



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:17 AM UTC

PDB ID : 1D2H / pdb_00001d2h
Title : CRYSTAL STRUCTURE OF R175K MUTANT GLYCINE N-METHYLTRANSFERASE COMPLEXED WITH S-ADENOSYLHOMOCYSTEINE
Authors : Huang, Y.; Komoto, J.; Takusagawa, F.; Konishi, K.; Takata, Y.
Deposited on : 1999-10-11
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

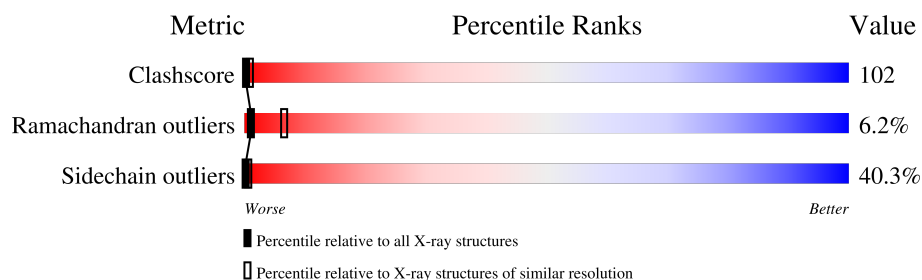
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	292	
1	B	292	
1	C	292	
1	D	292	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	A	1301	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8492 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.

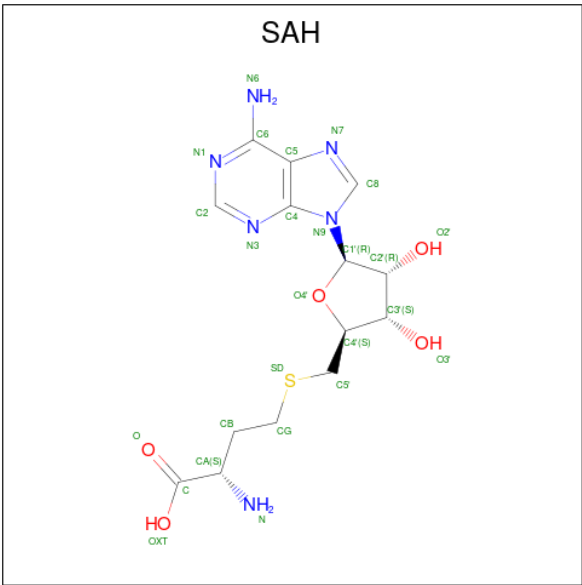
- Molecule 1 is a protein called GLYCINE N-METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1970	1257	339	363	11			
1	B	252	Total	C	N	O	S	0	0	0
			1970	1257	339	363	11			
1	C	252	Total	C	N	O	S	0	0	0
			1970	1257	339	363	11			
1	D	252	Total	C	N	O	S	0	0	0
			1970	1257	339	363	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	LYS	ARG	engineered mutation	UNP P13255
B	89	LYS	ARG	engineered mutation	UNP P13255
C	89	LYS	ARG	engineered mutation	UNP P13255
D	89	LYS	ARG	engineered mutation	UNP P13255

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

- Molecule 3 is water.

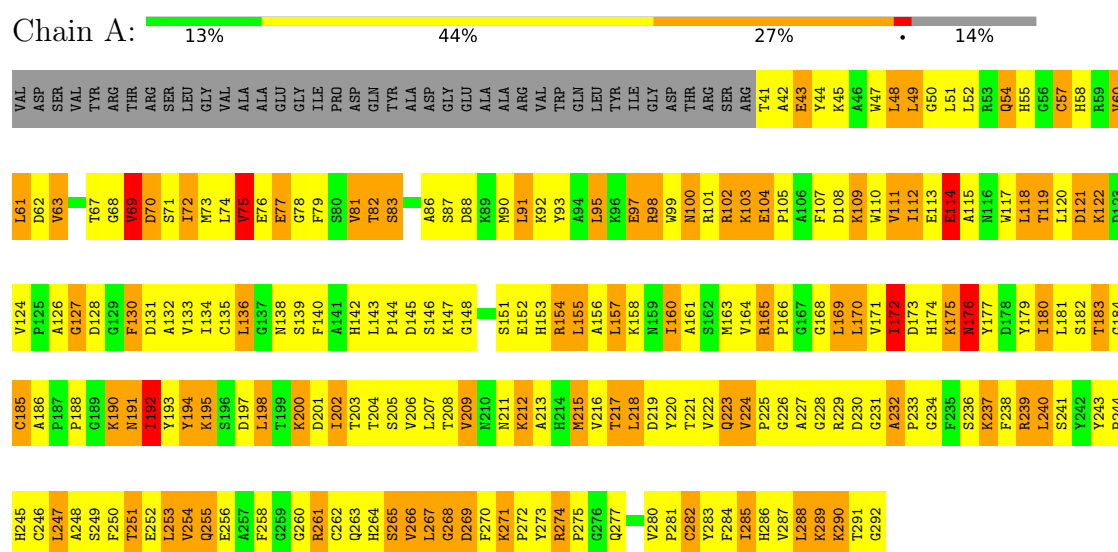
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	157	Total	O	0	0
			157	157		
3	B	119	Total	O	0	0
			119	119		
3	C	114	Total	O	0	0
			114	114		
3	D	118	Total	O	0	0
			118	118		

3 Residue-property plots

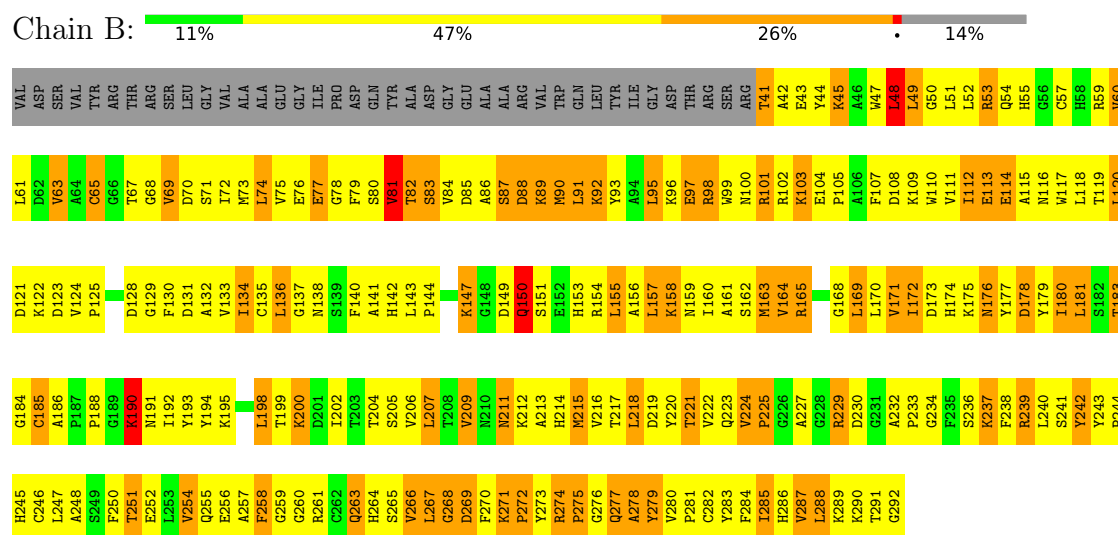
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: GLYCINE N-METHYLTRANSFERASE

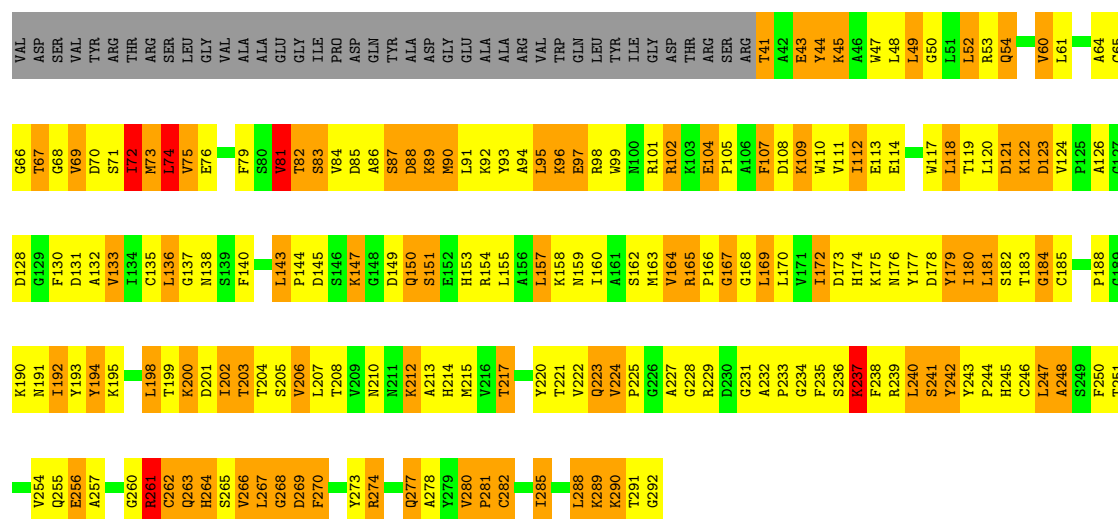


• Molecule 1: GLYCINE N-METHYLTRANSFERASE



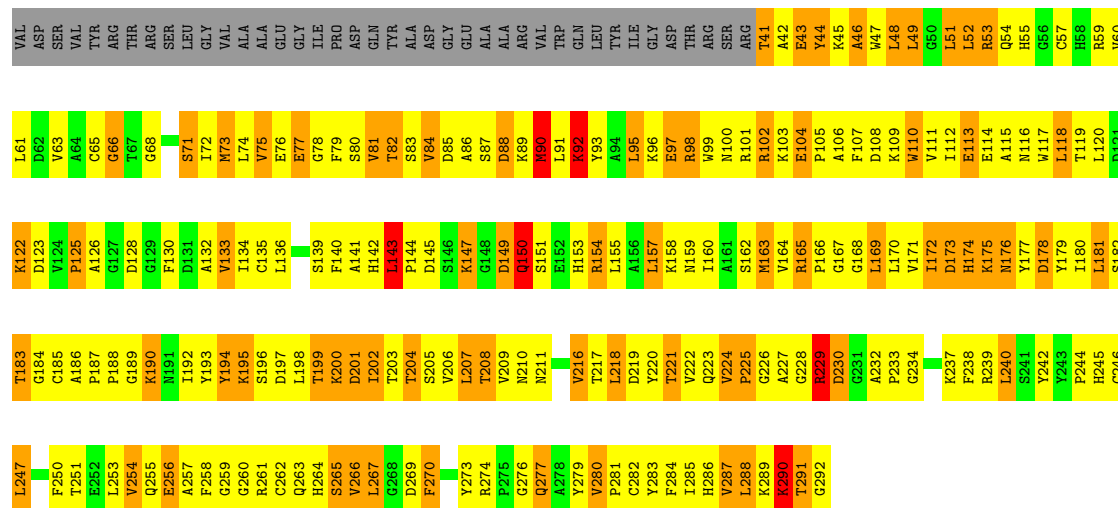
• Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain C: 20% 38% 27% 1% 14%



● Molecule 1: GLYCINE N-METHYLTRANSFERASE

Chain D: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	77.90Å 77.90Å 227.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	92.5 (10.00-3.00)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8492	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

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	0.37	0/2020	0.93	7/2737 (0.3%)
1	B	0.35	0/2020	0.90	6/2737 (0.2%)
1	C	0.36	0/2020	0.84	6/2737 (0.2%)
1	D	0.36	0/2020	0.86	4/2737 (0.1%)
All	All	0.36	0/8080	0.88	23/10948 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	GLY	N-CA-C	-10.28	95.03	112.30
1	A	268	GLY	N-CA-C	-8.98	97.22	112.30
1	D	81	VAL	N-CA-C	7.65	119.59	108.58
1	B	81	VAL	N-CA-C	6.99	118.19	107.99
1	C	81	VAL	N-CA-C	6.68	117.74	108.12
1	A	111	VAL	N-CA-C	6.65	118.69	107.18
1	A	172	ILE	N-CA-C	-6.54	102.92	110.05
1	B	178	ASP	N-CA-C	-5.96	103.95	111.11
1	A	87	SER	N-CA-C	5.92	118.18	108.52
1	B	282	CYS	N-CA-C	-5.86	104.97	111.36
1	A	290	LYS	N-CA-C	-5.80	102.06	110.24
1	B	232	ALA	CA-C-N	5.77	125.75	120.21
1	B	232	ALA	C-N-CA	5.77	125.75	120.21
1	C	87	SER	N-CA-C	5.69	117.93	108.20
1	D	143	LEU	CA-C-N	5.53	125.73	120.31
1	D	143	LEU	C-N-CA	5.53	125.73	120.31
1	D	178	ASP	N-CA-C	-5.52	104.28	111.02
1	A	114	GLU	N-CA-C	-5.48	103.16	110.55
1	C	237	LYS	N-CA-C	5.35	116.41	108.60
1	C	167	GLY	N-CA-C	-5.32	105.72	114.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	ILE	N-CA-C	5.16	117.27	108.86
1	C	204	THR	N-CA-C	5.14	116.99	108.20
1	C	67	THR	N-CA-C	-5.13	106.12	112.38

There are no chirality outliers.

There are no planarity outliers.

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	1970	0	1941	423	0
1	B	1970	0	1941	394	0
1	C	1970	0	1941	398	0
1	D	1970	0	1941	423	0
2	A	26	0	19	10	0
2	B	26	0	19	5	0
2	C	26	0	19	5	0
2	D	26	0	19	6	0
3	A	157	0	0	6	0
3	B	119	0	0	4	0
3	C	114	0	0	3	0
3	D	118	0	0	3	0
All	All	8492	0	7840	1610	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 102.

