Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:01 pm BST

PDB ID	:	4FSX
Title	:	crystal structure of Se-substituted Zea mays ZMET2 in complex with SAH
Authors	:	Du, J.; Patel, D.J.
Deposited on	:	2012-06-27
Resolution	:	3.20 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:

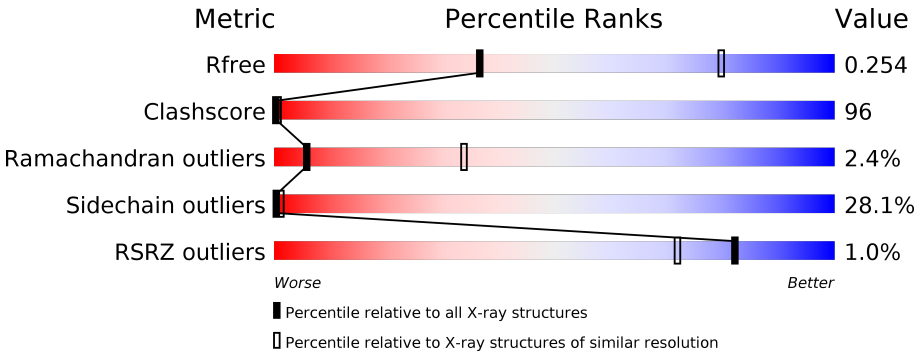
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	784	% 21% 47% 17% 13%
1	B	784	% 19% 48% 18% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10631 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.

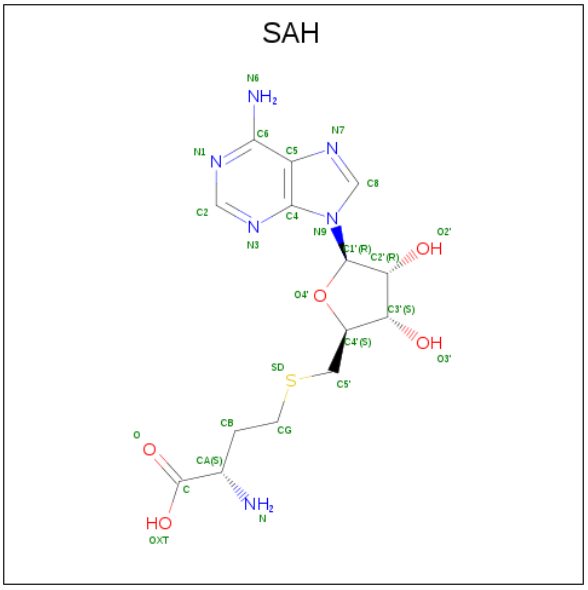
- Molecule 1 is a protein called DNA (cytosine-5)-methyltransferase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	680	Total	C	N	O	S	Se	0	0	0
			5331	3401	904	993	18	15			
1	B	675	Total	C	N	O	S	Se	0	0	0
			5248	3346	893	976	18	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	SER	-	EXPRESSION TAG	UNP Q9AXT8
B	129	SER	-	EXPRESSION TAG	UNP Q9AXT8

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

Continued on next page...

Continued from previous page...

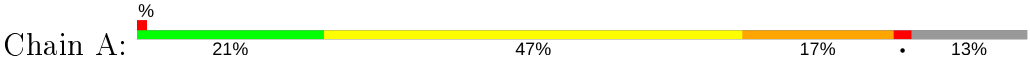
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

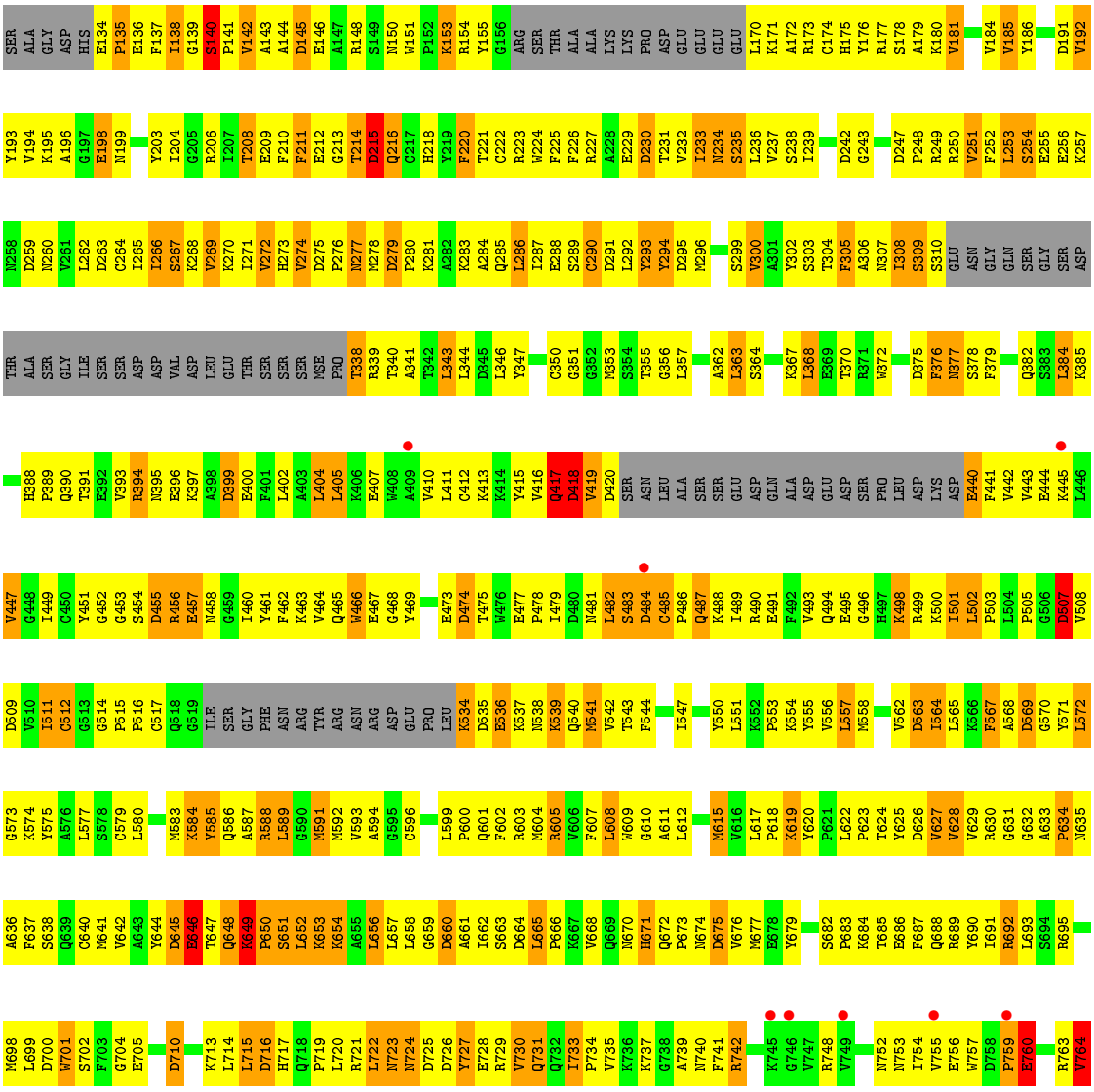
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA (cytosine-5)-methyltransferase 1

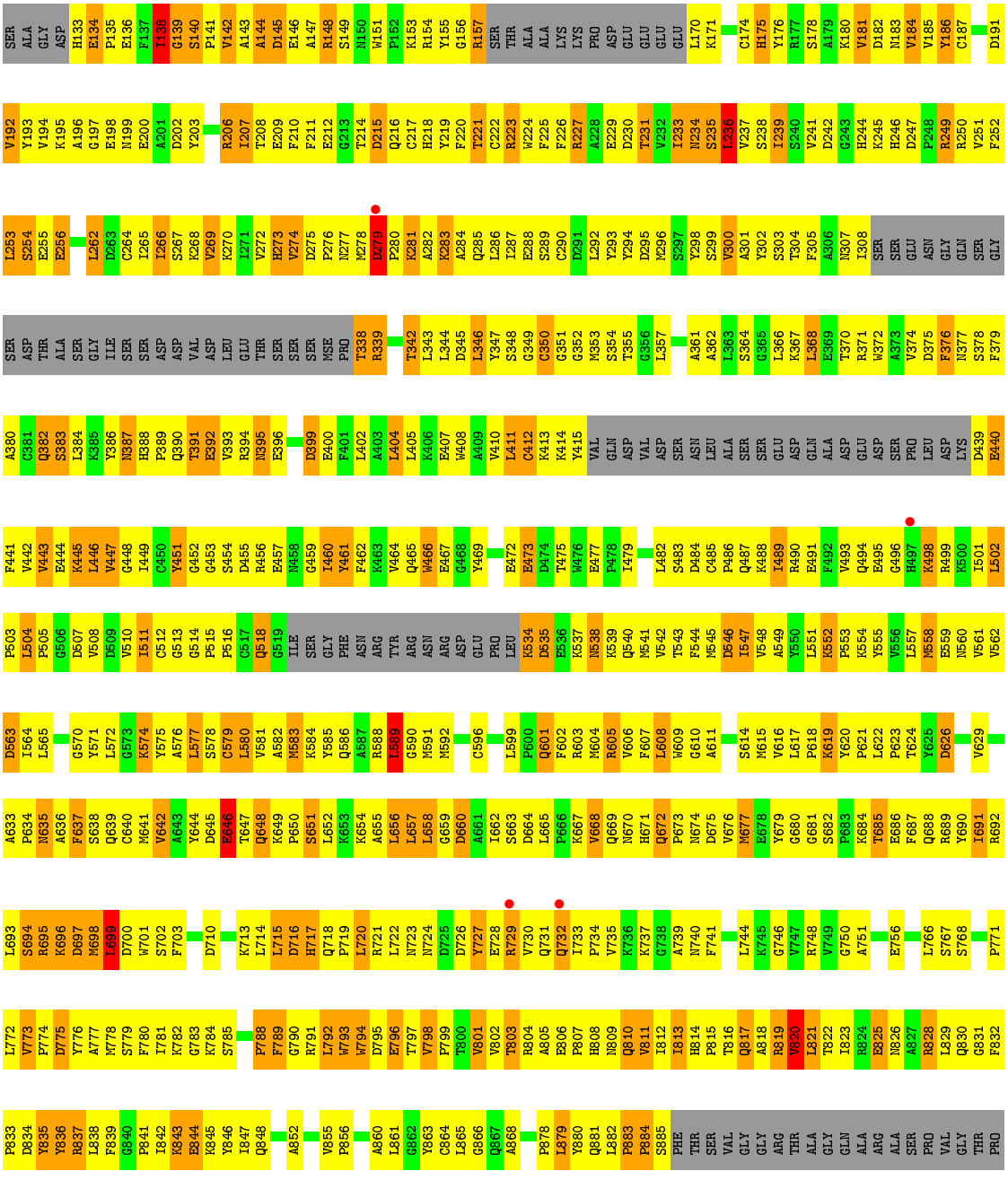
Chain A:





• Molecule 1: DNA (cytosine-5)-methyltransferase 1

Chain B:




ALA
GLY
GLU
VAL
VAL
GLU
GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	64.86Å 88.95Å 113.49Å 93.47° 95.53° 110.41°	Depositor
Resolution (Å)	40.25 – 3.20 48.87 – 3.19	Depositor EDS
% Data completeness (in resolution range)	97.6 (40.25-3.20) 98.9 (48.87-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.240 , 0.263 0.230 , 0.254	Depositor DCC
R_{free} test set	1946 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 69.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10631	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.64	0/5445	0.79	5/7358 (0.1%)
1	B	0.63	1/5362 (0.0%)	0.82	12/7252 (0.2%)
All	All	0.63	1/10807 (0.0%)	0.80	17/14610 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	579	CYS	CB-SG	-5.50	1.72	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	535	ASP	CB-CG-OD1	-9.04	110.17	118.30
1	A	632	GLY	N-CA-C	-8.60	91.61	113.10
1	B	535	ASP	N-CA-C	8.56	134.12	111.00
1	B	146	GLU	N-CA-C	-6.83	92.56	111.00
1	B	746	GLY	N-CA-C	-6.81	96.08	113.10
1	A	809	ASN	N-CA-C	6.74	129.18	111.00
1	B	680	GLY	N-CA-C	-6.54	96.76	113.10
1	B	699	LEU	CA-CB-CG	-6.52	100.31	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	810	GLN	N-CA-C	6.51	128.59	111.00
1	A	649	LYS	N-CA-C	-6.46	93.57	111.00
1	B	657	LEU	CA-CB-CG	-6.36	100.67	115.30
1	A	418	ASP	N-CA-C	-6.25	94.13	111.00
1	B	279	ASP	N-CA-CB	-6.17	99.50	110.60
1	B	139	GLY	N-CA-C	-5.96	98.19	113.10
1	B	279	ASP	C-N-CD	-5.96	107.49	120.60
1	B	589	LEU	CA-CB-CG	5.08	126.98	115.30
1	A	879	LEU	CB-CG-CD2	-5.05	102.41	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	ASP	Peptide
1	A	455	ASP	Peptide
1	A	507	ASP	Peptide
1	B	504	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5331	0	5166	987	0
1	B	5248	0	5023	1014	0
2	A	26	0	19	6	0
2	B	26	0	19	6	0
All	All	10631	0	10227	1998	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 96.

