:HG12	2:D:486:LEU:HD13	1.87	0.56
1:G:30:ARG:HH21	1:G:191:THR:CB	2.17	0.56
2:D:509:VAL:HG22	2:D:538:TYR:CD1	2.39	0.56
2:D:571:ASP:O	2:D:573:VAL:HG13	2.04	0.56
2:D:584:GLU:O	2:D:591:VAL:HG23	2.06	0.56
1:E:26:GLN:OE1	1:E:180:SER:HB2	2.04	0.56
2:F:451:LEU:HD11	2:F:498:ALA:HA	1.88	0.56
2:B:409:HIS:CD2	2:B:442:VAL:H	2.23	0.56
2:D:544:ASN:OD1	2:D:544:ASN:N	2.33	0.56
2:F:423:VAL:CG2	2:F:432:VAL:HG11	2.34	0.56
1:C:236:ARG:HG3	1:C:236:ARG:NH1	2.19	0.56
1:E:82:PRO:O	1:E:84:ARG:N	2.37	0.56
2:H:646:LEU:HD13	2:H:647:TYR:N	2.21	0.56
2:D:500:GLN:HE21	2:D:503:LYS:HE2	1.71	0.56
2:H:482:GLY:O	2:H:483:ASP:HB2	2.06	0.56
4:Y:20:DA:C6	4:Y:21:DA:C6	2.94	0.56
1:A:288:TYR:O	1:A:289:LEU:HD23	2.05	0.56
2:B:464:ASN:N	2:B:465:PRO:HD3	2.20	0.56
1:E:72:VAL:O	1:E:101:GLU:HA	2.05	0.56
1:G:54:THR:OG1	1:G:55:THR:HG23	2.06	0.56
1:A:187:ARG:O	1:A:189:PRO:HD3	2.06	0.56
1:A:273:ARG:O	1:A:275:PRO:HD3	2.06	0.56
1:C:30:ARG:NE	1:C:191:THR:HB	2.20	0.56
1:C:36:TYR:N	1:C:36:TYR:CD1	2.74	0.56
1:G:47:PRO:O	1:G:48:GLY:O	2.24	0.56
1:G:181:HIS:HB2	1:G:182:PRO:HD2	1.88	0.56
1:G:194:LEU:HD22	1:G:279:GLU:HG3	1.87	0.56
1:G:261:SER:O	1:G:262:LEU:C	2.48	0.56
3:X:6:DC:H42	4:Y:22:DG:H1	1.51	0.56
1:A:26:GLN:O	1:A:49:GLU:HB2	2.06	0.55
2:B:583:TYR:CD1	2:B:583:TYR:C	2.84	0.55
1:C:181:HIS:HB2	1:C:182:PRO:HD2	1.88	0.55
2:F:467:LEU:N	2:F:467:LEU:CD1	2.68	0.55
1:A:86:HIS:CG	1:A:157:VAL:HG12	2.40	0.55
1:A:88:HIS:CG	1:A:120:CYS:HA	2.41	0.55
1:A:222:GLU:CD	1:A:222:GLU:N	2.64	0.55
2:F:550:ILE:H	2:F:550:ILE:CD1	2.17	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:ILE:N	1:G:60:THR:O	2.39	0.55
3:I:21:DT:H6	3:I:21:DT:H5'	1.69	0.55
2:F:451:LEU:HD13	2:F:451:LEU:C	2.30	0.55
1:G:40:GLY:C	1:G:42:SER:N	2.60	0.55
2:B:508:SER:C	2:B:509:VAL:HG23	2.32	0.55
2:F:618:ASP:CG	2:F:621:ILE:HG22	2.31	0.55
1:A:282:GLU:HG2	1:A:283:PRO:HD2	1.87	0.55
2:B:511:ARG:HG2	2:B:536:ALA:HA	1.89	0.55
2:D:416:CYS:SG	2:D:421:CYS:HB2	2.46	0.55
1:E:30:ARG:HE	1:E:191:THR:HB	1.72	0.55
2:F:363:SER:HB3	3:X:26:DA:H3'	1.88	0.55
2:F:489:ARG:HD3	2:F:489:ARG:C	2.32	0.55
1:G:30:ARG:NE	1:G:191:THR:O	2.40	0.55
1:E:74:ILE:HB	1:E:100:TYR:HB3	1.89	0.55
1:G:27:PRO:HG2	1:G:183:ILE:HD11	1.89	0.55
3:I:23:DT:O2	4:J:6:DA:C2	2.58	0.55
1:A:77:VAL:CG2	1:A:158:ARG:HB2	2.36	0.55
1:A:262:LEU:O	1:A:290:PRO:HB3	2.07	0.55
2:D:477:GLN:O	2:D:482:GLY:HA3	2.07	0.55
1:E:46:ILE:HG22	1:E:47:PRO:O	2.06	0.55
2:F:631:LEU:O	2:F:639:THR:HA	2.07	0.55
1:G:51:SER:HB2	1:G:57:THR:H	1.69	0.55
2:H:584:GLU:O	2:H:591:VAL:HG23	2.07	0.55
3:X:14:DT:H2''	3:X:15:DG:H5'	1.88	0.55
4:Y:2:DT:H1'	4:Y:3:DG:H5''	1.89	0.55
1:A:82:PRO:O	1:A:84:ARG:N	2.39	0.55
2:D:568:LEU:C	2:D:568:LEU:HD23	2.30	0.55
2:F:464:ASN:N	2:F:465:PRO:HD3	2.21	0.55
2:F:632:ARG:HG3	2:F:639:THR:HG22	1.89	0.55
1:G:188:ALA:HB1	1:G:190:ASN:ND2	2.22	0.55
2:H:458:ALA:O	2:H:465:PRO:HG3	2.07	0.55
4:Y:24:DC:H2''	4:Y:25:DC:C5'	2.32	0.55
1:A:202:ASN:N	1:A:202:ASN:ND2	2.55	0.55
2:B:568:LEU:O	2:B:608:ALA:HA	2.06	0.55
1:E:158:ARG:HD3	1:E:179:LEU:CD2	2.37	0.55
1:E:237:GLY:HA2	1:E:255:PRO:HD3	1.89	0.55
2:F:545:ALA:C	2:F:633:ARG:NH2	2.64	0.55
1:A:27:PRO:CG	1:A:183:ILE:HD11	2.37	0.54
1:C:24:ILE:HD11	1:C:110:ILE:HG12	1.89	0.54
1:C:201:ARG:HB3	1:C:212:ILE:HD12	1.89	0.54
1:C:218:LYS:NZ	1:C:218:LYS:HB3	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:PHE:CZ	1:C:254:THR:HG22	2.42	0.54
2:D:353:PHE:CD2	2:D:367:LEU:HD21	2.41	0.54
1:E:60:THR:CG2	1:E:61:ILE:N	2.70	0.54
1:E:81:PRO:O	1:E:83:HIS:N	2.40	0.54
1:G:167:ASP:HB2	1:G:168:PRO:HD2	1.89	0.54
1:A:34:PHE:CD1	1:A:34:PHE:N	2.75	0.54
1:C:108:ARG:HD2	1:C:110:ILE:O	2.06	0.54
2:F:572:LYS:HZ3	2:F:606:GLN:HG2	1.63	0.54
2:F:633:ARG:O	2:F:637:LEU:HA	2.06	0.54
1:G:171:ARG:HE	1:G:171:ARG:HA	1.72	0.54
1:A:65:GLY:O	1:A:66:TYR:HB2	2.07	0.54
2:B:342:LEU:HD12	2:B:532:VAL:CG1	2.37	0.54
1:E:222:GLU:CD	1:E:222:GLU:N	2.65	0.54
1:G:171:ARG:HE	1:G:172:PRO:HD2	1.72	0.54
2:H:534:SER:C	2:H:535:ASP:O	2.50	0.54
1:C:59:PRO:O	1:C:112:SER:HA	2.07	0.54
2:F:550:ILE:N	2:F:550:ILE:CD1	2.66	0.54
2:H:393:VAL:HG21	2:H:432:VAL:HG21	1.89	0.54
2:H:402:LYS:H	2:H:402:LYS:HE3	1.73	0.54
1:A:51:SER:CB	1:A:57:THR:HB	2.32	0.54
1:A:144:PRO:O	1:A:148:GLN:HG3	2.07	0.54
1:A:246:ARG:HB3	2:B:607:PHE:CD2	2.41	0.54
1:C:58:HIS:HB3	1:C:59:PRO:CD	2.38	0.54
1:C:187:ARG:O	1:C:187:ARG:HG2	2.06	0.54
1:E:58:HIS:HB3	1:E:112:SER:HB2	1.90	0.54
1:E:282:GLU:HG2	1:E:283:PRO:HD2	1.90	0.54
4:Y:16:DC:H2''	4:Y:17:DG:C5'	2.35	0.54
1:A:88:HIS:CE1	1:A:120:CYS:CB	2.91	0.54
2:B:572:LYS:HD3	2:B:606:GLN:HB3	1.88	0.54
1:G:171:ARG:NE	1:G:172:PRO:HD2	2.23	0.54
2:F:346:GLU:OE1	2:F:378:SER:OG	2.26	0.54
2:H:397:LEU:HD21	2:H:411:LEU:HD13	1.88	0.54
4:J:4:DG:H2''	4:J:5:DA:H5''	1.90	0.54
1:A:88:HIS:CE1	1:A:121:VAL:H	2.25	0.54
2:B:425:ALA:O	2:B:426:GLY:O	2.25	0.54
2:B:443:THR:HA	4:Y:22:DG:OP2	2.08	0.54
1:C:27:PRO:O	1:C:181:HIS:HE1	1.91	0.54
2:D:559:CYS:SG	2:D:650:GLU:HB2	2.47	0.54
2:H:392:LYS:HB3	2:H:517:PHE:HB2	1.88	0.54
2:H:452:GLU:OE2	2:H:495:ARG:HG3	2.08	0.54
4:J:20:DA:C6	4:J:21:DA:N6	2.75	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:ARG:HG3	2:B:639:THR:HG22	1.89	0.54
2:D:414:LYS:O	2:D:415:HIS:HB2	2.08	0.54
2:F:448:PHE:HA	2:F:502:THR:HG21	1.89	0.54
2:H:568:LEU:HD23	2:H:568:LEU:C	2.31	0.54
1:A:26:GLN:HB3	1:A:181:HIS:NE2	2.23	0.54
2:D:398:VAL:HG23	2:D:511:ARG:HB2	1.90	0.54
1:G:194:LEU:HB3	1:G:281:SER:HB3	1.89	0.54
2:H:583:TYR:CD1	2:H:583:TYR:C	2.85	0.54
2:H:587:GLU:HA	2:H:587:GLU:OE1	2.08	0.54
1:C:88:HIS:CE1	1:C:120:CYS:CB	2.88	0.53
1:C:171:ARG:HE	1:C:172:PRO:HD2	1.71	0.53
1:E:48:GLY:H	1:E:57:THR:HG23	1.69	0.53
1:G:257:TYR:CG	1:G:258:ALA:N	2.75	0.53
2:H:346:GLU:OE2	2:H:379:TYR:O	2.26	0.53
3:I:21:DT:H2''	3:I:22:DT:H5'	1.90	0.53
1:C:19:ALA:HA	1:C:64:ASN:O	2.08	0.53
1:C:236:ARG:HH11	1:C:236:ARG:CG	2.20	0.53
1:C:261:SER:O	1:C:262:LEU:C	2.51	0.53
1:E:158:ARG:HG2	1:E:158:ARG:HH11	1.72	0.53
2:F:552:ARG:HG3	2:F:553:MET:N	2.24	0.53
1:G:51:SER:HA	1:G:57:THR:HG23	1.89	0.53
3:X:7:DT:H3	4:Y:22:DG:N2	2.06	0.53
2:B:402:LYS:H	2:B:402:LYS:CD	2.21	0.53
3:X:21:DT:H6	3:X:21:DT:H5'	1.73	0.53
1:C:86:HIS:CG	1:C:87:PRO:HD2	2.43	0.53
4:J:16:DC:H2'	4:J:17:DG:H5''	1.88	0.53
1:A:60:THR:HG21	1:A:110:ILE:HG23	1.90	0.53
2:D:572:LYS:HE2	2:D:606:GLN:HG2	1.88	0.53
2:F:646:LEU:C	2:F:646:LEU:CD1	2.81	0.53
2:H:375:ASN:O	2:H:376:LYS:CB	2.56	0.53
2:H:444:LYS:HA	2:H:447:VAL:HG23	1.90	0.53
4:J:17:DG:H5''	4:J:17:DG:H8	1.73	0.53