All (1610) 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:A:247:LEU:HD12	1:A:247:LEU:O	1.23	1.36
1:C:193:TYR:HB3	1:C:194:TYR:CE1	1.62	1.34
1:A:247:LEU:HD12	1:A:247:LEU:C	1.46	1.32
1:C:223:GLN:HB2	1:C:235:PHE:CE2	1.65	1.31
1:A:122:LYS:HA	1:A:122:LYS:NZ	1.49	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:HG21	1:C:194:TYR:CE2	1.69	1.26
1:D:136:LEU:CD1	1:D:171:VAL:HG12	1.67	1.24
1:D:136:LEU:HD11	1:D:171:VAL:CG1	1.67	1.24
1:D:175:LYS:HE3	1:D:282:CYS:SG	1.77	1.22
1:C:225:PRO:CA	1:C:233:PRO:HB3	1.71	1.20
1:D:227:ALA:HB3	1:D:234:GLY:CA	1.71	1.20
1:A:227:ALA:HB3	1:A:234:GLY:CA	1.72	1.19
1:D:82:THR:HG21	1:D:130:PHE:CE2	1.79	1.17
1:C:85:ASP:HB3	1:C:91:LEU:HD13	1.24	1.17
1:D:220:TYR:HB2	1:D:238:PHE:CE1	1.81	1.15
1:C:188:PRO:HB3	1:C:202:ILE:HD11	1.20	1.15
1:B:82:THR:HG21	1:B:130:PHE:HE2	1.09	1.15
1:D:227:ALA:HB3	1:D:234:GLY:N	1.59	1.15
1:A:77:GLU:HB3	1:A:79:PHE:HE1	1.09	1.15
1:B:258:PHE:CE2	1:B:288:LEU:HD12	1.83	1.14
1:A:102:ARG:HG2	1:A:102:ARG:HH21	0.99	1.13
1:A:227:ALA:HB3	1:A:234:GLY:N	1.65	1.12
1:D:192:ILE:HD11	1:D:283:TYR:HB2	1.32	1.12
1:A:188:PRO:HB3	1:A:202:ILE:HD12	1.29	1.11
1:D:90:MET:HE2	1:D:90:MET:HA	1.33	1.11
1:C:205:SER:HA	1:D:208:THR:O	1.49	1.10
1:A:77:GLU:OE2	1:A:77:GLU:HA	1.40	1.10
1:A:77:GLU:HB3	1:A:79:PHE:CE1	1.87	1.09
1:D:200:LYS:HB3	1:D:222:VAL:CA	1.81	1.09
1:C:193:TYR:HB3	1:C:194:TYR:CD1	1.88	1.08
1:A:220:TYR:CE1	1:A:240:LEU:HD12	1.89	1.08
1:A:60:VAL:HG13	1:A:132:ALA:HB3	1.36	1.08
1:A:211:ASN:HD22	1:B:184:GLY:HA3	1.16	1.08
1:B:188:PRO:HB3	1:B:202:ILE:CD1	1.83	1.07
1:C:273:TYR:C	1:C:274:ARG:HD3	1.79	1.07
1:C:261:ARG:HG2	1:C:292:GLY:HA3	1.27	1.07
1:C:223:GLN:HE21	1:C:225:PRO:HD3	1.17	1.07
1:D:188:PRO:HB3	1:D:202:ILE:HG13	1.36	1.07
1:C:41:THR:HG22	1:C:44:TYR:H	0.94	1.06
1:D:290:LYS:O	1:D:290:LYS:HG3	1.56	1.06
1:D:116:ASN:HD21	1:D:118:LEU:HB2	1.13	1.06
1:D:41:THR:HG22	1:D:44:TYR:H	1.19	1.06
1:C:85:ASP:CB	1:C:91:LEU:HD13	1.85	1.05
1:C:135:CYS:HB3	1:C:172:ILE:HG13	1.38	1.05
1:D:227:ALA:HB3	1:D:234:GLY:HA3	1.32	1.05
1:D:287:VAL:C	1:D:288:LEU:HD22	1.80	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:THR:HA	1:A:195:LYS:NZ	1.70	1.05
1:D:165:ARG:HH21	1:D:165:ARG:HG3	1.18	1.05
1:C:44:TYR:CE2	1:C:193:TYR:HD2	1.74	1.05
1:C:188:PRO:HB3	1:C:202:ILE:CD1	1.87	1.05
1:C:194:TYR:HD1	1:C:194:TYR:N	1.54	1.05
1:D:176:ASN:C	1:D:176:ASN:HD22	1.62	1.04
1:C:225:PRO:HA	1:C:233:PRO:CB	1.86	1.04
1:A:136:LEU:HD11	1:A:171:VAL:HG12	1.35	1.03
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.23	1.03
1:D:147:LYS:NZ	1:D:147:LYS:HB3	1.69	1.03
1:B:263:GLN:HE21	1:B:289:LYS:HD2	1.17	1.03
1:D:75:VAL:HG23	1:D:81:VAL:HG21	1.40	1.03
1:D:202:ILE:HD13	1:D:220:TYR:CD2	1.91	1.03
1:D:219:ASP:HB3	1:D:237:LYS:HE2	1.39	1.03
1:C:41:THR:HG22	1:C:44:TYR:N	1.73	1.03
1:B:95:LEU:HD13	1:B:112:ILE:HG21	1.37	1.02
1:B:188:PRO:HB3	1:B:202:ILE:HD12	1.42	1.02
1:A:169:LEU:HA	1:A:288:LEU:O	1.59	1.02
1:D:158:LYS:HA	1:D:257:ALA:HB1	1.40	1.02
1:A:95:LEU:HD13	1:A:112:ILE:HD13	1.02	1.01
1:A:95:LEU:CD1	1:A:112:ILE:HD13	1.91	1.01
1:A:154:ARG:HH11	1:A:154:ARG:CG	1.72	1.01
1:A:217:THR:HG21	1:A:239:ARG:NH1	1.74	1.01
1:A:193:TYR:HB3	1:A:194:TYR:CE2	1.95	1.01
1:A:247:LEU:C	1:A:247:LEU:CD1	2.26	1.01
1:B:136:LEU:HD11	1:B:171:VAL:CG1	1.90	1.01
1:B:147:LYS:HB3	1:B:149:ASP:OD2	1.60	1.01
1:A:136:LEU:HD11	1:A:171:VAL:CG1	1.91	1.01
1:A:95:LEU:HD13	1:A:112:ILE:CD1	1.90	1.00
1:D:176:ASN:O	1:D:176:ASN:ND2	1.92	1.00
1:C:224:VAL:HG21	1:C:227:ALA:HB2	1.41	1.00
1:D:207:LEU:HD12	1:D:208:THR:H	1.25	1.00
1:A:126:ALA:CB	1:A:130:PHE:HE1	1.74	1.00
1:B:261:ARG:HD3	1:B:292:GLY:HA3	1.42	1.00
1:B:263:GLN:NE2	1:B:289:LYS:HD2	1.77	0.99
1:C:198:LEU:HD21	1:C:222:VAL:HG11	1.39	0.99
1:A:191:ASN:OD1	1:A:193:TYR:HB2	1.62	0.99
1:A:227:ALA:HB3	1:A:234:GLY:HA3	1.39	0.99
1:B:82:THR:HG21	1:B:130:PHE:CE2	1.97	0.99
1:D:101:ARG:HD3	1:D:107:PHE:CE2	1.97	0.99
1:A:261:ARG:CD	1:A:292:GLY:HA3	1.92	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:TYR:C	1:C:194:TYR:HD1	1.70	0.98
1:A:188:PRO:HB3	1:A:202:ILE:CD1	1.93	0.98
1:A:267:LEU:N	1:A:267:LEU:HD23	1.75	0.98
1:D:200:LYS:CB	1:D:222:VAL:HA	1.92	0.98
1:D:207:LEU:HD12	1:D:208:THR:N	1.79	0.98
1:A:192:ILE:HG13	1:A:270:PHE:CE1	1.98	0.98
1:A:136:LEU:CD1	1:A:171:VAL:HG12	1.94	0.98
1:A:126:ALA:HB2	1:A:130:PHE:HE1	1.23	0.98
1:D:200:LYS:HB3	1:D:222:VAL:HA	0.98	0.98
1:A:211:ASN:HD22	1:B:184:GLY:CA	1.76	0.97
1:C:177:TYR:O	1:C:181:LEU:HD22	1.63	0.97
1:D:199:THR:HG22	1:D:199:THR:O	1.63	0.97
1:B:254:VAL:HG13	1:B:288:LEU:HD11	1.46	0.97
1:D:82:THR:HG21	1:D:130:PHE:HE2	1.11	0.97
1:A:247:LEU:O	1:A:247:LEU:CD1	2.12	0.96
1:A:217:THR:HG21	1:A:239:ARG:HH11	1.28	0.96
1:C:44:TYR:CZ	1:C:193:TYR:HD2	1.82	0.96
1:A:169:LEU:HD12	1:A:288:LEU:O	1.66	0.96
1:A:251:THR:HG22	1:A:264:HIS:CE1	2.01	0.95
1:A:102:ARG:HG2	1:A:102:ARG:NH2	1.75	0.95
1:A:122:LYS:HA	1:A:122:LYS:HZ2	1.22	0.95
1:B:87:SER:HB3	2:B:2301:SAH:O2'	1.64	0.95
1:C:133:VAL:CG2	1:C:164:VAL:HG22	1.97	0.95
1:B:274:ARG:O	1:B:277:GLN:HB3	1.64	0.95
1:C:194:TYR:CD1	1:C:194:TYR:N	2.30	0.95
1:C:99:TRP:O	1:C:102:ARG:HB3	1.64	0.95
1:B:82:THR:CG2	1:B:130:PHE:HE2	1.79	0.95
1:A:228:GLY:HA3	1:A:232:ALA:HB3	1.46	0.94
1:B:221:THR:HG22	1:B:221:THR:O	1.63	0.94
1:C:224:VAL:HG22	1:C:227:ALA:H	1.32	0.94
1:C:274:ARG:O	1:C:277:GLN:HB3	1.68	0.94
1:D:90:MET:HG3	2:D:4301:SAH:O3'	1.68	0.94
1:A:204:THR:HG23	1:A:218:LEU:HD11	1.48	0.94
1:A:224:VAL:HG13	1:A:234:GLY:H	1.32	0.94
1:C:143:LEU:HD12	1:C:144:PRO:N	1.82	0.94
1:C:200:LYS:HB3	1:C:222:VAL:HA	1.50	0.94
1:D:75:VAL:CG2	1:D:81:VAL:HG21	1.96	0.94
1:D:227:ALA:CB	1:D:234:GLY:HA3	1.97	0.94
1:C:193:TYR:HB3	1:C:194:TYR:HE1	1.13	0.93
1:C:181:LEU:HD23	1:C:246:CYS:SG	2.09	0.93
1:C:135:CYS:HB3	1:C:172:ILE:CG1	1.97	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:VAL:HG22	1:C:224:VAL:O	1.68	0.93
1:D:147:LYS:HB3	1:D:147:LYS:HZ1	1.27	0.93
1:A:188:PRO:CB	1:A:202:ILE:HD12	1.99	0.93
1:C:165:ARG:HH21	1:C:165:ARG:CG	1.81	0.93
1:C:225:PRO:HA	1:C:233:PRO:HB3	0.96	0.93
1:A:227:ALA:CB	1:A:234:GLY:HA3	1.97	0.93
1:C:108:ASP:C	1:C:109:LYS:HD2	1.94	0.93
1:A:190:LYS:HZ2	1:A:191:ASN:H	1.17	0.92
1:C:223:GLN:HE21	1:C:225:PRO:CD	1.82	0.92
1:B:73:MET:HE3	1:B:74:LEU:CD2	1.99	0.92
1:A:176:ASN:C	1:A:176:ASN:HD22	1.76	0.92
1:B:75:VAL:HG22	1:B:81:VAL:HG13	1.51	0.92
1:A:41:THR:HA	1:A:195:LYS:HZ1	1.35	0.92
1:D:263:GLN:NE2	1:D:291:THR:HG21	1.85	0.92
1:A:97:GLU:OE2	1:A:97:GLU:HA	1.67	0.92
1:B:227:ALA:HB3	1:B:234:GLY:HA3	1.52	0.92
1:C:44:TYR:HB2	1:C:270:PHE:CE1	2.05	0.92
1:A:274:ARG:HB3	1:A:274:ARG:HH11	1.35	0.91
1:D:204:THR:HA	1:D:218:LEU:HD12	1.48	0.91
1:B:85:ASP:HB3	1:B:91:LEU:HD22	1.53	0.91
1:C:111:VAL:C	1:C:112:ILE:HG12	1.93	0.91
1:A:269:ASP:O	1:A:285:ILE:HD13	1.70	0.91
1:C:85:ASP:HB3	1:C:91:LEU:CD1	2.00	0.91
1:A:122:LYS:HA	1:A:122:LYS:CE	1.90	0.91
1:B:222:VAL:HB	1:B:236:SER:O	1.70	0.91
1:D:175:LYS:CE	1:D:282:CYS:SG	2.59	0.90
1:A:82:THR:HG21	1:A:130:PHE:HE2	1.36	0.90
1:B:169:LEU:HA	1:B:288:LEU:O	1.71	0.90
1:A:142:HIS:CE1	2:A:1301:SAH:HG2	2.06	0.90
1:D:150:GLN:O	1:D:153:HIS:HB2	1.72	0.90
1:B:140:PHE:CZ	1:B:157:LEU:CD2	2.55	0.90
1:C:193:TYR:C	1:C:194:TYR:CD1	2.50	0.89
1:A:100:ASN:N	1:A:100:ASN:HD22	1.69	0.89
1:B:287:VAL:O	1:B:288:LEU:HD23	1.71	0.89
1:B:124:VAL:O	1:B:163:MET:HE1	1.71	0.89
1:B:75:VAL:HG23	1:B:81:VAL:HG11	1.53	0.89
1:C:201:ASP:C	1:C:202:ILE:HG12	1.97	0.89
1:C:133:VAL:HG21	1:C:164:VAL:HG22	1.55	0.89
1:A:261:ARG:HD3	1:A:292:GLY:HA3	1.53	0.89
1:C:164:VAL:HG12	1:C:168:GLY:HA3	1.55	0.89
1:C:193:TYR:CB	1:C:194:TYR:CE1	2.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:VAL:HG21	1:D:164:VAL:HG22	1.55	0.88
1:B:156:ALA:O	1:B:160:ILE:HG13	1.73	0.88
1:D:41:THR:HG22	1:D:44:TYR:N	1.88	0.88
1:B:116:ASN:OD1	1:B:118:LEU:HD13	1.72	0.88
1:C:169:LEU:HA	1:C:288:LEU:O	1.72	0.88
1:A:100:ASN:HD22	1:A:100:ASN:H	1.20	0.88
1:C:60:VAL:HG21	1:C:74:LEU:HD12	1.54	0.88
1:D:280:VAL:O	1:D:280:VAL:HG12	1.73	0.88
1:A:261:ARG:HD3	1:A:292:GLY:C	1.98	0.88
1:D:202:ILE:HD13	1:D:220:TYR:HD2	1.36	0.88
1:C:44:TYR:CZ	1:C:193:TYR:CD2	2.61	0.87
1:D:221:THR:OG1	1:D:237:LYS:HE3	1.72	0.87
1:B:140:PHE:CZ	1:B:157:LEU:HD22	2.08	0.87
1:D:77:GLU:HA	1:D:77:GLU:OE1	1.73	0.87
1:A:224:VAL:HG13	1:A:234:GLY:N	1.89	0.87
1:A:237:LYS:HG3	1:A:238:PHE:N	1.89	0.87
1:A:41:THR:N	1:A:195:LYS:HE2	1.90	0.87
1:B:287:VAL:C	1:B:288:LEU:HD23	1.99	0.87
1:C:224:VAL:CG2	1:C:227:ALA:HB2	2.04	0.87
1:D:168:GLY:O	1:D:289:LYS:HA	1.74	0.87
1:A:98:ARG:HD3	1:C:99:TRP:CZ2	2.10	0.87
1:C:203:THR:HG22	1:D:210:ASN:ND2	1.89	0.87
1:B:41:THR:HG23	1:B:43:GLU:OE1	1.75	0.87
1:A:83:SER:O	1:A:112:ILE:HA	1.74	0.86
1:D:68:GLY:O	1:D:72:ILE:HG13	1.75	0.86
1:B:136:LEU:HD13	1:B:171:VAL:O	1.74	0.86
1:C:143:LEU:HD12	1:C:143:LEU:C	1.99	0.86
1:D:41:THR:CG2	1:D:44:TYR:H	1.87	0.86
1:B:155:LEU:HD13	1:B:158:LYS:NZ	1.91	0.86
1:B:129:GLY:O	1:B:165:ARG:HB3	1.74	0.86
1:C:101:ARG:HD3	1:C:107:PHE:CE2	2.10	0.86
1:A:156:ALA:O	1:A:160:ILE:HD12	1.73	0.86
1:B:227:ALA:HB3	1:B:234:GLY:CA	2.05	0.86
1:A:228:GLY:HA3	1:A:232:ALA:CB	2.05	0.86
1:A:61:LEU:HD12	1:A:62:ASP:N	1.90	0.86
1:B:256:GLU:HB2	3:B:2394:HOH:O	1.76	0.86
1:C:135:CYS:CB	1:C:172:ILE:HG13	2.05	0.86
1:A:251:THR:CG2	1:A:264:HIS:CE1	2.58	0.85
1:C:198:LEU:HD21	1:C:222:VAL:CG1	2.05	0.85
1:B:55:HIS:CG	1:B:169:LEU:HD21	2.11	0.85
1:C:83:SER:O	1:C:112:ILE:HA	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ARG:HD3	1:A:292:GLY:CA	2.06	0.85
1:C:188:PRO:CB	1:C:202:ILE:HD11	2.05	0.85
1:C:201:ASP:O	1:C:202:ILE:HG12	1.74	0.85
1:B:142:HIS:O	1:B:144:PRO:HD3	1.77	0.85
1:D:90:MET:HA	1:D:90:MET:CE	2.06	0.85
1:C:167:GLY:C	1:C:289:LYS:HE2	2.00	0.85
1:A:192:ILE:HG13	1:A:270:PHE:HE1	1.37	0.85
1:D:258:PHE:HE2	1:D:288:LEU:CG	1.89	0.85
1:D:99:TRP:O	1:D:102:ARG:HB3	1.74	0.85
1:D:176:ASN:HD21	1:D:179:TYR:H	1.23	0.85
1:B:83:SER:O	1:B:112:ILE:HA	1.75	0.84
1:C:193:TYR:CB	1:C:194:TYR:CD1	2.60	0.84
1:D:51:LEU:HD12	1:D:51:LEU:C	2.03	0.84
1:C:203:THR:HG22	1:D:210:ASN:HD21	1.42	0.84
1:C:165:ARG:HH21	1:C:165:ARG:HG3	1.40	0.84
1:C:101:ARG:O	1:C:104:GLU:HG3	1.77	0.84
1:D:220:TYR:HB2	1:D:238:PHE:HE1	1.37	0.84
1:A:287:VAL:C	1:A:288:LEU:HD22	2.02	0.83
1:D:49:LEU:HD13	1:D:73:MET:HE1	1.59	0.83
1:D:134:ILE:HB	1:D:136:LEU:CD2	2.07	0.83
1:D:140:PHE:CZ	1:D:157:LEU:CD2	2.60	0.83
1:A:126:ALA:CB	1:A:130:PHE:CE1	2.60	0.83
1:C:44:TYR:CE2	1:C:193:TYR:CD2	2.63	0.83
1:A:190:LYS:HZ2	1:A:191:ASN:N	1.76	0.83
1:A:211:ASN:ND2	1:B:184:GLY:HA3	1.92	0.83
1:B:188:PRO:HB3	1:B:202:ILE:HD11	1.61	0.83
1:A:91:LEU:HD11	1:A:112:ILE:CG2	2.08	0.83
1:B:136:LEU:HD11	1:B:171:VAL:HG12	1.60	0.83
1:B:183:THR:CG2	1:B:185:CYS:H	1.91	0.83
1:D:154:ARG:HB3	1:D:256:GLU:OE2	1.78	0.83
1:D:258:PHE:HE2	1:D:288:LEU:CB	1.92	0.83
1:D:202:ILE:CD1	1:D:220:TYR:HD2	1.90	0.83
1:A:192:ILE:CG1	1:A:270:PHE:CE1	2.61	0.83
1:B:155:LEU:HD13	1:B:158:LYS:HZ1	1.44	0.83
1:D:133:VAL:CG2	1:D:164:VAL:HG22	2.09	0.83
1:D:202:ILE:CD1	1:D:220:TYR:CD2	2.61	0.83
1:B:242:TYR:N	1:B:242:TYR:CD2	2.48	0.82
1:D:288:LEU:N	1:D:288:LEU:CD2	2.42	0.82
1:B:136:LEU:HD22	1:B:136:LEU:H	1.45	0.82
1:B:280:VAL:HG13	1:B:280:VAL:O	1.78	0.82
1:C:274:ARG:HD3	1:C:274:ARG:N	1.94	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:CD2	1:C:246:CYS:SG	2.67	0.82
1:A:217:THR:HG23	1:A:241:SER:OG	1.80	0.82
1:B:41:THR:HG22	1:B:44:TYR:H	1.45	0.82
1:D:91:LEU:HD21	1:D:113:GLU:O	1.80	0.82
1:B:73:MET:HE3	1:B:74:LEU:HD21	1.60	0.82
1:A:224:VAL:CG1	1:A:234:GLY:CA	2.58	0.81
1:C:69:VAL:HG22	1:C:70:ASP:N	1.94	0.81
1:D:165:ARG:HH21	1:D:165:ARG:CG	1.90	0.81
1:A:204:THR:HG23	1:A:218:LEU:CD1	2.09	0.81
1:B:183:THR:HG22	1:B:185:CYS:H	1.44	0.81
1:C:201:ASP:HB3	1:C:221:THR:HB	1.62	0.81
1:C:264:HIS:HB2	1:C:288:LEU:HD11	1.60	0.81
1:D:267:LEU:HD12	1:D:267:LEU:N	1.95	0.81
1:C:61:LEU:HD23	1:C:133:VAL:CG1	2.10	0.81
1:A:270:PHE:HE2	1:A:285:ILE:HG12	1.45	0.81
1:C:178:ASP:OD2	1:C:246:CYS:HA	1.80	0.81
1:D:228:GLY:HA3	1:D:232:ALA:HB3	1.61	0.81
1:A:176:ASN:HD21	1:A:179:TYR:H	1.28	0.81
1:A:41:THR:HB	1:A:192:ILE:O	1.80	0.81
1:C:126:ALA:HB2	1:C:163:MET:HE2	1.62	0.81
1:D:170:LEU:O	1:D:287:VAL:HA	1.80	0.81
1:D:173:ASP:C	1:D:173:ASP:OD1	2.22	0.81
1:B:207:LEU:HD23	1:B:207:LEU:O	1.81	0.81
1:C:242:TYR:N	1:C:242:TYR:CD2	2.49	0.80
1:C:69:VAL:CG2	1:C:194:TYR:CE2	2.60	0.80
1:D:219:ASP:OD1	1:D:239:ARG:HB3	1.80	0.80
1:B:75:VAL:CG2	1:B:81:VAL:CG1	2.59	0.80
1:A:91:LEU:CD1	1:A:112:ILE:CG2	2.59	0.80
1:A:126:ALA:HB2	1:A:130:PHE:CE1	2.13	0.80
1:B:229:ARG:HE	1:B:229:ARG:HA	1.47	0.80
1:D:227:ALA:HB3	1:D:234:GLY:H	1.42	0.80
1:D:220:TYR:CB	1:D:238:PHE:CE1	2.64	0.80
1:C:85:ASP:CB	1:C:91:LEU:CD1	2.60	0.79
2:A:1301:SAH:H5'2	2:A:1301:SAH:HN1	1.46	0.79
1:B:241:SER:C	1:B:242:TYR:CD2	2.60	0.79
1:C:120:LEU:HD23	1:C:159:ASN:O	1.81	0.79
1:C:167:GLY:CA	1:C:289:LYS:HE2	2.12	0.79
1:A:72:ILE:HD12	1:A:110:TRP:CH2	2.18	0.79
1:A:118:LEU:O	1:A:119:THR:HG23	1.82	0.79
1:D:176:ASN:C	1:D:176:ASN:ND2	2.37	0.79
1:A:121:ASP:CG	1:A:122:LYS:H	1.91	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:220:TYR:CD1	1:D:238:PHE:CZ	2.71	0.79
1:D:192:ILE:CD1	1:D:283:TYR:HB2	2.11	0.79
1:D:258:PHE:CE2	1:D:288:LEU:CB	2.66	0.79
1:A:72:ILE:O	1:A:75:VAL:HB	1.83	0.79
1:A:224:VAL:HG13	1:A:234:GLY:CA	2.10	0.79
1:A:265:SER:OG	1:A:287:VAL:HG23	1.83	0.79
1:A:287:VAL:O	1:A:288:LEU:HD22	1.82	0.79
1:B:141:ALA:O	1:B:242:TYR:HB3	1.83	0.79
1:C:280:VAL:O	1:C:280:VAL:CG1	2.31	0.79
1:B:105:PRO:O	1:B:109:LYS:HD3	1.82	0.79
1:B:161:ALA:O	1:B:164:VAL:HG23	1.82	0.78
1:D:101:ARG:HD3	1:D:107:PHE:CZ	2.18	0.78
1:C:289:LYS:O	1:C:291:THR:HG23	1.83	0.78
1:B:97:GLU:OE2	1:B:101:ARG:HD2	1.83	0.78
1:C:41:THR:CG2	1:C:44:TYR:H	1.88	0.78
1:A:190:LYS:HG2	3:A:1359:HOH:O	1.82	0.78
1:C:75:VAL:HG12	1:C:76:GLU:N	1.98	0.78
1:C:223:GLN:NE2	1:C:225:PRO:HG3	1.99	0.78
1:B:221:THR:HA	1:B:237:LYS:HB2	1.63	0.78
1:B:277:GLN:HE21	1:B:279:TYR:HB3	1.49	0.78
1:A:201:ASP:HB2	3:A:1347:HOH:O	1.82	0.78
1:B:82:THR:CG2	1:B:130:PHE:CE2	2.64	0.78
1:C:44:TYR:HB2	1:C:270:PHE:CD1	2.19	0.78
1:D:41:THR:HB	1:D:44:TYR:HB3	1.66	0.78
1:A:220:TYR:HE1	1:A:240:LEU:HD12	1.45	0.78
1:C:242:TYR:N	1:C:242:TYR:HD2	1.80	0.78
1:D:60:VAL:HG21	1:D:74:LEU:HD13	1.65	0.78
1:B:193:TYR:HE1	1:B:283:TYR:CD2	2.01	0.77
1:B:269:ASP:O	1:B:285:ILE:HD11	1.84	0.77
1:A:41:THR:HA	1:A:195:LYS:CE	2.13	0.77
1:A:102:ARG:HH21	1:A:102:ARG:CG	1.89	0.77
1:D:157:LEU:HD11	1:D:172:ILE:CD1	2.14	0.77
1:D:219:ASP:CB	1:D:237:LYS:HE2	2.14	0.77
1:B:75:VAL:CG2	1:B:81:VAL:HG13	2.14	0.77
1:C:224:VAL:CG2	1:C:227:ALA:CB	2.61	0.77
1:D:116:ASN:ND2	1:D:118:LEU:HB2	1.96	0.77
1:C:140:PHE:CE2	1:C:250:PHE:HE1	2.03	0.77
1:D:140:PHE:CZ	1:D:157:LEU:HD22	2.20	0.77
1:B:75:VAL:HG23	1:B:81:VAL:CG1	2.14	0.77
1:D:288:LEU:HD22	1:D:288:LEU:N	1.99	0.77
1:D:262:CYS:HA	1:D:291:THR:H	1.50	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:GLN:NE2	1:B:289:LYS:CD	2.48	0.77
1:A:229:ARG:H	1:A:232:ALA:HB3	1.50	0.77
1:A:261:ARG:NE	1:A:292:GLY:HA3	1.99	0.77
1:B:218:LEU:HD22	1:B:242:TYR:CE2	2.20	0.77
1:C:143:LEU:CD1	1:C:144:PRO:HD2	2.15	0.77
1:A:287:VAL:C	1:A:288:LEU:CD2	2.58	0.76
1:D:258:PHE:CE2	1:D:288:LEU:HB3	2.20	0.76
1:B:85:ASP:O	1:B:114:GLU:HA	1.84	0.76
1:B:224:VAL:O	1:B:233:PRO:HB3	1.85	0.76
1:D:219:ASP:HB3	1:D:237:LYS:CE	2.16	0.76
1:B:54:GLN:O	1:B:54:GLN:HG2	1.85	0.76
1:B:242:TYR:N	1:B:242:TYR:HD2	1.84	0.76
1:D:190:LYS:HD3	1:D:190:LYS:N	2.01	0.76
1:B:191:ASN:HB3	1:B:194:TYR:O	1.85	0.75
1:C:109:LYS:HD2	1:C:109:LYS:N	1.99	0.75
1:C:126:ALA:HB2	1:C:163:MET:CE	2.15	0.75
1:A:176:ASN:ND2	1:A:179:TYR:H	1.84	0.75
1:B:258:PHE:CZ	1:B:288:LEU:HD12	2.20	0.75
1:C:167:GLY:HA2	1:C:289:LYS:HE2	1.68	0.75
1:A:136:LEU:HD13	1:A:171:VAL:O	1.86	0.75
1:A:267:LEU:HB3	1:A:271:LYS:O	1.86	0.75
1:C:95:LEU:HD11	1:C:112:ILE:HB	1.68	0.75
1:D:82:THR:CG2	1:D:130:PHE:CE2	2.67	0.75
1:A:193:TYR:HB3	1:A:194:TYR:CD2	2.22	0.75
1:A:154:ARG:CG	1:A:154:ARG:NH1	2.42	0.75
1:C:67:THR:O	1:C:94:ALA:HB2	1.87	0.75
1:D:280:VAL:O	1:D:280:VAL:CG1	2.35	0.75
1:B:188:PRO:CB	1:B:202:ILE:HD12	2.18	0.74
1:D:247:LEU:HD11	1:D:286:HIS:CE1	2.23	0.74
1:C:224:VAL:HG22	1:C:227:ALA:CB	2.17	0.74
1:B:95:LEU:CD1	1:B:112:ILE:HG21	2.16	0.74
1:C:69:VAL:HG21	1:C:194:TYR:CZ	2.23	0.74
1:C:280:VAL:O	1:C:280:VAL:HG12	1.88	0.74
1:D:122:LYS:HD2	1:D:123:ASP:OD2	1.87	0.74
1:B:69:VAL:HG23	1:B:70:ASP:H	1.53	0.74
1:D:192:ILE:HD11	1:D:283:TYR:CB	2.16	0.74
1:A:267:LEU:N	1:A:267:LEU:CD2	2.50	0.73
1:D:169:LEU:HA	1:D:288:LEU:O	1.88	0.73
1:A:135:CYS:HB3	1:A:172:ILE:HA	1.71	0.73
1:A:101:ARG:HB3	1:A:104:GLU:HG3	1.69	0.73
1:B:77:GLU:HB2	1:B:79:PHE:CE1	2.24	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLN:HG2	1:D:153:HIS:CD2	2.24	0.73
1:D:199:THR:O	1:D:199:THR:CG2	2.34	0.73
1:D:287:VAL:C	1:D:288:LEU:CD2	2.60	0.73
1:A:270:PHE:CE2	1:A:285:ILE:HG12	2.24	0.73
1:C:168:GLY:O	1:C:289:LYS:HA	1.88	0.73
1:C:179:TYR:CD1	1:C:180:ILE:N	2.56	0.73
1:D:247:LEU:HD11	1:D:286:HIS:HE1	1.52	0.73
1:A:172:ILE:HG21	1:A:250:PHE:HE2	1.52	0.73
1:C:69:VAL:HG11	1:C:194:TYR:HE2	1.54	0.73
1:C:75:VAL:HG11	1:C:107:PHE:CE1	2.24	0.73
1:D:83:SER:O	1:D:112:ILE:HA	1.88	0.73
1:A:100:ASN:H	1:A:100:ASN:ND2	1.86	0.72
1:B:220:TYR:O	1:B:237:LYS:HB2	1.88	0.72
1:D:116:ASN:HD21	1:D:118:LEU:CB	1.96	0.72
1:A:224:VAL:CG1	1:A:234:GLY:HA3	2.18	0.72
1:C:117:TRP:CD1	1:C:160:ILE:HD11	2.24	0.72
1:B:174:HIS:HD2	1:B:175:LYS:O	1.72	0.72
1:B:73:MET:CE	1:B:74:LEU:CD2	2.68	0.72
1:D:225:PRO:O	1:D:233:PRO:HB3	1.88	0.72
1:D:263:GLN:HE22	1:D:291:THR:HG21	1.54	0.72
1:D:41:THR:HB	1:D:44:TYR:CB	2.20	0.72
1:A:101:ARG:NE	1:A:107:PHE:CE1	2.58	0.72
1:A:224:VAL:HG12	1:A:234:GLY:C	2.15	0.72
1:A:264:HIS:CE1	1:A:286:HIS:ND1	2.58	0.72
1:B:264:HIS:ND1	1:B:288:LEU:HD21	2.04	0.72
1:C:101:ARG:HB2	1:C:107:PHE:CD2	2.25	0.72
1:B:136:LEU:CD1	1:B:171:VAL:HG12	2.19	0.72
1:B:209:VAL:HB	1:B:214:HIS:HB2	1.72	0.72
1:D:277:GLN:O	1:D:277:GLN:HG2	1.88	0.72
1:D:220:TYR:HB2	1:D:238:PHE:CD1	2.25	0.71
1:D:192:ILE:HD13	1:D:269:ASP:OD1	1.90	0.71
1:C:273:TYR:C	1:C:274:ARG:CD	2.62	0.71
1:D:174:HIS:HD2	1:D:174:HIS:O	1.72	0.71
1:A:289:LYS:HG2	1:A:289:LYS:O	1.90	0.71
1:C:203:THR:CG2	1:D:210:ASN:HD21	2.03	0.71
1:B:77:GLU:HB2	1:B:79:PHE:HE1	1.56	0.71
1:B:63:VAL:HG12	1:B:120:LEU:HD21	1.72	0.71
1:C:133:VAL:HG23	1:C:164:VAL:HG22	1.71	0.71
1:C:224:VAL:O	1:C:224:VAL:CG2	2.38	0.71
1:D:49:LEU:O	1:D:53:ARG:HB2	1.91	0.71
1:C:193:TYR:CB	1:C:194:TYR:HE1	1.97	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:CD2	1:C:222:VAL:CG1	2.69	0.71
1:C:223:GLN:HB2	1:C:235:PHE:CZ	2.23	0.71
1:A:124:VAL:O	1:A:163:MET:HE1	1.90	0.71
1:B:74:LEU:O	1:B:79:PHE:HD1	1.73	0.71
1:B:176:ASN:ND2	1:B:179:TYR:H	1.88	0.71
1:D:136:LEU:HB3	1:D:193:TYR:OH	1.91	0.71
1:A:252:GLU:OE1	1:A:253:LEU:HD23	1.91	0.71
1:C:225:PRO:C	1:C:233:PRO:HB3	2.15	0.71
1:B:136:LEU:HD11	1:B:171:VAL:CB	2.21	0.70
1:A:75:VAL:HG12	1:A:76:GLU:N	2.06	0.70
1:D:247:LEU:CD1	1:D:286:HIS:HE1	2.04	0.70
1:B:92:LYS:HD3	1:B:93:TYR:CD2	2.25	0.70
1:D:220:TYR:CD1	1:D:238:PHE:CE1	2.80	0.70
1:A:170:LEU:HD23	1:A:258:PHE:HZ	1.56	0.70
1:C:99:TRP:CZ2	1:C:102:ARG:NH1	2.59	0.70
1:D:195:LYS:NZ	1:D:195:LYS:HB3	2.06	0.70
1:B:227:ALA:HB3	1:B:234:GLY:N	2.07	0.70
1:C:224:VAL:HG22	1:C:227:ALA:N	2.04	0.70
1:D:176:ASN:ND2	1:D:179:TYR:H	1.90	0.70
1:C:192:ILE:O	1:C:192:ILE:CG1	2.38	0.70
1:C:69:VAL:HG21	1:C:194:TYR:HE2	1.45	0.70
1:C:268:GLY:N	1:C:273:TYR:HB2	2.06	0.70
1:B:209:VAL:O	1:B:209:VAL:HG12	1.90	0.70
1:D:111:VAL:HG12	1:D:111:VAL:O	1.92	0.70
1:C:143:LEU:HD12	1:C:144:PRO:CD	2.22	0.69
1:D:140:PHE:CZ	1:D:157:LEU:HD21	2.26	0.69
1:A:200:LYS:HG2	1:A:222:VAL:HG22	1.74	0.69
1:A:227:ALA:CB	1:A:234:GLY:CA	2.57	0.69
1:B:47:TRP:CZ3	1:B:48:LEU:HD12	2.27	0.69
1:B:200:LYS:HB3	1:B:222:VAL:HA	1.72	0.69
1:C:145:ASP:O	1:C:145:ASP:OD2	2.09	0.69
1:A:72:ILE:CD1	1:A:110:TRP:CH2	2.75	0.69
1:A:192:ILE:HD11	1:A:270:PHE:CE1	2.27	0.69
1:A:220:TYR:O	1:A:237:LYS:HB2	1.92	0.69
1:D:97:GLU:OE1	1:D:97:GLU:HA	1.91	0.69
1:A:77:GLU:OE2	1:A:77:GLU:CA	2.26	0.69
1:A:75:VAL:HG11	1:A:107:PHE:CE2	2.28	0.69
1:B:254:VAL:CG1	1:B:288:LEU:HD11	2.21	0.69
1:B:269:ASP:H	1:B:281:PRO:HB3	1.57	0.69
1:C:228:GLY:HA3	1:C:232:ALA:O	1.91	0.69
1:B:48:LEU:HD22	1:B:73:MET:HE1	1.75	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:TRP:O	1:B:102:ARG:HB3	1.91	0.69
1:B:136:LEU:HD22	1:B:136:LEU:N	2.08	0.69
1:B:140:PHE:CZ	1:B:157:LEU:HD21	2.26	0.69
1:D:49:LEU:CD1	1:D:73:MET:CE	2.71	0.69
1:D:175:LYS:NZ	1:D:283:TYR:CE1	2.60	0.69
1:A:221:THR:HA	1:A:237:LYS:HB2	1.75	0.69
1:A:274:ARG:HH11	1:A:274:ARG:CB	2.05	0.69
1:A:98:ARG:CD	1:C:99:TRP:CZ2	2.76	0.68
1:B:63:VAL:CG1	1:B:120:LEU:HD21	2.23	0.68
1:B:73:MET:HE3	1:B:74:LEU:HD23	1.75	0.68
1:C:210:ASN:OD1	1:D:203:THR:HG23	1.94	0.68
1:C:223:GLN:CB	1:C:235:PHE:CE2	2.60	0.68
1:B:112:ILE:O	1:B:112:ILE:HG22	1.92	0.68
1:A:41:THR:CA	1:A:195:LYS:HE2	2.23	0.68
1:B:221:THR:O	1:B:221:THR:CG2	2.35	0.68
1:C:45:LYS:HD2	1:C:73:MET:SD	2.33	0.68
1:C:223:GLN:HG3	1:C:235:PHE:CZ	2.29	0.68
1:A:192:ILE:CD1	1:A:270:PHE:CE1	2.77	0.68
1:C:86:ALA:HB2	2:C:3301:SAH:C2	2.23	0.68
1:C:67:THR:HG23	1:C:90:MET:CE	2.24	0.68
1:C:133:VAL:O	1:C:170:LEU:HA	1.94	0.68
1:D:99:TRP:CZ3	1:D:102:ARG:HD3	2.29	0.68
1:D:224:VAL:HG22	1:D:224:VAL:O	1.93	0.68
1:A:224:VAL:CG1	1:A:234:GLY:C	2.67	0.68
1:B:75:VAL:CG2	1:B:81:VAL:HG11	2.21	0.68
1:B:217:THR:HG23	1:B:241:SER:OG	1.93	0.68
1:D:77:GLU:HB3	1:D:79:PHE:CE1	2.28	0.68
1:A:117:TRP:CZ3	1:A:140:PHE:HA	2.29	0.68
1:C:220:TYR:O	1:C:237:LYS:HB3	1.94	0.68
1:B:73:MET:CE	1:B:74:LEU:HD21	2.23	0.68
1:D:95:LEU:CD1	1:D:112:ILE:HG21	2.23	0.68
1:A:41:THR:O	1:A:41:THR:HG22	1.93	0.67
1:A:254:VAL:CG1	1:A:255:GLN:N	2.57	0.67
1:C:82:THR:HG21	1:C:130:PHE:CE2	2.29	0.67
1:C:207:LEU:HD12	1:C:208:THR:H	1.59	0.67
1:B:99:TRP:O	1:B:102:ARG:HD3	1.95	0.67
1:B:200:LYS:HD2	1:B:200:LYS:O	1.93	0.67
1:A:217:THR:CG2	1:A:239:ARG:HH11	2.06	0.67
1:B:186:ALA:O	1:B:188:PRO:HD3	1.93	0.67
1:A:82:THR:HG21	1:A:130:PHE:CE2	2.25	0.67
1:B:207:LEU:HD23	1:B:214:HIS:HB3	1.75	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TRP:CE3	1:C:48:LEU:N	2.63	0.67
1:C:207:LEU:HD12	1:C:208:THR:N	2.09	0.67
1:D:136:LEU:HD13	1:D:171:VAL:O	1.94	0.67
1:C:49:LEU:HD11	1:C:73:MET:HE3	1.77	0.67
1:D:165:ARG:HG3	1:D:165:ARG:NH2	2.01	0.67
1:A:154:ARG:HG3	1:A:154:ARG:NH1	2.02	0.67
1:C:164:VAL:CG1	1:C:168:GLY:HA3	2.23	0.67
1:D:256:GLU:HG2	1:D:257:ALA:N	2.10	0.67
1:B:261:ARG:HD3	1:B:292:GLY:CA	2.21	0.67
1:B:254:VAL:CG1	1:B:255:GLN:N	2.58	0.67
1:D:158:LYS:NZ	3:D:4355:HOH:O	2.27	0.67
1:D:227:ALA:H	1:D:233:PRO:HA	1.59	0.67
1:A:98:ARG:NH1	1:A:112:ILE:HD12	2.10	0.66
1:B:215:MET:HA	1:B:244:PRO:HD3	1.77	0.66
1:C:111:VAL:CG1	1:C:112:ILE:N	2.59	0.66
1:D:175:LYS:HD2	1:D:282:CYS:O	1.95	0.66
1:A:219:ASP:OD1	1:A:239:ARG:HB2	1.95	0.66
1:B:149:ASP:C	1:B:151:SER:H	2.03	0.66
1:C:267:LEU:HD13	1:C:267:LEU:N	2.11	0.66
1:A:268:GLY:O	1:A:269:ASP:C	2.38	0.66
1:B:136:LEU:HA	1:B:173:ASP:OD2	1.95	0.66
1:C:281:PRO:C	1:C:282:CYS:SG	2.78	0.66
1:B:111:VAL:CG1	1:B:112:ILE:N	2.58	0.66
1:D:90:MET:HG3	2:D:4301:SAH:C3'	2.25	0.66
1:A:146:SER:HB2	1:A:152:GLU:OE1	1.95	0.66
1:D:254:VAL:CG1	1:D:255:GLN:N	2.59	0.66
1:B:108:ASP:O	1:B:108:ASP:OD2	2.13	0.66
1:D:95:LEU:HD11	1:D:112:ILE:CG2	2.25	0.66
1:B:155:LEU:CD1	1:B:158:LYS:HZ2	2.09	0.66
1:C:176:ASN:HD21	1:C:178:ASP:HB2	1.61	0.66
1:A:101:ARG:CZ	1:A:107:PHE:CE1	2.79	0.66
1:C:220:TYR:HB2	1:C:238:PHE:CE1	2.30	0.66
1:A:61:LEU:HD12	1:A:61:LEU:C	2.20	0.66
1:B:136:LEU:HD11	1:B:171:VAL:HB	1.77	0.66