All (1998) 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:695:ARG:HG2	1:B:835:TYR:CD1	1.50	1.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:LEU:C	1:B:657:LEU:HD12	1.33	1.45
1:A:134:GLU:HB3	1:A:135:PRO:CD	1.43	1.38
1:B:883:PRO:CG	1:B:884:PRO:HD2	1.53	1.37
1:B:695:ARG:HG2	1:B:835:TYR:CE1	1.64	1.32
1:B:699:LEU:HD12	1:B:701:TRP:NE1	1.44	1.31
1:B:142:VAL:HG11	1:B:174:CYS:SG	1.75	1.26
1:B:883:PRO:HG2	1:B:884:PRO:CD	1.66	1.25
1:B:457:GLU:HB2	1:B:461:TYR:OH	1.35	1.24
1:A:134:GLU:CB	1:A:135:PRO:HD2	1.64	1.23
1:A:784:LYS:C	1:A:786:LEU:HD12	1.58	1.23
1:B:656:LEU:O	1:B:657:LEU:HD12	1.39	1.22
1:A:404:LEU:O	1:A:404:LEU:HD12	1.34	1.22
1:B:142:VAL:CG1	1:B:174:CYS:SG	2.29	1.20
1:A:784:LYS:CA	1:A:786:LEU:HD12	1.72	1.20
1:B:279:ASP:O	1:B:283:LYS:HG3	1.38	1.18
1:A:822:THR:HG22	1:A:825:GLU:OE2	1.44	1.17
1:B:279:ASP:CB	1:B:280:PRO:HD3	1.74	1.17
1:A:781:ILE:N	1:A:781:ILE:HD13	1.57	1.16
1:A:209:GLU:HB2	1:A:221:THR:CG2	1.75	1.16
1:A:273:HIS:HB2	1:A:294:TYR:CE2	1.81	1.15
1:B:699:LEU:HD12	1:B:701:TRP:CD1	1.82	1.15
1:B:279:ASP:HB3	1:B:280:PRO:HD3	1.23	1.14
1:A:456:ARG:HH21	1:A:456:ARG:HG2	1.04	1.14
1:B:604:MSE:SE	1:B:641:MSE:HE1	1.97	1.14
1:B:134:GLU:OE1	1:B:135:PRO:HD3	1.44	1.14
1:B:695:ARG:CG	1:B:695:ARG:HH11	1.59	1.14
1:A:664:ASP:O	1:A:664:ASP:OD1	1.66	1.13
1:A:780:PHE:HE2	1:A:809:ASN:ND2	1.45	1.13
1:A:273:HIS:HB2	1:A:294:TYR:HE2	1.00	1.12
1:B:691:ILE:CD1	1:B:833:PRO:HA	1.78	1.12
1:B:699:LEU:HD11	1:B:701:TRP:CD2	1.83	1.12
1:A:209:GLU:CB	1:A:221:THR:HG22	1.79	1.12
1:B:691:ILE:HD11	1:B:833:PRO:HA	1.13	1.12
1:A:412:CYS:O	1:A:416:VAL:HG23	1.46	1.11
1:B:148:ARG:HH11	1:B:148:ARG:HG2	1.07	1.11
1:B:227:ARG:HB2	1:B:230:ASP:OD2	1.48	1.11
1:B:772:LEU:O	1:B:773:VAL:HG22	1.47	1.11
1:B:837:ARG:HH11	1:B:837:ARG:HG3	1.14	1.11
1:A:250:ARG:NH1	1:A:252:PHE:HE2	1.48	1.10
1:B:883:PRO:HB2	1:B:884:PRO:HD3	1.25	1.10
1:A:879:LEU:HD22	1:A:879:LEU:N	1.67	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ALA:HA	2:A:1000:SAH:OXT	1.49	1.09
1:A:195:LYS:NZ	1:A:264:CYS:HA	1.67	1.09
1:B:206:ARG:HH11	1:B:206:ARG:HG3	0.98	1.09
1:A:784:LYS:CB	1:A:786:LEU:CD1	2.30	1.09
1:B:645:ASP:O	1:B:646:GLU:HB3	1.45	1.09
1:A:440:GLU:HG2	1:A:441:PHE:H	1.09	1.09
1:B:667:LYS:HA	1:B:817:GLN:OE1	1.52	1.08
1:A:540:GLN:HA	1:A:540:GLN:NE2	1.47	1.08
1:B:226:PHE:CE2	1:B:254:SER:HB2	1.89	1.08
1:B:796:GLU:HG3	1:B:797:THR:H	1.19	1.08
1:A:781:ILE:HG12	1:A:786:LEU:HD21	1.34	1.08
1:A:279:ASP:HB2	1:A:280:PRO:HD2	1.31	1.07
1:B:143:ALA:O	1:B:144:ALA:HB3	1.54	1.07
1:B:649:LYS:HD2	1:B:652:LEU:HD12	1.36	1.07
1:A:154:ARG:HH22	1:A:209:GLU:CD	1.55	1.07
1:A:417:GLN:NE2	1:A:417:GLN:HA	1.66	1.07
1:A:592:MSE:HE1	1:A:861:LEU:HD21	1.11	1.06
1:B:699:LEU:CD1	1:B:701:TRP:CD1	2.38	1.06
1:B:883:PRO:CB	1:B:884:PRO:CD	2.34	1.06
1:A:784:LYS:O	1:A:786:LEU:HD12	1.53	1.06
1:B:685:THR:HG22	1:B:688:GLN:H	1.18	1.06
1:B:852:ALA:HA	2:B:1000:SAH:OXT	1.55	1.06
1:B:667:LYS:HG3	1:B:817:GLN:OE1	1.55	1.06
1:B:820:VAL:HG13	1:B:821:LEU:H	1.01	1.06
1:A:209:GLU:HB3	1:A:221:THR:HG22	1.38	1.05
1:A:214:THR:O	1:A:215:ASP:HB2	1.55	1.05
1:B:695:ARG:HG3	1:B:695:ARG:HH11	0.91	1.05
1:A:173:ARG:HH11	1:A:212:GLU:CD	1.56	1.05
1:A:733:ILE:CG2	1:A:791:ARG:HH21	1.68	1.05
1:A:733:ILE:HG22	1:A:791:ARG:HH21	1.22	1.05
1:B:134:GLU:OE1	1:B:134:GLU:HA	1.47	1.05
1:B:231:THR:OG1	1:B:233:ILE:HG23	1.55	1.05
1:A:478:PRO:HG2	1:A:481:ASN:HB2	1.06	1.05
1:B:278:MSE:HB3	1:B:282:ALA:HB3	1.39	1.05
1:B:791:ARG:HD2	1:B:792:LEU:H	1.16	1.05
1:A:154:ARG:HB3	1:A:170:LEU:HD23	1.34	1.04
1:A:250:ARG:NH1	1:A:252:PHE:CE2	2.24	1.04
1:B:699:LEU:CD1	1:B:701:TRP:CE2	2.41	1.04
1:B:748:ARG:CB	1:B:756:GLU:H	1.71	1.04
1:A:281:LYS:HA	1:A:284:ALA:HB3	1.37	1.04
1:A:652:LEU:O	1:A:653:LYS:C	1.96	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:VAL:CG1	1:B:713:LYS:CE	2.36	1.03
1:B:685:THR:CG2	1:B:688:GLN:H	1.70	1.03
1:B:656:LEU:C	1:B:657:LEU:CD1	2.27	1.03
1:B:676:VAL:HG13	1:B:713:LYS:CE	1.89	1.03
1:B:723:ASN:OD1	1:B:726:ASP:HB2	1.58	1.03
1:A:229:GLU:HG3	1:A:237:VAL:HG11	1.39	1.02
1:B:676:VAL:HG13	1:B:713:LYS:HE2	1.41	1.02
1:B:695:ARG:CG	1:B:835:TYR:CD1	2.43	1.02
1:A:596:CYS:HB3	1:A:623:PRO:HB3	1.39	1.02
1:A:273:HIS:CB	1:A:294:TYR:HE2	1.72	1.02
1:A:367:LYS:HE3	1:A:701:TRP:CH2	1.93	1.02
1:B:793:TRP:HB3	1:B:815:PRO:HB3	1.42	1.02
1:A:759:PRO:O	1:A:760:GLU:HB2	1.60	1.01
1:B:646:GLU:HG2	1:B:646:GLU:O	1.60	1.01
1:B:379:PHE:CD2	1:B:844:GLU:HG2	1.95	1.01
1:A:715:LEU:HD22	1:A:837:ARG:HG2	1.42	1.01
1:A:725:ASP:HA	1:A:766:LEU:CD1	1.90	1.00
1:A:772:LEU:HD13	1:A:773:VAL:HG22	1.38	1.00
1:B:339:ARG:HH11	1:B:339:ARG:HG2	1.23	1.00
1:B:772:LEU:C	1:B:774:PRO:CD	2.30	1.00
1:B:729:ARG:HH21	1:B:772:LEU:HA	1.25	1.00
1:A:879:LEU:HD22	1:A:879:LEU:H	1.17	0.99
1:B:695:ARG:HG2	1:B:835:TYR:HD1	1.16	0.99
1:A:541:MSE:SE	1:A:558:MSE:HE1	2.12	0.99
1:A:515:PRO:HG2	1:A:558:MSE:HE3	1.43	0.99
1:A:646:GLU:HA	1:A:646:GLU:OE2	1.58	0.99
1:B:699:LEU:HD12	1:B:701:TRP:CE2	1.96	0.99
1:B:549:ALA:HA	1:B:583:MSE:HE2	1.43	0.98
1:B:883:PRO:HB2	1:B:884:PRO:CD	1.90	0.98
1:A:803:THR:HA	1:A:850:GLY:HA3	1.39	0.98
1:A:300:VAL:O	1:A:300:VAL:HG23	1.63	0.98
1:A:784:LYS:CB	1:A:786:LEU:HD11	1.93	0.98
1:B:691:ILE:HD11	1:B:833:PRO:CA	1.93	0.98
1:B:206:ARG:CG	1:B:206:ARG:HH11	1.76	0.98
1:B:820:VAL:HG13	1:B:821:LEU:N	1.78	0.97
1:B:676:VAL:CG1	1:B:713:LYS:HE2	1.94	0.97
1:A:134:GLU:HB3	1:A:135:PRO:HD2	0.99	0.97
1:A:784:LYS:H	1:A:786:LEU:CD1	1.76	0.97
1:B:206:ARG:NH1	1:B:206:ARG:HG3	1.68	0.97
1:B:143:ALA:O	1:B:144:ALA:CB	2.12	0.97
1:B:134:GLU:CD	1:B:135:PRO:HD3	1.85	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:LEU:HD21	1:A:814:HIS:HE1	1.29	0.96
1:A:353:MSE:HB2	1:A:853:VAL:HG11	1.47	0.96
1:A:540:GLN:HA	1:A:540:GLN:HE21	1.25	0.96
1:B:445:LYS:O	1:B:446:LEU:HD23	1.65	0.96
1:B:773:VAL:N	1:B:774:PRO:HD2	1.79	0.95
1:A:502:LEU:HD23	1:A:503:PRO:HD2	1.45	0.95
1:A:784:LYS:CA	1:A:786:LEU:CD1	2.44	0.95
1:B:773:VAL:N	1:B:774:PRO:CD	2.29	0.95
1:B:518:GLN:HB2	1:B:537:LYS:HB3	1.48	0.95
1:A:787:LYS:N	1:A:788:PRO:HD3	1.81	0.95
1:A:727:TYR:HE2	1:A:731:GLN:OE1	1.48	0.95
1:B:685:THR:HG22	1:B:688:GLN:N	1.80	0.95
1:B:772:LEU:C	1:B:774:PRO:HD3	1.86	0.95
1:A:209:GLU:CB	1:A:221:THR:CG2	2.41	0.95
1:A:784:LYS:N	1:A:786:LEU:CD1	2.30	0.94
1:B:645:ASP:O	1:B:645:ASP:OD1	1.85	0.94
1:A:879:LEU:N	1:A:879:LEU:CD2	2.30	0.94
1:B:699:LEU:CD1	1:B:701:TRP:NE1	2.30	0.94
1:A:663:SER:HB3	1:A:688:GLN:HE22	1.31	0.94
1:B:379:PHE:HD2	1:B:844:GLU:HG2	1.30	0.94
1:B:814:HIS:CD2	1:B:816:THR:H	1.85	0.94
1:A:220:PHE:H	1:A:220:PHE:HD2	1.14	0.94
1:A:589:LEU:HA	1:A:620:TYR:OH	1.68	0.94
1:B:142:VAL:HG13	1:B:174:CYS:SG	2.06	0.94
1:B:279:ASP:CB	1:B:280:PRO:CD	2.43	0.94
1:B:226:PHE:HE2	1:B:254:SER:HB2	1.26	0.94
1:B:699:LEU:HD23	1:B:699:LEU:O	1.68	0.93
1:B:814:HIS:HD2	1:B:816:THR:H	1.10	0.93
1:A:714:LEU:HD21	1:A:717:HIS:HB2	1.48	0.93
1:A:404:LEU:C	1:A:404:LEU:HD12	1.72	0.93
1:A:772:LEU:O	1:A:774:PRO:HD3	1.68	0.93
1:A:220:PHE:CE2	1:A:260:ASN:HB2	2.03	0.93
1:A:772:LEU:HD13	1:A:773:VAL:H	1.33	0.93
1:A:764:VAL:HG21	1:A:772:LEU:HG	1.48	0.93
1:B:307:ASN:ND2	1:B:586:GLN:CD	2.22	0.93
1:B:355:THR:HG22	1:B:388:HIS:NE2	1.83	0.92
1:A:780:PHE:CE2	1:A:809:ASN:ND2	2.37	0.92
1:A:786:LEU:HB3	1:A:788:PRO:HD3	1.48	0.92
1:A:605:ARG:HG2	1:A:605:ARG:HH11	1.31	0.92
1:B:796:GLU:HG3	1:B:797:THR:N	1.79	0.92
1:A:154:ARG:CZ	1:A:170:LEU:HD21	1.98	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LYS:O	1:A:213:GLY:HA2	1.69	0.92
1:B:695:ARG:CG	1:B:835:TYR:CE1	2.53	0.92
1:A:572:LEU:HD22	1:A:572:LEU:H	1.35	0.92
1:A:668:VAL:H	1:A:817:GLN:HE22	1.01	0.92
1:B:814:HIS:HD2	1:B:816:THR:N	1.66	0.92
1:A:279:ASP:HB2	1:A:280:PRO:CD	1.99	0.92
1:B:685:THR:HG23	1:B:687:PHE:N	1.85	0.92
1:B:562:VAL:HG21	1:B:604:MSE:HE3	1.51	0.92
1:B:833:PRO:HB2	1:B:835:TYR:CE2	2.04	0.92
1:A:605:ARG:HH11	1:A:605:ARG:CG	1.83	0.91
1:A:648:GLN:OE1	1:A:648:GLN:HA	1.67	0.91
1:A:781:ILE:N	1:A:781:ILE:CD1	2.30	0.91
1:A:668:VAL:H	1:A:817:GLN:NE2	1.67	0.91
1:A:151:TRP:HE1	1:A:175:HIS:CE1	1.87	0.91
1:A:478:PRO:CG	1:A:481:ASN:HB2	1.99	0.91
1:B:236:LEU:HD13	1:B:574:LYS:HB2	1.51	0.91
1:B:676:VAL:O	1:B:676:VAL:HG12	1.68	0.91
1:B:599:LEU:HD11	1:B:856:PRO:HG2	1.50	0.91
1:A:727:TYR:CE2	1:A:731:GLN:OE1	2.24	0.90
1:A:740:ASN:ND2	1:A:742:ARG:HG3	1.87	0.90
1:B:820:VAL:CG1	1:B:821:LEU:H	1.85	0.90
1:B:881:GLN:OE1	1:B:882:LEU:N	2.05	0.90
1:A:555:TYR:HE2	1:A:618:PRO:HD3	1.37	0.89
1:A:781:ILE:CG1	1:A:786:LEU:HD21	2.02	0.89
1:A:171:LYS:HB2	1:A:214:THR:HG23	1.54	0.89
1:A:415:TYR:CD2	1:A:490:ARG:HG2	2.08	0.89
1:A:154:ARG:NH2	1:A:209:GLU:CD	2.26	0.89
1:B:699:LEU:CD1	1:B:701:TRP:CG	2.56	0.89
1:A:784:LYS:CB	1:A:786:LEU:HD12	1.99	0.89
1:A:173:ARG:HH11	1:A:212:GLU:CG	1.86	0.89
1:A:644:TYR:CE2	1:A:649:LYS:HG3	2.07	0.89
1:B:844:GLU:O	1:B:847:ILE:HG13	1.72	0.89
1:A:444:GLU:O	1:A:488:LYS:HE3	1.73	0.88
1:A:879:LEU:H	1:A:879:LEU:CD2	1.84	0.88
1:B:279:ASP:CG	1:B:280:PRO:HD3	1.93	0.88
1:B:279:ASP:O	1:B:283:LYS:CG	2.20	0.88
1:B:279:ASP:HB3	1:B:280:PRO:CD	2.01	0.88
1:B:695:ARG:HG3	1:B:695:ARG:NH1	1.63	0.88
1:B:748:ARG:CB	1:B:756:GLU:N	2.36	0.88
1:A:195:LYS:HZ3	1:A:264:CYS:HA	1.35	0.88
1:A:236:LEU:HD13	1:A:574:LYS:HB2	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PHE:CD2	1:A:844:GLU:HG2	2.09	0.88
1:B:226:PHE:CE2	1:B:254:SER:CB	2.55	0.88
1:B:883:PRO:CB	1:B:884:PRO:HD3	2.01	0.88
1:A:220:PHE:CD2	1:A:260:ASN:O	2.26	0.88
1:A:727:TYR:O	1:A:727:TYR:HD2	1.56	0.88
1:B:554:LYS:HD3	1:B:615:MSE:HE3	1.55	0.88
1:A:748:ARG:CB	1:A:755:VAL:HA	2.03	0.88
1:B:408:TRP:O	1:B:412:CYS:HB2	1.74	0.88
1:A:633:ALA:O	1:A:634:PRO:O	1.90	0.88
1:A:554:LYS:HB3	1:A:615:MSE:HE3	1.55	0.87
1:B:443:VAL:HG12	1:B:466:TRP:CE3	2.09	0.87
1:B:644:TYR:O	1:B:645:ASP:HB3	1.73	0.87
1:A:215:ASP:O	1:A:216:GLN:HG3	1.73	0.87
1:B:391:THR:CG2	1:B:392:GLU:N	2.37	0.87
1:B:692:ARG:O	1:B:693:LEU:HD12	1.74	0.87
1:B:671:HIS:HD2	1:B:721:ARG:NH1	1.72	0.87
1:B:814:HIS:ND1	1:B:819:ARG:NH2	2.23	0.87
1:A:599:LEU:HD11	1:A:856:PRO:HG2	1.55	0.87
1:B:695:ARG:HD3	1:B:700:ASP:CG	1.94	0.87
1:B:729:ARG:HH21	1:B:772:LEU:CA	1.85	0.87
1:A:577:LEU:HD22	1:A:589:LEU:HD21	1.54	0.87
1:A:725:ASP:HA	1:A:766:LEU:HD13	1.56	0.87
1:A:728:GLU:OE1	1:A:766:LEU:HD21	1.74	0.87
1:B:445:LYS:C	1:B:446:LEU:HD23	1.95	0.87
1:A:279:ASP:CB	1:A:280:PRO:CD	2.51	0.87
1:B:699:LEU:HD11	1:B:701:TRP:CG	2.08	0.87
1:B:619:LYS:HG3	1:B:880:TYR:HB2	1.57	0.86
1:B:657:LEU:HD12	1:B:657:LEU:N	1.70	0.86
1:A:714:LEU:HD21	1:A:717:HIS:CB	2.04	0.86
1:B:791:ARG:CD	1:B:792:LEU:H	1.88	0.86
1:A:672:GLN:NE2	1:A:674:ASN:HB2	1.90	0.86
1:B:714:LEU:HD21	1:B:717:HIS:HB2	1.55	0.86
1:A:351:GLY:O	1:A:355:THR:HG23	1.74	0.86
1:A:822:THR:CG2	1:A:825:GLU:OE2	2.23	0.86
1:B:699:LEU:CD1	1:B:701:TRP:CD2	2.56	0.86
1:A:174:CYS:SG	1:A:212:GLU:OE1	2.33	0.86
1:B:339:ARG:CG	1:B:339:ARG:HH11	1.87	0.86
1:A:209:GLU:HB2	1:A:221:THR:HG23	1.57	0.86
1:B:690:TYR:O	1:B:693:LEU:HD13	1.75	0.86
1:B:729:ARG:HE	1:B:773:VAL:HG22	1.41	0.86
1:B:456:ARG:HG2	1:B:456:ARG:HH21	1.40	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:CYS:HB3	1:B:623:PRO:HB3	1.56	0.86
1:B:212:GLU:OE1	1:B:216:GLN:HG2	1.75	0.85
1:A:136:GLU:OE2	1:A:137:PHE:HB2	1.75	0.85
1:B:140:SER:OG	1:B:141:PRO:HD3	1.77	0.85
1:B:837:ARG:NH1	1:B:837:ARG:HG3	1.88	0.85
1:B:791:ARG:HD2	1:B:792:LEU:N	1.91	0.85
1:A:154:ARG:HB3	1:A:170:LEU:CD2	2.06	0.85
1:A:725:ASP:HA	1:A:766:LEU:HD11	1.56	0.85
1:A:772:LEU:CD1	1:A:773:VAL:HG22	2.06	0.85
1:A:478:PRO:HG2	1:A:481:ASN:CB	2.01	0.85
1:A:780:PHE:HE2	1:A:809:ASN:CG	1.80	0.85
1:A:588:ARG:NH2	1:A:878:PRO:HA	1.91	0.85
1:A:772:LEU:CD1	1:A:773:VAL:H	1.89	0.85
1:B:656:LEU:O	1:B:657:LEU:CD1	2.23	0.85
1:B:695:ARG:HA	1:B:835:TYR:CE1	2.11	0.85
1:B:605:ARG:HG2	1:B:605:ARG:HH11	1.42	0.85
1:A:236:LEU:HD23	1:A:239:ILE:HD11	1.58	0.84
1:A:134:GLU:HB3	1:A:135:PRO:HD3	1.55	0.84
1:A:665:LEU:HD13	1:A:665:LEU:O	1.74	0.84
1:A:787:LYS:HB3	1:A:811:VAL:HG12	1.59	0.84
1:B:534:LYS:NZ	1:B:535:ASP:HB2	1.91	0.84
1:B:658:LEU:HB3	1:B:794:TRP:HA	1.58	0.84
1:B:814:HIS:CD2	1:B:817:GLN:H	1.95	0.84
1:A:440:GLU:HG2	1:A:441:PHE:N	1.92	0.84
1:B:676:VAL:HG22	1:B:713:LYS:HE2	1.60	0.84
1:A:353:MSE:HB2	1:A:853:VAL:CG1	2.06	0.84
1:A:220:PHE:CD2	1:A:220:PHE:O	2.30	0.84
1:A:659:GLY:O	1:A:663:SER:HB2	1.78	0.84
1:B:235:SER:OG	1:B:236:LEU:N	2.09	0.84
1:A:764:VAL:HG21	1:A:772:LEU:CD1	2.08	0.84
1:A:171:LYS:CB	1:A:214:THR:HG23	2.08	0.84
1:A:173:ARG:NH1	1:A:212:GLU:CG	2.40	0.84
1:A:764:VAL:HG21	1:A:772:LEU:CG	2.08	0.84
1:A:247:ASP:OD1	1:A:248:PRO:HD2	1.76	0.83
1:A:186:TYR:CE2	1:A:265:ILE:HG21	2.13	0.83
1:A:540:GLN:CA	1:A:540:GLN:NE2	2.30	0.83
1:B:466:TRP:HZ2	1:B:475:THR:HG22	1.42	0.83
1:A:134:GLU:N	1:A:180:LYS:HZ2	1.76	0.83
1:B:695:ARG:HD3	1:B:700:ASP:CB	2.09	0.83
1:A:668:VAL:HG21	1:A:677:MSE:HE1	1.61	0.83
1:A:728:GLU:OE1	1:A:766:LEU:CD2	2.26	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASN:HD22	1:B:586:GLN:CD	1.79	0.83
1:B:774:PRO:HB3	1:B:778:MSE:CE	2.08	0.83
1:A:173:ARG:NH1	1:A:212:GLU:HG2	1.91	0.83
1:B:193:TYR:CE1	1:B:269:VAL:HG13	2.14	0.83
1:A:154:ARG:NH1	1:A:211:PHE:CD2	2.47	0.83
1:B:676:VAL:CG1	1:B:713:LYS:HE3	2.08	0.83
1:B:879:LEU:H	1:B:879:LEU:HD22	1.42	0.83
1:B:379:PHE:HA	1:B:382:GLN:HG3	1.59	0.82
1:A:440:GLU:CG	1:A:441:PHE:H	1.92	0.82
1:B:774:PRO:HB3	1:B:778:MSE:HE2	1.58	0.82
1:A:624:THR:O	1:A:653:LYS:HG3	1.79	0.82
1:B:140:SER:CB	1:B:141:PRO:HD3	2.09	0.82
1:A:449:ILE:HD13	1:A:462:PHE:CE1	2.15	0.82
1:B:695:ARG:CG	1:B:835:TYR:HD1	1.85	0.82
1:B:880:TYR:CE2	1:B:881:GLN:O	2.33	0.82
1:B:236:LEU:O	1:B:239:ILE:HD11	1.79	0.82
1:B:553:PRO:HD2	1:B:585:TYR:OH	1.80	0.82
1:B:667:LYS:CA	1:B:817:GLN:OE1	2.27	0.82
1:B:222:CYS:SG	1:B:224:TRP:CH2	2.73	0.81
1:A:648:GLN:O	1:A:650:PRO:HD3	1.79	0.81
1:B:391:THR:HG23	1:B:392:GLU:N	1.92	0.81
1:A:151:TRP:NE1	1:A:175:HIS:CE1	2.46	0.81
1:B:685:THR:O	1:B:689:ARG:HG3	1.79	0.81
1:B:274:VAL:HG23	1:B:278:MSE:HG3	1.61	0.81
1:B:671:HIS:CD2	1:B:721:ARG:NH1	2.48	0.81
1:A:281:LYS:O	1:A:285:GLN:HG2	1.81	0.81
1:A:415:TYR:CD2	1:A:490:ARG:HA	2.16	0.81
1:A:412:CYS:O	1:A:416:VAL:CG2	2.29	0.81
1:A:484:ASP:N	1:A:484:ASP:OD1	2.11	0.81
1:B:676:VAL:CG2	1:B:713:LYS:HE2	2.10	0.81
1:B:883:PRO:CG	1:B:884:PRO:CD	2.30	0.81
1:A:456:ARG:NH2	1:A:456:ARG:HG2	1.79	0.81
1:B:134:GLU:CD	1:B:135:PRO:CD	2.48	0.81
1:A:220:PHE:HE2	1:A:260:ASN:C	1.84	0.81
1:A:564:ILE:HG22	1:A:565:LEU:HD23	1.62	0.81
1:A:784:LYS:O	1:A:786:LEU:CD1	2.29	0.81
1:A:291:ASP:O	1:A:292:LEU:HD23	1.81	0.80
1:A:733:ILE:HG22	1:A:791:ARG:NH2	1.96	0.80
1:B:484:ASP:O	1:B:486:PRO:HD3	1.81	0.80
1:B:817:GLN:HB3	1:B:819:ARG:HG2	1.63	0.80