2:D:375:ASN:O	2:D:376:LYS:CB	2.57	0.53
4:J:1:DT:H2''	4:J:2:DT:O5'	2.08	0.53
4:Y:9:DT:H2''	4:Y:10:DC:H5'	1.85	0.53
1:A:194:LEU:HB3	1:A:281:SER:HB3	1.90	0.53
2:B:342:LEU:HD12	2:B:532:VAL:HG11	1.90	0.53
2:D:377:LYS:O	2:D:377:LYS:CG	2.57	0.53
1:E:132:GLN:O	1:E:132:GLN:HG2	2.07	0.53
1:E:215:LEU:N	1:E:215:LEU:HD23	2.24	0.53
2:H:558:GLY:O	2:H:647:TYR:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:24:DC:H1'	4:J:25:DC:H5''	1.91	0.53
2:B:409:HIS:HD2	2:B:442:VAL:H	1.55	0.53
2:B:451:LEU:CD1	2:B:498:ALA:HA	2.39	0.53
1:C:27:PRO:HG2	1:C:183:ILE:HD11	1.90	0.53
2:D:616:TYR:CZ	2:D:617:LYS:HG2	2.44	0.53
1:E:65:GLY:O	1:E:66:TYR:HB2	2.09	0.53
4:J:17:DG:H2''	4:J:18:DG:H8	1.73	0.53
1:C:34:PHE:CD1	1:C:118:ILE:HG21	2.44	0.52
1:C:46:ILE:HD13	1:C:116:LEU:O	2.10	0.52
1:C:114:GLN:NE2	1:E:241:GLN:H	2.06	0.52
1:C:222:GLU:CD	1:C:222:GLU:H	2.17	0.52
2:D:470:HIS:HD2	2:D:472:ASP:OD1	1.91	0.52
2:D:482:GLY:O	2:D:483:ASP:HB2	2.09	0.52
1:E:79:LYS:O	1:E:158:ARG:NE	2.24	0.52
1:E:273:ARG:CD	1:E:280:LEU:HD21	2.39	0.52
2:F:508:SER:C	2:F:509:VAL:HG23	2.34	0.52
4:Y:17:DG:C8	4:Y:17:DG:C5'	2.92	0.52
4:J:22:DG:H2''	4:J:23:DT:OP2	2.09	0.52
2:D:545:ALA:CA	2:D:633:ARG:NH2	2.71	0.52
1:G:104:LEU:HD21	1:G:163:VAL:HG13	1.91	0.52
1:G:126:LEU:O	1:G:129:ALA:HB3	2.08	0.52
1:G:202:ASN:HD22	1:G:202:ASN:N	1.95	0.52
2:H:464:ASN:N	2:H:465:PRO:HD3	2.24	0.52
2:D:626:SER:OG	2:D:646:LEU:HD23	2.08	0.52
1:E:122:LYS:C	1:E:124:ARG:H	2.17	0.52
1:G:199:VAL:HG12	1:G:201:ARG:H	1.75	0.52
2:H:509:VAL:CG2	2:H:538:TYR:CD1	2.92	0.52
2:D:394:ILE:CG1	2:D:515:THR:HB	2.39	0.52
1:E:23:ILE:HD11	1:E:178:VAL:HG22	1.91	0.52
1:G:156:ALA:HA	1:G:183:ILE:O	2.10	0.52
1:G:198:ARG:HB3	2:H:567:TYR:OH	2.10	0.52
2:H:377:LYS:O	2:H:377:LYS:CG	2.57	0.52
2:H:402:LYS:H	2:H:402:LYS:CE	2.23	0.52
1:A:118:ILE:N	1:A:118:ILE:HD12	2.23	0.52
1:C:185:ASP:C	1:C:187:ARG:H	2.16	0.52
2:D:356:ARG:O	2:D:440:LEU:HD12	2.10	0.52
2:D:381:GLN:HA	2:D:432:VAL:O	2.10	0.52
2:D:621:ILE:HG12	2:D:623:LYS:O	2.10	0.52
1:G:196:ILE:HG12	1:G:272:LEU:CD2	2.39	0.52
3:X:15:DG:C3'	3:X:16:DG:H5''	2.39	0.52
1:C:75:SER:HB3	1:C:162:GLN:NE2	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:515:THR:OG1	2:F:531:PRO:HB3	2.09	0.52
4:J:17:DG:C2'	4:J:18:DG:H8	2.22	0.52
2:D:534:SER:C	2:D:535:ASP:O	2.52	0.52
2:F:636:ASP:OD2	2:F:638:GLU:HG2	2.10	0.52
2:H:534:SER:O	2:H:535:ASP:O	2.28	0.52
2:H:561:THR:O	2:H:615:LYS:NZ	2.42	0.52
2:B:578:ILE:HG12	2:B:579:GLN:N	2.25	0.52
1:C:30:ARG:NE	1:C:191:THR:O	2.42	0.52
1:C:144:PRO:O	1:C:148:GLN:HG3	2.10	0.52
1:C:156:ALA:O	1:C:157:VAL:CG1	2.58	0.52
2:F:500:GLN:HE21	2:F:503:LYS:HE2	1.74	0.52
1:E:60:THR:HG23	1:E:111:HIS:C	2.34	0.52
1:E:60:THR:HG23	1:E:111:HIS:O	2.10	0.52
1:E:185:ASP:OD2	1:E:187:ARG:CB	2.58	0.52
2:F:599:SER:C	2:F:601:THR:H	2.17	0.52
2:F:615:LYS:N	2:F:615:LYS:HD2	2.24	0.52
2:F:632:ARG:HG3	2:F:638:GLU:O	2.10	0.52
1:G:30:ARG:HH21	1:G:191:THR:CG2	2.22	0.52
2:H:384:ILE:N	2:H:384:ILE:HD12	2.24	0.52
2:B:508:SER:C	2:B:509:VAL:CG2	2.83	0.52
1:C:233:TRP:CZ2	1:C:257:TYR:HA	2.45	0.52
2:D:407:HIS:HD2	2:D:409:HIS:H	1.56	0.52
2:F:451:LEU:HD12	2:F:498:ALA:HA	1.92	0.52
2:H:548:LEU:HD11	2:H:633:ARG:HG3	1.91	0.52
4:Y:20:DA:C2	4:Y:21:DA:C6	2.98	0.52
1:C:37:LYS:HB2	1:C:37:LYS:NZ	2.25	0.51
1:C:88:HIS:ND1	1:C:120:CYS:HA	2.24	0.51
1:C:228:PHE:HZ	1:C:254:THR:HG22	1.74	0.51
2:F:387:TYR:CE2	2:F:518:LEU:HD22	2.44	0.51
1:G:36:TYR:CE1	1:G:120:CYS:SG	3.03	0.51
2:H:357:TYR:CE2	4:J:8:DG:H2'	2.45	0.51
2:H:571:ASP:O	2:H:572:LYS:C	2.52	0.51
4:J:5:DA:C2	4:J:6:DA:N1	2.79	0.51
1:A:171:ARG:HE	1:A:172:PRO:CD	2.23	0.51
1:C:261:SER:O	1:C:262:LEU:O	2.28	0.51
2:H:398:VAL:HG23	2:H:511:ARG:HB2	1.92	0.51
2:H:398:VAL:HG22	2:H:511:ARG:O	2.10	0.51
2:H:407:HIS:CG	2:H:510:VAL:HG23	2.44	0.51
4:J:19:DA:N3	4:J:20:DA:C4	2.78	0.51
2:B:581:ARG:HE	2:B:593:GLU:HG3	1.75	0.51
2:D:455:MET:SD	2:D:469:VAL:HG13	2.51	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:GLY:N	1:E:57:THR:CG2	2.67	0.51
1:E:88:HIS:CE1	1:E:120:CYS:CB	2.93	0.51
3:I:21:DT:H5'	3:I:21:DT:C6	2.45	0.51
2:B:409:HIS:CD2	2:B:441:HIS:HA	2.46	0.51
2:B:489:ARG:HD3	2:B:489:ARG:C	2.35	0.51
2:F:454:ARG:HG2	2:F:454:ARG:HH11	1.75	0.51
2:F:467:LEU:CD1	2:F:467:LEU:H	2.24	0.51
2:F:578:ILE:HG12	2:F:579:GLN:N	2.25	0.51
2:H:402:LYS:H	2:H:402:LYS:HD3	1.73	0.51
1:A:88:HIS:NE2	1:A:120:CYS:HB3	2.26	0.51
2:B:444:LYS:O	2:B:447:VAL:HG23	2.10	0.51
2:B:564:GLU:O	2:B:612:LYS:HA	2.10	0.51
1:C:239:PHE:HB3	1:C:252:PHE:HB3	1.92	0.51
2:D:618:ASP:OD2	2:D:621:ILE:HG22	2.10	0.51
1:G:58:HIS:HB3	1:G:59:PRO:CD	2.40	0.51
1:G:213:PHE:CE2	2:H:554:ASP:HB3	2.46	0.51
2:B:448:PHE:HA	2:B:502:THR:HG21	1.91	0.51
1:E:55:THR:CG2	1:E:56:LYS:N	2.74	0.51
2:H:402:LYS:HE3	2:H:402:LYS:N	2.26	0.51
1:C:79:LYS:HG2	1:C:80:ASP:OD1	2.11	0.51
1:E:78:THR:O	1:E:158:ARG:HD2	2.10	0.51
1:G:54:THR:OG1	1:G:55:THR:N	2.41	0.51
2:H:409:HIS:CD2	2:H:442:VAL:H	2.29	0.51
2:H:464:ASN:ND2	2:H:528:ARG:NH1	2.58	0.51
3:X:21:DT:H5'	3:X:21:DT:C6	2.45	0.51
4:J:17:DG:C2'	4:J:18:DG:C8	2.94	0.51
2:D:353:PHE:CE2	2:D:439:ILE:HG12	2.46	0.51
1:E:55:THR:HG22	1:E:56:LYS:N	2.26	0.51
1:E:226:VAL:CG1	1:E:228:PHE:CE1	2.94	0.51
2:B:632:ARG:HG3	2:B:639:THR:CG2	2.41	0.51
1:C:171:ARG:NE	1:C:172:PRO:HD2	2.27	0.51
1:C:202:ASN:ND2	1:C:202:ASN:N	2.55	0.51
1:E:24:ILE:HD11	1:E:62:LYS:HB2	1.92	0.51
1:A:36:TYR:CE2	3:X:8:DT:C2'	2.93	0.50
2:B:425:ALA:O	2:B:426:GLY:C	2.54	0.50
1:C:167:ASP:OD1	1:C:169:ALA:HB3	2.11	0.50
1:E:88:HIS:CG	1:E:120:CYS:HA	2.46	0.50
1:E:285:GLU:CD	1:E:285:GLU:H	2.19	0.50
2:B:573:VAL:HG22	2:B:606:GLN:O	2.11	0.50
1:C:49:GLU:O	1:C:49:GLU:HG2	2.11	0.50
1:E:202:ASN:H	1:E:202:ASN:ND2	2.05	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:5:DA:C2	4:Y:6:DA:N1	2.79	0.50
1:A:132:GLN:O	1:A:132:GLN:HG2	2.11	0.50
2:B:624:PRO:HB2	2:B:646:LEU:HD11	1.94	0.50
2:D:375:ASN:O	2:D:376:LYS:HB2	2.11	0.50
1:E:90:LEU:HD12	1:E:117:GLY:O	2.11	0.50
1:E:95:CYS:SG	1:E:100:TYR:HA	2.52	0.50
2:F:400:ASN:CG	2:F:400:ASN:O	2.54	0.50
2:F:565:GLU:C	2:F:566:ILE:HD12	2.36	0.50
2:F:641:GLU:O	2:F:642:PRO:C	2.55	0.50
1:G:236:ARG:CG	1:G:236:ARG:NH1	2.72	0.50
3:X:22:DT:N3	4:Y:7:DA:C2	2.78	0.50
2:B:423:VAL:CG2	2:B:432:VAL:HG11	2.40	0.50
2:D:633:ARG:NH1	2:D:638:GLU:HB2	2.26	0.50
2:F:606:GLN:NE2	4:J:19:DA:OP2	2.44	0.50
2:B:550:ILE:HG23	2:B:568:LEU:HD11	1.93	0.50
2:B:646:LEU:HD13	2:B:647:TYR:N	2.27	0.50
2:D:407:HIS:CG	2:D:510:VAL:HG23	2.46	0.50
