



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:40 am BST

PDB ID : 5LDH
Title : STRUCTURE OF THE ACTIVE TERNARY COMPLEX OF PIG HEART
LACTATE DEHYDROGENASE WITH S-LAC-NAD AT 2.7 ANGSTROMS
RESOLUTION
Authors : Grau, U.M.; Rossmann, M.G.
Deposited on : 1980-10-29
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

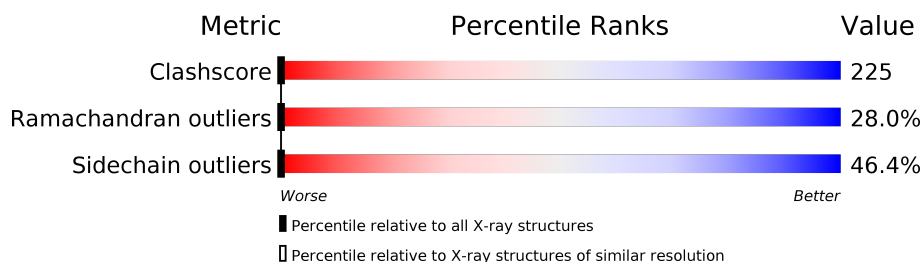
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	334	
1	B	334	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LNC	A	332	-	-	X	-
2	LNC	B	332	-	-	X	-
3	CIT	A	333	-	-	X	-
3	CIT	B	333	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5248 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.

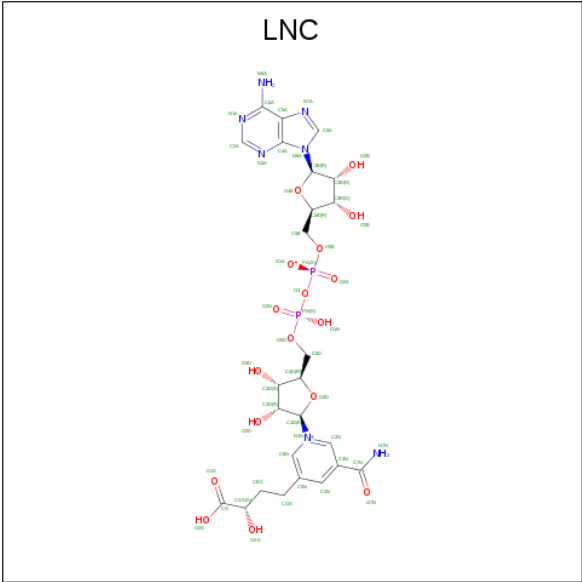
- Molecule 1 is a protein called LACTATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2560	1626	435	485	14			
1	B	334	Total	C	N	O	S	0	0	0
			2560	1626	435	485	14			

There are 18 discrepancies between the modelled and reference sequences:

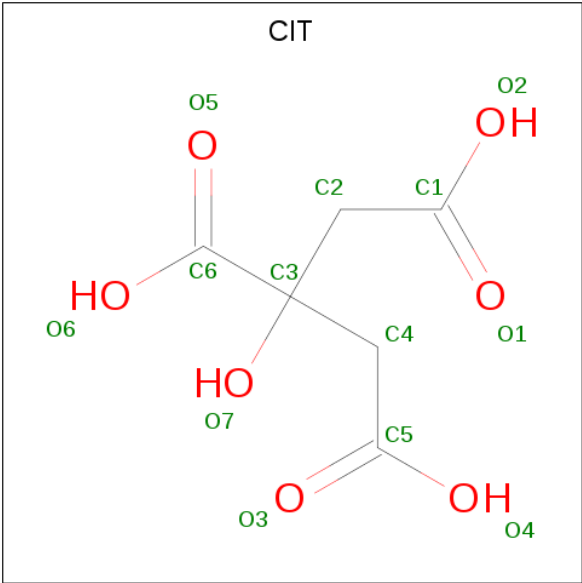
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLN	GLU	CONFLICT	UNP P00336
A	14	GLN	GLU	CONFLICT	UNP P00336
A	20	ASP	ASN	CONFLICT	UNP P00336
A	81	ASN	ASP	CONFLICT	UNP P00336
A	132B	ASN	ASP	CONFLICT	UNP P00336
A	149	ALA	THR	CONFLICT	UNP P00336
A	177	GLY	ALA	CONFLICT	UNP P00336
A	209C	VAL	SER	CONFLICT	UNP P00336
A	211	GLN	GLU	CONFLICT	UNP P00336
B	13	GLN	GLU	CONFLICT	UNP P00336
B	14	GLN	GLU	CONFLICT	UNP P00336
B	20	ASP	ASN	CONFLICT	UNP P00336
B	81	ASN	ASP	CONFLICT	UNP P00336
B	132B	ASN	ASP	CONFLICT	UNP P00336
B	149	ALA	THR	CONFLICT	UNP P00336
B	177	GLY	ALA	CONFLICT	UNP P00336
B	209C	VAL	SER	CONFLICT	UNP P00336
B	211	GLN	GLU	CONFLICT	UNP P00336

- Molecule 2 is (3S)-5-(3-CARBOXY-3-HYDROXYPROPYL) NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: LNC) (formula: C₂₅H₃₃N₇O₁₇P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0
			51	25	7	17	2	
2	B	1	Total	C	N	O	P	0
			51	25	7	17	2	

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).

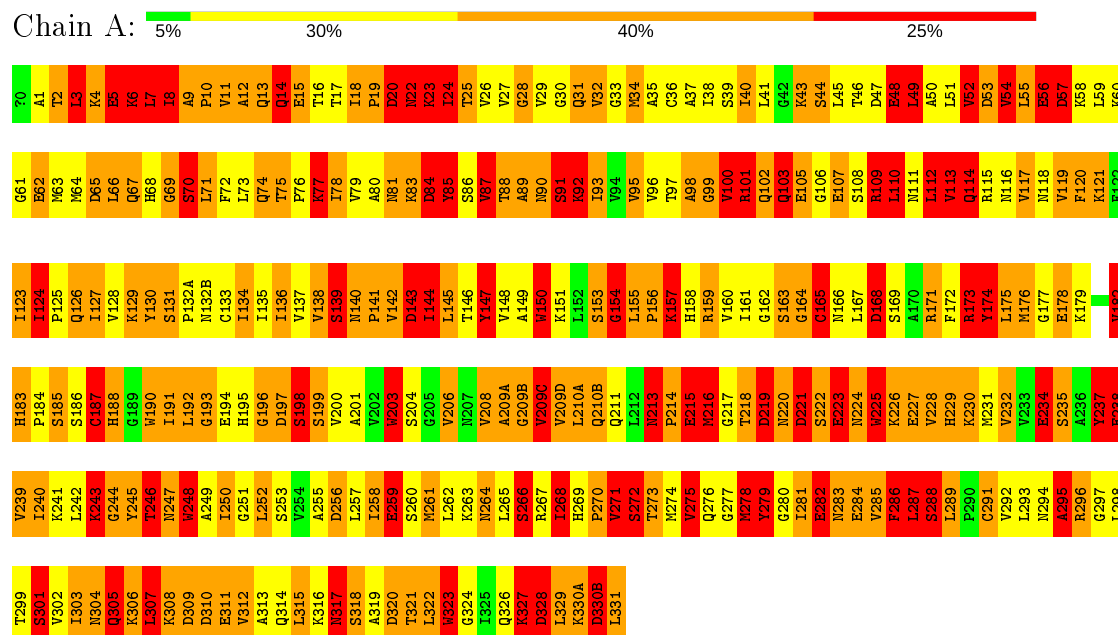


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

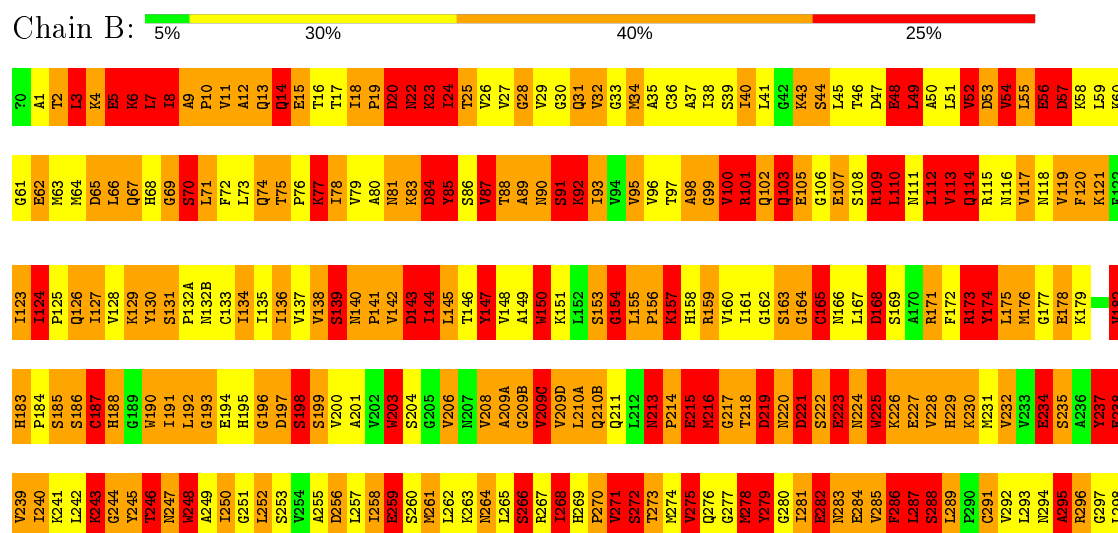
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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: LACTATE DEHYDROGENASE



• Molecule 1: LACTATE DEHYDROGENASE



T299	S301	V302	I303	N304	D305	K306	L307	K308	D309	D310	E311	V312	A313	Q314	L315	K316	N317	S318	A319	D320	T321	L322	K323	G324	F325	Q326	K327	D328	L329	K330A	D330B	L331
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-------	-------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.60Å 133.60Å 113.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.70 43.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.70) 69.4 (43.73-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.196 , (Not available) 0.429 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , -39.8	EDS
L-test for twinning ¹	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
F_o, F_c correlation	0.41	EDS
Total number of atoms	5248	wwPDB-VP
Average B, all atoms (Å ²)	0.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, LNC, CIT

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	1.11	24/2599 (0.9%)	1.88	150/3525 (4.3%)
1	B	1.11	24/2599 (0.9%)	1.88	150/3525 (4.3%)
All	All	1.11	48/5198 (0.9%)	1.88	300/7050 (4.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	TRP	NE1-CE2	-7.38	1.27	1.37
1	B	150	TRP	NE1-CE2	-7.38	1.27	1.37
1	A	203	TRP	NE1-CE2	-7.37	1.27	1.37
1	B	203	TRP	NE1-CE2	-7.37	1.27	1.37
1	A	190	TRP	NE1-CE2	-7.35	1.27	1.37
1	A	225	TRP	NE1-CE2	-7.35	1.27	1.37
1	B	190	TRP	NE1-CE2	-7.35	1.27	1.37
1	B	225	TRP	NE1-CE2	-7.35	1.27	1.37
1	A	323	TRP	NE1-CE2	-7.34	1.28	1.37
1	B	323	TRP	NE1-CE2	-7.34	1.28	1.37
1	A	248	TRP	NE1-CE2	-7.28	1.28	1.37
1	B	248	TRP	NE1-CE2	-7.28	1.28	1.37
1	A	194	GLU	CD-OE1	-5.28	1.19	1.25
1	B	194	GLU	CD-OE1	-5.28	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	GLU	CD-OE1	-5.28	1.19	1.25
1	B	238	GLU	CD-OE1	-5.28	1.19	1.25
1	A	311	GLU	CD-OE1	-5.28	1.19	1.25
1	B	311	GLU	CD-OE1	-5.28	1.19	1.25
1	A	215	GLU	CD-OE1	-5.26	1.19	1.25
1	B	215	GLU	CD-OE1	-5.26	1.19	1.25
1	A	5	GLU	CD-OE1	-5.25	1.19	1.25
1	B	5	GLU	CD-OE1	-5.25	1.19	1.25
1	A	105	GLU	CD-OE1	-5.25	1.19	1.25
1	B	105	GLU	CD-OE1	-5.25	1.19	1.25
1	A	259	GLU	CD-OE1	-5.25	1.19	1.25
1	B	259	GLU	CD-OE1	-5.25	1.19	1.25
1	A	284	GLU	CD-OE1	-5.24	1.19	1.25
1	B	284	GLU	CD-OE1	-5.24	1.19	1.25
1	A	48	GLU	CD-OE1	-5.23	1.20	1.25
1	B	48	GLU	CD-OE1	-5.23	1.20	1.25
1	A	223	GLU	CD-OE1	-5.22	1.20	1.25
1	A	227	GLU	CD-OE1	-5.22	1.20	1.25
1	B	223	GLU	CD-OE1	-5.22	1.20	1.25
1	B	227	GLU	CD-OE1	-5.22	1.20	1.25
1	A	234	GLU	CD-OE1	-5.21	1.20	1.25
1	B	234	GLU	CD-OE1	-5.21	1.20	1.25
1	A	282	GLU	CD-OE1	-5.20	1.20	1.25
1	B	282	GLU	CD-OE1	-5.20	1.20	1.25
1	A	178	GLU	CD-OE1	-5.20	1.20	1.25
1	B	178	GLU	CD-OE1	-5.20	1.20	1.25
1	A	62	GLU	CD-OE1	-5.19	1.20	1.25
1	B	62	GLU	CD-OE1	-5.19	1.20	1.25
1	A	15	GLU	CD-OE1	-5.18	1.20	1.25
1	B	15	GLU	CD-OE1	-5.18	1.20	1.25
1	A	107	GLU	CD-OE1	-5.17	1.20	1.25
1	B	107	GLU	CD-OE1	-5.17	1.20	1.25
1	A	56	GLU	CD-OE1	-5.16	1.20	1.25
1	B	56	GLU	CD-OE1	-5.16	1.20	1.25

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ASP	N-CA-C	-10.06	83.85	111.00
1	B	20	ASP	N-CA-C	-10.06	83.85	111.00
1	A	304	ASN	N-CA-C	9.96	137.88	111.00
1	B	304	ASN	N-CA-C	9.96	137.88	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209(C)	VAL	N-CA-C	-9.69	84.83	111.00
1	B	209(C)	VAL	N-CA-C	-9.69	84.83	111.00
1	A	188	HIS	N-CA-C	9.40	136.38	111.00
1	B	188	HIS	N-CA-C	9.40	136.38	111.00
1	A	246	THR	N-CA-C	-9.39	85.64	111.00
1	B	246	THR	N-CA-C	-9.39	85.64	111.00
1	A	185	SER	N-CA-C	9.37	136.31	111.00
1	B	185	SER	N-CA-C	9.37	136.31	111.00
1	A	154	GLY	N-CA-C	9.32	136.41	113.10
1	B	154	GLY	N-CA-C	9.32	136.41	113.10
1	A	190	TRP	N-CA-C	9.20	135.84	111.00
1	B	190	TRP	N-CA-C	9.20	135.84	111.00
1	A	216	MET	N-CA-C	9.17	135.76	111.00
1	B	216	MET	N-CA-C	9.17	135.76	111.00
1	A	91	SER	N-CA-C	8.88	134.98	111.00
1	B	91	SER	N-CA-C	8.88	134.98	111.00
1	A	271	VAL	N-CA-C	8.86	134.91	111.00
1	B	271	VAL	N-CA-C	8.86	134.91	111.00
1	A	305	GLN	N-CA-C	8.83	134.84	111.00
1	B	305	GLN	N-CA-C	8.83	134.84	111.00
1	A	209(B)	GLY	N-CA-C	-8.79	91.14	113.10
1	B	209(B)	GLY	N-CA-C	-8.79	91.14	113.10
1	A	282	GLU	N-CA-C	8.59	134.20	111.00
1	B	282	GLU	N-CA-C	8.59	134.20	111.00
1	A	112	LEU	N-CA-C	8.35	133.54	111.00
1	B	112	LEU	N-CA-C	8.35	133.54	111.00
1	A	47	ASP	N-CA-C	-8.31	88.56	111.00
1	A	215	GLU	N-CA-C	8.31	133.43	111.00
1	B	47	ASP	N-CA-C	-8.31	88.56	111.00
1	B	215	GLU	N-CA-C	8.31	133.43	111.00
1	A	100	VAL	N-CA-C	-8.17	88.93	111.00
1	B	100	VAL	N-CA-C	-8.17	88.93	111.00
1	A	185	SER	CB-CA-C	-8.10	94.72	110.10
1	B	185	SER	CB-CA-C	-8.10	94.72	110.10
1	A	295	ALA	N-CA-CB	-8.05	98.83	110.10
1	B	295	ALA	N-CA-CB	-8.05	98.83	110.10
1	A	307	LEU	N-CA-C	-7.92	89.61	111.00
1	B	307	LEU	N-CA-C	-7.92	89.61	111.00
1	A	282	GLU	CB-CA-C	-7.92	94.56	110.40
1	B	282	GLU	CB-CA-C	-7.92	94.56	110.40
1	A	28	GLY	N-CA-C	-7.84	93.49	113.10
1	B	28	GLY	N-CA-C	-7.84	93.49	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	LYS	N-CA-C	7.83	132.15	111.00
1	B	77	LYS	N-CA-C	7.83	132.15	111.00
1	A	271	VAL	CB-CA-C	-7.75	96.67	111.40
1	B	271	VAL	CB-CA-C	-7.75	96.67	111.40
1	A	295	ALA	N-CA-C	7.74	131.91	111.00
1	A	304	ASN	CB-CA-C	-7.74	94.91	110.40
1	B	295	ALA	N-CA-C	7.74	131.91	111.00
1	B	304	ASN	CB-CA-C	-7.74	94.91	110.40
1	A	215	GLU	CB-CA-C	-7.69	95.03	110.40
1	B	215	GLU	CB-CA-C	-7.69	95.03	110.40
1	A	25	THR	N-CA-C	7.67	131.70	111.00
1	B	25	THR	N-CA-C	7.67	131.70	111.00
1	A	91	SER	CB-CA-C	-7.64	95.59	110.10
1	B	91	SER	CB-CA-C	-7.64	95.59	110.10
1	A	216	MET	CB-CA-C	-7.45	95.50	110.40
1	B	216	MET	CB-CA-C	-7.45	95.50	110.40
1	A	173	ARG	N-CA-C	7.45	131.10	111.00
1	B	173	ARG	N-CA-C	7.45	131.10	111.00
1	A	143	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	143	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	53	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	53	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	57	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	57	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	165	CYS	N-CA-C	7.34	130.81	111.00
1	B	165	CYS	N-CA-C	7.34	130.81	111.00
1	A	320	ASP	CB-CG-OD1	7.33	124.90	118.30
1	B	320	ASP	CB-CG-OD1	7.33	124.90	118.30
1	A	256	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	256	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	328	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	328	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	20	ASP	CB-CG-OD1	7.32	124.89	118.30
1	B	20	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	330(B)	ASP	CB-CG-OD1	7.32	124.88	118.30
1	B	330(B)	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	219	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	219	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	47	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	47	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	221	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	221	ASP	CB-CG-OD1	7.30	124.87	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	197	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	309	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	65	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	197	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	309	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	168	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	168	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	83	LYS	N-CA-C	7.29	130.68	111.00
1	A	310	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	83	LYS	N-CA-C	7.29	130.68	111.00
1	B	310	ASP	CB-CG-OD1	7.29	124.86	118.30
1	A	84	ASP	CB-CG-OD1	7.25	124.82	118.30
1	B	84	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	112	LEU	CB-CA-C	-7.07	96.77	110.20
1	B	112	LEU	CB-CA-C	-7.07	96.77	110.20
1	A	75	THR	N-CA-C	-7.03	92.03	111.00
1	B	75	THR	N-CA-C	-7.03	92.03	111.00
1	A	188	HIS	CB-CA-C	-6.99	96.42	110.40
1	B	188	HIS	CB-CA-C	-6.99	96.42	110.40
1	A	77	LYS	CB-CA-C	-6.95	96.51	110.40
1	B	77	LYS	CB-CA-C	-6.95	96.51	110.40
1	A	124	ILE	CB-CA-C	-6.82	97.96	111.60
1	B	124	ILE	CB-CA-C	-6.82	97.96	111.60
1	A	5	GLU	N-CA-C	6.79	129.33	111.00
1	B	5	GLU	N-CA-C	6.79	129.33	111.00
1	A	22	ASN	N-CA-C	6.71	129.13	111.00
1	B	22	ASN	N-CA-C	6.71	129.13	111.00
1	A	173	ARG	CB-CA-C	-6.70	97.00	110.40
1	B	173	ARG	CB-CA-C	-6.70	97.00	110.40
1	A	101	ARG	N-CA-C	6.68	129.02	111.00
1	B	101	ARG	N-CA-C	6.68	129.02	111.00
1	A	23	LYS	N-CA-C	6.60	128.83	111.00
1	B	23	LYS	N-CA-C	6.60	128.83	111.00
1	A	190	TRP	CB-CA-C	-6.59	97.23	110.40
1	B	190	TRP	CB-CA-C	-6.59	97.23	110.40
1	A	83	LYS	CB-CA-C	-6.49	97.41	110.40
1	B	83	LYS	CB-CA-C	-6.49	97.41	110.40
1	A	5	GLU	CB-CA-C	-6.47	97.46	110.40
1	B	5	GLU	CB-CA-C	-6.47	97.46	110.40
1	A	113	VAL	N-CA-C	-6.29	94.01	111.00
1	A	124	ILE	N-CA-C	6.29	127.99	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	VAL	N-CA-C	-6.29	94.01	111.00
1	B	124	ILE	N-CA-C	6.29	127.99	111.00
1	A	165	CYS	CB-CA-C	-6.19	98.03	110.40
1	B	165	CYS	CB-CA-C	-6.19	98.03	110.40
1	A	8	ILE	CB-CA-C	-6.15	99.30	111.60
1	B	8	ILE	CB-CA-C	-6.15	99.30	111.60
1	A	305	GLN	CB-CA-C	-6.14	98.11	110.40
1	B	305	GLN	CB-CA-C	-6.14	98.11	110.40
1	A	101	ARG	CB-CA-C	-6.09	98.23	110.40
1	B	101	ARG	CB-CA-C	-6.09	98.23	110.40
1	A	193	GLY	N-CA-C	6.07	128.28	113.10
1	B	193	GLY	N-CA-C	6.07	128.28	113.10
1	A	279	TYR	N-CA-C	-6.02	94.75	111.00
1	B	279	TYR	N-CA-C	-6.02	94.75	111.00
1	A	20	ASP	CB-CA-C	5.97	122.34	110.40
1	B	20	ASP	CB-CA-C	5.97	122.34	110.40
1	A	23	LYS	CB-CA-C	-5.96	98.47	110.40
1	B	23	LYS	CB-CA-C	-5.96	98.47	110.40
1	A	266	SER	N-CA-C	-5.90	95.08	111.00
1	B	266	SER	N-CA-C	-5.90	95.08	111.00
1	A	297	GLY	N-CA-C	-5.87	98.42	113.10
1	B	297	GLY	N-CA-C	-5.87	98.42	113.10
1	A	49	LEU	N-CA-C	5.83	126.74	111.00
1	B	49	LEU	N-CA-C	5.83	126.74	111.00
1	A	237	TYR	N-CA-C	5.82	126.70	111.00
1	B	237	TYR	N-CA-C	5.82	126.70	111.00
1	A	62	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	234	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	B	62	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	B	234	GLU	OE1-CD-OE2	5.81	130.28	123.30
1	A	105	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	B	105	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	107	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	B	107	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	259	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	311	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	259	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	B	311	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	15	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	B	15	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	A	48	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	B	48	GLU	OE1-CD-OE2	5.78	130.23	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	B	223	GLU	OE1-CD-OE2	5.78	130.23	123.30
1	A	5	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	B	5	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	178	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	B	178	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	215	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	B	215	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	A	238	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	238	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	284	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	284	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	194	GLU	OE1-CD-OE2	5.75	130.21	123.30
1	B	194	GLU	OE1-CD-OE2	5.75	130.21	123.30
1	A	56	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	A	282	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	B	56	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	B	282	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	A	227	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	227	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	A	106	GLY	N-CA-C	5.70	127.34	113.10
1	B	106	GLY	N-CA-C	5.70	127.34	113.10
1	A	182	VAL	N-CA-C	5.66	126.29	111.00
1	B	182	VAL	N-CA-C	5.66	126.29	111.00
1	A	52	VAL	N-CA-C	5.61	126.16	111.00
1	B	52	VAL	N-CA-C	5.61	126.16	111.00
1	A	243	LYS	N-CA-C	5.59	126.09	111.00
1	B	243	LYS	N-CA-C	5.59	126.09	111.00
1	A	301	SER	N-CA-C	5.55	125.98	111.00
1	B	301	SER	N-CA-C	5.55	125.98	111.00
1	A	209(C)	VAL	CB-CA-C	5.54	121.93	111.40
1	B	209(C)	VAL	CB-CA-C	5.54	121.93	111.40
1	A	8	ILE	N-CA-C	5.45	125.72	111.00
1	B	8	ILE	N-CA-C	5.45	125.72	111.00
1	A	110	LEU	N-CA-C	5.41	125.61	111.00
1	A	317	ASN	N-CA-C	5.41	125.61	111.00
1	B	110	LEU	N-CA-C	5.41	125.61	111.00
1	B	317	ASN	N-CA-C	5.41	125.61	111.00
1	A	24	ILE	CB-CA-C	-5.39	100.81	111.60
1	B	24	ILE	CB-CA-C	-5.39	100.81	111.60
1	A	275	VAL	N-CA-C	-5.38	96.46	111.00
1	B	275	VAL	N-CA-C	-5.38	96.46	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLN	N-CA-C	5.36	125.46	111.00
1	B	14	GLN	N-CA-C	5.36	125.46	111.00
1	A	84	ASP	N-CA-C	-5.27	96.78	111.00
1	B	84	ASP	N-CA-C	-5.27	96.78	111.00
1	A	194	GLU	CB-CA-C	-5.26	99.88	110.40
1	B	194	GLU	CB-CA-C	-5.26	99.88	110.40
1	A	330(B)	ASP	N-CA-C	5.26	125.20	111.00
1	B	330(B)	ASP	N-CA-C	5.26	125.20	111.00
1	A	6	LYS	N-CA-C	5.25	125.16	111.00
1	B	6	LYS	N-CA-C	5.25	125.16	111.00
1	A	69	GLY	N-CA-C	-5.24	100.00	113.10
1	A	153	SER	N-CA-C	5.24	125.15	111.00
1	B	69	GLY	N-CA-C	-5.24	100.00	113.10
1	B	153	SER	N-CA-C	5.24	125.15	111.00
1	A	194	GLU	N-CA-C	5.24	125.15	111.00
1	B	194	GLU	N-CA-C	5.24	125.15	111.00
1	A	157	LYS	N-CA-C	5.21	125.08	111.00
1	B	157	LYS	N-CA-C	5.21	125.08	111.00
1	A	62	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	284	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	62	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	B	284	GLU	CG-CD-OE2	-5.16	107.98	118.30
1	A	48	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	234	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	238	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	B	48	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	B	234	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	B	238	GLU	CG-CD-OE2	-5.16	107.99	118.30
1	A	105	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	107	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	194	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	215	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	A	311	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	B	105	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	B	107	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	B	194	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	B	215	GLU	CG-CD-OE2	-5.15	107.99	118.30
1	B	311	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	178	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	B	178	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	A	5	GLU	CG-CD-OE2	-5.15	108.01	118.30
1	B	5	GLU	CG-CD-OE2	-5.15	108.01	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	A	259	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	B	15	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	B	259	GLU	CG-CD-OE2	-5.14	108.01	118.30
1	A	223	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	B	223	GLU	CG-CD-OE2	-5.14	108.02	118.30
1	A	243	LYS	CB-CA-C	-5.14	100.12	110.40
1	B	243	LYS	CB-CA-C	-5.14	100.12	110.40
1	A	121	LYS	N-CA-C	5.14	124.87	111.00
1	B	121	LYS	N-CA-C	5.14	124.87	111.00
1	A	56	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	85	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	A	227	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	282	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	56	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	85	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	227	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	B	282	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	22	ASN	CB-CA-C	-5.13	100.15	110.40
1	B	22	ASN	CB-CA-C	-5.13	100.15	110.40
1	A	279	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	B	279	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	A	245	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	B	245	TYR	CB-CG-CD1	-5.11	117.94	121.00
1	A	272	SER	N-CA-C	5.11	124.79	111.00
1	B	272	SER	N-CA-C	5.11	124.79	111.00
1	A	47	ASP	CB-CA-C	5.09	120.59	110.40
1	B	47	ASP	CB-CA-C	5.09	120.59	110.40
1	A	182	VAL	CB-CA-C	-5.09	101.72	111.40
1	B	182	VAL	CB-CA-C	-5.09	101.72	111.40
1	A	52	VAL	CB-CA-C	-5.06	101.79	111.40
1	B	52	VAL	CB-CA-C	-5.06	101.79	111.40
1	A	174	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	B	174	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	130	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	B	130	TYR	CB-CG-CD1	-5.04	117.98	121.00
1	A	284	GLU	N-CA-C	-5.02	97.44	111.00
1	B	284	GLU	N-CA-C	-5.02	97.44	111.00
1	A	288	SER	N-CA-C	5.02	124.55	111.00
1	B	288	SER	N-CA-C	5.02	124.55	111.00
1	A	237	TYR	CB-CG-CD1	-5.01	117.99	121.00
1	B	237	TYR	CB-CG-CD1	-5.01	117.99	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	TYR	CB-CG-CD1	-5.01	118.00	121.00
1	B	147	TYR	CB-CG-CD1	-5.01	118.00	121.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	173	ARG	Sidechain
1	B	109	ARG	Sidechain
1	B	171	ARG	Sidechain
1	B	173	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2560	0	2628	1248	1
1	B	2560	0	2628	1225	2
2	A	51	0	31	50	0
2	B	51	0	31	48	0
3	A	13	0	4	15	0
3	B	13	0	4	15	0
All	All	5248	0	5326	2375	3

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 225.