1:B:254:SER:OG	1:B:256:GLU:HB2	1.82	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:ASP:OD1	1:B:280:PRO:N	2.15	0.80
1:B:646:GLU:OE2	1:B:647:THR:CG2	2.30	0.80
1:B:487:GLN:N	1:B:487:GLN:OE1	2.15	0.80
1:B:148:ARG:NH1	1:B:148:ARG:HG2	1.86	0.80
1:B:696:LYS:CD	1:B:696:LYS:O	2.30	0.80
1:A:792:LEU:HD23	1:A:792:LEU:N	1.96	0.80
1:B:410:VAL:HG13	1:B:411:LEU:H	1.47	0.80
1:B:828:ARG:HH21	1:B:828:ARG:HG3	1.46	0.80
1:A:415:TYR:HD2	1:A:490:ARG:HG2	1.45	0.80
1:B:440:GLU:CA	1:B:440:GLU:OE1	2.30	0.80
1:B:447:VAL:O	1:B:447:VAL:CG2	2.30	0.80
1:B:577:LEU:O	1:B:581:VAL:HG12	1.81	0.80
1:A:273:HIS:NE2	1:A:274:VAL:O	2.15	0.80
1:A:456:ARG:HD2	1:A:458:ASN:OD1	1.81	0.80
1:B:227:ARG:O	1:B:230:ASP:HB2	1.82	0.79
1:B:656:LEU:N	1:B:656:LEU:HD23	1.95	0.79
1:A:787:LYS:N	1:A:788:PRO:CD	2.45	0.79
1:B:362:ALA:CB	1:B:699:LEU:HD22	2.13	0.79
1:B:646:GLU:O	1:B:646:GLU:CG	2.30	0.79
1:B:696:LYS:CE	1:B:696:LYS:O	2.30	0.79
1:B:278:MSE:O	1:B:279:ASP:HB3	1.80	0.79
1:B:699:LEU:CD2	1:B:699:LEU:O	2.30	0.79
1:A:294:TYR:HD2	1:A:294:TYR:O	1.66	0.79
1:A:355:THR:HG22	1:A:388:HIS:NE2	1.97	0.79
1:A:417:GLN:HE21	1:A:417:GLN:HA	1.46	0.79
1:A:648:GLN:CA	1:A:648:GLN:OE1	2.30	0.79
1:B:699:LEU:HD11	1:B:701:TRP:CE2	2.13	0.79
1:B:772:LEU:O	1:B:773:VAL:CG2	2.30	0.79
1:A:204:ILE:O	1:A:224:TRP:HE3	1.65	0.79
1:A:375:ASP:OD2	1:A:376:PHE:N	2.16	0.79
1:A:154:ARG:HD3	1:A:172:ALA:HB2	1.63	0.79
1:A:671:HIS:HD2	1:A:721:ARG:NH1	1.80	0.78
1:B:833:PRO:CB	1:B:835:TYR:HE2	1.96	0.78
1:B:134:GLU:HG3	1:B:135:PRO:HD2	1.63	0.78
1:B:278:MSE:HB3	1:B:282:ALA:CB	2.12	0.78
1:A:730:VAL:HG21	1:A:818:ALA:O	1.82	0.78
1:B:134:GLU:OE1	1:B:134:GLU:CA	2.30	0.78
1:B:772:LEU:CB	1:B:774:PRO:CD	2.61	0.78
1:B:667:LYS:CG	1:B:817:GLN:OE1	2.31	0.78
1:A:494:GLN:O	1:A:498:LYS:HD3	1.82	0.78
1:B:239:ILE:HD13	1:B:578:SER:HB3	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:657:LEU:CD1	1:B:657:LEU:N	2.41	0.78
1:B:554:LYS:HD3	1:B:615:MSE:CE	2.14	0.78
1:B:676:VAL:HG11	1:B:713:LYS:CE	2.14	0.78
1:B:715:LEU:HD22	1:B:837:ARG:HG2	1.65	0.78
1:A:852:ALA:CA	2:A:1000:SAH:OXT	2.32	0.78
1:A:646:GLU:CA	1:A:646:GLU:OE2	2.30	0.78
1:A:740:ASN:HD22	1:A:742:ARG:HG3	1.46	0.77
1:B:457:GLU:HB2	1:B:461:TYR:HH	1.49	0.77
1:B:828:ARG:HH22	1:B:834:ASP:CG	1.87	0.77
1:A:300:VAL:O	1:A:300:VAL:CG2	2.30	0.77
1:B:278:MSE:SE	1:B:282:ALA:HB1	2.34	0.77
1:A:569:ASP:N	1:A:569:ASP:OD2	2.17	0.77
1:B:675:ASP:HA	1:B:718:GLN:NE2	1.99	0.77
1:B:723:ASN:OD1	1:B:726:ASP:CB	2.33	0.77
1:A:250:ARG:HH21	1:A:584:LYS:HE2	1.47	0.77
1:B:549:ALA:HA	1:B:583:MSE:CE	2.13	0.77
1:B:772:LEU:C	1:B:774:PRO:HD2	2.00	0.77
1:B:880:TYR:CG	1:B:881:GLN:N	2.52	0.77
1:A:671:HIS:CD2	1:A:721:ARG:NH1	2.53	0.77
1:B:279:ASP:CG	1:B:280:PRO:CD	2.52	0.77
1:A:685:THR:O	1:A:689:ARG:HG3	1.85	0.77
1:A:784:LYS:N	1:A:786:LEU:HD12	1.96	0.77
1:A:220:PHE:HD2	1:A:260:ASN:O	1.67	0.77
1:B:220:PHE:CD2	1:B:262:LEU:HA	2.20	0.77
1:A:154:ARG:HD2	1:A:175:HIS:NE2	2.00	0.77
1:B:142:VAL:CG1	1:B:175:HIS:H	1.98	0.77
1:A:866:GLY:O	1:A:870:LEU:HD12	1.85	0.77
1:A:309:SER:O	1:A:310:SER:CB	2.33	0.76
1:B:135:PRO:CG	1:B:135:PRO:O	2.30	0.76
1:B:837:ARG:O	1:B:838:LEU:HD12	1.85	0.76
1:A:338:THR:HG21	1:A:367:LYS:NZ	1.99	0.76
1:A:690:TYR:O	1:A:693:LEU:HD13	1.86	0.76
1:A:134:GLU:CB	1:A:135:PRO:CD	2.30	0.76
1:A:449:ILE:HD13	1:A:462:PHE:CZ	2.21	0.76
1:A:294:TYR:O	1:A:294:TYR:CD2	2.37	0.76
1:B:659:GLY:CA	1:B:794:TRP:HB3	2.15	0.76
1:B:729:ARG:NH2	1:B:772:LEU:HA	2.00	0.76
1:A:728:GLU:CD	1:A:766:LEU:HG	2.06	0.76
1:B:699:LEU:CG	1:B:699:LEU:O	2.30	0.76
1:A:883:PRO:HB2	1:A:884:PRO:HD3	1.67	0.76
1:A:466:TRP:HZ2	1:A:475:THR:HG1	1.33	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:821:LEU:HG	1:B:825:GLU:OE1	1.84	0.76
1:B:138:ILE:HG12	1:B:139:GLY:H	1.51	0.76
1:B:457:GLU:CB	1:B:461:TYR:OH	2.27	0.76
1:B:227:ARG:CB	1:B:230:ASP:OD2	2.29	0.75
1:A:469:TYR:CE1	1:B:806:GLU:OE1	2.40	0.75
1:A:206:ARG:O	1:A:222:CYS:HB2	1.87	0.75
1:A:487:GLN:HA	1:A:487:GLN:NE2	2.01	0.75
1:B:676:VAL:HG13	1:B:713:LYS:HE3	1.65	0.75
1:A:748:ARG:CB	1:A:756:GLU:H	1.99	0.75
1:A:828:ARG:NH2	1:A:834:ASP:OD1	2.20	0.75
1:B:671:HIS:ND1	1:B:673:PRO:HD3	2.00	0.75
1:B:413:LYS:HZ2	1:B:414:LYS:HG2	1.51	0.75
1:B:535:ASP:O	1:B:535:ASP:OD1	2.04	0.75
1:A:289:SER:O	1:A:289:SER:OG	2.00	0.75
1:A:823:ILE:HD13	1:A:845:LYS:HG3	1.68	0.75
1:A:277:ASN:N	1:A:277:ASN:OD1	2.15	0.75
1:A:728:GLU:OE1	1:A:766:LEU:HG	1.86	0.75
1:A:717:HIS:CE1	1:A:822:THR:HG21	2.22	0.75
1:B:833:PRO:CG	1:B:835:TYR:HE2	2.00	0.75
1:A:134:GLU:HB2	1:A:135:PRO:HD2	1.68	0.75
1:A:564:ILE:O	1:A:570:GLY:HA2	1.86	0.75
1:A:781:ILE:H	1:A:781:ILE:HD13	1.52	0.75
1:B:685:THR:HG23	1:B:687:PHE:H	1.51	0.74
1:A:195:LYS:CE	1:A:264:CYS:HA	2.15	0.74
1:A:766:LEU:HD23	1:A:768:SER:H	1.50	0.74
1:A:763:ARG:O	1:A:764:VAL:HG13	1.87	0.74
1:B:599:LEU:HD23	1:B:829:LEU:O	1.86	0.74
1:A:141:PRO:O	1:A:142:VAL:HG22	1.85	0.74
1:B:605:ARG:HG2	1:B:605:ARG:NH1	2.02	0.74
1:B:626:ASP:OD2	1:B:655:ALA:N	2.21	0.74
1:B:774:PRO:O	1:B:777:ALA:N	2.21	0.74
1:B:729:ARG:HD3	1:B:773:VAL:HG21	1.69	0.74
1:A:225:PHE:CE1	1:A:294:TYR:CD1	2.76	0.74
1:A:811:VAL:O	1:A:811:VAL:HG22	1.86	0.74
1:B:134:GLU:OE1	1:B:135:PRO:CD	2.29	0.74
1:A:780:PHE:HB3	1:A:786:LEU:HD22	1.69	0.74
1:B:134:GLU:CG	1:B:135:PRO:HD2	2.17	0.74
1:B:696:LYS:O	1:B:696:LYS:HD2	1.86	0.74
1:B:811:VAL:O	1:B:811:VAL:HG22	1.87	0.74
1:A:666:PRO:HG3	1:A:679:TYR:O	1.87	0.74
1:B:502:LEU:HD23	1:B:503:PRO:HD2	1.67	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:SER:CB	1:A:688:GLN:HE22	2.00	0.74
1:A:780:PHE:CE2	1:A:809:ASN:CG	2.61	0.74
1:A:249:ARG:O	1:A:249:ARG:HG3	1.87	0.74
1:A:662:ILE:O	1:A:665:LEU:HG	1.88	0.74
1:B:462:PHE:O	1:B:464:VAL:HG12	1.88	0.73
1:B:143:ALA:CB	1:B:147:ALA:HB2	2.18	0.73
1:A:214:THR:O	1:A:215:ASP:CB	2.35	0.73
1:A:635:ASN:OD1	1:A:636:ALA:N	2.20	0.73
1:A:692:ARG:O	1:A:693:LEU:HD12	1.89	0.73
1:B:273:HIS:HD2	1:B:274:VAL:N	1.85	0.73
1:B:695:ARG:HG2	1:B:835:TYR:HE1	1.46	0.73
1:B:820:VAL:CG1	1:B:821:LEU:N	2.44	0.73
1:A:668:VAL:N	1:A:817:GLN:HE22	1.83	0.73
1:B:879:LEU:N	1:B:879:LEU:HD22	2.03	0.73
1:A:883:PRO:HB2	1:A:884:PRO:CD	2.19	0.73
1:B:197:GLY:HA3	1:B:200:GLU:OE2	1.89	0.73
1:A:276:PRO:HG2	1:A:277:ASN:OD1	1.88	0.73
1:B:741:PHE:N	1:B:789:PHE:O	2.21	0.73
1:A:221:THR:HB	1:A:259:ASP:OD1	1.88	0.73
1:A:557:LEU:HD21	1:A:861:LEU:HD13	1.69	0.73
1:A:220:PHE:CE2	1:A:260:ASN:O	2.42	0.73
1:B:135:PRO:O	1:B:135:PRO:HG2	1.89	0.73
1:A:677:MSE:HG3	1:A:714:LEU:HD22	1.71	0.72
1:A:733:ILE:CG2	1:A:791:ARG:NH2	2.50	0.72
1:A:151:TRP:NE1	1:A:175:HIS:ND1	2.37	0.72
1:B:454:SER:O	1:B:456:ARG:HG3	1.88	0.72
1:B:484:ASP:OD1	1:B:485:CYS:N	2.22	0.72
1:A:154:ARG:NE	1:A:170:LEU:HD21	2.03	0.72
1:A:557:LEU:HD12	1:A:558:MSE:N	2.05	0.72
1:A:812:ILE:HG23	1:A:820:VAL:HG22	1.71	0.72
1:A:838:LEU:C	1:A:839:PHE:HD1	1.93	0.72
1:B:218:HIS:CB	1:B:262:LEU:HD11	2.19	0.72
1:A:728:GLU:OE1	1:A:766:LEU:CG	2.37	0.72
1:B:249:ARG:NH2	1:B:287:ILE:O	2.21	0.72
1:B:443:VAL:O	1:B:488:LYS:HE2	1.89	0.72
1:B:791:ARG:CD	1:B:813:ILE:O	2.37	0.72
1:B:231:THR:HG1	1:B:233:ILE:HG23	1.55	0.72
1:A:588:ARG:HH21	1:A:878:PRO:HA	1.52	0.72
1:B:148:ARG:HB3	1:B:155:TYR:CD2	2.25	0.72
1:A:220:PHE:CE2	1:A:260:ASN:C	2.63	0.72
1:A:515:PRO:HG2	1:A:558:MSE:CE	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ARG:HD3	1:A:772:LEU:O	1.90	0.72
1:A:837:ARG:HB3	1:A:839:PHE:HE1	1.54	0.72
1:B:138:ILE:CG1	1:B:139:GLY:H	2.02	0.72
1:A:486:PRO:HB2	1:A:490:ARG:HD2	1.71	0.72
1:A:772:LEU:HD13	1:A:773:VAL:N	2.04	0.71
1:B:449:ILE:O	1:B:449:ILE:HG23	1.89	0.71
1:B:549:ALA:HB2	1:B:583:MSE:HE1	1.71	0.71
1:A:232:VAL:HG12	1:A:233:ILE:HG22	1.73	0.71
1:A:737:LYS:NZ	1:A:795:ASP:OD2	2.23	0.71
1:B:181:VAL:HG12	1:B:186:TYR:OH	1.90	0.71
1:B:460:ILE:CD1	1:B:460:ILE:N	2.53	0.71
1:B:793:TRP:CB	1:B:815:PRO:HB3	2.19	0.71
1:B:819:ARG:O	1:B:820:VAL:HG12	1.90	0.71
1:A:250:ARG:NH2	1:A:295:ASP:OD2	2.24	0.71
1:B:273:HIS:HB2	1:B:294:TYR:CE1	2.26	0.71
1:B:644:TYR:O	1:B:645:ASP:CB	2.36	0.71
1:A:605:ARG:NH1	1:A:605:ARG:HG2	1.99	0.71
1:A:724:ASN:O	1:A:728:GLU:HG3	1.89	0.71
1:B:143:ALA:HB3	1:B:147:ALA:HB2	1.72	0.71
1:A:442:VAL:HG13	1:A:467:GLU:HG3	1.71	0.71
1:B:814:HIS:N	1:B:820:VAL:O	2.22	0.71
1:A:138:ILE:HG23	1:A:139:GLY:N	2.05	0.71
1:A:215:ASP:C	1:A:216:GLN:CG	2.57	0.71
1:A:250:ARG:HH21	1:A:584:LYS:CE	2.04	0.71
1:A:670:ASN:ND2	1:A:722:LEU:HD22	2.06	0.71
1:B:226:PHE:HE2	1:B:254:SER:CB	1.96	0.71
1:B:413:LYS:NZ	1:B:414:LYS:HG2	2.04	0.70
1:B:518:GLN:NE2	1:B:518:GLN:HA	2.05	0.70
1:A:375:ASP:CG	2:A:1000:SAH:O2'	2.28	0.70
1:B:191:ASP:OD1	1:B:206:ARG:NH1	2.24	0.70
1:B:819:ARG:NH2	1:B:825:GLU:OE2	2.24	0.70
1:A:136:GLU:HG3	1:A:218:HIS:CE1	2.25	0.70
1:A:536:GLU:O	1:A:537:LYS:C	2.30	0.70
1:A:277:ASN:O	1:A:278:MSE:HG3	1.91	0.70
1:A:648:GLN:O	1:A:650:PRO:CD	2.40	0.70
1:B:440:GLU:C	1:B:440:GLU:OE1	2.30	0.70
1:B:603:ARG:CZ	1:B:830:GLN:HE22	2.05	0.70
1:A:644:TYR:CD2	1:A:649:LYS:HG3	2.25	0.70
1:A:695:ARG:HB3	1:A:700:ASP:HB3	1.73	0.70
1:B:646:GLU:OE2	1:B:647:THR:HG22	1.90	0.70
1:A:236:LEU:HD13	1:A:574:LYS:CB	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:GLU:OE1	1:A:221:THR:HG21	1.92	0.70
1:B:239:ILE:HD13	1:B:578:SER:CB	2.22	0.70
1:B:637:PHE:N	1:B:637:PHE:CD2	2.59	0.70
1:A:220:PHE:HE2	1:A:260:ASN:CB	2.04	0.70
1:A:733:ILE:HG21	1:A:791:ARG:HH21	1.54	0.70
1:B:774:PRO:O	1:B:775:ASP:C	2.30	0.70
1:B:467:GLU:O	1:B:469:TYR:CE2	2.45	0.70
1:A:215:ASP:O	1:A:216:GLN:CG	2.40	0.70
1:A:464:VAL:HG11	1:A:466:TRP:CH2	2.27	0.70
1:A:631:GLY:HA3	1:A:641:MSE:HE1	1.73	0.70
1:A:780:PHE:C	1:A:781:ILE:HD13	2.13	0.70
1:B:459:GLY:O	1:B:461:TYR:CD2	2.45	0.70
1:B:583:MSE:O	1:B:584:LYS:HB2	1.91	0.70
1:B:771:PRO:C	1:B:773:VAL:H	1.95	0.70
1:A:220:PHE:CE2	1:A:260:ASN:CB	2.75	0.69
1:A:279:ASP:CB	1:A:280:PRO:HD2	2.12	0.69
1:A:173:ARG:N	1:A:212:GLU:O	2.25	0.69
1:B:376:PHE:O	1:B:395:ASN:ND2	2.24	0.69
1:A:535:ASP:C	1:A:535:ASP:OD2	2.30	0.69
1:A:739:ALA:HB3	1:A:791:ARG:HG2	1.74	0.69
1:B:592:MSE:SE	1:B:861:LEU:HD21	2.42	0.69
1:B:339:ARG:NH1	1:B:339:ARG:HG2	1.96	0.69
1:A:649:LYS:O	1:A:649:LYS:HD3	1.93	0.69
1:A:727:TYR:O	1:A:727:TYR:CD2	2.45	0.69
1:A:140:SER:HB3	1:A:141:PRO:HD2	1.75	0.69
1:A:793:TRP:HB3	1:A:795:ASP:OD1	1.92	0.69
1:A:793:TRP:CE3	1:A:793:TRP:HA	2.27	0.69
1:B:220:PHE:CE2	1:B:262:LEU:HA	2.27	0.69
1:A:787:LYS:HB2	1:A:809:ASN:O	1.92	0.69
1:A:814:HIS:HD2	1:A:816:THR:H	1.41	0.69
1:B:144:ALA:C	1:B:145:ASP:OD2	2.30	0.69
1:B:833:PRO:HB2	1:B:835:TYR:HE2	1.47	0.69
1:B:440:GLU:OE1	1:B:440:GLU:HA	1.91	0.69
1:A:145:ASP:OD1	1:A:148:ARG:NH1	2.26	0.69
1:A:540:GLN:CA	1:A:540:GLN:HE21	1.89	0.69
1:A:274:VAL:HG23	1:A:295:ASP:HA	1.74	0.68
1:A:460:ILE:CG2	1:A:462:PHE:CE2	2.76	0.68
1:A:211:PHE:CD1	1:A:211:PHE:C	2.67	0.68
1:A:515:PRO:CG	1:A:558:MSE:HE3	2.21	0.68
1:B:273:HIS:CD2	1:B:274:VAL:N	2.60	0.68
1:B:700:ASP:OD1	1:B:702:SER:HB2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ASP:O	1:A:395:ASN:HA	1.94	0.68
1:B:404:LEU:HB2	1:B:451:TYR:HB3	1.75	0.68
1:B:575:TYR:O	1:B:579:CYS:SG	2.50	0.68
1:A:154:ARG:HB2	1:A:171:LYS:HA	1.75	0.68
1:A:176:TYR:HE1	1:A:212:GLU:HG3	1.57	0.68
1:A:231:THR:OG1	1:A:233:ILE:HG23	1.93	0.68
1:A:225:PHE:HE1	1:A:294:TYR:CD1	2.10	0.68
1:A:464:VAL:CG1	1:A:466:TRP:CZ2	2.77	0.68
1:B:729:ARG:NE	1:B:773:VAL:HG22	2.08	0.68
1:A:668:VAL:CG2	1:A:677:MSE:HE1	2.24	0.68
1:B:215:ASP:O	1:B:216:GLN:HB2	1.94	0.68
1:A:253:LEU:HD12	1:A:294:TYR:CE1	2.29	0.68
1:A:784:LYS:O	1:A:785:SER:C	2.30	0.68
1:B:467:GLU:O	1:B:469:TYR:CD2	2.47	0.68
1:B:802:VAL:HG12	1:B:804:ARG:H	1.59	0.68
1:B:805:ALA:HA	1:B:810:GLN:NE2	2.09	0.68
1:A:227:ARG:HB2	1:A:230:ASP:OD2	1.94	0.68
1:B:222:CYS:SG	1:B:224:TRP:CZ3	2.87	0.68
1:A:781:ILE:HG12	1:A:786:LEU:CD2	2.19	0.67
1:B:635:ASN:OD1	1:B:636:ALA:N	2.27	0.67
1:B:658:LEU:O	1:B:659:GLY:C	2.30	0.67
1:B:685:THR:HG23	1:B:686:GLU:N	2.06	0.67
1:A:648:GLN:O	1:A:649:LYS:C	2.30	0.67
1:B:646:GLU:OE2	1:B:647:THR:CA	2.42	0.67
1:A:641:MSE:HG3	1:A:642:VAL:N	2.08	0.67
1:B:699:LEU:HG	1:B:701:TRP:CD1	2.29	0.67
1:A:142:VAL:HA	1:A:175:HIS:O	1.95	0.67
1:A:786:LEU:CB	1:A:788:PRO:HD3	2.22	0.67
1:B:443:VAL:HG12	1:B:466:TRP:HE3	1.56	0.67
1:A:204:ILE:O	1:A:224:TRP:CE3	2.47	0.67
1:A:714:LEU:C	1:A:714:LEU:HD23	2.15	0.67
1:B:771:PRO:C	1:B:773:VAL:N	2.46	0.67
1:A:466:TRP:CD1	1:A:466:TRP:N	2.62	0.67
1:B:218:HIS:HB3	1:B:262:LEU:HD11	1.76	0.67
1:B:791:ARG:HG2	1:B:814:HIS:O	1.95	0.67
1:B:667:LYS:HG3	1:B:817:GLN:CD	2.14	0.67
1:A:220:PHE:HE2	1:A:260:ASN:HB2	1.60	0.67
1:A:377:ASN:OD1	1:A:379:PHE:N	2.28	0.67
1:A:691:ILE:HG23	1:A:834:ASP:OD1	1.95	0.67
1:A:879:LEU:O	1:A:879:LEU:HD23	1.95	0.67
1:A:154:ARG:NH1	1:A:175:HIS:CE1	2.63	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:HD23	1:A:829:LEU:O	1.95	0.67
1:A:672:GLN:HE21	1:A:674:ASN:HB2	1.60	0.67
1:B:469:TYR:HB3	1:B:473:GLU:HB2	1.76	0.67
1:B:696:LYS:HE3	1:B:696:LYS:O	1.95	0.67
1:A:255:GLU:HG3	1:A:255:GLU:O	1.95	0.67
1:B:273:HIS:HB2	1:B:294:TYR:CZ	2.30	0.67
1:B:657:LEU:O	1:B:660:ASP:HB2	1.94	0.67
1:A:651:SER:O	1:A:652:LEU:C	2.30	0.66
1:B:279:ASP:CG	1:B:280:PRO:N	2.47	0.66
1:B:345:ASP:CG	1:B:348:SER:HB3	2.15	0.66
1:B:646:GLU:OE2	1:B:647:THR:HA	1.96	0.66
1:A:788:PRO:O	1:A:789:PHE:C	2.30	0.66
1:B:239:ILE:HD12	1:B:239:ILE:H	1.61	0.66
1:B:599:LEU:HD23	1:B:601:GLN:HE21	1.59	0.66
1:B:662:ILE:HG21	1:B:825:GLU:HB3	1.77	0.66
1:B:884:PRO:O	1:B:885:SER:C	2.34	0.66
1:A:289:SER:O	1:A:290:CYS:HB3	1.95	0.66
1:A:729:ARG:HG3	1:A:729:ARG:HH11	1.60	0.66
1:A:171:LYS:HB3	1:A:214:THR:CG2	2.25	0.66
1:A:671:HIS:HD2	1:A:721:ARG:HH12	1.42	0.66
1:A:690:TYR:CE1	1:A:698:MSE:SE	2.99	0.66
1:A:220:PHE:CZ	1:A:260:ASN:HB2	2.31	0.66
1:A:449:ILE:HD11	1:A:460:ILE:HG23	1.77	0.66
1:A:874:GLU:HG3	1:A:875:GLY:H	1.61	0.66
1:B:699:LEU:O	1:B:699:LEU:HG	1.94	0.66
1:A:803:THR:CA	1:A:850:GLY:HA3	2.21	0.66
1:B:235:SER:O	1:B:237:VAL:HG23	1.96	0.66
1:B:344:LEU:HD12	1:B:372:TRP:HB2	1.78	0.66
1:B:447:VAL:O	1:B:447:VAL:HG22	1.96	0.66
1:B:648:GLN:O	1:B:650:PRO:HD3	1.96	0.66
1:B:599:LEU:HD11	1:B:856:PRO:CG	2.22	0.66
1:A:171:LYS:O	1:A:213:GLY:CA	2.44	0.66
1:B:290:CYS:HB2	1:B:292:LEU:O	1.96	0.66
1:B:449:ILE:CG2	1:B:449:ILE:O	2.44	0.66
1:A:456:ARG:HH21	1:A:456:ARG:CG	1.93	0.66
1:A:498:LYS:HD3	1:A:498:LYS:H	1.61	0.66
1:B:278:MSE:O	1:B:280:PRO:HD2	1.94	0.66
1:A:495:GLU:HA	1:A:495:GLU:OE1	1.96	0.65
1:B:226:PHE:CD2	1:B:254:SER:HB2	2.31	0.65
1:B:589:LEU:HA	1:B:620:TYR:OH	1.95	0.65
1:B:677:MSE:O	1:B:714:LEU:HB3	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ARG:CD	1:A:172:ALA:HB2	2.26	0.65
1:A:465:GLN:HG3	1:A:474:ASP:OD1	1.96	0.65
1:A:478:PRO:O	1:A:482:LEU:HD23	1.97	0.65
1:B:275:ASP:HB2	1:B:276:PRO:HD2	1.78	0.65