1:E:55:THR:CA	2:H:375:ASN:OD1	2.56	0.50
1:E:233:TRP:CZ3	1:E:268:VAL:HG11	2.39	0.50
1:G:25:GLU:O	1:G:59:PRO:HA	2.12	0.50
4:Y:1:DT:H2''	4:Y:2:DT:O5'	2.10	0.50
1:A:74:ILE:HD12	1:A:161:PHE:CD2	2.47	0.50
2:B:387:TYR:CE2	2:B:518:LEU:HD22	2.47	0.50
2:B:487:THR:O	2:B:491:LYS:HG3	2.11	0.50
2:D:357:TYR:OH	4:Y:8:DG:OP2	2.22	0.50
2:D:486:LEU:HA	2:D:490:GLU:OE1	2.11	0.50
2:D:561:THR:O	2:D:615:LYS:HG3	2.11	0.50
2:F:559:CYS:SG	2:F:650:GLU:HB2	2.52	0.50
1:G:187:ARG:HG3	1:G:187:ARG:HH11	1.77	0.50
1:G:273:ARG:HD2	1:G:280:LEU:HD21	1.93	0.50
2:B:400:ASN:CG	2:B:400:ASN:O	2.55	0.50
1:C:203:SER:OG	1:C:289:LEU:HD11	2.12	0.50
1:E:86:HIS:CE1	1:E:157:VAL:HG12	2.46	0.50
1:E:249:ALA:O	1:E:250:ILE:HD13	2.10	0.50
2:F:379:TYR:CD2	2:F:435:ALA:HB2	2.47	0.50
2:F:568:LEU:C	2:F:568:LEU:HD23	2.37	0.50
2:H:592:TRP:CD1	2:H:617:LYS:HB3	2.46	0.50
2:D:500:GLN:HE21	2:D:503:LYS:CE	2.25	0.50
2:H:412:VAL:HG22	2:H:413:GLY:N	2.27	0.50
3:X:21:DT:H2''	3:X:22:DT:H5'	1.93	0.50
1:A:48:GLY:N	1:A:57:THR:CG2	2.67	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:VAL:HB	2:D:421:CYS:HB3	1.93	0.50
1:G:23:ILE:HD12	1:G:23:ILE:N	2.26	0.50
1:G:37:LYS:HB2	1:G:37:LYS:NZ	2.27	0.50
1:G:229:THR:N	1:G:269:SER:O	2.42	0.50
2:D:583:TYR:HA	2:D:592:TRP:O	2.12	0.49
1:E:246:ARG:HB3	2:F:607:PHE:CD2	2.47	0.49
2:H:632:ARG:CG	2:H:639:THR:HG22	2.41	0.49
2:B:460:ILE:HG12	2:B:486:LEU:CD1	2.38	0.49
1:C:48:GLY:HA3	1:C:57:THR:OG1	2.11	0.49
1:E:25:GLU:CG	1:E:58:HIS:O	2.60	0.49
2:H:353:PHE:CD2	2:H:367:LEU:HD21	2.48	0.49
2:H:375:ASN:O	2:H:376:LYS:HB2	2.11	0.49
2:B:568:LEU:C	2:B:568:LEU:HD23	2.37	0.49
1:C:187:ARG:O	1:C:189:PRO:HD3	2.12	0.49
1:E:218:LYS:NZ	1:E:218:LYS:HB3	2.27	0.49
1:E:226:VAL:HG12	1:E:228:PHE:HE1	1.74	0.49
2:F:476:LEU:CD2	2:F:483:ASP:CG	2.86	0.49
1:C:156:ALA:HA	1:C:183:ILE:O	2.13	0.49
2:D:423:VAL:HG21	2:D:432:VAL:HG11	1.94	0.49
1:E:62:LYS:HE2	1:E:64:ASN:HD21	1.76	0.49
1:G:236:ARG:HG3	1:G:236:ARG:NH1	2.17	0.49
3:I:15:DG:C3'	3:I:16:DG:H5''	2.37	0.49
4:J:17:DG:C5'	4:J:17:DG:H8	2.24	0.49
4:J:20:DA:C6	4:J:21:DA:C6	3.00	0.49
2:B:379:TYR:O	2:B:380:PRO:C	2.54	0.49
2:B:571:ASP:O	2:B:572:LYS:C	2.56	0.49
2:B:460:ILE:CG1	2:B:486:LEU:HD13	2.40	0.49
2:B:467:LEU:N	2:B:467:LEU:CD1	2.75	0.49
2:B:550:ILE:HD12	2:B:550:ILE:H	1.77	0.49
1:C:51:SER:HB2	1:C:56:LYS:HA	1.94	0.49
2:D:439:ILE:N	2:D:439:ILE:HD13	2.26	0.49
2:D:558:GLY:O	2:D:647:TYR:HA	2.13	0.49
2:F:508:SER:C	2:F:509:VAL:CG2	2.86	0.49
3:X:5:DA:C2	3:X:6:DC:C2	3.01	0.49
1:A:158:ARG:HD3	1:A:179:LEU:HD23	1.93	0.49
1:A:202:ASN:H	1:A:202:ASN:ND2	2.02	0.49
1:A:236:ARG:CG	1:A:236:ARG:NH1	2.72	0.49
2:B:618:ASP:CG	2:B:621:ILE:HG22	2.37	0.49
2:D:412:VAL:HG22	2:D:413:GLY:H	1.77	0.49
2:D:552:ARG:HG3	2:D:553:MET:N	2.28	0.49
2:D:572:LYS:HD3	2:D:573:VAL:H	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:ARG:HG2	1:E:267:ARG:HH11	1.78	0.49
1:G:277:ASP:OD1	1:G:279:GLU:HB3	2.13	0.49
2:H:455:MET:SD	2:H:469:VAL:HG13	2.53	0.49
1:A:24:ILE:HG13	1:A:62:LYS:HB2	1.95	0.49
1:C:66:TYR:CD1	1:C:66:TYR:C	2.90	0.49
2:H:451:LEU:HD13	2:H:451:LEU:C	2.38	0.49
1:A:51:SER:CB	1:A:57:THR:CG2	2.73	0.49
1:A:60:THR:OG1	1:A:112:SER:CB	2.57	0.49
1:A:167:ASP:C	1:A:169:ALA:N	2.70	0.49
1:C:24:ILE:CD1	1:C:110:ILE:HG12	2.42	0.49
1:C:132:GLN:O	1:C:132:GLN:HG2	2.13	0.49
2:D:487:THR:O	2:D:491:LYS:HG3	2.12	0.49
2:F:550:ILE:CG2	2:F:568:LEU:HD11	2.43	0.49
1:G:24:ILE:HD11	1:G:110:ILE:HG12	1.95	0.49
1:G:49:GLU:HG2	1:G:49:GLU:O	2.11	0.49
2:H:566:ILE:N	2:H:566:ILE:CD1	2.75	0.49
2:H:571:ASP:O	2:H:572:LYS:O	2.31	0.49
1:A:72:VAL:HB	1:A:104:LEU:HD13	1.94	0.49
1:A:185:ASP:OD2	1:A:187:ARG:CB	2.61	0.49
1:C:228:PHE:CZ	1:C:255:PRO:HD2	2.48	0.49
2:D:464:ASN:N	2:D:465:PRO:HD3	2.28	0.49
1:E:51:SER:CB	1:E:57:THR:CG2	2.77	0.49
2:H:605:ARG:O	2:H:606:GLN:HB2	2.11	0.49
4:Y:10:DC:H2''	4:Y:11:DC:O5'	2.13	0.49
1:A:74:ILE:CB	1:A:100:TYR:HB3	2.42	0.48
2:B:346:GLU:OE1	2:B:378:SER:OG	2.29	0.48
2:F:477:GLN:O	2:F:479:GLU:N	2.46	0.48
2:F:517:PHE:HA	2:F:527:ARG:O	2.12	0.48
2:F:621:ILE:CD1	2:F:649:PRO:HB3	2.35	0.48
2:F:650:GLU:HG2	2:F:650:GLU:O	2.13	0.48
1:G:97:ASP:HB2	1:G:99:TYR:CE2	2.48	0.48
2:H:423:VAL:CG2	2:H:432:VAL:HG11	2.43	0.48
2:H:507:LEU:N	2:H:507:LEU:CD1	2.76	0.48
1:A:51:SER:HB2	1:A:57:THR:HG22	1.85	0.48
1:A:86:HIS:CE1	1:A:157:VAL:HG12	2.48	0.48
2:B:476:LEU:HD22	2:B:483:ASP:HB2	1.95	0.48
1:C:207:LEU:HG	1:C:291:ASP:OD1	2.13	0.48
1:E:122:LYS:C	1:E:124:ARG:N	2.69	0.48
4:J:20:DA:C2	4:J:21:DA:C6	3.02	0.48
1:A:236:ARG:HG3	1:A:236:ARG:NH1	2.21	0.48
2:B:608:ALA:O	2:B:609:ILE:HG13	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:631:LEU:O	2:B:639:THR:HA	2.13	0.48
2:D:354:ARG:HG2	2:D:355:PHE:N	2.27	0.48
1:E:194:LEU:HB3	1:E:281:SER:HB3	1.93	0.48
1:E:236:ARG:HG3	1:E:236:ARG:NH1	2.23	0.48
2:F:627:VAL:HG23	2:F:645:PHE:HB3	1.95	0.48
2:F:629:VAL:HG12	2:F:643:LYS:O	2.13	0.48
1:A:206:CYS:HA	1:A:288:TYR:CD1	2.48	0.48
2:B:477:GLN:O	2:B:479:GLU:N	2.46	0.48
2:B:552:ARG:CG	2:B:553:MET:N	2.76	0.48
1:C:34:PHE:CE2	1:C:185:ASP:HB2	2.48	0.48
1:C:104:LEU:HD21	1:C:163:VAL:HG13	1.96	0.48
1:C:171:ARG:O	1:C:172:PRO:C	2.56	0.48
1:C:273:ARG:HD2	1:C:280:LEU:HD21	1.94	0.48
1:E:88:HIS:CE1	1:E:120:CYS:HB2	2.49	0.48
1:E:246:ARG:C	1:E:247:GLN:HG3	2.39	0.48
3:I:7:DT:N3	4:J:22:DG:N2	2.61	0.48
1:A:229:THR:O	1:A:268:VAL:HG13	2.12	0.48
2:F:554:ASP:C	2:F:554:ASP:OD1	2.57	0.48
1:G:27:PRO:O	1:G:181:HIS:HE1	1.97	0.48
1:G:196:ILE:HG13	1:G:272:LEU:HD22	1.96	0.48
1:A:72:VAL:HB	1:A:104:LEU:CD1	2.43	0.48
2:F:632:ARG:CG	2:F:639:THR:HG22	2.42	0.48
1:G:36:TYR:N	1:G:36:TYR:HD1	2.09	0.48
4:Y:19:DA:N3	4:Y:20:DA:C4	2.82	0.48
4:J:17:DG:H5''	4:J:17:DG:C8	2.48	0.48
1:A:57:THR:CG2	1:A:57:THR:O	2.61	0.48
2:B:615:LYS:HD2	2:B:615:LYS:N	2.28	0.48
2:F:634:LYS:O	2:F:635:SER:C	2.56	0.48
1:G:207:LEU:HG	1:G:291:ASP:OD1	2.13	0.48
1:G:223:ASP:OD2	1:G:274:ARG:CG	2.59	0.48
1:G:228:PHE:CZ	1:G:254:THR:HG22	2.49	0.48
4:Y:16:DC:H2'	4:Y:17:DG:H5''	1.94	0.48
1:A:60:THR:CG2	1:A:61:ILE:N	2.75	0.48
1:A:88:HIS:NE2	1:A:120:CYS:CB	2.77	0.48
1:A:203:SER:OG	1:A:289:LEU:HD11	2.14	0.48
1:C:24:ILE:CG1	1:C:62:LYS:HB2	2.43	0.48
1:C:206:CYS:HA	1:C:288:TYR:HD1	1.78	0.48
2:D:467:LEU:N	2:D:467:LEU:HD12	2.28	0.48
1:G:88:HIS:CE1	1:G:121:VAL:H	2.31	0.48
2:H:583:TYR:O	2:H:627:VAL:HB	2.13	0.48
3:X:8:DT:O2	4:Y:21:DA:C2	2.60	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLY:N	1:A:57:THR:HG21	2.24	0.48