1:B:168:GLY:O	1:B:289:LYS:HA	1.96	0.66
1:C:193:TYR:CB	1:C:194:TYR:HD1	2.09	0.66
1:C:140:PHE:CD2	1:C:250:PHE:HE1	2.13	0.65
1:A:61:LEU:HB2	1:A:130:PHE:CE2	2.31	0.65
1:C:247:LEU:HD12	1:C:251:THR:OG1	1.96	0.65
1:C:191:ASN:OD1	1:C:193:TYR:HB2	1.96	0.65
1:A:191:ASN:HD21	1:A:194:TYR:HD2	1.43	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LEU:CD1	1:D:286:HIS:CE1	2.79	0.65
1:D:267:LEU:HD12	1:D:267:LEU:H	1.61	0.65
1:A:95:LEU:CD1	1:A:112:ILE:CD1	2.63	0.65
1:B:49:LEU:O	1:B:53:ARG:HG2	1.97	0.65
1:C:61:LEU:HD23	1:C:133:VAL:HG13	1.79	0.65
1:C:44:TYR:O	1:C:44:TYR:CD1	2.50	0.65
1:D:149:ASP:C	1:D:151:SER:H	2.05	0.65
1:A:161:ALA:O	1:A:164:VAL:HG23	1.96	0.65
1:A:165:ARG:O	1:A:165:ARG:HG2	1.97	0.65
1:D:192:ILE:HG21	1:D:269:ASP:OD1	1.96	0.65
1:B:101:ARG:NE	1:B:107:PHE:CE1	2.65	0.65
1:C:130:PHE:HB2	1:C:163:MET:O	1.97	0.65
1:D:60:VAL:HG12	1:D:132:ALA:HB3	1.78	0.65
1:A:265:SER:O	1:A:287:VAL:HG22	1.97	0.64
1:B:95:LEU:HD13	1:B:112:ILE:CG2	2.21	0.64
1:C:50:GLY:O	1:C:54:GLN:HB3	1.97	0.64
1:D:204:THR:HA	1:D:218:LEU:CD1	2.23	0.64
1:A:209:VAL:O	1:A:209:VAL:CG1	2.45	0.64
1:A:254:VAL:HG13	1:A:255:GLN:N	2.11	0.64
1:B:75:VAL:HG22	1:B:81:VAL:CG1	2.22	0.64
1:C:49:LEU:CD1	1:C:73:MET:HE3	2.26	0.64
1:A:190:LYS:NZ	1:A:191:ASN:H	1.94	0.64
1:A:60:VAL:HG12	1:A:132:ALA:O	1.98	0.64
1:A:209:VAL:O	1:A:209:VAL:HG13	1.98	0.64
1:B:98:ARG:CZ	1:D:99:TRP:CE2	2.81	0.64
1:B:134:ILE:HB	1:B:136:LEU:HD21	1.80	0.64
1:B:277:GLN:HG2	1:B:277:GLN:O	1.96	0.64
1:A:191:ASN:HB3	3:A:1310:HOH:O	1.97	0.64
1:A:280:VAL:HG13	1:A:280:VAL:O	1.96	0.64
1:C:223:GLN:HE22	1:C:225:PRO:HG3	1.62	0.64
1:A:138:ASN:ND2	1:A:175:LYS:HB2	2.13	0.64
1:B:101:ARG:O	1:B:107:PHE:HB2	1.98	0.64
1:B:48:LEU:CD2	1:B:73:MET:HE1	2.27	0.64
1:B:72:ILE:HG13	1:B:110:TRP:CH2	2.32	0.64
1:C:109:LYS:N	1:C:109:LYS:CD	2.61	0.64
1:A:133:VAL:O	1:A:170:LEU:HD12	1.97	0.64
1:A:251:THR:HG23	1:A:286:HIS:HE1	1.62	0.64
1:B:101:ARG:NE	1:B:107:PHE:CZ	2.66	0.64
1:B:243:TYR:CD2	1:B:245:HIS:CD2	2.86	0.64
1:C:143:LEU:CD1	1:C:144:PRO:CD	2.76	0.64
1:D:110:TRP:CH2	1:D:112:ILE:HD11	2.33	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ALA:HB1	1:A:130:PHE:CE1	2.32	0.63
1:B:157:LEU:HD13	1:B:160:ILE:HD12	1.79	0.63
1:B:73:MET:CE	1:B:74:LEU:HD23	2.29	0.63
1:A:136:LEU:HD11	1:A:171:VAL:HG11	1.79	0.63
1:A:173:ASP:OD1	1:A:193:TYR:HE1	1.81	0.63
1:B:155:LEU:CD1	1:B:158:LYS:NZ	2.60	0.63
1:D:170:LEU:HD12	1:D:171:VAL:N	2.13	0.63
1:A:92:LYS:HG2	1:A:93:TYR:CD2	2.33	0.63
1:C:112:ILE:O	1:C:113:GLU:HG2	1.98	0.63
1:A:75:VAL:HG23	1:A:81:VAL:HG11	1.81	0.63
1:D:247:LEU:HD12	1:D:251:THR:OG1	1.99	0.63
1:A:92:LYS:HD3	1:A:93:TYR:CE2	2.34	0.63
1:D:51:LEU:CD1	1:D:55:HIS:ND1	2.61	0.63
1:C:119:THR:HG1	1:C:123:ASP:CG	2.06	0.63
1:D:174:HIS:O	1:D:174:HIS:CD2	2.51	0.63
1:A:251:THR:HG23	1:A:264:HIS:CE1	2.34	0.63
1:D:225:PRO:C	1:D:233:PRO:HB3	2.24	0.63
1:A:188:PRO:CG	1:A:202:ILE:HD12	2.29	0.62
1:A:121:ASP:CG	1:A:122:LYS:N	2.55	0.62
1:C:75:VAL:CG1	1:C:107:PHE:CE1	2.83	0.62
1:C:143:LEU:HD13	1:C:144:PRO:HD2	1.80	0.62
1:C:44:TYR:CD1	1:C:44:TYR:C	2.77	0.62
1:C:215:MET:HE3	3:C:3394:HOH:O	1.98	0.62
1:D:174:HIS:CD2	1:D:174:HIS:C	2.77	0.62
1:D:175:LYS:HB2	1:D:177:TYR:CE2	2.34	0.62
1:A:99:TRP:CZ3	1:A:102:ARG:HD3	2.34	0.62
1:C:111:VAL:O	1:C:112:ILE:HG12	1.99	0.62
1:A:41:THR:N	1:A:194:TYR:HA	2.15	0.62
1:C:85:ASP:HB2	1:C:91:LEU:HD13	1.81	0.62
1:B:220:TYR:HD1	1:B:238:PHE:CZ	2.18	0.62
1:D:263:GLN:NE2	1:D:291:THR:CG2	2.60	0.62
1:C:107:PHE:HD1	1:C:107:PHE:N	1.97	0.62
1:D:140:PHE:CE1	1:D:157:LEU:HD22	2.35	0.62
1:D:220:TYR:CB	1:D:238:PHE:HE1	2.08	0.62
1:B:177:TYR:HA	1:B:180:ILE:HB	1.82	0.62
1:C:119:THR:HB	1:C:122:LYS:HD3	1.80	0.62
1:C:165:ARG:CG	1:C:165:ARG:NH2	2.50	0.62
1:A:122:LYS:CE	1:A:122:LYS:CA	2.67	0.61
1:B:100:ASN:C	1:B:102:ARG:H	2.08	0.61
1:B:268:GLY:O	1:B:269:ASP:C	2.43	0.61
1:D:193:TYR:HB3	1:D:194:TYR:CE1	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:GLN:O	1:D:258:PHE:HB2	1.99	0.61
1:B:178:ASP:OD2	1:B:246:CYS:HA	2.01	0.61
1:D:75:VAL:HG12	1:D:76:GLU:N	2.15	0.61
1:D:238:PHE:CG	1:D:238:PHE:O	2.52	0.61
1:D:263:GLN:HB2	1:D:289:LYS:HB3	1.81	0.61
1:C:225:PRO:CA	1:C:233:PRO:CB	2.62	0.61
1:B:69:VAL:HG23	1:B:70:ASP:N	2.15	0.61
1:A:101:ARG:O	1:A:104:GLU:HG3	2.00	0.61
1:B:261:ARG:CD	1:B:292:GLY:HA3	2.23	0.61
1:C:72:ILE:O	1:C:75:VAL:HB	2.01	0.61
1:C:101:ARG:HD3	1:C:107:PHE:HE2	1.63	0.61
1:D:258:PHE:HE2	1:D:288:LEU:HG	1.65	0.61
1:A:142:HIS:HE1	2:A:1301:SAH:HG2	1.58	0.61
1:A:264:HIS:CD2	1:A:265:SER:N	2.69	0.61
1:C:117:TRP:CG	1:C:160:ILE:HD11	2.36	0.61
1:D:77:GLU:HB3	1:D:79:PHE:CD1	2.35	0.61
1:A:207:LEU:HD12	1:A:208:THR:H	1.65	0.61
1:C:261:ARG:CG	1:C:292:GLY:HA3	2.18	0.61
1:B:190:LYS:CE	1:B:190:LYS:HA	2.30	0.61
1:A:192:ILE:CG1	1:A:270:PHE:HE1	2.04	0.60
2:A:1301:SAH:H5'2	2:A:1301:SAH:N	2.16	0.60
1:C:82:THR:CG2	1:C:130:PHE:HE2	2.14	0.60
1:C:140:PHE:CE2	1:C:250:PHE:CE1	2.87	0.60
1:C:223:GLN:NE2	1:C:225:PRO:CD	2.60	0.60
1:D:86:ALA:CB	2:D:4301:SAH:C2	2.79	0.60
1:A:177:TYR:HA	1:A:180:ILE:HB	1.82	0.60
1:C:69:VAL:HG11	1:C:194:TYR:CE2	2.36	0.60
1:C:89:LYS:O	1:C:93:TYR:HD2	1.84	0.60
1:C:120:LEU:CD2	1:C:160:ILE:HA	2.30	0.60
1:C:223:GLN:NE2	1:C:225:PRO:CG	2.63	0.60
1:A:108:ASP:OD2	1:A:109:LYS:HE3	2.01	0.60
1:A:151:SER:O	1:A:154:ARG:HB2	2.00	0.60
1:C:108:ASP:O	1:C:109:LYS:HD2	2.00	0.60
1:A:117:TRP:CH2	1:A:140:PHE:HA	2.36	0.60
1:B:188:PRO:CB	1:B:202:ILE:CD1	2.72	0.60
1:B:227:ALA:CB	1:B:234:GLY:HA3	2.28	0.60
1:D:87:SER:OG	1:D:90:MET:HB2	2.02	0.60
1:A:99:TRP:O	1:A:102:ARG:HB3	2.00	0.60
1:B:57:CYS:SG	1:B:169:LEU:HD22	2.41	0.60
1:C:48:LEU:HD23	1:C:73:MET:CE	2.32	0.60
1:C:184:GLY:O	1:C:185:CYS:SG	2.57	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:THR:HA	1:D:237:LYS:HA	1.81	0.60
1:C:108:ASP:C	1:C:109:LYS:CD	2.72	0.60
1:C:224:VAL:CG2	1:C:227:ALA:H	2.10	0.60
1:A:82:THR:CG2	1:A:130:PHE:HE2	2.10	0.60
1:C:105:PRO:HB2	3:C:3341:HOH:O	2.01	0.60
1:D:95:LEU:HD13	1:D:112:ILE:HG21	1.83	0.60
1:D:107:PHE:HD1	1:D:107:PHE:H	1.49	0.60
1:B:45:LYS:O	1:B:49:LEU:HD22	2.02	0.60
1:C:120:LEU:HD23	1:C:159:ASN:C	2.26	0.60
1:C:183:THR:HG22	1:C:183:THR:O	2.01	0.60
1:A:86:ALA:HB2	2:A:1301:SAH:C2	2.31	0.60
1:B:43:GLU:HB3	3:B:2390:HOH:O	2.01	0.60
1:B:209:VAL:O	1:B:209:VAL:CG1	2.49	0.60
1:D:155:LEU:HD12	1:D:158:LYS:HE2	1.84	0.60
1:D:136:LEU:HD11	1:D:171:VAL:HG12	0.77	0.60
1:A:269:ASP:O	1:A:270:PHE:CD2	2.56	0.59
1:C:82:THR:HG21	1:C:130:PHE:HE2	1.66	0.59
1:A:288:LEU:CD2	1:A:288:LEU:N	2.65	0.59
1:A:99:TRP:O	1:A:102:ARG:HG2	2.02	0.59
1:A:267:LEU:C	1:A:268:GLY:O	2.39	0.59
1:B:192:ILE:HD13	1:B:269:ASP:OD1	2.02	0.59
1:B:229:ARG:HE	1:B:229:ARG:CA	2.08	0.59
1:B:63:VAL:HB	1:B:117:TRP:HE1	1.67	0.59
1:D:49:LEU:HD11	1:D:73:MET:CE	2.32	0.59
1:D:133:VAL:HG21	1:D:164:VAL:CG2	2.31	0.59
1:A:142:HIS:CE1	2:A:1301:SAH:CG	2.83	0.59
1:B:193:TYR:CE1	1:B:283:TYR:CD2	2.89	0.59
1:C:117:TRP:CH2	1:C:140:PHE:HA	2.38	0.59
1:D:95:LEU:CD1	1:D:112:ILE:CG2	2.80	0.59
1:A:128:ASP:O	1:A:165:ARG:HB2	2.02	0.59
1:A:193:TYR:C	1:A:194:TYR:CG	2.79	0.59
1:A:229:ARG:N	1:A:232:ALA:HB3	2.17	0.59
1:B:177:TYR:HB2	1:B:245:HIS:O	2.02	0.59
1:C:97:GLU:N	1:C:97:GLU:OE2	2.35	0.59
1:C:277:GLN:HG3	1:C:278:ALA:N	2.18	0.59
1:D:87:SER:HB3	2:D:4301:SAH:O2'	2.02	0.59
1:B:98:ARG:HH22	1:D:99:TRP:CD1	2.20	0.59
1:D:134:ILE:HB	1:D:136:LEU:HD23	1.82	0.59
1:D:157:LEU:CD1	1:D:172:ILE:CD1	2.80	0.59
1:A:270:PHE:CE2	1:A:285:ILE:CD1	2.86	0.59
1:B:254:VAL:HG12	1:B:255:GLN:N	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASP:C	1:C:202:ILE:CG1	2.75	0.59
1:A:47:TRP:CE3	1:A:48:LEU:N	2.71	0.58
1:A:77:GLU:CB	1:A:79:PHE:CE1	2.77	0.58
1:C:89:LYS:O	1:C:93:TYR:CD2	2.56	0.58
1:C:178:ASP:OD1	1:C:246:CYS:HB3	2.03	0.58
1:C:202:ILE:HD13	1:C:220:TYR:CE2	2.38	0.58
1:D:95:LEU:HD13	1:D:112:ILE:HD13	1.85	0.58
1:A:60:VAL:CG1	1:A:132:ALA:HB3	2.23	0.58
1:A:74:LEU:O	1:A:79:PHE:HD1	1.86	0.58
1:C:107:PHE:N	1:C:107:PHE:CD1	2.68	0.58
1:D:172:ILE:CG2	1:D:250:PHE:HE2	2.16	0.58
1:D:172:ILE:CG2	1:D:172:ILE:O	2.50	0.58
1:D:279:TYR:O	1:D:281:PRO:HD3	2.02	0.58
1:A:91:LEU:HD11	1:A:112:ILE:HG22	1.83	0.58
1:A:145:ASP:O	1:A:145:ASP:OD2	2.21	0.58
1:B:98:ARG:HG2	1:B:99:TRP:N	2.18	0.58
1:B:172:ILE:CG2	1:B:172:ILE:O	2.51	0.58
1:C:206:VAL:H	1:D:208:THR:HG22	1.67	0.58
1:D:71:SER:OG	1:D:83:SER:HB3	2.01	0.58
1:A:207:LEU:HD12	1:B:206:VAL:O	2.04	0.58
1:B:88:ASP:OD1	1:B:88:ASP:N	2.36	0.58
1:C:48:LEU:HD23	1:C:73:MET:HE1	1.85	0.58
1:A:251:THR:HG23	1:A:286:HIS:CE1	2.38	0.58
1:B:111:VAL:O	1:B:112:ILE:HG13	2.04	0.58
1:B:129:GLY:C	1:B:165:ARG:HB3	2.28	0.58
1:C:44:TYR:CB	1:C:270:PHE:CE1	2.85	0.58
1:C:178:ASP:O	1:C:181:LEU:HB2	2.02	0.58
1:C:179:TYR:CD1	1:C:179:TYR:C	2.80	0.58
1:D:93:TYR:HA	1:D:96:LYS:HD2	1.84	0.58
1:D:122:LYS:HD3	1:D:122:LYS:O	2.03	0.58
1:D:263:GLN:HE21	1:D:291:THR:HG21	1.66	0.58
1:A:61:LEU:HB2	1:A:130:PHE:CD2	2.38	0.58
1:B:111:VAL:HG12	1:B:112:ILE:N	2.19	0.58
1:C:192:ILE:O	1:C:192:ILE:HG13	2.03	0.58
1:C:261:ARG:O	1:C:262:CYS:HB3	2.02	0.58
1:D:72:ILE:HG12	1:D:110:TRP:CH2	2.38	0.58
1:A:173:ASP:OD1	1:A:193:TYR:CE1	2.57	0.58
1:B:193:TYR:HE1	1:B:283:TYR:CG	2.21	0.58
1:A:193:TYR:C	1:A:194:TYR:CD2	2.82	0.58
1:C:173:ASP:OD1	1:C:173:ASP:C	2.46	0.58
1:D:264:HIS:HE1	1:D:286:HIS:ND1	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:NZ	1:B:149:ASP:CG	2.62	0.58
1:D:55:HIS:ND1	1:D:169:LEU:HD21	2.19	0.58
1:B:147:LYS:HZ2	1:B:149:ASP:CG	2.12	0.57
1:C:135:CYS:HB3	1:C:172:ILE:HG12	1.84	0.57
1:C:176:ASN:C	1:C:176:ASN:HD22	2.11	0.57
1:C:268:GLY:CA	1:C:273:TYR:HB2	2.34	0.57
1:D:206:VAL:HG22	1:D:216:VAL:HG22	1.84	0.57
1:A:91:LEU:CD1	1:A:112:ILE:HG21	2.34	0.57
1:A:98:ARG:NH2	1:C:99:TRP:CE2	2.72	0.57
1:D:105:PRO:O	1:D:108:ASP:HB3	2.04	0.57
1:C:136:LEU:HG	1:C:193:TYR:OH	2.04	0.57
1:B:98:ARG:NH2	1:D:99:TRP:CE2	2.72	0.57
1:C:198:LEU:CD2	1:C:222:VAL:HG13	2.34	0.57
1:D:49:LEU:CD1	1:D:73:MET:HE1	2.29	0.57
1:D:49:LEU:HD13	1:D:73:MET:CE	2.30	0.57
1:D:158:LYS:HA	1:D:257:ALA:CB	2.27	0.57
1:B:176:ASN:HD21	1:B:179:TYR:H	1.52	0.57
1:B:219:ASP:HA	1:B:239:ARG:HB2	1.86	0.57
1:C:73:MET:HG2	1:C:74:LEU:N	2.20	0.57
1:C:97:GLU:OE2	1:C:97:GLU:CA	2.50	0.57
1:D:49:LEU:HD21	1:D:77:GLU:HG2	1.86	0.57
1:A:122:LYS:HA	1:A:122:LYS:HZ1	1.58	0.57
1:A:170:LEU:HD23	1:A:258:PHE:CZ	2.39	0.57
1:B:176:ASN:OD1	1:B:284:PHE:CE1	2.58	0.57
1:C:170:LEU:HD23	1:C:288:LEU:HD23	1.85	0.57
1:C:41:THR:HB	1:C:44:TYR:HD2	1.70	0.57
1:C:247:LEU:CD1	1:C:251:THR:OG1	2.52	0.57
1:D:75:VAL:CG2	1:D:81:VAL:CG2	2.78	0.57
1:D:175:LYS:NZ	1:D:283:TYR:CZ	2.72	0.57
1:A:264:HIS:CD2	1:A:264:HIS:C	2.82	0.57
1:A:264:HIS:HE1	1:A:286:HIS:ND1	2.01	0.57
1:C:111:VAL:HG12	1:C:112:ILE:N	2.19	0.57
1:D:247:LEU:HD21	1:D:266:VAL:HG21	1.85	0.57
1:A:223:GLN:OE1	1:A:233:PRO:HG2	2.05	0.57
1:A:81:VAL:O	1:A:81:VAL:CG1	2.53	0.56
1:A:81:VAL:O	1:A:81:VAL:HG13	2.05	0.56
1:A:164:VAL:HG11	1:A:168:GLY:O	2.05	0.56
1:A:211:ASN:ND2	1:B:184:GLY:CA	2.59	0.56
1:B:237:LYS:HG3	1:B:238:PHE:N	2.17	0.56
1:C:82:THR:CG2	1:C:130:PHE:CE2	2.88	0.56
1:C:99:TRP:CE2	1:C:102:ARG:NH1	2.72	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:LEU:HD12	1:D:247:LEU:O	2.04	0.56
1:C:207:LEU:HD23	1:C:215:MET:HE2	1.87	0.56
1:A:130:PHE:CD1	1:A:130:PHE:N	2.73	0.56
1:A:261:ARG:CD	1:A:292:GLY:CA	2.71	0.56
1:B:190:LYS:HA	1:B:190:LYS:HE2	1.87	0.56
1:B:278:ALA:HB2	3:B:2325:HOH:O	2.05	0.56
1:D:254:VAL:HG13	1:D:255:GLN:N	2.20	0.56
1:A:228:GLY:CA	1:A:232:ALA:HB3	2.27	0.56
1:B:258:PHE:C	1:B:260:GLY:H	2.14	0.56
1:D:51:LEU:HD11	1:D:169:LEU:HD21	1.86	0.56
1:D:91:LEU:HD21	1:D:113:GLU:C	2.31	0.56
1:A:268:GLY:O	1:A:270:PHE:N	2.38	0.56
1:B:133:VAL:CG2	1:B:164:VAL:HG22	2.35	0.56
1:D:178:ASP:OD2	1:D:246:CYS:HA	2.05	0.56
1:A:157:LEU:HD11	1:A:172:ILE:HD13	1.87	0.56
1:A:183:THR:O	1:A:183:THR:HG23	2.05	0.56
1:B:86:ALA:HB2	1:B:115:ALA:O	2.06	0.56
1:C:85:ASP:HB2	1:C:91:LEU:CD1	2.34	0.56
1:C:277:GLN:CG	1:C:278:ALA:N	2.69	0.56
1:D:228:GLY:HA3	1:D:232:ALA:CB	2.34	0.56
1:D:193:TYR:O	1:D:194:TYR:CD2	2.59	0.56
1:B:117:TRP:CE2	2:B:2301:SAH:C2	2.89	0.56
1:C:95:LEU:CD1	1:C:112:ILE:HB	2.33	0.56
1:C:135:CYS:CB	1:C:172:ILE:CG1	2.74	0.56
1:A:258:PHE:C	1:A:260:GLY:H	2.12	0.55
1:A:273:TYR:C	1:A:273:TYR:CD2	2.83	0.55
1:D:99:TRP:CE2	1:D:102:ARG:NH2	2.73	0.55
1:B:55:HIS:CD2	1:B:169:LEU:HD21	2.41	0.55
1:C:98:ARG:NH1	1:C:111:VAL:HA	2.22	0.55
1:D:269:ASP:O	1:D:270:PHE:CG	2.58	0.55
1:A:165:ARG:HH21	1:A:165:ARG:CG	2.20	0.55
1:A:217:THR:CG2	1:A:239:ARG:NH1	2.59	0.55
1:B:193:TYR:O	1:B:194:TYR:CD1	2.60	0.55
1:D:192:ILE:HG12	1:D:283:TYR:CD1	2.40	0.55
1:A:62:ASP:HB3	1:A:83:SER:HB3	1.88	0.55
1:A:102:ARG:NH2	1:A:102:ARG:CG	2.54	0.55
1:C:220:TYR:CB	1:C:238:PHE:CE1	2.89	0.55
1:C:243:TYR:CD2	1:C:244:PRO:O	2.59	0.55
1:C:269:ASP:O	1:C:285:ILE:HG13	2.06	0.55
1:D:143:LEU:HD12	1:D:143:LEU:C	2.31	0.55
1:A:44:TYR:CD2	1:A:193:TYR:O	2.60	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASP:CB	1:A:193:TYR:OH	2.54	0.55
1:B:225:PRO:O	1:B:233:PRO:CA	2.55	0.55
1:C:223:GLN:NE2	1:C:225:PRO:HD3	2.02	0.55
1:D:227:ALA:CB	1:D:234:GLY:N	2.50	0.55
1:B:76:GLU:C	1:B:78:GLY:H	2.15	0.55
1:B:63:VAL:HG23	1:B:135:CYS:HB2	1.89	0.55
1:B:254:VAL:HG11	1:B:264:HIS:CE1	2.42	0.55
1:B:266:VAL:HG22	1:B:266:VAL:O	2.07	0.55
1:C:281:PRO:O	1:C:282:CYS:SG	2.65	0.55
1:B:136:LEU:H	1:B:136:LEU:CD2	2.18	0.55
1:B:191:ASN:OD1	1:B:193:TYR:HB2	2.06	0.55
1:C:101:ARG:NH2	1:C:104:GLU:OE1	2.39	0.55
1:C:222:VAL:HG12	1:C:223:GLN:N	2.22	0.55
1:C:223:GLN:HB2	1:C:235:PHE:CD2	2.36	0.55
1:C:264:HIS:HB2	1:C:288:LEU:CD1	2.34	0.55
1:C:267:LEU:N	1:C:267:LEU:CD1	2.69	0.55
1:D:51:LEU:CD1	1:D:55:HIS:CE1	2.90	0.55
1:A:267:LEU:HD23	1:A:267:LEU:H	1.63	0.55
1:C:183:THR:O	1:C:183:THR:CG2	2.55	0.55
1:D:110:TRP:CZ2	1:D:112:ILE:HD11	2.42	0.55
1:A:91:LEU:CD1	1:A:112:ILE:HG22	2.36	0.55
1:A:130:PHE:N	1:A:130:PHE:HD1	2.05	0.55
1:A:134:ILE:HB	1:A:136:LEU:HD22	1.88	0.55
1:A:138:ASN:H	1:A:173:ASP:CG	2.14	0.55
1:B:218:LEU:HD13	1:B:218:LEU:N	2.21	0.55
1:C:69:VAL:CG1	1:C:194:TYR:HE2	2.20	0.55
1:D:165:ARG:CG	1:D:165:ARG:NH2	2.56	0.55
1:A:188:PRO:HG3	1:A:202:ILE:HD12	1.88	0.54
1:D:195:LYS:HB3	1:D:195:LYS:HZ3	1.72	0.54
1:D:210:ASN:O	1:D:211:ASN:HB3	2.05	0.54
1:A:98:ARG:HH11	1:A:112:ILE:H	1.54	0.54
1:A:126:ALA:O	1:A:127:GLY:C	2.51	0.54
1:A:224:VAL:HG11	1:A:234:GLY:HA3	1.88	0.54
1:B:140:PHE:CE1	1:B:157:LEU:HD22	2.41	0.54
1:B:229:ARG:HA	1:B:229:ARG:NE	2.18	0.54
1:C:74:LEU:O	1:C:79:PHE:HB2	2.08	0.54
1:C:112:ILE:C	1:C:113:GLU:HG2	2.33	0.54
1:D:173:ASP:OD2	1:D:193:TYR:CE1	2.60	0.54
1:D:193:TYR:C	1:D:194:TYR:CG	2.85	0.54
1:C:41:THR:CG2	1:C:44:TYR:N	2.58	0.54
1:C:44:TYR:CD1	1:C:270:PHE:CZ	2.95	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TRP:CZ3	1:A:48:LEU:HB2	2.43	0.54
1:A:101:ARG:CZ	1:A:107:PHE:CZ	2.91	0.54
1:A:280:VAL:O	1:A:280:VAL:CG1	2.56	0.54
1:B:101:ARG:HB3	1:B:107:PHE:CD1	2.42	0.54
1:C:165:ARG:O	1:C:166:PRO:C	2.48	0.54
1:D:48:LEU:O	1:D:49:LEU:C	2.51	0.54
1:D:86:ALA:HB2	2:D:4301:SAH:C2	2.38	0.54
1:D:126:ALA:HB2	1:D:163:MET:CE	2.37	0.54
1:B:99:TRP:O	1:B:102:ARG:CB	2.56	0.54
1:B:258:PHE:H	1:B:258:PHE:HD2	1.55	0.54
1:B:263:GLN:HB2	1:B:289:LYS:HB3	1.89	0.54
1:C:101:ARG:CD	1:C:107:PHE:CE2	2.88	0.54
1:C:223:GLN:HG2	1:C:224:VAL:N	2.23	0.54
1:D:51:LEU:O	1:D:54:GLN:HG2	2.06	0.54
1:D:140:PHE:C	1:D:142:HIS:H	2.16	0.54
1:A:172:ILE:HG21	1:A:250:PHE:CE2	2.39	0.54
1:B:267:LEU:C	1:B:268:GLY:O	2.47	0.54
1:C:264:HIS:HA	1:C:288:LEU:CD1	2.38	0.54
1:A:231:GLY:O	1:A:232:ALA:C	2.51	0.54
1:C:227:ALA:HB3	1:C:234:GLY:H	1.72	0.54
1:B:176:ASN:ND2	1:B:179:TYR:HB3	2.23	0.53
1:C:149:ASP:C	1:C:151:SER:H	2.16	0.53
1:D:170:LEU:HB3	1:D:288:LEU:HB2	1.90	0.53
1:D:267:LEU:N	1:D:267:LEU:CD1	2.68	0.53
1:D:238:PHE:CD1	1:D:238:PHE:O	2.61	0.53
1:A:61:LEU:CD2	1:A:163:MET:SD	2.96	0.53
1:C:223:GLN:CG	1:C:235:PHE:CZ	2.91	0.53
1:A:142:HIS:O	1:A:144:PRO:HD3	2.08	0.53
1:D:164:VAL:O	1:D:290:LYS:CE	2.56	0.53
1:D:164:VAL:HG12	1:D:168:GLY:HA3	1.90	0.53
1:D:172:ILE:CG2	1:D:250:PHE:CE2	2.91	0.53
1:A:154:ARG:HH11	1:A:154:ARG:HG2	1.65	0.53
1:B:137:GLY:H	1:B:173:ASP:CG	2.16	0.53
1:B:225:PRO:O	1:B:233:PRO:HA	2.08	0.53
1:D:51:LEU:HD11	1:D:55:HIS:CE1	2.43	0.53
1:D:85:ASP:CB	1:D:91:LEU:HD13	2.39	0.53
1:D:86:ALA:HB3	2:D:4301:SAH:C2	2.38	0.53
1:D:97:GLU:OE1	1:D:97:GLU:CA	2.56	0.53
1:D:149:ASP:O	1:D:151:SER:N	2.41	0.53
1:D:211:ASN:CG	1:D:211:ASN:O	2.51	0.53
1:A:220:TYR:O	1:A:237:LYS:CB	2.57	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:CE1	1:B:281:PRO:HG3	2.43	0.53
1:B:280:VAL:O	1:B:280:VAL:CG1	2.51	0.53
1:D:175:LYS:NZ	1:D:282:CYS:SG	2.82	0.53
1:A:98:ARG:CZ	1:A:112:ILE:HD12	2.39	0.53
1:A:287:VAL:C	1:A:288:LEU:HD23	2.33	0.53
1:B:261:ARG:HB3	1:B:292:GLY:CA	2.38	0.53
1:C:143:LEU:C	1:C:143:LEU:CD1	2.71	0.53
1:A:183:THR:HG22	1:A:185:CYS:H	1.74	0.53
1:C:149:ASP:CG	1:C:151:SER:HB3	2.34	0.53
1:C:266:VAL:HA	1:C:285:ILE:O	2.09	0.53
1:D:157:LEU:CD1	1:D:172:ILE:HD12	2.39	0.53
1:D:220:TYR:CG	1:D:238:PHE:CE1	2.96	0.53
1:C:179:TYR:HD1	1:C:180:ILE:N	2.07	0.53
1:D:200:LYS:CG	1:D:222:VAL:HG22	2.39	0.53
1:A:57:CYS:HB3	1:A:131:ASP:HB3	1.91	0.52
1:B:115:ALA:HA	1:B:123:ASP:OD2	2.09	0.52
1:B:218:LEU:CD2	1:B:242:TYR:CE2	2.92	0.52
1:B:225:PRO:O	1:B:233:PRO:CB	2.57	0.52
1:B:257:ALA:C	1:B:259:GLY:H	2.17	0.52
1:C:69:VAL:CG2	1:C:194:TYR:HE2	2.13	0.52
1:C:221:THR:HA	1:C:237:LYS:HB3	1.91	0.52
1:D:164:VAL:CG1	1:D:168:GLY:HA3	2.39	0.52
1:D:247:LEU:HD12	1:D:247:LEU:C	2.34	0.52
1:A:91:LEU:HD12	1:A:112:ILE:HG21	1.91	0.52
1:A:142:HIS:HE1	2:A:1301:SAH:SD	2.32	0.52
1:A:289:LYS:O	1:A:291:THR:HG23	2.09	0.52
1:B:224:VAL:CG1	1:B:234:GLY:O	2.58	0.52
1:D:49:LEU:HG	1:D:53:ARG:NH1	2.25	0.52
1:A:206:VAL:HG12	1:A:207:LEU:N	2.24	0.52
1:C:131:ASP:OD2	1:C:165:ARG:NE	2.43	0.52
1:D:177:TYR:CD1	1:D:180:ILE:HD12	2.45	0.52
1:D:193:TYR:HB3	1:D:194:TYR:CD1	2.45	0.52
1:A:41:THR:CA	1:A:195:LYS:NZ	2.60	0.52
1:B:57:CYS:HA	1:B:131:ASP:HB3	1.90	0.52
1:B:61:LEU:HB2	1:B:130:PHE:CD2	2.45	0.52
1:B:191:ASN:C	1:B:193:TYR:H	2.16	0.52
1:B:224:VAL:HG12	1:B:234:GLY:O	2.09	0.52
1:A:190:LYS:HE3	1:A:192:ILE:N	2.24	0.52
1:B:49:LEU:HD13	1:B:49:LEU:H	1.74	0.52
1:A:61:LEU:HD23	1:A:163:MET:SD	2.49	0.52
1:A:99:TRP:CD1	1:C:98:ARG:NH2	2.77	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLY:O	1:A:232:ALA:O	2.28	0.52
1:A:261:ARG:HG3	1:A:292:GLY:O	2.09	0.52
1:A:269:ASP:O	1:A:270:PHE:CG	2.62	0.52
1:B:110:TRP:CD1	1:B:111:VAL:N	2.78	0.52
1:C:122:LYS:HE2	1:C:123:ASP:OD2	2.10	0.52
1:C:220:TYR:O	1:C:237:LYS:CB	2.58	0.52
1:D:55:HIS:CE1	1:D:169:LEU:HD21	2.45	0.52
1:D:258:PHE:CE2	1:D:288:LEU:HG	2.45	0.52
1:A:154:ARG:NH1	1:A:154:ARG:HG2	2.25	0.52
1:C:108:ASP:HB3	1:C:109:LYS:HD3	1.90	0.52
1:D:51:LEU:HD12	1:D:51:LEU:O	2.08	0.52
1:D:183:THR:HG23	1:D:183:THR:O	2.09	0.52
1:A:111:VAL:O	1:A:111:VAL:HG12	2.10	0.52
1:A:122:LYS:HZ2	1:A:122:LYS:CA	2.09	0.52
1:A:142:HIS:HE1	2:A:1301:SAH:CG	2.21	0.52
1:C:47:TRP:CZ3	1:C:270:PHE:HE2	2.27	0.52
1:B:49:LEU:O	1:B:53:ARG:CG	2.57	0.52
1:C:254:VAL:O	1:C:257:ALA:HB3	2.09	0.52
1:D:259:GLY:C	1:D:261:ARG:H	2.18	0.52
1:A:60:VAL:CG1	1:A:132:ALA:O	2.58	0.51
1:A:224:VAL:HG22	1:A:226:GLY:H	1.74	0.51
1:B:88:ASP:O	1:B:89:LYS:C	2.53	0.51
1:B:99:TRP:O	1:B:102:ARG:CG	2.57	0.51
1:B:170:LEU:O	1:B:287:VAL:HA	2.10	0.51
1:B:220:TYR:CD1	1:B:238:PHE:CZ	2.97	0.51
1:C:50:GLY:O	1:C:54:GLN:CB	2.58	0.51
1:C:165:ARG:NH2	1:C:165:ARG:HG2	2.24	0.51
1:C:223:GLN:HG3	1:C:235:PHE:CE1	2.45	0.51
1:D:186:ALA:HB3	1:D:204:THR:OG1	2.09	0.51
1:D:223:GLN:O	1:D:225:PRO:HD3	2.10	0.51
1:C:145:ASP:O	1:C:145:ASP:CG	2.53	0.51
1:C:212:LYS:NZ	1:C:214:HIS:ND1	2.52	0.51
1:D:113:GLU:HA	1:D:113:GLU:OE1	2.10	0.51
1:D:210:ASN:N	1:D:210:ASN:HD22	2.07	0.51
1:D:247:LEU:HD22	1:D:284:PHE:CG	2.45	0.51
1:B:246:CYS:O	1:B:247:LEU:C	2.53	0.51
1:B:274:ARG:O	1:B:274:ARG:HG2	2.09	0.51
1:C:174:HIS:CD2	1:C:174:HIS:O	2.63	0.51
1:C:224:VAL:HG22	1:C:227:ALA:HB3	1.92	0.51
1:D:51:LEU:C	1:D:51:LEU:CD1	2.74	0.51
1:D:288:LEU:N	1:D:288:LEU:HD23	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:TRP:CE3	1:C:48:LEU:CA	2.93	0.51
1:D:71:SER:OG	1:D:83:SER:CB	2.58	0.51
1:A:172:ILE:HG22	1:A:286:HIS:HB2	1.92	0.51
1:A:251:THR:O	1:A:254:VAL:HG12	2.11	0.51
1:B:85:ASP:OD2	2:B:2301:SAH:H1'	2.10	0.51
1:B:140:PHE:CD2	1:B:250:PHE:HE1	2.28	0.51
1:B:164:VAL:HG12	1:B:168:GLY:HA3	1.93	0.51
1:D:173:ASP:OD2	1:D:193:TYR:HE1	1.92	0.51
1:C:203:THR:CG2	1:D:210:ASN:ND2	2.66	0.51
1:C:223:GLN:HE21	1:C:225:PRO:CG	2.23	0.51
1:D:200:LYS:HG2	1:D:222:VAL:HG22	1.92	0.51
1:B:247:LEU:HD12	1:B:286:HIS:HE2	1.75	0.51
1:C:222:VAL:CG1	1:C:223:GLN:N	2.73	0.51
1:D:269:ASP:O	1:D:270:PHE:CD2	2.63	0.51
1:A:114:GLU:O	1:A:115:ALA:HB2	2.10	0.51
1:B:95:LEU:HD12	1:B:112:ILE:HD13	1.92	0.51
1:B:258:PHE:N	1:B:258:PHE:CD2	2.78	0.51
1:C:140:PHE:CD2	1:C:250:PHE:CE1	2.97	0.51
1:D:175:LYS:CB	1:D:177:TYR:CE2	2.93	0.51
1:A:42:ALA:O	1:A:45:LYS:HB3	2.11	0.51
1:A:98:ARG:HD3	1:C:99:TRP:CH2	2.44	0.51
1:A:266:VAL:C	1:A:267:LEU:HD23	2.33	0.51
1:B:48:LEU:HD23	1:B:74:LEU:HD21	1.93	0.51
1:C:60:VAL:HA	1:C:132:ALA:O	2.11	0.51
1:C:67:THR:O	1:C:94:ALA:CB	2.56	0.51
1:A:41:THR:O	1:A:42:ALA:C	2.54	0.51
1:B:258:PHE:CD2	1:B:288:LEU:HD12	2.39	0.51
1:C:67:THR:C	1:C:94:ALA:HB2	2.35	0.51
1:B:63:VAL:CG2	1:B:135:CYS:HB2	2.41	0.50
1:C:198:LEU:CD2	1:C:222:VAL:HG11	2.22	0.50
1:D:41:THR:CB	1:D:44:TYR:HB3	2.39	0.50
1:D:57:CYS:SG	1:D:132:ALA:HB2	2.51	0.50
1:D:172:ILE:O	1:D:172:ILE:HG22	2.11	0.50
1:D:228:GLY:CA	1:D:232:ALA:HB3	2.39	0.50
1:A:193:TYR:O	1:A:194:TYR:CG	2.64	0.50
1:B:261:ARG:HB3	1:B:292:GLY:HA3	1.92	0.50
1:D:98:ARG:HB2	1:D:110:TRP:CE3	2.46	0.50
1:D:200:LYS:HD3	1:D:220:TYR:HB3	1.93	0.50
1:A:207:LEU:HD12	1:A:208:THR:N	2.26	0.50
1:C:147:LYS:HE3	1:C:149:ASP:OD2	2.12	0.50
1:A:223:GLN:OE1	1:A:233:PRO:CG	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HG13	1:C:110:TRP:CH2	2.45	0.50
1:D:65:CYS:O	1:D:65:CYS:SG	2.69	0.50
1:D:221:THR:CA	1:D:237:LYS:HG3	2.42	0.50
1:A:72:ILE:HG22	1:A:73:MET:N	2.27	0.50
1:B:98:ARG:NH2	1:D:99:TRP:CD1	2.79	0.50
1:D:41:THR:O	1:D:42:ALA:C	2.55	0.50
1:A:110:TRP:CD1	1:A:111:VAL:N	2.79	0.50
1:A:243:TYR:HD2	1:A:245:HIS:CD2	2.29	0.50
1:B:47:TRP:HH2	1:B:171:VAL:CG1	2.24	0.50
1:B:72:ILE:CG1	1:B:110:TRP:CH2	2.94	0.50
1:B:241:SER:C	1:B:242:TYR:HD2	2.13	0.50
1:C:254:VAL:HG13	1:C:255:GLN:N	2.27	0.50
1:C:273:TYR:O	1:C:274:ARG:CD	2.60	0.50
1:D:247:LEU:CD1	1:D:251:THR:OG1	2.59	0.50
1:A:72:ILE:CD1	1:A:110:TRP:HH2	2.23	0.50
1:A:237:LYS:CG	1:A:238:PHE:N	2.66	0.50
1:A:270:PHE:CE2	1:A:285:ILE:CG1	2.93	0.50
1:B:87:SER:OG	1:B:90:MET:HG3	2.11	0.50
1:B:192:ILE:HD11	1:B:283:TYR:HB2	1.94	0.50
1:B:258:PHE:CE1	1:B:288:LEU:HB3	2.47	0.50
1:A:98:ARG:NH2	1:C:99:TRP:NE1	2.59	0.50
1:C:145:ASP:OD2	1:C:145:ASP:C	2.54	0.50
1:B:168:GLY:O	1:B:169:LEU:CD1	2.60	0.50
1:B:277:GLN:O	1:B:277:GLN:CG	2.60	0.50
1:A:169:LEU:HD12	1:A:288:LEU:C	2.34	0.49
1:D:186:ALA:CB	1:D:204:THR:OG1	2.60	0.49
1:A:220:TYR:CD1	1:A:238:PHE:CE2	2.99	0.49
1:D:49:LEU:HD21	1:D:77:GLU:CG	2.43	0.49
1:D:202:ILE:HD13	1:D:220:TYR:CE2	2.43	0.49
1:A:176:ASN:C	1:A:176:ASN:ND2	2.49	0.49
1:A:192:ILE:HG13	1:A:270:PHE:CD1	2.43	0.49
1:A:246:CYS:O	1:A:247:LEU:C	2.55	0.49
1:B:61:LEU:HD12	1:B:82:THR:O	2.11	0.49
1:D:88:ASP:O	1:D:89:LYS:C	2.55	0.49
1:B:101:ARG:CZ	1:B:107:PHE:CZ	2.96	0.49
1:B:101:ARG:HD3	1:B:107:PHE:CZ	2.47	0.49
1:B:138:ASN:OD1	1:B:141:ALA:HB2	2.11	0.49
1:B:178:ASP:OD2	1:B:246:CYS:CA	2.60	0.49
1:C:85:ASP:O	1:C:91:LEU:HD22	2.12	0.49
1:D:141:ALA:O	1:D:242:TYR:HA	2.11	0.49
1:A:175:LYS:O	1:A:177:TYR:CD2	2.65	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:TYR:O	1:B:237:LYS:CB	2.59	0.49