All (2375) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:TRP:CB	1:B:160:VAL:HG21	1.22	1.65
3:B:333:CIT:C4	3:B:333:CIT:C3	1.75	1.62
1:A:150:TRP:CB	1:A:160:VAL:HG21	1.22	1.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:HB2	1:A:160:VAL:CG2	1.21	1.62
1:B:150:TRP:HB2	1:B:160:VAL:CG2	1.21	1.62
1:B:275:VAL:CG2	1:B:285:VAL:HG11	1.31	1.61
3:A:333:CIT:C3	3:A:333:CIT:C4	1.75	1.57
1:A:275:VAL:CG2	1:A:285:VAL:HG11	1.31	1.55
1:B:145:LEU:HA	1:B:148:VAL:CG1	1.37	1.53
1:A:145:LEU:HA	1:A:148:VAL:CG1	1.37	1.50
1:B:163:SER:N	1:B:271:VAL:HG13	1.25	1.47
1:B:265:LEU:HD13	1:B:267:ARG:NH2	1.30	1.41
1:A:163:SER:N	1:A:271:VAL:HG13	1.25	1.39
1:A:265:LEU:HD13	1:A:267:ARG:NH2	1.30	1.38
1:B:28:GLY:O	1:B:33:GLY:CA	1.74	1.35
1:A:145:LEU:CA	1:A:148:VAL:HG13	1.57	1.34
1:A:203:TRP:NE1	1:A:311:GLU:OE1	1.56	1.34
2:A:332:LNC:H4	2:A:332:LNC:CAS	1.55	1.34
1:A:275:VAL:HG21	1:A:285:VAL:CG1	1.57	1.34
1:A:275:VAL:CG1	1:A:285:VAL:CG1	2.06	1.34
1:A:120:PHE:O	1:A:123:ILE:HG22	1.25	1.34
1:B:145:LEU:CA	1:B:148:VAL:HG13	1.57	1.34
1:B:275:VAL:CG2	1:B:285:VAL:CG1	2.06	1.33
1:B:275:VAL:CG1	1:B:285:VAL:CG1	2.06	1.32
1:B:275:VAL:HG21	1:B:285:VAL:CG1	1.57	1.32
1:A:28:GLY:O	1:A:33:GLY:CA	1.74	1.32
1:B:124:ILE:HG12	1:B:125:PRO:CD	1.57	1.32
1:B:203:TRP:NE1	1:B:311:GLU:OE1	1.56	1.32
1:B:78:ILE:HD13	1:B:78:ILE:O	1.26	1.32
1:A:291:CYS:SG	1:A:302:VAL:HG23	1.69	1.32
1:A:275:VAL:CG2	1:A:285:VAL:CG1	2.06	1.32
1:B:291:CYS:SG	1:B:302:VAL:HG23	1.69	1.32
1:A:24:ILE:HD13	1:A:25:THR:N	1.43	1.31
1:A:144:ILE:O	1:A:148:VAL:HG12	1.22	1.31
1:B:120:PHE:O	1:B:124:ILE:HD13	1.22	1.31
1:A:143:ASP:OD2	1:A:287:LEU:HA	1.16	1.31
2:B:332:LNC:C4N	2:B:332:LNC:HAS	1.38	1.31
1:B:24:ILE:HD13	1:B:25:THR:N	1.43	1.31
1:A:124:ILE:HG12	1:A:125:PRO:CD	1.57	1.30
1:A:279:TYR:O	1:A:279:TYR:CD2	1.83	1.30
1:B:120:PHE:O	1:B:123:ILE:HG22	1.25	1.30
1:A:32:VAL:HG21	2:A:332:LNC:C5D	1.60	1.30
1:B:279:TYR:O	1:B:279:TYR:CD2	1.83	1.30
1:B:32:VAL:HG21	2:B:332:LNC:C5D	1.60	1.30