1:G:28:LYS:N	1:G:48:GLY:O	2.47	0.48
1:G:262:LEU:CD2	1:G:266:VAL:HG12	2.39	0.48
1:A:185:ASP:O	1:A:187:ARG:N	2.42	0.48
1:C:36:TYR:CE1	1:C:120:CYS:SG	3.07	0.48
2:D:435:ALA:O	2:D:436:ASN:C	2.56	0.48
1:G:202:ASN:ND2	1:G:202:ASN:N	2.52	0.48
2:H:572:LYS:HZ1	2:H:606:GLN:CG	2.10	0.48
1:E:206:CYS:HA	1:E:288:TYR:HD1	1.77	0.47
2:F:577:ASP:OD1	2:F:634:LYS:HB2	2.13	0.47
1:G:203:SER:OG	1:G:289:LEU:HD11	2.13	0.47
1:A:167:ASP:CB	1:A:168:PRO:HD2	2.34	0.47
1:C:82:PRO:O	1:C:84:ARG:HG3	2.14	0.47
2:D:624:PRO:CB	2:D:646:LEU:HD11	2.39	0.47
2:D:632:ARG:HG3	2:D:639:THR:HG22	1.94	0.47
1:E:32:MET:HG3	1:E:47:PRO:HD3	1.96	0.47
1:E:88:HIS:NE2	1:E:120:CYS:CB	2.76	0.47
1:G:72:VAL:HB	1:G:104:LEU:HD11	1.95	0.47
1:C:156:ALA:C	1:C:157:VAL:HG13	2.39	0.47
1:E:236:ARG:CG	1:E:236:ARG:NH1	2.74	0.47
2:F:355:PHE:CE2	2:F:539:ASP:HB2	2.50	0.47
2:F:509:VAL:HA	2:F:537:ILE:O	2.13	0.47
2:F:578:ILE:O	2:F:598:PHE:HZ	1.97	0.47
2:H:506:ASP:C	2:H:508:SER:H	2.21	0.47
1:C:30:ARG:HH21	1:C:191:THR:CG2	2.27	0.47
1:E:86:HIS:CG	1:E:157:VAL:HG12	2.50	0.47
2:F:405:HIS:HB3	2:F:501:GLN:OE1	2.15	0.47
1:G:122:LYS:C	1:G:124:ARG:N	2.71	0.47
1:C:51:SER:HA	1:C:57:THR:HG23	1.96	0.47
1:C:88:HIS:CE1	1:C:120:CYS:HA	2.50	0.47
1:C:199:VAL:HG12	1:C:201:ARG:H	1.78	0.47
1:G:86:HIS:CG	1:G:87:PRO:CD	2.97	0.47
1:G:158:ARG:CZ	1:G:182:PRO:HD3	2.45	0.47
4:J:19:DA:H2''	4:J:20:DA:N7	2.29	0.47
2:B:402:LYS:HG2	2:B:403:ASN:OD1	2.14	0.47
2:B:456:THR:HG23	2:B:486:LEU:HD22	1.97	0.47
1:C:86:HIS:CG	1:C:87:PRO:CD	2.97	0.47
2:D:476:LEU:HD22	2:D:483:ASP:HB2	1.95	0.47
2:D:632:ARG:CG	2:D:639:THR:HG22	2.45	0.47
1:E:171:ARG:HE	1:E:172:PRO:HD3	1.80	0.47
1:E:226:VAL:CG1	1:E:228:PHE:HE1	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:8:DT:N3	4:Y:21:DA:C2	2.83	0.47
4:Y:19:DA:N3	4:Y:20:DA:C5	2.83	0.47
1:A:29:GLN:HG2	1:A:182:PRO:O	2.15	0.47
1:A:73:ARG:HA	1:A:100:TYR:O	2.14	0.47
1:C:30:ARG:HH21	1:C:191:THR:CB	2.28	0.47
1:C:95:CYS:SG	1:C:100:TYR:HB2	2.55	0.47
1:C:200:ASN:O	1:C:201:ARG:HB2	2.14	0.47
2:D:583:TYR:CE1	2:D:628:PHE:HB2	2.50	0.47
1:E:240:SER:C	1:E:242:ALA:N	2.69	0.47
2:F:425:ALA:O	2:F:426:GLY:C	2.58	0.47
2:F:454:ARG:HG2	2:F:454:ARG:NH1	2.30	0.47
1:G:65:GLY:O	1:G:66:TYR:HB2	2.14	0.47
2:H:550:ILE:HD11	2:H:640:SER:OG	2.13	0.47
2:H:646:LEU:C	2:H:646:LEU:CD1	2.87	0.47
1:C:86:HIS:CD2	1:C:157:VAL:HG12	2.50	0.47
2:D:646:LEU:C	2:D:646:LEU:CD1	2.87	0.47
1:E:74:ILE:HG12	1:E:100:TYR:HD1	1.78	0.47
1:E:200:ASN:O	1:E:201:ARG:HB2	2.15	0.47
1:E:265:PRO:HB3	1:E:289:LEU:HD23	1.97	0.47
1:G:105:CYS:SG	1:G:107:ASP:OD1	2.73	0.47
1:G:273:ARG:O	1:G:275:PRO:HD3	2.15	0.47
2:H:355:PHE:HB3	2:H:441:HIS:HB2	1.97	0.47
2:H:459:CYS:SG	2:H:494:ILE:HD11	2.55	0.47
3:I:8:DT:O2	4:J:21:DA:H2	1.98	0.47
4:J:5:DA:H2''	4:J:6:DA:C8	2.50	0.47
2:B:604:HIS:O	2:B:605:ARG:C	2.58	0.47
2:F:467:LEU:HD12	2:F:467:LEU:H	1.77	0.47
2:F:550:ILE:HD11	2:F:640:SER:HG	1.78	0.47
2:F:613:THR:HG23	2:F:614:PRO:CD	2.42	0.47
2:F:614:PRO:HG2	2:F:647:TYR:OH	2.14	0.47
1:G:25:GLU:HA	1:G:25:GLU:OE1	2.14	0.47
3:I:9:DT:H2''	3:I:10:DC:O5'	2.15	0.47
2:B:565:GLU:C	2:B:566:ILE:HD12	2.41	0.47
1:C:40:GLY:O	1:C:42:SER:N	2.48	0.47
2:D:641:GLU:O	2:D:642:PRO:C	2.58	0.47
1:E:158:ARG:HH12	1:E:182:PRO:HD3	1.77	0.47
2:H:478:ALA:O	2:H:526:THR:HB	2.14	0.47
4:Y:17:DG:OP1	4:Y:17:DG:C4'	2.61	0.47
1:E:113:PHE:CE2	1:E:161:PHE:HE2	2.33	0.46
1:E:202:ASN:N	1:E:202:ASN:ND2	2.59	0.46
2:F:552:ARG:HG3	2:F:553:MET:H	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:632:ARG:HG3	2:F:639:THR:CG2	2.45	0.46
1:G:66:TYR:CD2	1:G:165:VAL:HB	2.50	0.46
1:G:187:ARG:O	1:G:187:ARG:CG	2.61	0.46
2:H:405:HIS:HB3	2:H:501:GLN:OE1	2.14	0.46
2:H:467:LEU:HD12	2:H:467:LEU:N	2.30	0.46
3:X:8:DT:C2	4:Y:21:DA:C2	3.02	0.46
1:A:22:GLU:OE2	1:A:62:LYS:HD3	2.14	0.46
2:B:354:ARG:HD2	2:B:356:ARG:CZ	2.44	0.46
2:B:580:ILE:N	2:B:580:ILE:CD1	2.78	0.46
1:C:229:THR:N	1:C:269:SER:O	2.47	0.46
2:D:572:LYS:HZ3	2:D:606:GLN:CG	2.25	0.46
1:E:60:THR:CG2	1:E:61:ILE:H	2.26	0.46
1:E:277:ASP:C	1:E:277:ASP:OD1	2.58	0.46
1:G:40:GLY:O	1:G:41:ARG:C	2.56	0.46
2:B:555:ARG:HH11	2:B:555:ARG:CG	2.28	0.46
2:B:613:THR:CG2	2:B:614:PRO:N	2.79	0.46
1:C:194:LEU:HD22	1:C:279:GLU:HG3	1.96	0.46
1:E:233:TRP:CD1	1:E:258:ALA:HB2	2.49	0.46
2:F:593:GLU:HG2	2:F:595:PHE:CE1	2.50	0.46
1:G:66:TYR:OH	1:G:69:PRO:O	2.34	0.46
1:G:74:ILE:HD11	1:G:161:PHE:HD2	1.76	0.46
1:G:122:LYS:O	1:G:123:LYS:C	2.58	0.46
1:G:210:ASP:O	1:G:253:ARG:HA	2.15	0.46
2:H:367:LEU:HG	2:H:437:LEU:O	2.16	0.46
2:B:384:ILE:CD1	2:B:430:MET:HE3	2.45	0.46
1:E:58:HIS:CE1	1:E:114:GLN:NE2	2.81	0.46
2:F:398:VAL:HG23	2:F:511:ARG:HB2	1.96	0.46
2:F:564:GLU:O	2:F:612:LYS:HA	2.16	0.46
4:J:2:DT:H2''	4:J:3:DG:H5'	1.96	0.46
2:B:451:LEU:HD11	2:B:498:ALA:HA	1.97	0.46
2:B:593:GLU:HG2	2:B:595:PHE:CE1	2.51	0.46
1:C:198:ARG:HD2	2:D:567:TYR:OH	2.16	0.46
2:D:520:ASP:HA	2:D:527:ARG:HD3	1.98	0.46
2:F:456:THR:HG23	2:F:486:LEU:HD22	1.98	0.46
2:F:508:SER:O	2:F:509:VAL:CG2	2.64	0.46
2:F:511:ARG:HG2	2:F:536:ALA:HA	1.98	0.46
1:G:171:ARG:O	1:G:172:PRO:C	2.58	0.46
1:G:239:PHE:HB3	1:G:252:PHE:CB	2.46	0.46
2:H:423:VAL:HG21	2:H:432:VAL:CG1	2.45	0.46
1:C:171:ARG:HE	1:C:171:ARG:HA	1.79	0.46
2:D:451:LEU:O	2:D:455:MET:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ARG:HD2	1:E:280:LEU:CD2	2.41	0.46
2:F:490:GLU:O	2:F:494:ILE:HG12	2.16	0.46
2:H:574:GLN:HB3	2:H:577:ASP:HB3	1.98	0.46
1:A:43:ALA:C	1:A:44:GLY:O	2.56	0.46
1:A:213:PHE:CZ	2:B:554:ASP:HB3	2.51	0.46
2:B:554:ASP:C	2:B:554:ASP:OD1	2.58	0.46
2:B:605:ARG:HA	2:B:606:GLN:NE2	2.31	0.46
1:C:198:ARG:O	1:C:199:VAL:CG2	2.63	0.46
1:C:201:ARG:HB3	1:C:212:ILE:CD1	2.46	0.46
1:C:277:ASP:OD1	1:C:279:GLU:HB3	2.16	0.46
2:D:581:ARG:NH1	2:D:583:TYR:CD2	2.84	0.46
2:H:464:ASN:HD22	2:H:528:ARG:NH1	2.13	0.46
2:D:392:LYS:HB3	2:D:517:PHE:HB2	1.98	0.46
1:E:34:PHE:N	1:E:34:PHE:CD1	2.83	0.46
1:G:46:ILE:HA	1:G:47:PRO:HD3	1.75	0.46
2:H:391:ALA:HB3	2:H:425:ALA:HB3	1.98	0.46
1:C:122:LYS:HG2	3:X:22:DT:H3'	1.98	0.46
1:E:29:GLN:NE2	1:E:181:HIS:HB2	2.30	0.46
1:E:167:ASP:C	1:E:169:ALA:N	2.69	0.46
2:F:500:GLN:HE21	2:F:503:LYS:CE	2.28	0.46
1:A:51:SER:CB	1:A:57:THR:HG21	2.39	0.46
1:A:265:PRO:HB3	1:A:287:GLN:OE1	2.16	0.46
2:B:354:ARG:HD2	2:B:356:ARG:NE	2.31	0.46
2:B:650:GLU:O	2:B:650:GLU:HG2	2.16	0.46
1:C:21:VAL:CG2	1:C:163:VAL:HG21	2.38	0.46
1:C:223:ASP:OD2	1:C:274:ARG:HG3	2.15	0.46
2:D:569:LEU:HD23	2:D:608:ALA:HB2	1.98	0.46
1:E:167:ASP:O	1:E:168:PRO:C	2.58	0.46