1:B:286:LEU:O	1:B:289:SER:N	2.28	0.65
1:B:518:GLN:HB2	1:B:537:LYS:CB	2.24	0.65
1:B:806:GLU:H	1:B:810:GLN:HE21	1.44	0.65
1:A:154:ARG:CD	1:A:172:ALA:CB	2.74	0.65
1:A:464:VAL:HG11	1:A:466:TRP:CZ2	2.30	0.65
1:B:235:SER:O	1:B:237:VAL:N	2.29	0.65
1:B:410:VAL:O	1:B:413:LYS:N	2.29	0.65
1:B:534:LYS:HZ2	1:B:535:ASP:HB2	1.60	0.65
1:B:671:HIS:HE1	1:B:673:PRO:HB3	1.62	0.65
1:B:353:MSE:HE2	1:B:512:CYS:HB3	1.79	0.65
1:B:676:VAL:HG21	1:B:713:LYS:NZ	2.12	0.65
1:B:272:VAL:CG1	1:B:273:HIS:N	2.60	0.65
1:A:309:SER:O	1:A:310:SER:HB3	1.96	0.65
1:A:752:ASN:C	1:A:754:ILE:H	2.00	0.65
1:B:549:ALA:CA	1:B:583:MSE:CE	2.75	0.65
1:B:660:ASP:O	1:B:688:GLN:NE2	2.30	0.65
1:B:685:THR:CG2	1:B:688:GLN:N	2.45	0.65
1:A:723:ASN:HD22	1:A:723:ASN:C	2.01	0.65
1:B:564:ILE:HG23	1:B:572:LEU:HB2	1.77	0.65
1:B:686:GLU:HA	1:B:689:ARG:NH2	2.11	0.65
1:A:557:LEU:HD12	1:A:558:MSE:H	1.60	0.64
1:B:646:GLU:OE2	1:B:647:THR:N	2.30	0.64
1:A:145:ASP:CG	1:A:148:ARG:NH1	2.49	0.64
1:A:541:MSE:HG3	1:A:541:MSE:O	1.95	0.64
1:B:699:LEU:CG	1:B:701:TRP:CD1	2.79	0.64
1:B:347:TYR:CD2	1:B:516:PRO:HD3	2.32	0.64
1:B:648:GLN:N	1:B:648:GLN:OE1	2.30	0.64
1:B:413:LYS:HZ1	1:B:414:LYS:HE2	1.62	0.64
1:B:254:SER:HG	1:B:256:GLU:HB2	1.61	0.64
1:B:649:LYS:C	1:B:651:SER:H	2.00	0.64
1:A:195:LYS:HG2	1:A:266:ILE:HD11	1.80	0.64
1:B:388:HIS:HA	1:B:702:SER:HG	1.62	0.64
1:B:657:LEU:HB3	1:B:794:TRP:O	1.98	0.64
1:A:585:TYR:CD1	1:A:610:GLY:O	2.50	0.64
1:A:781:ILE:O	1:A:782:LYS:CB	2.44	0.64
1:B:626:ASP:OD2	1:B:655:ALA:HB2	1.98	0.64
1:A:279:ASP:OD1	1:A:279:ASP:N	2.29	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:TYR:HE2	1:A:618:PRO:CD	2.10	0.64
1:A:729:ARG:CD	1:A:772:LEU:O	2.45	0.64
1:A:838:LEU:C	1:A:839:PHE:CD1	2.71	0.64
1:B:883:PRO:HG2	1:B:884:PRO:HD2	0.71	0.64
1:A:592:MSE:HE2	1:A:620:TYR:CD1	2.33	0.64
1:A:631:GLY:CA	1:A:641:MSE:HE1	2.28	0.64
1:B:508:VAL:CG1	1:B:511:ILE:HG22	2.28	0.64
1:A:376:PHE:CD2	1:A:376:PHE:C	2.70	0.64
1:A:417:GLN:HE21	1:A:417:GLN:CA	2.09	0.64
1:A:490:ARG:O	1:A:494:GLN:HG3	1.98	0.64
1:B:229:GLU:HG3	1:B:237:VAL:HG21	1.79	0.64
1:A:287:ILE:HD12	1:A:288:GLU:N	2.13	0.63
1:A:603:ARG:CZ	1:A:830:GLN:HE22	2.10	0.63
1:B:804:ARG:O	1:B:810:GLN:NE2	2.30	0.63
1:B:466:TRP:NE1	1:B:473:GLU:O	2.31	0.63
1:A:247:ASP:OD1	1:A:248:PRO:CD	2.46	0.63
1:A:809:ASN:CG	1:A:809:ASN:O	2.35	0.63
1:A:664:ASP:OD1	1:A:828:ARG:NH1	2.29	0.63
1:B:695:ARG:CG	1:B:835:TYR:HE1	2.07	0.63
1:A:665:LEU:O	1:A:666:PRO:C	2.37	0.63
1:A:822:THR:HG22	1:A:825:GLU:CD	2.19	0.63
1:A:884:PRO:O	1:A:885:SER:C	2.36	0.63
1:B:250:ARG:HH21	1:B:295:ASP:CG	2.01	0.63
1:B:383:SER:HB3	1:B:838:LEU:HA	1.80	0.63
1:B:464:VAL:HG13	1:B:475:THR:O	1.99	0.63
1:B:676:VAL:HG11	1:B:713:LYS:HE3	1.78	0.63
1:B:791:ARG:HG3	1:B:792:LEU:O	1.97	0.63
1:A:727:TYR:C	1:A:727:TYR:CD2	2.67	0.63
1:B:349:GLY:HA2	1:B:380:ALA:HB1	1.80	0.63
1:B:469:TYR:HB3	1:B:473:GLU:CB	2.28	0.63
1:B:687:PHE:O	1:B:690:TYR:N	2.31	0.63
1:A:757:TRP:HZ3	1:A:773:VAL:CG2	2.11	0.63
1:A:469:TYR:HB3	1:A:473:GLU:HB2	1.80	0.63
1:B:540:GLN:OE1	1:B:540:GLN:HA	1.99	0.63
1:B:735:VAL:HG22	1:B:735:VAL:O	1.99	0.63
1:B:828:ARG:CG	1:B:828:ARG:HH21	2.12	0.63
1:B:348:SER:HA	2:B:1000:SAH:N	2.13	0.63
1:B:659:GLY:N	1:B:794:TRP:HB3	2.13	0.63
1:A:664:ASP:OD2	1:A:692:ARG:NH1	2.32	0.62
1:B:609:TRP:CD1	1:B:620:TYR:CE1	2.86	0.62
1:B:802:VAL:CG1	1:B:803:THR:N	2.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:TYR:CE2	1:A:618:PRO:HD3	2.26	0.62
1:A:726:ASP:OD1	1:A:729:ARG:NH1	2.32	0.62
1:B:448:GLY:O	1:B:462:PHE:HA	1.99	0.62
1:B:691:ILE:O	1:B:691:ILE:HD12	1.99	0.62
1:A:137:PHE:CE2	1:A:218:HIS:HB3	2.34	0.62
1:A:138:ILE:HG21	1:A:178:SER:HB2	1.79	0.62
1:A:668:VAL:O	1:A:817:GLN:NE2	2.33	0.62
1:B:572:LEU:H	1:B:572:LEU:HD12	1.64	0.62
1:B:578:SER:HA	1:B:581:VAL:CG1	2.29	0.62
1:B:648:GLN:N	1:B:648:GLN:CD	2.49	0.62
1:B:847:ILE:HD12	1:B:848:GLN:N	2.13	0.62
1:A:587:ALA:HA	1:A:609:TRP:O	1.99	0.62
1:B:364:SER:CB	1:B:866:GLY:HA3	2.29	0.62
1:B:549:ALA:HB2	1:B:583:MSE:CE	2.28	0.62
1:A:171:LYS:CB	1:A:214:THR:CG2	2.77	0.62
1:A:242:ASP:OD1	1:A:243:GLY:N	2.32	0.62
1:B:135:PRO:CD	1:B:135:PRO:O	2.48	0.62
1:B:440:GLU:CG	1:B:440:GLU:O	2.44	0.62
1:B:714:LEU:HD23	1:B:715:LEU:N	2.15	0.62
1:B:792:LEU:CD2	1:B:796:GLU:HB3	2.29	0.62
1:A:788:PRO:HA	1:A:808:HIS:O	1.98	0.62
1:B:411:LEU:C	1:B:411:LEU:HD23	2.20	0.62
1:B:445:LYS:O	1:B:446:LEU:CD2	2.43	0.62
1:B:464:VAL:HG21	1:B:466:TRP:CH2	2.35	0.62
1:A:541:MSE:SE	1:A:558:MSE:CE	2.94	0.62
1:A:727:TYR:C	1:A:727:TYR:HD2	2.02	0.62
1:A:776:TYR:CD2	1:A:777:ALA:N	2.68	0.62
1:B:733:ILE:HG13	1:B:734:PRO:HD2	1.82	0.62
1:A:710:ASP:HB3	1:A:715:LEU:HD21	1.82	0.62
1:B:272:VAL:HG12	1:B:273:HIS:N	2.14	0.62
1:B:772:LEU:O	1:B:774:PRO:HD3	1.98	0.62
1:B:833:PRO:HB2	1:B:835:TYR:CD2	2.34	0.62
1:A:225:PHE:CE1	1:A:294:TYR:HD1	2.18	0.62
1:A:449:ILE:HD12	1:A:461:TYR:O	2.00	0.62
1:A:784:LYS:H	1:A:786:LEU:HD13	1.62	0.62
1:B:648:GLN:OE1	1:B:648:GLN:CA	2.48	0.62
1:B:813:ILE:HA	1:B:820:VAL:HA	1.82	0.62
1:B:343:LEU:HD12	1:B:344:LEU:H	1.65	0.61
1:A:154:ARG:HD3	1:A:172:ALA:CB	2.29	0.61
1:A:195:LYS:HG2	1:A:266:ILE:CD1	2.31	0.61
1:A:254:SER:OG	1:A:256:GLU:HB2	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:CYS:O	1:A:583:MSE:HG3	2.00	0.61
1:A:879:LEU:C	1:A:879:LEU:HD23	2.19	0.61
1:A:787:LYS:H	1:A:788:PRO:HD3	1.65	0.61
1:A:249:ARG:O	1:A:293:TYR:HE2	1.82	0.61
1:B:601:GLN:OE1	1:B:801:VAL:HG12	2.00	0.61
1:B:805:ALA:HA	1:B:810:GLN:HE22	1.65	0.61
1:B:791:ARG:HD3	1:B:813:ILE:O	2.00	0.61
1:B:821:LEU:CG	1:B:825:GLU:OE1	2.48	0.61
1:A:280:PRO:O	1:A:281:LYS:HB2	2.01	0.61
1:A:377:ASN:OD1	1:A:377:ASN:C	2.38	0.61
1:B:570:GLY:O	1:B:574:LYS:HG2	2.01	0.61
1:A:250:ARG:NH1	1:A:252:PHE:CZ	2.67	0.61
1:A:453:GLY:O	1:A:456:ARG:HB2	1.99	0.61
1:A:664:ASP:CG	1:A:692:ARG:HH11	2.03	0.61
1:B:236:LEU:O	1:B:239:ILE:CD1	2.48	0.61
1:B:589:LEU:HD23	1:B:608:LEU:HD12	1.83	0.61
1:A:272:VAL:O	1:A:293:TYR:HA	2.00	0.61
1:B:153:LYS:O	1:B:171:LYS:NZ	2.28	0.61
1:B:443:VAL:HG12	1:B:466:TRP:CZ3	2.35	0.61
1:B:549:ALA:CB	1:B:583:MSE:CE	2.79	0.61
1:B:671:HIS:HD2	1:B:721:ARG:CZ	2.13	0.61
1:A:415:TYR:HD2	1:A:490:ARG:HA	1.65	0.61
1:A:726:ASP:HA	1:A:729:ARG:HH11	1.65	0.61
1:A:584:LYS:HB3	1:A:584:LYS:HZ3	1.65	0.61
1:B:695:ARG:CG	1:B:695:ARG:NH1	2.30	0.61
1:A:407:GLU:O	1:A:411:LEU:HD13	2.01	0.60
1:A:663:SER:OG	1:A:684:LYS:HE2	2.01	0.60
1:B:250:ARG:NH2	1:B:295:ASP:OD2	2.29	0.60
1:B:714:LEU:CD2	1:B:717:HIS:HB2	2.28	0.60
1:A:338:THR:HB	1:A:367:LYS:HD3	1.82	0.60
1:A:791:ARG:NH1	1:A:815:PRO:O	2.34	0.60
1:B:181:VAL:CG1	1:B:186:TYR:OH	2.49	0.60
1:B:273:HIS:CD2	1:B:273:HIS:C	2.74	0.60
1:B:675:ASP:OD1	1:B:675:ASP:N	2.34	0.60
1:B:710:ASP:OD2	1:B:837:ARG:NH1	2.34	0.60
1:B:880:TYR:CZ	1:B:881:GLN:O	2.53	0.60
1:A:154:ARG:CZ	1:A:175:HIS:CE1	2.83	0.60
1:A:601:GLN:NE2	1:A:830:GLN:OE1	2.34	0.60
1:A:700:ASP:O	1:A:702:SER:N	2.34	0.60
1:A:580:LEU:HD22	1:A:608:LEU:CD2	2.31	0.60
1:A:726:ASP:HA	1:A:729:ARG:NH1	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:VAL:O	1:B:488:LYS:CE	2.49	0.60
1:A:410:VAL:O	1:A:413:LYS:HB3	2.01	0.60
1:A:652:LEU:O	1:A:654:LYS:N	2.34	0.60
1:B:138:ILE:CG1	1:B:139:GLY:N	2.65	0.60
1:B:445:LYS:HB3	1:B:465:GLN:HB2	1.82	0.60
1:B:772:LEU:CB	1:B:774:PRO:HD3	2.31	0.60
1:A:154:ARG:HH12	1:A:211:PHE:HD2	1.45	0.60
1:B:649:LYS:O	1:B:651:SER:N	2.30	0.60
1:B:740:ASN:HA	1:B:789:PHE:O	2.01	0.60
1:A:772:LEU:H	1:A:772:LEU:HD12	1.66	0.60
1:A:792:LEU:H	1:A:792:LEU:HD23	1.67	0.60
1:A:344:LEU:HD12	1:A:372:TRP:HB2	1.84	0.60
1:A:338:THR:HG21	1:A:367:LYS:HZ3	1.66	0.60
1:B:405:LEU:HD21	1:B:503:PRO:HG2	1.84	0.60
1:A:379:PHE:HD2	1:A:844:GLU:HG2	1.63	0.60
1:A:394:ARG:NE	1:A:396:GLU:OE1	2.34	0.60
1:B:649:LYS:HD2	1:B:652:LEU:CD1	2.21	0.60
1:A:226:PHE:O	1:A:251:VAL:HG12	2.02	0.59
1:A:384:LEU:HD13	1:A:388:HIS:HD2	1.67	0.59
1:A:763:ARG:NH1	1:A:771:PRO:CB	2.64	0.59
1:B:604:MSE:O	1:B:605:ARG:NH1	2.35	0.59
1:B:785:SER:O	1:B:788:PRO:CD	2.50	0.59
1:B:833:PRO:CB	1:B:835:TYR:CE2	2.76	0.59
1:A:698:MSE:C	1:A:699:LEU:HD12	2.22	0.59
1:A:780:PHE:O	1:A:783:GLY:N	2.29	0.59
1:A:657:LEU:HD23	1:A:795:ASP:HA	1.84	0.59
1:B:459:GLY:O	1:B:461:TYR:CE2	2.55	0.59
1:B:646:GLU:C	1:B:646:GLU:OE2	2.41	0.59
1:B:410:VAL:HG13	1:B:411:LEU:N	2.16	0.59
1:B:561:VAL:HG23	1:B:563:ASP:H	1.65	0.59
1:B:676:VAL:CG2	1:B:713:LYS:CE	2.80	0.59
1:B:790:GLY:O	1:B:811:VAL:HA	2.01	0.59
1:B:830:GLN:HA	1:B:830:GLN:OE1	2.01	0.59
1:B:586:GLN:NE2	1:B:615:MSE:O	2.35	0.59
1:B:734:PRO:O	1:B:735:VAL:CG1	2.51	0.59
1:A:469:TYR:HE1	1:B:806:GLU:OE1	1.85	0.59
1:A:498:LYS:HD3	1:A:498:LYS:N	2.17	0.59
1:B:170:LEU:HD21	1:B:211:PHE:CE1	2.37	0.59
1:A:279:ASP:CB	1:A:280:PRO:HD3	2.32	0.59
1:A:664:ASP:OD2	1:A:683:PRO:HA	2.02	0.59
1:A:737:LYS:HE3	1:A:796:GLU:OE1	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ARG:HB3	1:B:155:TYR:CE2	2.37	0.59
1:B:414:LYS:O	1:B:415:TYR:HB2	2.03	0.59
1:B:343:LEU:HD13	1:B:510:VAL:HB	1.85	0.59
1:B:362:ALA:HB1	1:B:699:LEU:HD22	1.83	0.59
1:B:788:PRO:CB	1:B:808:HIS:O	2.50	0.59
1:B:196:ALA:HB1	1:B:203:TYR:CZ	2.37	0.59
1:B:649:LYS:CD	1:B:652:LEU:HD12	2.24	0.59
1:A:544:PHE:CD1	1:A:558:MSE:SE	3.06	0.59
1:A:752:ASN:C	1:A:754:ILE:N	2.53	0.59
1:B:212:GLU:HG3	1:B:216:GLN:HA	1.85	0.59
1:B:246:HIS:CE1	1:B:582:ALA:HB2	2.36	0.59
1:B:475:THR:HG23	1:B:477:GLU:HG2	1.84	0.59
1:B:484:ASP:C	1:B:486:PRO:HD3	2.21	0.59
1:B:553:PRO:HD2	1:B:585:TYR:HH	1.67	0.59
1:A:211:PHE:CD1	1:A:211:PHE:O	2.56	0.59
1:A:580:LEU:HD22	1:A:608:LEU:HD21	1.84	0.59
1:A:586:GLN:NE2	1:A:615:MSE:O	2.35	0.59
1:A:362:ALA:HB1	1:A:699:LEU:HD22	1.84	0.59
1:A:823:ILE:HD11	1:A:842:ILE:HG23	1.84	0.59
1:B:227:ARG:N	1:B:230:ASP:OD2	2.29	0.59
1:B:453:GLY:O	1:B:456:ARG:HG2	2.03	0.59
1:B:454:SER:OG	1:B:455:ASP:N	2.36	0.59
1:B:686:GLU:HA	1:B:689:ARG:HH21	1.67	0.59
1:B:233:ILE:CG1	1:B:233:ILE:O	2.50	0.58
1:B:285:GLN:O	1:B:288:GLU:HB2	2.02	0.58
1:B:772:LEU:CA	1:B:774:PRO:HD2	2.33	0.58
1:B:830:GLN:HB3	1:B:832:PHE:HD2	1.68	0.58
1:B:881:GLN:HA	1:B:881:GLN:OE1	2.03	0.58
1:A:280:PRO:O	1:A:280:PRO:CG	2.51	0.58
1:A:772:LEU:CD1	1:A:773:VAL:N	2.64	0.58
1:B:209:GLU:HB2	1:B:221:THR:CG2	2.34	0.58
1:B:278:MSE:CB	1:B:282:ALA:HB3	2.26	0.58
1:B:542:VAL:O	1:B:546:ASP:OD1	2.21	0.58
1:B:791:ARG:HG2	1:B:814:HIS:C	2.23	0.58
1:A:347:TYR:CD1	1:A:515:PRO:HA	2.38	0.58
1:A:562:VAL:HG21	1:A:604:MSE:SE	2.53	0.58
1:B:233:ILE:HG13	1:B:233:ILE:O	2.03	0.58
1:B:648:GLN:H	1:B:648:GLN:CD	2.05	0.58
1:A:220:PHE:CD2	1:A:220:PHE:N	2.59	0.58
1:A:413:LYS:CG	1:A:420:ASP:HB3	2.34	0.58
1:A:677:MSE:CG	1:A:714:LEU:HD22	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASP:OD1	2:B:1000:SAH:O2'	2.21	0.58
1:B:207:ILE:HD11	1:B:209:GLU:O	2.03	0.58
1:B:387:ASN:H	1:B:387:ASN:HD22	1.51	0.58
1:B:343:LEU:HD21	1:B:512:CYS:SG	2.43	0.58
1:B:728:GLU:HA	1:B:731:GLN:NE2	2.17	0.58
1:A:281:LYS:HA	1:A:284:ALA:CB	2.24	0.58
1:A:341:ALA:O	1:A:368:LEU:HD23	2.04	0.58
1:A:364:SER:CB	1:A:866:GLY:HA3	2.34	0.58
1:A:367:LYS:HE3	1:A:701:TRP:HH2	1.64	0.58
1:A:146:GLU:O	1:A:150:ASN:N	2.24	0.58
1:A:195:LYS:CG	1:A:266:ILE:HD11	2.33	0.58
1:A:416:VAL:O	1:A:417:GLN:NE2	2.30	0.58
1:B:342:THR:HB	1:B:371:ARG:HG3	1.85	0.58
1:B:664:ASP:HB2	1:B:688:GLN:OE1	2.04	0.58
1:A:567:PHE:HD2	1:A:572:LEU:HD21	1.68	0.58
1:B:649:LYS:C	1:B:651:SER:N	2.57	0.58
1:A:572:LEU:CD2	1:A:572:LEU:H	2.11	0.58
1:A:600:PRO:HG2	1:A:661:ALA:HB2	1.85	0.58
1:A:729:ARG:HG3	1:A:729:ARG:NH1	2.17	0.58
1:B:504:LEU:O	1:B:507:ASP:N	2.29	0.58
1:B:508:VAL:HG21	1:B:551:LEU:HD13	1.86	0.58
1:B:590:GLY:HA2	1:B:640:CYS:HB3	1.86	0.58
1:B:142:VAL:HG12	1:B:175:HIS:H	1.68	0.58
1:B:485:CYS:HB3	1:B:488:LYS:HD2	1.84	0.58
1:B:534:LYS:C	1:B:534:LYS:HZ3	2.07	0.58
1:B:621:PRO:HG3	1:B:860:ALA:HB1	1.86	0.58
1:A:814:HIS:CD2	1:A:816:THR:H	2.22	0.57
1:B:732:GLN:HG3	1:B:732:GLN:O	2.02	0.57
1:A:154:ARG:HH22	1:A:209:GLU:CG	2.15	0.57
1:A:215:ASP:C	1:A:216:GLN:HG3	2.20	0.57
1:A:186:TYR:HE2	1:A:265:ILE:HG21	1.66	0.57
1:A:464:VAL:O	1:A:474:ASP:CG	2.42	0.57
1:B:599:LEU:CD1	1:B:856:PRO:HG2	2.27	0.57
1:A:250:ARG:HG3	1:A:293:TYR:CZ	2.38	0.57
1:A:226:PHE:HB2	1:A:252:PHE:O	2.04	0.57
1:B:440:GLU:O	1:B:440:GLU:CD	2.42	0.57
1:B:685:THR:HG21	1:B:687:PHE:HB3	1.85	0.57
1:A:670:ASN:HD21	1:A:722:LEU:HD22	1.68	0.57
1:A:781:ILE:HG12	1:A:786:LEU:HD11	1.85	0.57
1:A:786:LEU:HB3	1:A:788:PRO:CD	2.27	0.57
1:B:404:LEU:HB2	1:B:451:TYR:CB	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:PHE:HB3	1:B:789:PHE:HB2	1.87	0.57
1:A:192:VAL:HA	1:A:268:LYS:HA	1.86	0.57
1:A:220:PHE:HE2	1:A:260:ASN:CA	2.18	0.57
1:B:170:LEU:HD21	1:B:211:PHE:HE1	1.69	0.57
1:B:439:ASP:OD1	1:B:440:GLU:N	2.38	0.57
1:B:456:ARG:HH21	1:B:456:ARG:CG	2.16	0.57
1:B:879:LEU:H	1:B:879:LEU:CD2	2.14	0.57
1:A:170:LEU:HD12	1:A:259:ASP:OD2	2.05	0.57
1:A:273:HIS:CD2	1:A:274:VAL:O	2.57	0.57
1:A:338:THR:HG21	1:A:367:LYS:HZ2	1.70	0.57
1:A:541:MSE:CE	1:A:572:LEU:O	2.52	0.57
1:B:192:VAL:N	1:B:269:VAL:HG23	2.20	0.57
1:B:302:TYR:HB3	1:B:588:ARG:HG3	1.85	0.57
1:A:764:VAL:CG2	1:A:772:LEU:CD1	2.83	0.57
1:A:809:ASN:O	1:A:809:ASN:OD1	2.22	0.57
1:B:513:GLY:HA3	1:B:558:MSE:HA	1.87	0.57
1:B:535:ASP:O	1:B:535:ASP:CG	2.43	0.57
1:B:672:GLN:NE2	1:B:673:PRO:HD2	2.19	0.57
1:A:236:LEU:CD1	1:A:574:LYS:HB2	2.32	0.57
1:A:792:LEU:CD2	1:A:792:LEU:N	2.64	0.57
1:B:134:GLU:CG	1:B:135:PRO:CD	2.80	0.57
1:B:788:PRO:O	1:B:807:PRO:O	2.23	0.57
1:B:142:VAL:HG12	1:B:143:ALA:H	1.70	0.57
1:B:622:LEU:HD12	1:B:880:TYR:O	2.05	0.57
1:A:236:LEU:HD23	1:A:239:ILE:CD1	2.32	0.56
1:A:455:ASP:CB	1:A:461:TYR:HE2	2.18	0.56
1:A:671:HIS:C	1:A:671:HIS:ND1	2.58	0.56
1:B:225:PHE:HE1	1:B:294:TYR:CD2	2.23	0.56
1:B:472:GLU:O	1:B:473:GLU:HB2	2.05	0.56
1:B:617:LEU:HD12	1:B:618:PRO:HD2	1.86	0.56
1:B:637:PHE:HB3	1:B:640:CYS:SG	2.44	0.56
1:B:715:LEU:HD12	1:B:715:LEU:H	1.69	0.56
1:A:247:ASP:HB3	1:A:250:ARG:HB2	1.86	0.56
1:A:460:ILE:HG21	1:A:462:PHE:CE2	2.39	0.56
1:A:517:CYS:SG	1:A:517:CYS:O	2.63	0.56
1:A:670:ASN:ND2	1:A:722:LEU:CD2	2.68	0.56
1:B:460:ILE:HD13	1:B:460:ILE:N	2.20	0.56
1:B:785:SER:O	1:B:788:PRO:HD3	2.06	0.56
1:B:351:GLY:O	1:B:355:THR:HG23	2.06	0.56
1:A:757:TRP:HZ3	1:A:773:VAL:HG21	1.70	0.56
1:B:443:VAL:O	1:B:488:LYS:NZ	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:GLU:O	1:B:495:GLU:OE1	2.24	0.56
1:A:141:PRO:HB2	1:A:143:ALA:H	1.69	0.56
1:A:154:ARG:O	1:A:155:TYR:HB2	2.05	0.56
1:A:555:TYR:CE1	1:A:615:MSE:HG2	2.41	0.56
1:A:714:LEU:HD11	1:A:717:HIS:HD2	1.70	0.56
1:A:722:LEU:N	1:A:722:LEU:HD13	2.20	0.56
1:A:803:THR:OG1	1:A:847:ILE:HA	2.05	0.56
1:A:592:MSE:CE	1:A:861:LEU:HD21	2.07	0.56
1:A:136:GLU:CG	1:A:218:HIS:CE1	2.88	0.56
1:A:137:PHE:CD2	1:A:218:HIS:HB3	2.40	0.56
1:A:136:GLU:HG2	1:A:137:PHE:H	1.71	0.56
