



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:45 am GMT

PDB ID : 1D4F
Title : CRYSTAL STRUCTURE OF RECOMBINANT RAT-LIVER D244E MUTANT S-ADENOSYLHOMOCYSTEINE HYDROLASE
Authors : Komoto, J.; Huang, Y.; Takusagawa, F.; Gomi, T.; Ogawa, H.; Takata, Y.; Fujioka, M.
Deposited on : 2000-06-22
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

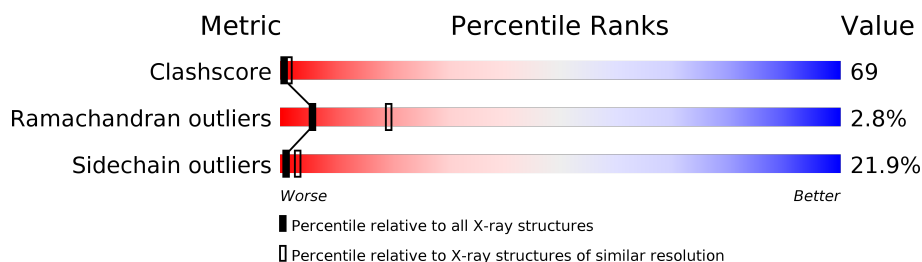
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>31%</div> <div>55%</div> <div>14%</div> </div>
1	B	431	<div> <div>35%</div> <div>49%</div> <div>15%</div> <div>.</div> </div>
1	C	431	<div> <div>27%</div> <div>55%</div> <div>16%</div> <div>.</div> </div>
1	D	431	<div> <div>31%</div> <div>52%</div> <div>16%</div> </div>

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	NAD	A	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14005 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 S-ADENOSYLHOMOCYSTEINE HYDROLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	B	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	C	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			
1	D	430	Total	C	N	O	S	0	0	0
			3320	2109	571	615	25			

There are 4 discrepancies between the modelled and reference sequences:

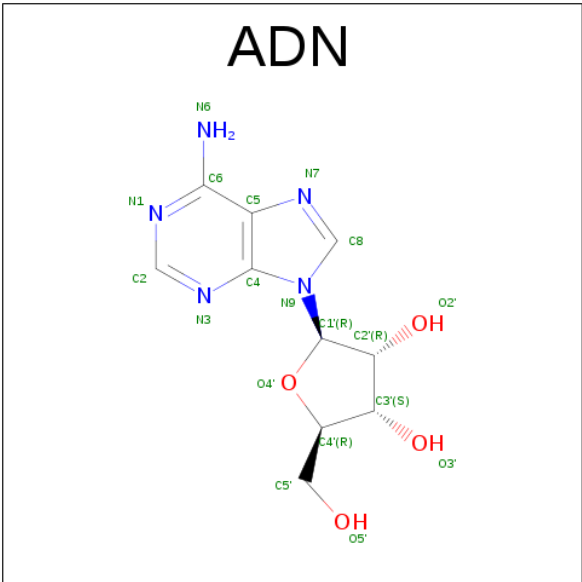
Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLU	ASP	ENGINEERED	UNP P10760
B	244	GLU	ASP	ENGINEERED	UNP P10760
C	244	GLU	ASP	ENGINEERED	UNP P10760
D	244	GLU	ASP	ENGINEERED	UNP P10760

- Molecule 2 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
2	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 3 is ADENOSINE (three-letter code: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		
3	C	1	Total	C	N	O	0	0
			19	10	5	4		
3	D	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is water.