2:F:599:SER:O	2:F:601:THR:N	2.48	0.46
2:B:379:TYR:CD2	2:B:435:ALA:HB2	2.50	0.45
2:B:579:GLN:NE2	2:B:632:ARG:HE	2.15	0.45
2:B:584:GLU:O	2:B:591:VAL:HG23	2.16	0.45
1:C:30:ARG:NH2	1:C:191:THR:HB	2.30	0.45
1:C:185:ASP:C	1:C:187:ARG:N	2.74	0.45
1:C:246:ARG:C	1:C:247:GLN:HG3	2.42	0.45
2:D:353:PHE:CD2	2:D:367:LEU:CD2	2.98	0.45
1:E:26:GLN:HB3	1:E:181:HIS:CE1	2.50	0.45
2:F:580:ILE:N	2:F:580:ILE:CD1	2.79	0.45
1:G:132:GLN:HA	1:G:135:GLN:HG2	1.97	0.45
2:H:460:ILE:HG12	2:H:486:LEU:HD13	1.99	0.45
4:Y:20:DA:N1	4:Y:21:DA:N1	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:HG23	1:A:111:HIS:O	2.17	0.45
1:C:46:ILE:HA	1:C:47:PRO:HD3	1.67	0.45
1:C:88:HIS:CE1	1:C:120:CYS:CA	2.99	0.45
1:C:237:GLY:HA2	1:C:255:PRO:HD3	1.98	0.45
2:D:425:ALA:O	2:D:426:GLY:C	2.58	0.45
2:D:464:ASN:ND2	2:D:528:ARG:HH11	2.14	0.45
2:D:509:VAL:CG2	2:D:538:TYR:CD1	2.99	0.45
2:D:509:VAL:CG2	2:D:538:TYR:HD1	2.27	0.45
1:E:54:THR:C	2:H:375:ASN:OD1	2.58	0.45
1:E:180:SER:O	1:E:181:HIS:C	2.59	0.45
2:F:408:ALA:O	2:F:442:VAL:HG11	2.16	0.45
1:G:246:ARG:C	1:G:247:GLN:HG3	2.40	0.45
2:B:634:LYS:O	2:B:635:SER:C	2.60	0.45
1:C:122:LYS:C	1:C:124:ARG:N	2.74	0.45
2:D:387:TYR:OH	2:D:519:PRO:HD2	2.15	0.45
1:G:157:VAL:O	1:G:182:PRO:HA	2.15	0.45
1:G:214:LEU:O	1:G:249:ALA:HA	2.17	0.45
1:A:229:THR:N	1:A:269:SER:O	2.50	0.45
1:C:268:VAL:HG12	1:C:269:SER:N	2.30	0.45
2:D:481:GLY:O	2:D:483:ASP:N	2.49	0.45
2:F:575:LYS:HD2	2:F:600:PRO:O	2.17	0.45
1:A:68:GLY:CA	1:A:106:PRO:O	2.64	0.45
1:A:141:PHE:CE1	1:A:177:PRO:HG2	2.52	0.45
1:A:285:GLU:H	1:A:285:GLU:CD	2.25	0.45
2:B:455:MET:CE	2:B:469:VAL:HG13	2.43	0.45
2:B:556:THR:O	2:B:645:PHE:HA	2.16	0.45
2:B:577:ASP:CG	2:B:577:ASP:O	2.58	0.45
1:E:171:ARG:HA	1:E:171:ARG:NE	2.28	0.45
1:G:258:ALA:O	1:G:260:PRO:HD3	2.16	0.45
2:H:349:LYS:NZ	2:H:372:SER:OG	2.37	0.45
2:H:487:THR:O	2:H:491:LYS:HG3	2.17	0.45
2:H:627:VAL:HG23	2:H:628:PHE:N	2.31	0.45
1:A:261:SER:O	1:A:262:LEU:C	2.59	0.45
2:D:434:PHE:CE2	2:D:514:PHE:HE2	2.35	0.45
1:G:24:ILE:HD12	1:G:60:THR:HG22	1.97	0.45
1:G:59:PRO:O	1:G:112:SER:HA	2.16	0.45
1:E:25:GLU:HB3	1:E:60:THR:H	1.82	0.45
1:E:39:GLU:O	1:E:40:GLY:C	2.59	0.45
1:G:199:VAL:C	1:G:201:ARG:H	2.24	0.45
1:A:51:SER:H	1:A:57:THR:HB	1.82	0.45
2:B:500:GLN:HE21	2:B:503:LYS:HE2	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:H	1:C:23:ILE:CD1	2.29	0.45
1:C:259:ASP:HB3	1:C:262:LEU:HD13	1.99	0.45
2:D:354:ARG:HG2	2:D:355:PHE:O	2.17	0.45
1:G:66:TYR:CD1	1:G:66:TYR:C	2.94	0.45
1:A:259:ASP:HB3	1:A:262:LEU:HD13	1.98	0.45
1:A:259:ASP:OD1	1:A:259:ASP:C	2.60	0.45
2:B:518:LEU:O	2:B:527:ARG:HB2	2.17	0.45
1:C:132:GLN:HA	1:C:135:GLN:CG	2.47	0.45
2:D:603:VAL:O	2:D:603:VAL:HG12	2.16	0.45
1:G:213:PHE:CD2	2:H:554:ASP:HB3	2.51	0.45
2:B:500:GLN:O	2:B:503:LYS:HG2	2.16	0.45
2:B:608:ALA:C	2:B:609:ILE:HG13	2.42	0.45
2:B:613:THR:HG23	2:B:614:PRO:CD	2.47	0.45
1:C:214:LEU:HD22	1:C:250:ILE:HG13	1.99	0.45
1:E:22:GLU:OE2	1:E:62:LYS:HD3	2.16	0.45
1:E:126:LEU:HD21	1:E:154:LEU:HD21	1.99	0.45
2:F:584:GLU:C	2:F:591:VAL:HG23	2.42	0.45
2:B:517:PHE:HA	2:B:527:ARG:O	2.17	0.44
1:C:66:TYR:CE2	1:C:165:VAL:HB	2.51	0.44
1:E:23:ILE:H	1:E:23:ILE:CD1	2.28	0.44
1:E:201:ARG:HB3	1:E:212:ILE:HD12	1.99	0.44
2:F:354:ARG:HD2	2:F:356:ARG:HD3	1.98	0.44
2:F:571:ASP:O	2:F:573:VAL:HG13	2.17	0.44
1:G:116:LEU:HA	1:G:116:LEU:HD23	1.70	0.44
4:J:20:DA:C2	4:J:21:DA:C5	3.06	0.44
1:A:167:ASP:HB2	1:A:168:PRO:CD	2.38	0.44
2:B:411:LEU:HD12	2:B:411:LEU:HA	1.75	0.44
1:C:236:ARG:NH1	1:C:236:ARG:CG	2.79	0.44
1:E:213:PHE:CZ	2:F:554:ASP:HB3	2.52	0.44
1:E:229:THR:O	1:E:268:VAL:HG13	2.18	0.44
2:B:529:LEU:O	2:B:530:GLU:C	2.60	0.44
1:C:233:TRP:CD1	1:C:258:ALA:HB2	2.52	0.44
2:D:344:ILE:O	2:D:344:ILE:HG22	2.17	0.44
1:E:46:ILE:CG1	1:E:118:ILE:HD11	2.46	0.44
1:E:254:THR:O	1:E:255:PRO:C	2.61	0.44
1:G:130:ILE:CD1	1:G:152:TYR:HE1	2.30	0.44
2:H:454:ARG:HG2	2:H:454:ARG:HH11	1.82	0.44
2:H:636:ASP:CG	2:H:638:GLU:HG2	2.40	0.44
4:J:16:DC:H6	4:J:16:DC:H5'	1.83	0.44
4:J:19:DA:C2	4:J:20:DA:C4	3.05	0.44
1:A:39:GLU:O	1:A:40:GLY:C	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:HIS:CD2	2:B:409:HIS:H	2.16	0.44
2:B:464:ASN:ND2	2:B:528:ARG:NH1	2.65	0.44
2:B:508:SER:O	2:B:509:VAL:CG2	2.65	0.44
2:B:555:ARG:HA	2:B:555:ARG:HD2	1.74	0.44
2:B:631:LEU:HB2	2:B:640:SER:HB3	1.99	0.44
1:C:34:PHE:CD1	1:C:118:ILE:CG2	3.01	0.44
1:C:40:GLY:C	1:C:42:SER:H	2.25	0.44
2:D:367:LEU:HD23	2:D:367:LEU:HA	1.87	0.44
2:D:434:PHE:CE2	2:D:514:PHE:CE2	3.05	0.44
1:E:214:LEU:C	1:E:215:LEU:HD23	2.43	0.44
1:E:245:HIS:CD2	2:F:569:LEU:HB3	2.52	0.44
2:B:409:HIS:CD2	2:B:442:VAL:HG22	2.52	0.44
1:C:76:LEU:HA	1:C:76:LEU:HD12	1.71	0.44
1:C:244:VAL:O	1:C:244:VAL:HG12	2.17	0.44
1:E:43:ALA:C	1:E:44:GLY:O	2.61	0.44
1:E:156:ALA:HA	1:E:183:ILE:O	2.18	0.44
2:F:347:GLN:O	2:F:370:ALA:N	2.50	0.44
4:Y:2:DT:H2''	4:Y:3:DG:H5'	1.99	0.44
4:Y:20:DA:C2	4:Y:21:DA:C2	3.05	0.44
1:A:48:GLY:N	1:A:57:THR:HG23	2.28	0.44
1:A:218:LYS:HB3	1:A:218:LYS:HZ2	1.79	0.44
2:B:633:ARG:O	2:B:637:LEU:HA	2.17	0.44
1:C:274:ARG:NH2	1:C:279:GLU:HG2	2.33	0.44
1:G:30:ARG:CZ	1:G:191:THR:HB	2.48	0.44
2:H:506:ASP:C	2:H:508:SER:N	2.76	0.44
1:A:24:ILE:CG1	1:A:62:LYS:HB2	2.48	0.44
2:D:504:GLU:HA	2:D:504:GLU:OE1	2.17	0.44
1:E:24:ILE:CD1	1:E:62:LYS:HB2	2.48	0.44
2:F:411:LEU:HD12	2:F:411:LEU:HA	1.77	0.44
1:G:114:GLN:H	1:G:114:GLN:HG2	1.57	0.44
1:G:206:CYS:HA	1:G:288:TYR:CD1	2.53	0.44
2:H:476:LEU:CD2	2:H:483:ASP:CG	2.91	0.44
2:H:603:VAL:O	2:H:603:VAL:HG12	2.16	0.44
1:A:63:ILE:O	1:A:109:SER:OG	2.36	0.44
1:C:266:VAL:O	1:C:266:VAL:HG13	2.17	0.44
1:E:158:ARG:CZ	1:E:182:PRO:HD3	2.47	0.44
2:F:402:LYS:H	2:F:402:LYS:HD3	1.82	0.44
1:G:222:GLU:CD	1:G:222:GLU:H	2.26	0.44
2:H:380:PRO:C	2:H:381:GLN:HG3	2.40	0.44
3:X:8:DT:C2'	3:X:9:DT:OP2	2.61	0.44
1:A:226:VAL:HG12	1:A:228:PHE:CE1	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:LEU:O	1:C:249:ALA:HA	2.18	0.44
2:D:423:VAL:HG21	2:D:432:VAL:CG1	2.48	0.44
2:D:559:CYS:SG	2:D:650:GLU:CB	3.05	0.44
2:F:346:GLU:O	2:F:380:PRO:HA	2.18	0.44
2:F:489:ARG:NH1	2:F:489:ARG:HG2	2.32	0.44
1:G:60:THR:OG1	1:G:112:SER:HB3	2.17	0.44
1:G:88:HIS:CG	1:G:120:CYS:HA	2.53	0.44
2:H:394:ILE:CG1	2:H:515:THR:HB	2.48	0.44
1:A:74:ILE:N	1:A:100:TYR:O	2.50	0.43
1:A:240:SER:C	1:A:242:ALA:N	2.71	0.43
1:C:75:SER:HB3	1:C:162:GLN:HE22	1.83	0.43
2:D:478:ALA:O	2:D:526:THR:HB	2.17	0.43
2:D:507:LEU:N	2:D:507:LEU:HD12	2.32	0.43
2:D:615:LYS:HD2	2:D:615:LYS:N	2.33	0.43