1:B:95:LEU:CD1	1:B:112:ILE:CG2	2.84	0.49
1:B:141:ALA:O	1:B:242:TYR:CB	2.59	0.49
1:D:147:LYS:NZ	1:D:147:LYS:CB	2.56	0.49
1:A:86:ALA:CB	2:A:1301:SAH:C2	2.91	0.49
1:B:258:PHE:C	1:B:260:GLY:N	2.70	0.49
1:C:73:MET:O	1:C:74:LEU:C	2.55	0.49
1:D:49:LEU:HD11	1:D:73:MET:HE2	1.95	0.49
1:A:91:LEU:HD11	1:A:112:ILE:HG23	1.93	0.49
1:B:41:THR:HG22	1:B:41:THR:O	2.13	0.49
1:B:92:LYS:HD3	1:B:93:TYR:CE2	2.48	0.49
1:B:117:TRP:CD2	2:B:2301:SAH:N1	2.81	0.49
1:B:213:ALA:HB1	1:B:244:PRO:CG	2.43	0.49
1:C:87:SER:CB	2:C:3301:SAH:O2'	2.61	0.49
1:C:176:ASN:C	1:C:176:ASN:ND2	2.71	0.49
1:D:92:LYS:HA	1:D:95:LEU:HD23	1.95	0.49
1:D:130:PHE:O	1:D:165:ARG:HD3	2.13	0.49
1:B:99:TRP:O	1:B:102:ARG:CD	2.60	0.49
1:B:140:PHE:HZ	1:B:157:LEU:HD22	1.72	0.49
1:B:176:ASN:HD22	1:B:176:ASN:C	2.21	0.49
1:C:124:VAL:O	1:C:124:VAL:HG12	2.13	0.49
1:C:266:VAL:HG22	1:C:266:VAL:O	2.12	0.49
1:D:63:VAL:HB	1:D:117:TRP:HE1	1.77	0.49
1:D:65:CYS:O	1:D:66:GLY:C	2.54	0.49
1:D:75:VAL:HG22	1:D:81:VAL:CG2	2.42	0.49
1:D:164:VAL:O	1:D:290:LYS:HE2	2.13	0.49
1:A:207:LEU:HD23	1:A:215:MET:HE2	1.94	0.49
1:A:227:ALA:H	1:A:233:PRO:HA	1.78	0.49
1:C:263:GLN:HB2	1:C:289:LYS:HB3	1.95	0.49
1:B:254:VAL:HG12	1:B:255:GLN:H	1.77	0.48
1:C:85:ASP:O	1:C:114:GLU:HA	2.13	0.48
1:D:164:VAL:O	1:D:290:LYS:HE3	2.13	0.48
1:D:263:GLN:HE21	1:D:291:THR:CG2	2.24	0.48
1:D:133:VAL:HG23	1:D:164:VAL:HG22	1.93	0.48
1:D:227:ALA:N	1:D:233:PRO:HA	2.26	0.48
1:A:92:LYS:HD3	1:A:93:TYR:CZ	2.49	0.48
1:B:169:LEU:HD12	1:B:289:LYS:HA	1.94	0.48
1:B:193:TYR:O	1:B:194:TYR:CG	2.66	0.48
1:B:251:THR:HG22	1:B:252:GLU:N	2.28	0.48
1:B:289:LYS:O	1:B:290:LYS:C	2.55	0.48
1:A:74:LEU:HA	1:A:77:GLU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLU:HB3	1:A:79:PHE:CD1	2.45	0.48
1:D:61:LEU:HA	1:D:82:THR:O	2.13	0.48
1:D:116:ASN:ND2	1:D:118:LEU:N	2.61	0.48
1:A:92:LYS:CG	1:A:93:TYR:N	2.77	0.48
1:A:101:ARG:HB3	1:A:104:GLU:CG	2.38	0.48
1:A:133:VAL:O	1:A:170:LEU:CD1	2.61	0.48
1:A:140:PHE:CZ	1:A:157:LEU:HD22	2.47	0.48
1:B:269:ASP:H	1:B:281:PRO:CB	2.24	0.48
1:D:264:HIS:CD2	1:D:264:HIS:C	2.91	0.48
1:D:273:TYR:C	1:D:273:TYR:CD2	2.90	0.48
1:A:72:ILE:HD11	1:A:110:TRP:CH2	2.49	0.48
1:A:264:HIS:HD2	1:A:265:SER:N	2.12	0.48
1:B:176:ASN:ND2	1:B:179:TYR:CB	2.77	0.48
1:D:91:LEU:O	1:D:95:LEU:HD22	2.13	0.48
1:A:99:TRP:O	1:A:102:ARG:CB	2.60	0.48
1:D:256:GLU:C	1:D:258:PHE:N	2.68	0.48
1:D:282:CYS:SG	1:D:283:TYR:CE1	3.03	0.48
1:C:66:GLY:C	1:C:68:GLY:N	2.70	0.48
1:C:188:PRO:HB3	1:C:202:ILE:HD12	1.87	0.48
1:D:84:VAL:HG21	1:D:115:ALA:HB3	1.95	0.48
1:C:71:SER:O	1:C:72:ILE:C	2.57	0.48
1:C:176:ASN:ND2	1:C:178:ASP:HB2	2.27	0.48
1:D:87:SER:OG	1:D:90:MET:CG	2.61	0.48
1:D:250:PHE:O	1:D:251:THR:C	2.56	0.48
1:A:197:ASP:O	1:A:198:LEU:HD13	2.14	0.48
1:B:49:LEU:HD13	1:B:49:LEU:N	2.29	0.48
1:B:174:HIS:C	1:B:174:HIS:CD2	2.91	0.48
1:C:236:SER:C	1:C:237:LYS:HG3	2.36	0.48
1:D:44:TYR:CD1	1:D:44:TYR:C	2.90	0.48
1:D:166:PRO:HB3	1:D:292:GLY:OXT	2.14	0.48
1:A:98:ARG:O	1:A:99:TRP:C	2.56	0.47
1:A:175:LYS:HE3	1:A:283:TYR:CE2	2.49	0.47
1:A:176:ASN:ND2	1:A:176:ASN:O	2.47	0.47
1:B:81:VAL:O	1:B:81:VAL:HG22	2.13	0.47
1:B:181:LEU:HD12	1:B:181:LEU:HA	1.70	0.47
1:B:183:THR:HG22	1:B:184:GLY:N	2.28	0.47
1:B:258:PHE:CZ	1:B:288:LEU:CB	2.97	0.47
1:C:87:SER:HB3	2:C:3301:SAH:O2'	2.14	0.47
1:C:207:LEU:HB3	1:C:215:MET:HB3	1.96	0.47
1:C:220:TYR:HB2	1:C:238:PHE:CD1	2.49	0.47
1:D:163:MET:HA	1:D:163:MET:HE2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:HB3	3:D:4306:HOH:O	2.13	0.47
1:D:202:ILE:CD1	1:D:220:TYR:CE2	2.96	0.47
1:D:217:THR:O	1:D:217:THR:HG22	2.12	0.47
1:D:219:ASP:HB3	1:D:237:LYS:CD	2.44	0.47
1:A:254:VAL:CG1	1:A:255:GLN:H	2.26	0.47
1:A:261:ARG:HE	1:A:261:ARG:HB3	1.37	0.47
1:B:118:LEU:HD12	1:B:118:LEU:N	2.28	0.47
1:D:207:LEU:HD12	1:D:207:LEU:C	2.37	0.47
1:A:117:TRP:HH2	1:A:139:SER:O	1.97	0.47
1:C:84:VAL:HA	1:C:113:GLU:O	2.13	0.47
1:C:212:LYS:HZ2	1:C:214:HIS:CE1	2.32	0.47
1:D:136:LEU:CD1	1:D:171:VAL:O	2.62	0.47
1:A:75:VAL:HG11	1:A:107:PHE:CZ	2.48	0.47
1:B:176:ASN:ND2	1:B:176:ASN:O	2.38	0.47
1:B:274:ARG:HG2	1:B:277:GLN:CB	2.44	0.47
1:C:111:VAL:HG13	1:C:112:ILE:H	1.79	0.47
1:A:71:SER:O	1:A:72:ILE:C	2.57	0.47
1:A:100:ASN:N	1:A:100:ASN:ND2	2.42	0.47
1:A:261:ARG:HD3	1:A:292:GLY:O	2.12	0.47
1:B:117:TRP:HD1	1:B:120:LEU:HD22	1.80	0.47
1:D:107:PHE:CD1	1:D:107:PHE:N	2.79	0.47
1:D:216:VAL:O	1:D:216:VAL:HG12	2.15	0.47
1:D:264:HIS:CD2	1:D:265:SER:N	2.82	0.47
1:D:274:ARG:O	1:D:277:GLN:HB3	2.15	0.47
1:A:117:TRP:HH2	1:A:139:SER:C	2.22	0.47
1:B:97:GLU:OE2	1:B:101:ARG:CD	2.60	0.47
1:C:41:THR:HG23	1:C:43:GLU:H	1.79	0.47
1:C:97:GLU:O	1:C:101:ARG:HG3	2.15	0.47
1:C:223:GLN:CB	1:C:235:PHE:CZ	2.94	0.47
1:C:289:LYS:O	1:C:290:LYS:C	2.58	0.47
1:D:224:VAL:O	1:D:225:PRO:C	2.57	0.47
1:A:289:LYS:HB2	1:A:289:LYS:HE3	1.55	0.47
1:B:41:THR:HG23	1:B:43:GLU:CD	2.38	0.47
1:B:98:ARG:NH2	1:D:99:TRP:CD2	2.83	0.47
1:B:277:GLN:O	1:B:278:ALA:C	2.56	0.47
1:D:166:PRO:C	1:D:168:GLY:N	2.71	0.47
1:D:177:TYR:O	1:D:178:ASP:C	2.56	0.47
1:D:258:PHE:CE2	1:D:288:LEU:CG	2.82	0.47
1:A:90:MET:O	1:A:91:LEU:C	2.58	0.47
1:A:192:ILE:HG12	1:A:193:TYR:N	2.26	0.47
1:B:190:LYS:HZ3	1:B:190:LYS:C	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ARG:HH21	1:C:104:GLU:CD	2.23	0.47
1:C:118:LEU:HG	1:C:155:LEU:HD23	1.96	0.47
1:C:246:CYS:O	1:C:247:LEU:C	2.58	0.47
1:D:175:LYS:CE	1:D:282:CYS:HG	2.25	0.47
1:A:237:LYS:HG3	1:A:238:PHE:H	1.72	0.47
1:C:91:LEU:HD12	1:C:91:LEU:HA	1.68	0.47
1:D:41:THR:HG22	1:D:43:GLU:N	2.29	0.47
1:D:43:GLU:O	1:D:46:ALA:HB3	2.15	0.47
1:D:97:GLU:CD	1:D:97:GLU:N	2.73	0.47
1:D:183:THR:CG2	1:D:185:CYS:H	2.28	0.47
1:D:258:PHE:HD2	1:D:262:CYS:HG	1.59	0.47
1:A:81:VAL:HG13	1:A:110:TRP:CD1	2.50	0.47
1:A:281:PRO:HG2	1:A:284:PHE:CZ	2.50	0.47
1:B:261:ARG:HB3	1:B:292:GLY:N	2.30	0.47
1:C:41:THR:CG2	1:C:44:TYR:HB3	2.44	0.47
1:A:172:ILE:CG2	1:A:250:PHE:HE2	2.24	0.46
1:B:136:LEU:HD11	1:B:171:VAL:HG11	1.91	0.46
1:B:279:TYR:CG	1:B:280:VAL:N	2.83	0.46
1:C:107:PHE:HD1	1:C:107:PHE:H	1.62	0.46
1:D:41:THR:HB	1:D:44:TYR:HB2	1.95	0.46
1:D:85:ASP:HB3	1:D:91:LEU:HD13	1.97	0.46
1:A:70:ASP:O	1:A:71:SER:C	2.59	0.46
1:A:101:ARG:CB	1:A:104:GLU:HG3	2.40	0.46
1:A:261:ARG:H	1:A:261:ARG:HG2	1.54	0.46
1:B:45:LYS:HG2	1:B:49:LEU:CD2	2.46	0.46
1:B:207:LEU:CD2	1:B:214:HIS:HB3	2.43	0.46
1:C:165:ARG:HH21	1:C:165:ARG:HG2	1.68	0.46
1:A:43:GLU:O	1:A:44:TYR:C	2.58	0.46
1:A:99:TRP:CE3	1:A:102:ARG:HD3	2.50	0.46
1:A:135:CYS:HB3	1:A:172:ILE:HG13	1.95	0.46
1:B:44:TYR:O	1:B:45:LYS:C	2.58	0.46
1:B:90:MET:HG3	2:B:2301:SAH:O3'	2.14	0.46
1:B:103:LYS:HA	1:B:103:LYS:HD3	1.44	0.46
1:B:191:ASN:C	1:B:193:TYR:N	2.71	0.46
1:A:41:THR:HA	1:A:195:LYS:HZ3	1.73	0.46
1:A:191:ASN:O	1:A:191:ASN:ND2	2.49	0.46
1:A:209:VAL:CG1	1:A:212:LYS:HE3	2.45	0.46
1:B:111:VAL:HG13	1:B:112:ILE:H	1.80	0.46
1:D:65:CYS:O	1:D:68:GLY:N	2.48	0.46
1:D:77:GLU:HB3	1:D:79:PHE:HE1	1.74	0.46
1:A:118:LEU:O	1:A:119:THR:CG2	2.59	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ARG:CG	1:A:165:ARG:NH2	2.78	0.46
1:D:99:TRP:CZ2	1:D:102:ARG:CZ	2.99	0.46
1:D:114:GLU:O	1:D:115:ALA:HB2	2.16	0.46
1:D:117:TRP:HA	1:D:120:LEU:HB2	1.97	0.46
1:D:240:LEU:HD12	1:D:240:LEU:HA	1.60	0.46
1:A:73:MET:O	1:A:74:LEU:C	2.59	0.46
1:A:120:LEU:O	1:A:121:ASP:C	2.57	0.46
1:A:191:ASN:O	1:A:191:ASN:CG	2.58	0.46
1:A:252:GLU:OE1	1:A:253:LEU:CD2	2.60	0.46
1:A:76:GLU:C	1:A:78:GLY:N	2.74	0.46
1:A:186:ALA:O	1:A:188:PRO:HD3	2.16	0.46
1:A:202:ILE:HG22	1:A:203:THR:N	2.31	0.46
1:B:183:THR:HG22	1:B:185:CYS:N	2.22	0.46
1:C:203:THR:HA	1:D:210:ASN:HD21	1.79	0.46
1:C:238:PHE:HE2	1:C:240:LEU:HD22	1.80	0.46
1:B:60:VAL:HG13	1:B:132:ALA:O	2.15	0.46
1:B:176:ASN:ND2	1:B:176:ASN:C	2.74	0.46
1:B:183:THR:HG23	1:B:185:CYS:H	1.77	0.46
1:D:201:ASP:CG	1:D:202:ILE:N	2.73	0.46
1:A:48:LEU:O	1:A:49:LEU:C	2.59	0.46
1:A:288:LEU:N	1:A:288:LEU:HD23	2.31	0.46
1:B:216:VAL:HG23	1:B:244:PRO:HB3	1.97	0.46
1:C:49:LEU:O	1:C:53:ARG:HB2	2.16	0.46
1:C:99:TRP:CE3	1:C:102:ARG:HD3	2.51	0.46
1:C:224:VAL:CG2	1:C:227:ALA:N	2.73	0.46
1:B:110:TRP:CD1	1:B:111:VAL:O	2.69	0.46
1:B:114:GLU:H	1:B:114:GLU:HG3	1.53	0.46
1:C:111:VAL:CG1	1:C:112:ILE:H	2.29	0.46
1:C:120:LEU:O	1:C:121:ASP:C	2.58	0.46
1:D:158:LYS:CA	1:D:257:ALA:HB1	2.29	0.46
1:D:227:ALA:CB	1:D:234:GLY:H	2.19	0.46
1:A:104:GLU:HA	1:A:105:PRO:HD2	1.81	0.45
1:A:188:PRO:CB	1:A:202:ILE:CD1	2.76	0.45
1:B:110:TRP:HD1	1:B:111:VAL:N	2.13	0.45
1:C:44:TYR:CE2	1:C:193:TYR:HA	2.51	0.45
1:D:99:TRP:CE2	1:D:102:ARG:CZ	3.00	0.45
1:D:202:ILE:HD11	1:D:220:TYR:HD2	1.76	0.45
1:B:63:VAL:HB	1:B:117:TRP:NE1	2.31	0.45
1:C:61:LEU:HB3	1:C:133:VAL:HG13	1.98	0.45
1:C:201:ASP:CB	1:C:221:THR:HB	2.39	0.45
1:D:42:ALA:HB2	3:D:4360:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD12	1:D:256:GLU:OE1	2.15	0.45
1:D:264:HIS:CE1	1:D:286:HIS:ND1	2.84	0.45
1:A:58:HIS:CE1	3:A:1312:HOH:O	2.70	0.45
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.43	0.45
1:C:44:TYR:CG	1:C:270:PHE:CE1	3.04	0.45
1:D:149:ASP:C	1:D:151:SER:N	2.73	0.45
1:A:156:ALA:C	1:A:160:ILE:HD12	2.40	0.45
1:A:268:GLY:H	1:A:273:TYR:HB2	1.81	0.45
1:B:48:LEU:HD23	1:B:73:MET:CE	2.47	0.45
1:B:172:ILE:O	1:B:172:ILE:HG23	2.14	0.45
1:B:177:TYR:O	1:B:178:ASP:C	2.57	0.45
1:B:215:MET:HG3	1:B:216:VAL:N	2.30	0.45
1:C:149:ASP:C	1:C:151:SER:N	2.75	0.45
1:D:174:HIS:HD2	1:D:174:HIS:C	2.21	0.45
1:D:258:PHE:CE2	1:D:288:LEU:HD12	2.52	0.45
1:B:87:SER:OG	1:B:90:MET:CG	2.65	0.45
1:B:113:GLU:HG3	3:B:2310:HOH:O	2.16	0.45
1:B:157:LEU:O	1:B:158:LYS:C	2.59	0.45
1:C:44:TYR:O	1:C:44:TYR:HD1	1.98	0.45
1:D:116:ASN:ND2	1:D:118:LEU:CB	2.70	0.45
1:C:179:TYR:CD1	1:C:180:ILE:HG12	2.51	0.45
1:D:195:LYS:HB3	1:D:195:LYS:HZ2	1.81	0.45
1:D:237:LYS:HG2	1:D:238:PHE:H	1.81	0.45
1:C:44:TYR:CZ	1:C:193:TYR:CE2	3.05	0.45
1:C:90:MET:HB3	1:C:90:MET:HE2	1.65	0.45
1:A:41:THR:CA	1:A:195:LYS:CE	2.81	0.45
1:A:165:ARG:O	1:A:166:PRO:C	2.58	0.45
1:B:97:GLU:HA	1:B:100:ASN:HD22	1.81	0.45
1:B:150:GLN:HG2	1:B:153:HIS:CD2	2.52	0.45
1:B:164:VAL:HG11	1:B:169:LEU:O	2.16	0.45
1:B:183:THR:CG2	1:B:185:CYS:O	2.65	0.45
1:D:136:LEU:HD21	1:D:171:VAL:CG1	2.47	0.45
1:D:179:TYR:O	1:D:180:ILE:C	2.59	0.45
1:A:81:VAL:CG1	1:A:110:TRP:CD1	3.00	0.45
1:A:174:HIS:CD2	1:A:284:PHE:HB2	2.52	0.45
1:A:184:GLY:HA3	1:B:211:ASN:ND2	2.32	0.45
1:B:149:ASP:O	1:B:151:SER:N	2.50	0.45
1:D:51:LEU:O	1:D:52:LEU:C	2.57	0.45
1:A:258:PHE:C	1:A:260:GLY:N	2.73	0.45
1:C:119:THR:O	1:C:120:LEU:C	2.60	0.45
1:C:163:MET:HE2	1:C:163:MET:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LYS:O	1:C:291:THR:CG2	2.62	0.45
1:C:217:THR:HG23	1:C:241:SER:CB	2.47	0.44
1:C:260:GLY:O	1:C:262:CYS:N	2.50	0.44
1:D:139:SER:O	1:D:142:HIS:HB2	2.18	0.44
1:A:91:LEU:HG	1:A:112:ILE:HG22	1.98	0.44
1:A:265:SER:OG	1:A:287:VAL:CG2	2.60	0.44
1:C:67:THR:HG23	1:C:90:MET:HE1	1.97	0.44
1:C:183:THR:O	1:C:184:GLY:C	2.60	0.44
1:C:212:LYS:O	1:C:213:ALA:C	2.61	0.44
1:D:134:ILE:HB	1:D:136:LEU:HD22	1.93	0.44
1:D:166:PRO:O	1:D:167:GLY:C	2.58	0.44
1:A:60:VAL:HG13	1:A:132:ALA:CB	2.26	0.44
1:A:289:LYS:O	1:A:289:LYS:CG	2.54	0.44
1:C:41:THR:HG21	1:C:43:GLU:HG2	1.98	0.44
1:D:224:VAL:HG13	1:D:234:GLY:C	2.43	0.44
1:D:254:VAL:HG12	1:D:255:GLN:H	1.82	0.44
1:A:133:VAL:O	1:A:170:LEU:HA	2.18	0.44
1:A:243:TYR:CD2	1:A:245:HIS:CD2	3.06	0.44
1:A:261:ARG:HB2	1:A:292:GLY:N	2.33	0.44
1:B:111:VAL:CG1	1:B:112:ILE:H	2.31	0.44
1:B:118:LEU:O	1:B:119:THR:HG23	2.18	0.44
1:B:120:LEU:HB3	1:B:159:ASN:HB3	1.99	0.44
1:B:164:VAL:O	1:B:290:LYS:CD	2.66	0.44
1:C:140:PHE:CZ	1:C:157:LEU:CD2	3.01	0.44
1:C:150:GLN:O	1:C:151:SER:C	2.60	0.44
1:D:49:LEU:HD12	1:D:49:LEU:HA	1.75	0.44
1:D:90:MET:CE	1:D:90:MET:CA	2.87	0.44
1:D:101:ARG:O	1:D:102:ARG:C	2.61	0.44
1:D:109:LYS:O	1:D:110:TRP:C	2.61	0.44
1:D:201:ASP:O	1:D:220:TYR:HA	2.18	0.44
1:A:191:ASN:CG	1:A:193:TYR:HB2	2.38	0.44
1:C:73:MET:HG2	1:C:74:LEU:HD23	1.99	0.44
1:C:95:LEU:HD13	1:C:112:ILE:HG21	2.00	0.44
1:C:120:LEU:HD21	1:C:160:ILE:HA	1.99	0.44
1:C:188:PRO:CB	1:C:202:ILE:CD1	2.77	0.44
1:A:142:HIS:CE1	2:A:1301:SAH:SD	3.10	0.44
1:A:169:LEU:HD12	1:A:289:LYS:HA	2.00	0.44
1:B:168:GLY:O	1:B:169:LEU:HD13	2.18	0.44
1:B:185:CYS:HA	1:B:204:THR:HB	2.00	0.44
1:B:218:LEU:HB3	1:B:220:TYR:CE2	2.53	0.44
1:C:95:LEU:CD1	1:C:112:ILE:CB	2.96	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:GLU:O	1:C:105:PRO:C	2.58	0.44
1:D:77:GLU:OE1	1:D:77:GLU:CA	2.53	0.44
1:B:43:GLU:O	1:B:44:TYR:C	2.61	0.44
1:B:279:TYR:CD2	1:B:280:VAL:N	2.79	0.44
1:C:65:CYS:HB3	1:C:85:ASP:HB2	1.99	0.44
1:C:88:ASP:O	1:C:89:LYS:C	2.60	0.44
1:C:198:LEU:HD23	1:C:222:VAL:HG13	1.98	0.44
1:C:217:THR:HG23	1:C:241:SER:OG	2.18	0.44
1:A:269:ASP:OD1	1:A:282:CYS:SG	2.73	0.44
1:B:100:ASN:C	1:B:102:ARG:N	2.73	0.44
1:D:186:ALA:CB	1:D:218:LEU:HD21	2.47	0.44
1:B:48:LEU:O	1:B:49:LEU:C	2.60	0.44
1:B:137:GLY:N	1:B:173:ASP:OD2	2.51	0.44
1:B:155:LEU:O	1:B:155:LEU:HD12	2.18	0.44
1:B:195:LYS:HB2	1:B:195:LYS:HE2	1.53	0.44
1:B:247:LEU:O	1:B:248:ALA:C	2.60	0.44
1:B:274:ARG:O	1:B:274:ARG:CG	2.65	0.44
1:D:143:LEU:HD12	1:D:144:PRO:N	2.33	0.44
1:D:256:GLU:O	1:D:257:ALA:C	2.61	0.44
1:D:287:VAL:O	1:D:288:LEU:HD22	2.13	0.44
1:A:173:ASP:CG	1:A:193:TYR:OH	2.61	0.43
1:A:211:ASN:HD22	1:B:184:GLY:HA2	1.73	0.43
1:B:82:THR:HA	1:B:111:VAL:HB	2.00	0.43
1:C:94:ALA:C	1:C:96:LYS:N	2.75	0.43
1:D:85:ASP:HB2	1:D:91:LEU:HD13	1.99	0.43
1:D:227:ALA:CB	1:D:234:GLY:CA	2.60	0.43
1:A:194:TYR:CD2	1:A:194:TYR:N	2.85	0.43
1:A:254:VAL:HG12	1:A:255:GLN:H	1.83	0.43
1:A:274:ARG:O	1:A:274:ARG:HG2	2.17	0.43
1:B:109:LYS:HD2	1:B:109:LYS:N	2.33	0.43
1:B:118:LEU:C	1:B:119:THR:HG23	2.43	0.43
1:B:138:ASN:OD1	1:B:141:ALA:CB	2.66	0.43
1:D:195:LYS:HE2	1:D:197:ASP:OD2	2.18	0.43
1:A:164:VAL:O	1:A:290:LYS:HD2	2.18	0.43
1:B:133:VAL:HG21	1:B:164:VAL:HG22	1.99	0.43
1:B:168:GLY:C	1:B:169:LEU:HD13	2.43	0.43
1:A:49:LEU:HD11	1:A:77:GLU:HG3	1.99	0.43
1:B:55:HIS:CD2	1:B:169:LEU:HD11	2.53	0.43
1:C:81:VAL:HG22	1:C:110:TRP:CD1	2.54	0.43
1:D:72:ILE:HG23	1:D:107:PHE:HE2	1.82	0.43
1:D:180:ILE:O	1:D:184:GLY:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:LEU:CG	1:A:112:ILE:HG22	2.49	0.43
1:A:98:ARG:O	1:A:102:ARG:N	2.51	0.43
1:B:140:PHE:CD2	1:B:250:PHE:CE1	3.06	0.43
1:B:168:GLY:O	1:B:169:LEU:HD12	2.19	0.43
1:C:200:LYS:HB3	1:C:222:VAL:HG22	2.00	0.43
1:C:228:GLY:CA	1:C:232:ALA:O	2.64	0.43
1:C:244:PRO:O	1:C:245:HIS:CG	2.71	0.43
1:D:136:LEU:HD21	1:D:171:VAL:HB	2.00	0.43
1:B:220:TYR:HD1	1:B:238:PHE:CE2	2.37	0.43
1:C:82:THR:HA	1:C:111:VAL:HB	2.01	0.43
1:D:72:ILE:HG23	1:D:107:PHE:CE2	2.54	0.43
1:A:98:ARG:HH11	1:A:111:VAL:HA	1.83	0.43
1:A:280:VAL:HG12	3:A:1341:HOH:O	2.17	0.43
1:B:84:VAL:CB	1:B:113:GLU:O	2.67	0.43
1:B:105:PRO:O	1:B:109:LYS:CD	2.59	0.43
1:B:281:PRO:HB2	1:B:283:TYR:O	2.18	0.43
1:C:247:LEU:O	1:C:248:ALA:C	2.60	0.43
1:A:231:GLY:C	1:A:232:ALA:O	2.62	0.43
1:A:262:CYS:HA	1:A:291:THR:HG23	2.01	0.43
1:B:263:GLN:CB	1:B:289:LYS:HB3	2.48	0.43
1:C:192:ILE:HD11	1:C:270:PHE:CD1	2.54	0.43
1:A:202:ILE:CG2	1:A:203:THR:N	2.81	0.43
1:B:76:GLU:C	1:B:78:GLY:N	2.75	0.43
1:C:47:TRP:CE3	1:C:48:LEU:HA	2.53	0.43
1:C:264:HIS:HA	1:C:288:LEU:HD13	2.01	0.43
1:D:227:ALA:HB1	1:D:234:GLY:HA3	1.94	0.43
1:A:50:GLY:O	1:A:51:LEU:C	2.62	0.43
1:A:289:LYS:O	1:A:290:LYS:C	2.62	0.43
1:B:157:LEU:HD13	1:B:157:LEU:HA	1.77	0.43
1:C:119:THR:C	1:C:123:ASP:OD1	2.62	0.43
1:C:212:LYS:NZ	1:C:214:HIS:CE1	2.87	0.43
1:D:46:ALA:O	1:D:47:TRP:C	2.60	0.43
1:D:87:SER:O	1:D:88:ASP:C	2.60	0.43
1:D:224:VAL:HG13	1:D:234:GLY:CA	2.49	0.43
1:D:224:VAL:CG2	1:D:227:ALA:HB2	2.49	0.43
1:A:54:GLN:HG2	1:A:55:HIS:HD1	1.84	0.42
1:A:247:LEU:HD11	1:A:251:THR:OG1	2.18	0.42
1:A:268:GLY:N	1:A:273:TYR:HB2	2.34	0.42
1:B:104:GLU:HA	1:B:105:PRO:HD2	1.89	0.42
1:C:76:GLU:OE1	1:C:101:ARG:NH1	2.52	0.42
1:D:98:ARG:HB2	1:D:110:TRP:HE3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:CYS:HB3	1:D:172:ILE:HG13	2.01	0.42
1:A:98:ARG:CD	1:C:99:TRP:CH2	3.02	0.42
1:A:98:ARG:NH2	1:C:99:TRP:CD1	2.87	0.42
1:B:101:ARG:CD	1:B:107:PHE:CZ	3.02	0.42
1:C:69:VAL:CB	1:C:194:TYR:HE2	2.31	0.42
1:C:263:GLN:NE2	3:C:3306:HOH:O	2.53	0.42
1:D:101:ARG:C	1:D:103:LYS:N	2.77	0.42
1:D:276:GLY:O	1:D:277:GLN:C	2.62	0.42
1:B:134:ILE:HG13	1:B:136:LEU:CD2	2.50	0.42
1:C:86:ALA:CB	2:C:3301:SAH:C2	2.94	0.42
1:C:192:ILE:HG21	1:C:269:ASP:OD1	2.20	0.42
1:D:95:LEU:CD1	1:D:112:ILE:HB	2.50	0.42
1:A:54:GLN:HG2	1:A:55:HIS:ND1	2.34	0.42
1:A:68:GLY:O	1:A:69:VAL:C	2.62	0.42
1:B:101:ARG:O	1:B:107:PHE:CB	2.67	0.42
1:B:103:LYS:O	1:B:104:GLU:HG3	2.19	0.42
1:C:231:GLY:O	1:C:232:ALA:C	2.63	0.42
1:D:195:LYS:HD2	1:D:195:LYS:C	2.43	0.42
1:A:264:HIS:CE1	1:A:286:HIS:CE1	3.07	0.42
1:B:136:LEU:CD1	1:B:171:VAL:O	2.56	0.42
1:B:179:TYR:O	1:B:180:ILE:C	2.63	0.42
1:B:200:LYS:HD2	1:B:200:LYS:C	2.44	0.42
1:C:88:ASP:OD1	1:C:114:GLU:CD	2.63	0.42
1:C:154:ARG:HG3	1:C:256:GLU:OE1	2.20	0.42
1:D:76:GLU:C	1:D:78:GLY:H	2.27	0.42
1:D:193:TYR:O	1:D:194:TYR:CG	2.73	0.42
1:D:221:THR:HG23	1:D:237:LYS:HB2	2.01	0.42
1:D:290:LYS:O	1:D:290:LYS:CG	2.39	0.42
1:A:76:GLU:C	1:A:78:GLY:H	2.28	0.42
1:B:142:HIS:O	1:B:144:PRO:CD	2.60	0.42
1:C:49:LEU:HD13	1:C:73:MET:HE3	1.99	0.42
1:C:147:LYS:HE3	1:C:147:LYS:HB3	1.23	0.42
1:C:207:LEU:HD23	1:C:215:MET:CE	2.47	0.42
1:D:258:PHE:HE2	1:D:288:LEU:CD1	2.31	0.42
1:A:101:ARG:HB3	1:A:104:GLU:CD	2.45	0.42
1:A:247:LEU:CD1	1:A:251:THR:OG1	2.68	0.42
1:B:121:ASP:HA	1:B:163:MET:HE3	2.02	0.42
1:B:138:ASN:H	1:B:173:ASP:CG	2.28	0.42
1:C:117:TRP:O	1:C:159:ASN:HB2	2.19	0.42
1:C:217:THR:HG23	1:C:241:SER:HB3	2.02	0.42
1:D:166:PRO:HG3	1:D:292:GLY:OXT	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PRO:HG3	1:C:202:ILE:HG13	2.02	0.42
1:C:268:GLY:C	1:C:281:PRO:HB3	2.44	0.42
1:D:177:TYR:O	1:D:181:LEU:HB2	2.19	0.42
1:A:91:LEU:O	1:A:92:LYS:C	2.63	0.42
1:B:97:GLU:CD	1:B:101:ARG:HD2	2.41	0.42
1:B:136:LEU:HA	1:B:173:ASP:CG	2.44	0.42
1:B:149:ASP:OD2	1:B:149:ASP:N	2.52	0.42
1:D:187:PRO:HA	1:D:188:PRO:HD3	1.82	0.42
1:B:60:VAL:CG1	1:B:132:ALA:O	2.68	0.42
1:B:149:ASP:C	1:B:151:SER:N	2.69	0.42
1:B:269:ASP:N	1:B:281:PRO:HB3	2.30	0.42
1:D:140:PHE:CE2	1:D:157:LEU:HD21	2.55	0.42
1:D:218:LEU:HD12	1:D:218:LEU:HA	1.85	0.42
1:A:92:LYS:CD	1:A:93:TYR:CE2	3.00	0.41
1:A:107:PHE:HD2	1:A:110:TRP:HE3	1.67	0.41
1:A:145:ASP:OD2	1:A:145:ASP:C	2.63	0.41
1:A:145:ASP:OD2	1:A:148:GLY:C	2.63	0.41
1:B:42:ALA:O	1:B:43:GLU:C	2.63	0.41
1:B:92:LYS:NZ	1:D:88:ASP:OD2	2.53	0.41
1:B:119:THR:O	1:B:120:LEU:C	2.63	0.41
1:B:138:ASN:HA	1:B:173:ASP:O	2.20	0.41
1:B:268:GLY:O	1:B:270:PHE:N	2.53	0.41
1:B:271:LYS:O	1:B:272:PRO:C	2.61	0.41
1:D:43:GLU:O	1:D:44:TYR:C	2.64	0.41
1:D:91:LEU:HG	1:D:112:ILE:CG2	2.50	0.41
1:D:99:TRP:CZ3	1:D:102:ARG:CD	3.01	0.41
1:A:224:VAL:O	1:A:226:GLY:N	2.52	0.41
1:B:261:ARG:HB2	1:B:292:GLY:O	2.20	0.41
1:C:75:VAL:HG11	1:C:107:PHE:CD1	2.54	0.41
1:C:210:ASN:HD21	1:D:203:THR:HA	1.85	0.41
1:C:238:PHE:CE2	1:C:240:LEU:HD22	2.55	0.41
1:A:119:THR:O	1:A:120:LEU:C	2.64	0.41
1:B:121:ASP:HA	1:B:163:MET:CE	2.50	0.41
1:B:188:PRO:CG	1:B:202:ILE:HD12	2.51	0.41
1:C:176:ASN:O	1:C:180:ILE:HG13	2.20	0.41
1:A:271:LYS:HB3	1:A:272:PRO:CD	2.51	0.41
1:B:124:VAL:HA	1:B:125:PRO:HD3	1.90	0.41
1:C:212:LYS:O	1:C:212:LYS:HG2	2.17	0.41
1:D:71:SER:HB3	1:D:110:TRP:CZ2	2.55	0.41
1:D:126:ALA:HB2	1:D:163:MET:HE1	2.01	0.41
1:A:153:HIS:CD2	1:A:245:HIS:NE2	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD12	1:A:171:VAL:N	2.36	0.41
1:B:45:LYS:HG3	1:B:73:MET:SD	2.61	0.41
1:C:98:ARG:O	1:C:102:ARG:N	2.54	0.41
1:D:76:GLU:C	1:D:78:GLY:N	2.77	0.41
1:D:87:SER:OG	1:D:90:MET:CB	2.68	0.41
1:D:136:LEU:HD22	1:D:136:LEU:N	2.35	0.41
1:D:155:LEU:O	1:D:158:LYS:HB3	2.19	0.41
1:A:76:GLU:H	1:A:76:GLU:HG3	1.68	0.41
1:A:145:ASP:HA	3:A:1455:HOH:O	2.20	0.41
1:A:155:LEU:HD12	1:A:158:LYS:HD2	2.02	0.41
1:A:252:GLU:O	1:A:256:GLU:HB2	2.20	0.41
1:B:213:ALA:HB1	1:B:244:PRO:HG3	2.02	0.41
1:B:243:TYR:HD2	1:B:245:HIS:CD2	2.35	0.41
1:C:48:LEU:CD1	1:C:52:LEU:HD22	2.50	0.41
1:C:157:LEU:HB3	1:C:257:ALA:HB2	2.03	0.41
1:D:183:THR:HG23	1:D:185:CYS:H	1.86	0.41
1:A:61:LEU:HA	1:A:82:THR:HG23	2.03	0.41
1:A:120:LEU:O	1:A:124:VAL:N	2.54	0.41
1:B:118:LEU:N	1:B:118:LEU:CD1	2.84	0.41
1:C:241:SER:C	1:C:242:TYR:CD2	2.98	0.41
1:D:145:ASP:CG	1:D:145:ASP:O	2.61	0.41
1:D:247:LEU:HD13	1:D:247:LEU:HA	1.72	0.41
1:D:264:HIS:HB2	1:D:288:LEU:HD13	2.02	0.41
1:A:191:ASN:C	1:A:193:TYR:N	2.79	0.41
1:B:65:CYS:O	1:B:68:GLY:N	2.49	0.41
1:B:98:ARG:NH2	1:D:99:TRP:CG	2.89	0.41
1:B:190:LYS:CE	1:B:190:LYS:CA	2.99	0.41
1:B:198:LEU:HD21	1:B:222:VAL:HG13	2.03	0.41
1:B:268:GLY:N	1:B:271:LYS:O	2.53	0.41
1:B:275:PRO:O	1:B:276:GLY:C	2.62	0.41
1:C:41:THR:HG22	1:C:41:THR:O	2.18	0.41
1:C:149:ASP:OD2	1:C:151:SER:HB3	2.21	0.41
2:C:3301:SAH:HB2	2:C:3301:SAH:H5'2	1.70	0.41
1:A:191:ASN:O	1:A:193:TYR:N	2.54	0.41
1:B:47:TRP:CH2	1:B:171:VAL:HG11	2.56	0.41
1:B:136:LEU:CD1	1:B:171:VAL:HB	2.49	0.41
1:B:138:ASN:CG	1:B:138:ASN:O	2.63	0.41
1:B:155:LEU:HD12	1:B:155:LEU:C	2.46	0.41
1:B:157:LEU:HD11	1:B:172:ILE:HD13	2.02	0.41
1:B:264:HIS:HA	1:B:288:LEU:HD22	2.03	0.41
1:C:137:GLY:O	1:C:138:ASN:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HA	1:C:240:LEU:HD12	1.68	0.41
1:C:242:TYR:HD2	1:C:242:TYR:H	1.60	0.41
1:C:267:LEU:O	1:C:268:GLY:C	2.64	0.41
1:D:125:PRO:O	1:D:126:ALA:C	2.64	0.41
1:A:142:HIS:O	1:A:144:PRO:CD	2.69	0.41
1:B:47:TRP:O	1:B:48:LEU:C	2.64	0.41
1:C:64:ALA:O	1:C:65:CYS:C	2.64	0.41
1:C:153:HIS:O	1:C:157:LEU:HD22	2.21	0.41
1:D:101:ARG:HD3	1:D:107:PHE:CD2	2.53	0.41
1:A:266:VAL:O	1:A:266:VAL:HG22	2.21	0.40
1:B:188:PRO:HG3	1:B:202:ILE:HG13	2.02	0.40
1:A:95:LEU:HD13	1:A:95:LEU:HA	1.78	0.40
1:A:102:ARG:HG3	1:A:103:LYS:N	2.34	0.40
1:A:165:ARG:HH21	1:A:165:ARG:HG3	1.85	0.40
1:A:174:HIS:HD2	1:A:174:HIS:O	2.04	0.40
1:A:228:GLY:H	1:A:232:ALA:C	2.28	0.40
1:A:270:PHE:CE2	1:A:285:ILE:HD13	2.56	0.40
1:B:50:GLY:O	1:B:54:GLN:HB2	2.20	0.40
1:B:118:LEU:O	1:B:119:THR:CG2	2.69	0.40
1:B:136:LEU:CA	1:B:173:ASP:OD2	2.67	0.40
1:C:85:ASP:HB3	1:C:91:LEU:HD22	2.03	0.40
1:D:157:LEU:HD11	1:D:172:ILE:HD13	1.96	0.40
1:D:189:GLY:C	1:D:190:LYS:HD3	2.46	0.40
1:A:289:LYS:HG2	1:A:291:THR:HG22	2.03	0.40
1:B:44:TYR:CE1	1:B:48:LEU:HD13	2.57	0.40
1:B:274:ARG:O	1:B:275:PRO:C	2.63	0.40
1:C:49:LEU:HA	1:C:49:LEU:HD12	1.82	0.40
1:C:179:TYR:HD1	1:C:180:ILE:HG12	1.86	0.40
1:D:103:LYS:O	1:D:104:GLU:C	2.63	0.40
1:D:186:ALA:HA	1:D:187:PRO:HD3	1.89	0.40
1:D:204:THR:OG1	1:D:218:LEU:HD11	2.21	0.40
1:D:208:THR:O	1:D:208:THR:HG22	2.21	0.40
1:D:209:VAL:O	1:D:209:VAL:HG12	2.20	0.40
1:D:224:VAL:HG21	1:D:227:ALA:HB2	2.03	0.40
1:D:229:ARG:HB3	1:D:230:ASP:H	1.75	0.40
1:A:99:TRP:O	1:A:102:ARG:CG	2.67	0.40
1:B:63:VAL:HG11	1:B:120:LEU:HD21	1.97	0.40
1:C:45:LYS:HG3	1:C:49:LEU:HD22	2.02	0.40
1:C:122:LYS:CE	1:C:123:ASP:OD2	2.69	0.40
1:C:140:PHE:HZ	1:C:157:LEU:CD2	2.33	0.40
1:C:202:ILE:HD13	1:C:220:TYR:CD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:PHE:C	1:D:142:HIS:N	2.77	0.40
1:D:159:ASN:O	1:D:162:SER:HB3	2.21	0.40
1:D:224:VAL:O	1:D:226:GLY:N	2.54	0.40
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.85	0.40
1:D:153:HIS:CD2	1:D:245:HIS:NE2	2.90	0.40
1:D:254:VAL:HG12	1:D:255:GLN:N	2.36	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	250/292 (86%)	185 (74%)	49 (20%)	16 (6%)	1	6
1	B	250/292 (86%)	186 (74%)	49 (20%)	15 (6%)	1	7
1	C	250/292 (86%)	187 (75%)	50 (20%)	13 (5%)	1	9
1	D	250/292 (86%)	184 (74%)	48 (19%)	18 (7%)	1	4
All	All	1000/1168 (86%)	742 (74%)	196 (20%)	62 (6%)	1	6