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:CD1	1:A:156:PRO:HA	1.67	1.29
1:A:277:GLY:O	1:A:278:MET:SD	1.91	1.29
1:B:150:TRP:CD1	1:B:156:PRO:HA	1.67	1.29
1:B:277:GLY:O	1:B:278:MET:SD	1.91	1.29
1:B:275:VAL:HG11	1:B:285:VAL:CG1	1.60	1.28
2:B:332:LNC:CAS	2:B:332:LNC:H4	1.55	1.28
1:B:203:TRP:CH2	1:B:226:LYS:HE2	1.68	1.28
1:A:120:PHE:O	1:A:124:ILE:HD13	1.22	1.27
1:B:143:ASP:OD2	1:B:287:LEU:HA	1.16	1.27
1:B:144:ILE:O	1:B:148:VAL:HG12	1.22	1.27
1:A:275:VAL:HG11	1:A:285:VAL:CG1	1.60	1.27
1:B:243:LYS:N	1:B:243:LYS:HD3	1.32	1.27
2:A:332:LNC:HAS	2:A:332:LNC:C4N	1.38	1.27
1:A:203:TRP:CH2	1:A:226:LYS:HE2	1.68	1.26
1:A:245:TYR:O	1:B:65:ASP:OD2	1.52	1.26
1:A:8:ILE:O	1:A:10:PRO:HD2	1.13	1.26
1:A:65:ASP:OD2	1:B:245:TYR:O	1.52	1.25
1:A:34:MET:CE	1:A:66:LEU:HD21	1.65	1.25
1:B:229:HIS:O	1:B:232:VAL:CG2	1.84	1.25
1:B:203:TRP:CZ3	1:B:218:THR:HG21	1.72	1.25
1:B:246:THR:CG2	2:B:332:LNC:HGS2	1.66	1.25
1:B:34:MET:CE	1:B:66:LEU:HD21	1.65	1.25
1:B:144:ILE:CG2	1:B:145:LEU:HD13	1.66	1.25
1:A:246:THR:CG2	2:A:332:LNC:HGS2	1.66	1.25
1:B:8:ILE:O	1:B:10:PRO:HD2	1.13	1.24
1:A:78:ILE:HD13	1:A:78:ILE:O	1.26	1.24
1:A:124:ILE:CG1	1:A:125:PRO:HD3	1.68	1.24
1:A:144:ILE:CG2	1:A:145:LEU:HD13	1.66	1.24
1:B:124:ILE:CG1	1:B:125:PRO:HD3	1.68	1.24
1:A:209(B):GLY:O	1:A:209(C):VAL:HG12	1.08	1.23
1:A:229:HIS:O	1:A:232:VAL:CG2	1.84	1.23
1:B:209(B):GLY:O	1:B:209(C):VAL:CG1	1.85	1.23
1:A:28:GLY:O	1:A:33:GLY:HA3	1.09	1.23
1:A:203:TRP:CZ3	1:A:218:THR:HG21	1.72	1.23
1:A:209(B):GLY:O	1:A:209(C):VAL:CG1	1.85	1.23
1:B:28:GLY:O	1:B:33:GLY:HA3	1.09	1.22
1:B:209(B):GLY:O	1:B:209(C):VAL:HG12	1.08	1.22
1:A:101:ARG:HG2	1:A:102:GLN:N	1.18	1.21
1:A:245:TYR:O	1:B:65:ASP:CB	1.88	1.21
1:A:65:ASP:CG	1:B:248:TRP:HB2	1.61	1.21
1:A:248:TRP:HB2	1:B:65:ASP:CG	1.61	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:SER:O	1:A:271:VAL:HG22	1.40	1.21
1:A:65:ASP:CG	1:B:245:TYR:O	1.79	1.20
1:A:41:LEU:O	1:A:73:LEU:CD2	1.90	1.20
1:A:95:VAL:HG12	1:A:136:ILE:HB	1.20	1.20
1:B:273:THR:HG21	1:B:298:LEU:CD1	1.70	1.20
1:B:101:ARG:HG2	1:B:102:GLN:N	1.18	1.20
1:B:163:SER:O	1:B:271:VAL:HG22	1.40	1.20
1:A:273:THR:HG21	1:A:298:LEU:CD1	1.70	1.19
1:A:245:TYR:O	1:B:65:ASP:CG	1.79	1.19
1:A:65:ASP:CB	1:B:245:TYR:O	1.88	1.19
1:B:213:ASN:HB2	1:B:214:PRO:CD	1.72	1.19
1:B:41:LEU:O	1:B:73:LEU:CD2	1.90	1.19
1:B:238:GLU:O	1:B:240:ILE:N	1.76	1.19
1:A:245:TYR:O	1:B:65:ASP:HB2	1.42	1.19
1:B:144:ILE:HG22	1:B:145:LEU:N	1.57	1.18
1:A:121:LYS:O	1:A:125:PRO:CD	1.91	1.18
1:A:238:GLU:O	1:A:240:ILE:N	1.76	1.18
1:A:243:LYS:HD3	1:A:243:LYS:N	1.32	1.18
1:A:165:CYS:CB	1:A:270:PRO:HB2	1.74	1.18
1:A:25:THR:HG22	1:A:50:ALA:HB3	1.18	1.17
1:B:121:LYS:HA	1:B:124:ILE:HD11	1.17	1.17
1:B:165:CYS:HB3	1:B:270:PRO:CG	1.73	1.17
1:B:121:LYS:O	1:B:125:PRO:CD	1.91	1.17
1:A:271:VAL:CG1	1:A:271:VAL:O	1.89	1.17
1:A:193:GLY:HA2	1:A:287:LEU:HD21	1.19	1.17
1:A:213:ASN:HB2	1:A:214:PRO:CD	1.72	1.17
1:A:203:TRP:HH2	1:A:226:LYS:CE	1.57	1.16
1:B:140:ASN:CB	1:B:141:PRO:CD	2.23	1.16
1:A:165:CYS:HB3	1:A:270:PRO:CG	1.73	1.16
1:A:229:HIS:O	1:A:232:VAL:HG23	1.44	1.16
1:A:275:VAL:HG22	1:A:285:VAL:HG11	1.27	1.15
1:B:165:CYS:CB	1:B:270:PRO:HB2	1.74	1.15
1:B:203:TRP:HH2	1:B:226:LYS:CE	1.57	1.15
1:A:101:ARG:CG	1:A:102:GLN:N	2.05	1.15
1:A:102:GLN:O	1:A:110:LEU:CD2	1.94	1.15
1:B:110:LEU:HD23	1:B:140:ASN:ND2	1.62	1.15
1:A:110:LEU:HD23	1:A:140:ASN:ND2	1.62	1.15
1:B:95:VAL:HG12	1:B:136:ILE:HB	1.20	1.15
1:B:275:VAL:CB	1:B:285:VAL:HG11	1.76	1.15
1:B:102:GLN:O	1:B:110:LEU:CD2	1.94	1.14
1:A:275:VAL:CB	1:A:285:VAL:HG11	1.76	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HG22	1:B:50:ALA:HB3	1.18	1.14
1:B:32:VAL:CG2	2:B:332:LNC:H5'2	1.78	1.14
1:B:9:ALA:HB3	1:B:10:PRO:CD	1.76	1.14
1:A:188:HIS:CD2	3:A:333:CIT:C5	2.31	1.14
1:B:165:CYS:CB	1:B:270:PRO:CB	2.26	1.14
1:A:210(B):GLN:O	1:A:214:PRO:HD2	1.44	1.14
1:B:271:VAL:CG1	1:B:271:VAL:O	1.89	1.14
1:A:143:ASP:O	1:A:146:THR:HG22	1.45	1.13
1:A:165:CYS:CB	1:A:270:PRO:CB	2.26	1.13
1:A:9:ALA:HB3	1:A:10:PRO:CD	1.76	1.13
1:B:210(B):GLN:O	1:B:214:PRO:HD2	1.44	1.13
1:B:229:HIS:O	1:B:232:VAL:HG23	1.44	1.13
1:B:143:ASP:O	1:B:146:THR:HG22	1.45	1.13
1:A:65:ASP:HB2	1:B:245:TYR:O	1.42	1.13
1:A:140:ASN:HB3	1:A:141:PRO:CD	1.78	1.12
1:A:145:LEU:HA	1:A:148:VAL:HG11	1.22	1.12
1:A:58:LYS:HA	1:B:242:LEU:HG	1.31	1.12
1:A:144:ILE:HG22	1:A:145:LEU:N	1.57	1.12
1:B:3:LEU:HD22	1:B:4:LYS:HG2	1.30	1.12
1:A:121:LYS:HA	1:A:124:ILE:HD11	1.17	1.12
1:A:32:VAL:CG2	2:A:332:LNC:H5'2	1.78	1.12
1:A:140:ASN:CB	1:A:141:PRO:CD	2.23	1.12
1:B:32:VAL:HG21	2:B:332:LNC:H5'1	1.28	1.12
1:B:188:HIS:CD2	3:B:333:CIT:C5	2.31	1.12
1:B:145:LEU:HA	1:B:148:VAL:HG11	1.22	1.12
1:B:34:MET:HE3	1:B:66:LEU:HD21	1.12	1.12
1:A:34:MET:HE3	1:A:66:LEU:HD21	1.14	1.11
1:B:247:ASN:HA	1:B:250:ILE:CG2	1.80	1.11
1:A:95:VAL:CG1	1:A:136:ILE:HB	1.78	1.11
1:A:32:VAL:CG2	2:A:332:LNC:C5D	2.28	1.11
1:A:183:HIS:HE1	1:A:209(A):ALA:HB2	1.16	1.11
1:A:188:HIS:HD2	3:A:333:CIT:C5	1.63	1.11
1:B:95:VAL:CG1	1:B:136:ILE:HB	1.78	1.11
1:A:242:LEU:HG	1:B:58:LYS:HA	1.31	1.11
1:A:93:ILE:HD11	1:A:261:MET:HG2	1.32	1.11
1:B:140:ASN:HB3	1:B:141:PRO:CD	1.78	1.10
1:B:140:ASN:HB3	1:B:141:PRO:HD3	1.25	1.10
1:B:275:VAL:CG1	1:B:285:VAL:HG12	1.77	1.10
1:A:24:ILE:HD13	1:A:25:THR:CA	1.80	1.10
1:A:144:ILE:O	1:A:148:VAL:CG1	1.98	1.10
1:A:140:ASN:HB3	1:A:141:PRO:HD3	1.25	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:HB2	1:A:214:PRO:HD3	1.19	1.10
1:B:144:ILE:O	1:B:148:VAL:CG1	1.98	1.10
1:A:275:VAL:CG1	1:A:285:VAL:HG12	1.77	1.10
1:B:49:LEU:HD12	1:B:50:ALA:N	1.67	1.10
1:A:188:HIS:HD2	3:A:333:CIT:O4	1.30	1.10
1:A:49:LEU:HD12	1:A:50:ALA:N	1.67	1.10
1:B:250:ILE:HG23	1:B:251:GLY:N	1.63	1.10
1:B:188:HIS:HD2	3:B:333:CIT:O4	1.30	1.09
1:A:146:THR:OG1	1:A:160:VAL:CG1	2.00	1.09
1:A:247:ASN:HA	1:A:250:ILE:CG2	1.80	1.09
1:B:101:ARG:CG	1:B:102:GLN:N	2.05	1.09
1:B:121:LYS:O	1:B:125:PRO:HD2	1.48	1.09
1:B:146:THR:OG1	1:B:160:VAL:CG1	2.00	1.09
1:B:213:ASN:HB2	1:B:214:PRO:HD3	1.19	1.09
1:A:203:TRP:HE1	1:A:311:GLU:CD	1.55	1.09
1:A:9:ALA:HB3	1:A:10:PRO:HD3	1.30	1.09
1:B:32:VAL:CG2	2:B:332:LNC:C5D	2.28	1.09
1:A:281:ILE:CG2	1:A:285:VAL:HG13	1.83	1.09
1:B:24:ILE:HD13	1:B:25:THR:CA	1.80	1.09
1:B:192:LEU:HD23	1:B:315:LEU:CD1	1.82	1.09
1:A:265:LEU:CD1	1:A:267:ARG:HH21	1.66	1.09
1:A:192:LEU:HD23	1:A:315:LEU:CD1	1.82	1.09
1:B:145:LEU:CA	1:B:148:VAL:CG1	2.22	1.09
1:B:102:GLN:O	1:B:110:LEU:HD22	1.53	1.09
1:B:197:ASP:OD1	1:B:237:TYR:OH	1.68	1.09
1:A:145:LEU:C	1:A:148:VAL:HG13	1.72	1.08
1:A:197:ASP:OD1	1:A:237:TYR:OH	1.68	1.08
1:A:271:VAL:HG12	1:A:271:VAL:O	1.28	1.08
1:A:3:LEU:HD22	1:A:4:LYS:CG	1.84	1.08
1:B:203:TRP:HE1	1:B:311:GLU:CD	1.55	1.08
1:B:273:THR:CG2	1:B:274:MET:H	1.65	1.08
1:A:24:ILE:CD1	1:A:25:THR:N	2.16	1.08
1:B:145:LEU:C	1:B:148:VAL:HG13	1.72	1.08
1:B:24:ILE:CD1	1:B:25:THR:N	2.16	1.08
1:B:265:LEU:CD1	1:B:267:ARG:NH2	2.17	1.08
1:B:143:ASP:OD2	1:B:287:LEU:CA	2.02	1.08
1:A:273:THR:CG2	1:A:298:LEU:HD11	1.84	1.08
1:B:265:LEU:CD1	1:B:267:ARG:HH21	1.66	1.08
1:A:8:ILE:O	1:A:10:PRO:CD	2.01	1.08
1:B:193:GLY:HA2	1:B:287:LEU:HD21	1.19	1.08
1:B:8:ILE:O	1:B:10:PRO:CD	2.01	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:CG2	1:B:285:VAL:HG13	1.83	1.07
1:A:165:CYS:CB	1:A:270:PRO:CG	2.32	1.07
1:B:188:HIS:HD2	3:B:333:CIT:C5	1.63	1.07
1:A:121:LYS:O	1:A:125:PRO:HD2	1.48	1.07
1:A:93:ILE:HD12	1:A:258:ILE:HG12	1.23	1.07
1:B:93:ILE:HD12	1:B:258:ILE:HG12	1.23	1.07
1:A:18:ILE:CG2	1:A:18:ILE:O	2.03	1.07
1:B:157:LYS:H	1:B:157:LYS:HD2	1.17	1.07
1:A:265:LEU:CD1	1:A:267:ARG:NH2	2.17	1.07
1:B:183:HIS:HE1	1:B:209(A):ALA:HB2	1.16	1.07
1:B:247:ASN:O	1:B:250:ILE:HG22	1.54	1.07
1:A:123:ILE:HG23	1:A:124:ILE:N	1.67	1.07
1:A:250:ILE:HG23	1:A:251:GLY:N	1.63	1.07
1:B:273:THR:CG2	1:B:298:LEU:HD11	1.84	1.07
1:B:3:LEU:HD22	1:B:4:LYS:CG	1.84	1.06
1:A:273:THR:HG22	1:A:274:MET:N	1.65	1.06
1:A:143:ASP:OD2	1:A:287:LEU:CA	2.02	1.06
1:A:3:LEU:HD22	1:A:4:LYS:HG2	1.30	1.06
1:A:49:LEU:HD12	1:A:49:LEU:C	1.75	1.06
1:A:8:ILE:O	1:A:8:ILE:HG12	1.51	1.06
1:B:13:GLN:O	1:B:14:GLN:OE1	1.72	1.06
1:B:281:ILE:HG21	1:B:285:VAL:HG13	1.08	1.06
1:B:165:CYS:CB	1:B:270:PRO:CG	2.32	1.06
1:A:175:LEU:HG	1:A:176:MET:H	1.18	1.06
1:B:102:GLN:CA	1:B:110:LEU:HD21	1.85	1.06
1:B:192:LEU:HD22	1:B:315:LEU:HD13	1.37	1.06
1:A:102:GLN:CA	1:A:110:LEU:HD21	1.85	1.05
1:B:192:LEU:CD2	1:B:315:LEU:HD13	1.85	1.05
1:B:209(D):VAL:CG1	1:B:210(A):LEU:H	1.68	1.05
1:A:13:GLN:O	1:A:14:GLN:OE1	1.72	1.05
1:A:296:ARG:HG3	1:A:296:ARG:NH1	1.54	1.05
1:A:192:LEU:CD2	1:A:315:LEU:HD13	1.85	1.05
1:B:144:ILE:CG2	1:B:145:LEU:N	2.17	1.05
1:B:271:VAL:HG12	1:B:271:VAL:O	1.28	1.05
1:B:273:THR:HG22	1:B:274:MET:N	1.65	1.05
1:B:49:LEU:HD12	1:B:49:LEU:C	1.75	1.05
1:B:9:ALA:HB3	1:B:10:PRO:HD3	1.30	1.05
1:A:140:ASN:HB2	1:A:141:PRO:HD2	1.34	1.05
1:A:145:LEU:CA	1:A:148:VAL:CG1	2.22	1.05
1:B:154:GLY:O	1:B:155:LEU:HG	1.57	1.05
1:B:203:TRP:HH2	1:B:226:LYS:HE2	0.89	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ASP:O	1:B:85:TYR:CG	2.10	1.05
1:A:72:PHE:CE1	1:B:253:SER:HA	1.91	1.05
1:B:275:VAL:HG22	1:B:285:VAL:HG11	1.27	1.05
1:A:144:ILE:CG2	1:A:145:LEU:N	2.17	1.05
1:A:32:VAL:HG21	2:A:332:LNC:H5'1	1.28	1.05
1:B:102:GLN:HA	1:B:110:LEU:HD21	1.39	1.05
1:B:203:TRP:HZ3	1:B:218:THR:HG21	1.00	1.05
1:A:157:LYS:HD2	1:A:157:LYS:H	1.17	1.04
1:A:209(D):VAL:CG1	1:A:210(A):LEU:H	1.68	1.04
1:B:123:ILE:HG23	1:B:124:ILE:N	1.67	1.04
1:A:84:ASP:O	1:A:85:TYR:CG	2.10	1.04
1:B:165:CYS:HB3	1:B:270:PRO:HG3	1.37	1.04
1:B:32:VAL:HG21	2:B:332:LNC:H5'2	1.29	1.04
1:B:93:ILE:HD11	1:B:261:MET:HG2	1.32	1.04
1:A:247:ASN:O	1:A:250:ILE:HG22	1.54	1.04
1:A:253:SER:HA	1:B:72:PHE:CE1	1.91	1.04
1:A:273:THR:CG2	1:A:274:MET:H	1.65	1.04
1:B:246:THR:HG21	2:B:332:LNC:HGS2	1.36	1.04
1:B:296:ARG:NH1	1:B:296:ARG:HG3	1.54	1.04
1:A:209(D):VAL:HG13	1:A:210(A):LEU:N	1.72	1.04
1:A:209(D):VAL:HG13	1:A:210(A):LEU:H	0.88	1.04
1:A:51:LEU:HD12	1:A:51:LEU:O	1.58	1.04
1:B:291:CYS:SG	1:B:302:VAL:CG2	2.45	1.04
1:B:279:TYR:HE1	1:B:306:LYS:HE2	1.22	1.03
1:B:140:ASN:HB2	1:B:141:PRO:HD2	1.34	1.03
1:A:92:LYS:O	1:A:133:CYS:HB2	1.58	1.03
1:A:246:THR:HG21	2:A:332:LNC:HGS2	1.36	1.03
1:A:65:ASP:OD2	1:B:248:TRP:N	1.92	1.03
1:A:243:LYS:CD	1:A:243:LYS:N	2.21	1.03
1:A:248:TRP:N	1:B:65:ASP:OD2	1.92	1.03
1:A:248:TRP:HB2	1:B:65:ASP:CB	1.89	1.03
1:A:281:ILE:HG21	1:A:285:VAL:HG13	1.08	1.03
1:B:121:LYS:HA	1:B:124:ILE:CD1	1.89	1.03
1:B:245:TYR:HA	1:B:248:TRP:CD1	1.94	1.03
1:A:147:TYR:HA	1:A:150:TRP:HE3	1.22	1.03
1:A:165:CYS:HB3	1:A:270:PRO:HG3	1.37	1.03
1:A:203:TRP:HH2	1:A:226:LYS:HE2	0.89	1.03
1:A:296:ARG:HG3	1:A:296:ARG:HH11	0.90	1.03
1:A:330(A):LYS:C	1:A:330(A):LYS:HD2	1.79	1.03
1:A:163:SER:N	1:A:271:VAL:CG1	2.21	1.03
1:A:18:ILE:O	1:A:18:ILE:HG22	1.22	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:VAL:O	1:A:53:ASP:OD1	1.77	1.03
1:A:79:VAL:HG11	1:A:87:VAL:HG11	1.41	1.03
1:B:296:ARG:HH11	1:B:296:ARG:HG3	0.90	1.03
1:A:192:LEU:HD22	1:A:315:LEU:HD13	1.37	1.02
1:A:93:ILE:HG12	1:A:261:MET:HE3	1.41	1.02
1:B:18:ILE:O	1:B:18:ILE:CG2	2.03	1.02
1:A:102:GLN:O	1:A:110:LEU:HD22	1.53	1.02
1:A:291:CYS:SG	1:A:302:VAL:CG2	2.45	1.02
1:B:163:SER:N	1:B:271:VAL:CG1	2.21	1.02
1:A:145:LEU:HA	1:A:148:VAL:HG13	1.05	1.02
1:B:330(A):LYS:HD2	1:B:330(A):LYS:C	1.79	1.02
1:B:19:PRO:HB3	1:B:48:GLU:HG3	1.42	1.02
1:A:279:TYR:HE1	1:A:306:LYS:HE2	1.22	1.02
1:A:154:GLY:O	1:A:155:LEU:HG	1.57	1.02
1:A:245:TYR:HA	1:A:248:TRP:CD1	1.94	1.02
1:B:120:PHE:C	1:B:124:ILE:HD13	1.79	1.02
1:B:147:TYR:HA	1:B:150:TRP:HE3	1.22	1.02
1:B:175:LEU:HG	1:B:176:MET:H	1.18	1.02
1:B:92:LYS:O	1:B:133:CYS:HB2	1.58	1.02
1:B:40:ILE:CG2	1:B:41:LEU:N	2.23	1.02
1:B:51:LEU:O	1:B:51:LEU:HD12	1.58	1.02
1:A:248:TRP:CH2	1:B:34:MET:HB3	1.94	1.02
1:B:203:TRP:CE2	1:B:311:GLU:OE1	2.12	1.02
1:A:65:ASP:CB	1:B:248:TRP:HB2	1.89	1.01
1:B:133:CYS:O	1:B:159:ARG:HD2	1.59	1.01
1:B:18:ILE:O	1:B:18:ILE:HG22	1.22	1.01
1:B:8:ILE:O	1:B:8:ILE:HG12	1.51	1.01
1:A:121:LYS:HA	1:A:124:ILE:CD1	1.89	1.01
1:A:34:MET:HB3	1:B:248:TRP:CH2	1.94	1.01
1:A:110:LEU:HD23	1:A:140:ASN:CG	1.81	1.01
1:A:40:ILE:CG2	1:A:41:LEU:N	2.23	1.01
1:A:41:LEU:O	1:A:73:LEU:HD21	1.60	1.01
1:A:3:LEU:HD13	1:A:4:LYS:H	1.24	1.01
1:B:145:LEU:HA	1:B:148:VAL:HG13	1.05	1.01
1:B:209(D):VAL:HG13	1:B:210(A):LEU:N	1.72	1.01
1:B:209(D):VAL:HG13	1:B:210(A):LEU:H	0.88	1.01
1:A:203:TRP:CE2	1:A:311:GLU:OE1	2.12	1.01
1:B:79:VAL:HG11	1:B:87:VAL:HG11	1.41	1.01
1:A:120:PHE:C	1:A:124:ILE:HD13	1.79	1.01
1:B:246:THR:HG23	2:B:332:LNC:HGS2	1.40	1.01
1:B:93:ILE:HG12	1:B:261:MET:HE3	1.39	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:HA	1:A:110:LEU:HD21	1.39	1.00
1:A:25:THR:CG2	1:A:50:ALA:HB3	1.92	1.00
1:B:243:LYS:N	1:B:243:LYS:CD	2.21	1.00
1:B:247:ASN:HA	1:B:250:ILE:HG21	1.41	1.00
1:A:19:PRO:HB3	1:A:48:GLU:HG3	1.42	1.00
1:B:110:LEU:HD23	1:B:140:ASN:CG	1.81	1.00
1:B:55:LEU:O	1:B:59:LEU:HD13	1.61	1.00
1:A:175:LEU:HG	1:A:176:MET:N	1.74	1.00
1:A:273:THR:HG22	1:A:274:MET:H	0.83	1.00
1:A:133:CYS:O	1:A:159:ARG:HD2	1.59	1.00
1:A:218:THR:O	1:A:219:ASP:HB2	1.61	1.00
1:A:32:VAL:HG21	2:A:332:LNC:H5'2	1.29	1.00
1:A:296:ARG:HH11	1:A:296:ARG:CG	1.75	1.00
1:B:3:LEU:HD13	1:B:4:LYS:H	1.24	1.00
1:B:52:VAL:O	1:B:53:ASP:OD1	1.77	1.00
1:A:246:THR:HG23	2:A:332:LNC:HGS2	1.40	1.00
1:A:55:LEU:O	1:A:59:LEU:HD13	1.61	1.00
1:B:279:TYR:O	1:B:279:TYR:HD2	1.30	1.00
1:B:102:GLN:O	1:B:103:GLN:HB2	1.59	0.99
1:B:210(B):GLN:O	1:B:214:PRO:CD	2.09	0.99
1:A:247:ASN:HA	1:A:250:ILE:HG21	1.41	0.99
1:A:120:PHE:O	1:A:123:ILE:CG2	2.11	0.99
1:A:192:LEU:CD2	1:A:315:LEU:CD1	2.40	0.99
1:A:188:HIS:CD2	3:A:333:CIT:O5	2.15	0.99
1:B:102:GLN:HA	1:B:110:LEU:CD2	1.92	0.99
1:B:53:ASP:HB3	1:B:55:LEU:HD23	1.43	0.99
1:A:203:TRP:HZ3	1:A:218:THR:HG21	1.00	0.99
1:A:210(B):GLN:O	1:A:214:PRO:CD	2.09	0.99
1:B:241:LYS:HE2	1:B:241:LYS:CA	1.91	0.99
1:B:188:HIS:CD2	3:B:333:CIT:O5	2.15	0.99
1:B:41:LEU:O	1:B:73:LEU:HD21	1.60	0.99
1:B:165:CYS:SG	1:B:270:PRO:HB2	2.02	0.99
1:B:296:ARG:HH11	1:B:296:ARG:CG	1.75	0.99
1:A:286:PHE:HD1	1:A:286:PHE:O	1.45	0.99
1:B:120:PHE:O	1:B:123:ILE:CG2	2.11	0.99
1:A:53:ASP:HB3	1:A:55:LEU:HD23	1.43	0.99
1:B:308:LYS:HA	1:B:312:VAL:CG1	1.93	0.99
1:A:102:GLN:O	1:A:103:GLN:HB2	1.59	0.99
1:A:110:LEU:CD1	1:A:112:LEU:HD21	1.92	0.99
1:A:209(B):GLY:C	1:A:209(C):VAL:HG12	1.83	0.99
1:B:25:THR:CG2	1:B:50:ALA:HB3	1.92	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LYS:HE2	1:A:241:LYS:CA	1.91	0.98
1:A:308:LYS:HA	1:A:312:VAL:CG1	1.93	0.98
1:B:224:ASN:HB3	1:B:227:GLU:HB3	1.45	0.98
1:A:101:ARG:HG2	1:A:102:GLN:H	1.20	0.98
1:A:224:ASN:HB3	1:A:227:GLU:HB3	1.45	0.98
1:A:304:ASN:O	1:A:305:GLN:OE1	1.81	0.98
1:B:218:THR:O	1:B:219:ASP:HB2	1.61	0.98
1:B:275:VAL:CG1	1:B:285:VAL:HG11	1.83	0.98
1:B:250:ILE:HG23	1:B:251:GLY:H	1.23	0.98
1:A:165:CYS:SG	1:A:270:PRO:HB2	2.02	0.98
1:B:110:LEU:CD1	1:B:112:LEU:HD21	1.92	0.98
1:B:146:THR:OG1	1:B:160:VAL:HG12	1.64	0.98
1:B:286:PHE:HD1	1:B:286:PHE:O	1.45	0.98
1:B:304:ASN:O	1:B:305:GLN:OE1	1.81	0.98
1:B:171:ARG:O	1:B:175:LEU:HD23	1.63	0.98
1:A:102:GLN:HA	1:A:110:LEU:CD2	1.92	0.97
1:B:140:ASN:CB	1:B:141:PRO:HD2	1.91	0.97
1:A:183:HIS:CE1	1:A:209(A):ALA:HB2	1.99	0.97
1:A:140:ASN:CB	1:A:141:PRO:HD2	1.91	0.97
1:A:40:ILE:HG22	1:A:41:LEU:N	1.78	0.97
1:B:10:PRO:O	1:B:11:VAL:HG13	1.64	0.97
1:B:273:THR:HG22	1:B:274:MET:H	0.83	0.97
1:A:279:TYR:O	1:A:279:TYR:HD2	1.30	0.97
1:A:250:ILE:CG2	1:A:251:GLY:H	1.78	0.97
1:B:192:LEU:CD2	1:B:315:LEU:CD1	2.40	0.97
1:A:171:ARG:O	1:A:175:LEU:HD23	1.63	0.97
1:A:134:ILE:HG21	1:A:296:ARG:O	1.65	0.97
1:B:250:ILE:CG2	1:B:251:GLY:H	1.78	0.97
1:B:3:LEU:HD13	1:B:4:LYS:N	1.80	0.96
1:A:10:PRO:O	1:A:11:VAL:HG13	1.64	0.96
1:A:55:LEU:HB2	1:A:59:LEU:CD1	1.95	0.96
1:B:209(B):GLY:C	1:B:209(C):VAL:HG12	1.83	0.96
1:A:150:TRP:CD1	1:A:156:PRO:CA	2.48	0.96
1:A:238:GLU:O	1:A:240:ILE:HD13	1.65	0.96
1:A:241:LYS:HA	1:A:241:LYS:HE2	1.46	0.96
1:B:120:PHE:O	1:B:124:ILE:CD1	2.14	0.96
1:B:238:GLU:O	1:B:240:ILE:HD13	1.65	0.96
1:B:55:LEU:C	1:B:59:LEU:HD13	1.86	0.96
1:A:242:LEU:CG	1:B:58:LYS:HA	1.94	0.96
1:A:229:HIS:O	1:A:232:VAL:HG22	1.65	0.96
1:A:3:LEU:HD13	1:A:4:LYS:N	1.80	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:HIS:CE1	1:B:209(A):ALA:HB2	1.99	0.96
1:A:165:CYS:HB2	1:A:270:PRO:HB2	1.47	0.96
1:B:163:SER:H	1:B:271:VAL:CG1	1.79	0.96
1:B:165:CYS:HB2	1:B:270:PRO:HB2	1.47	0.96
1:B:55:LEU:HB2	1:B:59:LEU:CD1	1.95	0.96
1:B:97:THR:HG21	2:B:332:LNC:H5'1	1.47	0.96
1:B:40:ILE:HG22	1:B:41:LEU:N	1.78	0.96
1:B:283:ASN:O	1:B:285:VAL:HG23	1.66	0.96
1:B:175:LEU:HG	1:B:176:MET:N	1.74	0.95
1:A:283:ASN:O	1:A:285:VAL:HG23	1.66	0.95
1:A:58:LYS:HA	1:B:242:LEU:CG	1.94	0.95
1:B:229:HIS:O	1:B:232:VAL:HG22	1.65	0.95
1:B:275:VAL:HG11	1:B:285:VAL:HG12	0.96	0.95
1:A:275:VAL:HG11	1:A:285:VAL:HG12	0.96	0.95
1:B:134:ILE:HG21	1:B:296:ARG:O	1.65	0.95
1:B:150:TRP:CD1	1:B:156:PRO:CA	2.48	0.95
1:A:55:LEU:C	1:A:59:LEU:HD13	1.86	0.95
1:A:19:PRO:O	1:A:20:ASP:HB2	1.65	0.95
1:A:34:MET:CE	1:A:66:LEU:CD2	2.44	0.95
1:B:193:GLY:O	1:B:287:LEU:HG	1.67	0.95
1:A:120:PHE:O	1:A:124:ILE:CD1	2.14	0.94
1:B:227:GLU:HG2	1:B:231:MET:SD	2.07	0.94
1:A:53:ASP:CB	1:A:55:LEU:HD23	1.97	0.94
1:B:275:VAL:HG21	1:B:285:VAL:HG13	1.50	0.94
1:B:40:ILE:CG2	1:B:41:LEU:HD22	1.98	0.94
1:A:97:THR:HG21	2:A:332:LNC:H5'1	1.47	0.94
1:B:286:PHE:O	1:B:287:LEU:HB2	1.67	0.94
1:B:34:MET:CE	1:B:66:LEU:CD2	2.44	0.94
1:A:146:THR:OG1	1:A:160:VAL:HG12	1.64	0.94
1:A:102:GLN:O	1:A:110:LEU:HD21	1.67	0.94
1:A:121:LYS:CA	1:A:124:ILE:HD11	1.98	0.94
1:A:193:GLY:HA2	1:A:287:LEU:CD2	1.98	0.94
1:A:193:GLY:O	1:A:287:LEU:HG	1.67	0.94
1:A:227:GLU:HG2	1:A:231:MET:SD	2.07	0.94
1:A:250:ILE:HG23	1:A:251:GLY:H	1.23	0.94
1:B:147:TYR:HA	1:B:150:TRP:CE3	2.03	0.94
1:B:18:ILE:CG2	1:B:20:ASP:OD2	2.16	0.93
1:B:78:ILE:CD1	1:B:78:ILE:O	2.16	0.93
1:A:40:ILE:CG2	1:A:41:LEU:HD22	1.98	0.93
1:A:163:SER:H	1:A:271:VAL:CG1	1.79	0.93
1:A:286:PHE:O	1:A:287:LEU:HB2	1.67	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:LEU:O	1:A:73:LEU:HD22	1.66	0.93
1:B:53:ASP:CB	1:B:55:LEU:HD23	1.97	0.93
1:A:6:LYS:C	1:A:7:LEU:HD23	1.88	0.93
1:B:102:GLN:C	1:B:110:LEU:HD21	1.89	0.93
1:A:102:GLN:C	1:A:110:LEU:HD21	1.89	0.93
1:A:18:ILE:CG2	1:A:20:ASP:OD2	2.16	0.93
1:B:150:TRP:HB2	1:B:160:VAL:HG23	1.51	0.93
1:B:193:GLY:HA2	1:B:287:LEU:CD2	1.98	0.93
1:A:147:TYR:HA	1:A:150:TRP:CE3	2.03	0.93
1:B:19:PRO:O	1:B:20:ASP:HB2	1.65	0.93
1:B:6:LYS:C	1:B:7:LEU:HD23	1.88	0.93
1:B:147:TYR:C	1:B:147:TYR:CD2	2.41	0.93
1:B:41:LEU:O	1:B:73:LEU:HD22	1.66	0.93
1:B:96:VAL:HG22	1:B:120:PHE:CE2	2.04	0.92
1:B:229:HIS:C	1:B:232:VAL:HG22	1.90	0.92
1:A:96:VAL:HG22	1:A:120:PHE:CE2	2.04	0.92
1:B:121:LYS:CA	1:B:124:ILE:HD11	1.98	0.92
1:A:144:ILE:HG23	1:A:145:LEU:HD13	1.50	0.92
1:B:102:GLN:O	1:B:110:LEU:HD21	1.67	0.92
1:A:114:GLN:O	1:A:117:VAL:HG22	1.69	0.92
1:B:136:ILE:HD13	1:B:257:LEU:HD21	1.51	0.92
1:A:250:ILE:CG2	1:A:251:GLY:N	2.32	0.92
1:B:241:LYS:HA	1:B:241:LYS:HE2	1.46	0.92
1:A:288:SER:O	1:A:289:LEU:HB2	1.69	0.92
1:B:135:ILE:HG23	1:B:135:ILE:O	1.70	0.92
1:B:250:ILE:CG2	1:B:251:GLY:N	2.32	0.92
1:B:120:PHE:C	1:B:124:ILE:CD1	2.38	0.91
1:B:288:SER:O	1:B:289:LEU:HB2	1.69	0.91
1:B:144:ILE:HG23	1:B:145:LEU:HD13	1.50	0.91
1:A:275:VAL:CG1	1:A:285:VAL:HG11	1.83	0.91
1:A:244:GLY:O	1:A:247:ASN:HB3	1.71	0.91
1:B:114:GLN:O	1:B:117:VAL:HG22	1.69	0.91
1:B:85:TYR:OH	1:B:123:ILE:HG12	1.71	0.91
1:B:247:ASN:C	1:B:250:ILE:HG22	1.91	0.91
1:A:85:TYR:OH	1:A:123:ILE:HG12	1.71	0.91
1:A:144:ILE:HG22	1:A:145:LEU:H	1.31	0.91
1:A:229:HIS:C	1:A:232:VAL:HG22	1.90	0.91
1:A:316:LYS:HG2	1:A:317:ASN:H	1.34	0.91
1:A:85:TYR:OH	1:A:123:ILE:CG1	2.19	0.91
1:A:273:THR:HG21	1:A:298:LEU:HD11	0.92	0.91
1:A:282:GLU:HG2	1:A:282:GLU:O	1.69	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ASN:C	1:A:250:ILE:HG22	1.91	0.91
1:A:203:TRP:NE1	1:A:311:GLU:CD	2.18	0.91
1:A:129:LYS:O	1:A:132(A):PRO:HD3	1.70	0.90
1:A:136:ILE:HD13	1:A:257:LEU:HD21	1.51	0.90
1:B:244:GLY:O	1:B:247:ASN:HB3	1.71	0.90
1:B:129:LYS:O	1:B:132(A):PRO:HD3	1.70	0.90
1:B:93:ILE:CG1	1:B:261:MET:HE3	2.00	0.90
1:B:282:GLU:O	1:B:282:GLU:HG2	1.69	0.90
1:B:28:GLY:C	1:B:33:GLY:HA3	1.90	0.90
1:A:120:PHE:C	1:A:124:ILE:CD1	2.38	0.90
1:A:316:LYS:CG	1:A:317:ASN:N	2.33	0.90
1:A:28:GLY:C	1:A:33:GLY:HA3	1.90	0.90
1:B:85:TYR:OH	1:B:123:ILE:CG1	2.19	0.90
1:B:123:ILE:CG2	1:B:124:ILE:H	1.85	0.90
1:A:246:THR:HG21	2:A:332:LNC:CGS	2.02	0.90
1:B:144:ILE:HG22	1:B:145:LEU:H	1.31	0.90
1:B:1:ALA:O	1:B:2:THR:HG22	1.71	0.90
1:A:123:ILE:CG2	1:A:124:ILE:N	2.35	0.90
1:B:101:ARG:HG2	1:B:102:GLN:H	1.20	0.90
1:A:4:LYS:HG3	1:A:5:GLU:H	1.36	0.90
1:B:4:LYS:HG3	1:B:5:GLU:H	1.36	0.90
1:A:78:ILE:CD1	1:A:78:ILE:O	2.16	0.90
1:A:245:TYR:C	1:B:65:ASP:OD2	2.09	0.90
1:A:275:VAL:HG21	1:A:285:VAL:HG13	1.50	0.90
1:A:65:ASP:OD2	1:B:245:TYR:C	2.09	0.90
1:A:24:ILE:HD13	1:A:25:THR:HA	1.52	0.90
1:B:24:ILE:HD13	1:B:25:THR:HA	1.52	0.89
1:A:123:ILE:CG2	1:A:124:ILE:H	1.85	0.89
1:A:273:THR:CG2	1:A:274:MET:N	2.31	0.89
1:B:316:LYS:HG2	1:B:317:ASN:H	1.34	0.89
1:A:123:ILE:HG23	1:A:124:ILE:H	1.35	0.89
1:A:147:TYR:C	1:A:147:TYR:CD2	2.41	0.89
1:A:238:GLU:O	1:A:239:VAL:C	2.11	0.89
1:B:40:ILE:HG22	1:B:41:LEU:HD22	1.53	0.89
1:A:135:ILE:O	1:A:135:ILE:HG23	1.70	0.89
1:A:150:TRP:HB2	1:A:160:VAL:HG23	1.51	0.89
1:A:38:ILE:HG21	1:B:38:ILE:HG21	1.55	0.89
1:A:40:ILE:HG22	1:A:41:LEU:HD22	1.53	0.89
1:B:123:ILE:CG2	1:B:124:ILE:N	2.35	0.89
1:A:169:SER:N	1:A:191:ILE:HD11	1.87	0.89
1:B:54:VAL:C	1:B:55:LEU:HD22	1.94	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ALA:O	1:A:2:THR:HG22	1.71	0.89
1:B:238:GLU:O	1:B:239:VAL:C	2.11	0.89
1:B:330(A):LYS:CD	1:B:330(A):LYS:C	2.41	0.89
1:B:101:ARG:NH1	2:B:332:LNC:O1N	2.05	0.89
1:A:97:THR:HG23	2:A:332:LNC:H4'	1.55	0.88
1:B:246:THR:HG21	2:B:332:LNC:CGS	2.02	0.88
1:B:258:ILE:HG23	1:B:259:GLU:N	1.87	0.88
1:B:203:TRP:NE1	1:B:311:GLU:CD	2.18	0.88
1:A:147:TYR:HD2	1:A:148:VAL:N	1.72	0.88
1:A:163:SER:CA	1:A:271:VAL:HG13	2.02	0.88
1:B:163:SER:CA	1:B:271:VAL:HG13	2.02	0.88
1:B:308:LYS:HA	1:B:312:VAL:HG11	1.54	0.88
1:A:27:VAL:HG11	1:A:123:ILE:HD11	1.55	0.88
1:A:54:VAL:C	1:A:55:LEU:HD22	1.94	0.88
1:B:136:ILE:HD13	1:B:257:LEU:CD2	2.04	0.88
1:B:316:LYS:CG	1:B:317:ASN:N	2.33	0.88
1:A:215:GLU:C	1:A:216:MET:SD	2.52	0.88
1:A:308:LYS:HA	1:A:312:VAL:HG11	1.54	0.88
1:B:169:SER:N	1:B:191:ILE:HD11	1.87	0.88
1:B:273:THR:HG21	1:B:298:LEU:HD11	0.92	0.88
1:B:171:ARG:HH22	2:B:332:LNC:CS	1.86	0.88
1:A:65:ASP:CG	1:B:248:TRP:CB	2.42	0.88
1:B:215:GLU:C	1:B:216:MET:SD	2.52	0.88
1:A:16:THR:O	1:A:17:THR:CG2	2.22	0.88
1:A:221:ASP:O	1:A:222:SER:OG	1.91	0.88
1:A:258:ILE:HG23	1:A:259:GLU:N	1.87	0.87
1:A:284:GLU:O	1:A:285:VAL:HG23	1.75	0.87
1:B:247:ASN:HA	1:B:250:ILE:HG22	1.55	0.87
1:A:8:ILE:C	1:A:10:PRO:HD2	1.93	0.87
1:A:101:ARG:NH1	2:A:332:LNC:O1N	2.05	0.87
1:B:284:GLU:O	1:B:285:VAL:HG23	1.75	0.87
1:A:110:LEU:HD12	1:A:112:LEU:HD21	1.56	0.87
1:A:171:ARG:HH22	2:A:332:LNC:CS	1.86	0.87
1:B:221:ASP:O	1:B:222:SER:OG	1.91	0.87
1:B:16:THR:O	1:B:17:THR:CG2	2.22	0.87
1:B:6:LYS:HB3	1:B:7:LEU:HD23	1.56	0.87
1:B:165:CYS:HB3	1:B:270:PRO:CB	1.99	0.87
1:B:9:ALA:CB	1:B:10:PRO:CD	2.53	0.87
1:A:134:ILE:HG13	1:A:261:MET:CE	2.05	0.87
1:B:97:THR:HG23	2:B:332:LNC:H4'	1.55	0.87
1:A:136:ILE:HD13	1:A:257:LEU:CD2	2.04	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330(A):LYS:CD	1:A:330(A):LYS:C	2.41	0.87
1:B:8:ILE:C	1:B:10:PRO:HD2	1.93	0.87
1:B:161:ILE:HD13	1:B:293:LEU:CD2	2.05	0.86
1:B:28:GLY:O	1:B:33:GLY:HA2	1.75	0.86
1:A:124:ILE:HG12	1:A:125:PRO:HD3	0.87	0.86
1:B:243:LYS:H	1:B:243:LYS:CD	1.81	0.86
1:A:124:ILE:O	1:A:127:ILE:HG23	1.75	0.86
1:A:154:GLY:O	1:A:155:LEU:CG	2.23	0.86
1:A:247:ASN:HA	1:A:250:ILE:HG22	1.55	0.86
1:A:275:VAL:HG13	1:A:285:VAL:HB	1.56	0.86
1:A:188:HIS:NE2	3:A:333:CIT:H41	1.91	0.86
1:B:101:ARG:HG3	1:B:102:GLN:CD	1.96	0.86
1:B:147:TYR:HD2	1:B:148:VAL:N	1.72	0.86
1:B:289:LEU:O	1:B:291:CYS:SG	2.33	0.86
1:B:188:HIS:NE2	3:B:333:CIT:H41	1.91	0.86
1:B:27:VAL:HG11	1:B:123:ILE:HD11	1.55	0.86
1:A:289:LEU:O	1:A:291:CYS:SG	2.33	0.86
1:B:110:LEU:HD12	1:B:112:LEU:HD21	1.56	0.86
1:B:157:LYS:N	1:B:157:LYS:HD2	1.90	0.86
1:B:223:GLU:O	1:B:224:ASN:HB2	1.75	0.86
1:B:2:THR:HG23	1:B:3:LEU:H	1.41	0.86
1:A:248:TRP:CB	1:B:65:ASP:CG	2.42	0.86
1:A:223:GLU:CD	1:A:225:TRP:CH2	2.49	0.86
1:A:2:THR:HG23	1:A:3:LEU:H	1.41	0.86
1:B:223:GLU:CD	1:B:225:TRP:CH2	2.49	0.86
1:A:101:ARG:HG3	1:A:102:GLN:CD	1.96	0.86
1:A:161:ILE:HD13	1:A:293:LEU:CD2	2.05	0.86
1:B:96:VAL:CG2	1:B:120:PHE:CE2	2.59	0.86
1:B:124:ILE:O	1:B:127:ILE:HG23	1.75	0.86
1:B:25:THR:HG22	1:B:50:ALA:CB	2.05	0.86
1:B:316:LYS:CG	1:B:317:ASN:H	1.88	0.86
1:A:96:VAL:CG2	1:A:120:PHE:CE2	2.59	0.86
1:A:109:ARG:NH1	1:A:195:HIS:CD2	2.44	0.86
1:A:24:ILE:HG12	1:A:93:ILE:O	1.76	0.86
1:B:154:GLY:O	1:B:155:LEU:CG	2.23	0.86
1:B:203:TRP:HZ3	1:B:218:THR:CG2	1.88	0.86
1:A:11:VAL:HG22	1:A:11:VAL:O	1.75	0.85
1:A:223:GLU:O	1:A:224:ASN:HB2	1.75	0.85
1:A:203:TRP:CH2	1:A:226:LYS:CE	2.43	0.85
1:B:11:VAL:HG22	1:B:11:VAL:O	1.75	0.85
1:A:110:LEU:CD2	1:A:140:ASN:ND2	2.39	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:LYS:H	1:B:243:LYS:HD3	1.05	0.85
1:A:243:LYS:HD3	1:A:243:LYS:H	1.05	0.85
1:A:6:LYS:HB3	1:A:7:LEU:HD23	1.56	0.85
1:B:109:ARG:NH1	1:B:195:HIS:CD2	2.44	0.85
1:B:275:VAL:HG13	1:B:285:VAL:HB	1.56	0.85
1:A:11:VAL:CG2	1:A:11:VAL:O	2.25	0.85
1:A:89:ALA:O	1:A:131:SER:HB3	1.76	0.85
1:B:210(B):GLN:O	1:B:214:PRO:CG	2.24	0.85
1:B:134:ILE:HG13	1:B:261:MET:CE	2.05	0.85
1:B:19:PRO:HB3	1:B:48:GLU:CG	2.06	0.85
1:A:279:TYR:CE1	1:A:306:LYS:HE2	2.11	0.85
1:A:168:ASP:HB3	1:A:191:ILE:HD12	1.59	0.85
1:B:101:ARG:HG2	1:B:102:GLN:CA	2.07	0.85
1:B:11:VAL:CG2	1:B:11:VAL:O	2.25	0.85
1:B:24:ILE:HG12	1:B:93:ILE:O	1.76	0.85
1:A:157:LYS:HD2	1:A:157:LYS:N	1.90	0.85
1:B:89:ALA:O	1:B:131:SER:HB3	1.76	0.85
1:A:316:LYS:CG	1:A:317:ASN:H	1.88	0.85
1:B:63:MET:SD	1:B:78:ILE:HD11	2.17	0.85
1:A:243:LYS:CD	1:A:243:LYS:H	1.81	0.85
1:A:28:GLY:O	1:A:33:GLY:HA2	1.75	0.85
1:A:65:ASP:HB3	1:B:248:TRP:HB2	1.55	0.84
1:A:19:PRO:HB3	1:A:48:GLU:CG	2.06	0.84
1:B:203:TRP:CH2	1:B:226:LYS:CE	2.43	0.84
1:B:247:ASN:CA	1:B:250:ILE:HG22	2.08	0.84
1:B:279:TYR:CE1	1:B:306:LYS:HE2	2.11	0.84
1:A:248:TRP:HB2	1:B:65:ASP:HB3	1.55	0.84
1:A:210(B):GLN:O	1:A:214:PRO:CG	2.24	0.84
1:B:124:ILE:HG12	1:B:125:PRO:HD3	0.87	0.84
1:B:168:ASP:HB3	1:B:191:ILE:HD12	1.59	0.84
1:A:63:MET:SD	1:A:78:ILE:HD11	2.17	0.84
1:B:110:LEU:HD13	1:B:112:LEU:HD21	1.60	0.84
1:A:147:TYR:CA	1:A:150:TRP:HE3	1.91	0.84
1:A:26:VAL:HG22	1:A:28:GLY:H	1.42	0.84
1:A:1:ALA:O	1:A:2:THR:CG2	2.26	0.84
1:B:27:VAL:HG11	1:B:123:ILE:CD1	2.08	0.84
1:B:306:LYS:HZ3	1:B:315:LEU:CD2	1.90	0.84
1:A:150:TRP:HB3	1:A:160:VAL:HG21	1.54	0.83
1:B:84:ASP:O	1:B:85:TYR:CD1	2.31	0.83
1:A:101:ARG:HG2	1:A:102:GLN:CA	2.07	0.83
1:A:150:TRP:NE1	1:A:156:PRO:HA	1.93	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:VAL:HG11	1:A:123:ILE:CD1	2.08	0.83
1:A:97:THR:O	1:A:98:ALA:HB3	1.79	0.83
1:B:110:LEU:CD2	1:B:140:ASN:ND2	2.39	0.83
1:B:150:TRP:NE1	1:B:156:PRO:HA	1.93	0.83
1:A:247:ASN:CA	1:A:250:ILE:HG22	2.08	0.83
1:B:223:GLU:OE2	1:B:225:TRP:CZ2	2.31	0.83
1:A:255:ALA:O	1:A:258:ILE:HG22	1.77	0.83
1:A:306:LYS:HZ3	1:A:315:LEU:CD2	1.91	0.83
1:A:84:ASP:O	1:A:85:TYR:CD1	2.31	0.83
1:B:255:ALA:O	1:B:258:ILE:HG22	1.77	0.83
1:B:26:VAL:HG22	1:B:28:GLY:H	1.42	0.83
1:A:203:TRP:HZ3	1:A:218:THR:CG2	1.88	0.83
1:A:25:THR:HG22	1:A:50:ALA:CB	2.05	0.83
1:B:183:HIS:HE1	1:B:209(A):ALA:CB	1.91	0.83
1:B:85:TYR:O	1:B:130:TYR:CD2	2.32	0.83
1:A:223:GLU:OE2	1:A:225:TRP:CZ2	2.31	0.83
1:A:40:ILE:HG22	1:A:41:LEU:H	1.43	0.83
1:B:16:THR:O	1:B:17:THR:HG22	1.79	0.83
1:B:163:SER:O	1:B:271:VAL:CG2	2.27	0.83
1:A:85:TYR:O	1:A:130:TYR:CD2	2.32	0.82
1:B:147:TYR:CA	1:B:150:TRP:HE3	1.91	0.82
1:A:195:HIS:NE2	2:A:332:LNC:OAS	2.13	0.82
1:B:265:LEU:HD13	1:B:267:ARG:HH21	0.83	0.82
1:B:134:ILE:HA	1:B:159:ARG:HG3	1.61	0.82
1:A:9:ALA:CB	1:A:10:PRO:CD	2.53	0.82
1:B:195:HIS:NE2	2:B:332:LNC:OAS	2.13	0.82
1:A:110:LEU:HD13	1:A:112:LEU:HD21	1.60	0.82
1:A:32:VAL:CG2	2:A:332:LNC:H5'1	2.03	0.82
1:A:93:ILE:CG1	1:A:261:MET:HE3	2.09	0.82
1:A:183:HIS:HE1	1:A:209(A):ALA:CB	1.91	0.82
1:B:246:THR:CG2	2:B:332:LNC:CGS	2.53	0.82
1:A:253:SER:CA	1:B:72:PHE:CE1	2.63	0.82
1:A:281:ILE:HG21	1:A:285:VAL:CG1	2.03	0.82
1:B:263:LYS:O	1:B:264:ASN:HB2	1.78	0.82
1:B:273:THR:CG2	1:B:274:MET:N	2.31	0.82
1:A:229:HIS:CD2	1:A:229:HIS:C	2.53	0.82
1:B:281:ILE:HG21	1:B:285:VAL:CG1	2.03	0.82
1:B:1:ALA:O	1:B:2:THR:CG2	2.26	0.82
1:A:275:VAL:HG13	1:A:285:VAL:CG1	2.10	0.81
1:A:3:LEU:CD2	1:A:4:LYS:HG2	2.09	0.81
1:B:229:HIS:C	1:B:229:HIS:CD2	2.53	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:LEU:HD13	1:B:267:ARG:HH22	1.45	0.81
1:B:1:ALA:O	1:B:2:THR:CB	2.27	0.81
1:A:263:LYS:O	1:A:264:ASN:HB2	1.78	0.81
1:A:1:ALA:O	1:A:2:THR:CB	2.27	0.81
1:A:246:THR:CG2	2:A:332:LNC:CGS	2.53	0.81
1:A:16:THR:O	1:A:17:THR:HG22	1.79	0.81
1:A:303:ILE:N	1:A:303:ILE:HD13	1.95	0.81
1:B:143:ASP:O	1:B:146:THR:CG2	2.27	0.81
1:A:165:CYS:HB3	1:A:270:PRO:CB	1.99	0.81
1:A:72:PHE:CE1	1:B:253:SER:CA	2.63	0.81
1:B:8:ILE:CG1	1:B:8:ILE:O	2.27	0.81
1:A:93:ILE:CD1	1:A:258:ILE:HG12	2.08	0.81
1:B:218:THR:O	1:B:219:ASP:CB	2.29	0.81
1:A:128:VAL:O	1:A:132(A):PRO:CA	2.29	0.81
1:B:128:VAL:O	1:B:132(A):PRO:CA	2.29	0.81
1:A:143:ASP:O	1:A:146:THR:CG2	2.27	0.81
1:B:222:SER:O	1:B:224:ASN:ND2	2.14	0.81
1:A:10:PRO:C	1:A:11:VAL:HG13	2.01	0.81
1:A:24:ILE:CG1	1:A:25:THR:N	2.44	0.81
1:B:303:ILE:HD13	1:B:303:ILE:N	1.95	0.81
1:B:200:VAL:HG21	1:B:314:GLN:HB3	1.62	0.81
1:B:275:VAL:HG13	1:B:285:VAL:CG1	2.10	0.81
1:B:192:LEU:HD21	1:B:289:LEU:CD1	2.11	0.81
1:B:55:LEU:O	1:B:59:LEU:CD1	2.29	0.81
1:B:56:GLU:OE1	1:B:56:GLU:N	2.15	0.81
1:A:34:MET:HE3	1:A:66:LEU:CD2	2.06	0.80
1:B:150:TRP:HB3	1:B:160:VAL:HG21	1.54	0.80
1:A:135:ILE:O	1:A:135:ILE:CG2	2.29	0.80
1:A:19:PRO:O	1:A:20:ASP:CB	2.29	0.80
1:A:200:VAL:HG21	1:A:314:GLN:HB3	1.62	0.80
1:A:171:ARG:NH2	2:A:332:LNC:O2S	2.14	0.80
1:A:55:LEU:O	1:A:59:LEU:CD1	2.29	0.80
1:A:85:TYR:CZ	1:A:123:ILE:HG12	2.16	0.80
1:B:245:TYR:HA	1:B:248:TRP:HD1	1.46	0.80
1:B:32:VAL:CG2	2:B:332:LNC:H5'1	2.03	0.80
1:B:5:GLU:OE2	1:B:6:LYS:HG2	1.81	0.80
1:B:97:THR:O	1:B:98:ALA:HB3	1.79	0.80
1:B:41:LEU:HD11	1:B:49:LEU:CD2	2.11	0.80
1:B:10:PRO:C	1:B:11:VAL:HG13	2.01	0.80
1:A:165:CYS:HB2	1:A:270:PRO:CG	2.10	0.80
1:A:209(B):GLY:O	1:A:209(C):VAL:CB	2.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:THR:O	1:A:219:ASP:CB	2.29	0.80
1:B:49:LEU:CD1	1:B:49:LEU:C	2.46	0.80
1:B:24:ILE:CG1	1:B:25:THR:N	2.44	0.80
1:B:3:LEU:CD2	1:B:4:LYS:HG2	2.09	0.80
1:A:176:MET:HG2	1:A:177:GLY:N	1.95	0.80
1:A:222:SER:O	1:A:224:ASN:ND2	2.14	0.80
1:A:134:ILE:HA	1:A:159:ARG:HG3	1.61	0.80
1:A:265:LEU:HD13	1:A:267:ARG:HH21	0.83	0.80
1:A:192:LEU:HD21	1:A:289:LEU:CD1	2.11	0.80
1:A:5:GLU:OE2	1:A:6:LYS:HG2	1.81	0.80
1:A:163:SER:O	1:A:271:VAL:CG2	2.27	0.80
1:B:135:ILE:CG2	1:B:135:ILE:O	2.29	0.80
1:A:128:VAL:O	1:A:132(A):PRO:HA	1.82	0.80
1:A:41:LEU:HD11	1:A:49:LEU:CD2	2.11	0.80
1:B:85:TYR:CZ	1:B:123:ILE:HG12	2.16	0.80
1:B:123:ILE:HG23	1:B:124:ILE:H	1.35	0.80
1:B:209(B):GLY:O	1:B:209(C):VAL:CB	2.29	0.80
1:B:171:ARG:NH2	2:B:332:LNC:O2S	2.14	0.80
1:B:282:GLU:O	1:B:283:ASN:CB	2.30	0.79
1:A:275:VAL:HG22	1:A:281:ILE:HB	1.63	0.79
1:A:56:GLU:N	1:A:56:GLU:OE1	2.15	0.79
1:A:265:LEU:O	1:A:266:SER:O	2.01	0.79
1:B:128:VAL:O	1:B:132(A):PRO:HA	1.82	0.79
1:B:187:CYS:O	1:B:188:HIS:ND1	2.16	0.79
1:A:52:VAL:HG23	1:A:53:ASP:N	1.98	0.79
1:B:154:GLY:O	1:B:155:LEU:CB	2.30	0.79
1:B:40:ILE:HG22	1:B:41:LEU:H	1.43	0.79
1:A:154:GLY:O	1:A:155:LEU:CB	2.30	0.79
1:A:165:CYS:HB2	1:A:270:PRO:CB	2.06	0.79
1:A:187:CYS:O	1:A:188:HIS:ND1	2.16	0.79
1:A:203:TRP:CZ3	1:A:218:THR:CG2	2.63	0.79
1:A:71:LEU:HD13	1:B:173:ARG:HH12	1.46	0.79
1:B:176:MET:HG2	1:B:177:GLY:N	1.95	0.79
1:A:173:ARG:HH12	1:B:71:LEU:HD13	1.46	0.79
1:A:29:VAL:HG23	1:A:53:ASP:OD1	1.83	0.79
1:A:144:ILE:HG22	1:A:145:LEU:HD13	1.65	0.79
1:B:165:CYS:HB2	1:B:270:PRO:CG	2.10	0.79
1:B:265:LEU:O	1:B:266:SER:O	2.01	0.79
1:B:275:VAL:CB	1:B:285:VAL:CG1	2.46	0.79
1:B:29:VAL:HG23	1:B:53:ASP:OD1	1.83	0.79
1:B:55:LEU:HD22	1:B:55:LEU:N	1.98	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LYS:NZ	1:A:315:LEU:CD2	2.45	0.78
1:B:203:TRP:CZ3	1:B:218:THR:CG2	2.63	0.78
1:A:11:VAL:O	1:A:12:ALA:CB	2.31	0.78
1:B:306:LYS:NZ	1:B:315:LEU:CD2	2.45	0.78
1:A:95:VAL:HG12	1:A:136:ILE:CB	2.09	0.78
1:B:11:VAL:O	1:B:12:ALA:CB	2.31	0.78
1:B:1:ALA:O	1:B:2:THR:HB	1.84	0.78
1:B:275:VAL:HG22	1:B:281:ILE:HB	1.63	0.78
1:B:19:PRO:O	1:B:20:ASP:CB	2.29	0.78
1:A:121:LYS:O	1:A:125:PRO:CG	2.32	0.78
1:A:41:LEU:O	1:A:73:LEU:CD1	2.32	0.78
1:B:93:ILE:CD1	1:B:258:ILE:HG12	2.08	0.78
1:A:282:GLU:O	1:A:283:ASN:CB	2.30	0.78
1:A:203:TRP:HH2	1:A:226:LYS:CD	1.97	0.78
1:A:284:GLU:C	1:A:285:VAL:HG23	2.04	0.78
1:B:241:LYS:N	1:B:241:LYS:CE	2.47	0.78
2:B:332:LNC:C4N	2:B:332:LNC:CAS	2.27	0.78
1:A:245:TYR:HA	1:A:248:TRP:HD1	1.46	0.77
1:B:241:LYS:N	1:B:241:LYS:HE2	1.99	0.77
1:A:275:VAL:HG13	1:A:285:VAL:CB	2.15	0.77
1:A:55:LEU:N	1:A:55:LEU:HD22	1.98	0.77
1:B:146:THR:OG1	1:B:160:VAL:HG11	1.83	0.77
1:A:62:GLU:HA	1:B:245:TYR:CD1	2.20	0.77
1:B:25:THR:HG21	1:B:88:THR:OG1	1.84	0.77
1:B:41:LEU:O	1:B:73:LEU:CD1	2.32	0.77
1:A:23:LYS:HD3	1:A:90:ASN:CB	2.14	0.77
1:A:25:THR:HG21	1:A:88:THR:OG1	1.84	0.77
1:A:37:ALA:O	1:A:40:ILE:HG22	1.84	0.77
1:B:23:LYS:HD3	1:B:90:ASN:CB	2.14	0.77
1:A:110:LEU:H	1:A:110:LEU:CD2	1.98	0.77
1:A:241:LYS:CE	1:A:241:LYS:N	2.47	0.77
1:B:203:TRP:HH2	1:B:226:LYS:CD	1.97	0.77
1:B:37:ALA:O	1:B:41:LEU:HD23	1.84	0.77