1:A:839:PHE:HD1	1:A:839:PHE:N	2.03	0.56
1:A:635:ASN:O	1:A:638:SER:N	2.36	0.56
1:B:194:VAL:HB	1:B:203:TYR:HB2	1.87	0.56
1:A:609:TRP:CD1	1:A:620:TYR:CE1	2.93	0.56
1:A:780:PHE:HB3	1:A:786:LEU:CD2	2.35	0.56
1:B:236:LEU:HD23	1:B:239:ILE:CG1	2.36	0.56
1:B:220:PHE:HD2	1:B:262:LEU:HA	1.69	0.56
1:B:351:GLY:N	1:B:384:LEU:HD12	2.20	0.56
1:B:695:ARG:HH11	1:B:835:TYR:HD1	1.53	0.56
1:A:236:LEU:O	1:A:239:ILE:HD13	2.05	0.56
1:A:541:MSE:HE2	1:A:572:LEU:HB3	1.88	0.56
1:A:302:TYR:CD2	1:A:878:PRO:HB3	2.41	0.56
1:B:218:HIS:HB2	1:B:262:LEU:HD11	1.87	0.56
1:B:388:HIS:HA	1:B:702:SER:OG	2.06	0.56
1:B:508:VAL:HG11	1:B:511:ILE:HG22	1.88	0.56
1:A:495:GLU:CG	1:A:499:ARG:HH21	2.19	0.56
1:A:714:LEU:HD21	1:A:717:HIS:HB3	1.84	0.56
1:B:281:LYS:O	1:B:284:ALA:HB3	2.05	0.56
1:B:675:ASP:HA	1:B:718:GLN:HE21	1.70	0.56
1:A:355:THR:HG22	1:A:388:HIS:CE1	2.41	0.56
1:A:347:TYR:OH	1:A:540:GLN:NE2	2.39	0.56
1:A:784:LYS:N	1:A:786:LEU:HD11	2.18	0.56
1:B:658:LEU:HD21	1:B:791:ARG:NH2	2.21	0.55
1:B:374:VAL:HG22	1:B:394:ARG:HB2	1.88	0.55
1:B:483:SER:O	1:B:486:PRO:HG3	2.06	0.55
1:B:485:CYS:SG	1:B:488:LYS:NZ	2.77	0.55
1:A:338:THR:HG22	1:A:339:ARG:H	1.72	0.55
1:A:407:GLU:O	1:A:410:VAL:HB	2.06	0.55
1:A:817:GLN:O	1:A:818:ALA:HB3	2.05	0.55
1:B:645:ASP:O	1:B:645:ASP:CG	2.45	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:PHE:O	1:B:744:LEU:N	2.29	0.55
1:A:664:ASP:CG	1:A:664:ASP:O	2.44	0.55
1:A:723:ASN:ND2	1:A:723:ASN:C	2.58	0.55
1:B:599:LEU:CD2	1:B:601:GLN:HE21	2.19	0.55
1:B:664:ASP:HB2	1:B:688:GLN:CD	2.26	0.55
1:B:791:ARG:CG	1:B:792:LEU:N	2.69	0.55
1:B:823:ILE:CD1	1:B:845:LYS:HD2	2.36	0.55
1:A:444:GLU:HG3	1:A:445:LYS:N	2.20	0.55
1:A:511:ILE:CG2	1:A:553:PRO:HB3	2.36	0.55
1:A:652:LEU:O	1:A:653:LYS:O	2.23	0.55
1:A:665:LEU:HD21	1:A:814:HIS:CE1	2.22	0.55
1:A:735:VAL:O	1:A:735:VAL:CG1	2.55	0.55
1:B:278:MSE:O	1:B:280:PRO:CD	2.54	0.55
1:B:391:THR:HG23	1:B:392:GLU:H	1.68	0.55
1:B:879:LEU:N	1:B:879:LEU:CD2	2.70	0.55
1:A:558:MSE:O	1:A:607:PHE:HA	2.06	0.55
1:A:631:GLY:HA3	1:A:641:MSE:CE	2.35	0.55
1:A:704:GLY:O	1:A:705:GLU:HB3	2.07	0.55
1:B:176:TYR:O	1:B:210:PHE:HB2	2.07	0.55
1:B:796:GLU:CG	1:B:797:THR:N	2.58	0.55
1:B:802:VAL:CG1	1:B:803:THR:H	2.20	0.55
1:B:814:HIS:ND1	1:B:819:ARG:CZ	2.69	0.55
1:A:535:ASP:OD2	1:A:536:GLU:N	2.39	0.55
1:B:147:ALA:O	1:B:151:TRP:N	2.39	0.55
1:B:543:THR:O	1:B:547:ILE:HG12	2.07	0.55
1:A:652:LEU:N	1:A:652:LEU:HD23	2.21	0.55
1:A:704:GLY:O	1:A:705:GLU:CB	2.55	0.55
1:B:672:GLN:OE1	1:B:674:ASN:O	2.25	0.55
1:B:772:LEU:CB	1:B:774:PRO:HD2	2.35	0.55
1:A:142:VAL:HG12	1:A:176:TYR:CE2	2.42	0.55
1:A:273:HIS:CB	1:A:294:TYR:CE2	2.62	0.55
1:A:280:PRO:HG2	1:A:280:PRO:O	2.07	0.55
1:A:568:ALA:O	1:A:569:ASP:C	2.44	0.55
1:A:605:ARG:NH1	1:A:605:ARG:CG	2.53	0.55
1:A:596:CYS:O	1:A:625:TYR:N	2.40	0.55
1:A:780:PHE:C	1:A:782:LYS:N	2.60	0.55
1:A:786:LEU:C	1:A:788:PRO:HD3	2.27	0.55
1:B:281:LYS:HG3	1:B:282:ALA:N	2.22	0.54
1:B:349:GLY:O	1:B:350:CYS:SG	2.65	0.54
1:B:645:ASP:O	1:B:646:GLU:CB	2.30	0.54
1:A:555:TYR:OH	1:A:868:ALA:HB1	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:C	1:A:845:LYS:HE2	2.27	0.54
1:B:206:ARG:CG	1:B:206:ARG:NH1	2.45	0.54
1:B:239:ILE:HG21	1:B:575:TYR:CE1	2.43	0.54
1:B:667:LYS:CB	1:B:817:GLN:OE1	2.55	0.54
1:A:234:ASN:O	1:A:235:SER:HB3	2.07	0.54
1:A:394:ARG:NH2	1:A:396:GLU:OE1	2.38	0.54
1:A:839:PHE:N	1:A:839:PHE:CD1	2.74	0.54
1:A:154:ARG:CZ	1:A:175:HIS:HE1	2.21	0.54
1:A:249:ARG:CG	1:A:249:ARG:O	2.56	0.54
1:A:195:LYS:CG	1:A:266:ILE:CD1	2.85	0.54
1:A:269:VAL:HG22	1:A:271:ILE:HG13	1.90	0.54
1:A:585:TYR:HD1	1:A:610:GLY:O	1.89	0.54
1:B:387:ASN:CB	1:B:836:TYR:CE2	2.90	0.54
1:A:186:TYR:CE2	1:A:265:ILE:CG2	2.89	0.54
1:A:415:TYR:CD2	1:A:490:ARG:CG	2.88	0.54
1:A:413:LYS:HG2	1:A:420:ASP:HB3	1.90	0.54
1:A:505:PRO:HD3	1:A:550:TYR:CE1	2.42	0.54
1:A:772:LEU:N	1:A:772:LEU:HD12	2.22	0.54
1:B:139:GLY:HA3	1:B:178:SER:HB3	1.88	0.54
1:A:280:PRO:O	1:A:281:LYS:CB	2.56	0.54
1:A:599:LEU:HD11	1:A:856:PRO:CG	2.33	0.54
1:A:644:TYR:CE1	1:A:649:LYS:HB3	2.42	0.54
1:A:727:TYR:CE2	1:A:731:GLN:CD	2.80	0.54
1:B:266:ILE:HG22	1:B:267:SER:HB3	1.89	0.54
1:B:459:GLY:O	1:B:461:TYR:HD2	1.88	0.54
1:B:690:TYR:C	1:B:693:LEU:HD13	2.27	0.54
1:A:253:LEU:HD12	1:A:294:TYR:HE1	1.70	0.54
1:A:538:ASN:C	1:A:540:GLN:N	2.55	0.54
1:A:793:TRP:HE3	1:A:793:TRP:HA	1.68	0.54
1:A:716:ASP:OD2	1:A:838:LEU:HB2	2.08	0.54
1:B:156:GLY:O	1:B:157:ARG:C	2.46	0.54
1:B:151:TRP:CE3	1:B:175:HIS:CE1	2.96	0.54
1:B:223:ARG:HA	1:B:256:GLU:O	2.08	0.54
1:B:387:ASN:ND2	1:B:387:ASN:N	2.56	0.54
1:B:404:LEU:O	1:B:404:LEU:HD22	2.07	0.54
1:B:685:THR:CG2	1:B:687:PHE:N	2.66	0.54
1:B:691:ILE:HG23	1:B:692:ARG:HG3	1.89	0.54
1:A:173:ARG:NH1	1:A:212:GLU:CD	2.41	0.54
1:A:405:LEU:HD21	1:A:503:PRO:HG2	1.89	0.54
1:A:785:SER:O	1:A:786:LEU:HB2	2.06	0.54
1:B:139:GLY:CA	1:B:178:SER:HB3	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:PHE:HE1	1:A:210:PHE:HB3	1.73	0.53
1:A:449:ILE:CD1	1:A:460:ILE:HG23	2.36	0.53
1:A:502:LEU:CD2	1:A:503:PRO:HD2	2.30	0.53
1:A:766:LEU:HD23	1:A:767:SER:N	2.23	0.53
1:B:676:VAL:CB	1:B:713:LYS:HE2	2.38	0.53
1:A:134:GLU:O	1:A:136:GLU:N	2.41	0.53
1:A:285:GLN:HA	1:A:285:GLN:OE1	2.08	0.53
1:B:714:LEU:HD23	1:B:714:LEU:C	2.29	0.53
1:A:220:PHE:HD2	1:A:220:PHE:N	1.87	0.53
1:A:227:ARG:N	1:A:230:ASP:OD2	2.38	0.53
1:A:757:TRP:CH2	1:A:763:ARG:NH2	2.76	0.53
1:B:456:ARG:HG2	1:B:456:ARG:NH2	2.17	0.53
1:B:834:ASP:C	1:B:836:TYR:H	2.10	0.53
1:A:198:GLU:O	1:A:199:ASN:HB2	2.07	0.53
1:A:273:HIS:CE1	1:A:274:VAL:O	2.62	0.53
1:A:250:ARG:CZ	1:A:295:ASP:OD2	2.56	0.53
1:A:715:LEU:HD22	1:A:837:ARG:CG	2.29	0.53
1:B:447:VAL:O	1:B:447:VAL:HG23	2.06	0.53
1:B:389:PRO:HD2	1:B:702:SER:OG	2.08	0.53
1:A:619:LYS:HB3	1:A:878:PRO:O	2.08	0.53
1:A:730:VAL:CG2	1:A:818:ALA:O	2.53	0.53
1:B:247:ASP:C	1:B:247:ASP:OD1	2.47	0.53
1:B:578:SER:O	1:B:579:CYS:C	2.44	0.53
1:B:802:VAL:HG13	1:B:803:THR:H	1.72	0.53
1:A:195:LYS:HE2	1:A:264:CYS:HA	1.89	0.53
1:A:367:LYS:HE3	1:A:701:TRP:CZ3	2.40	0.53
1:A:633:ALA:C	1:A:634:PRO:O	2.42	0.53
1:A:148:ARG:CG	1:A:155:TYR:CD1	2.91	0.53
1:A:375:ASP:OD2	2:A:1000:SAH:O2'	2.27	0.53
1:A:814:HIS:CD2	1:A:815:PRO:HD2	2.42	0.53
1:B:443:VAL:CG1	1:B:466:TRP:CE3	2.89	0.53
1:B:404:LEU:HD11	1:B:502:LEU:HD21	1.91	0.53
1:B:622:LEU:HB3	1:B:623:PRO:HD2	1.90	0.53
1:B:672:GLN:CD	1:B:674:ASN:H	2.11	0.53
1:A:136:GLU:CD	1:A:137:PHE:N	2.62	0.53
1:A:417:GLN:O	1:A:418:ASP:C	2.45	0.53
1:A:617:LEU:HD12	1:A:618:PRO:HD2	1.91	0.53
1:A:729:ARG:NE	1:A:772:LEU:O	2.41	0.53
1:B:209:GLU:HB2	1:B:221:THR:HB	1.90	0.53
1:B:352:GLY:N	2:B:1000:SAH:O	2.41	0.53
1:B:602:PHE:O	1:B:799:PRO:O	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:PRO:CG	1:B:835:TYR:CE2	2.88	0.53
1:A:140:SER:HB3	1:A:141:PRO:CD	2.38	0.53
1:A:375:ASP:C	1:A:375:ASP:OD2	2.46	0.53
1:B:148:ARG:HH11	1:B:148:ARG:CG	1.97	0.53
1:B:695:ARG:NH1	1:B:835:TYR:CD1	2.77	0.53
1:A:232:VAL:CG1	1:A:233:ILE:HG22	2.38	0.52
1:A:622:LEU:HD12	1:A:880:TYR:O	2.09	0.52
1:A:672:GLN:HE22	1:A:674:ASN:HB2	1.71	0.52
1:A:822:THR:CG2	1:A:825:GLU:CD	2.78	0.52
1:B:828:ARG:NH2	1:B:834:ASP:OD1	2.42	0.52
1:A:223:ARG:HD2	1:A:255:GLU:HA	1.92	0.52
1:A:399:ASP:N	1:A:399:ASP:OD1	2.35	0.52
1:A:763:ARG:NH1	1:A:771:PRO:HB2	2.24	0.52
1:A:176:TYR:OH	1:A:212:GLU:OE2	2.28	0.52
1:A:716:ASP:N	1:A:716:ASP:OD1	2.40	0.52
1:A:740:ASN:N	1:A:740:ASN:OD1	2.42	0.52
1:B:347:TYR:HD2	1:B:516:PRO:HD3	1.72	0.52
1:B:772:LEU:CA	1:B:774:PRO:CD	2.87	0.52
1:B:443:VAL:CG1	1:B:466:TRP:CZ3	2.92	0.52
1:B:605:ARG:CG	1:B:605:ARG:HH11	2.16	0.52
1:B:729:ARG:NH2	1:B:771:PRO:O	2.43	0.52
1:A:284:ALA:HA	1:A:287:ILE:CG1	2.40	0.52
1:A:340:THR:HA	1:A:367:LYS:O	2.09	0.52
1:A:464:VAL:HG13	1:A:466:TRP:CZ2	2.43	0.52
1:A:495:GLU:CG	1:A:499:ARG:NH2	2.73	0.52
1:A:671:HIS:HE1	1:A:673:PRO:CG	2.23	0.52
1:A:714:LEU:HD23	1:A:715:LEU:N	2.24	0.52
1:A:837:ARG:HB3	1:A:839:PHE:CE1	2.39	0.52
1:B:411:LEU:HD21	1:B:493:VAL:CG2	2.39	0.52
1:B:534:LYS:HZ1	1:B:535:ASP:HB2	1.73	0.52
1:B:544:PHE:CE1	1:B:558:MSE:HE3	2.45	0.52
1:B:549:ALA:CB	1:B:583:MSE:HE1	2.38	0.52
1:B:729:ARG:CZ	1:B:729:ARG:HB3	2.38	0.52
1:B:252:PHE:HD2	1:B:296:MSE:HB3	1.74	0.52
1:A:148:ARG:HH11	1:A:148:ARG:HG3	1.75	0.52
1:A:180:LYS:HB2	1:A:185:VAL:HG13	1.92	0.52
1:A:624:THR:O	1:A:624:THR:HG22	2.09	0.52
1:A:763:ARG:HH11	1:A:771:PRO:CB	2.23	0.52
1:A:384:LEU:HD13	1:A:388:HIS:CD2	2.44	0.52
1:A:723:ASN:HD21	1:A:725:ASP:HB2	1.75	0.52
1:B:489:ILE:HG12	1:B:490:ARG:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ASP:HB3	1:A:461:TYR:HE2	1.75	0.52
1:A:215:ASP:O	1:A:216:GLN:CB	2.57	0.52
1:A:391:THR:CG2	1:A:393:VAL:HG23	2.40	0.52
1:A:601:GLN:HB3	1:A:798:VAL:HG23	1.91	0.52
1:A:140:SER:O	1:A:141:PRO:C	2.48	0.51
1:A:154:ARG:HD2	1:A:172:ALA:HB3	1.93	0.51
1:B:511:ILE:HD11	1:B:548:VAL:HG22	1.92	0.51
1:B:766:LEU:C	1:B:768:SER:O	2.48	0.51
1:A:136:GLU:CG	1:A:137:PHE:N	2.73	0.51
1:A:272:VAL:HG21	1:A:286:LEU:CD2	2.39	0.51
1:B:209:GLU:HB2	1:B:221:THR:HG22	1.92	0.51
1:B:619:LYS:HB2	1:B:878:PRO:O	2.10	0.51
1:A:605:ARG:HG3	1:A:605:ARG:HH11	1.74	0.51
1:A:763:ARG:C	1:A:764:VAL:HG22	2.31	0.51
1:A:700:ASP:HB2	1:A:835:TYR:OH	2.10	0.51
1:B:538:ASN:N	1:B:538:ASN:ND2	2.57	0.51
1:B:555:TYR:HE2	1:B:618:PRO:HD3	1.74	0.51
1:B:720:LEU:HD12	1:B:805:ALA:O	2.11	0.51
1:A:211:PHE:HD1	1:A:211:PHE:C	2.14	0.51
1:A:273:HIS:CG	1:A:294:TYR:HE2	2.26	0.51
1:A:580:LEU:HD23	1:A:587:ALA:CB	2.41	0.51
1:A:727:TYR:CE2	1:A:731:GLN:NE2	2.78	0.51
1:A:764:VAL:HG21	1:A:772:LEU:HD12	1.89	0.51
1:A:691:ILE:CG2	1:A:834:ASP:OD1	2.58	0.51
1:B:729:ARG:CD	1:B:773:VAL:HG21	2.38	0.51
1:B:622:LEU:HD11	1:B:879:LEU:HB2	1.92	0.51
1:A:656:LEU:C	1:A:657:LEU:HD12	2.30	0.51
1:B:195:LYS:HE2	1:B:264:CYS:HA	1.92	0.51
1:B:665:LEU:HB3	1:B:717:HIS:HE2	1.76	0.51
1:A:501:ILE:HG12	1:A:502:LEU:N	2.24	0.51
1:A:596:CYS:HA	1:A:627:VAL:CG1	2.41	0.51
1:B:229:GLU:OE1	1:B:229:GLU:N	2.29	0.51
1:B:404:LEU:HD13	1:B:404:LEU:C	2.30	0.51
1:B:572:LEU:N	1:B:572:LEU:HD12	2.25	0.51
1:A:154:ARG:CD	1:A:172:ALA:HB3	2.39	0.51
1:A:154:ARG:HD2	1:A:172:ALA:CB	2.40	0.51
1:A:172:ALA:HA	1:A:213:GLY:HA2	1.92	0.51
1:B:192:VAL:CA	1:B:269:VAL:HG23	2.41	0.51
1:B:217:CYS:HB2	1:B:219:TYR:CE2	2.46	0.51
1:B:266:ILE:HG22	1:B:267:SER:N	2.25	0.51
1:A:151:TRP:CD1	1:A:175:HIS:CE1	2.98	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:ND2	1:A:234:ASN:O	2.43	0.51
1:A:415:TYR:CE2	1:A:490:ARG:HG2	2.46	0.51
1:B:186:TYR:HD1	1:B:268:LYS:HG3	1.76	0.51
1:B:362:ALA:HB2	1:B:699:LEU:HD22	1.90	0.51
1:B:814:HIS:CD2	1:B:815:PRO:N	2.78	0.51
1:A:249:ARG:O	1:A:293:TYR:CE2	2.64	0.51
1:A:564:ILE:HG23	1:A:573:GLY:N	2.26	0.51
1:B:231:THR:OG1	1:B:233:ILE:CG2	2.44	0.51
1:B:274:VAL:HA	1:B:278:MSE:HE3	1.93	0.51
1:B:241:VAL:HG21	1:B:579:CYS:HB3	1.93	0.51
1:B:676:VAL:HG21	1:B:713:LYS:HZ1	1.76	0.51
1:A:575:TYR:CE1	1:A:579:CYS:SG	3.04	0.51
1:A:648:GLN:C	1:A:649:LYS:O	2.43	0.51
1:B:304:THR:HG21	1:B:588:ARG:NH2	2.25	0.51
1:B:671:HIS:CE1	1:B:673:PRO:HD3	2.46	0.51
1:A:671:HIS:HE1	1:A:673:PRO:HG3	1.75	0.50
1:B:272:VAL:CG1	1:B:273:HIS:H	2.24	0.50
1:B:460:ILE:HD12	1:B:460:ILE:N	2.26	0.50
1:B:508:VAL:HG11	1:B:511:ILE:CG2	2.41	0.50
1:A:609:TRP:HD1	1:A:620:TYR:CE1	2.29	0.50
1:B:154:ARG:HH21	1:B:209:GLU:CD	2.15	0.50
1:B:464:VAL:HG23	1:B:465:GLN:N	2.24	0.50
1:A:675:ASP:OD1	1:A:675:ASP:N	2.43	0.50
1:B:224:TRP:O	1:B:254:SER:HB3	2.11	0.50
1:B:642:VAL:O	1:B:642:VAL:CG2	2.59	0.50
1:B:695:ARG:NE	1:B:703:PHE:HE2	2.08	0.50
1:A:253:LEU:HD22	1:A:254:SER:O	2.11	0.50
1:A:544:PHE:HD1	1:A:558:MSE:SE	2.43	0.50
1:A:715:LEU:HD12	1:A:834:ASP:O	2.11	0.50
1:B:140:SER:CB	1:B:141:PRO:CD	2.85	0.50
1:B:411:LEU:HD23	1:B:412:CYS:N	2.26	0.50
1:B:413:LYS:HZ1	1:B:414:LYS:CE	2.23	0.50
1:B:766:LEU:O	1:B:768:SER:O	2.29	0.50
1:A:196:ALA:HB2	1:A:203:TYR:CE1	2.47	0.50
1:A:505:PRO:HD3	1:A:550:TYR:HE1	1.76	0.50
1:A:557:LEU:HD22	1:A:609:TRP:CH2	2.47	0.50
1:A:733:ILE:CG2	1:A:791:ARG:HE	2.25	0.50
1:A:757:TRP:CZ3	1:A:773:VAL:CG2	2.95	0.50
1:A:814:HIS:HD2	1:A:816:THR:N	2.06	0.50
1:B:250:ARG:NH2	1:B:295:ASP:OD1	2.44	0.50
1:B:402:LEU:O	1:B:405:LEU:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ASN:ND2	1:B:586:GLN:NE2	2.60	0.50
1:B:685:THR:HG21	1:B:688:GLN:H	1.67	0.50
1:B:821:LEU:CB	1:B:825:GLU:OE1	2.60	0.50
1:B:622:LEU:CD1	1:B:879:LEU:HB2	2.41	0.50
1:A:195:LYS:NZ	1:A:263:ASP:O	2.28	0.50
1:A:370:THR:O	1:A:391:THR:OG1	2.24	0.50
1:A:412:CYS:C	1:A:416:VAL:HG23	2.28	0.50
1:A:690:TYR:HE1	1:A:698:MSE:SE	2.45	0.50
1:A:823:ILE:HG12	1:A:846:TYR:CE2	2.47	0.50
1:B:410:VAL:O	1:B:413:LYS:HB3	2.11	0.50
1:A:136:GLU:CG	1:A:137:PHE:H	2.24	0.50
1:A:141:PRO:O	1:A:142:VAL:HG13	2.11	0.50
1:A:148:ARG:HG2	1:A:155:TYR:CD1	2.46	0.50
1:A:154:ARG:NH1	1:A:211:PHE:CG	2.80	0.50
1:A:148:ARG:HG2	1:A:155:TYR:CG	2.45	0.50
1:A:397:LYS:HB2	1:A:400:GLU:OE1	2.11	0.50
1:A:456:ARG:NH2	1:A:456:ARG:CG	2.59	0.50
1:A:495:GLU:HG3	1:A:499:ARG:NH2	2.26	0.50
1:A:584:LYS:HB3	1:A:584:LYS:NZ	2.25	0.50
1:A:665:LEU:O	1:A:665:LEU:CD1	2.53	0.50
1:A:670:ASN:O	1:A:670:ASN:OD1	2.30	0.50
1:B:186:TYR:CZ	1:B:265:ILE:HG21	2.47	0.50
1:B:186:TYR:CD1	1:B:268:LYS:HG3	2.47	0.50
1:B:413:LYS:NZ	1:B:414:LYS:CE	2.75	0.50
1:B:646:GLU:OE2	1:B:647:THR:HG23	2.09	0.50
1:B:728:GLU:O	1:B:731:GLN:HG2	2.12	0.50
1:B:814:HIS:HA	1:B:821:LEU:HD13	1.93	0.50
1:A:287:ILE:CD1	1:A:288:GLU:HG2	2.42	0.50
1:A:455:ASP:HB3	1:A:461:TYR:CE2	2.47	0.50
1:A:591:MSE:HG3	1:A:640:CYS:O	2.12	0.50
1:B:591:MSE:CE	1:B:640:CYS:HB2	2.42	0.50
1:B:774:PRO:O	1:B:776:TYR:N	2.45	0.50
1:A:447:VAL:HG13	1:A:463:LYS:HG2	1.93	0.50
1:A:474:ASP:C	1:A:475:THR:HG23	2.32	0.50
1:B:192:VAL:HG13	1:B:193:TYR:N	2.27	0.50
1:B:375:ASP:OD1	1:B:376:PHE:N	2.45	0.50
1:B:791:ARG:CG	1:B:813:ILE:O	2.59	0.50
1:B:658:LEU:CD2	1:B:791:ARG:NH2	2.74	0.50
1:A:250:ARG:NH2	1:A:584:LYS:HE2	2.23	0.49
1:A:657:LEU:HD23	1:A:795:ASP:CA	2.42	0.49
1:A:780:PHE:C	1:A:782:LYS:H	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:LEU:O	1:A:868:ALA:N	2.45	0.49
1:B:208:THR:OG1	1:B:221:THR:CG2	2.60	0.49
1:B:378:SER:O	1:B:382:GLN:CG	2.60	0.49
1:B:884:PRO:O	1:B:885:SER:O	2.30	0.49
1:A:204:ILE:HB	1:A:225:PHE:HB2	1.94	0.49
1:A:242:ASP:CG	1:A:243:GLY:H	2.15	0.49
1:A:364:SER:OG	1:A:863:TYR:O	2.30	0.49
1:A:823:ILE:HG12	1:A:846:TYR:CD2	2.46	0.49
1:B:207:ILE:HD12	1:B:221:THR:O	2.12	0.49
1:B:281:LYS:HA	1:B:284:ALA:HB3	1.94	0.49
1:B:535:ASP:OD2	1:B:539:LYS:HE3	2.12	0.49
1:B:679:TYR:O	1:B:681:GLY:N	2.43	0.49
1:B:774:PRO:CB	1:B:778:MSE:CE	2.86	0.49
1:B:791:ARG:HG2	1:B:813:ILE:O	2.12	0.49
1:B:810:GLN:O	1:B:811:VAL:HG13	2.11	0.49
1:A:140:SER:CB	1:A:141:PRO:CD	2.90	0.49
1:A:389:PRO:CD	1:A:390:GLN:H	2.26	0.49
1:B:143:ALA:N	1:B:175:HIS:O	2.44	0.49