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	269	ASP
1	B	269	ASP
1	C	261	ARG
1	D	48	LEU
1	A	127	GLY
1	B	48	LEU
1	D	150	GLN
1	A	121	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	176	ASN
1	A	192	ILE
1	A	248	ALA
1	B	65	CYS
1	B	112	ILE
1	B	190	LYS
1	C	88	ASP
1	D	46	ALA
1	D	92	LYS
1	D	118	LEU
1	D	229	ARG
1	D	290	LYS
1	B	77	GLU
1	B	225	PRO
1	B	258	PHE
1	B	272	PRO
1	C	73	MET
1	C	281	PRO
1	D	88	ASP
1	D	110	TRP
1	D	125	PRO
1	A	213	ALA
1	A	275	PRO
1	B	150	GLN
1	B	278	ALA
1	B	279	TYR
1	C	89	LYS
1	C	150	GLN
1	C	248	ALA
1	C	282	CYS
1	D	66	GLY
1	D	106	ALA
1	D	244	PRO
1	A	119	THR
1	A	225	PRO
1	A	244	PRO
1	B	101	ARG
1	C	74	LEU
1	C	262	CYS
1	D	44	TYR
1	D	90	MET
1	D	270	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	63	VAL
1	A	75	VAL
1	A	216	VAL
1	B	69	VAL
1	C	184	GLY
1	C	268	GLY
1	D	225	PRO
1	D	260	GLY
1	A	232	ALA
1	C	72	ILE
1	B	275	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	211/242 (87%)	121 (57%)	90 (43%)	0	0
1	B	211/242 (87%)	124 (59%)	87 (41%)	0	0
1	C	211/242 (87%)	127 (60%)	84 (40%)	0	1
1	D	211/242 (87%)	132 (63%)	79 (37%)	0	1
All	All	844/968 (87%)	504 (60%)	340 (40%)	0	0