1:A:275:VAL:CG1	1:A:285:VAL:CB	2.62	0.77
1:B:121:LYS:O	1:B:125:PRO:CG	2.32	0.77
1:B:1:ALA:C	1:B:2:THR:HG22	2.04	0.77
1:B:275:VAL:CG1	1:B:285:VAL:CB	2.62	0.77
1:A:37:ALA:O	1:A:41:LEU:HD23	1.84	0.77
1:B:37:ALA:O	1:B:40:ILE:HG22	1.84	0.77
1:A:99:GLY:O	1:A:100:VAL:HG13	1.85	0.77
1:A:1:ALA:C	1:A:2:THR:HG22	2.04	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLU:HB2	1:B:225:TRP:CZ3	2.20	0.77
1:A:38:ILE:HG21	1:B:38:ILE:CG2	2.15	0.77
3:A:333:CIT:C1	3:A:333:CIT:O6	2.33	0.76
1:A:20:ASP:O	1:A:22:ASN:HB2	1.84	0.76
1:A:313:ALA:HA	1:A:316:LYS:CD	2.16	0.76
1:B:247:ASN:O	1:B:250:ILE:CG2	2.33	0.76
1:B:52:VAL:HG23	1:B:53:ASP:N	1.98	0.76
1:A:1:ALA:O	1:A:2:THR:HB	1.84	0.76
1:A:35:ALA:CB	1:A:247:ASN:OD1	2.33	0.76
1:A:38:ILE:CG2	1:B:38:ILE:HG21	2.15	0.76
1:B:121:LYS:N	1:B:124:ILE:HD11	2.01	0.76
1:A:121:LYS:N	1:A:124:ILE:HD11	2.01	0.76
1:A:18:ILE:HG23	1:A:20:ASP:OD2	1.85	0.76
1:B:110:LEU:H	1:B:110:LEU:CD2	1.98	0.76
1:A:146:THR:OG1	1:A:160:VAL:HG11	1.83	0.76
1:B:99:GLY:O	1:B:100:VAL:HG13	1.85	0.76
1:A:265:LEU:HD13	1:A:267:ARG:HH22	1.45	0.76
1:B:73:LEU:HG	1:B:75:THR:HG23	1.68	0.76
1:B:229:HIS:C	1:B:232:VAL:CG2	2.53	0.76
1:B:282:GLU:O	1:B:283:ASN:HB2	1.84	0.76
1:B:286:PHE:CD1	1:B:286:PHE:O	2.35	0.76
1:B:31:GLN:HB2	2:B:332:LNC:O2N	1.85	0.76
1:A:241:LYS:N	1:A:241:LYS:HE2	1.99	0.76
1:A:93:ILE:HD11	1:A:261:MET:CE	2.15	0.76
1:A:38:ILE:HD11	1:B:248:TRP:CE3	2.21	0.76
1:B:284:GLU:C	1:B:285:VAL:HG23	2.04	0.76
1:B:8:ILE:O	1:B:9:ALA:HB3	1.84	0.76
1:A:163:SER:H	1:A:271:VAL:HG13	0.93	0.76
1:A:31:GLN:HB2	2:A:332:LNC:O2N	1.85	0.76
3:A:333:CIT:C2	3:A:333:CIT:C4	2.63	0.76
1:B:213:ASN:C	1:B:215:GLU:H	1.90	0.76
1:B:275:VAL:HG13	1:B:285:VAL:CB	2.15	0.76
3:B:333:CIT:C1	3:B:333:CIT:O6	2.33	0.76
1:B:165:CYS:HB2	1:B:270:PRO:CB	2.06	0.75
1:B:93:ILE:HD11	1:B:261:MET:CE	2.15	0.75
1:A:248:TRP:CE3	1:B:38:ILE:HD11	2.21	0.75
3:B:333:CIT:C2	3:B:333:CIT:C4	2.63	0.75
1:A:275:VAL:CG2	1:A:281:ILE:HB	2.16	0.75
1:A:275:VAL:CB	1:A:285:VAL:CG1	2.46	0.75
1:B:93:ILE:CD1	1:B:261:MET:HE3	2.16	0.75
2:A:332:LNC:CAS	2:A:332:LNC:C4N	2.27	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:O	1:A:9:ALA:HB3	1.84	0.75
1:B:275:VAL:CG2	1:B:281:ILE:HB	2.16	0.75
1:A:245:TYR:CD1	1:B:62:GLU:HA	2.20	0.75
1:A:99:GLY:O	1:A:100:VAL:CG1	2.34	0.75
1:A:282:GLU:O	1:A:283:ASN:HB2	1.84	0.75
1:A:286:PHE:CD1	1:A:286:PHE:O	2.35	0.75
1:B:313:ALA:HA	1:B:316:LYS:CD	2.16	0.75
1:B:316:LYS:HG3	1:B:317:ASN:N	2.00	0.75
1:B:35:ALA:CB	1:B:247:ASN:OD1	2.33	0.75
1:A:223:GLU:HB2	1:A:225:TRP:CZ3	2.20	0.75
1:A:161:ILE:HD13	1:A:293:LEU:HD21	1.67	0.75
1:B:20:ASP:O	1:B:22:ASN:HB2	1.84	0.75
1:A:19:PRO:CB	1:A:48:GLU:HG3	2.16	0.75
1:B:165:CYS:SG	1:B:270:PRO:CB	2.72	0.75
1:B:306:LYS:NZ	1:B:315:LEU:HD22	2.02	0.75
1:B:24:ILE:HD13	1:B:24:ILE:C	2.07	0.75
1:B:284:GLU:O	1:B:285:VAL:CG2	2.35	0.75
1:A:247:ASN:O	1:A:250:ILE:CG2	2.33	0.74
1:A:24:ILE:HD13	1:A:24:ILE:C	2.07	0.74
1:A:313:ALA:O	1:A:316:LYS:HG2	1.87	0.74
1:A:73:LEU:HG	1:A:75:THR:HG23	1.68	0.74
1:B:18:ILE:HG23	1:B:20:ASP:OD2	1.85	0.74
1:B:99:GLY:O	1:B:100:VAL:CG1	2.34	0.74
1:A:213:ASN:C	1:A:215:GLU:H	1.90	0.74
1:B:101:ARG:CG	1:B:102:GLN:H	1.85	0.74
1:B:16:THR:C	1:B:17:THR:HG23	2.07	0.74
1:A:150:TRP:CB	1:A:160:VAL:CG2	2.09	0.74
1:A:229:HIS:C	1:A:232:VAL:CG2	2.53	0.74
1:A:49:LEU:HD12	1:A:50:ALA:CA	2.18	0.74
1:B:150:TRP:CA	1:B:160:VAL:CG2	2.64	0.74
1:B:203:TRP:HA	1:B:206:VAL:CG2	2.17	0.74
1:B:313:ALA:O	1:B:316:LYS:HG2	1.87	0.74
1:A:210(B):GLN:HG3	1:A:214:PRO:HG3	1.68	0.74
1:A:308:LYS:C	1:A:312:VAL:CG2	2.55	0.74
1:B:218:THR:CG2	1:B:225:TRP:HB2	2.17	0.74
1:B:326:GLN:O	1:B:327:LYS:C	2.24	0.74
1:A:150:TRP:CA	1:A:160:VAL:HG21	2.16	0.74
1:A:218:THR:CG2	1:A:225:TRP:HB2	2.17	0.74
1:A:306:LYS:NZ	1:A:315:LEU:HD22	2.02	0.74
1:B:308:LYS:C	1:B:312:VAL:CG2	2.55	0.74
1:B:150:TRP:CA	1:B:160:VAL:HG21	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:SER:H	1:B:271:VAL:HG13	0.93	0.74
1:A:248:TRP:CZ2	1:B:34:MET:HB3	2.22	0.74
1:B:49:LEU:HD12	1:B:50:ALA:CA	2.18	0.74
1:A:165:CYS:SG	1:A:270:PRO:CB	2.72	0.74
1:A:203:TRP:CH2	1:A:226:LYS:CD	2.70	0.74
1:A:284:GLU:O	1:A:285:VAL:CG2	2.35	0.74
1:A:316:LYS:HG3	1:A:317:ASN:N	2.00	0.74
1:B:171:ARG:O	1:B:175:LEU:CD2	2.36	0.74
1:A:198:SER:O	1:A:199:SER:C	2.26	0.74
1:A:247:ASN:CA	1:A:250:ILE:CG2	2.62	0.74
1:A:275:VAL:CG1	1:A:285:VAL:HB	2.18	0.74
1:A:97:THR:O	1:A:98:ALA:CB	2.36	0.74
1:B:161:ILE:HD13	1:B:293:LEU:HD21	1.67	0.74
1:B:210(B):GLN:HG3	1:B:214:PRO:HG3	1.68	0.74
1:B:222:SER:O	1:B:223:GLU:C	2.26	0.74
1:A:203:TRP:HA	1:A:206:VAL:CG2	2.17	0.74
1:A:53:ASP:HB3	1:A:55:LEU:CD2	2.18	0.74
1:A:6:LYS:C	1:A:7:LEU:CD2	2.56	0.74
1:B:102:GLN:O	1:B:103:GLN:CB	2.36	0.74
1:A:218:THR:HB	1:A:226:LYS:HD3	1.69	0.74
1:A:326:GLN:O	1:A:327:LYS:C	2.24	0.74
1:B:124:ILE:CG1	1:B:125:PRO:CD	2.44	0.74
1:B:203:TRP:CH2	1:B:226:LYS:CD	2.70	0.74
1:B:6:LYS:C	1:B:7:LEU:CD2	2.56	0.74
1:A:134:ILE:HG13	1:A:261:MET:SD	2.28	0.73
1:B:121:LYS:HE3	1:B:331:LEU:HD12	1.70	0.73
1:B:198:SER:O	1:B:199:SER:C	2.26	0.73
1:A:121:LYS:HE3	1:A:331:LEU:HD12	1.70	0.73
1:A:171:ARG:O	1:A:175:LEU:CD2	2.36	0.73
1:A:40:ILE:HG23	1:A:41:LEU:N	2.03	0.73
1:B:188:HIS:NE2	3:B:333:CIT:C4	2.51	0.73
1:B:309:ASP:O	1:B:309:ASP:OD1	2.06	0.73
1:B:19:PRO:CB	1:B:48:GLU:HG3	2.16	0.73
1:B:97:THR:O	1:B:98:ALA:CB	2.36	0.73
1:B:134:ILE:HG13	1:B:261:MET:SD	2.28	0.73
1:B:53:ASP:HB3	1:B:55:LEU:CD2	2.18	0.73
1:A:150:TRP:CA	1:A:160:VAL:CG2	2.64	0.73
1:A:193:GLY:CA	1:A:287:LEU:HD21	2.10	0.73
1:B:11:VAL:O	1:B:12:ALA:HB2	1.88	0.73
1:A:161:ILE:CG2	1:A:271:VAL:HG11	2.18	0.73
1:A:4:LYS:HG3	1:A:5:GLU:N	2.03	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:LEU:O	1:A:148:VAL:HG13	1.88	0.73
1:A:223:GLU:CD	1:A:225:TRP:CZ2	2.62	0.73
1:B:275:VAL:CG1	1:B:285:VAL:HB	2.18	0.73
1:B:23:LYS:CD	1:B:90:ASN:O	2.36	0.73
1:A:309:ASP:O	1:A:309:ASP:OD1	2.06	0.73
1:B:4:LYS:HG3	1:B:5:GLU:N	2.03	0.73
1:A:16:THR:C	1:A:17:THR:HG23	2.07	0.73
1:A:222:SER:O	1:A:223:GLU:C	2.26	0.73
1:A:188:HIS:NE2	3:A:333:CIT:C4	2.51	0.73
1:A:3:LEU:CD2	1:A:4:LYS:CG	2.67	0.73
1:B:223:GLU:CD	1:B:225:TRP:CZ2	2.62	0.73
1:A:149:ALA:O	1:A:153:SER:CB	2.37	0.73
1:A:23:LYS:CD	1:A:90:ASN:O	2.36	0.73
1:A:242:LEU:C	1:A:243:LYS:HD3	2.08	0.73
1:A:34:MET:HB3	1:B:248:TRP:CZ2	2.22	0.73
1:B:242:LEU:C	1:B:243:LYS:HD3	2.08	0.73
1:A:150:TRP:NE1	1:A:156:PRO:CA	2.52	0.72
1:B:149:ALA:O	1:B:153:SER:CB	2.37	0.72
1:B:218:THR:HB	1:B:226:LYS:HD3	1.69	0.72
1:A:58:LYS:HG3	1:B:242:LEU:HD11	1.70	0.72
1:A:8:ILE:O	1:A:8:ILE:CG1	2.27	0.72
1:B:134:ILE:CG2	1:B:296:ARG:O	2.37	0.72
1:B:144:ILE:HG22	1:B:145:LEU:HD13	1.65	0.72
1:A:80:ALA:O	1:A:81:ASN:HB2	1.89	0.72
1:A:101:ARG:HB2	2:A:332:LNC:H122	1.72	0.72
1:A:241:LYS:CE	1:A:241:LYS:CA	2.67	0.72
1:B:210(B):GLN:O	1:B:214:PRO:HG2	1.89	0.72
1:A:11:VAL:O	1:A:12:ALA:HB2	1.88	0.72
1:B:161:ILE:CG2	1:B:271:VAL:HG11	2.18	0.72
1:A:210(B):GLN:O	1:A:214:PRO:HG2	1.89	0.72
1:B:145:LEU:O	1:B:148:VAL:HG13	1.88	0.72
1:B:3:LEU:HD22	1:B:4:LYS:HG3	1.71	0.72
1:A:242:LEU:HD11	1:B:58:LYS:HG3	1.70	0.72
1:B:150:TRP:CB	1:B:160:VAL:CG2	2.09	0.72
1:B:230:LYS:HG2	1:B:231:MET:H	1.55	0.72
1:B:6:LYS:CB	1:B:7:LEU:HD23	2.19	0.72
1:A:134:ILE:CG2	1:A:296:ARG:O	2.37	0.71
1:B:193:GLY:CA	1:B:287:LEU:HD21	2.10	0.71
1:B:95:VAL:HG12	1:B:136:ILE:CB	2.09	0.71
1:A:34:MET:HG2	1:A:62:GLU:OE2	1.89	0.71
1:B:34:MET:HG2	1:B:62:GLU:OE2	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:ALA:O	1:B:81:ASN:HB2	1.89	0.71
1:A:9:ALA:CB	1:A:10:PRO:HD3	2.15	0.71
1:B:144:ILE:HG21	1:B:145:LEU:HD13	1.71	0.71
1:B:101:ARG:HB2	2:B:332:LNC:H122	1.72	0.71
1:A:230:LYS:HG2	1:A:231:MET:H	1.55	0.71
1:B:64:MET:O	1:B:68:HIS:CG	2.44	0.71
1:A:330(A):LYS:O	1:A:330(A):LYS:HD2	1.90	0.71
1:A:34:MET:CG	1:A:62:GLU:OE2	2.39	0.71
1:B:213:ASN:CB	1:B:214:PRO:CD	2.55	0.71
1:B:330(A):LYS:HD2	1:B:330(A):LYS:O	1.90	0.71
1:B:330(A):LYS:O	1:B:330(B):ASP:HB3	1.90	0.71
1:A:61:GLY:HA3	1:B:242:LEU:HB2	1.73	0.71
1:B:100:VAL:HG11	1:B:119:VAL:HG21	1.71	0.71
1:B:162:GLY:O	1:B:163:SER:CB	2.39	0.71
1:A:101:ARG:HG3	1:A:102:GLN:OE1	1.91	0.71
1:B:97:THR:CG2	2:B:332:LNC:H5'1	2.21	0.71
1:A:100:VAL:HG11	1:A:119:VAL:HG21	1.71	0.71
1:A:188:HIS:CD2	3:A:333:CIT:C4	2.74	0.71
1:A:23:LYS:CG	1:A:90:ASN:O	2.39	0.71
1:A:93:ILE:HD11	1:A:261:MET:HE2	1.72	0.71
1:A:162:GLY:O	1:A:163:SER:CB	2.39	0.70
1:A:330(A):LYS:O	1:A:330(B):ASP:HB3	1.90	0.70
1:B:150:TRP:NE1	1:B:156:PRO:CA	2.52	0.70
1:B:23:LYS:CG	1:B:90:ASN:O	2.39	0.70
1:A:147:TYR:C	1:A:147:TYR:HD2	1.90	0.70
1:A:243:LYS:O	1:A:246:THR:HB	1.92	0.70
1:A:64:MET:O	1:A:68:HIS:CG	2.44	0.70
1:A:6:LYS:CB	1:A:7:LEU:HD23	2.19	0.70
1:B:109:ARG:NH1	1:B:195:HIS:NE2	2.39	0.70
1:B:243:LYS:O	1:B:246:THR:HB	1.92	0.70
1:B:288:SER:O	1:B:289:LEU:CB	2.39	0.70
1:A:284:GLU:O	1:A:285:VAL:CB	2.39	0.70
1:A:209(D):VAL:CG1	1:A:210(A):LEU:N	2.39	0.70
1:A:49:LEU:CD1	1:A:49:LEU:C	2.46	0.70
1:A:93:ILE:CD1	1:A:261:MET:CE	2.69	0.70
1:B:188:HIS:CD2	3:B:333:CIT:C4	2.74	0.70
1:B:258:ILE:CG2	1:B:259:GLU:N	2.54	0.70
1:B:308:LYS:C	1:B:312:VAL:HG21	2.12	0.70
1:A:242:LEU:HB2	1:B:61:GLY:HA3	1.73	0.70
1:B:161:ILE:HD13	1:B:293:LEU:HD23	1.73	0.70
1:B:284:GLU:O	1:B:285:VAL:CB	2.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HB3	1:A:7:LEU:CD2	2.22	0.70
1:A:54:VAL:HG13	1:A:54:VAL:O	1.92	0.70
1:A:55:LEU:HB2	1:A:59:LEU:HD11	1.73	0.70
1:A:248:TRP:CZ2	1:B:34:MET:CG	2.75	0.70
1:B:3:LEU:CD2	1:B:4:LYS:CG	2.67	0.70
1:B:34:MET:CG	1:B:62:GLU:OE2	2.39	0.70
1:B:93:ILE:CD1	1:B:261:MET:CE	2.69	0.70
1:A:109:ARG:NH1	1:A:195:HIS:NE2	2.39	0.70
1:A:24:ILE:CG1	1:A:25:THR:H	2.05	0.70
1:A:163:SER:C	1:A:271:VAL:HG22	2.12	0.70
1:A:4:LYS:CG	1:A:5:GLU:H	2.04	0.70
1:B:54:VAL:O	1:B:54:VAL:HG13	1.92	0.70
1:A:144:ILE:HG21	1:A:145:LEU:HD13	1.71	0.69
1:A:258:ILE:CG2	1:A:259:GLU:N	2.54	0.69
1:A:258:ILE:HD13	1:A:262:LEU:HB2	1.74	0.69
1:B:32:VAL:HG22	2:B:332:LNC:C5D	2.22	0.69
3:B:333:CIT:C3	3:B:333:CIT:C5	2.70	0.69
1:A:210(B):GLN:HG3	1:A:214:PRO:CG	2.22	0.69
1:A:32:VAL:HG22	2:A:332:LNC:C5D	2.22	0.69
1:B:109:ARG:CZ	1:B:195:HIS:CD2	2.75	0.69
1:B:40:ILE:HG23	1:B:41:LEU:N	2.03	0.69
1:A:72:PHE:CZ	1:B:253:SER:HA	2.27	0.69
1:B:78:ILE:HD13	1:B:78:ILE:C	2.12	0.69
1:A:3:LEU:HD22	1:A:4:LYS:HG3	1.71	0.69
1:B:6:LYS:HB3	1:B:7:LEU:CD2	2.22	0.69
1:A:109:ARG:CZ	1:A:195:HIS:CD2	2.75	0.69
1:A:97:THR:CG2	2:A:332:LNC:H5'1	2.21	0.69
1:B:101:ARG:CG	1:B:102:GLN:CD	2.60	0.69
1:B:241:LYS:CE	1:B:241:LYS:CA	2.67	0.69
1:B:165:CYS:CB	1:B:270:PRO:HG2	2.23	0.69
1:A:308:LYS:C	1:A:312:VAL:HG21	2.12	0.69
1:B:112:LEU:O	1:B:113:VAL:CG1	2.41	0.69
1:A:218:THR:CG2	1:A:226:LYS:HD3	2.23	0.69
1:A:308:LYS:O	1:A:312:VAL:HG21	1.92	0.69
1:A:34:MET:CG	1:B:248:TRP:CZ2	2.75	0.69
1:A:78:ILE:C	1:A:78:ILE:HD13	2.12	0.69
1:B:165:CYS:HB2	1:B:270:PRO:HG2	1.74	0.69
1:B:284:GLU:O	1:B:285:VAL:HB	1.93	0.69
1:A:101:ARG:CG	1:A:102:GLN:CD	2.60	0.69
1:A:279:TYR:HE1	1:A:306:LYS:CE	2.03	0.69
1:B:210(B):GLN:HG3	1:B:214:PRO:CG	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:SER:C	1:B:271:VAL:HG22	2.12	0.69
1:B:308:LYS:O	1:B:312:VAL:HG21	1.92	0.69
1:A:209(D):VAL:O	1:A:210(A):LEU:HG	1.93	0.69
1:B:9:ALA:CB	1:B:10:PRO:HD3	2.15	0.69
1:B:218:THR:CG2	1:B:226:LYS:HD3	2.23	0.69
1:A:101:ARG:HD2	1:A:102:GLN:HB2	1.75	0.69
1:A:102:GLN:O	1:A:103:GLN:CB	2.36	0.69
1:A:112:LEU:O	1:A:113:VAL:CG1	2.41	0.69
1:B:23:LYS:HE3	1:B:50:ALA:HB2	1.75	0.69
1:B:34:MET:HE3	1:B:66:LEU:CD2	2.07	0.68
1:B:7:LEU:N	1:B:7:LEU:CD2	2.56	0.68
1:A:165:CYS:HB2	1:A:270:PRO:HG2	1.74	0.68
1:A:330(A):LYS:CD	1:A:330(B):ASP:N	2.57	0.68
1:B:101:ARG:HG3	1:B:102:GLN:OE1	1.91	0.68
1:B:101:ARG:HD2	1:B:102:GLN:HB2	1.75	0.68
1:B:199:SER:O	1:B:229:HIS:CE1	2.46	0.68
1:B:258:ILE:HD13	1:B:262:LEU:HB2	1.74	0.68
1:A:109:ARG:CA	1:A:140:ASN:OD1	2.42	0.68
1:A:161:ILE:HD13	1:A:293:LEU:HD23	1.73	0.68
1:B:101:ARG:HB2	2:B:332:LNC:C3D	2.24	0.68
1:B:288:SER:O	1:B:289:LEU:HD23	1.94	0.68
1:B:23:LYS:HD3	1:B:90:ASN:O	1.93	0.68
1:B:24:ILE:HG12	1:B:25:THR:H	1.59	0.68
1:B:264:ASN:ND2	1:B:295:ALA:HB2	2.09	0.68
1:A:199:SER:O	1:A:229:HIS:CE1	2.46	0.68
1:A:288:SER:O	1:A:289:LEU:CB	2.39	0.68
1:A:288:SER:O	1:A:289:LEU:HD23	1.94	0.68
1:A:248:TRP:CZ2	1:B:34:MET:CB	2.76	0.68
1:A:229:HIS:HD2	1:A:229:HIS:C	1.96	0.68
1:A:7:LEU:CD2	1:A:7:LEU:N	2.56	0.68
1:B:124:ILE:O	1:B:128:VAL:HG12	1.94	0.68
1:B:109:ARG:CA	1:B:140:ASN:OD1	2.42	0.68
1:B:55:LEU:HB2	1:B:59:LEU:HD11	1.73	0.68
1:A:101:ARG:HB2	2:A:332:LNC:C3D	2.24	0.68
1:B:229:HIS:CA	1:B:232:VAL:HG22	2.23	0.68
1:B:24:ILE:CG1	1:B:25:THR:H	2.05	0.68
1:A:124:ILE:O	1:A:128:VAL:HG12	1.94	0.68
1:A:24:ILE:HG12	1:A:25:THR:H	1.59	0.68
1:A:134:ILE:CG1	1:A:261:MET:CE	2.71	0.68
1:A:275:VAL:HG23	1:A:281:ILE:HG13	1.76	0.68
1:A:308:LYS:HE2	1:A:312:VAL:HG11	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB2	1:A:247:ASN:OD1	1.93	0.68
1:B:218:THR:HG22	1:B:225:TRP:HB2	1.75	0.68
1:B:272:SER:HA	1:B:288:SER:HA	1.74	0.68
1:B:330(A):LYS:HD3	1:B:330(B):ASP:N	2.09	0.68
1:A:218:THR:HG22	1:A:225:TRP:HB2	1.75	0.68
1:A:264:ASN:ND2	1:A:295:ALA:HB2	2.09	0.68
1:A:165:CYS:CB	1:A:270:PRO:HG2	2.23	0.68
1:A:272:SER:HA	1:A:288:SER:HA	1.74	0.68
1:B:10:PRO:C	1:B:11:VAL:CG1	2.62	0.68
1:B:109:ARG:HB3	1:B:140:ASN:OD1	1.94	0.68
1:B:192:LEU:HD23	1:B:315:LEU:HD11	1.76	0.68
1:A:229:HIS:CD2	1:A:229:HIS:O	2.47	0.68
1:B:209(D):VAL:O	1:B:210(A):LEU:HG	1.93	0.68
1:B:229:HIS:O	1:B:229:HIS:CD2	2.47	0.68
1:A:248:TRP:CZ2	1:B:34:MET:HG3	2.29	0.68
1:B:6:LYS:O	1:B:7:LEU:HB2	1.95	0.68
1:A:229:HIS:CA	1:A:232:VAL:HG22	2.23	0.67
1:A:284:GLU:O	1:A:285:VAL:HB	1.93	0.67
1:A:34:MET:CB	1:B:248:TRP:CZ2	2.76	0.67
1:A:9:ALA:HB3	1:A:10:PRO:HD2	1.75	0.67
1:B:93:ILE:HD11	1:B:261:MET:CG	2.19	0.67
1:A:23:LYS:HE3	1:A:50:ALA:HB2	1.75	0.67
1:A:253:SER:HA	1:B:72:PHE:CZ	2.27	0.67
1:A:32:VAL:HG22	2:A:332:LNC:PN	2.34	0.67
1:B:110:LEU:HD23	1:B:140:ASN:OD1	1.94	0.67
1:A:6:LYS:O	1:A:7:LEU:HB2	1.95	0.67
1:B:134:ILE:CG1	1:B:261:MET:CE	2.71	0.67
1:A:187:CYS:C	1:A:188:HIS:ND1	2.48	0.67
1:A:23:LYS:HD3	1:A:90:ASN:O	1.93	0.67
1:B:187:CYS:C	1:B:188:HIS:ND1	2.48	0.67
1:B:44:SER:C	1:B:45:LEU:HD12	2.15	0.67
1:B:203:TRP:CZ3	1:B:226:LYS:HD3	2.30	0.67
1:B:223:GLU:OE2	1:B:225:TRP:HZ2	1.75	0.67
1:B:275:VAL:HG23	1:B:281:ILE:HG13	1.76	0.67
1:A:49:LEU:O	1:A:78:ILE:HA	1.94	0.67
1:A:56:GLU:CD	1:A:56:GLU:H	1.98	0.67
1:B:227:GLU:HA	1:B:230:LYS:NZ	2.09	0.67
1:B:35:ALA:HB2	1:B:247:ASN:OD1	1.93	0.67
1:B:49:LEU:O	1:B:78:ILE:HA	1.94	0.67
1:A:10:PRO:C	1:A:11:VAL:CG1	2.62	0.67
1:A:330(A):LYS:HD3	1:A:330(B):ASP:N	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:MET:HG3	1:B:248:TRP:CZ2	2.29	0.67
1:B:113:VAL:HG11	1:B:144:ILE:CD1	2.25	0.67
1:B:283:ASN:O	1:B:285:VAL:CG2	2.43	0.67
1:A:198:SER:O	1:A:199:SER:O	2.13	0.67
1:B:198:SER:O	1:B:199:SER:O	2.13	0.67
1:B:306:LYS:HZ2	1:B:315:LEU:HD22	1.60	0.67
1:B:308:LYS:HE2	1:B:312:VAL:HG11	1.76	0.67
1:B:195:HIS:CE1	2:B:332:LNC:OAS	2.48	0.67
1:A:16:THR:C	1:A:17:THR:CG2	2.62	0.67
1:A:84:ASP:O	1:A:85:TYR:CD2	2.48	0.67
1:A:88:THR:O	1:A:89:ALA:C	2.33	0.67
1:B:147:TYR:C	1:B:147:TYR:HD2	1.90	0.67
1:B:32:VAL:HG22	2:B:332:LNC:PN	2.34	0.67
1:A:113:VAL:HG11	1:A:144:ILE:CD1	2.25	0.66
1:A:192:LEU:HD23	1:A:315:LEU:HD11	1.76	0.66
1:A:223:GLU:OE2	1:A:225:TRP:HZ2	1.75	0.66
1:A:228:VAL:CG1	1:A:229:HIS:N	2.58	0.66
1:A:93:ILE:HD11	1:A:261:MET:CG	2.19	0.66
1:B:228:VAL:CG1	1:B:229:HIS:N	2.58	0.66
1:B:199:SER:O	1:B:229:HIS:HE1	1.78	0.66
1:B:281:ILE:O	1:B:285:VAL:HG22	1.96	0.66
1:B:330(A):LYS:CD	1:B:330(B):ASP:N	2.57	0.66
1:A:101:ARG:CG	1:A:102:GLN:H	1.85	0.66
1:A:109:ARG:HB3	1:A:140:ASN:OD1	1.94	0.66
1:A:13:GLN:O	1:A:14:GLN:CD	2.33	0.66
1:A:195:HIS:CE1	2:A:332:LNC:OAS	2.48	0.66
1:A:32:VAL:HA	1:A:247:ASN:OD1	1.95	0.66
3:A:333:CIT:C5	3:A:333:CIT:C3	2.70	0.66
1:B:221:ASP:OD1	1:B:223:GLU:HG3	1.96	0.66
1:A:245:TYR:CD2	1:A:248:TRP:NE1	2.64	0.66
1:A:44:SER:C	1:A:45:LEU:HD12	2.15	0.66
1:B:53:ASP:HB2	1:B:55:LEU:HD23	1.77	0.66
1:B:56:GLU:H	1:B:56:GLU:CD	1.98	0.66
1:A:124:ILE:CG1	1:A:125:PRO:CD	2.44	0.66
1:A:227:GLU:HA	1:A:230:LYS:NZ	2.09	0.66
1:A:265:LEU:HD22	1:A:267:ARG:CZ	2.26	0.66
1:B:229:HIS:HA	1:B:232:VAL:CG2	2.26	0.66
1:B:88:THR:O	1:B:89:ALA:C	2.33	0.66
1:B:32:VAL:HA	1:B:247:ASN:OD1	1.95	0.66
1:B:3:LEU:O	1:B:4:LYS:CB	2.44	0.66
1:B:245:TYR:CD2	1:B:248:TRP:NE1	2.64	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:O	1:A:4:LYS:CB	2.44	0.66
1:B:44:SER:O	1:B:45:LEU:HD12	1.96	0.66
1:B:41:LEU:HD11	1:B:49:LEU:HD23	1.78	0.66
1:B:84:ASP:O	1:B:85:TYR:CD2	2.48	0.66
1:A:133:CYS:O	1:A:159:ARG:CD	2.40	0.66
1:A:221:ASP:OD1	1:A:223:GLU:HG3	1.96	0.66
1:B:101:ARG:HG2	1:B:102:GLN:CB	2.25	0.66
1:B:13:GLN:O	1:B:14:GLN:CD	2.33	0.66
1:A:110:LEU:HD23	1:A:140:ASN:OD1	1.94	0.66
1:A:267:ARG:O	1:A:268:ILE:CG1	2.44	0.66
1:A:192:LEU:HD21	1:A:289:LEU:HD11	1.76	0.66
1:B:16:THR:C	1:B:17:THR:CG2	2.62	0.66
1:B:223:GLU:CB	1:B:225:TRP:CH2	2.79	0.66
1:B:192:LEU:HD21	1:B:289:LEU:HD11	1.76	0.66
1:A:138:VAL:HG12	2:A:332:LNC:HN72	1.61	0.65
1:A:199:SER:O	1:A:229:HIS:HE1	1.78	0.65
1:A:230:LYS:HG2	1:A:231:MET:N	2.11	0.65
1:B:13:GLN:O	1:B:14:GLN:HB2	1.95	0.65
1:B:161:ILE:CD1	1:B:293:LEU:HD23	2.26	0.65
1:B:4:LYS:CG	1:B:5:GLU:H	2.04	0.65
1:A:306:LYS:HZ2	1:A:315:LEU:HD22	1.58	0.65
1:A:3:LEU:O	1:A:4:LYS:HB3	1.96	0.65
1:B:229:HIS:C	1:B:229:HIS:HD2	1.96	0.65
1:B:3:LEU:O	1:B:4:LYS:HB3	1.96	0.65
1:B:267:ARG:O	1:B:268:ILE:CG1	2.44	0.65
1:A:101:ARG:HG2	1:A:102:GLN:CB	2.25	0.65
1:A:215:GLU:HB3	1:A:216:MET:SD	2.36	0.65
1:B:147:TYR:CD2	1:B:148:VAL:N	2.58	0.65
1:B:238:GLU:C	1:B:240:ILE:N	2.50	0.65
1:A:229:HIS:HA	1:A:232:VAL:CG2	2.26	0.65
1:A:97:THR:HG23	2:A:332:LNC:C4D	2.26	0.65
1:B:230:LYS:HG2	1:B:231:MET:N	2.11	0.65
1:A:213:ASN:CB	1:A:214:PRO:CD	2.55	0.65
1:A:223:GLU:CB	1:A:225:TRP:CH2	2.79	0.65
1:A:281:ILE:O	1:A:285:VAL:HG22	1.96	0.65
1:A:13:GLN:O	1:A:14:GLN:HB2	1.95	0.65
1:A:203:TRP:CZ3	1:A:226:LYS:HD3	2.30	0.65
1:A:222:SER:O	1:A:224:ASN:N	2.30	0.65
1:A:238:GLU:C	1:A:240:ILE:N	2.50	0.65
1:B:16:THR:O	1:B:17:THR:HG23	1.97	0.65
1:B:227:GLU:HA	1:B:230:LYS:CE	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:N	1:B:242:LEU:HD21	2.12	0.65
1:B:23:LYS:HA	1:B:48:GLU:O	1.97	0.65
1:A:221:ASP:C	1:A:222:SER:OG	2.34	0.65
1:A:44:SER:O	1:A:45:LEU:HD12	1.96	0.65
1:A:245:TYR:CE1	1:B:62:GLU:HG2	2.32	0.65
1:B:102:GLN:C	1:B:110:LEU:CD2	2.57	0.65
1:A:161:ILE:CD1	1:A:293:LEU:HD23	2.26	0.64
1:B:222:SER:O	1:B:224:ASN:N	2.30	0.64
1:B:24:ILE:CD1	1:B:25:THR:CA	2.67	0.64
1:A:121:LYS:HE3	1:A:331:LEU:CD1	2.27	0.64
1:B:215:GLU:HB3	1:B:216:MET:SD	2.36	0.64
1:A:156:PRO:HB2	1:A:157:LYS:HD2	1.80	0.64
1:A:308:LYS:C	1:A:312:VAL:HG22	2.18	0.64
1:B:279:TYR:HE1	1:B:306:LYS:CE	2.03	0.64
1:B:121:LYS:HE3	1:B:331:LEU:CD1	2.27	0.64
1:B:51:LEU:C	1:B:51:LEU:HD12	2.18	0.64
1:A:227:GLU:HA	1:A:230:LYS:CE	2.27	0.64
1:A:283:ASN:O	1:A:285:VAL:CG2	2.43	0.64
1:A:23:LYS:HA	1:A:48:GLU:O	1.97	0.64
1:A:242:LEU:HD21	1:B:58:LYS:N	2.12	0.64
1:A:203:TRP:CD1	1:A:203:TRP:N	2.65	0.64
1:A:229:HIS:HD2	1:A:229:HIS:O	1.81	0.64
1:A:96:VAL:HG21	1:A:120:PHE:CE2	2.32	0.64
1:B:168:ASP:HB3	1:B:191:ILE:CD1	2.27	0.64
1:B:223:GLU:CB	1:B:225:TRP:CZ3	2.81	0.64
3:B:333:CIT:C6	3:B:333:CIT:C4	2.73	0.64
1:B:55:LEU:CD2	1:B:55:LEU:N	2.60	0.64
1:B:97:THR:HG23	2:B:332:LNC:C4D	2.26	0.64
1:B:138:VAL:HG12	2:B:332:LNC:HN72	1.61	0.64
1:B:225:TRP:O	1:B:228:VAL:HB	1.98	0.64
1:B:265:LEU:HD22	1:B:267:ARG:CZ	2.26	0.64
1:A:53:ASP:HB2	1:A:55:LEU:HD23	1.77	0.64
1:A:55:LEU:N	1:A:55:LEU:CD2	2.60	0.64
1:A:62:GLU:HG2	1:B:245:TYR:CE1	2.32	0.64
1:B:238:GLU:O	1:B:240:ILE:CA	2.46	0.64
1:A:306:LYS:HZ3	1:A:315:LEU:HD21	1.63	0.64
1:A:41:LEU:HD11	1:A:49:LEU:HD23	1.78	0.64
1:B:96:VAL:HG21	1:B:120:PHE:CE2	2.32	0.64
1:B:209(D):VAL:CG1	1:B:210(A):LEU:N	2.39	0.64
1:A:23:LYS:HD3	1:A:90:ASN:HB3	1.80	0.64
1:A:250:ILE:HG12	2:A:332:LNC:C7N	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:TRP:CD1	1:B:203:TRP:N	2.65	0.64
1:B:229:HIS:O	1:B:229:HIS:HD2	1.81	0.64
1:B:308:LYS:C	1:B:312:VAL:HG22	2.18	0.64
1:A:269:HIS:N	1:A:291:CYS:O	2.31	0.63
1:A:43:LYS:O	1:A:44:SER:HB2	1.97	0.63
1:A:51:LEU:HD12	1:A:51:LEU:C	2.18	0.63
1:B:43:LYS:O	1:B:44:SER:HB2	1.97	0.63
1:B:133:CYS:O	1:B:159:ARG:CD	2.40	0.63
1:B:277:GLY:C	1:B:278:MET:SD	2.75	0.63
1:A:83:LYS:O	1:A:84:ASP:HB2	1.97	0.63
1:B:144:ILE:CG2	1:B:145:LEU:CD1	2.61	0.63
1:B:291:CYS:CB	1:B:302:VAL:HG23	2.28	0.63
1:A:213:ASN:O	1:A:215:GLU:N	2.31	0.63
1:A:223:GLU:CB	1:A:225:TRP:CZ3	2.81	0.63
1:B:213:ASN:O	1:B:215:GLU:N	2.31	0.63
1:B:303:ILE:N	1:B:303:ILE:CD1	2.62	0.63
1:B:156:PRO:HB2	1:B:157:LYS:HD2	1.80	0.63
1:B:109:ARG:CZ	1:B:195:HIS:HD2	2.12	0.63
1:B:250:ILE:HG12	2:B:332:LNC:C7N	2.28	0.63
1:A:144:ILE:C	1:A:148:VAL:CG1	2.67	0.63
1:A:281:ILE:HG22	1:A:285:VAL:HG22	1.81	0.63
1:A:97:THR:CG2	2:A:332:LNC:H4'	2.29	0.63
1:A:230:LYS:CG	1:A:231:MET:N	2.62	0.63
1:B:109:ARG:HA	1:B:140:ASN:OD1	1.99	0.63
1:A:238:GLU:O	1:A:240:ILE:CA	2.46	0.63
1:A:255:ALA:O	1:A:258:ILE:CG2	2.47	0.63
1:A:292:VAL:HG22	1:A:299:THR:O	1.98	0.63
1:B:306:LYS:HZ3	1:B:315:LEU:HD21	1.62	0.63
1:A:154:GLY:O	1:A:155:LEU:HB2	1.99	0.63
1:A:225:TRP:O	1:A:228:VAL:HB	1.98	0.63
1:A:277:GLY:C	1:A:278:MET:SD	2.75	0.63
1:B:229:HIS:HA	1:B:232:VAL:HG22	1.80	0.63
1:A:291:CYS:CB	1:A:302:VAL:HG23	2.28	0.62
1:A:279:TYR:OH	1:A:315:LEU:HD21	1.99	0.62
1:B:281:ILE:HG22	1:B:285:VAL:HG22	1.81	0.62
1:A:140:ASN:CB	1:A:141:PRO:HD3	2.04	0.62
1:A:281:ILE:CG2	1:A:285:VAL:CG1	2.71	0.62
1:B:154:GLY:O	1:B:155:LEU:HB2	1.99	0.62
1:B:9:ALA:HB3	1:B:10:PRO:HD2	1.75	0.62
1:A:292:VAL:CG2	1:A:299:THR:O	2.47	0.62
1:B:113:VAL:HG11	1:B:144:ILE:HD12	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:HA	1:A:140:ASN:OD1	1.99	0.62
1:B:100:VAL:CG2	1:B:101:ARG:H	2.13	0.62
1:B:156:PRO:O	1:B:158:HIS:N	2.33	0.62
1:B:218:THR:HB	1:B:226:LYS:CD	2.29	0.62
1:B:275:VAL:HG11	1:B:286:PHE:N	2.15	0.62
1:B:52:VAL:C	1:B:53:ASP:OD1	2.37	0.62
1:A:2:THR:HG23	1:A:3:LEU:N	2.13	0.62
1:B:292:VAL:CG2	1:B:299:THR:O	2.47	0.62
1:B:292:VAL:HG22	1:B:299:THR:O	1.98	0.62
1:B:30:GLY:O	1:B:34:MET:N	2.26	0.62
1:B:279:TYR:OH	1:B:315:LEU:HD21	1.99	0.62
1:A:227:GLU:O	1:A:230:LYS:HG2	1.99	0.62
1:B:187:CYS:C	1:B:188:HIS:HD1	2.03	0.62
1:A:213:ASN:ND2	1:B:5:GLU:OE1	2.33	0.62
1:A:187:CYS:C	1:A:188:HIS:HD1	2.03	0.62
1:A:93:ILE:CD1	1:A:261:MET:HE2	2.29	0.62
1:B:247:ASN:CA	1:B:250:ILE:CG2	2.62	0.62
1:B:255:ALA:O	1:B:258:ILE:CG2	2.47	0.62
1:B:83:LYS:O	1:B:84:ASP:HB2	1.97	0.62
1:A:41:LEU:C	1:A:73:LEU:CD2	2.68	0.62
1:A:113:VAL:HG11	1:A:144:ILE:HD12	1.80	0.62
1:B:97:THR:CG2	2:B:332:LNC:H4'	2.29	0.62
1:A:16:THR:O	1:A:17:THR:HG23	1.97	0.62
1:A:52:VAL:C	1:A:53:ASP:OD1	2.37	0.62
1:B:127:ILE:HD13	1:B:128:VAL:N	2.14	0.61
1:B:144:ILE:C	1:B:148:VAL:CG1	2.67	0.61
1:B:20:ASP:O	1:B:22:ASN:CB	2.48	0.61
1:B:27:VAL:HG21	1:B:123:ILE:HD11	1.82	0.61
1:B:269:HIS:N	1:B:291:CYS:O	2.31	0.61
1:B:2:THR:HG23	1:B:3:LEU:N	2.13	0.61
1:B:56:GLU:N	1:B:56:GLU:CD	2.54	0.61
1:A:100:VAL:CG2	1:A:101:ARG:H	2.13	0.61
1:A:127:ILE:HD13	1:A:128:VAL:N	2.14	0.61
1:A:275:VAL:CG2	1:A:281:ILE:HG13	2.30	0.61
1:A:64:MET:HG3	1:A:68:HIS:CE1	2.36	0.61
1:B:134:ILE:HG13	1:B:261:MET:HE1	1.82	0.61
1:A:103:GLN:O	1:A:105:GLU:HB2	1.99	0.61
1:A:168:ASP:HB3	1:A:191:ILE:CD1	2.27	0.61
1:A:196:GLY:O	1:A:197:ASP:HB2	2.01	0.61
1:A:229:HIS:HA	1:A:232:VAL:HG22	1.80	0.61
1:B:221:ASP:C	1:B:222:SER:OG	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:TRP:CZ3	1:B:327:LYS:HD3	2.36	0.61
1:A:109:ARG:CZ	1:A:195:HIS:HD2	2.12	0.61
1:A:5:GLU:OE1	1:B:213:ASN:ND2	2.33	0.61
1:B:203:TRP:CZ2	1:B:311:GLU:OE1	2.54	0.61
1:B:227:GLU:O	1:B:230:LYS:HG2	1.99	0.61
1:B:192:LEU:HD21	1:B:289:LEU:HD13	1.81	0.61
1:A:218:THR:HB	1:A:226:LYS:CD	2.29	0.61
3:A:333:CIT:C6	3:A:333:CIT:C4	2.73	0.61
1:B:51:LEU:C	1:B:52:VAL:HG12	2.21	0.61
1:A:203:TRP:HD1	1:A:203:TRP:H	1.49	0.61
1:A:134:ILE:CG1	1:A:261:MET:HE3	2.31	0.61
1:A:303:ILE:CD1	1:A:303:ILE:N	2.62	0.61
1:B:275:VAL:CG2	1:B:281:ILE:HG13	2.30	0.61
1:B:281:ILE:CG2	1:B:285:VAL:CG1	2.71	0.61
1:B:37:ALA:O	1:B:41:LEU:CD2	2.48	0.61
1:A:275:VAL:HG11	1:A:286:PHE:N	2.15	0.61
1:A:71:LEU:O	1:A:71:LEU:HD12	2.01	0.61
1:A:7:LEU:N	1:A:7:LEU:HD22	2.15	0.61
1:B:27:VAL:CG1	1:B:123:ILE:HD11	2.30	0.61
1:B:230:LYS:CG	1:B:231:MET:N	2.62	0.61
1:B:136:ILE:CD1	1:B:257:LEU:CD2	2.78	0.61
1:A:102:GLN:HA	1:A:110:LEU:HD23	1.82	0.61
1:A:156:PRO:O	1:A:158:HIS:N	2.33	0.61
1:A:20:ASP:O	1:A:22:ASN:CB	2.48	0.61
1:A:41:LEU:C	1:A:73:LEU:HD22	2.21	0.61
1:B:103:GLN:O	1:B:105:GLU:HB2	1.99	0.61
1:A:72:PHE:HE1	1:B:253:SER:HG	1.41	0.61
1:A:117:VAL:O	1:A:121:LYS:HG3	2.01	0.61
1:A:136:ILE:CD1	1:A:257:LEU:CD2	2.78	0.61
1:A:279:TYR:HE2	1:A:281:ILE:CG1	2.14	0.61
1:A:323:TRP:HA	1:A:326:GLN:HB3	1.83	0.61
1:A:51:LEU:C	1:A:52:VAL:HG12	2.21	0.61
1:A:146:THR:O	1:A:150:TRP:HB3	2.01	0.61
1:A:161:ILE:HG23	1:A:271:VAL:HG11	1.83	0.61
1:A:261:MET:HG3	1:A:262:LEU:N	2.09	0.61
1:B:71:LEU:O	1:B:71:LEU:HD12	2.01	0.61
1:B:41:LEU:C	1:B:73:LEU:HD22	2.21	0.61
1:B:7:LEU:N	1:B:7:LEU:HD22	2.15	0.61
1:B:84:ASP:C	1:B:85:TYR:CG	2.74	0.61
1:B:23:LYS:HG2	1:B:90:ASN:O	2.01	0.61
1:B:279:TYR:C	1:B:279:TYR:CD2	2.72	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLU:O	1:B:283:ASN:OD1	2.19	0.60
1:B:23:LYS:HD3	1:B:90:ASN:HB3	1.80	0.60
1:A:147:TYR:O	1:A:151:LYS:HB2	2.00	0.60
1:A:192:LEU:HD21	1:A:289:LEU:HD13	1.81	0.60
1:A:248:TRP:HB2	1:B:65:ASP:OD2	1.99	0.60
1:A:330(B):ASP:O	1:A:330(B):ASP:CG	2.39	0.60
1:A:32:VAL:HG22	2:A:332:LNC:H5'2	1.79	0.60
1:A:37:ALA:O	1:A:41:LEU:CD2	2.48	0.60
1:A:65:ASP:CG	1:B:248:TRP:CA	2.69	0.60
1:A:23:LYS:HG2	1:A:90:ASN:O	2.01	0.60
1:B:85:TYR:OH	1:B:123:ILE:HG13	1.99	0.60
1:A:27:VAL:HG21	1:A:123:ILE:HD11	1.82	0.60
1:A:34:MET:HE2	1:A:66:LEU:HD21	1.75	0.60
1:B:112:LEU:O	1:B:113:VAL:HG12	2.01	0.60
1:B:147:TYR:O	1:B:151:LYS:HB2	2.00	0.60
1:B:261:MET:HG3	1:B:262:LEU:N	2.09	0.60
1:B:279:TYR:HE2	1:B:281:ILE:CG1	2.14	0.60
1:A:144:ILE:CG2	1:A:145:LEU:CD1	2.61	0.60
1:A:67:GLN:O	1:A:70:SER:CB	2.49	0.60
1:B:143:ASP:C	1:B:146:THR:HG22	2.21	0.60
1:B:168:ASP:C	1:B:191:ILE:HD11	2.22	0.60
1:A:13:GLN:O	1:A:14:GLN:CB	2.50	0.60
1:A:24:ILE:CD1	1:A:25:THR:CA	2.67	0.60
1:B:67:GLN:O	1:B:70:SER:CB	2.49	0.60
1:A:54:VAL:CG1	1:A:54:VAL:O	2.49	0.60
1:B:100:VAL:CG2	1:B:101:ARG:N	2.65	0.60
1:B:146:THR:O	1:B:150:TRP:HB3	2.01	0.60
1:B:291:CYS:HB3	1:B:302:VAL:HA	1.84	0.60
1:B:8:ILE:O	1:B:9:ALA:CB	2.50	0.60
1:A:149:ALA:O	1:A:153:SER:HB3	2.02	0.60
1:B:209(B):GLY:C	1:B:209(C):VAL:CG1	2.54	0.60
1:B:265:LEU:HD22	1:B:267:ARG:NH2	2.17	0.60
1:B:67:GLN:O	1:B:70:SER:OG	2.18	0.60
1:A:265:LEU:HD22	1:A:267:ARG:NH2	2.17	0.60
1:A:291:CYS:HB3	1:A:302:VAL:HA	1.84	0.60
1:A:32:VAL:CG1	2:A:332:LNC:H5'2	2.31	0.60
1:A:62:GLU:CG	1:B:245:TYR:CE1	2.84	0.60
1:B:32:VAL:CG1	2:B:332:LNC:H5'2	2.31	0.60
1:B:55:LEU:HB2	1:B:59:LEU:HD12	1.82	0.60
1:A:308:LYS:CA	1:A:312:VAL:HG21	2.32	0.60
1:A:85:TYR:O	1:A:130:TYR:CE2	2.55	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:TYR:CE1	1:B:62:GLU:CG	2.84	0.60
1:A:110:LEU:H	1:A:110:LEU:HD22	1.67	0.59
1:A:112:LEU:O	1:A:113:VAL:HG12	2.01	0.59
1:A:136:ILE:HD13	1:A:257:LEU:HD23	1.84	0.59
1:A:203:TRP:CZ2	1:A:311:GLU:OE1	2.54	0.59
1:A:323:TRP:CZ3	1:A:327:LYS:HD3	2.36	0.59
1:B:117:VAL:O	1:B:121:LYS:HG3	2.01	0.59
1:B:196:GLY:O	1:B:197:ASP:HB2	2.01	0.59
1:B:282:GLU:O	1:B:283:ASN:CG	2.41	0.59
1:B:323:TRP:HA	1:B:326:GLN:HB3	1.83	0.59
1:A:100:VAL:CG2	1:A:101:ARG:N	2.65	0.59
1:A:124:ILE:HG12	1:A:125:PRO:HD2	1.76	0.59
1:B:125:PRO:HA	1:B:128:VAL:CG1	2.32	0.59
1:A:242:LEU:HD21	1:B:57:ASP:C	2.23	0.59
1:A:282:GLU:O	1:A:283:ASN:CG	2.41	0.59
1:A:8:ILE:O	1:A:9:ALA:CB	2.50	0.59
1:A:57:ASP:C	1:B:242:LEU:HD21	2.23	0.59
1:A:65:ASP:OD2	1:B:248:TRP:HB2	1.99	0.59
1:B:64:MET:HG3	1:B:68:HIS:CE1	2.36	0.59
1:A:125:PRO:HA	1:A:128:VAL:CG1	2.32	0.59
1:A:308:LYS:HA	1:A:312:VAL:HG13	1.81	0.59
1:B:54:VAL:O	1:B:54:VAL:CG1	2.49	0.59
1:A:109:ARG:CB	1:A:140:ASN:OD1	2.50	0.59
1:B:85:TYR:O	1:B:130:TYR:CE2	2.55	0.59
1:B:203:TRP:CE3	1:B:218:THR:HG21	2.34	0.59
1:B:41:LEU:C	1:B:73:LEU:CD2	2.68	0.59
1:B:109:ARG:CB	1:B:140:ASN:OD1	2.50	0.59
1:B:24:ILE:CD1	1:B:25:THR:H	2.12	0.59
1:A:168:ASP:C	1:A:191:ILE:HD11	2.22	0.59
1:A:277:GLY:O	1:A:278:MET:CG	2.51	0.59
1:B:149:ALA:O	1:B:153:SER:HB3	2.02	0.59
1:B:238:GLU:O	1:B:240:ILE:CD1	2.47	0.59
1:A:62:GLU:CA	1:B:245:TYR:CD1	2.86	0.59
1:B:23:LYS:HD3	1:B:90:ASN:HB2	1.84	0.59
1:A:248:TRP:CA	1:B:65:ASP:CG	2.69	0.59
1:A:282:GLU:O	1:A:283:ASN:OD1	2.19	0.59
1:A:299:THR:O	1:A:301:SER:CB	2.51	0.59
1:A:85:TYR:OH	1:A:123:ILE:HG13	1.99	0.59
1:B:203:TRP:H	1:B:203:TRP:HD1	1.49	0.59
1:B:299:THR:O	1:B:301:SER:CB	2.51	0.59
1:B:330(B):ASP:CG	1:B:330(B):ASP:O	2.39	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ASN:O	1:A:215:GLU:HG3	2.03	0.59
1:B:232:VAL:HA	1:B:235:SER:HB2	1.85	0.59
1:A:121:LYS:N	1:A:124:ILE:CD1	2.64	0.58
1:A:23:LYS:HD3	1:A:90:ASN:HB2	1.84	0.58
1:B:110:LEU:H	1:B:110:LEU:HD22	1.67	0.58
1:B:161:ILE:HG23	1:B:271:VAL:HG11	1.83	0.58
1:B:283:ASN:ND2	1:B:323:TRP:CZ2	2.72	0.58
1:B:91:SER:OG	1:B:92:LYS:N	2.33	0.58
1:B:213:ASN:O	1:B:215:GLU:HG3	2.03	0.58
1:A:102:GLN:C	1:A:110:LEU:CD2	2.57	0.58
1:A:84:ASP:C	1:A:85:TYR:CG	2.74	0.58
1:B:136:ILE:CD1	1:B:257:LEU:HD23	2.33	0.58
1:A:157:LYS:N	1:A:157:LYS:CD	2.65	0.58
1:A:308:LYS:O	1:A:312:VAL:CG2	2.52	0.58
1:A:56:GLU:CD	1:A:56:GLU:N	2.54	0.58
1:B:13:GLN:O	1:B:14:GLN:CB	2.50	0.58
1:B:308:LYS:CA	1:B:312:VAL:HG21	2.32	0.58
1:A:110:LEU:H	1:A:110:LEU:HD23	1.68	0.58
1:A:218:THR:CB	1:A:226:LYS:HD3	2.34	0.58
1:A:63:MET:O	1:A:67:GLN:N	2.32	0.58
1:A:227:GLU:CG	1:A:231:MET:SD	2.89	0.58
1:A:245:TYR:CD1	1:B:62:GLU:CA	2.86	0.58
1:A:93:ILE:CD1	1:A:261:MET:HE3	2.33	0.58
1:B:124:ILE:HG12	1:B:125:PRO:HD2	1.76	0.58
1:B:32:VAL:HG22	2:B:332:LNC:H5'2	1.79	0.58
1:A:136:ILE:CD1	1:A:257:LEU:HD23	2.33	0.58
1:A:248:TRP:CA	1:B:65:ASP:OD2	2.52	0.58
1:B:277:GLY:O	1:B:278:MET:CG	2.51	0.58
1:B:157:LYS:N	1:B:157:LYS:CD	2.65	0.58
1:A:147:TYR:CA	1:A:150:TRP:CE3	2.77	0.57
1:A:272:SER:HA	1:A:287:LEU:O	2.04	0.57
1:A:51:LEU:O	1:A:52:VAL:HG12	2.04	0.57
1:B:112:LEU:H	1:B:112:LEU:HD23	1.69	0.57
1:B:183:HIS:CD2	1:B:183:HIS:N	2.71	0.57
1:B:40:ILE:HG22	1:B:41:LEU:CD2	2.31	0.57
1:B:89:ALA:O	1:B:90:ASN:C	2.43	0.57
1:A:232:VAL:HA	1:A:235:SER:HB2	1.85	0.57
1:B:213:ASN:C	1:B:215:GLU:N	2.57	0.57
1:B:215:GLU:O	1:B:216:MET:SD	2.62	0.57
1:B:281:ILE:O	1:B:281:ILE:HG22	2.01	0.57
1:A:253:SER:CA	1:B:72:PHE:HE1	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:PRO:O	1:A:11:VAL:CG1	2.46	0.57
1:A:55:LEU:HA	1:A:56:GLU:OE1	2.05	0.57
1:A:91:SER:OG	1:A:92:LYS:N	2.33	0.57
1:B:228:VAL:HG12	1:B:229:HIS:N	2.20	0.57
1:B:308:LYS:HA	1:B:312:VAL:HG13	1.81	0.57
1:B:37:ALA:C	1:B:41:LEU:HD23	2.25	0.57
1:A:228:VAL:HG12	1:A:229:HIS:N	2.20	0.57
1:B:223:GLU:HB2	1:B:225:TRP:CH2	2.40	0.57
1:B:218:THR:CB	1:B:226:LYS:HD3	2.34	0.57
1:B:272:SER:HA	1:B:287:LEU:O	2.04	0.57
1:B:51:LEU:O	1:B:52:VAL:HG12	2.04	0.57
1:A:283:ASN:ND2	1:A:323:TRP:CZ2	2.72	0.57
1:A:30:GLY:O	1:A:34:MET:N	2.26	0.57
1:B:288:SER:C	1:B:289:LEU:CD2	2.73	0.57
1:A:121:LYS:O	1:A:125:PRO:HD3	2.01	0.57
1:B:110:LEU:H	1:B:110:LEU:HD23	1.68	0.57
1:B:245:TYR:CB	1:B:248:TRP:HD1	2.18	0.57
1:B:308:LYS:O	1:B:312:VAL:CG2	2.52	0.57
1:A:134:ILE:HD13	1:A:134:ILE:N	2.19	0.57
1:B:134:ILE:HD13	1:B:134:ILE:N	2.19	0.57
1:A:215:GLU:O	1:A:216:MET:SD	2.62	0.57
1:A:275:VAL:HG11	1:A:285:VAL:CB	2.30	0.57
1:A:288:SER:C	1:A:289:LEU:CD2	2.73	0.57
1:A:37:ALA:C	1:A:41:LEU:HD23	2.25	0.57
1:A:112:LEU:H	1:A:112:LEU:HD23	1.69	0.57
1:A:110:LEU:N	1:A:140:ASN:OD1	2.37	0.57
1:A:183:HIS:CD2	1:A:183:HIS:N	2.71	0.57
1:A:288:SER:O	1:A:289:LEU:CD2	2.53	0.57
1:A:268:ILE:HG12	1:A:292:VAL:HG12	1.87	0.57
1:B:147:TYR:CA	1:B:150:TRP:CE3	2.77	0.57
1:A:248:TRP:CE2	1:B:34:MET:HG3	2.40	0.56
1:A:304:ASN:O	1:A:305:GLN:HB2	2.05	0.56
1:A:308:LYS:HA	1:A:312:VAL:CG2	2.35	0.56
1:A:67:GLN:O	1:A:70:SER:OG	2.18	0.56
1:A:62:GLU:N	1:B:245:TYR:HD1	2.03	0.56
1:B:304:ASN:O	1:B:305:GLN:HB2	2.05	0.56
1:A:210(B):GLN:O	1:A:210(B):GLN:HG3	2.06	0.56
1:A:223:GLU:O	1:A:224:ASN:CB	2.52	0.56
1:B:210(B):GLN:HG3	1:B:210(B):GLN:O	2.06	0.56
1:B:308:LYS:HA	1:B:312:VAL:CG2	2.35	0.56
1:B:55:LEU:HA	1:B:56:GLU:OE1	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:O	1:A:7:LEU:CB	2.53	0.56
1:B:265:LEU:O	1:B:266:SER:C	2.44	0.56
1:B:110:LEU:N	1:B:140:ASN:OD1	2.37	0.56
1:A:96:VAL:HG22	1:A:120:PHE:CZ	2.41	0.56
1:B:134:ILE:CG1	1:B:261:MET:HE1	2.34	0.56
1:B:32:VAL:O	1:B:36:CYS:SG	2.64	0.56
1:B:96:VAL:HG22	1:B:120:PHE:CZ	2.41	0.56
1:A:245:TYR:CB	1:A:248:TRP:HD1	2.18	0.56
1:A:35:ALA:HB3	1:A:247:ASN:OD1	2.05	0.56
1:A:55:LEU:HB2	1:A:59:LEU:HD12	1.82	0.56
1:B:282:GLU:O	1:B:282:GLU:CG	2.33	0.56
1:A:65:ASP:HB2	1:B:245:TYR:C	2.23	0.56
1:A:69:GLY:O	1:A:71:LEU:N	2.39	0.56
1:A:99:GLY:C	1:A:100:VAL:HG13	2.26	0.56
1:B:101:ARG:HH12	2:B:332:LNC:PN	2.28	0.56
1:A:65:ASP:OD2	1:B:248:TRP:CA	2.52	0.56
1:B:288:SER:O	1:B:289:LEU:CD2	2.53	0.56
1:A:40:ILE:HG22	1:A:41:LEU:CD2	2.31	0.56
1:A:72:PHE:HE1	1:B:253:SER:CA	2.17	0.56
1:A:87:VAL:O	1:A:89:ALA:N	2.39	0.56
1:B:268:ILE:HG12	1:B:292:VAL:HG12	1.87	0.56
1:B:87:VAL:O	1:B:89:ALA:N	2.39	0.56
1:A:27:VAL:CG1	1:A:123:ILE:HD11	2.30	0.56
1:A:49:LEU:CD1	1:A:50:ALA:N	2.57	0.56
1:B:241:LYS:N	1:B:241:LYS:HE3	2.20	0.56
1:A:241:LYS:HE3	1:A:241:LYS:N	2.20	0.56
1:A:304:ASN:C	1:A:305:GLN:OE1	2.44	0.56
1:A:101:ARG:HH12	2:A:332:LNC:PN	2.28	0.56
1:A:246:THR:HG23	2:A:332:LNC:CGS	2.25	0.56
1:A:89:ALA:O	1:A:90:ASN:C	2.43	0.56
1:B:175:LEU:CG	1:B:176:MET:H	2.06	0.56
1:B:227:GLU:CG	1:B:231:MET:SD	2.89	0.56
1:A:143:ASP:C	1:A:146:THR:HG22	2.21	0.55
1:A:245:TYR:HD1	1:B:62:GLU:N	2.03	0.55
1:A:282:GLU:HG2	1:A:283:ASN:OD1	2.06	0.55