1:E:48:GLY:CA	1:E:57:THR:OG1	2.60	0.43
2:H:379:TYR:O	2:H:381:GLN:HG3	2.17	0.43
2:H:435:ALA:O	2:H:436:ASN:C	2.61	0.43
2:H:578:ILE:HG12	2:H:579:GLN:N	2.32	0.43
3:X:17:DG:H2''	3:X:18:DG:OP2	2.17	0.43
3:I:22:DT:C2	4:J:7:DA:H2	2.31	0.43
1:C:245:HIS:HB3	1:C:249:ALA:HB3	2.00	0.43
2:D:549:LYS:HB3	2:D:571:ASP:OD1	2.18	0.43
1:E:167:ASP:CG	1:E:169:ALA:HB3	2.41	0.43
1:E:196:ILE:HG12	1:E:272:LEU:HD22	2.00	0.43
1:G:88:HIS:CE1	1:G:120:CYS:CA	3.01	0.43
2:H:423:VAL:HG21	2:H:432:VAL:HG11	2.00	0.43
3:I:16:DG:H2''	3:I:17:DG:H8	1.84	0.43
2:D:581:ARG:HD2	2:D:632:ARG:NH1	2.33	0.43
2:F:464:ASN:HD21	2:F:528:ARG:NH1	2.16	0.43
1:G:100:TYR:CD1	1:G:100:TYR:C	2.97	0.43
2:H:381:GLN:HA	2:H:432:VAL:O	2.18	0.43
2:H:385:CYS:O	2:H:386:ASN:HB2	2.16	0.43
2:H:444:LYS:HA	2:H:447:VAL:CG2	2.48	0.43
1:A:245:HIS:CD2	2:B:569:LEU:HB3	2.54	0.43
2:B:353:PHE:HE2	2:B:439:ILE:HG12	1.83	0.43
2:D:443:THR:O	2:D:447:VAL:HG23	2.18	0.43
2:D:629:VAL:O	2:D:629:VAL:HG13	2.16	0.43
1:E:126:LEU:HD13	1:E:126:LEU:O	2.17	0.43
2:F:425:ALA:O	2:F:426:GLY:O	2.36	0.43
2:H:573:VAL:HG22	2:H:606:GLN:O	2.18	0.43
4:J:10:DC:H2''	4:J:11:DC:O5'	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HG22	1:A:47:PRO:O	2.18	0.43
1:C:36:TYR:N	1:C:36:TYR:HD1	2.15	0.43
2:D:367:LEU:HA	2:D:368:PRO:HD3	1.69	0.43
2:D:587:GLU:OE1	2:D:587:GLU:HA	2.18	0.43
2:F:624:PRO:CB	2:F:646:LEU:HD11	2.48	0.43
1:A:29:GLN:NE2	1:A:181:HIS:HB2	2.34	0.43
1:A:86:HIS:CE1	1:A:157:VAL:CG1	3.01	0.43
2:B:469:VAL:HG11	2:B:494:ILE:HD13	2.01	0.43
2:B:641:GLU:H	2:B:641:GLU:CD	2.25	0.43
2:B:646:LEU:C	2:B:646:LEU:CD1	2.90	0.43
2:D:577:ASP:O	2:D:577:ASP:CG	2.61	0.43
2:H:480:GLY:H	2:H:526:THR:HG22	1.84	0.43
2:H:487:THR:HG1	2:H:490:GLU:HG3	1.82	0.43
4:Y:1:DT:C6	4:Y:2:DT:H72	2.54	0.43
4:J:17:DG:C5'	4:J:17:DG:C8	3.02	0.43
2:B:508:SER:O	2:B:509:VAL:HG22	2.19	0.43
2:B:574:GLN:OE1	4:Y:20:DA:OP1	2.37	0.43
2:B:632:ARG:CG	2:B:639:THR:HG22	2.47	0.43
2:B:641:GLU:O	2:B:642:PRO:C	2.61	0.43
1:C:54:THR:OG1	1:C:55:THR:N	2.49	0.43
1:C:246:ARG:HB3	2:D:607:PHE:CD2	2.54	0.43
2:D:380:PRO:C	2:D:381:GLN:HG3	2.41	0.43
1:G:58:HIS:HB3	1:G:59:PRO:HD2	1.98	0.43
1:G:156:ALA:O	1:G:157:VAL:HG13	2.18	0.43
1:G:268:VAL:HG12	1:G:269:SER:N	2.33	0.43
2:H:477:GLN:O	2:H:479:GLU:N	2.52	0.43
4:J:23:DT:H1'	4:J:24:DC:H5''	2.00	0.43
1:A:34:PHE:N	1:A:34:PHE:HD1	2.16	0.43
2:B:412:VAL:HG22	2:B:413:GLY:N	2.34	0.43
1:C:20:TYR:CD1	1:C:20:TYR:N	2.87	0.43
1:C:202:ASN:HD22	1:C:202:ASN:C	2.25	0.43
2:D:354:ARG:HD2	2:D:356:ARG:HD3	2.01	0.43
2:D:409:HIS:CD2	2:D:442:VAL:H	2.37	0.43
2:D:633:ARG:HB2	2:D:636:ASP:OD1	2.18	0.43
1:E:51:SER:CB	1:E:57:THR:HG21	2.42	0.43
2:F:574:GLN:NE2	4:J:20:DA:OP1	2.51	0.43
2:H:476:LEU:HD22	2:H:483:ASP:CB	2.47	0.43
4:J:17:DG:H2''	4:J:18:DG:C8	2.52	0.43
1:A:23:ILE:H	1:A:23:ILE:CD1	2.28	0.43
1:A:43:ALA:O	1:A:44:GLY:O	2.37	0.43
1:A:130:ILE:O	1:A:134:ILE:HG12	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:464:ASN:HD22	2:D:528:ARG:NH1	2.17	0.43
2:D:479:GLU:C	2:D:481:GLY:N	2.76	0.43
2:F:543:PRO:C	2:F:545:ALA:H	2.27	0.43
1:G:75:SER:HB3	1:G:162:GLN:NE2	2.34	0.43
1:E:86:HIS:ND1	1:E:157:VAL:HG12	2.34	0.43
1:G:35:ARG:NH2	1:G:39:GLU:OE2	2.45	0.43
2:H:354:ARG:HG2	2:H:355:PHE:N	2.33	0.43
1:A:22:GLU:HG3	1:A:62:LYS:HB3	2.01	0.42
1:A:86:HIS:CD2	1:A:157:VAL:HG12	2.53	0.42
2:B:616:TYR:CG	2:B:617:LYS:N	2.87	0.42
2:D:464:ASN:HD21	2:D:528:ARG:HH11	1.67	0.42
2:F:621:ILE:HG12	2:F:622:THR:N	2.33	0.42
1:G:86:HIS:CD2	1:G:157:VAL:HG12	2.54	0.42
2:H:548:LEU:O	2:H:640:SER:HB2	2.19	0.42
3:X:22:DT:C2	4:Y:7:DA:C2	3.05	0.42
2:B:357:TYR:O	2:B:358:VAL:C	2.61	0.42
1:C:257:TYR:CG	1:C:258:ALA:N	2.87	0.42
2:D:444:LYS:O	2:D:447:VAL:HG23	2.19	0.42
1:E:61:ILE:HG21	1:E:161:PHE:CD2	2.54	0.42
2:F:492:GLU:O	2:F:496:GLN:HG3	2.19	0.42
2:H:418:ASP:HB3	2:H:457:GLU:OE1	2.20	0.42
2:H:454:ARG:HG2	2:H:454:ARG:NH1	2.33	0.42
1:A:153:ASP:OD2	1:A:156:ALA:HB3	2.19	0.42
1:A:156:ALA:HA	1:A:183:ILE:O	2.18	0.42
2:B:444:LYS:HB2	4:Y:22:DG:OP1	2.19	0.42
2:D:425:ALA:O	2:D:426:GLY:O	2.36	0.42
1:E:144:PRO:O	1:E:148:GLN:HG3	2.19	0.42
1:E:165:VAL:HG22	1:E:175:LEU:HD21	2.00	0.42
2:F:583:TYR:HA	2:F:592:TRP:O	2.19	0.42
2:F:599:SER:C	2:F:601:THR:N	2.77	0.42
1:G:24:ILE:CD1	1:G:110:ILE:HG12	2.49	0.42
1:G:113:PHE:CD2	1:G:113:PHE:N	2.87	0.42
1:A:23:ILE:HD11	1:A:178:VAL:HG22	2.00	0.42
1:A:60:THR:CG2	1:A:61:ILE:H	2.33	0.42
2:B:455:MET:HE2	2:B:469:VAL:HA	2.01	0.42
2:F:476:LEU:HD22	2:F:483:ASP:CG	2.45	0.42
2:H:387:TYR:HD2	2:H:430:MET:HE2	1.83	0.42
1:A:143:VAL:HA	1:A:144:PRO:HD3	1.83	0.42
2:B:341:TYR:N	2:B:341:TYR:CD1	2.87	0.42
2:B:574:GLN:NE2	4:Y:20:DA:OP1	2.53	0.42
1:C:24:ILE:HD12	1:C:60:THR:HG22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:487:THR:N	2:D:490:GLU:OE1	2.44	0.42
2:F:353:PHE:HE2	2:F:439:ILE:HG12	1.83	0.42
2:F:555:ARG:HA	2:F:555:ARG:HD2	1.85	0.42
1:G:88:HIS:CE1	1:G:120:CYS:HA	2.53	0.42
3:X:5:DA:N1	4:Y:23:DT:O4	2.53	0.42
1:A:25:GLU:HB2	1:A:60:THR:H	1.85	0.42
1:A:55:THR:HA	2:D:375:ASN:OD1	2.20	0.42
1:A:167:ASP:O	1:A:168:PRO:C	2.63	0.42
1:E:213:PHE:CE1	2:F:554:ASP:HB3	2.55	0.42
2:F:362:PRO:O	2:F:363:SER:O	2.36	0.42
2:F:476:LEU:HD22	2:F:483:ASP:HB2	2.01	0.42
1:G:156:ALA:O	1:G:157:VAL:CG1	2.67	0.42
3:I:8:DT:O2	4:J:21:DA:C2	2.72	0.42
1:A:51:SER:N	1:A:57:THR:HB	2.34	0.42
1:A:200:ASN:O	1:A:201:ARG:CB	2.63	0.42
2:B:408:ALA:O	2:B:442:VAL:HG11	2.20	0.42
2:B:492:GLU:OE1	2:B:495:ARG:NH2	2.51	0.42
2:D:407:HIS:CE1	2:D:510:VAL:HG23	2.54	0.42
1:E:178:VAL:HG13	1:E:178:VAL:O	2.20	0.42
1:E:221:LYS:HG2	1:E:222:GLU:OE2	2.20	0.42
2:F:460:ILE:CG1	2:F:486:LEU:HD13	2.43	0.42
2:F:616:TYR:CG	2:F:617:LYS:N	2.87	0.42
2:H:387:TYR:CE2	2:H:518:LEU:CD2	2.99	0.42
2:H:425:ALA:O	2:H:426:GLY:C	2.63	0.42
1:A:55:THR:CG2	1:A:56:LYS:H	2.31	0.42
1:C:158:ARG:CZ	1:C:182:PRO:HD3	2.50	0.42
4:J:2:DT:H2''	4:J:3:DG:C5'	2.49	0.42
4:J:17:DG:OP1	4:J:17:DG:C4'	2.64	0.42
1:A:188:ALA:HA	1:A:189:PRO:HD3	1.85	0.42
2:B:572:LYS:HZ2	2:B:606:GLN:CG	2.24	0.42
1:C:24:ILE:N	1:C:60:THR:O	2.47	0.42
2:D:448:PHE:HA	2:D:502:THR:HG21	2.02	0.42
2:D:500:GLN:HE21	2:D:503:LYS:NZ	2.17	0.42
2:D:583:TYR:O	2:D:627:VAL:HB	2.20	0.42
1:E:165:VAL:CG2	1:E:175:LEU:HD21	2.50	0.42
1:E:254:THR:O	1:E:255:PRO:O	2.38	0.42
1:G:21:VAL:CG2	1:G:163:VAL:HG21	2.47	0.42
1:G:132:GLN:HA	1:G:135:GLN:CG	2.50	0.42
4:J:20:DA:H2''	4:J:21:DA:O5'	2.20	0.42
1:A:136:THR:HG23	1:A:138:ASN:HB2	2.01	0.42