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	GLU
1	A	48	LEU
1	A	49	LEU
1	A	52	LEU
1	A	54	GLN
1	A	57	CYS
1	A	60	VAL
1	A	61	LEU
1	A	63	VAL
1	A	67	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	VAL
1	A	70	ASP
1	A	72	ILE
1	A	75	VAL
1	A	77	GLU
1	A	81	VAL
1	A	82	THR
1	A	83	SER
1	A	88	ASP
1	A	91	LEU
1	A	95	LEU
1	A	97	GLU
1	A	98	ARG
1	A	100	ASN
1	A	102	ARG
1	A	103	LYS
1	A	104	GLU
1	A	109	LYS
1	A	112	ILE
1	A	113	GLU
1	A	114	GLU
1	A	118	LEU
1	A	122	LYS
1	A	130	PHE
1	A	136	LEU
1	A	143	LEU
1	A	147	LYS
1	A	154	ARG
1	A	155	LEU
1	A	157	LEU
1	A	160	ILE
1	A	165	ARG
1	A	169	LEU
1	A	170	LEU
1	A	172	ILE
1	A	175	LYS
1	A	176	ASN
1	A	180	ILE
1	A	181	LEU
1	A	182	SER
1	A	183	THR
1	A	185	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	190	LYS
1	A	191	ASN
1	A	192	ILE
1	A	194	TYR
1	A	195	LYS
1	A	198	LEU
1	A	200	LYS
1	A	205	SER
1	A	209	VAL
1	A	212	LYS
1	A	215	MET
1	A	217	THR
1	A	218	LEU
1	A	223	GLN
1	A	224	VAL
1	A	230	ASP
1	A	236	SER
1	A	237	LYS
1	A	239	ARG
1	A	240	LEU
1	A	247	LEU
1	A	249	SER
1	A	251	THR
1	A	253	LEU
1	A	254	VAL
1	A	255	GLN
1	A	261	ARG
1	A	263	GLN
1	A	265	SER
1	A	266	VAL
1	A	267	LEU
1	A	271	LYS
1	A	274	ARG
1	A	277	GLN
1	A	282	CYS
1	A	285	ILE
1	A	288	LEU
1	A	289	LYS
1	B	41	THR
1	B	45	LYS
1	B	48	LEU
1	B	49	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	LEU
1	B	52	LEU
1	B	53	ARG
1	B	59	ARG
1	B	60	VAL
1	B	63	VAL
1	B	67	THR
1	B	71	SER
1	B	74	LEU
1	B	80	SER
1	B	81	VAL
1	B	82	THR
1	B	83	SER
1	B	87	SER
1	B	88	ASP
1	B	89	LYS
1	B	90	MET
1	B	91	LEU
1	B	92	LYS
1	B	95	LEU
1	B	96	LYS
1	B	97	GLU
1	B	98	ARG
1	B	103	LYS
1	B	113	GLU
1	B	114	GLU
1	B	120	LEU
1	B	122	LYS
1	B	128	ASP
1	B	134	ILE
1	B	136	LEU
1	B	143	LEU
1	B	147	LYS
1	B	150	GLN
1	B	154	ARG
1	B	155	LEU
1	B	157	LEU
1	B	158	LYS
1	B	162	SER
1	B	163	MET
1	B	164	VAL
1	B	165	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	LEU
1	B	171	VAL
1	B	172	ILE
1	B	176	ASN
1	B	180	ILE
1	B	181	LEU
1	B	183	THR
1	B	185	CYS
1	B	190	LYS
1	B	198	LEU
1	B	199	THR
1	B	200	LYS
1	B	205	SER
1	B	207	LEU
1	B	209	VAL
1	B	211	ASN
1	B	212	LYS
1	B	215	MET
1	B	218	LEU
1	B	221	THR
1	B	223	GLN
1	B	224	VAL
1	B	229	ARG
1	B	230	ASP
1	B	237	LYS
1	B	239	ARG
1	B	240	LEU
1	B	242	TYR
1	B	251	THR
1	B	254	VAL
1	B	263	GLN
1	B	265	SER
1	B	266	VAL
1	B	267	LEU
1	B	271	LYS
1	B	274	ARG
1	B	277	GLN
1	B	285	ILE
1	B	287	VAL
1	B	288	LEU
1	B	291	THR
1	C	41	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	43	GLU
1	C	44	TYR
1	C	45	LYS
1	C	49	LEU
1	C	52	LEU
1	C	54	GLN
1	C	60	VAL
1	C	69	VAL
1	C	72	ILE
1	C	74	LEU
1	C	75	VAL
1	C	81	VAL
1	C	82	THR
1	C	83	SER
1	C	90	MET
1	C	92	LYS
1	C	95	LEU
1	C	96	LYS
1	C	97	GLU
1	C	102	ARG
1	C	104	GLU
1	C	107	PHE
1	C	109	LYS
1	C	112	ILE
1	C	118	LEU
1	C	121	ASP
1	C	122	LYS
1	C	123	ASP
1	C	128	ASP
1	C	133	VAL
1	C	136	LEU
1	C	143	LEU
1	C	147	LYS
1	C	151	SER
1	C	157	LEU
1	C	158	LYS
1	C	162	SER
1	C	164	VAL
1	C	165	ARG
1	C	169	LEU
1	C	172	ILE
1	C	175	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	179	TYR
1	C	180	ILE
1	C	181	LEU
1	C	182	SER
1	C	190	LYS
1	C	192	ILE
1	C	194	TYR
1	C	195	LYS
1	C	198	LEU
1	C	199	THR
1	C	200	LYS
1	C	202	ILE
1	C	203	THR
1	C	206	VAL
1	C	212	LYS
1	C	217	THR
1	C	223	GLN
1	C	224	VAL
1	C	229	ARG
1	C	237	LYS
1	C	239	ARG
1	C	240	LEU
1	C	241	SER
1	C	242	TYR
1	C	247	LEU
1	C	256	GLU
1	C	261	ARG
1	C	263	GLN
1	C	264	HIS
1	C	265	SER
1	C	266	VAL
1	C	267	LEU
1	C	269	ASP
1	C	270	PHE
1	C	274	ARG
1	C	277	GLN
1	C	280	VAL
1	C	285	ILE
1	C	288	LEU
1	C	289	LYS
1	C	290	LYS
1	D	41	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	43	GLU
1	D	45	LYS
1	D	49	LEU
1	D	51	LEU
1	D	52	LEU
1	D	53	ARG
1	D	59	ARG
1	D	71	SER
1	D	73	MET
1	D	75	VAL
1	D	77	GLU
1	D	80	SER
1	D	82	THR
1	D	84	VAL
1	D	90	MET
1	D	92	LYS
1	D	95	LEU
1	D	97	GLU
1	D	98	ARG
1	D	100	ASN
1	D	102	ARG
1	D	104	GLU
1	D	113	GLU
1	D	119	THR
1	D	122	LYS
1	D	128	ASP
1	D	133	VAL
1	D	143	LEU
1	D	147	LYS
1	D	149	ASP
1	D	150	GLN
1	D	154	ARG
1	D	157	LEU
1	D	160	ILE
1	D	163	MET
1	D	165	ARG
1	D	169	LEU
1	D	172	ILE
1	D	173	ASP
1	D	174	HIS
1	D	175	LYS
1	D	176	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	181	LEU
1	D	182	SER
1	D	183	THR
1	D	190	LYS
1	D	194	TYR
1	D	195	LYS
1	D	196	SER
1	D	198	LEU
1	D	199	THR
1	D	200	LYS
1	D	201	ASP
1	D	202	ILE
1	D	204	THR
1	D	205	SER
1	D	207	LEU
1	D	208	THR
1	D	216	VAL
1	D	218	LEU
1	D	221	THR
1	D	224	VAL
1	D	229	ARG
1	D	230	ASP
1	D	240	LEU
1	D	247	LEU
1	D	254	VAL
1	D	256	GLU
1	D	265	SER
1	D	266	VAL
1	D	267	LEU
1	D	277	GLN
1	D	280	VAL
1	D	285	ILE
1	D	287	VAL
1	D	288	LEU
1	D	290	LYS
1	D	291	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	55	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	58	HIS
1	A	100	ASN
1	A	142	HIS
1	A	153	HIS
1	A	159	ASN
1	A	174	HIS
1	A	176	ASN
1	A	211	ASN
1	A	255	GLN
1	A	264	HIS
1	B	58	HIS
1	B	100	ASN
1	B	142	HIS
1	B	150	GLN
1	B	153	HIS
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN
1	B	211	ASN
1	B	214	HIS
1	B	245	HIS
1	B	255	GLN
1	B	263	GLN
1	C	54	GLN
1	C	159	ASN
1	C	174	HIS
1	C	176	ASN
1	C	210	ASN
1	C	211	ASN
1	C	223	GLN
1	C	263	GLN
1	C	264	HIS
1	C	286	HIS
1	D	116	ASN
1	D	153	HIS
1	D	159	ASN
1	D	176	ASN
1	D	210	ASN
1	D	223	GLN
1	D	255	GLN
1	D	263	GLN
1	D	264	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SAH	D	4301	-	27,28,28	1.11	2 (7%)	36,40,40	2.30	9 (25%)
2	SAH	C	3301	-	27,28,28	1.02	1 (3%)	36,40,40	2.46	13 (36%)
2	SAH	A	1301	-	27,28,28	1.09	2 (7%)	36,40,40	2.63	12 (33%)
2	SAH	B	2301	-	27,28,28	1.09	1 (3%)	36,40,40	2.25	6 (16%)