1:A:89:ALA:O	1:A:91:SER:N	2.39	0.55
1:B:121:LYS:CA	1:B:124:ILE:CD1	2.70	0.55
1:B:263:LYS:O	1:B:264:ASN:CB	2.53	0.55
1:B:29:VAL:O	1:B:34:MET:SD	2.64	0.55
1:A:191:ILE:HG22	1:A:201:ALA:HA	1.88	0.55
1:A:29:VAL:O	1:A:34:MET:SD	2.64	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:O	1:A:7:LEU:HD23	2.06	0.55
1:B:136:ILE:HD13	1:B:257:LEU:HD23	1.84	0.55
1:A:34:MET:HG3	1:B:248:TRP:CE2	2.40	0.55
1:B:69:GLY:O	1:B:71:LEU:N	2.39	0.55
1:A:27:VAL:HB	1:A:96:VAL:HA	1.88	0.55
1:B:191:ILE:HG22	1:B:201:ALA:HA	1.88	0.55
1:B:102:GLN:HE22	2:B:332:LNC:H6	1.72	0.55
1:B:46:THR:OG1	1:B:75:THR:HG22	2.06	0.55
1:B:89:ALA:O	1:B:91:SER:N	2.39	0.55
1:A:203:TRP:CE3	1:A:218:THR:HG21	2.34	0.55
1:A:234:GLU:HA	1:A:237:TYR:HB2	1.88	0.55
1:B:304:ASN:C	1:B:305:GLN:OE1	2.44	0.55
1:B:35:ALA:HB3	1:B:247:ASN:OD1	2.05	0.55
1:A:245:TYR:CD1	1:B:62:GLU:N	2.75	0.55
1:B:27:VAL:HB	1:B:96:VAL:HA	1.88	0.55
1:B:55:LEU:C	1:B:59:LEU:CD1	2.70	0.55
1:B:41:LEU:O	1:B:73:LEU:HD11	2.07	0.55
1:A:140:ASN:HB2	1:A:141:PRO:CD	2.04	0.55
1:A:247:ASN:O	1:A:248:TRP:C	2.44	0.55
1:A:62:GLU:N	1:B:245:TYR:CD1	2.75	0.55
1:B:6:LYS:O	1:B:7:LEU:CB	2.53	0.55
1:B:99:GLY:C	1:B:100:VAL:HG13	2.26	0.55
1:A:223:GLU:HB2	1:A:225:TRP:CH2	2.40	0.55
1:A:229:HIS:CA	1:A:232:VAL:CG2	2.84	0.55
1:A:245:TYR:CA	1:A:248:TRP:HD1	2.17	0.55
1:A:302:VAL:C	1:A:303:ILE:HD13	2.27	0.55
1:B:102:GLN:HA	1:B:110:LEU:HD23	1.82	0.55
1:B:234:GLU:HA	1:B:237:TYR:HB2	1.88	0.55
1:A:102:GLN:HE22	2:A:332:LNC:H6	1.72	0.55
1:A:32:VAL:O	1:A:36:CYS:SG	2.64	0.55
1:B:282:GLU:HG2	1:B:283:ASN:OD1	2.06	0.55
1:A:93:ILE:O	1:A:93:ILE:HG22	2.03	0.54
1:B:229:HIS:CA	1:B:232:VAL:CG2	2.84	0.54
1:A:58:LYS:HG3	1:B:242:LEU:CD1	2.38	0.54
1:B:292:VAL:O	1:B:292:VAL:HG23	2.07	0.54
1:A:149:ALA:O	1:A:153:SER:HB2	2.05	0.54
1:A:265:LEU:O	1:A:266:SER:C	2.44	0.54
1:A:282:GLU:O	1:A:282:GLU:CG	2.33	0.54
1:B:93:ILE:O	1:B:93:ILE:HG22	2.03	0.54
1:A:281:ILE:HG22	1:A:281:ILE:O	2.01	0.54
1:A:97:THR:HG22	1:A:98:ALA:N	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:TYR:CD2	1:A:148:VAL:N	2.58	0.54
1:A:313:ALA:HA	1:A:316:LYS:HD3	1.90	0.54
1:A:323:TRP:O	1:A:324:GLY:C	2.45	0.54
1:A:46:THR:OG1	1:A:75:THR:HG22	2.06	0.54
1:B:112:LEU:C	1:B:113:VAL:HG13	2.28	0.54
1:B:192:LEU:HD23	1:B:315:LEU:HD12	1.85	0.54
1:A:116:ASN:O	1:A:117:VAL:C	2.46	0.54
1:A:250:ILE:HG22	1:A:251:GLY:H	1.71	0.54
1:B:100:VAL:HG22	1:B:101:ARG:H	1.72	0.54
1:B:270:PRO:O	1:B:271:VAL:HB	2.08	0.54
1:B:93:ILE:HD11	1:B:261:MET:HE2	1.89	0.54
1:A:83:LYS:O	1:A:84:ASP:CB	2.56	0.54
1:A:242:LEU:CD1	1:B:58:LYS:HG3	2.38	0.54
1:A:112:LEU:C	1:A:113:VAL:HG13	2.28	0.54
1:A:258:ILE:CG2	1:A:259:GLU:H	2.19	0.54
1:A:263:LYS:O	1:A:264:ASN:CB	2.53	0.54
1:A:270:PRO:O	1:A:271:VAL:HB	2.08	0.54
1:B:258:ILE:CG2	1:B:259:GLU:H	2.19	0.54
1:B:6:LYS:O	1:B:7:LEU:HD23	2.06	0.54
1:B:223:GLU:OE1	1:B:225:TRP:HH2	1.91	0.54
1:B:323:TRP:O	1:B:324:GLY:C	2.45	0.54
1:B:68:HIS:O	1:B:69:GLY:C	2.45	0.54
1:A:253:SER:OG	1:B:72:PHE:CE1	2.59	0.54
1:A:150:TRP:NE1	1:A:156:PRO:HB3	2.23	0.54
1:B:222:SER:C	1:B:224:ASN:N	2.61	0.54
1:B:83:LYS:O	1:B:84:ASP:CB	2.56	0.54
1:A:292:VAL:O	1:A:292:VAL:HG23	2.07	0.54
1:A:69:GLY:HA3	1:B:252:LEU:HD22	1.90	0.54
1:A:85:TYR:HD2	1:A:126:GLN:HG2	1.73	0.54
1:B:247:ASN:O	1:B:248:TRP:C	2.44	0.54
1:A:55:LEU:CB	1:A:59:LEU:CD1	2.80	0.53
1:B:149:ALA:O	1:B:153:SER:HB2	2.05	0.53
1:B:171:ARG:HH11	1:B:171:ARG:HG3	1.73	0.53
1:B:275:VAL:HG11	1:B:285:VAL:CB	2.30	0.53
1:A:43:LYS:O	1:A:44:SER:CB	2.56	0.53
1:A:223:GLU:OE1	1:A:225:TRP:HH2	1.91	0.53
1:A:68:HIS:O	1:A:69:GLY:C	2.45	0.53
1:B:110:LEU:N	1:B:110:LEU:CD2	2.67	0.53
1:B:2:THR:CG2	1:B:3:LEU:H	2.18	0.53
1:A:197:ASP:O	1:A:198:SER:CB	2.57	0.53
1:B:302:VAL:C	1:B:303:ILE:HD13	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASN:O	1:B:305:GLN:CB	2.57	0.53
1:B:308:LYS:CA	1:B:312:VAL:CG2	2.87	0.53
1:B:328:ASP:CG	1:B:329:LEU:N	2.61	0.53
1:B:55:LEU:CB	1:B:59:LEU:CD1	2.80	0.53
1:A:252:LEU:HD22	1:B:69:GLY:HA3	1.90	0.53
1:B:97:THR:HG22	1:B:98:ALA:N	2.23	0.53
1:B:9:ALA:O	1:B:10:PRO:O	2.27	0.53
1:B:116:ASN:O	1:B:117:VAL:C	2.46	0.53
1:B:121:LYS:N	1:B:124:ILE:CD1	2.64	0.53
1:B:123:ILE:HG22	1:B:124:ILE:H	1.71	0.53
1:A:171:ARG:HH11	1:A:171:ARG:HG3	1.73	0.53
1:A:174:TYR:CZ	1:B:67:GLN:OE1	2.62	0.53
1:A:258:ILE:HG23	1:A:259:GLU:H	1.69	0.53
1:A:308:LYS:CA	1:A:312:VAL:CG2	2.87	0.53
1:A:57:ASP:O	1:A:58:LYS:C	2.47	0.53
1:A:242:LEU:CD2	1:B:58:LYS:HA	2.38	0.53
1:B:64:MET:O	1:B:68:HIS:ND1	2.42	0.53
1:B:74:GLN:C	1:B:75:THR:HG23	2.29	0.53
1:A:100:VAL:HG22	1:A:101:ARG:H	1.72	0.53
1:A:155:LEU:O	1:A:156:PRO:O	2.27	0.53
1:A:238:GLU:O	1:A:240:ILE:CD1	2.47	0.53
1:A:265:LEU:CG	1:A:267:ARG:HH21	2.21	0.53
1:A:57:ASP:N	1:A:57:ASP:OD2	2.42	0.53
1:A:9:ALA:O	1:A:10:PRO:O	2.27	0.53
1:B:155:LEU:O	1:B:156:PRO:O	2.27	0.53
1:B:203:TRP:HZ3	1:B:226:LYS:HD3	1.71	0.53
1:B:208:VAL:O	1:B:209(A):ALA:C	2.47	0.53
1:A:58:LYS:HA	1:B:242:LEU:CD2	2.38	0.53
1:A:213:ASN:C	1:A:215:GLU:N	2.57	0.53
1:B:121:LYS:O	1:B:125:PRO:HD3	2.01	0.53
1:B:275:VAL:CG2	1:B:281:ILE:CB	2.86	0.53
1:B:43:LYS:O	1:B:44:SER:CB	2.56	0.53
1:A:67:GLN:OE1	1:B:174:TYR:CZ	2.62	0.53
1:B:309:ASP:O	1:B:310:ASP:HB3	2.09	0.53
1:B:313:ALA:HA	1:B:316:LYS:HD3	1.90	0.53
1:B:85:TYR:HD2	1:B:126:GLN:HG2	1.73	0.53
1:A:275:VAL:CG2	1:A:281:ILE:CB	2.86	0.53
1:A:304:ASN:O	1:A:305:GLN:CB	2.57	0.53
1:B:10:PRO:O	1:B:11:VAL:CG1	2.46	0.53
1:B:24:ILE:C	1:B:24:ILE:CD1	2.74	0.53
1:B:299:THR:O	1:B:301:SER:HB3	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASP:O	1:B:58:LYS:C	2.47	0.53
1:A:163:SER:CA	1:A:271:VAL:CG1	2.83	0.52
1:A:64:MET:O	1:A:68:HIS:ND1	2.42	0.52
1:B:188:HIS:CD2	3:B:333:CIT:H41	2.40	0.52
1:B:3:LEU:CD2	1:B:4:LYS:HG3	2.38	0.52
1:A:123:ILE:HG22	1:A:124:ILE:H	1.71	0.52
1:B:150:TRP:NE1	1:B:156:PRO:HB3	2.23	0.52
1:A:169:SER:CA	1:A:191:ILE:HD11	2.39	0.52
1:A:328:ASP:CG	1:A:329:LEU:N	2.61	0.52
1:A:2:THR:O	1:A:4:LYS:N	2.42	0.52
1:B:203:TRP:CH2	1:B:226:LYS:HD3	2.44	0.52
1:A:188:HIS:CD2	3:A:333:CIT:H41	2.40	0.52
1:A:299:THR:O	1:A:301:SER:HB3	2.09	0.52
1:A:74:GLN:C	1:A:75:THR:HG23	2.29	0.52
1:B:246:THR:HG23	2:B:332:LNC:CGS	2.25	0.52
1:B:245:TYR:CA	1:B:248:TRP:HD1	2.17	0.52
1:A:134:ILE:HG22	1:A:159:ARG:HA	1.92	0.52
1:A:203:TRP:HZ3	1:A:226:LYS:HD3	1.71	0.52
1:A:220:ASN:O	1:A:221:ASP:HB2	2.10	0.52
1:A:222:SER:C	1:A:224:ASN:N	2.61	0.52
1:A:93:ILE:CD1	1:A:261:MET:HG2	2.23	0.52
1:B:134:ILE:HG22	1:B:159:ARG:HA	1.92	0.52
1:A:15:GLU:O	1:A:16:THR:HB	2.09	0.52
2:A:332:LNC:HAS	2:A:332:LNC:H4	0.59	0.52
1:B:3:LEU:O	1:B:4:LYS:HG2	2.10	0.52
1:A:307:LEU:C	1:A:308:LYS:HG2	2.31	0.52
1:B:2:THR:O	1:B:4:LYS:N	2.42	0.52
1:A:174:TYR:CG	1:A:175:LEU:N	2.78	0.52
1:A:294:ASN:O	1:A:296:ARG:N	2.43	0.52
1:A:264:ASN:OD1	1:A:295:ALA:HA	2.10	0.52
1:A:328:ASP:OD2	1:A:329:LEU:N	2.43	0.52
1:A:2:THR:CG2	1:A:3:LEU:H	2.18	0.52
1:A:3:LEU:O	1:A:4:LYS:HG2	2.10	0.52
1:B:101:ARG:HG2	1:B:102:GLN:HB2	1.92	0.52
1:B:101:ARG:HG3	1:B:102:GLN:NE2	2.25	0.52
1:B:150:TRP:HE1	1:B:156:PRO:HB3	1.75	0.52
1:B:150:TRP:HA	1:B:160:VAL:CG2	2.40	0.52
1:B:163:SER:CA	1:B:271:VAL:CG1	2.83	0.52
1:B:307:LEU:C	1:B:308:LYS:HG2	2.31	0.52
1:A:245:TYR:CG	1:B:62:GLU:OE1	2.35	0.51
1:A:32:VAL:HG22	2:A:332:LNC:O2N	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HG12	2:A:332:LNC:C3N	2.40	0.51
1:B:250:ILE:HG12	2:B:332:LNC:C3N	2.40	0.51
1:A:150:TRP:HE1	1:A:156:PRO:HB3	1.75	0.51
1:B:112:LEU:C	1:B:113:VAL:CG1	2.79	0.51
1:B:15:GLU:O	1:B:16:THR:HB	2.09	0.51
1:B:169:SER:CA	1:B:191:ILE:HD11	2.39	0.51
1:B:203:TRP:CZ2	1:B:226:LYS:HE2	2.37	0.51
1:B:264:ASN:OD1	1:B:295:ALA:HA	2.10	0.51
1:B:51:LEU:C	1:B:52:VAL:CG1	2.79	0.51
1:B:63:MET:O	1:B:67:GLN:N	2.32	0.51
1:A:110:LEU:O	1:A:111:ASN:C	2.49	0.51
1:A:150:TRP:HA	1:A:160:VAL:CG2	2.40	0.51
1:B:209(B):GLY:O	1:B:209(C):VAL:HB	2.08	0.51
1:B:294:ASN:O	1:B:296:ARG:N	2.43	0.51
1:B:328:ASP:OD2	1:B:329:LEU:N	2.43	0.51
1:A:208:VAL:O	1:A:209(A):ALA:C	2.47	0.51
1:B:245:TYR:CD2	1:B:248:TRP:CD1	2.98	0.51
1:A:101:ARG:HG2	1:A:102:GLN:HB2	1.92	0.51
1:A:101:ARG:HG3	1:A:102:GLN:NE2	2.25	0.51
1:A:275:VAL:CG2	1:A:281:ILE:CG1	2.89	0.51
1:A:330(A):LYS:HD2	1:A:330(B):ASP:N	2.23	0.51
1:A:51:LEU:C	1:A:52:VAL:CG1	2.79	0.51
1:B:220:ASN:O	1:B:221:ASP:HB2	2.10	0.51
1:A:203:TRP:CH2	1:A:226:LYS:HD3	2.44	0.51
1:A:267:ARG:O	1:A:268:ILE:HG12	2.10	0.51
1:A:309:ASP:O	1:A:310:ASP:HB3	2.09	0.51
1:B:100:VAL:HG23	1:B:101:ARG:N	2.26	0.51
1:A:209(D):VAL:C	1:A:210(A):LEU:HG	2.30	0.51
1:A:234:GLU:O	1:A:237:TYR:HB2	2.11	0.51
1:B:41:LEU:O	1:B:73:LEU:CG	2.57	0.51
1:A:114:GLN:O	1:A:117:VAL:CG2	2.51	0.51
1:A:245:TYR:CD2	1:A:248:TRP:CD1	2.98	0.51
1:A:313:ALA:O	1:A:314:GLN:C	2.49	0.51
1:A:41:LEU:O	1:A:73:LEU:CG	2.57	0.51
1:B:57:ASP:OD2	1:B:57:ASP:N	2.42	0.51
1:A:24:ILE:CD1	1:A:25:THR:H	2.12	0.51
1:B:224:ASN:HB3	1:B:227:GLU:CB	2.31	0.51
1:B:275:VAL:CG2	1:B:281:ILE:CG1	2.89	0.51
1:B:313:ALA:O	1:B:314:GLN:C	2.49	0.51
1:A:203:TRP:HA	1:A:206:VAL:HG21	1.92	0.51
1:A:209(B):GLY:C	1:A:209(C):VAL:CG1	2.54	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:CG1	1:A:286:PHE:H	2.24	0.51
1:B:166:ASN:N	1:B:270:PRO:HG2	2.26	0.51
1:B:197:ASP:O	1:B:198:SER:CB	2.57	0.51
1:B:49:LEU:HG	1:B:78:ILE:HB	1.93	0.51
1:A:112:LEU:C	1:A:113:VAL:CG1	2.79	0.50
1:A:166:ASN:N	1:A:270:PRO:HG2	2.26	0.50
1:B:110:LEU:O	1:B:111:ASN:C	2.49	0.50
1:B:190:TRP:HZ3	1:B:270:PRO:HD3	1.75	0.50
1:B:192:LEU:CD2	1:B:315:LEU:HD11	2.37	0.50
1:A:287:LEU:HD13	1:A:319:ALA:HB2	1.93	0.50
1:B:191:ILE:HA	1:B:201:ALA:HA	1.92	0.50
1:B:218:THR:HG23	1:B:225:TRP:HB2	1.92	0.50
1:B:265:LEU:CG	1:B:267:ARG:HH21	2.21	0.50
1:B:267:ARG:O	1:B:268:ILE:HG12	2.10	0.50
1:A:187:CYS:O	1:A:188:HIS:CG	2.64	0.50
1:A:249:ALA:HB2	1:B:65:ASP:HA	1.93	0.50
1:A:260:SER:HA	1:A:267:ARG:NH2	2.26	0.50
1:A:272:SER:HB3	1:A:287:LEU:O	2.11	0.50
1:B:89:ALA:HB2	1:B:130:TYR:HB3	1.93	0.50
1:B:128:VAL:O	1:B:132(A):PRO:N	2.44	0.50
1:B:32:VAL:HG22	2:B:332:LNC:O2N	2.10	0.50
1:A:128:VAL:O	1:A:132(A):PRO:N	2.44	0.50
1:A:190:TRP:HZ3	1:A:270:PRO:HD3	1.75	0.50
1:A:272:SER:CA	1:A:288:SER:HA	2.41	0.50
1:A:92:LYS:O	1:A:134:ILE:HD13	2.12	0.50
1:B:259:GLU:CD	1:B:259:GLU:C	2.70	0.50
1:A:100:VAL:HG23	1:A:101:ARG:N	2.26	0.50
1:A:209(B):GLY:O	1:A:209(C):VAL:HB	2.08	0.50
1:A:163:SER:HA	1:A:271:VAL:HG22	1.94	0.50
1:A:89:ALA:HB2	1:A:130:TYR:HB3	1.93	0.50
1:B:187:CYS:O	1:B:188:HIS:CG	2.64	0.50
1:B:209(D):VAL:C	1:B:210(A):LEU:HG	2.30	0.50
1:B:234:GLU:O	1:B:237:TYR:HB2	2.11	0.50
1:B:282:GLU:C	1:B:283:ASN:OD1	2.50	0.50
1:B:275:VAL:CG1	1:B:286:PHE:H	2.24	0.50
1:A:55:LEU:O	1:A:59:LEU:HD22	2.12	0.50
1:B:162:GLY:O	1:B:163:SER:HB3	2.11	0.50
1:B:203:TRP:HA	1:B:206:VAL:HG21	1.92	0.50
1:B:49:LEU:CD1	1:B:50:ALA:N	2.57	0.50
1:A:134:ILE:HG12	1:A:261:MET:HE3	1.92	0.50
1:A:261:MET:CG	1:A:262:LEU:N	2.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HG	1:A:78:ILE:HB	1.93	0.50
1:B:288:SER:C	1:B:289:LEU:HD22	2.32	0.50
1:A:162:GLY:O	1:A:163:SER:HB2	2.10	0.50
1:A:218:THR:C	1:A:226:LYS:HG2	2.33	0.50
1:A:282:GLU:C	1:A:283:ASN:OD1	2.50	0.50
1:A:296:ARG:CG	1:A:296:ARG:NH1	2.41	0.50
1:A:41:LEU:O	1:A:73:LEU:HD11	2.07	0.50
1:B:272:SER:HB3	1:B:287:LEU:O	2.11	0.50
2:B:332:LNC:HAS	2:B:332:LNC:H4	0.59	0.50
1:B:92:LYS:O	1:B:134:ILE:HD13	2.12	0.50
1:A:288:SER:C	1:A:289:LEU:HD22	2.32	0.50
1:B:163:SER:HA	1:B:271:VAL:HG22	1.94	0.50
1:B:174:TYR:CG	1:B:175:LEU:N	2.78	0.50
1:B:218:THR:C	1:B:226:LYS:HG2	2.33	0.50
1:B:240:ILE:CG2	1:B:240:ILE:O	2.55	0.50
1:B:298:LEU:H	1:B:298:LEU:HD23	1.77	0.50
1:B:121:LYS:CE	1:B:331:LEU:HD12	2.39	0.50
1:A:85:TYR:CE1	1:A:123:ILE:HG12	2.47	0.49
1:A:191:ILE:HA	1:A:201:ALA:HA	1.92	0.49
1:A:275:VAL:HG22	1:A:275:VAL:O	2.12	0.49
1:B:110:LEU:HD22	1:B:110:LEU:N	2.27	0.49
1:B:162:GLY:O	1:B:163:SER:HB2	2.10	0.49
1:B:260:SER:HA	1:B:267:ARG:NH2	2.26	0.49
1:B:287:LEU:HD13	1:B:319:ALA:HB2	1.93	0.49
1:B:74:GLN:O	1:B:75:THR:CG2	2.61	0.49
1:A:272:SER:CA	1:A:287:LEU:O	2.61	0.49
1:A:298:LEU:HD23	1:A:298:LEU:H	1.77	0.49
1:A:41:LEU:HB3	1:A:73:LEU:CD2	2.42	0.49
1:B:85:TYR:CE1	1:B:123:ILE:HG12	2.47	0.49
1:A:41:LEU:C	1:A:73:LEU:HD21	2.31	0.49
1:B:275:VAL:HG22	1:B:275:VAL:O	2.12	0.49
1:B:34:MET:HE1	1:B:66:LEU:CD2	2.38	0.49
1:A:162:GLY:O	1:A:163:SER:HB3	2.11	0.49
1:A:65:ASP:HA	1:B:249:ALA:HB2	1.93	0.49
1:B:272:SER:CA	1:B:288:SER:HA	2.41	0.49
1:B:55:LEU:O	1:B:59:LEU:HD22	2.12	0.49
1:A:245:TYR:C	1:B:65:ASP:HB2	2.23	0.49
1:B:41:LEU:HB3	1:B:73:LEU:CD2	2.42	0.49
1:A:240:ILE:CG2	1:A:240:ILE:O	2.55	0.49
1:B:244:GLY:C	1:B:247:ASN:HB3	2.33	0.49
1:B:250:ILE:HG22	1:B:251:GLY:H	1.71	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:GLU:CD	1:A:259:GLU:C	2.70	0.49
1:A:3:LEU:CD2	1:A:4:LYS:HG3	2.38	0.49
1:A:62:GLU:OE1	1:B:245:TYR:CG	2.35	0.49
1:B:272:SER:CA	1:B:287:LEU:O	2.61	0.49
1:B:281:ILE:CB	1:B:285:VAL:HG13	2.41	0.49
1:B:299:THR:O	1:B:299:THR:HG23	2.12	0.49
1:A:163:SER:CA	1:A:271:VAL:HG22	2.43	0.49
1:A:121:LYS:CE	1:A:331:LEU:HD12	2.39	0.49
1:A:269:HIS:O	1:A:270:PRO:O	2.31	0.49
1:A:306:LYS:C	1:A:307:LEU:O	2.48	0.49
1:B:101:ARG:CD	1:B:102:GLN:HB2	2.43	0.49
1:B:73:LEU:HD21	1:B:75:THR:HG21	1.94	0.49
1:A:245:TYR:CA	1:A:248:TRP:CD1	2.82	0.49
1:A:311:GLU:HA	1:A:314:GLN:HB2	1.95	0.49
1:B:269:HIS:O	1:B:270:PRO:O	2.31	0.49
1:A:216:MET:N	1:A:216:MET:SD	2.86	0.48
1:A:96:VAL:HG21	1:A:120:PHE:CD2	2.48	0.48
1:B:311:GLU:HA	1:B:314:GLN:HB2	1.95	0.48
1:A:74:GLN:O	1:A:75:THR:CG2	2.61	0.48
1:B:161:ILE:HG23	1:B:271:VAL:CG1	2.43	0.48
1:B:245:TYR:CA	1:B:248:TRP:CD1	2.82	0.48
1:A:121:LYS:CA	1:A:124:ILE:CD1	2.70	0.48
1:A:218:THR:HG23	1:A:225:TRP:HB2	1.92	0.48
1:A:253:SER:OG	1:B:72:PHE:HE1	1.95	0.48
1:A:73:LEU:HD21	1:A:75:THR:HG21	1.94	0.48
1:A:243:LYS:C	1:A:245:TYR:H	2.16	0.48
1:A:244:GLY:C	1:A:247:ASN:HB3	2.33	0.48
1:A:24:ILE:C	1:A:24:ILE:CD1	2.74	0.48
1:A:257:LEU:O	1:A:260:SER:HB3	2.14	0.48
1:A:299:THR:O	1:A:299:THR:HG23	2.12	0.48
1:A:69:GLY:O	1:A:70:SER:C	2.52	0.48
1:B:114:GLN:O	1:B:117:VAL:CG2	2.51	0.48
1:B:62:GLU:O	1:B:66:LEU:HD22	2.14	0.48
1:A:283:ASN:O	1:A:284:GLU:C	2.51	0.48
1:A:161:ILE:CD1	1:A:293:LEU:CD2	2.83	0.48
1:A:53:ASP:O	1:A:83:LYS:HG3	2.14	0.48
1:A:72:PHE:HE1	1:B:253:SER:OG	1.95	0.48
1:B:240:ILE:HG22	1:B:241:LYS:CE	2.43	0.48
1:B:56:GLU:O	1:B:59:LEU:HB2	2.14	0.48
1:B:67:GLN:O	1:B:70:SER:HB2	2.13	0.48
1:A:161:ILE:HG23	1:A:271:VAL:CG1	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:ASP:O	1:A:309:ASP:CG	2.50	0.48
1:A:85:TYR:CD2	1:A:126:GLN:HB3	2.49	0.48
1:B:121:LYS:HA	1:B:124:ILE:CG1	2.43	0.48
1:B:243:LYS:C	1:B:245:TYR:H	2.16	0.48
1:B:283:ASN:O	1:B:284:GLU:C	2.51	0.48
1:A:229:HIS:HA	1:A:232:VAL:HG21	1.94	0.48
1:A:67:GLN:O	1:A:70:SER:HB2	2.13	0.48
1:B:34:MET:O	1:B:38:ILE:HG12	2.13	0.48
1:B:85:TYR:CD2	1:B:126:GLN:HB3	2.49	0.48
1:B:96:VAL:HG21	1:B:120:PHE:CD2	2.48	0.48
1:A:166:ASN:N	1:A:270:PRO:CG	2.77	0.48
1:A:101:ARG:HB2	2:A:332:LNC:C2D	2.44	0.48
1:A:86:SER:HA	1:A:130:TYR:CZ	2.49	0.48
1:B:216:MET:N	1:B:216:MET:SD	2.86	0.48
1:A:110:LEU:N	1:A:110:LEU:CD2	2.67	0.48
1:A:144:ILE:HG23	1:A:145:LEU:N	2.16	0.48
1:A:223:GLU:OE1	1:A:225:TRP:CH2	2.65	0.48
1:A:23:LYS:CG	1:A:24:ILE:N	2.76	0.48
1:A:306:LYS:HG3	1:A:312:VAL:CG1	2.44	0.48
1:B:23:LYS:CG	1:B:24:ILE:N	2.76	0.48
1:B:93:ILE:CD1	1:B:261:MET:HG2	2.23	0.48
1:B:309:ASP:O	1:B:309:ASP:CG	2.50	0.48
1:A:228:VAL:HG12	1:A:229:HIS:H	1.79	0.48
1:B:166:ASN:N	1:B:270:PRO:CG	2.77	0.48
1:B:163:SER:CA	1:B:271:VAL:HG22	2.43	0.48
1:B:292:VAL:O	1:B:292:VAL:CG2	2.62	0.48
1:B:306:LYS:HG3	1:B:312:VAL:CG1	2.44	0.48
1:A:121:LYS:HA	1:A:124:ILE:CG1	2.43	0.47
1:A:125:PRO:O	1:A:129:LYS:CG	2.61	0.47
1:A:240:ILE:HG22	1:A:241:LYS:CE	2.43	0.47
1:A:41:LEU:O	1:A:73:LEU:HD13	2.14	0.47
1:B:125:PRO:O	1:B:129:LYS:CG	2.61	0.47
1:A:148:VAL:HG22	1:A:149:ALA:N	2.30	0.47
1:A:268:ILE:HA	1:A:291:CYS:O	2.14	0.47
1:A:294:ASN:ND2	1:A:299:THR:HG21	2.30	0.47
1:A:38:ILE:CG2	1:B:38:ILE:CG2	2.85	0.47
1:A:38:ILE:O	1:A:39:SER:C	2.52	0.47
1:A:65:ASP:HB3	1:B:248:TRP:CB	2.38	0.47
1:B:227:GLU:HA	1:B:230:LYS:HZ2	1.79	0.47
1:B:276:GLN:O	1:B:277:GLY:C	2.52	0.47
1:B:69:GLY:O	1:B:70:SER:C	2.52	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:CG	1:A:176:MET:H	2.06	0.47
1:A:253:SER:HG	1:B:72:PHE:HZ	1.52	0.47
1:A:252:LEU:O	1:A:255:ALA:HB3	2.15	0.47
1:A:92:LYS:O	1:A:133:CYS:CB	2.48	0.47
1:B:268:ILE:HA	1:B:291:CYS:O	2.14	0.47
1:B:294:ASN:ND2	1:B:299:THR:HG21	2.30	0.47
1:A:145:LEU:CA	1:A:148:VAL:HG11	2.16	0.47
1:A:166:ASN:H	1:A:270:PRO:HG2	1.80	0.47
1:A:230:LYS:O	1:A:231:MET:C	2.52	0.47
1:B:112:LEU:HB2	1:B:114:GLN:HG2	1.97	0.47
1:B:261:MET:CG	1:B:262:LEU:N	2.74	0.47
1:B:32:VAL:HG11	2:B:332:LNC:H5'2	1.96	0.47
1:B:53:ASP:O	1:B:83:LYS:HG3	2.14	0.47
1:A:110:LEU:N	1:A:110:LEU:HD22	2.27	0.47
1:A:112:LEU:O	1:A:113:VAL:HG13	2.15	0.47
1:A:273:THR:CG2	1:A:298:LEU:CD1	2.65	0.47
1:A:34:MET:O	1:A:38:ILE:HG12	2.13	0.47
1:A:93:ILE:HD12	1:A:258:ILE:CG1	2.17	0.47
1:B:112:LEU:O	1:B:113:VAL:HG13	2.15	0.47
1:B:150:TRP:NE1	1:B:156:PRO:CB	2.78	0.47
1:B:257:LEU:O	1:B:260:SER:HB3	2.14	0.47
1:B:231:MET:O	1:B:235:SER:N	2.39	0.47
1:B:19:PRO:HB2	1:B:48:GLU:HB2	1.97	0.47
1:A:276:GLN:O	1:A:277:GLY:C	2.52	0.47
1:A:277:GLY:HA3	1:A:304:ASN:HD21	1.80	0.47
1:B:229:HIS:HA	1:B:232:VAL:HG21	1.94	0.47
1:B:230:LYS:O	1:B:231:MET:C	2.52	0.47
1:A:62:GLU:O	1:A:66:LEU:HD22	2.14	0.47
1:B:215:GLU:CB	1:B:216:MET:SD	3.03	0.47
1:B:31:GLN:O	1:B:32:VAL:C	2.53	0.47
1:B:33:GLY:O	1:B:36:CYS:HB2	2.15	0.47
1:A:32:VAL:HG11	2:A:332:LNC:H5'2	1.96	0.47
1:A:56:GLU:O	1:A:59:LEU:HB2	2.14	0.47
1:A:34:MET:HE1	1:A:66:LEU:CD2	2.43	0.47
1:B:102:GLN:CA	1:B:110:LEU:CD2	2.62	0.47
1:B:24:ILE:C	1:B:25:THR:HG23	2.36	0.47
1:A:163:SER:O	1:A:164:GLY:O	2.33	0.47
1:A:182:VAL:HG23	1:A:183:HIS:N	2.30	0.47
1:A:215:GLU:CB	1:A:216:MET:SD	3.03	0.47
1:B:163:SER:HA	1:B:271:VAL:CG1	2.45	0.47
1:B:163:SER:O	1:B:164:GLY:O	2.33	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:SER:O	1:B:224:ASN:CG	2.53	0.47
1:B:252:LEU:O	1:B:255:ALA:HB3	2.15	0.47
1:B:265:LEU:CD2	1:B:267:ARG:NH2	2.78	0.47
1:B:163:SER:HA	1:B:271:VAL:CG2	2.45	0.47
1:B:306:LYS:C	1:B:307:LEU:O	2.48	0.47
1:B:38:ILE:O	1:B:39:SER:C	2.52	0.47
1:B:86:SER:HA	1:B:130:TYR:CZ	2.49	0.46
1:A:65:ASP:O	1:B:249:ALA:HB2	2.16	0.46
1:A:112:LEU:HB2	1:A:114:GLN:HG2	1.97	0.46
1:A:131:SER:N	1:A:132(A):PRO:CD	2.78	0.46
1:A:292:VAL:O	1:A:292:VAL:CG2	2.62	0.46
1:A:33:GLY:O	1:A:36:CYS:HB2	2.15	0.46
1:B:146:THR:O	1:B:160:VAL:HG11	2.16	0.46
1:B:223:GLU:OE1	1:B:225:TRP:CH2	2.65	0.46
1:B:138:VAL:CG1	2:B:332:LNC:HN72	2.27	0.46
1:A:248:TRP:CB	1:B:65:ASP:HB3	2.38	0.46
1:A:222:SER:O	1:A:224:ASN:CG	2.53	0.46
1:A:265:LEU:CD2	1:A:267:ARG:NH2	2.78	0.46
1:B:145:LEU:HD12	1:B:148:VAL:HG11	1.98	0.46
1:B:148:VAL:HG22	1:B:149:ALA:N	2.30	0.46
1:B:182:VAL:HG23	1:B:183:HIS:N	2.30	0.46
1:B:190:TRP:CZ3	1:B:270:PRO:HD3	2.51	0.46
1:B:59:LEU:O	1:B:60:LYS:C	2.54	0.46
1:A:203:TRP:CZ2	1:A:226:LYS:HE2	2.37	0.46
1:A:161:ILE:HG22	1:A:271:VAL:HG11	1.98	0.46
1:B:228:VAL:HG12	1:B:229:HIS:H	1.79	0.46
1:B:240:ILE:HG23	1:B:240:ILE:O	2.16	0.46
1:B:101:ARG:HB2	2:B:332:LNC:C2D	2.44	0.46
1:A:102:GLN:CA	1:A:110:LEU:CD2	2.62	0.46
1:A:163:SER:HA	1:A:271:VAL:CG1	2.45	0.46
1:A:281:ILE:CB	1:A:285:VAL:HG13	2.41	0.46
1:A:313:ALA:HA	1:A:316:LYS:CG	2.46	0.46
1:A:59:LEU:O	1:A:60:LYS:C	2.54	0.46
1:B:102:GLN:NE2	2:B:332:LNC:HGS1	2.31	0.46
1:A:224:ASN:O	1:A:225:TRP:C	2.54	0.46
1:A:267:ARG:HB3	1:A:268:ILE:H	1.56	0.46
1:A:190:TRP:CZ3	1:A:270:PRO:HD3	2.51	0.46
1:A:102:GLN:NE2	2:A:332:LNC:HGS1	2.31	0.46
1:A:53:ASP:OD2	2:A:332:LNC:O2B	2.20	0.46
1:B:277:GLY:HA3	1:B:304:ASN:HD21	1.80	0.46
1:A:101:ARG:CD	1:A:102:GLN:HB2	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:VAL:CG1	2:A:332:LNC:HN72	2.27	0.46
1:A:192:LEU:HD23	1:A:315:LEU:HD12	1.85	0.46
1:A:242:LEU:HG	1:B:58:LYS:CA	2.23	0.46
1:A:163:SER:HA	1:A:271:VAL:CG2	2.45	0.46
1:A:65:ASP:OD2	1:B:248:TRP:CB	2.59	0.46
1:B:131:SER:N	1:B:132(A):PRO:CD	2.78	0.46
1:A:31:GLN:O	1:A:32:VAL:C	2.53	0.46
1:B:140:ASN:O	1:B:142:VAL:N	2.49	0.46
1:B:286:PHE:CD1	1:B:286:PHE:C	2.88	0.46
1:B:307:LEU:O	1:B:312:VAL:HG13	2.16	0.46
1:A:173:ARG:NH1	1:B:71:LEU:HD13	2.24	0.46
1:A:146:THR:HG1	1:A:160:VAL:HG12	1.74	0.46
1:A:240:ILE:HG23	1:A:240:ILE:O	2.16	0.46
1:A:245:TYR:CG	1:B:62:GLU:HA	2.50	0.46
1:B:93:ILE:HD12	1:B:258:ILE:CG1	2.17	0.46
1:A:150:TRP:NE1	1:A:156:PRO:CB	2.78	0.45
1:B:166:ASN:H	1:B:270:PRO:HG2	1.80	0.45
1:B:307:LEU:HD13	1:B:309:ASP:OD2	2.17	0.45
1:B:313:ALA:HA	1:B:316:LYS:CG	2.46	0.45
1:B:327:LYS:HA	1:B:327:LYS:HD2	1.62	0.45
1:B:74:GLN:C	1:B:75:THR:CG2	2.84	0.45
1:A:145:LEU:HD12	1:A:148:VAL:HG11	1.98	0.45
1:A:146:THR:O	1:A:160:VAL:HG11	2.16	0.45
1:A:74:GLN:C	1:A:75:THR:CG2	2.84	0.45
1:B:224:ASN:O	1:B:225:TRP:C	2.54	0.45
1:A:62:GLU:HA	1:B:245:TYR:CG	2.50	0.45
1:B:53:ASP:OD2	2:B:332:LNC:O2B	2.20	0.45
1:A:249:ALA:HB2	1:B:65:ASP:O	2.16	0.45
1:A:103:GLN:HE21	1:A:103:GLN:HA	1.82	0.45
1:A:107:GLU:HB3	1:A:108:SER:H	1.27	0.45
1:A:174:TYR:CD1	1:A:175:LEU:N	2.85	0.45
1:A:224:ASN:HB3	1:A:227:GLU:CB	2.31	0.45
1:A:24:ILE:C	1:A:25:THR:HG23	2.36	0.45
1:A:255:ALA:C	1:A:258:ILE:HG22	2.37	0.45
1:B:103:GLN:HA	1:B:103:GLN:HE21	1.82	0.45
1:A:140:ASN:O	1:A:142:VAL:N	2.49	0.45
1:A:225:TRP:O	1:A:228:VAL:CB	2.64	0.45
1:B:150:TRP:HB2	1:B:160:VAL:HG21	0.49	0.45
1:B:273:THR:CG2	1:B:298:LEU:CD1	2.65	0.45
1:B:48:GLU:OE2	1:B:77:LYS:HB3	2.17	0.45
1:A:279:TYR:HE2	1:A:281:ILE:HG12	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LEU:HA	1:B:307:LEU:HD23	1.73	0.45
1:A:174:TYR:OH	1:B:67:GLN:OE1	2.34	0.45
1:A:182:VAL:HB	1:A:183:HIS:CD2	2.51	0.45
1:A:35:ALA:HB2	1:A:247:ASN:ND2	2.32	0.45
1:A:55:LEU:HG	2:A:332:LNC:H2'	1.99	0.45
1:A:32:VAL:CB	2:A:332:LNC:H5'2	2.45	0.45
1:A:3:LEU:O	1:A:4:LYS:CG	2.65	0.45
1:A:19:PRO:HB2	1:A:48:GLU:HB2	1.97	0.45
1:A:55:LEU:C	1:A:59:LEU:CD1	2.70	0.45
1:B:138:VAL:O	1:B:139:SER:HB2	2.17	0.45
1:B:150:TRP:HD1	1:B:156:PRO:CA	2.22	0.45
1:B:174:TYR:CD1	1:B:175:LEU:N	2.85	0.45
1:B:230:LYS:HE3	1:B:230:LYS:HB3	1.59	0.45
1:A:58:LYS:CA	1:B:242:LEU:HG	2.23	0.45
1:B:41:LEU:C	1:B:73:LEU:HD21	2.31	0.45
1:A:1:ALA:C	1:A:2:THR:CG2	2.71	0.45
1:A:35:ALA:HB2	1:A:247:ASN:HD21	1.82	0.45
1:A:67:GLN:OE1	1:B:174:TYR:OH	2.34	0.45
1:B:323:TRP:CA	1:B:326:GLN:HB3	2.47	0.45
1:B:331:LEU:HD23	1:B:331:LEU:O	2.16	0.45
1:B:41:LEU:HD11	1:B:49:LEU:HD21	1.96	0.45
1:B:40:ILE:HG21	1:B:41:LEU:HD22	1.94	0.45
1:A:307:LEU:O	1:A:312:VAL:HG13	2.16	0.45
1:A:331:LEU:HD23	1:A:331:LEU:O	2.16	0.45
1:B:35:ALA:HB2	1:B:247:ASN:ND2	2.32	0.45
1:A:192:LEU:CD2	1:A:289:LEU:HD13	2.46	0.44
1:B:182:VAL:HB	1:B:183:HIS:CD2	2.51	0.44
1:B:225:TRP:O	1:B:228:VAL:CB	2.64	0.44
1:B:55:LEU:HG	2:B:332:LNC:H2'	1.99	0.44
1:B:3:LEU:O	1:B:4:LYS:CG	2.65	0.44
1:A:150:TRP:CD1	1:A:156:PRO:N	2.85	0.44
1:A:307:LEU:HD13	1:A:309:ASP:OD2	2.17	0.44
1:B:168:ASP:C	1:B:191:ILE:CD1	2.85	0.44
1:B:275:VAL:HG13	1:B:285:VAL:HG11	1.83	0.44
1:B:288:SER:HB2	1:B:289:LEU:H	1.36	0.44
1:B:93:ILE:CD1	1:B:261:MET:HE2	2.46	0.44
1:A:110:LEU:HD12	1:A:112:LEU:CD2	2.37	0.44
1:A:48:GLU:OE2	1:A:77:LYS:HB3	2.17	0.44
1:B:101:ARG:CG	1:B:102:GLN:HB2	2.48	0.44
1:B:150:TRP:CD1	1:B:156:PRO:N	2.85	0.44
1:B:161:ILE:HG22	1:B:271:VAL:HG11	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ALA:HB2	1:B:247:ASN:HD21	1.82	0.44
1:B:3:LEU:CD1	1:B:3:LEU:N	2.80	0.44
1:A:168:ASP:C	1:A:191:ILE:CD1	2.85	0.44
1:A:192:LEU:CD2	1:A:315:LEU:HD11	2.37	0.44
1:A:262:LEU:C	1:A:262:LEU:HD13	2.38	0.44
1:A:313:ALA:HA	1:A:316:LYS:HD2	1.98	0.44
1:B:186:SER:HB2	1:B:187:CYS:H	1.62	0.44
1:A:101:ARG:O	1:A:110:LEU:CD2	2.66	0.44
1:A:267:ARG:HE	1:A:267:ARG:HB2	1.54	0.44
1:A:51:LEU:CD1	1:A:51:LEU:C	2.86	0.44
1:A:188:HIS:NE2	3:A:333:CIT:C6	2.74	0.44
1:A:85:TYR:CG	1:A:126:GLN:HB3	2.53	0.44
1:B:129:LYS:O	1:B:132(A):PRO:CD	2.56	0.44
1:B:188:HIS:NE2	3:B:333:CIT:C6	2.74	0.44
1:B:26:VAL:HG22	1:B:28:GLY:N	2.22	0.44
1:A:138:VAL:O	1:A:139:SER:HB2	2.17	0.44
1:A:322:LEU:HA	1:A:322:LEU:HD23	1.88	0.44
1:A:327:LYS:HA	1:A:327:LYS:HD2	1.62	0.44
1:A:3:LEU:CD1	1:A:3:LEU:N	2.80	0.44
1:B:109:ARG:HH11	1:B:195:HIS:CD2	2.33	0.44
1:B:275:VAL:CG1	1:B:286:PHE:N	2.80	0.44
1:B:85:TYR:CD2	1:B:126:GLN:CB	3.01	0.44
1:A:85:TYR:CZ	1:A:123:ILE:HA	2.53	0.44
1:B:163:SER:O	1:B:164:GLY:C	2.56	0.44
1:B:262:LEU:HD13	1:B:262:LEU:C	2.38	0.44
1:B:51:LEU:C	1:B:51:LEU:CD1	2.86	0.44
1:A:163:SER:O	1:A:164:GLY:C	2.56	0.44
1:A:203:TRP:HA	1:A:206:VAL:HG22	1.98	0.44
1:A:306:LYS:HG3	1:A:312:VAL:HG13	2.00	0.44
1:B:85:TYR:CZ	1:B:123:ILE:HA	2.53	0.44
1:B:125:PRO:O	1:B:129:LYS:HG3	2.18	0.44
1:A:117:VAL:HG23	1:A:118:ASN:H	1.83	0.43
1:A:125:PRO:O	1:A:129:LYS:HG3	2.18	0.43
1:A:134:ILE:HG13	1:A:261:MET:HE3	1.89	0.43
1:A:145:LEU:N	1:A:148:VAL:CG1	2.80	0.43
1:A:165:CYS:HB2	1:A:271:VAL:H	1.83	0.43
1:A:58:LYS:O	1:A:59:LEU:C	2.57	0.43
1:B:101:ARG:O	1:B:110:LEU:CD2	2.66	0.43
1:B:258:ILE:CD1	1:B:262:LEU:HB2	2.45	0.43
1:B:306:LYS:HG3	1:B:312:VAL:HG13	2.00	0.43
1:A:101:ARG:CG	1:A:102:GLN:HB2	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:C	1:A:279:TYR:CD2	2.72	0.43
1:A:85:TYR:CD2	1:A:126:GLN:CB	3.01	0.43
1:B:165:CYS:HB2	1:B:271:VAL:H	1.83	0.43
1:A:134:ILE:HG13	1:A:261:MET:HE1	1.97	0.43
1:B:107:GLU:HG2	1:B:237:TYR:CZ	2.53	0.43
1:B:23:LYS:HE2	1:B:88:THR:O	2.18	0.43
1:B:85:TYR:CG	1:B:126:GLN:HB3	2.53	0.43
1:A:107:GLU:HG2	1:A:237:TYR:CZ	2.53	0.43
1:A:23:LYS:HE2	1:A:88:THR:O	2.18	0.43
1:A:240:ILE:HA	1:A:240:ILE:HD12	1.83	0.43
1:A:318:SER:O	1:A:319:ALA:C	2.57	0.43
1:A:55:LEU:CG	2:A:332:LNC:H2'	2.48	0.43
1:A:71:LEU:HD13	1:B:173:ARG:NH1	2.24	0.43
1:B:24:ILE:C	1:B:25:THR:CG2	2.87	0.43
1:B:264:ASN:ND2	1:B:295:ALA:CB	2.80	0.43
1:B:41:LEU:CD1	1:B:49:LEU:HD23	2.48	0.43
1:A:323:TRP:CA	1:A:326:GLN:HB3	2.47	0.43
1:B:117:VAL:HG23	1:B:118:ASN:H	1.83	0.43
1:B:192:LEU:CD2	1:B:289:LEU:HD13	2.46	0.43
1:A:182:VAL:CG2	1:A:183:HIS:N	2.81	0.43
1:A:271:VAL:HG13	1:A:271:VAL:O	2.06	0.43
1:A:275:VAL:CG1	1:A:286:PHE:N	2.80	0.43
1:A:279:TYR:O	1:A:279:TYR:CG	2.57	0.43
1:A:282:GLU:CG	1:A:283:ASN:OD1	2.67	0.43
1:A:288:SER:HB2	1:A:289:LEU:H	1.36	0.43
1:B:41:LEU:O	1:B:73:LEU:HD13	2.14	0.43
1:A:150:TRP:HE1	1:A:156:PRO:CB	2.32	0.43
1:B:150:TRP:HE1	1:B:156:PRO:CB	2.32	0.43
1:B:203:TRP:CZ3	1:B:226:LYS:CD	2.98	0.43
1:A:226:LYS:HA	1:A:226:LYS:HD2	1.67	0.43
1:B:330(A):LYS:HD2	1:B:330(B):ASP:N	2.23	0.43
1:A:258:ILE:O	1:A:259:GLU:C	2.57	0.43
1:A:258:ILE:CD1	1:A:262:LEU:HB2	2.45	0.43
1:A:55:LEU:O	1:A:59:LEU:CD2	2.67	0.43
1:B:208:VAL:O	1:B:209(B):GLY:N	2.52	0.43
1:B:279:TYR:HE2	1:B:281:ILE:HG12	1.82	0.43
1:A:129:LYS:O	1:A:132(A):PRO:CD	2.56	0.42
1:A:23:LYS:HE3	1:A:50:ALA:CB	2.47	0.42
1:A:32:VAL:CG2	2:A:332:LNC:O3	2.67	0.42
1:A:58:LYS:HA	1:B:242:LEU:CD1	2.48	0.42
1:A:63:MET:SD	1:A:78:ILE:CD1	3.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ILE:CG1	1:B:261:MET:HE3	2.48	0.42
1:A:11:VAL:HG23	1:A:11:VAL:O	2.17	0.42
1:A:323:TRP:HA	1:A:326:GLN:OE1	2.19	0.42
1:B:142:VAL:O	1:B:143:ASP:C	2.58	0.42
1:B:216:MET:HB2	1:B:217:GLY:H	1.17	0.42
1:B:258:ILE:O	1:B:259:GLU:C	2.57	0.42
1:B:264:ASN:HD21	1:B:295:ALA:HB2	1.82	0.42
1:B:32:VAL:CG2	2:B:332:LNC:O3	2.67	0.42
1:A:248:TRP:CB	1:B:65:ASP:OD2	2.59	0.42
1:A:231:MET:O	1:A:235:SER:N	2.39	0.42
1:A:30:GLY:HA3	2:A:332:LNC:H11	2.02	0.42
1:B:265:LEU:CG	1:B:267:ARG:NH2	2.81	0.42
1:A:109:ARG:HH11	1:A:195:HIS:CD2	2.33	0.42
1:A:208:VAL:O	1:A:209(B):GLY:N	2.52	0.42
1:B:150:TRP:HD1	1:B:155:LEU:C	2.22	0.42
1:B:55:LEU:CG	2:B:332:LNC:H2'	2.48	0.42
1:A:110:LEU:HB3	1:A:112:LEU:HG	2.01	0.42
1:A:147:TYR:O	1:A:150:TRP:CE3	2.72	0.42
1:A:150:TRP:HD1	1:A:155:LEU:C	2.22	0.42
1:A:264:ASN:ND2	1:A:295:ALA:CB	2.80	0.42
1:A:284:GLU:C	1:A:285:VAL:CG2	2.73	0.42
1:B:150:TRP:HD1	1:B:155:LEU:O	2.02	0.42
1:B:220:ASN:HD22	1:B:220:ASN:HA	1.45	0.42
1:B:323:TRP:HA	1:B:326:GLN:OE1	2.19	0.42
1:B:30:GLY:HA3	2:B:332:LNC:H11	2.02	0.42
1:A:146:THR:C	1:A:160:VAL:HG11	2.40	0.42
1:A:190:TRP:HB3	1:A:191:ILE:H	1.71	0.42
1:B:147:TYR:O	1:B:150:TRP:CE3	2.72	0.42
1:B:146:THR:C	1:B:160:VAL:HG11	2.40	0.42
1:B:165:CYS:O	1:B:166:ASN:C	2.58	0.42
1:B:18:ILE:HG21	1:B:20:ASP:OD2	2.14	0.42
1:B:255:ALA:C	1:B:258:ILE:HG22	2.37	0.42
1:B:282:GLU:CG	1:B:283:ASN:OD1	2.67	0.42
1:B:305:GLN:OE1	1:B:305:GLN:CA	2.68	0.42
1:B:19:PRO:CB	1:B:48:GLU:HB2	2.50	0.42
1:B:99:GLY:O	1:B:100:VAL:HG12	2.18	0.42
1:A:165:CYS:O	1:A:166:ASN:C	2.58	0.42
1:A:41:LEU:CD1	1:A:49:LEU:HD23	2.48	0.42
1:B:182:VAL:HB	1:B:183:HIS:H	1.38	0.42
1:B:234:GLU:O	1:B:237:TYR:N	2.53	0.42
1:B:241:LYS:HB2	1:B:242:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CE2	1:A:281:ILE:HG12	2.55	0.42
1:A:264:ASN:HD21	1:A:295:ALA:HB2	1.82	0.42
1:A:307:LEU:CD1	1:A:309:ASP:OD2	2.68	0.42
1:A:58:LYS:CA	1:B:242:LEU:HD21	2.50	0.42
1:B:172:PHE:O	1:B:176:MET:HB3	2.20	0.42
1:B:307:LEU:CD1	1:B:309:ASP:OD2	2.68	0.42
1:B:318:SER:O	1:B:319:ALA:C	2.57	0.42
1:A:241:LYS:HB2	1:A:242:LEU:HD22	2.02	0.42
1:A:24:ILE:C	1:A:25:THR:CG2	2.87	0.42
1:A:41:LEU:HD11	1:A:49:LEU:HD21	1.96	0.42
1:B:182:VAL:CG2	1:B:183:HIS:N	2.81	0.42
1:B:221:ASP:O	1:B:222:SER:CB	2.67	0.42
1:B:58:LYS:O	1:B:59:LEU:C	2.57	0.42
1:A:135:ILE:HD13	1:A:137:VAL:HG23	2.01	0.42
1:A:150:TRP:HB2	1:A:160:VAL:HG21	0.49	0.42
1:A:308:LYS:CA	1:A:312:VAL:HG11	2.38	0.42
1:A:321:THR:CG2	1:A:322:LEU:N	2.83	0.42
1:B:135:ILE:HD13	1:B:137:VAL:HG23	2.01	0.42
1:B:308:LYS:CA	1:B:312:VAL:HG11	2.38	0.42
1:A:108:SER:O	1:A:109:ARG:C	2.58	0.41
1:A:307:LEU:O	1:A:312:VAL:CG1	2.68	0.41
1:B:3:LEU:C	1:B:3:LEU:HD22	2.41	0.41
1:A:13:GLN:HB3	1:A:14:GLN:H	1.69	0.41
1:A:230:LYS:HE3	1:A:230:LYS:HB3	1.59	0.41
1:A:3:LEU:HD22	1:A:3:LEU:C	2.41	0.41
1:B:110:LEU:HB3	1:B:112:LEU:HG	2.01	0.41
1:B:149:ALA:O	1:B:153:SER:N	2.46	0.41
1:A:131:SER:C	1:A:132(B):ASN:N	2.74	0.41
1:A:191:ILE:HG22	1:A:201:ALA:CA	2.51	0.41
1:B:103:GLN:HA	1:B:103:GLN:NE2	2.35	0.41
1:B:143:ASP:O	1:B:144:ILE:C	2.59	0.41
1:B:149:ALA:O	1:B:150:TRP:C	2.59	0.41
1:B:307:LEU:O	1:B:312:VAL:CG1	2.68	0.41
1:A:103:GLN:HA	1:A:103:GLN:NE2	2.35	0.41
1:A:143:ASP:O	1:A:144:ILE:C	2.59	0.41
1:A:19:PRO:CB	1:A:48:GLU:HB2	2.50	0.41
1:A:221:ASP:O	1:A:222:SER:CB	2.67	0.41
1:B:27:VAL:HA	1:B:52:VAL:O	2.21	0.41
1:A:110:LEU:HD12	1:A:112:LEU:HD11	2.03	0.41
1:A:234:GLU:O	1:A:237:TYR:N	2.53	0.41
1:A:99:GLY:O	1:A:100:VAL:HG12	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:LYS:HB3	1:B:83:LYS:HE2	1.89	0.41
1:A:142:VAL:O	1:A:143:ASP:C	2.58	0.41
1:A:223:GLU:HB3	1:A:225:TRP:CZ3	2.55	0.41
1:A:275:VAL:HG13	1:A:285:VAL:HG11	1.83	0.41
1:A:27:VAL:HA	1:A:52:VAL:O	2.21	0.41
1:B:138:VAL:O	1:B:139:SER:CB	2.68	0.41
1:B:308:LYS:HE2	1:B:312:VAL:CG1	2.49	0.41
1:B:322:LEU:HA	1:B:322:LEU:HD23	1.88	0.41
1:B:92:LYS:O	1:B:133:CYS:CB	2.48	0.41
1:A:138:VAL:O	1:A:139:SER:CB	2.68	0.41
1:A:182:VAL:HB	1:A:183:HIS:H	1.38	0.41
1:A:242:LEU:HD21	1:B:58:LYS:CA	2.50	0.41
1:A:277:GLY:O	1:A:278:MET:CB	2.69	0.41
3:A:333:CIT:C5	3:A:333:CIT:C6	2.99	0.41
1:A:78:ILE:CD1	1:A:78:ILE:C	2.76	0.41
1:B:108:SER:O	1:B:109:ARG:C	2.58	0.41
1:B:231:MET:O	1:B:234:GLU:HB2	2.21	0.41
1:B:279:TYR:CE2	1:B:281:ILE:HG12	2.55	0.41
1:B:193:GLY:CA	1:B:287:LEU:CD2	2.86	0.41
1:A:150:TRP:HD1	1:A:155:LEU:O	2.02	0.41
1:A:133:CYS:O	1:A:159:ARG:CG	2.69	0.41
1:A:172:PHE:O	1:A:176:MET:HB3	2.20	0.41
1:A:183:HIS:CE1	1:A:209(A):ALA:CB	2.80	0.41
1:A:26:VAL:HG22	1:A:28:GLY:N	2.22	0.41
1:A:308:LYS:HA	1:A:312:VAL:HG21	2.00	0.41
1:B:53:ASP:C	1:B:55:LEU:H	2.24	0.41
1:B:55:LEU:O	1:B:59:LEU:CD2	2.67	0.41
1:A:279:TYR:CE2	1:A:281:ILE:CG1	3.01	0.41
1:A:3:LEU:C	1:A:4:LYS:HG2	2.41	0.41
1:B:85:TYR:CD2	1:B:126:GLN:HG2	2.55	0.41
1:B:23:LYS:HE3	1:B:50:ALA:CB	2.47	0.41
3:B:333:CIT:C6	3:B:333:CIT:C5	2.99	0.41
1:A:113:VAL:HA	1:A:116:ASN:HB3	2.03	0.41
1:A:164:GLY:O	1:A:166:ASN:N	2.54	0.41
1:A:264:ASN:HD21	1:A:295:ALA:CB	2.34	0.41
1:A:31:GLN:H	1:A:31:GLN:HG2	1.46	0.41
1:A:31:GLN:HB2	1:A:32:VAL:H	1.78	0.41
1:A:53:ASP:C	1:A:55:LEU:H	2.24	0.41
1:A:89:ALA:O	1:A:91:SER:HB3	2.21	0.41
1:A:97:THR:CG2	2:A:332:LNC:C5D	2.95	0.41
1:B:110:LEU:HD12	1:B:112:LEU:HD11	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:CYS:O	1:B:159:ARG:CG	2.69	0.41
1:B:164:GLY:O	1:B:166:ASN:N	2.54	0.41
1:B:271:VAL:HG13	1:B:271:VAL:O	2.06	0.41
1:B:321:THR:CG2	1:B:322:LEU:N	2.83	0.41
1:B:89:ALA:O	1:B:91:SER:HB3	2.21	0.41
1:A:286:PHE:O	1:A:287:LEU:CB	2.50	0.41
1:B:113:VAL:HA	1:B:116:ASN:HB3	2.03	0.41
1:A:117:VAL:HG23	1:A:118:ASN:N	2.36	0.40
1:A:146:THR:HG23	1:A:147:TYR:H	1.86	0.40
1:A:133:CYS:O	1:A:159:ARG:HG3	2.21	0.40
1:A:309:ASP:O	1:A:310:ASP:CB	2.69	0.40
1:A:52:VAL:CG2	1:A:53:ASP:N	2.63	0.40
1:B:107:GLU:HB3	1:B:108:SER:H	1.27	0.40
1:B:131:SER:C	1:B:132(B):ASN:N	2.74	0.40
1:B:133:CYS:O	1:B:159:ARG:HG3	2.21	0.40
1:B:264:ASN:HD21	1:B:295:ALA:CB	2.34	0.40
1:A:246:THR:C	1:B:65:ASP:OD2	2.60	0.40
1:A:193:GLY:CA	1:A:287:LEU:CD2	2.86	0.40
1:A:137:VAL:HG11	1:A:145:LEU:HB3	2.04	0.40
1:A:305:GLN:OE1	1:A:305:GLN:CA	2.68	0.40
1:B:131:SER:C	1:B:132(B):ASN:H	2.25	0.40
1:A:149:ALA:O	1:A:150:TRP:C	2.59	0.40
1:A:193:GLY:O	1:A:287:LEU:CG	2.54	0.40
1:A:275:VAL:HG22	1:A:285:VAL:CG1	2.12	0.40
1:A:309:ASP:C	1:A:311:GLU:H	2.25	0.40
1:B:117:VAL:HG23	1:B:118:ASN:N	2.36	0.40
1:B:145:LEU:N	1:B:148:VAL:CG1	2.80	0.40
1:B:279:TYR:CE1	1:B:306:LYS:CE	2.91	0.40
1:B:3:LEU:C	1:B:4:LYS:HG2	2.41	0.40
1:A:131:SER:C	1:A:132(B):ASN:H	2.25	0.40
1:B:110:LEU:HD12	1:B:112:LEU:CD2	2.37	0.40
1:B:174:TYR:O	1:B:175:LEU:C	2.59	0.40
1:B:226:LYS:HA	1:B:226:LYS:HD2	1.67	0.40
1:A:65:ASP:OD2	1:B:246:THR:C	2.60	0.40
1:B:291:CYS:HB3	1:B:302:VAL:HG23	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ILE:CD1	1:B:107:GLU:OE2[3_565]	2.02	0.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:HIS:CB	1:B:266:SER:O[6_555]	2.14	0.06
1:A:183:HIS:CB	1:A:266:SER:O[6_555]	2.14	0.06