2:D:546:SER:O	2:D:548:LEU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:357:TYR:O	2:F:358:VAL:C	2.63	0.42
1:G:90:LEU:HA	1:G:117:GLY:O	2.20	0.42
1:A:32:MET:HG3	1:A:47:PRO:HD2	2.00	0.41
1:A:61:ILE:HG21	1:A:161:PHE:CD2	2.55	0.41
2:B:464:ASN:HD21	2:B:528:ARG:HH11	1.67	0.41
1:C:134:ILE:HD11	1:C:148:GLN:OE1	2.20	0.41
2:D:463:TYR:C	2:D:465:PRO:HD3	2.45	0.41
1:E:58:HIS:CE1	1:E:114:GLN:CD	2.99	0.41
1:E:229:THR:HG22	1:E:269:SER:HB3	1.99	0.41
2:F:354:ARG:HD2	2:F:356:ARG:NE	2.34	0.41
2:F:524:SER:O	2:F:526:THR:HG23	2.20	0.41
1:G:21:VAL:HG23	1:G:175:LEU:HD12	2.01	0.41
2:H:572:LYS:HE2	2:H:606:GLN:HG2	2.02	0.41
1:A:122:LYS:C	1:A:124:ARG:N	2.76	0.41
2:B:409:HIS:HD2	2:B:442:VAL:HG22	1.85	0.41
1:E:54:THR:O	1:E:54:THR:CG2	2.66	0.41
1:E:158:ARG:NH1	1:E:158:ARG:HG2	2.33	0.41
2:F:464:ASN:HD21	2:F:528:ARG:HH11	1.67	0.41
1:G:40:GLY:O	1:G:42:SER:N	2.53	0.41
1:G:267:ARG:HG2	1:G:267:ARG:HH11	1.84	0.41
2:H:559:CYS:SG	2:H:650:GLU:CB	3.03	0.41
1:A:56:LYS:CB	2:D:375:ASN:HD21	2.25	0.41
1:A:60:THR:HG22	1:A:61:ILE:H	1.84	0.41
1:C:65:GLY:O	1:C:66:TYR:HB2	2.20	0.41
1:C:104:LEU:HD12	1:C:104:LEU:HA	1.87	0.41
2:D:423:VAL:CG2	2:D:432:VAL:HG11	2.50	0.41
1:E:95:CYS:HA	1:E:99:TYR:O	2.21	0.41
1:E:171:ARG:HE	1:E:172:PRO:HD2	1.85	0.41
1:E:185:ASP:CG	1:E:187:ARG:HB2	2.46	0.41
1:E:285:GLU:CD	1:E:285:GLU:N	2.78	0.41
2:F:558:GLY:O	2:F:647:TYR:HA	2.20	0.41
1:G:218:LYS:HB3	1:G:218:LYS:HZ2	1.83	0.41
2:H:521:SER:OG	2:H:522:THR:HG23	2.20	0.41
2:H:621:ILE:HG12	2:H:623:LYS:O	2.20	0.41
1:A:62:LYS:HE2	1:A:64:ASN:HD21	1.85	0.41
2:B:545:ALA:C	2:B:633:ARG:NH2	2.79	0.41
2:B:605:ARG:C	2:B:606:GLN:NE2	2.79	0.41
1:C:39:GLU:HB3	1:C:40:GLY:H	1.67	0.41
1:C:216:CYS:HB2	1:C:217:ASP:H	1.72	0.41
2:D:346:GLU:HB2	2:D:381:GLN:H	1.85	0.41
1:E:60:THR:HG22	1:E:61:ILE:H	1.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ILE:HD13	1:G:152:TYR:HE1	1.86	0.41
1:G:226:VAL:O	1:G:236:ARG:HA	2.21	0.41
1:A:185:ASP:CG	1:A:187:ARG:HB2	2.45	0.41
1:A:272:LEU:O	1:A:280:LEU:HA	2.21	0.41
2:B:392:LYS:HB3	2:B:517:PHE:HB2	2.03	0.41
2:B:458:ALA:O	2:B:465:PRO:HG3	2.20	0.41
1:C:78:THR:OG1	1:C:83:HIS:HA	2.21	0.41
2:D:466:GLY:HA2	2:D:470:HIS:O	2.20	0.41
1:E:39:GLU:O	1:E:40:GLY:O	2.39	0.41
2:H:347:GLN:OE1	2:H:348:PRO:HD2	2.20	0.41
2:H:392:LYS:O	2:H:516:ALA:HA	2.20	0.41
2:H:633:ARG:HB2	2:H:636:ASP:OD1	2.20	0.41
4:Y:2:DT:H2''	4:Y:3:DG:C5'	2.51	0.41
2:D:350:GLN:HB3	2:D:536:ALA:O	2.20	0.41
2:D:512:LEU:HB2	2:D:534:SER:OG	2.21	0.41
2:D:566:ILE:N	2:D:566:ILE:CD1	2.82	0.41
1:G:239:PHE:HB3	1:G:252:PHE:HB3	2.03	0.41
2:H:402:LYS:HG2	2:H:403:ASN:N	2.35	0.41
4:Y:22:DG:H1'	4:Y:23:DT:C5'	2.51	0.41
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.21	0.41
1:A:86:HIS:ND1	1:A:157:VAL:HG12	2.36	0.41
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.78	0.41
2:B:441:HIS:HE1	2:B:507:LEU:HD23	1.85	0.41
1:C:144:PRO:HB2	1:C:147:GLU:OE1	2.20	0.41
1:C:264:ALA:HA	1:C:265:PRO:HD3	1.94	0.41
2:D:605:ARG:O	2:D:606:GLN:HB2	2.20	0.41
2:F:397:LEU:HD12	2:F:409:HIS:O	2.21	0.41
2:F:508:SER:O	2:F:509:VAL:HG22	2.20	0.41
2:F:542:ALA:HA	2:F:543:PRO:HD3	1.94	0.41
1:G:122:LYS:O	1:G:124:ARG:N	2.54	0.41
2:H:613:THR:HG22	2:H:614:PRO:O	2.21	0.41
2:H:616:TYR:CZ	2:H:617:LYS:HG2	2.55	0.41
1:A:26:GLN:HB3	1:A:181:HIS:CE1	2.55	0.41
1:A:206:CYS:SG	1:A:290:PRO:HA	2.61	0.41
2:B:573:VAL:HG11	2:B:578:ILE:HD12	2.01	0.41
2:F:358:VAL:C	2:F:360:GLU:H	2.29	0.41
1:G:156:ALA:C	1:G:157:VAL:HG13	2.46	0.41
2:H:412:VAL:HG22	2:H:413:GLY:H	1.85	0.41
2:B:558:GLY:O	2:B:647:TYR:HA	2.21	0.41
1:C:22:GLU:HG2	1:C:64:ASN:OD1	2.20	0.41
1:C:277:ASP:O	1:C:278:ARG:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:616:TYR:CG	2:D:617:LYS:N	2.89	0.41
1:E:35:ARG:NH2	1:E:39:GLU:OE2	2.51	0.41
1:E:52:THR:CG2	1:E:53:ASP:H	2.14	0.41
1:E:68:GLY:CA	1:E:106:PRO:O	2.68	0.41
1:E:126:LEU:HD22	1:E:126:LEU:HA	1.95	0.41
1:E:180:SER:C	1:E:181:HIS:O	2.60	0.41
1:E:229:THR:CG2	1:E:269:SER:CB	2.97	0.41
1:E:233:TRP:O	1:E:234:GLU:HB2	2.21	0.41
1:E:240:SER:C	1:E:242:ALA:H	2.29	0.41
2:H:481:GLY:O	2:H:483:ASP:N	2.53	0.41
1:A:70:GLY:O	1:A:104:LEU:HB2	2.21	0.41
1:A:88:HIS:ND1	1:A:120:CYS:HA	2.35	0.41
1:E:95:CYS:SG	1:E:100:TYR:CA	3.09	0.41
1:E:221:LYS:CG	1:E:222:GLU:OE2	2.69	0.41
2:F:555:ARG:NH1	2:F:555:ARG:CG	2.84	0.41
1:G:268:VAL:CG1	1:G:269:SER:N	2.84	0.41
2:H:409:HIS:HA	2:H:442:VAL:HG13	2.03	0.41
2:H:479:GLU:C	2:H:481:GLY:N	2.74	0.41
4:Y:23:DT:H1'	4:Y:24:DC:H5''	2.03	0.41
4:Y:25:DC:H2''	4:Y:26:DC:C6	2.55	0.41
1:A:178:VAL:O	1:A:178:VAL:HG13	2.21	0.40
1:A:199:VAL:C	1:A:201:ARG:H	2.28	0.40
1:C:222:GLU:CD	1:C:222:GLU:N	2.79	0.40
2:D:412:VAL:HG22	2:D:413:GLY:N	2.34	0.40
1:E:72:VAL:HB	1:E:104:LEU:CD1	2.50	0.40
2:F:356:ARG:HA	2:F:360:GLU:OE2	2.21	0.40
2:F:613:THR:CG2	2:F:614:PRO:N	2.84	0.40
1:G:76:LEU:HA	1:G:76:LEU:HD12	1.77	0.40
1:G:213:PHE:HD2	2:H:567:TYR:HB3	1.85	0.40
3:I:7:DT:H3	4:J:22:DG:N2	2.18	0.40
3:I:22:DT:C2	4:J:7:DA:C2	3.08	0.40
4:J:23:DT:H6	4:J:23:DT:H2'	1.75	0.40
2:B:346:GLU:OE2	2:B:378:SER:HB2	2.21	0.40
1:C:115:ASN:HD22	1:C:115:ASN:HA	1.51	0.40
1:C:128:GLN:O	1:C:131:SER:OG	2.30	0.40
2:D:405:HIS:HB3	2:D:501:GLN:OE1	2.21	0.40
1:E:117:GLY:C	1:E:118:ILE:HD12	2.46	0.40
1:E:218:LYS:HB3	1:E:218:LYS:HZ2	1.86	0.40
2:F:538:TYR:CD2	2:F:538:TYR:N	2.89	0.40
1:G:24:ILE:CG1	1:G:62:LYS:HB2	2.52	0.40
1:G:39:GLU:O	1:G:40:GLY:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:12:DG:O5'	3:X:12:DG:H2'	2.21	0.40
4:J:20:DA:O5'	4:J:20:DA:H8	2.04	0.40
1:A:26:GLN:OE1	1:A:180:SER:HB2	2.22	0.40
1:C:221:LYS:HB3	1:C:244:VAL:HG11	2.02	0.40
1:C:223:ASP:OD2	1:C:274:ARG:CG	2.69	0.40
2:D:348:PRO:CB	2:D:537:ILE:HD11	2.51	0.40
2:D:402:LYS:HG2	2:D:403:ASN:OD1	2.21	0.40
2:D:500:GLN:NE2	2:D:503:LYS:NZ	2.69	0.40
1:E:23:ILE:HG22	1:E:25:GLU:O	2.21	0.40
1:E:73:ARG:HA	1:E:100:TYR:O	2.22	0.40
1:E:132:GLN:HA	1:E:135:GLN:HG2	2.03	0.40
2:F:412:VAL:CG2	2:F:413:GLY:N	2.84	0.40
2:F:525:PHE:CD1	2:F:525:PHE:N	2.89	0.40
2:F:572:LYS:HA	2:F:607:PHE:CE1	2.57	0.40
1:G:72:VAL:HB	1:G:104:LEU:CD1	2.51	0.40
2:H:451:LEU:CD1	2:H:498:ALA:HA	2.52	0.40
2:H:577:ASP:O	2:H:577:ASP:CG	2.62	0.40
2:H:643:LYS:HA	2:H:644:PRO:HD3	1.97	0.40
2:B:402:LYS:NZ	2:B:403:ASN:H	2.19	0.40
1:C:68:GLY:HA2	1:C:106:PRO:O	2.21	0.40
1:E:43:ALA:O	1:E:44:GLY:O	2.39	0.40
1:E:95:CYS:SG	1:E:100:TYR:CB	3.07	0.40
1:E:171:ARG:NE	1:E:172:PRO:HD2	2.36	0.40
1:E:268:VAL:HG12	1:E:269:SER:N	2.37	0.40
1:G:228:PHE:HZ	1:G:254:THR:HG22	1.86	0.40