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	D	4301	-	-	6/15/31/31	0/3/3/3
2	SAH	C	3301	-	-	7/15/31/31	0/3/3/3
2	SAH	A	1301	-	-	3/15/31/31	0/3/3/3
2	SAH	B	2301	-	-	4/15/31/31	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2301	SAH	C5-N7	-3.66	1.32	1.39
2	D	4301	SAH	C5-N7	-3.63	1.32	1.39
2	A	1301	SAH	C5-N7	-3.58	1.32	1.39
2	C	3301	SAH	C5-N7	-3.23	1.33	1.39
2	D	4301	SAH	C4-N9	-2.12	1.33	1.37
2	A	1301	SAH	C4-N9	-2.10	1.33	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	SAH	C5-C4-N3	-7.25	116.74	126.72
2	B	2301	SAH	C5-C4-N3	-7.08	116.97	126.72
2	D	4301	SAH	C5-C4-N3	-6.93	117.18	126.72
2	C	3301	SAH	C5-C4-N3	-6.75	117.42	126.72
2	A	1301	SAH	N3-C4-N9	6.45	138.13	127.17
2	B	2301	SAH	N3-C4-N9	6.06	137.47	127.17
2	C	3301	SAH	N3-C4-N9	5.73	136.91	127.17
2	A	1301	SAH	C4'-O4'-C1'	-5.57	97.17	109.47
2	D	4301	SAH	N3-C4-N9	5.25	136.10	127.17
2	B	2301	SAH	C6-C5-C4	5.18	124.25	117.18
2	D	4301	SAH	C6-C5-C4	5.06	124.08	117.18
2	A	1301	SAH	C6-C5-C4	5.02	124.04	117.18
2	D	4301	SAH	C6-C5-N7	-4.69	123.05	132.09
2	C	3301	SAH	C6-C5-C4	4.67	123.56	117.18
2	C	3301	SAH	C4'-O4'-C1'	-4.60	99.31	109.47
2	A	1301	SAH	C6-C5-N7	-4.41	123.59	132.09
2	A	1301	SAH	O4'-C1'-N9	4.27	116.28	108.09
2	B	2301	SAH	C6-C5-N7	-4.24	123.92	132.09
2	D	4301	SAH	O4'-C1'-N9	4.20	116.15	108.09
2	C	3301	SAH	O4'-C4'-C5'	4.06	119.29	108.83
2	C	3301	SAH	C6-C5-N7	-3.75	124.87	132.09
2	A	1301	SAH	N3-C2-N1	-3.54	123.22	128.58
2	B	2301	SAH	N3-C2-N1	-3.52	123.26	128.58
2	C	3301	SAH	N3-C2-N1	-3.38	123.47	128.58
2	A	1301	SAH	C2-N3-C4	3.28	119.85	111.83
2	A	1301	SAH	O4'-C1'-C2'	-3.23	99.70	106.62
2	B	2301	SAH	C2-N3-C4	3.12	119.45	111.83
2	C	3301	SAH	C2-N3-C4	3.09	119.37	111.83
2	D	4301	SAH	N3-C2-N1	-3.07	123.94	128.58
2	C	3301	SAH	O4'-C1'-N9	3.03	113.91	108.09
2	D	4301	SAH	O3'-C3'-C2'	-3.00	102.19	111.82
2	D	4301	SAH	C2-N3-C4	2.90	118.92	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3301	SAH	O4'-C1'-C2'	-2.44	101.39	106.62
2	C	3301	SAH	N9-C8-N7	-2.26	110.72	113.94
2	C	3301	SAH	C2'-C1'-N9	2.24	118.86	113.30
2	A	1301	SAH	C4-N9-C8	2.17	108.01	105.74
2	C	3301	SAH	C4-N9-C8	2.15	108.00	105.74
2	D	4301	SAH	O2'-C2'-C3'	-2.14	104.95	111.82
2	A	1301	SAH	O4'-C4'-C5'	2.06	114.14	108.83
2	A	1301	SAH	N9-C8-N7	-2.05	111.03	113.94