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	332/334 (99%)	167 (50%)	72 (22%)	93 (28%)	0	0
1	B	332/334 (99%)	167 (50%)	72 (22%)	93 (28%)	0	0
All	All	664/668 (99%)	334 (50%)	144 (22%)	186 (28%)	0	0

All (186) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	LEU
1	A	4	LYS
1	A	6	LYS
1	A	9	ALA
1	A	10	PRO
1	A	12	ALA
1	A	14	GLN
1	A	20	ASP
1	A	44	SER
1	A	70	SER
1	A	84	ASP
1	A	85	TYR
1	A	88	THR
1	A	100	VAL
1	A	103	GLN
1	A	110	LEU
1	A	139	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	140	ASN
1	A	155	LEU
1	A	156	PRO
1	A	157	LYS
1	A	163	SER
1	A	165	CYS
1	A	187	CYS
1	A	198	SER
1	A	199	SER
1	A	209(C)	VAL
1	A	219	ASP
1	A	221	ASP
1	A	237	TYR
1	A	239	VAL
1	A	268	ILE
1	A	270	PRO
1	A	272	SER
1	A	278	MET
1	A	282	GLU
1	A	283	ASN
1	A	285	VAL
1	A	286	PHE
1	A	287	LEU
1	A	295	ALA
1	A	330(B)	ASP
1	B	2	THR
1	B	3	LEU
1	B	4	LYS
1	B	6	LYS
1	B	9	ALA
1	B	10	PRO
1	B	12	ALA
1	B	14	GLN
1	B	20	ASP
1	B	44	SER
1	B	70	SER
1	B	84	ASP
1	B	85	TYR
1	B	88	THR
1	B	100	VAL
1	B	103	GLN
1	B	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	139	SER
1	B	140	ASN
1	B	155	LEU
1	B	156	PRO
1	B	157	LYS
1	B	163	SER
1	B	165	CYS
1	B	187	CYS
1	B	198	SER
1	B	199	SER
1	B	209(C)	VAL
1	B	219	ASP
1	B	221	ASP
1	B	237	TYR
1	B	239	VAL
1	B	268	ILE
1	B	270	PRO
1	B	272	SER
1	B	278	MET
1	B	282	GLU
1	B	283	ASN
1	B	285	VAL
1	B	286	PHE
1	B	287	LEU
1	B	295	ALA
1	B	330(B)	ASP
1	A	8	ILE
1	A	19	PRO
1	A	22	ASN
1	A	31	GLN
1	A	87	VAL
1	A	89	ALA
1	A	101	ARG
1	A	113	VAL
1	A	114	GLN
1	A	144	ILE
1	A	164	GLY
1	A	182	VAL
1	A	196	GLY
1	A	209(A)	ALA
1	A	209(D)	VAL
1	A	217	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	224	ASN
1	A	238	GLU
1	A	280	GLY
1	B	8	ILE
1	B	19	PRO
1	B	22	ASN
1	B	31	GLN
1	B	87	VAL
1	B	89	ALA
1	B	101	ARG
1	B	113	VAL
1	B	114	GLN
1	B	144	ILE
1	B	164	GLY
1	B	182	VAL
1	B	196	GLY
1	B	209(A)	ALA
1	B	209(D)	VAL
1	B	217	GLY
1	B	224	ASN
1	B	238	GLU
1	B	280	GLY
1	A	43	LYS
1	A	57	ASP
1	A	76	PRO
1	A	81	ASN
1	A	90	ASN
1	A	92	LYS
1	A	98	ALA
1	A	143	ASP
1	A	154	GLY
1	A	244	GLY
1	A	264	ASN
1	A	266	SER
1	A	288	SER
1	A	289	LEU
1	A	305	GLN
1	B	43	LYS
1	B	57	ASP
1	B	76	PRO
1	B	81	ASN
1	B	90	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	92	LYS
1	B	98	ALA
1	B	143	ASP
1	B	154	GLY
1	B	244	GLY
1	B	264	ASN
1	B	266	SER
1	B	288	SER
1	B	289	LEU
1	B	305	GLN
1	A	23	LYS
1	A	99	GLY
1	A	112	LEU
1	A	213	ASN
1	A	214	PRO
1	A	223	GLU
1	A	248	TRP
1	A	301	SER
1	A	327	LYS
1	B	23	LYS
1	B	99	GLY
1	B	112	LEU
1	B	213	ASN
1	B	214	PRO
1	B	223	GLU
1	B	248	TRP
1	B	301	SER
1	B	327	LYS
1	A	7	LEU
1	A	141	PRO
1	A	215	GLU
1	B	7	LEU
1	B	141	PRO
1	B	215	GLU
1	A	184	PRO
1	B	184	PRO
1	A	271	VAL
1	B	271	VAL
1	A	11	VAL
1	B	11	VAL
1	A	54	VAL
1	B	54	VAL