1:B:413:LYS:NZ	1:B:414:LYS:NZ	2.60	0.49
1:B:472:GLU:H	1:B:472:GLU:CD	2.16	0.49
1:B:791:ARG:CG	1:B:792:LEU:H	2.25	0.49
1:A:174:CYS:O	1:A:212:GLU:N	2.26	0.49
1:A:176:TYR:O	1:A:210:PHE:HB2	2.12	0.49
1:A:206:ARG:O	1:A:222:CYS:CB	2.57	0.49
1:A:195:LYS:HB2	1:A:264:CYS:HB3	1.94	0.49
1:A:343:LEU:HD21	1:A:512:CYS:SG	2.52	0.49
1:A:394:ARG:HH21	1:A:396:GLU:CD	2.16	0.49
1:A:536:GLU:O	1:A:538:ASN:OD1	2.30	0.49
1:A:837:ARG:O	1:A:838:LEU:HD12	2.11	0.49
1:B:275:ASP:OD2	1:B:277:ASN:HB2	2.12	0.49
1:B:387:ASN:HB2	1:B:836:TYR:CE2	2.46	0.49
1:B:387:ASN:HD22	1:B:387:ASN:N	2.10	0.49
1:B:394:ARG:NH2	1:B:396:GLU:OE2	2.42	0.49
1:B:696:LYS:C	1:B:698:MSE:N	2.64	0.49
1:A:250:ARG:NH2	1:A:584:LYS:HD2	2.28	0.49
1:B:272:VAL:HG11	1:B:286:LEU:HD23	1.95	0.49
1:A:874:GLU:HG3	1:A:875:GLY:N	2.26	0.49
1:B:140:SER:HB3	1:B:141:PRO:HD3	1.91	0.49
1:B:375:ASP:O	1:B:395:ASN:HA	2.12	0.49
1:B:672:GLN:HE21	1:B:672:GLN:HA	1.78	0.49
1:B:687:PHE:C	1:B:687:PHE:CD2	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:O	1:A:185:VAL:HA	2.13	0.49
1:A:645:ASP:O	1:A:646:GLU:OE2	2.30	0.49
1:A:843:LYS:O	1:A:847:ILE:HD12	2.13	0.49
1:B:535:ASP:OD1	1:B:539:LYS:HE3	2.13	0.49
1:B:547:ILE:O	1:B:548:VAL:C	2.50	0.49
1:B:679:TYR:C	1:B:681:GLY:N	2.65	0.49
1:B:723:ASN:OD1	1:B:726:ASP:OD2	2.30	0.49
1:A:339:ARG:O	1:A:367:LYS:HB2	2.13	0.49
1:A:376:PHE:C	1:A:395:ASN:OD1	2.51	0.49
1:A:454:SER:C	1:A:456:ARG:N	2.66	0.49
1:B:180:LYS:CE	1:B:183:ASN:HA	2.42	0.49
1:B:207:ILE:HD13	1:B:220:PHE:HB2	1.94	0.49
1:B:378:SER:O	1:B:382:GLN:HG2	2.13	0.49
1:B:561:VAL:HG23	1:B:563:ASP:HB2	1.95	0.49
1:B:622:LEU:CD1	1:B:880:TYR:O	2.60	0.49
1:B:626:ASP:OD2	1:B:655:ALA:CB	2.61	0.49
1:A:537:LYS:C	1:A:539:LYS:H	2.15	0.49
1:A:757:TRP:CZ3	1:A:773:VAL:HG21	2.48	0.49
1:B:343:LEU:HB2	1:B:368:LEU:CD2	2.43	0.49
1:B:624:THR:O	1:B:624:THR:HG22	2.13	0.49
1:B:668:VAL:O	1:B:817:GLN:HG2	2.13	0.49
1:B:671:HIS:CE1	1:B:673:PRO:HB3	2.44	0.49
1:B:692:ARG:C	1:B:693:LEU:HD12	2.32	0.49
1:A:151:TRP:CD1	1:A:151:TRP:O	2.66	0.49
1:A:785:SER:OG	1:A:786:LEU:N	2.43	0.49
1:B:349:GLY:C	1:B:351:GLY:H	2.16	0.49
1:B:361:ALA:CB	1:B:368:LEU:HB2	2.43	0.49
1:B:565:LEU:HD11	1:B:606:VAL:HG21	1.95	0.49
1:A:413:LYS:HG3	1:A:420:ASP:HB3	1.95	0.48
1:A:442:VAL:HG11	1:A:467:GLU:OE2	2.13	0.48
1:A:585:TYR:CE1	1:A:612:LEU:HG	2.48	0.48
1:A:555:TYR:CE2	1:A:618:PRO:CG	2.95	0.48
1:B:349:GLY:CA	1:B:380:ALA:HB1	2.42	0.48
1:B:227:ARG:O	1:B:230:ASP:CB	2.58	0.48
1:B:346:LEU:O	1:B:347:TYR:HB2	2.12	0.48
1:B:457:GLU:O	1:B:461:TYR:OH	2.30	0.48
1:B:812:ILE:HG12	1:B:812:ILE:O	2.13	0.48
1:A:456:ARG:O	1:A:456:ARG:HG3	2.13	0.48
1:A:464:VAL:HG12	1:A:475:THR:O	2.13	0.48
1:A:728:GLU:CD	1:A:766:LEU:CG	2.78	0.48
1:B:553:PRO:O	1:B:553:PRO:CD	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:HIS:HE1	1:B:673:PRO:CB	2.27	0.48
1:B:802:VAL:HG12	1:B:803:THR:N	2.27	0.48
1:B:603:ARG:NH2	1:B:830:GLN:HE22	2.11	0.48
1:B:603:ARG:NH1	1:B:852:ALA:O	2.45	0.48
1:A:465:GLN:CG	1:A:474:ASP:OD1	2.62	0.48
1:A:496:GLY:O	1:A:501:ILE:HG23	2.13	0.48
1:A:733:ILE:HG21	1:A:791:ARG:NH2	2.22	0.48
1:B:144:ALA:O	1:B:145:ASP:CB	2.60	0.48
1:B:235:SER:O	1:B:236:LEU:C	2.50	0.48
1:B:621:PRO:HD3	1:B:864:CYS:SG	2.53	0.48
1:B:676:VAL:CG2	1:B:713:LYS:NZ	2.76	0.48
1:B:689:ARG:O	1:B:693:LEU:CD1	2.62	0.48
1:B:717:HIS:C	1:B:718:GLN:HG3	2.32	0.48
1:A:141:PRO:CB	1:A:143:ALA:H	2.26	0.48
1:A:347:TYR:HD1	1:A:516:PRO:HD3	1.77	0.48
1:A:367:LYS:CE	1:A:701:TRP:CH2	2.82	0.48
1:B:170:LEU:CD2	1:B:211:PHE:CZ	2.97	0.48
1:B:562:VAL:HG21	1:B:604:MSE:CE	2.34	0.48
1:B:621:PRO:CG	1:B:860:ALA:HB1	2.43	0.48
1:B:785:SER:O	1:B:788:PRO:HD2	2.12	0.48
1:A:309:SER:O	1:A:310:SER:OG	2.30	0.48
1:B:171:LYS:O	1:B:214:THR:HG23	2.13	0.48
1:B:239:ILE:HD12	1:B:239:ILE:N	2.28	0.48
1:B:841:PRO:HB2	1:B:843:LYS:HE3	1.95	0.48
1:A:248:PRO:HD2	1:A:249:ARG:H	1.78	0.48
1:B:195:LYS:HG3	1:B:266:ILE:HD12	1.95	0.48
1:B:229:GLU:H	1:B:229:GLU:CD	2.13	0.48
1:B:345:ASP:OD2	1:B:348:SER:HB3	2.13	0.48
1:B:362:ALA:HA	1:B:366:LEU:O	2.13	0.48
1:B:814:HIS:CE1	1:B:819:ARG:NH2	2.80	0.48
1:A:379:PHE:HA	1:A:382:GLN:HG2	1.96	0.48
1:A:757:TRP:HZ3	1:A:773:VAL:HG23	1.79	0.48
1:A:866:GLY:O	1:A:870:LEU:CD1	2.60	0.48
1:B:345:ASP:HA	1:B:512:CYS:HB2	1.95	0.48
1:B:588:ARG:NH1	1:B:618:PRO:O	2.47	0.48
1:B:607:PHE:CD2	1:B:861:LEU:HD11	2.49	0.48
1:A:191:ASP:HB2	1:A:269:VAL:O	2.14	0.48
1:B:538:ASN:O	1:B:541:MSE:HB3	2.13	0.48
1:B:601:GLN:OE1	1:B:801:VAL:CG1	2.62	0.48
1:B:673:PRO:HG2	1:B:674:ASN:ND2	2.29	0.48
1:B:695:ARG:CD	1:B:700:ASP:CB	2.85	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:ALA:O	1:B:790:GLY:HA3	2.13	0.48
1:A:175:HIS:HA	1:A:211:PHE:HA	1.95	0.48
1:A:415:TYR:HD2	1:A:490:ARG:CG	2.21	0.48
1:A:498:LYS:CD	1:A:498:LYS:N	2.76	0.48
1:A:514:GLY:O	1:A:515:PRO:C	2.53	0.48
1:A:787:LYS:HB2	1:A:809:ASN:C	2.34	0.48
1:B:387:ASN:HB2	1:B:836:TYR:HE2	1.78	0.48
1:B:599:LEU:HD12	1:B:599:LEU:N	2.28	0.48
1:B:601:GLN:HB3	1:B:798:VAL:O	2.14	0.48
1:B:689:ARG:O	1:B:693:LEU:HD11	2.14	0.48
1:B:790:GLY:C	1:B:813:ILE:HG13	2.35	0.48
1:A:220:PHE:CD2	1:A:220:PHE:C	2.84	0.47
1:A:811:VAL:O	1:A:811:VAL:CG2	2.58	0.47
1:B:695:ARG:HG2	1:B:695:ARG:HH11	1.68	0.47
1:B:729:ARG:HD3	1:B:773:VAL:CG2	2.38	0.47
1:B:741:PHE:CD2	1:B:788:PRO:HG2	2.49	0.47
1:A:724:ASN:OD1	1:A:724:ASN:N	2.41	0.47
1:A:807:PRO:HA	1:A:812:ILE:HG22	1.96	0.47
1:B:236:LEU:HD23	1:B:239:ILE:HG13	1.95	0.47
1:B:440:GLU:HG3	1:B:440:GLU:O	2.13	0.47
1:B:834:ASP:C	1:B:836:TYR:N	2.68	0.47
1:A:137:PHE:CD1	1:A:176:TYR:CD1	3.02	0.47
1:A:763:ARG:HB3	1:A:764:VAL:H	1.37	0.47
1:A:599:LEU:CD1	1:A:856:PRO:HG2	2.36	0.47
1:B:464:VAL:HG21	1:B:466:TRP:CZ2	2.49	0.47
1:B:729:ARG:HG2	1:B:729:ARG:H	1.51	0.47
1:B:830:GLN:HB3	1:B:832:PHE:CD2	2.49	0.47
1:A:179:ALA:HB1	1:A:262:LEU:CD2	2.44	0.47
1:A:404:LEU:C	1:A:404:LEU:CD1	2.49	0.47
1:A:554:LYS:HA	1:A:612:LEU:HD12	1.96	0.47
1:B:225:PHE:CE1	1:B:294:TYR:CD2	3.03	0.47
1:B:414:LYS:O	1:B:415:TYR:CB	2.62	0.47
1:A:220:PHE:CE2	1:A:260:ASN:CA	2.98	0.47
1:A:305:PHE:N	1:A:305:PHE:CD2	2.83	0.47
1:A:544:PHE:CE1	1:A:558:MSE:SE	3.17	0.47
1:A:563:ASP:O	1:A:564:ILE:C	2.49	0.47
1:A:619:LYS:CD	1:A:877:ASP:O	2.62	0.47
1:B:252:PHE:CD2	1:B:296:MSE:HB3	2.49	0.47
1:B:274:VAL:HG23	1:B:278:MSE:CG	2.38	0.47
1:B:514:GLY:N	1:B:515:PRO:CD	2.78	0.47
1:A:154:ARG:NH2	1:A:209:GLU:OE1	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:HD12	1:A:288:GLU:HG2	1.97	0.47
1:B:364:SER:OG	1:B:863:TYR:O	2.32	0.47
1:B:515:PRO:O	1:B:560:ASN:ND2	2.48	0.47
1:A:455:ASP:CB	1:A:461:TYR:CE2	2.97	0.47
1:A:719:PRO:HB3	1:A:820:VAL:O	2.14	0.47
1:B:246:HIS:HE1	1:B:581:VAL:HG13	1.80	0.47
1:B:394:ARG:NE	1:B:396:GLU:OE2	2.42	0.47
1:B:591:MSE:CG	1:B:606:VAL:HG22	2.44	0.47
1:B:669:GLN:OE1	1:B:669:GLN:N	2.42	0.47
1:B:774:PRO:CB	1:B:778:MSE:HE3	2.44	0.47
1:B:774:PRO:HB3	1:B:778:MSE:HE3	1.96	0.47
1:B:779:SER:O	1:B:780:PHE:C	2.52	0.47
1:A:220:PHE:O	1:A:220:PHE:CG	2.68	0.47
1:A:641:MSE:HG3	1:A:642:VAL:H	1.78	0.47
1:B:174:CYS:SG	1:B:175:HIS:N	2.87	0.47
1:B:440:GLU:OE1	1:B:440:GLU:O	2.33	0.47
1:A:394:ARG:HB3	1:A:394:ARG:HE	1.53	0.47
1:B:375:ASP:OD1	1:B:377:ASN:N	2.48	0.47
1:B:456:ARG:O	1:B:457:GLU:C	2.51	0.47
1:B:565:LEU:HD11	1:B:606:VAL:CG2	2.45	0.47
1:B:659:GLY:HA2	1:B:794:TRP:HB3	1.95	0.47
1:A:508:VAL:HG11	1:A:551:LEU:HB3	1.97	0.47
1:A:591:MSE:HE1	1:A:634:PRO:HD2	1.96	0.47
1:B:235:SER:O	1:B:237:VAL:CG2	2.63	0.47
1:B:250:ARG:NH2	1:B:295:ASP:CG	2.68	0.47
1:B:771:PRO:HB2	1:B:773:VAL:H	1.80	0.47
1:B:806:GLU:HA	1:B:807:PRO:HD3	1.72	0.47
1:A:464:VAL:HG13	1:A:466:TRP:CE2	2.50	0.47
1:A:550:TYR:HD1	1:A:551:LEU:HG	1.80	0.47
1:A:664:ASP:HB3	1:A:688:GLN:OE1	2.15	0.47
1:A:717:HIS:ND1	1:A:822:THR:HG21	2.29	0.47
1:B:301:ALA:C	1:B:302:TYR:CD2	2.88	0.47
1:B:387:ASN:CB	1:B:836:TYR:HE2	2.28	0.47
1:A:208:THR:OG1	1:A:221:THR:O	2.24	0.46
1:A:280:PRO:O	1:A:280:PRO:CD	2.62	0.46
1:A:468:GLY:HA3	1:B:808:HIS:CE1	2.50	0.46
1:A:483:SER:OG	1:A:484:ASP:N	2.48	0.46
1:A:589:LEU:HA	1:A:620:TYR:HH	1.78	0.46
1:A:787:LYS:HG3	1:A:809:ASN:O	2.16	0.46
1:B:349:GLY:O	1:B:351:GLY:N	2.46	0.46
1:B:558:MSE:HE3	1:B:558:MSE:HB2	1.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:819:ARG:O	1:B:820:VAL:CG1	2.62	0.46
1:A:150:ASN:HB3	1:A:151:TRP:CE3	2.50	0.46
1:A:384:LEU:C	1:A:384:LEU:HD12	2.36	0.46
1:A:389:PRO:HD2	1:A:390:GLN:H	1.80	0.46
1:B:346:LEU:HB3	1:B:347:TYR:HD1	1.80	0.46
1:B:561:VAL:CG2	1:B:563:ASP:HB2	2.46	0.46
1:B:695:ARG:HA	1:B:835:TYR:CD1	2.48	0.46
1:A:404:LEU:O	1:A:404:LEU:CD1	2.30	0.46
1:A:542:VAL:HG12	1:A:543:THR:N	2.28	0.46
1:A:555:TYR:CZ	1:A:615:MSE:HG2	2.49	0.46
1:A:700:ASP:C	1:A:702:SER:H	2.18	0.46
1:A:741:PHE:CD1	1:A:741:PHE:C	2.88	0.46
1:B:411:LEU:HD21	1:B:493:VAL:HG21	1.97	0.46
1:A:296:MSE:HE3	1:A:306:ALA:HA	1.97	0.46
1:A:413:LYS:O	1:A:420:ASP:HB2	2.15	0.46
1:A:487:GLN:O	1:A:491:GLU:HB3	2.16	0.46
1:A:725:ASP:OD2	1:A:766:LEU:HD22	2.15	0.46
1:A:659:GLY:HA2	1:A:794:TRP:HE3	1.81	0.46
1:A:829:LEU:HA	1:A:829:LEU:HD12	1.74	0.46
1:B:716:ASP:N	1:B:716:ASP:OD1	2.49	0.46
1:A:233:ILE:O	1:A:234:ASN:C	2.54	0.46
1:A:347:TYR:CD1	1:A:516:PRO:HD3	2.50	0.46
1:A:486:PRO:HB2	1:A:490:ARG:CD	2.45	0.46
1:A:670:ASN:HD21	1:A:722:LEU:CD2	2.28	0.46
1:A:727:TYR:O	1:A:730:VAL:HG13	2.15	0.46
1:B:353:MSE:HE2	1:B:512:CYS:CB	2.45	0.46
1:B:676:VAL:HG22	1:B:713:LYS:CE	2.39	0.46
1:A:233:ILE:CG1	1:A:233:ILE:O	2.63	0.46
1:A:252:PHE:HA	1:A:296:MSE:O	2.15	0.46
1:A:284:ALA:HA	1:A:287:ILE:HD11	1.97	0.46
1:A:303:SER:OG	1:A:640:CYS:SG	2.68	0.46
1:B:202:ASP:O	1:B:227:ARG:NH2	2.49	0.46
1:B:241:VAL:O	1:B:242:ASP:C	2.53	0.46
1:B:477:GLU:HB2	1:B:482:LEU:HD21	1.98	0.46
1:B:715:LEU:N	1:B:715:LEU:HD12	2.31	0.46
1:B:788:PRO:HG2	1:B:789:PHE:H	1.79	0.46
1:B:817:GLN:O	1:B:818:ALA:HB3	2.15	0.46
1:B:345:ASP:C	1:B:346:LEU:HD13	2.35	0.46
1:B:684:LYS:HB2	1:B:688:GLN:OE1	2.16	0.46
1:B:695:ARG:CD	1:B:700:ASP:HB3	2.46	0.46
1:B:729:ARG:CD	1:B:773:VAL:CG2	2.93	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:GLY:HA3	1:B:856:PRO:HD3	1.97	0.46
1:A:339:ARG:O	1:A:367:LYS:N	2.32	0.46
1:A:644:TYR:CD1	1:A:649:LYS:HB3	2.50	0.46
1:B:215:ASP:HB2	1:B:217:CYS:SG	2.56	0.46
1:B:221:THR:O	1:B:221:THR:HG22	2.16	0.46
1:B:231:THR:HB	1:B:298:TYR:CE1	2.51	0.46
1:B:535:ASP:OD1	1:B:539:LYS:CE	2.64	0.46
1:B:583:MSE:O	1:B:584:LYS:CB	2.61	0.46
1:B:729:ARG:HH21	1:B:772:LEU:C	2.18	0.46
1:A:344:LEU:HD21	1:A:346:LEU:HD21	1.96	0.46
1:A:509:ASP:OD1	1:A:509:ASP:N	2.46	0.46
1:A:511:ILE:HG23	1:A:553:PRO:CB	2.46	0.46
1:A:593:VAL:HG11	1:A:602:PHE:CD1	2.50	0.46
1:A:687:PHE:O	1:A:690:TYR:N	2.47	0.46
1:A:725:ASP:CA	1:A:766:LEU:HD13	2.38	0.46
1:B:547:ILE:HG12	1:B:547:ILE:H	1.49	0.46
1:B:589:LEU:CD1	1:B:589:LEU:C	2.84	0.46
1:B:828:ARG:NH2	1:B:834:ASP:OD2	2.29	0.46
1:A:505:PRO:HA	1:A:551:LEU:HD23	1.97	0.46
1:A:653:LYS:HA	1:A:653:LYS:HE3	1.97	0.46
1:B:209:GLU:HB2	1:B:221:THR:CB	2.45	0.46
1:B:464:VAL:CG2	1:B:466:TRP:CZ2	2.98	0.46
1:B:343:LEU:HB2	1:B:368:LEU:HD22	1.97	0.45
1:B:699:LEU:HG	1:B:701:TRP:CG	2.51	0.45
1:B:783:GLY:O	1:B:784:LYS:C	2.54	0.45
1:B:805:ALA:HB1	1:B:812:ILE:HD13	1.97	0.45
1:A:411:LEU:CD1	1:A:411:LEU:N	2.80	0.45
1:A:642:VAL:O	1:A:642:VAL:HG23	2.15	0.45
1:A:663:SER:CB	1:A:688:GLN:NE2	2.75	0.45
1:B:279:ASP:H	1:B:283:LYS:HD3	1.81	0.45
1:B:460:ILE:HD13	1:B:460:ILE:H	1.80	0.45
1:A:415:TYR:N	1:A:415:TYR:CD1	2.85	0.45
1:B:144:ALA:O	1:B:145:ASP:HB2	2.17	0.45
1:B:580:LEU:HD22	1:B:608:LEU:HD21	1.98	0.45
1:A:186:TYR:CD1	1:A:268:LYS:HD2	2.51	0.45
1:A:233:ILE:O	1:A:233:ILE:HG13	2.16	0.45
1:A:449:ILE:HD13	1:A:462:PHE:CD1	2.51	0.45
1:A:626:ASP:C	1:A:626:ASP:OD1	2.55	0.45
1:A:686:GLU:HA	1:A:689:ARG:CZ	2.46	0.45
1:B:180:LYS:HE3	1:B:183:ASN:HA	1.97	0.45
1:B:670:ASN:HD21	1:B:722:LEU:H	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:729:ARG:NE	1:B:773:VAL:CG2	2.76	0.45
1:B:733:ILE:CG1	1:B:734:PRO:HD2	2.46	0.45
1:B:779:SER:O	1:B:782:LYS:N	2.48	0.45
1:B:805:ALA:O	1:B:806:GLU:HG3	2.15	0.45
1:A:145:ASP:OD2	1:A:148:ARG:NH1	2.50	0.45
1:A:174:CYS:C	1:A:175:HIS:HD2	2.20	0.45
1:A:723:ASN:ND2	1:A:723:ASN:O	2.50	0.45
1:A:810:GLN:O	1:A:811:VAL:CG1	2.64	0.45
1:B:535:ASP:CG	1:B:539:LYS:HE3	2.36	0.45
1:B:307:ASN:HD21	1:B:586:GLN:CD	2.12	0.45
1:B:687:PHE:O	1:B:690:TYR:HB3	2.17	0.45
1:B:739:ALA:HB3	1:B:791:ARG:H	1.81	0.45
1:B:805:ALA:HB2	1:B:846:TYR:CE1	2.51	0.45
1:A:619:LYS:HD3	1:A:877:ASP:O	2.15	0.45
1:A:772:LEU:HD12	1:A:773:VAL:H	1.78	0.45
1:A:741:PHE:HD2	1:A:788:PRO:HB2	1.82	0.45
1:B:170:LEU:CD2	1:B:211:PHE:CE1	2.98	0.45
1:B:734:PRO:O	1:B:735:VAL:HG13	2.16	0.45
1:A:285:GLN:O	1:A:286:LEU:C	2.55	0.45
1:A:347:TYR:CD2	1:A:347:TYR:N	2.83	0.45
1:A:801:VAL:HG21	1:A:829:LEU:HB3	1.99	0.45
1:A:787:LYS:CB	1:A:809:ASN:O	2.62	0.45
1:B:223:ARG:HD2	1:B:253:LEU:HD22	1.98	0.45
1:B:469:TYR:HD1	1:B:473:GLU:HB3	1.82	0.45
1:B:776:TYR:O	1:B:779:SER:N	2.49	0.45
1:B:740:ASN:CA	1:B:789:PHE:O	2.64	0.45
1:B:811:VAL:CG2	1:B:811:VAL:O	2.58	0.45
1:A:660:ASP:OD2	1:A:660:ASP:N	2.50	0.45
1:A:683:PRO:HB2	1:A:689:ARG:HA	1.99	0.45
1:A:676:VAL:HA	1:A:714:LEU:O	2.17	0.45
1:B:171:LYS:HA	1:B:171:LYS:HE2	1.99	0.45
1:B:218:HIS:O	1:B:262:LEU:HG	2.17	0.45
1:B:446:LEU:HD23	1:B:446:LEU:N	2.22	0.45
1:B:730:VAL:O	1:B:733:ILE:HB	2.17	0.45
1:B:823:ILE:O	1:B:826:ASN:N	2.49	0.45
1:A:447:VAL:CG2	1:A:447:VAL:O	2.64	0.45
1:A:553:PRO:HB2	1:A:555:TYR:O	2.16	0.45
1:A:555:TYR:CE2	1:A:618:PRO:CD	2.94	0.45
1:A:672:GLN:HG3	1:A:672:GLN:O	2.16	0.45
1:A:787:LYS:HB3	1:A:811:VAL:CG1	2.41	0.45
1:A:363:LEU:HB3	1:A:863:TYR:CD1	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ASP:CG	2:B:1000:SAH:HO2'	2.21	0.45
1:B:343:LEU:HD12	1:B:344:LEU:N	2.30	0.45
1:B:349:GLY:C	1:B:350:CYS:SG	2.96	0.45
1:B:565:LEU:HB3	1:B:637:PHE:CE2	2.52	0.45
1:B:791:ARG:CD	1:B:792:LEU:N	2.64	0.45
1:B:718:GLN:N	1:B:822:THR:HB	2.32	0.45
1:B:691:ILE:HD11	1:B:832:PHE:O	2.17	0.45
1:A:281:LYS:O	1:A:285:GLN:CG	2.60	0.45
1:A:596:CYS:HB3	1:A:623:PRO:CB	2.28	0.45
1:B:287:ILE:HD11	1:B:293:TYR:CE2	2.52	0.45
1:B:646:GLU:CD	1:B:646:GLU:C	2.74	0.45
1:B:791:ARG:NE	1:B:813:ILE:O	2.50	0.45
1:B:793:TRP:HB2	1:B:794:TRP:CD1	2.52	0.45
1:B:823:ILE:HD13	1:B:845:LYS:CB	2.47	0.45
1:A:173:ARG:NH2	1:A:216:GLN:HA	2.32	0.44
1:A:451:TYR:HD1	1:A:460:ILE:HD12	1.81	0.44
1:A:484:ASP:O	1:A:485:CYS:C	2.55	0.44
1:A:483:SER:C	1:A:485:CYS:H	2.21	0.44
1:A:487:GLN:O	1:A:491:GLU:CB	2.65	0.44
1:A:570:GLY:O	1:A:571:TYR:C	2.54	0.44
1:A:653:LYS:HD2	1:A:653:LYS:H	1.83	0.44
1:B:395:ASN:HD22	1:B:395:ASN:C	2.20	0.44
1:B:793:TRP:N	1:B:793:TRP:CD1	2.84	0.44
1:B:820:VAL:O	1:B:821:LEU:HD13	2.17	0.44
1:B:557:LEU:HD21	1:B:861:LEU:HD13	1.99	0.44
1:B:364:SER:HA	1:B:863:TYR:HE1	1.83	0.44