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	SAH	O4'-C4'-C5'-SD
2	A	1301	SAH	C3'-C4'-C5'-SD
2	C	3301	SAH	N-CA-CB-CG
2	C	3301	SAH	C-CA-CB-CG
2	C	3301	SAH	O-C-CA-N
2	C	3301	SAH	CB-CG-SD-C5'
2	D	4301	SAH	N-CA-CB-CG
2	D	4301	SAH	C-CA-CB-CG
2	A	1301	SAH	CA-CB-CG-SD
2	C	3301	SAH	OXT-C-CA-N
2	D	4301	SAH	OXT-C-CA-N
2	B	2301	SAH	C2'-C1'-N9-C8
2	D	4301	SAH	CA-CB-CG-SD
2	C	3301	SAH	O-C-CA-CB
2	C	3301	SAH	OXT-C-CA-CB
2	B	2301	SAH	O4'-C1'-N9-C8
2	D	4301	SAH	CB-CG-SD-C5'
2	B	2301	SAH	OXT-C-CA-CB
2	D	4301	SAH	C2'-C1'-N9-C8
2	B	2301	SAH	O-C-CA-CB

There are no ring outliers.

4 monomers are involved in 26 short contacts:

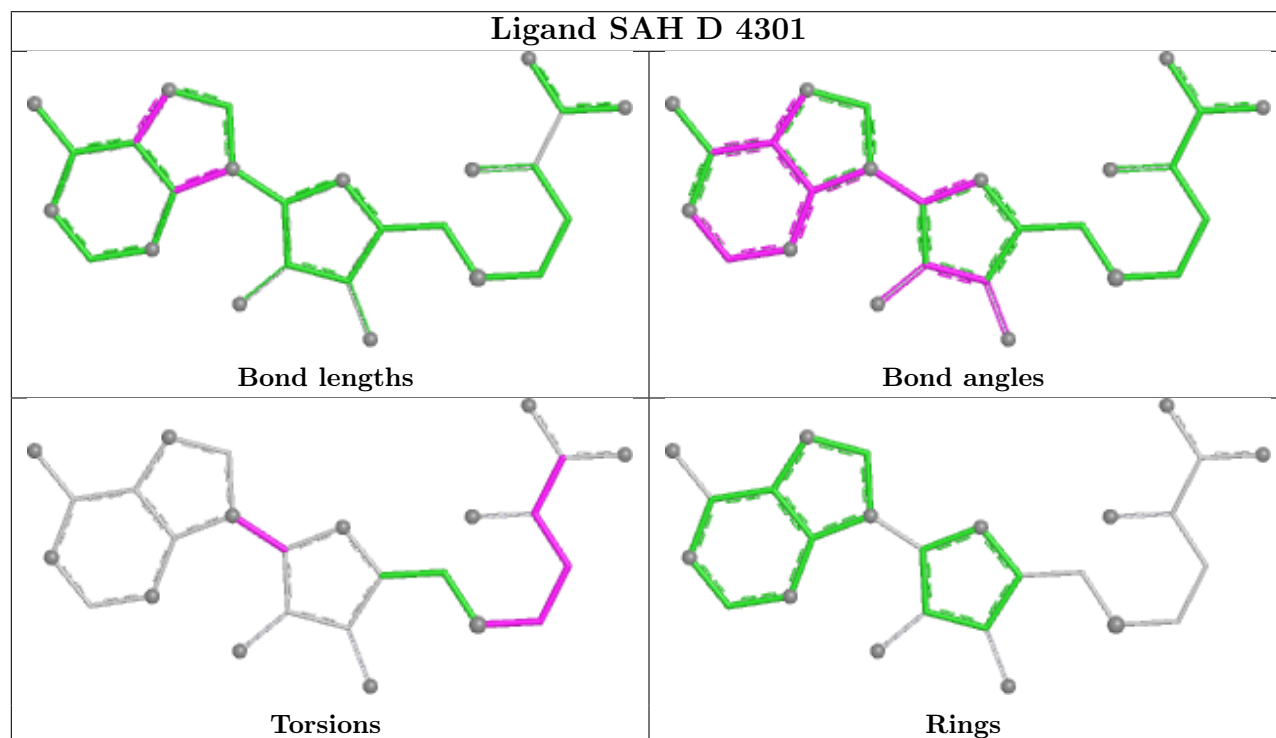
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4301	SAH	6	0
2	C	3301	SAH	5	0
2	A	1301	SAH	10	0

Continued on next page...

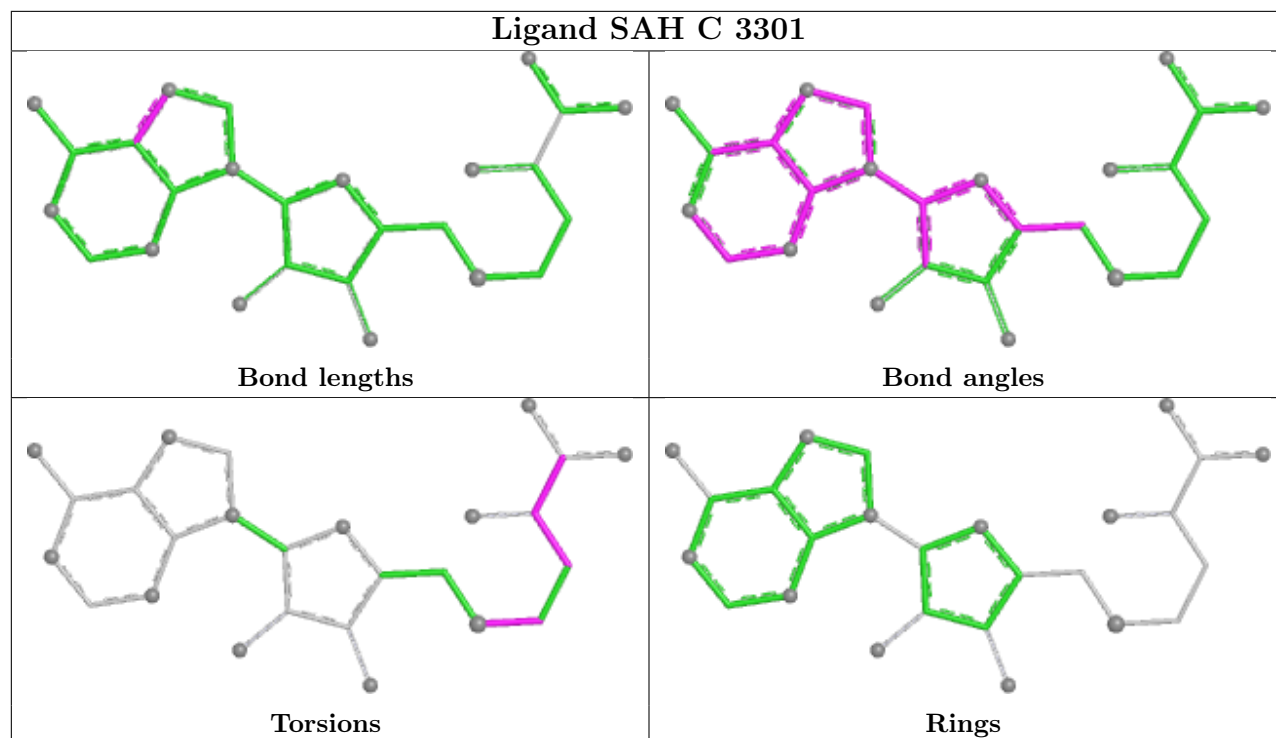
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2301	SAH	5	0

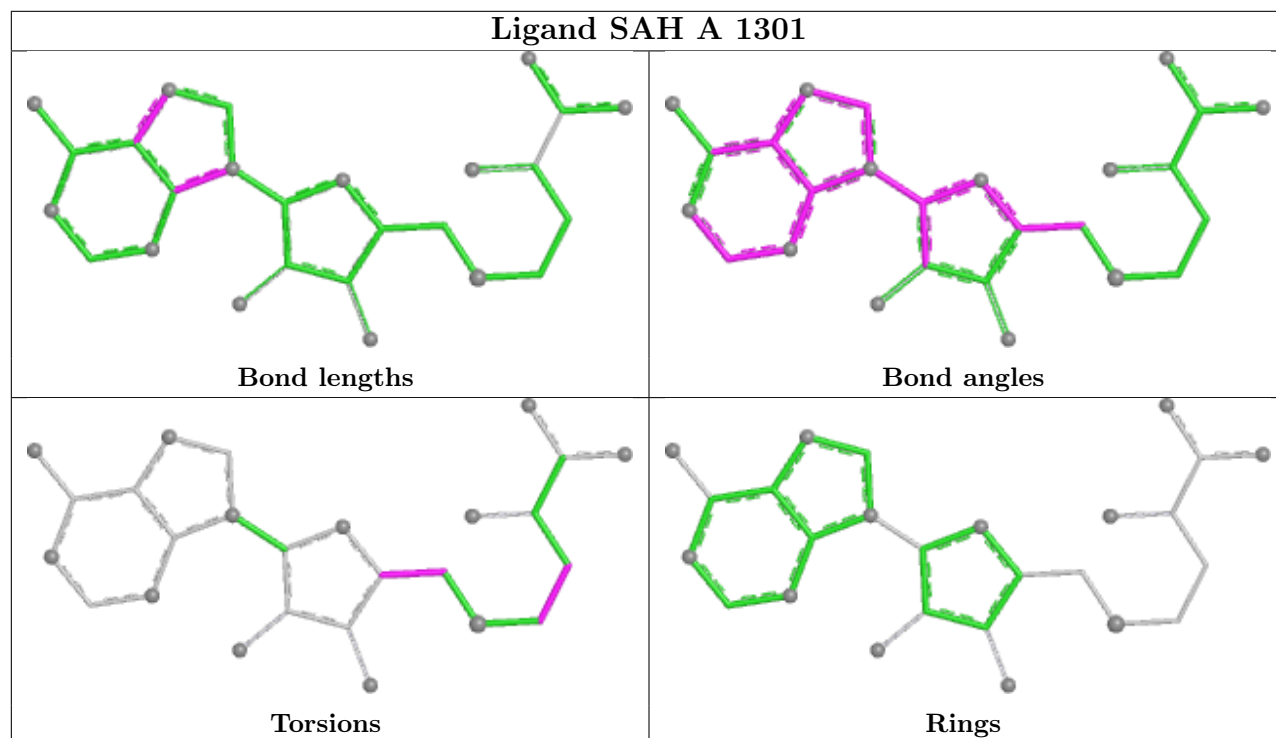
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

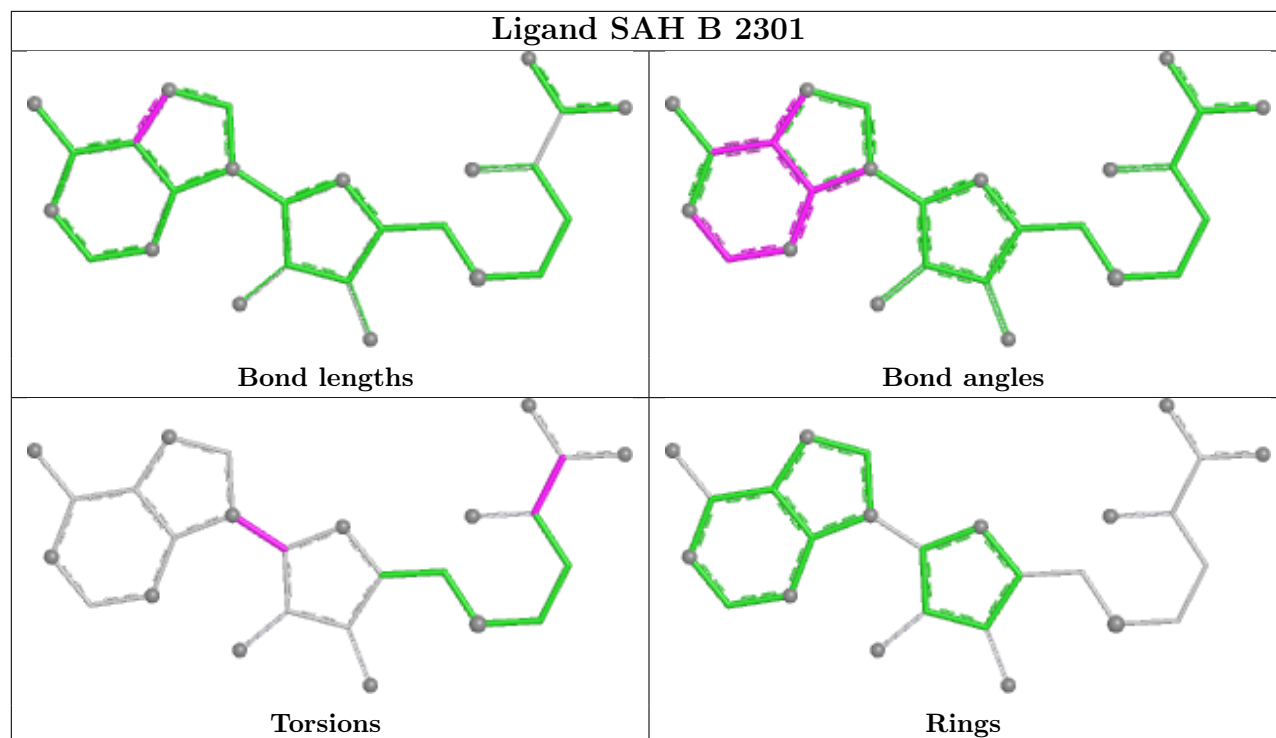


Ligand SAH C 3301



Ligand SAH A 1301





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.