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	289/289 (100%)	155 (54%)	134 (46%)	0	0
1	B	289/289 (100%)	155 (54%)	134 (46%)	0	0
All	All	578/578 (100%)	310 (54%)	268 (46%)	0	0

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	5	GLU
1	A	7	LEU
1	A	13	GLN
1	A	14	GLN
1	A	18	ILE
1	A	20	ASP
1	A	24	ILE
1	A	32	VAL
1	A	34	MET
1	A	40	ILE
1	A	48	GLU
1	A	49	LEU
1	A	52	VAL
1	A	54	VAL
1	A	55	LEU
1	A	56	GLU
1	A	66	LEU
1	A	67	GLN
1	A	70	SER
1	A	71	LEU
1	A	74	GLN
1	A	77	LYS
1	A	78	ILE
1	A	87	VAL
1	A	91	SER
1	A	92	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	93	ILE
1	A	95	VAL
1	A	101	ARG
1	A	102	GLN
1	A	103	GLN
1	A	109	ARG
1	A	110	LEU
1	A	112	LEU
1	A	114	GLN
1	A	115	ARG
1	A	117	VAL
1	A	119	VAL
1	A	120	PHE
1	A	123	ILE
1	A	124	ILE
1	A	126	GLN
1	A	127	ILE
1	A	129	LYS
1	A	131	SER
1	A	134	ILE
1	A	136	ILE
1	A	138	VAL
1	A	139	SER
1	A	142	VAL
1	A	144	ILE
1	A	145	LEU
1	A	147	TYR
1	A	150	TRP
1	A	157	LYS
1	A	159	ARG
1	A	167	LEU
1	A	168	ASP
1	A	174	TYR
1	A	175	LEU
1	A	176	MET
1	A	178	GLU
1	A	179	LYS
1	A	183	HIS
1	A	185	SER
1	A	186	SER
1	A	187	CYS
1	A	191	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	LEU
1	A	198	SER
1	A	203	TRP
1	A	204	SER
1	A	206	VAL
1	A	208	VAL
1	A	210(A)	LEU
1	A	210(B)	GLN
1	A	211	GLN
1	A	213	ASN
1	A	215	GLU
1	A	216	MET
1	A	218	THR
1	A	220	ASN
1	A	222	SER
1	A	225	TRP
1	A	226	LYS
1	A	228	VAL
1	A	229	HIS
1	A	230	LYS
1	A	232	VAL
1	A	234	GLU
1	A	235	SER
1	A	237	TYR
1	A	238	GLU
1	A	240	ILE
1	A	243	LYS
1	A	246	THR
1	A	247	ASN
1	A	250	ILE
1	A	252	LEU
1	A	256	ASP
1	A	258	ILE
1	A	259	GLU
1	A	261	MET
1	A	268	ILE
1	A	272	SER
1	A	273	THR
1	A	275	VAL
1	A	278	MET
1	A	279	TYR
1	A	281	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	286	PHE
1	A	287	LEU
1	A	288	SER
1	A	291	CYS
1	A	296	ARG
1	A	303	ILE
1	A	305	GLN
1	A	306	LYS
1	A	307	LEU
1	A	308	LYS
1	A	312	VAL
1	A	315	LEU
1	A	317	ASN
1	A	318	SER
1	A	320	ASP
1	A	321	THR
1	A	322	LEU
1	A	323	TRP
1	A	327	LYS
1	A	328	ASP
1	A	329	LEU
1	A	330(A)	LYS
1	A	331	LEU
1	B	3	LEU
1	B	5	GLU
1	B	7	LEU
1	B	13	GLN
1	B	14	GLN
1	B	18	ILE
1	B	20	ASP
1	B	24	ILE
1	B	32	VAL
1	B	34	MET
1	B	40	ILE
1	B	48	GLU
1	B	49	LEU
1	B	52	VAL
1	B	54	VAL
1	B	55	LEU
1	B	56	GLU
1	B	66	LEU
1	B	67	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	70	SER
1	B	71	LEU
1	B	74	GLN
1	B	77	LYS
1	B	78	ILE
1	B	87	VAL
1	B	91	SER
1	B	92	LYS
1	B	93	ILE
1	B	95	VAL
1	B	101	ARG
1	B	102	GLN
1	B	103	GLN
1	B	109	ARG
1	B	110	LEU
1	B	112	LEU
1	B	114	GLN
1	B	115	ARG
1	B	117	VAL
1	B	119	VAL
1	B	120	PHE
1	B	123	ILE
1	B	124	ILE
1	B	126	GLN
1	B	127	ILE
1	B	129	LYS
1	B	131	SER
1	B	134	ILE
1	B	136	ILE
1	B	138	VAL
1	B	139	SER
1	B	142	VAL
1	B	144	ILE
1	B	145	LEU
1	B	147	TYR
1	B	150	TRP
1	B	157	LYS
1	B	159	ARG
1	B	167	LEU
1	B	168	ASP
1	B	174	TYR
1	B	175	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	MET
1	B	178	GLU
1	B	179	LYS
1	B	183	HIS
1	B	185	SER
1	B	186	SER
1	B	187	CYS
1	B	191	ILE
1	B	192	LEU
1	B	198	SER
1	B	203	TRP
1	B	204	SER
1	B	206	VAL
1	B	208	VAL
1	B	210(A)	LEU
1	B	210(B)	GLN
1	B	211	GLN
1	B	213	ASN
1	B	215	GLU
1	B	216	MET
1	B	218	THR
1	B	220	ASN
1	B	222	SER
1	B	225	TRP
1	B	226	LYS
1	B	228	VAL
1	B	229	HIS
1	B	230	LYS
1	B	232	VAL
1	B	234	GLU
1	B	235	SER
1	B	237	TYR
1	B	238	GLU
1	B	240	ILE
1	B	243	LYS
1	B	246	THR
1	B	247	ASN
1	B	250	ILE
1	B	252	LEU
1	B	256	ASP
1	B	258	ILE
1	B	259	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	261	MET
1	B	268	ILE
1	B	272	SER
1	B	273	THR
1	B	275	VAL
1	B	278	MET
1	B	279	TYR
1	B	281	ILE
1	B	286	PHE
1	B	287	LEU
1	B	288	SER
1	B	291	CYS
1	B	296	ARG
1	B	303	ILE
1	B	305	GLN
1	B	306	LYS
1	B	307	LEU
1	B	308	LYS
1	B	312	VAL
1	B	315	LEU
1	B	317	ASN
1	B	318	SER
1	B	320	ASP
1	B	321	THR
1	B	322	LEU
1	B	323	TRP
1	B	327	LYS
1	B	328	ASP
1	B	329	LEU
1	B	330(A)	LYS
1	B	331	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	111	ASN
1	A	114	GLN
1	A	220	ASN
1	A	224	ASN
1	A	229	HIS
1	A	317	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	103	GLN
1	B	111	ASN
1	B	114	GLN
1	B	220	ASN
1	B	224	ASN
1	B	229	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CIT	B	333	1	3,12,12	11.32	2 (66%)	3,17,17	4.98	2 (66%)
2	LNC	A	332	-	46,55,55	1.98	3 (6%)	58,83,83	2.17	11 (18%)
2	LNC	B	332	-	46,55,55	1.98	3 (6%)	58,83,83	2.17	11 (18%)
3	CIT	A	333	1	3,12,12	11.32	2 (66%)	3,17,17	4.98	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CIT	B	333	1	-	1/6/16/16	-
2	LNC	A	332	-	-	19/31/71/71	0/5/5/5
2	LNC	B	332	-	-	19/31/71/71	0/5/5/5
3	CIT	A	333	1	-	1/6/16/16	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	333	CIT	C4-C3	14.36	1.75	1.54
3	A	333	CIT	C4-C3	14.36	1.75	1.54
3	B	333	CIT	O7-C3	-13.29	1.22	1.43
3	A	333	CIT	O7-C3	-13.29	1.22	1.43
2	A	332	LNC	C2N-N1N	-12.15	1.20	1.35
2	B	332	LNC	C2N-N1N	-12.15	1.20	1.35
2	A	332	LNC	C4N-C3N	-3.30	1.34	1.39
2	B	332	LNC	C4N-C3N	-3.30	1.34	1.39
2	A	332	LNC	C8A-N7A	-2.57	1.30	1.34
2	B	332	LNC	C8A-N7A	-2.57	1.30	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	LNC	PA-O3-PN	-9.17	101.37	132.83
2	B	332	LNC	PA-O3-PN	-9.17	101.37	132.83
2	A	332	LNC	C3N-C2N-N1N	8.29	128.53	120.43
2	B	332	LNC	C3N-C2N-N1N	8.29	128.53	120.43
3	B	333	CIT	C3-C2-C1	-7.00	103.77	114.98
3	A	333	CIT	C3-C2-C1	-7.00	103.77	114.98
3	B	333	CIT	C3-C4-C5	-4.79	107.31	114.98
3	A	333	CIT	C3-C4-C5	-4.79	107.31	114.98
2	A	332	LNC	C3N-C7N-N7N	4.21	122.80	117.75
2	B	332	LNC	C3N-C7N-N7N	4.21	122.80	117.75
2	A	332	LNC	C2N-N1N-C6N	-4.05	118.28	121.97
2	B	332	LNC	C2N-N1N-C6N	-4.05	118.28	121.97
2	A	332	LNC	O7N-C7N-N7N	-3.78	117.21	122.58
2	B	332	LNC	O7N-C7N-N7N	-3.78	117.21	122.58
2	A	332	LNC	C5N-C6N-N1N	-3.25	118.99	121.03
2	B	332	LNC	C5N-C6N-N1N	-3.25	118.99	121.03
2	A	332	LNC	C2N-C3N-C4N	-2.99	115.48	118.67
2	B	332	LNC	C2N-C3N-C4N	-2.99	115.48	118.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	LNC	O4D-C1D-C2D	-2.93	102.64	106.93
2	B	332	LNC	O4D-C1D-C2D	-2.93	102.64	106.93
2	A	332	LNC	CGS-CBS-CAS	-2.73	110.41	114.44
2	B	332	LNC	CGS-CBS-CAS	-2.73	110.41	114.44
2	A	332	LNC	C6N-C5N-C4N	2.19	120.76	117.07
2	B	332	LNC	C6N-C5N-C4N	2.19	120.76	117.07
2	A	332	LNC	C3N-C4N-C5N	-2.09	117.96	120.86
2	B	332	LNC	C3N-C4N-C5N	-2.09	117.96	120.86