2:H:375:ASN:C	2:H:376:LYS:HG3	2.46	0.40
3:I:22:DT:H2''	3:I:23:DT:OP2	2.20	0.40
2:B:613:THR:CG2	2:B:614:PRO:O	2.65	0.40
1:C:245:HIS:CD2	2:D:569:LEU:HB3	2.56	0.40
1:E:128:GLN:O	1:E:128:GLN:HG2	2.21	0.40
1:G:217:ASP:O	1:G:219:VAL:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	271/273 (99%)	231 (85%)	29 (11%)	11 (4%)	2	19
1	C	271/273 (99%)	231 (85%)	29 (11%)	11 (4%)	2	19
1	E	271/273 (99%)	229 (84%)	31 (11%)	11 (4%)	2	19
1	G	271/273 (99%)	231 (85%)	31 (11%)	9 (3%)	3	24
2	B	310/312 (99%)	274 (88%)	25 (8%)	11 (4%)	3	23
2	D	310/312 (99%)	264 (85%)	34 (11%)	12 (4%)	2	20
2	F	310/312 (99%)	272 (88%)	29 (9%)	9 (3%)	3	26
2	H	310/312 (99%)	261 (84%)	36 (12%)	13 (4%)	2	19
All	All	2324/2340 (99%)	1993 (86%)	244 (10%)	87 (4%)	2	21

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	83	HIS
1	A	192	ALA
1	A	246	ARG
2	B	363	SER
2	B	367	LEU
2	B	368	PRO
2	B	426	GLY
2	B	478	ALA
2	B	606	GLN
1	C	81	PRO
1	C	262	LEU
2	D	368	PRO
2	D	377	LYS
1	E	81	PRO
1	E	83	HIS
1	E	142	HIS
1	E	192	ALA
2	F	363	SER
2	F	478	ALA
1	G	81	PRO
2	H	368	PRO
2	H	377	LYS
2	H	478	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	482	GLY
2	H	535	ASP
2	H	572	LYS
1	A	142	HIS
1	A	201	ARG
2	B	359	CYS
2	B	482	GLY
1	C	199	VAL
2	D	371	SER
2	D	426	GLY
2	D	478	ALA
2	D	482	GLY
2	D	535	ASP
2	D	545	ALA
2	D	547	ASN
1	E	40	GLY
1	E	246	ARG
2	F	359	CYS
2	F	426	GLY
1	G	48	GLY
1	G	199	VAL
1	G	200	ASN
2	H	371	SER
2	H	426	GLY
2	H	545	ALA
2	H	547	ASN
1	A	40	GLY
1	A	66	TYR
1	C	48	GLY
2	D	572	LYS
1	E	66	TYR
1	E	186	ASN
2	F	600	PRO
1	G	186	ASN
1	G	262	LEU
1	A	96	ARG
1	C	142	HIS
1	C	172	PRO
1	E	51	SER
2	F	482	GLY
2	F	635	SER
1	A	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	545	ALA
1	C	49	GLU
1	C	200	ASN
1	E	201	ARG
1	G	66	TYR
1	G	165	VAL
1	G	172	PRO
2	H	483	ASP
2	B	600	PRO
1	C	43	ALA
2	F	545	ALA
1	C	165	VAL
2	H	481	GLY
2	D	481	GLY
1	E	44	GLY
2	D	382	VAL
2	H	382	VAL
1	A	44	GLY
1	C	157	VAL
2	F	481	GLY
2	B	481	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/242 (100%)	225 (93%)	17 (7%)	14	41
1	C	242/242 (100%)	219 (90%)	23 (10%)	8	32
1	E	242/242 (100%)	225 (93%)	17 (7%)	14	41
1	G	242/242 (100%)	222 (92%)	20 (8%)	10	35
2	B	268/268 (100%)	247 (92%)	21 (8%)	11	38
2	D	268/268 (100%)	254 (95%)	14 (5%)	21	48
2	F	268/268 (100%)	253 (94%)	15 (6%)	19	47
2	H	268/268 (100%)	254 (95%)	14 (5%)	21	48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2040/2040 (100%)	1899 (93%)	141 (7%)	14	41

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	37	LYS
1	A	76	LEU
1	A	81	PRO
1	A	104	LEU
1	A	126	LEU
1	A	130	ILE
1	A	135	GLN
1	A	145	ILE
1	A	167	ASP
1	A	198	ARG
1	A	199	VAL
1	A	202	ASN
1	A	214	LEU
1	A	222	GLU
1	A	272	LEU
1	A	284	MET
2	B	345	LEU
2	B	362	PRO
2	B	367	LEU
2	B	380	PRO
2	B	402	LYS
2	B	411	LEU
2	B	451	LEU
2	B	495	ARG
2	B	502	THR
2	B	504	GLU
2	B	510	VAL
2	B	550	ILE
2	B	551	VAL
2	B	579	GLN
2	B	580	ILE
2	B	584	GLU
2	B	586	GLU
2	B	600	PRO
2	B	606	GLN
2	B	621	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	644	PRO
1	C	28	LYS
1	C	33	ARG
1	C	37	LYS
1	C	54	THR
1	C	76	LEU
1	C	81	PRO
1	C	104	LEU
1	C	114	GLN
1	C	115	ASN
1	C	118	ILE
1	C	126	LEU
1	C	135	GLN
1	C	145	ILE
1	C	179	LEU
1	C	198	ARG
1	C	202	ASN
1	C	214	LEU
1	C	216	CYS
1	C	246	ARG
1	C	250	ILE
1	C	272	LEU
1	C	284	MET
1	C	291	ASP
2	D	345	LEU
2	D	402	LYS
2	D	410	SER
2	D	488	ASP
2	D	494	ILE
2	D	495	ARG
2	D	510	VAL
2	D	544	ASN
2	D	552	ARG
2	D	568	LEU
2	D	584	GLU
2	D	586	GLU
2	D	600	PRO
2	D	621	ILE
1	E	23	ILE
1	E	32	MET
1	E	37	LYS
1	E	76	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	81	PRO
1	E	104	LEU
1	E	114	GLN
1	E	126	LEU
1	E	135	GLN
1	E	145	ILE
1	E	198	ARG
1	E	202	ASN
1	E	214	LEU
1	E	222	GLU
1	E	272	LEU
1	E	284	MET
1	E	290	PRO
2	F	345	LEU
2	F	363	SER
2	F	402	LYS
2	F	411	LEU
2	F	488	ASP
2	F	495	ARG
2	F	502	THR
2	F	510	VAL
2	F	550	ILE
2	F	551	VAL
2	F	579	GLN
2	F	580	ILE
2	F	584	GLU
2	F	586	GLU
2	F	621	ILE
1	G	28	LYS
1	G	33	ARG
1	G	37	LYS
1	G	54	THR
1	G	76	LEU
1	G	81	PRO
1	G	104	LEU
1	G	114	GLN
1	G	126	LEU
1	G	135	GLN
1	G	145	ILE
1	G	179	LEU
1	G	202	ASN
1	G	203	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	214	LEU
1	G	246	ARG
1	G	247	GLN
1	G	272	LEU
1	G	284	MET
1	G	291	ASP
2	H	345	LEU
2	H	402	LYS
2	H	494	ILE
2	H	495	ARG
2	H	504	GLU
2	H	510	VAL
2	H	544	ASN
2	H	568	LEU
2	H	584	GLU
2	H	586	GLU
2	H	600	PRO
2	H	612	LYS
2	H	613	THR
2	H	621	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	111	HIS
1	A	115	ASN
1	A	128	GLN
1	A	137	ASN
1	A	155	ASN
1	A	181	HIS
1	A	202	ASN
1	A	241	GLN
1	A	271	GLN
2	B	350	GLN
2	B	407	HIS
2	B	409	HIS
2	B	436	ASN
2	B	464	ASN
2	B	470	HIS
2	B	500	GLN
2	B	574	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	579	GLN
2	B	606	GLN
2	B	630	GLN
1	C	114	GLN
1	C	115	ASN
1	C	128	GLN
1	C	137	ASN
1	C	162	GLN
1	C	202	ASN
1	C	220	GLN
1	C	247	GLN
1	C	271	GLN
2	D	375	ASN
2	D	396	GLN
2	D	407	HIS
2	D	409	HIS
2	D	436	ASN
2	D	464	ASN
2	D	470	HIS
2	D	500	GLN
1	E	58	HIS
1	E	114	GLN
1	E	115	ASN
1	E	119	GLN
1	E	128	GLN
1	E	137	ASN
1	E	155	ASN
1	E	162	GLN
1	E	181	HIS
1	E	202	ASN
1	E	247	GLN
1	E	271	GLN
2	F	343	GLN
2	F	350	GLN
2	F	407	HIS
2	F	436	ASN
2	F	464	ASN
2	F	470	HIS
2	F	500	GLN
2	F	574	GLN
2	F	579	GLN
2	F	606	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	83	HIS
1	G	115	ASN
1	G	128	GLN
1	G	137	ASN
1	G	155	ASN
1	G	162	GLN
1	G	202	ASN
1	G	220	GLN
1	G	247	GLN
2	H	396	GLN
2	H	407	HIS
2	H	409	HIS
2	H	436	ASN
2	H	464	ASN
2	H	500	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	273/273 (100%)	-0.71	1 (0%) 88 70	76, 176, 199, 200	0
1	C	273/273 (100%)	-0.98	0 100 100	67, 142, 189, 199	0
1	E	273/273 (100%)	-0.73	1 (0%) 88 70	77, 177, 199, 200	0
1	G	273/273 (100%)	-1.00	0 100 100	66, 144, 190, 200	0
2	B	312/312 (100%)	-0.77	0 100 100	75, 155, 198, 200	0
2	D	312/312 (100%)	-0.75	0 100 100	75, 164, 199, 200	0
2	F	312/312 (100%)	-0.84	1 (0%) 90 75	66, 156, 199, 200	0
2	H	312/312 (100%)	-0.74	0 100 100	74, 169, 199, 200	0
3	I	26/26 (100%)	-1.12	0 100 100	84, 106, 119, 122	0
3	X	26/26 (100%)	-1.07	0 100 100	90, 103, 116, 130	0
4	J	26/26 (100%)	-1.08	0 100 100	85, 108, 118, 127	0
4	Y	26/26 (100%)	-1.11	0 100 100	79, 104, 115, 129	0
All	All	2444/2444 (100%)	-0.83	3 (0%) 92 85	66, 157, 199, 200	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ASP	2.5
2	F	482	GLY	2.3
1	E	174	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.