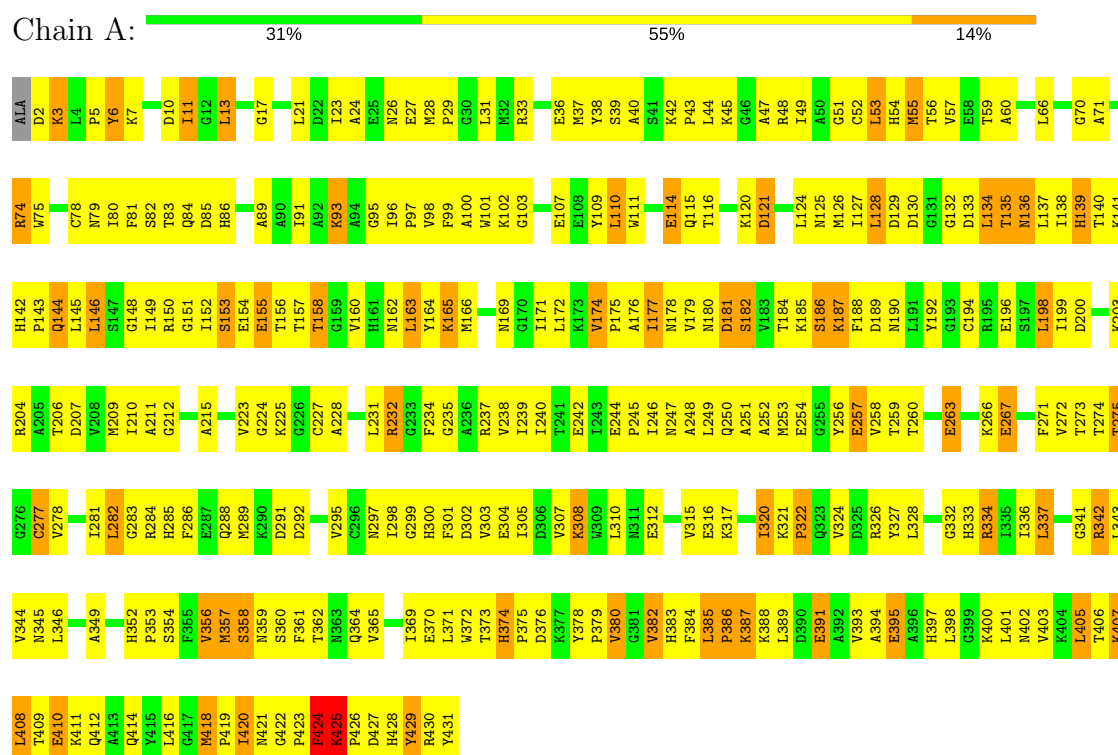
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	137	Total	O	0	0
			137	137		
4	B	118	Total	O	0	0
			118	118		
4	C	120	Total	O	0	0
			120	120		
4	D	98	Total	O	0	0
			98	98		

3 Residue-property plots

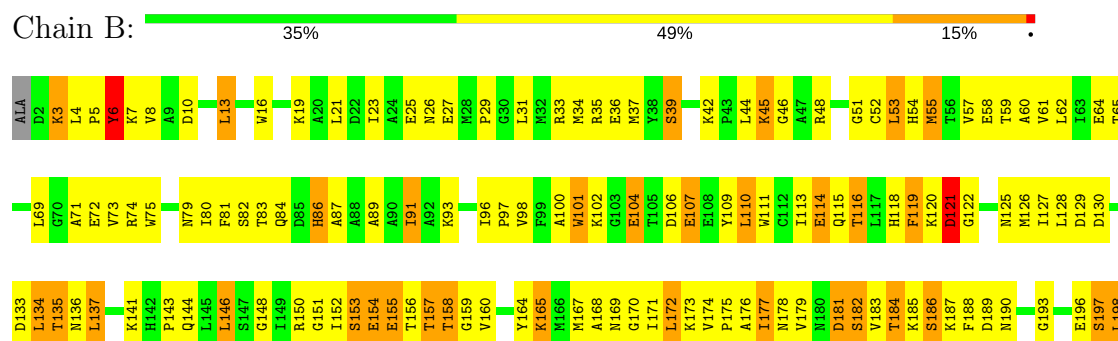
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

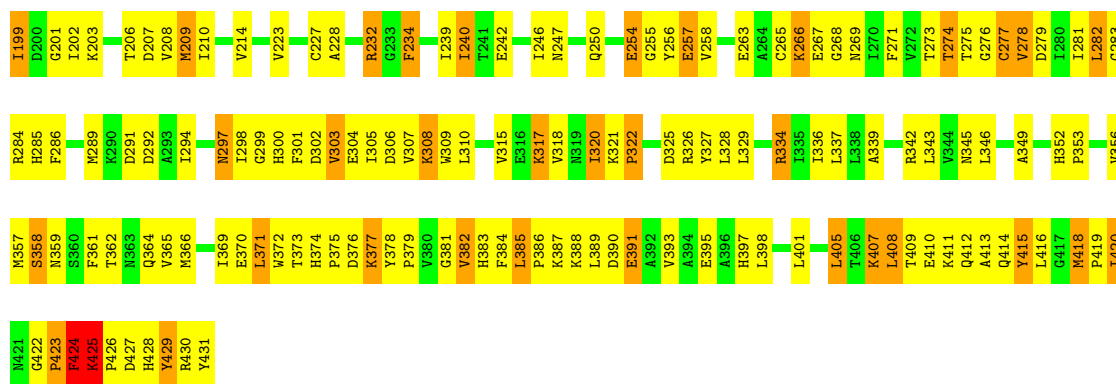
Note EDS was not executed.

• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE



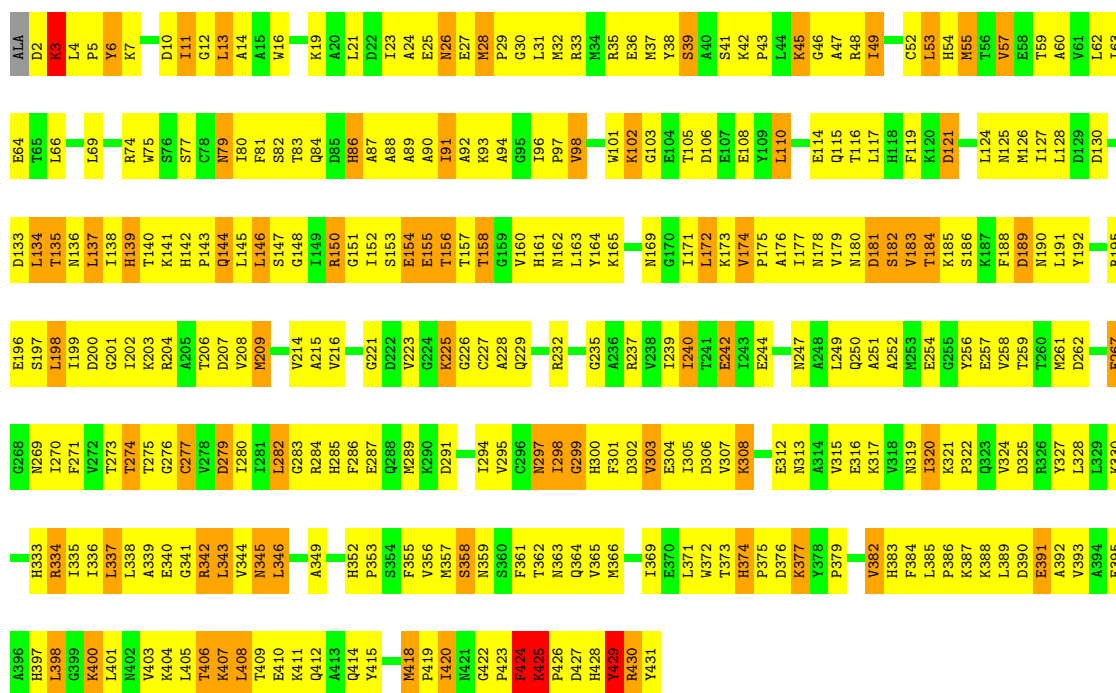
• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE





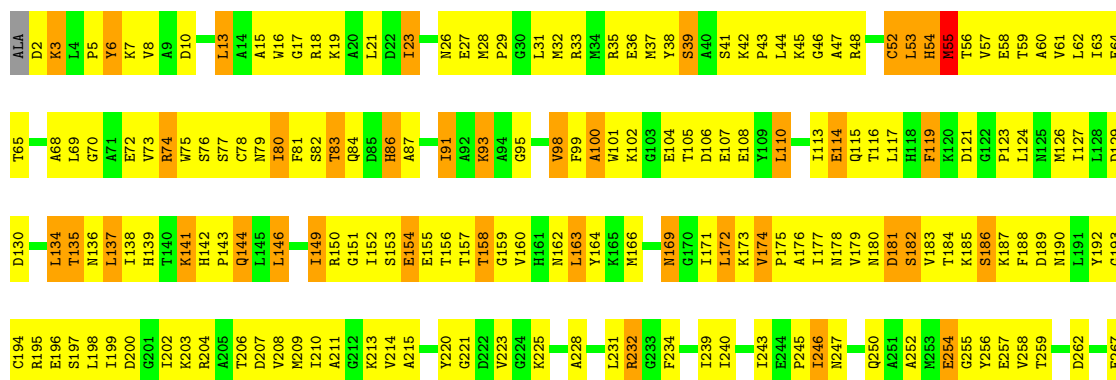
• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE

Chain C: 27% 55% 16%



• Molecule 1: S-ADENOSYLHOMOCYSTEINE HYDROLASE

Chain D: 31% 52% 16%



T406	A339	G268
K407	E340	N269
L408	G341	
T409	R342	T273
E410	L343	T274
K411	V344	T275
Q412	N345	G276
A413		G277
Q414	A349	V278
Y415		T279
L416	H352	T280
G417	P353	T281
M418		L282
P419	V356	G283
I420	M357	R284
N421	S358	H285
G422		F286
P423	F361	E287
F424	T362	
K425	N363	D291
P426	Q364	D292
D427	V365	
H428	M366	V295
Y429		G296
R430	I369	N297
Y431	E370	T298
	L371	G299
	W372	H300
	T373	F301
	H374	
	P375	E304
	G376	L305
	K377	D306
	Y378	V307
	P379	K308
	V380	W309
	G381	L310
	H382	N311
	K383	E312
	F384	
	L385	K317
	P386	V318
	K387	N319
	K388	T320
	L389	K321
	D390	P322
	E391	Q323
	A392	V324
	V393	D325
	A394	R326
	E395	Y327
	A396	L328
	H397	
	L398	N331
	L401	R334
	M402	T335
	V403	T336
	K404	L337
	L405	T338

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.00Å 223.00Å 91.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (8.00-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.197 , 0.248	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14005	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/3385	0.59	0/4580
1	B	0.31	0/3385	0.59	0/4580
1	C	0.32	0/3385	0.59	0/4580
1	D	0.32	0/3385	0.58	0/4580
All	All	0.32	0/13540	0.59	0/18320

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3343	465	0
1	B	3320	0	3343	480	0
1	C	3320	0	3343	497	0
1	D	3320	0	3343	513	0
2	A	44	0	26	22	0
2	B	44	0	26	16	0
2	C	44	0	26	7	0
2	D	44	0	26	9	0
3	A	19	0	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	19	0	13	2	0
3	C	19	0	13	1	0
3	D	19	0	13	1	0
4	A	137	0	0	3	0
4	B	118	0	0	8	0
4	C	120	0	0	7	0
4	D	98	0	0	3	0
All	All	14005	0	13528	1856	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 69.