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	332	LNC	CAS-CBS-CGS-C5N
2	A	332	LNC	OAS-CAS-CBS-CGS
2	A	332	LNC	CS-CAS-CBS-CGS
2	A	332	LNC	O4D-C1D-N1N-C6N
2	A	332	LNC	C2D-C1D-N1N-C6N
2	A	332	LNC	O4D-C1D-N1N-C2N
2	A	332	LNC	C2D-C1D-N1N-C2N
2	A	332	LNC	C5D-O5D-PN-O2N
2	A	332	LNC	C5D-O5D-PN-O3
2	A	332	LNC	O4B-C4B-C5B-O5B
2	A	332	LNC	C3B-C4B-C5B-O5B
2	B	332	LNC	CAS-CBS-CGS-C5N
2	B	332	LNC	OAS-CAS-CBS-CGS
2	B	332	LNC	CS-CAS-CBS-CGS
2	B	332	LNC	O4D-C1D-N1N-C6N
2	B	332	LNC	C2D-C1D-N1N-C6N
2	B	332	LNC	O4D-C1D-N1N-C2N
2	B	332	LNC	C2D-C1D-N1N-C2N
2	B	332	LNC	C5D-O5D-PN-O2N
2	B	332	LNC	C5D-O5D-PN-O3
2	B	332	LNC	O4B-C4B-C5B-O5B
2	B	332	LNC	C3B-C4B-C5B-O5B
3	B	333	CIT	O7-C3-C4-C5
3	A	333	CIT	O7-C3-C4-C5
2	A	332	LNC	O4D-C4D-C5D-O5D
2	B	332	LNC	O4D-C4D-C5D-O5D
2	A	332	LNC	PA-O3-PN-O1N
2	B	332	LNC	PA-O3-PN-O1N
2	A	332	LNC	C4N-C5N-CGS-CBS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	332	LNC	C4N-C5N-CGS-CBS
2	A	332	LNC	C3D-C4D-C5D-O5D
2	B	332	LNC	C3D-C4D-C5D-O5D
2	A	332	LNC	C5B-O5B-PA-O3
2	B	332	LNC	C5B-O5B-PA-O3
2	A	332	LNC	PA-O3-PN-O2N
2	B	332	LNC	PA-O3-PN-O2N
2	A	332	LNC	C5D-O5D-PN-O1N
2	A	332	LNC	C5B-O5B-PA-O2A
2	B	332	LNC	C5D-O5D-PN-O1N
2	B	332	LNC	C5B-O5B-PA-O2A

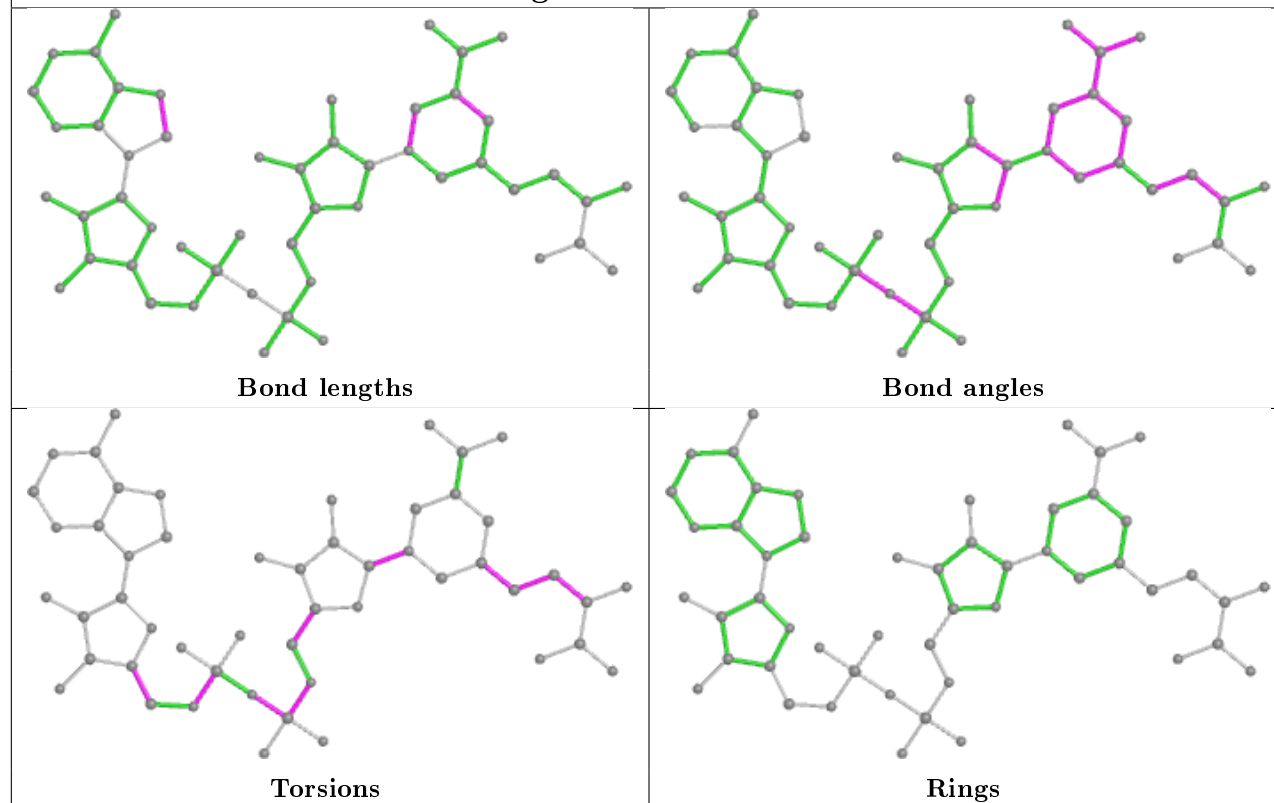
There are no ring outliers.

4 monomers are involved in 128 short contacts:

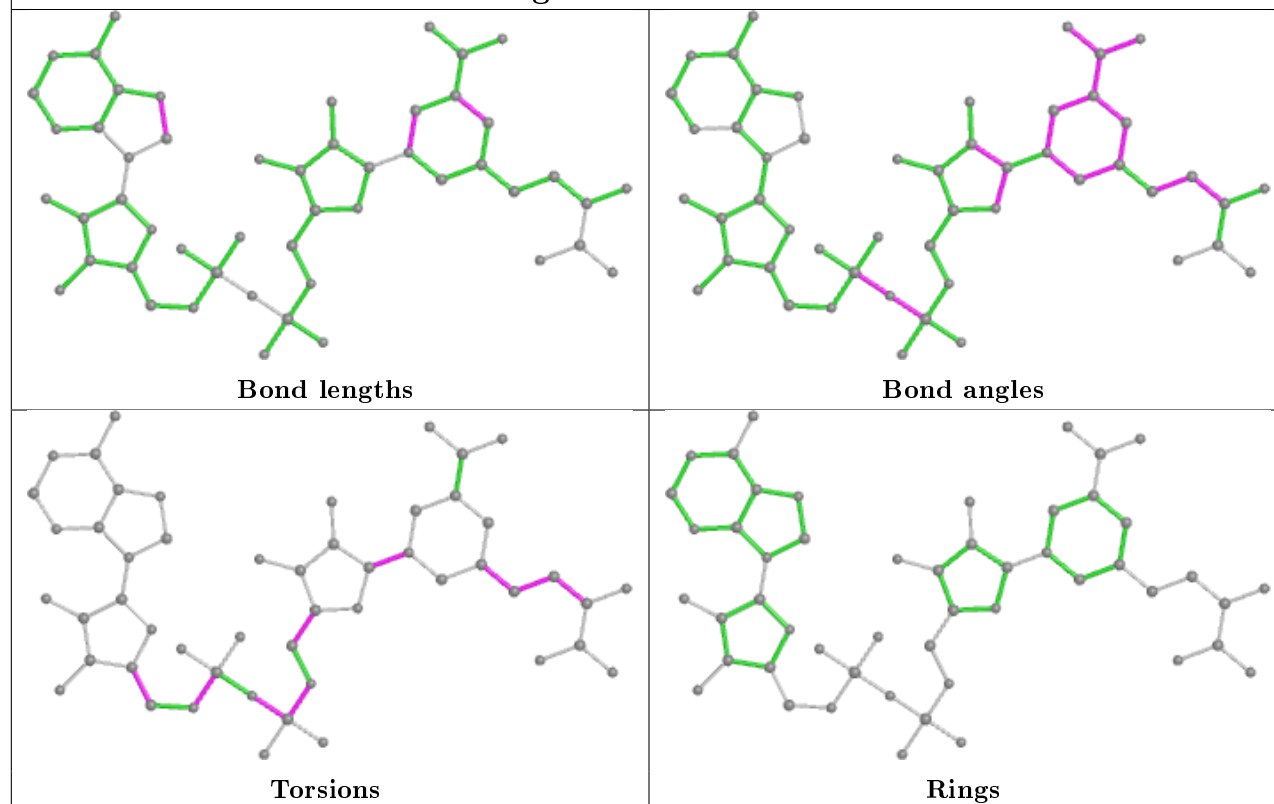
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	333	CIT	15	0
2	A	332	LNC	50	0
2	B	332	LNC	48	0
3	A	333	CIT	15	0

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

Ligand LNC A 332



Ligand LNC B 332



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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

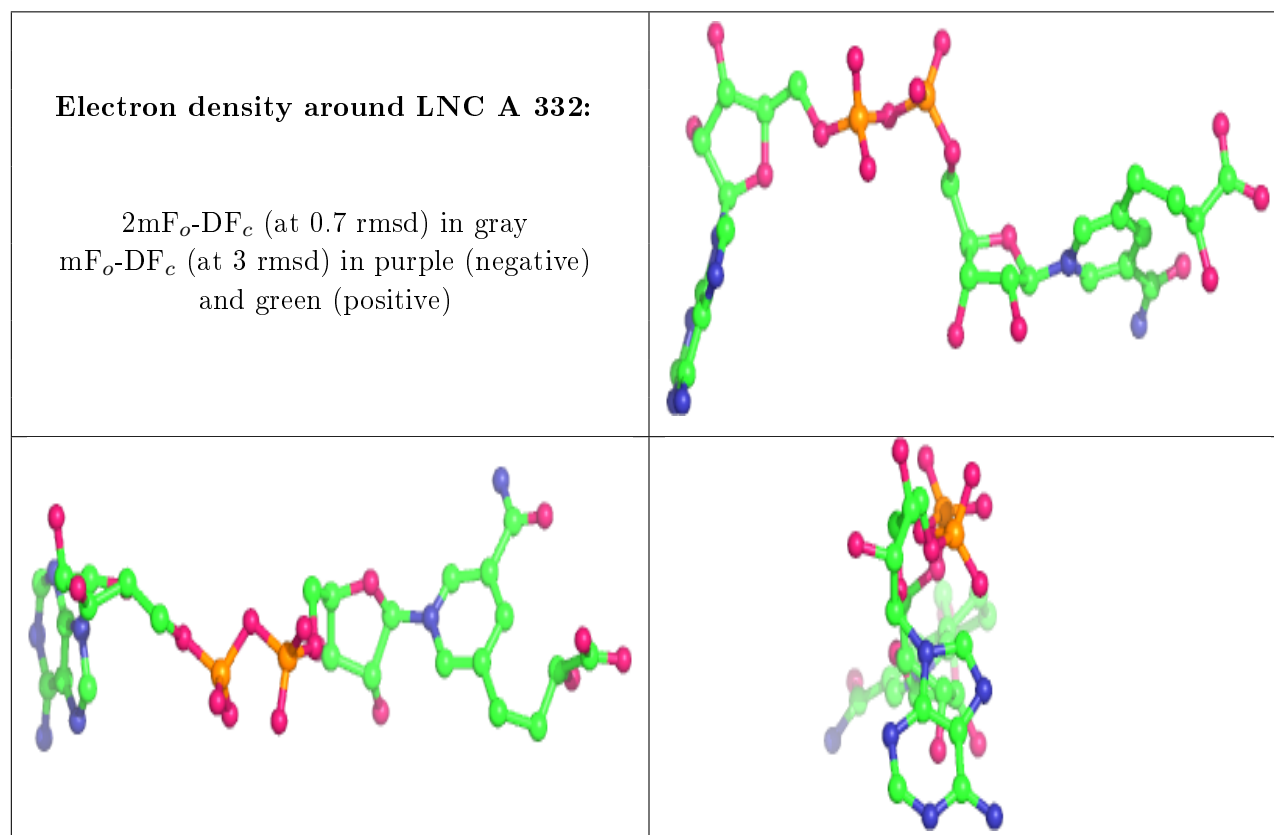
6.3 Carbohydrates [i](#)

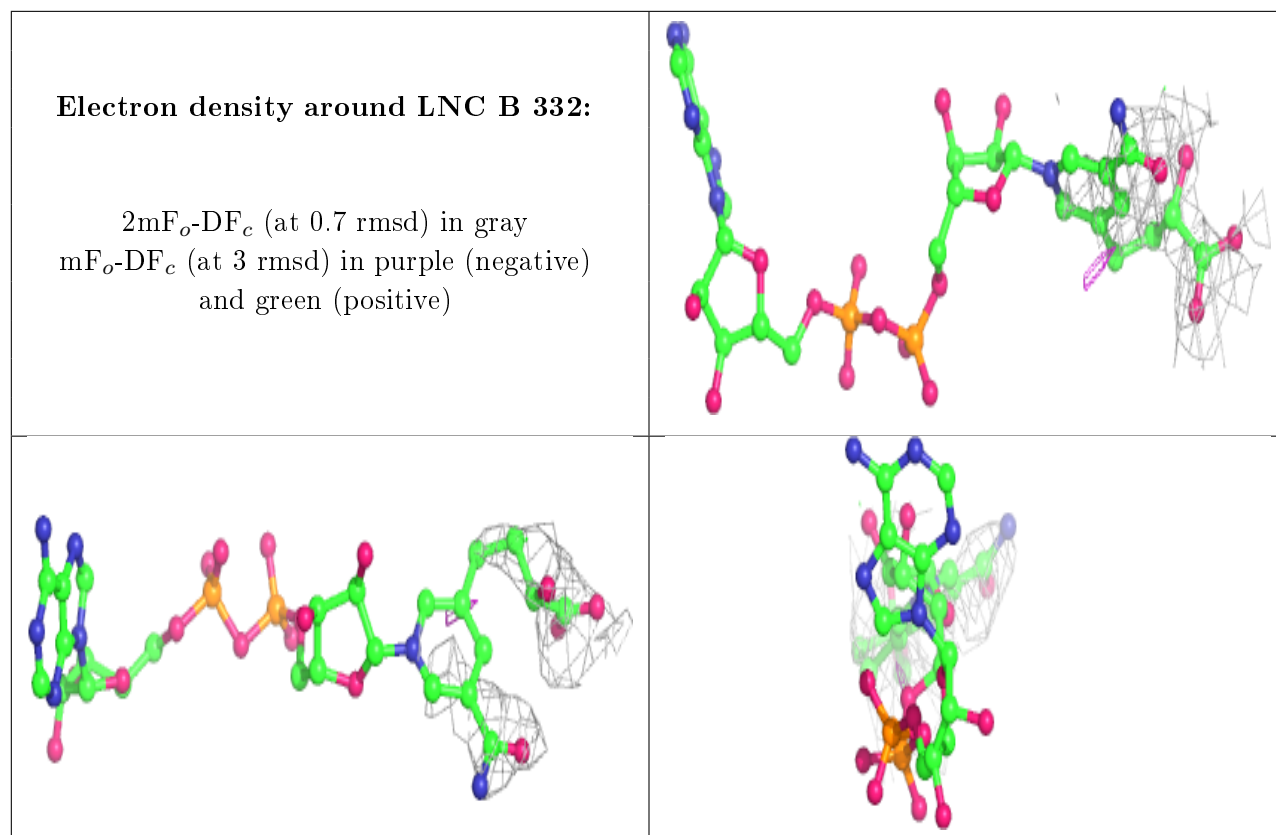
Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.