1:A:516:PRO:O	1:A:517:CYS:C	2.56	0.44
1:A:596:CYS:N	1:A:627:VAL:HG11	2.32	0.44
1:B:186:TYR:HD1	1:B:268:LYS:CG	2.29	0.44
1:B:670:ASN:OD1	1:B:670:ASN:C	2.55	0.44
1:B:675:ASP:CA	1:B:718:GLN:NE2	2.75	0.44
1:A:143:ALA:CB	1:A:177:ARG:HH21	2.30	0.44
1:A:278:MSE:C	1:A:279:ASP:OD1	2.55	0.44
1:A:376:PHE:CD2	1:A:377:ASN:N	2.86	0.44
1:A:602:PHE:O	1:A:799:PRO:O	2.35	0.44
1:A:752:ASN:O	1:A:753:ASN:CB	2.66	0.44
1:A:780:PHE:HD2	1:A:786:LEU:CD2	2.30	0.44
1:B:142:VAL:HG12	1:B:175:HIS:O	2.17	0.44
1:B:577:LEU:HD12	1:B:577:LEU:HA	1.77	0.44
1:A:355:THR:OG1	1:A:356:GLY:N	2.51	0.44
1:A:792:LEU:O	1:A:815:PRO:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ARG:HB3	1:B:157:ARG:HE	1.42	0.44
1:B:589:LEU:HD12	1:B:589:LEU:O	2.18	0.44
1:B:591:MSE:HE2	1:B:640:CYS:HB2	2.00	0.44
1:B:718:GLN:C	1:B:822:THR:HB	2.38	0.44
1:A:173:ARG:CB	1:A:212:GLU:O	2.66	0.44
1:A:479:ILE:O	1:A:482:LEU:HB2	2.18	0.44
1:A:653:LYS:HD2	1:A:653:LYS:N	2.32	0.44
1:A:812:ILE:CG2	1:A:820:VAL:HG22	2.45	0.44
1:B:338:THR:O	1:B:338:THR:CG2	2.66	0.44
1:B:549:ALA:CA	1:B:583:MSE:HE1	2.48	0.44
1:B:616:VAL:O	1:B:868:ALA:HB1	2.17	0.44
1:A:193:TYR:CE1	1:A:269:VAL:HB	2.53	0.44
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.98	0.44
1:A:542:VAL:HG22	1:A:575:TYR:OH	2.17	0.44
1:B:298:TYR:HD1	1:B:305:PHE:CE1	2.35	0.44
1:B:496:GLY:CA	1:B:501:ILE:HD13	2.46	0.44
1:B:579:CYS:O	1:B:583:MSE:HB2	2.18	0.44
1:B:772:LEU:N	1:B:774:PRO:HD2	2.32	0.44
1:A:302:TYR:O	1:A:303:SER:C	2.50	0.44
1:A:757:TRP:CD2	1:A:778:MSE:HE3	2.53	0.44
1:B:391:THR:HG22	1:B:393:VAL:HG23	2.00	0.44
1:B:451:TYR:CD2	1:B:452:GLY:N	2.86	0.44
1:B:304:THR:HG23	1:B:588:ARG:HB2	2.00	0.44
1:B:589:LEU:CD1	1:B:640:CYS:SG	3.05	0.44
1:B:821:LEU:HD12	1:B:821:LEU:HA	1.80	0.44
1:B:837:ARG:NH1	1:B:837:ARG:CG	2.65	0.44
1:A:456:ARG:HD3	1:A:456:ARG:HA	1.78	0.44
1:A:557:LEU:HD22	1:A:609:TRP:CZ2	2.52	0.44
1:B:457:GLU:CB	1:B:461:TYR:HH	2.17	0.44
1:B:686:GLU:CA	1:B:689:ARG:NH2	2.79	0.44
1:B:791:ARG:HB2	1:B:813:ILE:HG13	2.00	0.44
1:B:657:LEU:HD23	1:B:795:ASP:O	2.18	0.44
1:B:812:ILE:HG23	1:B:820:VAL:HG22	1.99	0.44
1:A:179:ALA:O	1:A:185:VAL:HG12	2.18	0.44
1:A:232:VAL:HG12	1:A:233:ILE:CG2	2.46	0.44
1:A:593:VAL:CG1	1:A:602:PHE:CD1	3.01	0.44
1:A:787:LYS:CG	1:A:809:ASN:O	2.66	0.44
1:B:143:ALA:HB1	1:B:147:ALA:HB2	1.96	0.44
1:B:207:ILE:HD12	1:B:209:GLU:H	1.83	0.44
1:B:233:ILE:HD12	1:B:578:SER:OG	2.18	0.44
1:B:663:SER:HB2	1:B:688:GLN:HE22	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LYS:O	1:B:785:SER:C	2.55	0.43
1:B:828:ARG:CG	1:B:828:ARG:NH2	2.73	0.43
1:A:444:GLU:CG	1:A:445:LYS:N	2.81	0.43
1:A:722:LEU:HB3	1:A:726:ASP:HB2	1.99	0.43
1:A:737:LYS:HZ1	1:A:795:ASP:CG	2.21	0.43
1:B:142:VAL:CG1	1:B:175:HIS:N	2.76	0.43
1:B:184:VAL:CG1	1:B:186:TYR:CE1	3.00	0.43
1:B:554:LYS:O	1:B:611:ALA:HA	2.17	0.43
1:B:603:ARG:CZ	1:B:830:GLN:NE2	2.79	0.43
1:A:194:VAL:HG12	1:A:195:LYS:N	2.33	0.43
1:A:733:ILE:HD12	1:A:739:ALA:HB1	2.00	0.43
1:B:386:TYR:HB2	1:B:839:PHE:CE2	2.53	0.43
1:B:781:ILE:O	1:B:782:LYS:C	2.55	0.43
1:A:254:SER:OG	1:A:256:GLU:N	2.51	0.43
1:A:347:TYR:O	2:A:1000:SAH:HG1	2.18	0.43
1:A:384:LEU:C	1:A:384:LEU:CD1	2.87	0.43
1:A:645:ASP:N	1:A:645:ASP:OD1	2.29	0.43
1:B:139:GLY:O	1:B:140:SER:HB3	2.17	0.43
1:B:580:LEU:O	1:B:585:TYR:HB2	2.17	0.43
1:B:589:LEU:HD12	1:B:589:LEU:C	2.39	0.43
1:B:719:PRO:HB3	1:B:820:VAL:HG12	1.99	0.43
1:B:790:GLY:N	1:B:813:ILE:HD11	2.33	0.43
1:A:143:ALA:O	1:A:144:ALA:C	2.56	0.43
1:A:154:ARG:NH2	1:A:170:LEU:HD21	2.33	0.43
1:A:308:ILE:HG23	1:A:309:SER:N	2.32	0.43
1:A:343:LEU:HB3	1:A:370:THR:HA	2.00	0.43
1:A:586:GLN:N	1:A:611:ALA:O	2.51	0.43
1:A:763:ARG:HH11	1:A:771:PRO:HB3	1.82	0.43
1:B:227:ARG:O	1:B:230:ASP:N	2.51	0.43
1:B:391:THR:CG2	1:B:393:VAL:HG23	2.49	0.43
1:B:446:LEU:HA	1:B:446:LEU:HD22	1.71	0.43
1:B:734:PRO:O	1:B:735:VAL:HG12	2.16	0.43
1:B:772:LEU:CB	1:B:774:PRO:CG	2.97	0.43
1:A:274:VAL:HG23	1:A:295:ASP:CA	2.47	0.43
1:A:615:MSE:HE2	1:A:615:MSE:HB2	1.83	0.43
1:B:175:HIS:HE1	1:B:209:GLU:HG2	1.83	0.43
1:B:439:ASP:O	1:B:440:GLU:HB3	2.19	0.43
1:B:546:ASP:O	1:B:549:ALA:HB3	2.19	0.43
1:B:703:PHE:N	1:B:703:PHE:CD2	2.87	0.43
1:A:151:TRP:HD1	1:A:151:TRP:O	2.01	0.43
1:A:564:ILE:CG2	1:A:573:GLY:CA	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:GLU:O	1:B:234:ASN:OD1	2.37	0.43
1:B:237:VAL:HG13	1:B:246:HIS:CD2	2.53	0.43
1:B:286:LEU:HA	1:B:289:SER:OG	2.17	0.43
1:B:694:SER:OG	1:B:697:ASP:OD2	2.37	0.43
1:B:740:ASN:C	1:B:789:PHE:O	2.57	0.43
1:B:806:GLU:O	1:B:810:GLN:HG2	2.18	0.43
1:A:172:ALA:CB	1:A:175:HIS:NE2	2.82	0.43
1:A:155:TYR:CE2	1:A:172:ALA:HB3	2.54	0.43
1:A:247:ASP:HA	1:A:248:PRO:HD3	1.72	0.43
1:A:556:VAL:HB	1:A:610:GLY:HA3	2.00	0.43
1:A:635:ASN:O	1:A:637:PHE:N	2.51	0.43
1:A:806:GLU:O	1:A:810:GLN:HG2	2.19	0.43
1:B:413:LYS:NZ	1:B:414:LYS:CG	2.80	0.43
1:B:498:LYS:HA	1:B:498:LYS:HD3	1.50	0.43
1:B:504:LEU:HB3	1:B:505:PRO:CD	2.49	0.43
1:B:672:GLN:HE21	1:B:673:PRO:HD2	1.84	0.43
1:B:672:GLN:NE2	1:B:674:ASN:H	2.15	0.43
1:A:155:TYR:OH	1:A:175:HIS:CD2	2.72	0.43
1:A:580:LEU:HD23	1:A:587:ALA:HB1	2.01	0.43
1:B:621:PRO:HG3	1:B:860:ALA:CB	2.48	0.43
1:B:817:GLN:HB2	1:B:817:GLN:HE21	1.57	0.43
1:A:278:MSE:HB2	1:A:283:LYS:HE3	2.01	0.43
1:A:389:PRO:CG	1:A:390:GLN:N	2.81	0.43
1:A:452:GLY:HA3	1:A:455:ASP:HB2	2.01	0.43
1:A:482:LEU:N	1:A:482:LEU:CD2	2.82	0.43
1:A:625:TYR:HA	1:A:653:LYS:HB2	2.01	0.43
1:B:249:ARG:O	1:B:293:TYR:CE2	2.71	0.43
1:B:658:LEU:O	1:B:660:ASP:N	2.52	0.43
1:A:186:TYR:HE2	1:A:265:ILE:CG2	2.29	0.42
1:B:237:VAL:CG1	1:B:246:HIS:HD2	2.31	0.42
1:B:300:VAL:HG23	1:B:300:VAL:O	2.19	0.42
1:B:559:GLU:OE2	1:B:605:ARG:HD2	2.19	0.42
1:A:658:LEU:HD11	1:A:662:ILE:HD13	2.00	0.42
1:B:221:THR:O	1:B:221:THR:CG2	2.63	0.42
1:B:237:VAL:CG1	1:B:246:HIS:CD2	3.02	0.42
1:B:656:LEU:CD2	1:B:656:LEU:N	2.69	0.42
1:B:675:ASP:O	1:B:715:LEU:HA	2.19	0.42
1:A:376:PHE:HD2	1:A:377:ASN:N	2.16	0.42
1:A:474:ASP:C	1:A:475:THR:CG2	2.87	0.42
1:B:574:LYS:HG2	1:B:574:LYS:H	1.50	0.42
1:B:699:LEU:CG	1:B:701:TRP:CG	3.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:HIS:CD2	1:B:815:PRO:HD2	2.54	0.42
1:B:302:TYR:CD2	1:B:878:PRO:HB3	2.55	0.42
1:A:493:VAL:O	1:A:494:GLN:C	2.55	0.42
1:A:588:ARG:HH11	1:A:617:LEU:HG	1.85	0.42
1:A:624:THR:O	1:A:653:LYS:CG	2.60	0.42
1:A:665:LEU:CD2	1:A:814:HIS:HE1	2.17	0.42
1:B:186:TYR:N	1:B:186:TYR:CD2	2.87	0.42
1:B:410:VAL:CG1	1:B:411:LEU:H	2.26	0.42
1:B:750:GLY:O	1:B:751:ALA:C	2.58	0.42
1:A:249:ARG:HB2	1:A:292:LEU:CD2	2.49	0.42
1:A:537:LYS:C	1:A:539:LYS:N	2.72	0.42
1:A:603:ARG:NH1	1:A:852:ALA:O	2.52	0.42
1:B:138:ILE:CD1	1:B:139:GLY:H	2.32	0.42
1:B:170:LEU:HD22	1:B:211:PHE:HZ	1.85	0.42
1:B:790:GLY:H	1:B:813:ILE:HD11	1.84	0.42
1:A:343:LEU:HD22	1:A:344:LEU:N	2.33	0.42
1:A:411:LEU:N	1:A:411:LEU:HD12	2.35	0.42
1:A:589:LEU:HD23	1:A:589:LEU:N	2.34	0.42
1:A:653:LYS:O	1:A:654:LYS:C	2.58	0.42
1:A:759:PRO:O	1:A:760:GLU:CB	2.43	0.42
1:A:786:LEU:C	1:A:788:PRO:CD	2.88	0.42
1:B:589:LEU:HD12	1:B:640:CYS:SG	2.59	0.42
1:B:624:THR:CG2	1:B:624:THR:O	2.68	0.42
1:A:375:ASP:OD1	2:A:1000:SAH:O2'	2.36	0.42
1:A:137:PHE:C	1:A:138:ILE:O	2.55	0.42
1:A:211:PHE:HD1	1:A:213:GLY:N	2.17	0.42
1:A:580:LEU:HD12	1:A:580:LEU:HA	1.76	0.42
1:A:628:VAL:O	1:A:628:VAL:CG1	2.67	0.42
1:A:763:ARG:NH1	1:A:773:VAL:O	2.44	0.42
1:A:757:TRP:CE3	1:A:778:MSE:HE3	2.55	0.42
1:B:250:ARG:HH22	1:B:296:MSE:HE2	1.84	0.42
1:B:586:GLN:O	1:B:610:GLY:HA2	2.19	0.42
1:B:735:VAL:CG2	1:B:735:VAL:O	2.65	0.42
1:B:737:LYS:HA	1:B:793:TRP:CE2	2.55	0.42
1:A:181:VAL:CG2	1:A:186:TYR:CE2	3.02	0.42
1:A:272:VAL:HG21	1:A:286:LEU:HD23	2.02	0.42
1:A:343:LEU:CD2	1:A:344:LEU:N	2.83	0.42
1:A:764:VAL:CG2	1:A:772:LEU:HD12	2.49	0.42
1:A:734:PRO:O	1:A:791:ARG:NE	2.52	0.42
1:A:880:TYR:HD1	1:A:881:GLN:H	1.68	0.42
1:B:347:TYR:OH	1:B:540:GLN:OE1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:HD21	1:B:791:ARG:HH21	1.85	0.42
1:B:727:TYR:O	1:B:730:VAL:CG1	2.68	0.42
1:A:139:GLY:O	1:A:140:SER:HB2	2.19	0.42
1:A:141:PRO:O	1:A:142:VAL:CG2	2.62	0.42
1:A:575:TYR:C	1:A:575:TYR:CD1	2.93	0.42
1:A:812:ILE:HG13	1:A:812:ILE:O	2.20	0.42
1:B:198:GLU:O	1:B:199:ASN:C	2.57	0.42
1:B:832:PHE:CZ	1:B:852:ALA:CB	3.02	0.42
1:A:273:HIS:ND1	1:A:294:TYR:CE2	2.88	0.42
1:A:272:VAL:CG1	1:A:286:LEU:HD22	2.50	0.42
1:A:447:VAL:O	1:A:447:VAL:HG22	2.20	0.42
1:A:477:GLU:OE1	1:A:481:ASN:ND2	2.52	0.42
1:A:500:LYS:NZ	1:A:507:ASP:OD2	2.38	0.42
1:B:229:GLU:O	1:B:234:ASN:CG	2.58	0.42
1:B:822:THR:H	1:B:825:GLU:CD	2.23	0.42
1:B:838:LEU:C	1:B:839:PHE:CD2	2.94	0.42
1:A:225:PHE:CZ	1:A:294:TYR:CD1	3.08	0.41
1:B:247:ASP:O	1:B:249:ARG:N	2.53	0.41
1:B:596:CYS:O	1:B:624:THR:N	2.53	0.41
1:B:633:ALA:HA	1:B:634:PRO:HD3	1.86	0.41
1:B:741:PHE:HB3	1:B:789:PHE:CB	2.49	0.41
1:A:148:ARG:HG3	1:A:155:TYR:CD1	2.55	0.41
1:A:338:THR:CG2	1:A:367:LYS:HZ3	2.31	0.41
1:A:419:VAL:HG12	1:A:419:VAL:O	2.20	0.41
1:A:440:GLU:CG	1:A:441:PHE:N	2.64	0.41
1:A:635:ASN:O	1:A:636:ALA:C	2.58	0.41
1:A:793:TRP:N	1:A:796:GLU:OE2	2.36	0.41
1:B:180:LYS:HE2	1:B:182:ASP:O	2.20	0.41
1:B:391:THR:HG22	1:B:392:GLU:N	2.20	0.41
1:A:737:LYS:NZ	1:A:795:ASP:CG	2.73	0.41
1:B:278:MSE:SE	1:B:282:ALA:CB	3.13	0.41
1:B:659:GLY:H	1:B:794:TRP:HB3	1.85	0.41
1:A:180:LYS:HB2	1:A:185:VAL:CG1	2.51	0.41
1:A:302:TYR:O	1:A:303:SER:HB2	2.20	0.41
1:A:512:CYS:HA	1:A:557:LEU:O	2.20	0.41
1:A:692:ARG:C	1:A:693:LEU:HD12	2.39	0.41
1:A:757:TRP:CH2	1:A:763:ARG:CZ	3.04	0.41
1:A:803:THR:OG1	1:A:847:ILE:HG13	2.21	0.41
1:B:154:ARG:NE	1:B:209:GLU:OE1	2.52	0.41
1:B:353:MSE:O	1:B:357:LEU:HB2	2.20	0.41
1:B:793:TRP:HA	1:B:815:PRO:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:TYR:CD2	1:B:837:ARG:HB2	2.56	0.41
1:A:402:LEU:HD22	1:A:547:ILE:HG12	2.02	0.41
1:A:447:VAL:HG13	1:A:463:LYS:HB3	2.01	0.41
1:A:555:TYR:CE2	1:A:618:PRO:HG3	2.56	0.41
1:A:656:LEU:HD22	1:A:656:LEU:HA	1.90	0.41
1:A:735:VAL:O	1:A:735:VAL:HG12	2.19	0.41
1:B:280:PRO:CG	1:B:281:LYS:N	2.84	0.41
1:B:513:GLY:N	1:B:557:LEU:O	2.53	0.41
1:B:545:MSE:HE3	1:B:576:ALA:HA	2.01	0.41
1:B:772:LEU:C	1:B:773:VAL:HG22	2.31	0.41
1:B:814:HIS:CD2	1:B:816:THR:N	2.55	0.41
1:B:695:ARG:CA	1:B:835:TYR:CE1	2.96	0.41
1:B:841:PRO:HG2	1:B:843:LYS:HE3	2.02	0.41
1:A:154:ARG:NE	1:A:170:LEU:CD2	2.80	0.41
1:A:486:PRO:O	1:A:487:GLN:C	2.58	0.41
1:A:781:ILE:CD1	1:A:786:LEU:HD21	2.49	0.41
1:A:838:LEU:O	1:A:845:LYS:HE2	2.19	0.41
1:A:865:LEU:CD2	1:A:865:LEU:C	2.88	0.41
1:A:876:SER:OG	1:A:876:SER:O	2.30	0.41
1:B:154:ARG:O	1:B:171:LYS:HE2	2.21	0.41
1:B:617:LEU:HD12	1:B:618:PRO:CD	2.51	0.41
1:B:810:GLN:O	1:B:811:VAL:CG1	2.69	0.41
1:A:266:ILE:H	1:A:266:ILE:HG12	1.31	0.41
1:A:267:SER:OG	1:A:268:LYS:N	2.52	0.41
1:A:269:VAL:CG2	1:A:270:LYS:N	2.84	0.41
1:A:543:THR:O	1:A:544:PHE:C	2.57	0.41
1:A:593:VAL:HG21	1:A:602:PHE:HE1	1.85	0.41
1:A:557:LEU:HD11	1:A:607:PHE:HB3	2.03	0.41
1:A:652:LEU:H	1:A:652:LEU:HD23	1.85	0.41
1:A:739:ALA:HB3	1:A:791:ARG:CG	2.47	0.41
1:B:134:GLU:CD	1:B:135:PRO:HD2	2.29	0.41
1:B:180:LYS:HE2	1:B:183:ASN:HA	2.03	0.41
1:B:445:LYS:HB3	1:B:465:GLN:OE1	2.19	0.41
1:B:462:PHE:HE2	1:B:479:ILE:HD13	1.85	0.41
1:B:554:LYS:HD3	1:B:615:MSE:HE2	1.99	0.41
1:B:571:TYR:CD2	1:B:571:TYR:C	2.94	0.41
1:B:659:GLY:O	1:B:663:SER:OG	2.37	0.41
1:B:806:GLU:N	1:B:810:GLN:HE21	2.13	0.41
1:B:819:ARG:CZ	1:B:825:GLU:OE2	2.69	0.41
1:A:822:THR:HG23	1:A:825:GLU:CG	2.50	0.41
1:B:144:ALA:O	1:B:145:ASP:OD2	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:HB2	1:B:262:LEU:CD1	2.48	0.41
1:B:510:VAL:HG12	1:B:511:ILE:N	2.35	0.41
1:B:604:MSE:SE	1:B:641:MSE:CE	2.92	0.41
1:A:249:ARG:HB2	1:A:292:LEU:HD22	2.02	0.41
1:A:541:MSE:HE3	1:A:572:LEU:O	2.21	0.41
1:A:580:LEU:HD23	1:A:587:ALA:HB2	2.03	0.41
1:A:686:GLU:HA	1:A:689:ARG:NH1	2.36	0.41
1:B:400:GLU:H	1:B:400:GLU:HG3	1.70	0.41
1:B:455:ASP:O	1:B:456:ARG:HB2	2.21	0.41
1:B:855:VAL:N	1:B:856:PRO:CD	2.84	0.41
1:A:204:ILE:HG21	1:A:204:ILE:HD13	1.78	0.41
1:A:657:LEU:HD23	1:A:795:ASP:C	2.42	0.41
1:A:814:HIS:CD2	1:A:815:PRO:N	2.89	0.41
1:B:135:PRO:HD2	1:B:135:PRO:O	2.19	0.41
1:B:138:ILE:HG12	1:B:139:GLY:N	2.24	0.41
1:B:223:ARG:HD2	1:B:253:LEU:CD2	2.50	0.41
1:B:457:GLU:O	1:B:461:TYR:CE2	2.74	0.41
1:B:343:LEU:HD12	1:B:511:ILE:HA	2.03	0.41
1:A:153:LYS:HE3	1:A:153:LYS:HB2	1.40	0.41
1:A:307:ASN:ND2	1:A:586:GLN:NE2	2.69	0.41
1:A:629:VAL:HG23	1:A:629:VAL:O	2.21	0.41
1:A:776:TYR:C	1:A:776:TYR:CD2	2.95	0.41
1:B:353:MSE:N	2:B:1000:SAH:O	2.47	0.41
1:B:491:GLU:O	1:B:494:GLN:HB2	2.21	0.41
1:B:733:ILE:HA	1:B:734:PRO:HD3	1.92	0.41
1:B:842:ILE:N	1:B:842:ILE:HD12	2.36	0.41
1:A:284:ALA:O	1:A:288:GLU:HG2	2.21	0.40
1:A:454:SER:C	1:A:456:ARG:H	2.22	0.40
1:A:457:GLU:O	1:A:458:ASN:C	2.56	0.40
1:A:714:LEU:C	1:A:714:LEU:CD2	2.87	0.40
1:B:145:ASP:O	1:B:148:ARG:HG3	2.21	0.40
1:B:272:VAL:HG13	1:B:273:HIS:H	1.84	0.40
1:B:362:ALA:HB2	1:B:699:LEU:CD2	2.51	0.40
1:B:404:LEU:HD13	1:B:405:LEU:N	2.36	0.40
1:B:622:LEU:HB3	1:B:623:PRO:CD	2.51	0.40
1:B:637:PHE:N	1:B:637:PHE:HD2	2.13	0.40
1:B:865:LEU:O	1:B:865:LEU:HD12	2.20	0.40
1:A:184:VAL:HG22	1:A:185:VAL:N	2.35	0.40
1:A:273:HIS:C	1:A:273:HIS:CD2	2.92	0.40
1:A:534:LYS:HB3	1:A:534:LYS:HE2	1.64	0.40
1:A:568:ALA:C	1:A:569:ASP:OD2	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:O	1:A:699:LEU:N	2.54	0.40
1:A:763:ARG:HD3	1:A:763:ARG:HA	1.93	0.40
1:B:347:TYR:N	1:B:347:TYR:CD1	2.89	0.40
1:B:244:HIS:CE1	1:B:552:LYS:NZ	2.89	0.40
1:B:733:ILE:HG13	1:B:739:ALA:HB1	2.03	0.40
1:B:819:ARG:O	1:B:820:VAL:CB	2.68	0.40
1:B:798:VAL:HG21	1:B:829:LEU:HD21	2.02	0.40
1:A:176:TYR:OH	1:A:212:GLU:CD	2.60	0.40
1:A:495:GLU:OE1	1:A:495:GLU:CA	2.66	0.40
1:A:594:ALA:HA	1:A:857:VAL:CG2	2.51	0.40
1:A:814:HIS:CD2	1:A:815:PRO:CD	3.05	0.40
1:B:287:ILE:HD11	1:B:293:TYR:CZ	2.56	0.40
1:B:399:ASP:N	1:B:399:ASP:OD1	2.50	0.40
1:B:466:TRP:HZ2	1:B:475:THR:CG2	2.24	0.40
1:B:794:TRP:N	1:B:794:TRP:CD1	2.83	0.40
1:B:803:THR:HG22	1:B:847:ILE:HA	2.03	0.40
1:A:296:MSE:HE2	1:A:305:PHE:HB3	2.02	0.40
1:A:486:PRO:HG2	1:A:487:GLN:H	1.87	0.40
1:A:580:LEU:HD22	1:A:608:LEU:HD23	2.02	0.40
1:B:231:THR:C	1:B:233:ILE:N	2.75	0.40
1:B:723:ASN:OD1	1:B:726:ASP:CG	2.58	0.40
1:A:173:ARG:HH22	1:A:216:GLN:HA	1.87	0.40
1:A:741:PHE:O	1:A:742:ARG:C	2.59	0.40
1:A:659:GLY:HA3	1:A:794:TRP:HB3	2.03	0.40
1:A:865:LEU:O	1:A:866:GLY:C	2.60	0.40
1:B:534:LYS:C	1:B:534:LYS:NZ	2.73	0.40
1:B:722:LEU:O	1:B:723:ASN:C	2.60	0.40
1:B:728:GLU:OE2	1:B:767:SER:CB	2.69	0.40
1:B:791:ARG:HG3	1:B:792:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	670/784 (86%)	591 (88%)	62 (9%)	17 (2%)	5 32
1	B	665/784 (85%)	607 (91%)	43 (6%)	15 (2%)	6 34
All	All	1335/1568 (85%)	1198 (90%)	105 (8%)	32 (2%)	6 34

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	634	PRO
1	A	646	GLU
1	B	140	SER
1	B	279	ASP
1	B	773	VAL
1	B	775	ASP
1	B	883	PRO
1	A	764	VAL
1	B	646	GLU
1	B	820	VAL
1	A	135	PRO
1	A	417	GLN
1	A	567	PHE
1	A	650	PRO
1	A	760	GLU
1	A	883	PRO
1	A	653	LYS
1	A	781	ILE
1	B	144	ALA
1	B	350	CYS
1	A	140	SER
1	B	236	LEU
1	B	884	PRO
1	A	215	ASP
1	A	290	CYS
1	B	138	ILE
1	B	788	PRO
1	A	759	PRO
1	A	787	LYS
1	B	142	VAL
1	B	266	ILE

5.3.2 Protein sidechains (i)

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	564/652 (86%)	413 (73%)	151 (27%)	0 2
1	B	544/652 (83%)	384 (71%)	160 (29%)	0 1
All	All	1108/1304 (85%)	797 (72%)	311 (28%)	0 1

All (311) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	A	140	SER
1	A	153	LYS
1	A	181	VAL
1	A	185	VAL
1	A	192	VAL
1	A	198	GLU
1	A	208	THR
1	A	211	PHE
1	A	214	THR
1	A	215	ASP
1	A	216	GLN
1	A	220	PHE
1	A	230	ASP
1	A	233	ILE
1	A	234	ASN
1	A	235	SER
1	A	238	SER
1	A	251	VAL
1	A	253	LEU
1	A	254	SER
1	A	257	LYS
1	A	266	ILE
1	A	267	SER
1	A	269	VAL
1	A	272	VAL
1	A	274	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	275	ASP
1	A	277	ASN
1	A	279	ASP
1	A	286	LEU
1	A	293	TYR
1	A	294	TYR
1	A	299	SER
1	A	300	VAL
1	A	304	THR
1	A	305	PHE
1	A	308	ILE
1	A	309	SER
1	A	338	THR
1	A	343	LEU
1	A	350	CYS
1	A	357	LEU
1	A	363	LEU
1	A	368	LEU
1	A	376	PHE
1	A	377	ASN
1	A	378	SER
1	A	384	LEU
1	A	385	LYS
1	A	394	ARG
1	A	399	ASP
1	A	404	LEU
1	A	405	LEU
1	A	417	GLN
1	A	418	ASP
1	A	419	VAL
1	A	440	GLU
1	A	443	VAL
1	A	447	VAL
1	A	456	ARG
1	A	457	GLU
1	A	466	TRP
1	A	474	ASP
1	A	482	LEU
1	A	483	SER
1	A	484	ASP
1	A	485	CYS
1	A	487	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	489	ILE
1	A	498	LYS
1	A	501	ILE
1	A	502	LEU
1	A	507	ASP
1	A	511	ILE
1	A	512	CYS
1	A	534	LYS
1	A	536	GLU
1	A	539	LYS
1	A	541	MSE
1	A	557	LEU
1	A	563	ASP
1	A	564	ILE
1	A	569	ASP
1	A	572	LEU
1	A	584	LYS
1	A	585	TYR
1	A	588	ARG
1	A	589	LEU
1	A	591	MSE
1	A	605	ARG
1	A	608	LEU
1	A	615	MSE
1	A	619	LYS
1	A	627	VAL
1	A	628	VAL
1	A	630	ARG
1	A	645	ASP
1	A	646	GLU
1	A	647	THR
1	A	648	GLN
1	A	649	LYS
1	A	651	SER
1	A	652	LEU
1	A	654	LYS
1	A	656	LEU
1	A	660	ASP
1	A	665	LEU
1	A	671	HIS
1	A	675	ASP
1	A	682	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	692	ARG
1	A	701	TRP
1	A	710	ASP
1	A	713	LYS
1	A	715	LEU
1	A	716	ASP
1	A	720	LEU
1	A	722	LEU
1	A	723	ASN
1	A	724	ASN
1	A	727	TYR
1	A	730	VAL
1	A	731	GLN
1	A	733	ILE
1	A	742	ARG
1	A	760	GLU
1	A	764	VAL
1	A	772	LEU
1	A	773	VAL
1	A	781	ILE
1	A	785	SER
1	A	786	LEU
1	A	787	LYS
1	A	791	ARG
1	A	792	LEU
1	A	793	TRP
1	A	796	GLU
1	A	797	THR
1	A	800	THR
1	A	813	ILE
1	A	821	LEU
1	A	822	THR
1	A	837	ARG
1	A	839	PHE
1	A	846	TYR
1	A	849	VAL
1	A	865	LEU
1	A	870	LEU
1	A	879	LEU
1	A	880	TYR
1	B	133	HIS
1	B	134	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	136	GLU
1	B	138	ILE
1	B	145	ASP
1	B	148	ARG
1	B	149	SER
1	B	157	ARG
1	B	175	HIS
1	B	181	VAL
1	B	184	VAL
1	B	185	VAL
1	B	186	TYR
1	B	187	CYS
1	B	192	VAL
1	B	206	ARG
1	B	207	ILE
1	B	215	ASP
1	B	221	THR
1	B	223	ARG
1	B	227	ARG
1	B	231	THR
1	B	233	ILE
1	B	234	ASN
1	B	235	SER
1	B	236	LEU
1	B	238	SER
1	B	239	ILE
1	B	245	LYS
1	B	249	ARG
1	B	251	VAL
1	B	253	LEU
1	B	254	SER
1	B	255	GLU
1	B	256	GLU
1	B	262	LEU
1	B	269	VAL
1	B	270	LYS
1	B	273	HIS
1	B	274	VAL
1	B	281	LYS
1	B	283	LYS
1	B	299	SER
1	B	300	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	303	SER
1	B	308	ILE
1	B	338	THR
1	B	339	ARG
1	B	342	THR
1	B	346	LEU
1	B	354	SER
1	B	367	LYS
1	B	368	LEU
1	B	370	THR
1	B	376	PHE
1	B	382	GLN
1	B	383	SER
1	B	387	ASN
1	B	390	GLN
1	B	391	THR
1	B	392	GLU
1	B	395	ASN
1	B	399	ASP
1	B	404	LEU
1	B	407	GLU
1	B	411	LEU
1	B	412	CYS
1	B	440	GLU
1	B	441	PHE
1	B	442	VAL
1	B	443	VAL
1	B	444	GLU
1	B	445	LYS
1	B	446	LEU
1	B	447	VAL
1	B	451	TYR
1	B	460	ILE
1	B	461	TYR
1	B	466	TRP
1	B	473	GLU
1	B	489	ILE
1	B	498	LYS
1	B	499	ARG
1	B	502	LEU
1	B	511	ILE
1	B	518	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	534	LYS
1	B	538	ASN
1	B	546	ASP
1	B	547	ILE
1	B	552	LYS
1	B	558	MSE
1	B	563	ASP
1	B	574	LYS
1	B	577	LEU
1	B	580	LEU
1	B	583	MSE
1	B	589	LEU
1	B	601	GLN
1	B	605	ARG
1	B	608	LEU
1	B	614	SER
1	B	619	LYS
1	B	626	ASP
1	B	629	VAL
1	B	635	ASN
1	B	637	PHE
1	B	638	SER
1	B	639	GLN
1	B	642	VAL
1	B	646	GLU
1	B	648	GLN
1	B	651	SER
1	B	654	LYS
1	B	656	LEU
1	B	658	LEU
1	B	660	ASP
1	B	668	VAL
1	B	672	GLN
1	B	677	MSE
1	B	682	SER
1	B	685	THR
1	B	691	ILE
1	B	694	SER
1	B	695	ARG
1	B	696	LYS
1	B	697	ASP
1	B	698	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	699	LEU
1	B	715	LEU
1	B	716	ASP
1	B	717	HIS
1	B	720	LEU
1	B	724	ASN
1	B	727	TYR
1	B	729	ARG
1	B	732	GLN
1	B	789	PHE
1	B	792	LEU
1	B	793	TRP
1	B	794	TRP
1	B	796	GLU
1	B	798	VAL
1	B	801	VAL
1	B	803	THR
1	B	809	ASN
1	B	811	VAL
1	B	813	ILE
1	B	817	GLN
1	B	819	ARG
1	B	820	VAL
1	B	821	LEU
1	B	825	GLU
1	B	828	ARG
1	B	835	TYR
1	B	836	TYR
1	B	837	ARG
1	B	843	LYS
1	B	844	GLU
1	B	879	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	216	GLN
1	A	234	ASN
1	A	540	GLN
1	A	586	GLN
1	A	670	ASN
1	A	671	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	672	GLN
1	A	674	ASN
1	A	717	HIS
1	A	723	ASN
1	A	814	HIS
1	A	817	GLN
1	B	175	HIS
1	B	183	ASN
1	B	244	HIS
1	B	246	HIS
1	B	273	HIS
1	B	307	ASN
1	B	395	ASN
1	B	518	GLN
1	B	671	HIS
1	B	674	ASN
1	B	810	GLN
1	B	814	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

2 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	$\#\|Z\| > 2$
2	SAH	B	1000	-	21,28,28	1.70	5 (23%)	20,40,40	1.93	5 (25%)
2	SAH	A	1000	-	21,28,28	1.70	5 (23%)	20,40,40	1.93	5 (25%)

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
2	SAH	B	1000	-	-	3/7/31/31	0/3/3/3
2	SAH	A	1000	-	-	5/7/31/31	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	SAH	C2-N3	5.02	1.40	1.32
2	B	1000	SAH	C2-N3	4.97	1.40	1.32
2	B	1000	SAH	C2-N1	3.27	1.40	1.33
2	A	1000	SAH	C2-N1	3.26	1.40	1.33
2	B	1000	SAH	C5-C4	-2.68	1.33	1.40
2	A	1000	SAH	C5-C4	-2.68	1.33	1.40
2	A	1000	SAH	C6-C5	-2.62	1.33	1.43
2	B	1000	SAH	C6-C5	-2.62	1.33	1.43
2	B	1000	SAH	O4'-C1'	2.08	1.44	1.41
2	A	1000	SAH	O4'-C1'	2.04	1.43	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	SAH	N3-C2-N1	-6.76	118.11	128.68
2	B	1000	SAH	N3-C2-N1	-6.72	118.18	128.68
2	B	1000	SAH	C5-C6-N6	-2.69	116.26	120.35
2	A	1000	SAH	C5-C6-N6	-2.69	116.27	120.35
2	B	1000	SAH	C5'-C4'-C3'	-2.22	109.50	115.06
2	A	1000	SAH	C5'-C4'-C3'	-2.21	109.52	115.06
2	B	1000	SAH	C3'-C2'-C1'	2.09	104.12	100.98
2	B	1000	SAH	O4'-C1'-C2'	-2.07	103.91	106.93
2	A	1000	SAH	C3'-C2'-C1'	2.06	104.08	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1000	SAH	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1000	SAH	O4'-C4'-C5'-SD
2	A	1000	SAH	N-CA-CB-CG
2	A	1000	SAH	C-CA-CB-CG
2	A	1000	SAH	O4'-C4'-C5'-SD
2	A	1000	SAH	C3'-C4'-C5'-SD
2	B	1000	SAH	CA-CB-CG-SD
2	B	1000	SAH	C3'-C4'-C5'-SD
2	A	1000	SAH	C4'-C5'-SD-CG

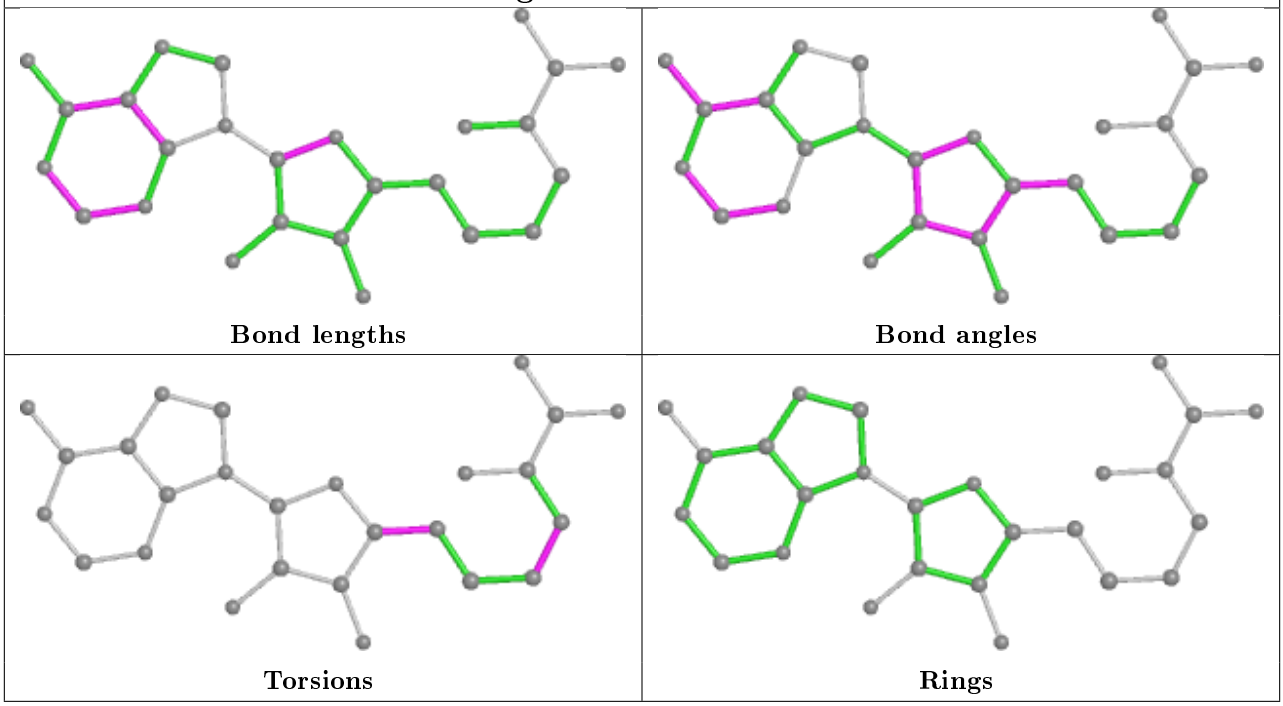
There are no ring outliers.

2 monomers are involved in 12 short contacts:

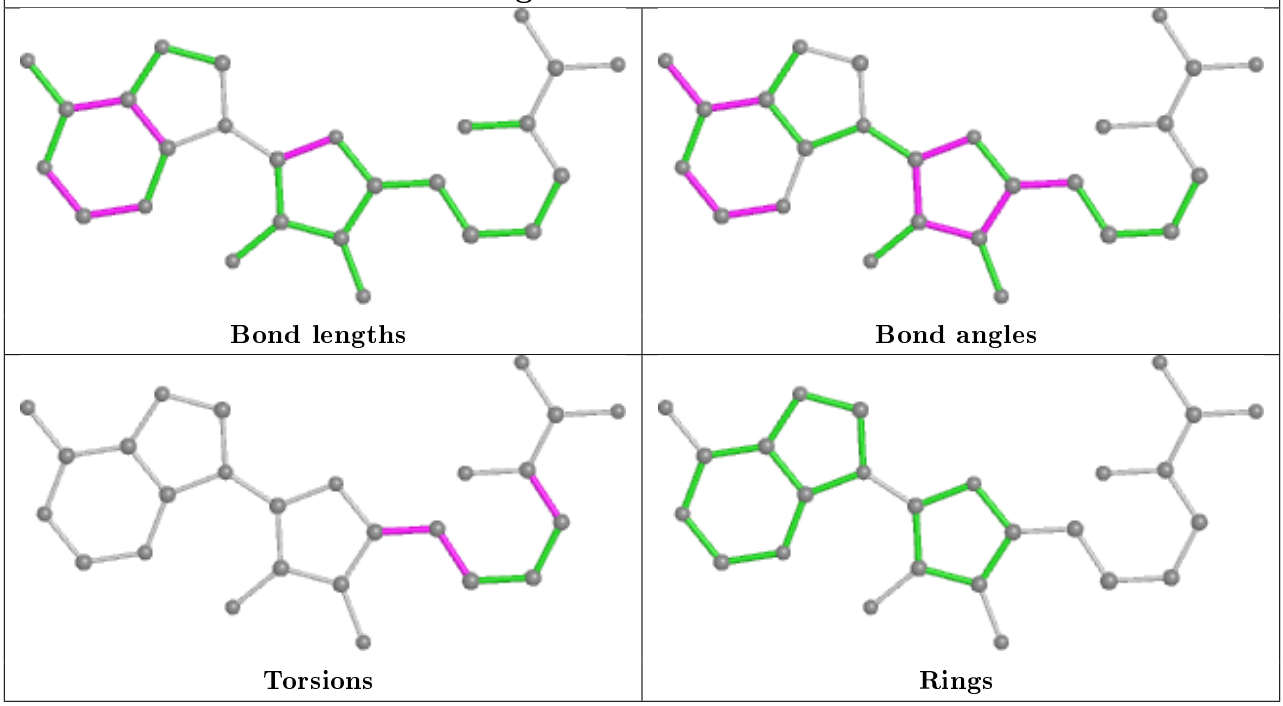
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1000	SAH	6	0
2	A	1000	SAH	6	0

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 then 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 SAH B 1000



Ligand SAH A 1000



5.7 Other polymers (i)

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	665/784 (84%)	-0.17	9 (1%) 75 63	21, 62, 129, 200	0
1	B	660/784 (84%)	-0.25	4 (0%) 89 83	17, 69, 134, 285	0
All	All	1325/1568 (84%)	-0.21	13 (0%) 82 72	17, 65, 132, 285	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	PRO	3.8
1	A	746	GLY	3.3
1	A	484	ASP	3.1
1	A	445	LYS	2.6
1	B	729	ARG	2.5
1	A	409	ALA	2.4
1	A	755	VAL	2.3
1	B	497	HIS	2.2
1	B	732	GLN	2.1
1	A	809	ASN	2.1
1	A	749	VAL	2.1
1	B	279	ASP	2.1
1	A	745	LYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

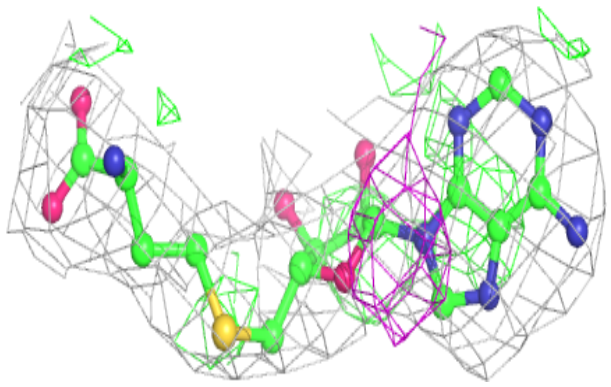
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

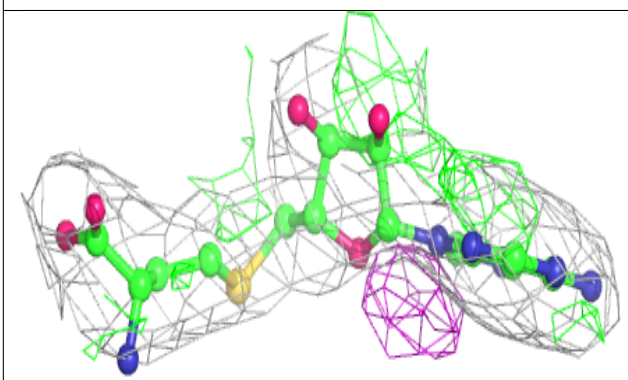
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	A	1000	26/26	0.91	0.29	42,53,71,112	0
2	SAH	B	1000	26/26	0.95	0.19	31,55,87,93	0

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

Electron density around SAH A 1000:

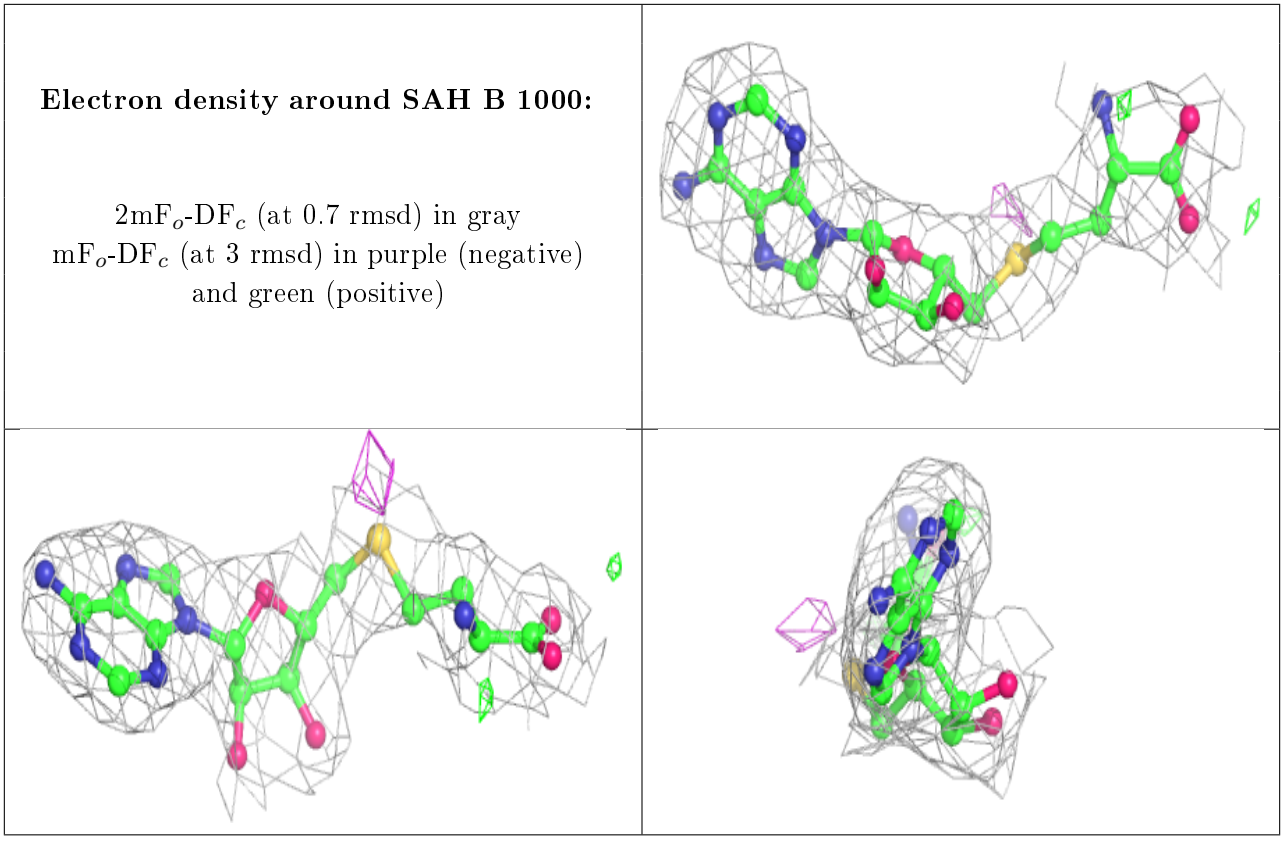
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around SAH B 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.