All (1856) 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:419:PRO:CG	1:A:422:GLY:HA3	1.36	1.53
1:A:419:PRO:HG2	1:A:422:GLY:C	1.23	1.52
1:A:419:PRO:HG2	1:A:422:GLY:CA	1.40	1.51
1:D:419:PRO:HG2	1:D:422:GLY:C	1.31	1.45
1:A:419:PRO:CG	1:A:422:GLY:CA	1.91	1.40
1:D:178:ASN:ND2	1:D:181:ASP:HB2	1.40	1.34
1:C:137:LEU:O	1:C:137:LEU:HD12	1.23	1.33
1:D:419:PRO:HG2	1:D:422:GLY:CA	1.56	1.33
1:A:91:ILE:HG22	1:A:98:VAL:CG2	1.61	1.29
1:A:225:LYS:NZ	1:A:250:GLN:HE22	1.31	1.29
1:A:387:LYS:NZ	1:A:425:LYS:HG3	1.43	1.28
1:D:408:LEU:O	1:D:420:ILE:HD12	1.35	1.27
1:B:158:THR:HG21	1:B:301:PHE:CE2	1.70	1.25
1:A:425:LYS:HA	1:A:425:LYS:NZ	1.49	1.25
1:A:425:LYS:HD3	1:A:431:TYR:OH	1.22	1.24
1:B:424:PHE:O	1:B:426:PRO:HD3	1.11	1.24
1:D:169:ASN:HB2	1:D:171:ILE:CD1	1.68	1.24
1:D:419:PRO:CG	1:D:422:GLY:HA3	1.67	1.23
1:C:244:GLU:OE2	1:D:425:LYS:HD2	1.37	1.21
1:D:81:PHE:CE2	1:D:342:ARG:HD2	1.75	1.21
1:D:418:MET:HG3	1:D:424:PHE:CD1	1.75	1.20
1:D:407:LYS:HB2	1:D:407:LYS:NZ	1.42	1.19
1:A:419:PRO:CB	1:A:422:GLY:HA3	1.72	1.19
1:D:373:THR:HG22	1:D:374:HIS:ND1	1.57	1.19
1:A:424:PHE:O	1:A:426:PRO:HD3	1.39	1.18
1:C:419:PRO:HB2	1:C:422:GLY:N	1.58	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HD3	1:B:431:TYR:OH	1.43	1.17
1:A:373:THR:HG22	1:A:374:HIS:CE1	1.81	1.16
1:D:373:THR:HG22	1:D:374:HIS:CE1	1.80	1.16
1:B:424:PHE:O	1:B:426:PRO:CD	1.95	1.15
1:D:178:ASN:HD21	1:D:181:ASP:CB	1.59	1.15
1:C:275:THR:HG21	1:C:280:ILE:HD11	1.16	1.14
1:D:386:PRO:HG2	1:D:389:LEU:HD12	1.29	1.14
1:A:419:PRO:CG	1:A:422:GLY:C	2.08	1.14
1:A:291:ASP:OD2	1:A:334:ARG:NH2	1.78	1.14
1:A:419:PRO:HG3	1:A:422:GLY:HA3	1.28	1.14
1:A:373:THR:HG22	1:A:374:HIS:ND1	1.63	1.13
1:B:419:PRO:HG2	1:B:422:GLY:C	1.69	1.13
1:B:177:ILE:HG13	1:B:371:LEU:HD21	1.30	1.12
1:A:91:ILE:CG2	1:A:98:VAL:HG21	1.79	1.12
1:C:419:PRO:HB2	1:C:422:GLY:CA	1.78	1.12
1:A:91:ILE:CG2	1:A:98:VAL:CG2	2.28	1.11
1:C:430:ARG:NH1	1:D:187:LYS:HE3	1.64	1.11
1:B:278:VAL:HG12	1:B:303:VAL:HB	1.21	1.10
1:C:299:GLY:O	1:C:343:LEU:CD1	1.99	1.10
1:D:419:PRO:CG	1:D:422:GLY:CA	2.24	1.10
1:B:362:THR:O	1:B:366:MET:HG3	1.49	1.09
1:C:110:LEU:HD13	1:C:110:LEU:O	1.50	1.09
1:A:126:MET:HE3	1:A:150:ARG:HB3	1.24	1.09
1:A:419:PRO:HB2	1:A:422:GLY:N	1.68	1.09
1:D:169:ASN:HB2	1:D:171:ILE:HD12	1.32	1.08
1:B:419:PRO:HG2	1:B:422:GLY:CA	1.82	1.08
1:C:27:GLU:O	1:C:29:PRO:HD3	1.51	1.08
1:D:419:PRO:CB	1:D:422:GLY:HA3	1.82	1.08
1:D:419:PRO:HB2	1:D:422:GLY:H	1.17	1.08
1:A:91:ILE:HG22	1:A:98:VAL:HG21	1.12	1.08
1:A:419:PRO:HB2	1:A:422:GLY:H	1.16	1.07
1:D:408:LEU:O	1:D:420:ILE:CD1	2.01	1.07
1:D:419:PRO:HB2	1:D:422:GLY:N	1.69	1.07
1:A:387:LYS:HZ1	1:A:425:LYS:HG3	0.93	1.07
1:A:199:ILE:HD11	1:A:231:LEU:HD23	1.35	1.06
1:A:425:LYS:CD	1:A:431:TYR:OH	2.01	1.06
1:A:373:THR:CG2	1:A:374:HIS:CE1	2.38	1.06
1:D:317:LYS:HG3	1:D:327:TYR:CE2	1.90	1.06
1:C:177:ILE:CG1	1:C:371:LEU:HD21	1.85	1.05
1:D:158:THR:HG21	1:D:301:PHE:HE2	1.18	1.05
1:D:21:LEU:HD23	1:D:57:VAL:HG13	1.38	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:C	1:C:137:LEU:HD12	1.74	1.05
1:B:158:THR:HG21	1:B:301:PHE:HE2	0.91	1.05
1:D:158:THR:HG21	1:D:301:PHE:CE2	1.91	1.05
1:A:10:ASP:HB3	1:A:13:LEU:HD22	1.37	1.04
1:C:425:LYS:NZ	1:C:426:PRO:CD	2.20	1.04
1:B:317:LYS:HD2	1:B:327:TYR:CE2	1.91	1.04
1:C:177:ILE:HG13	1:C:371:LEU:HD21	1.08	1.04
1:D:221:GLY:O	1:D:225:LYS:HG3	1.55	1.03
1:A:48:ARG:HD3	1:A:121:ASP:OD2	1.55	1.03
1:A:277:CYS:HB3	1:B:416:LEU:HD21	1.36	1.03
1:A:425:LYS:HA	1:A:425:LYS:HZ2	0.91	1.03
1:A:126:MET:CE	1:A:150:ARG:HB3	1.89	1.03
1:A:169:ASN:HB2	1:A:171:ILE:HD12	1.38	1.03
1:A:410:GLU:OE2	1:A:414:GLN:HG3	1.58	1.03
1:D:419:PRO:CG	1:D:422:GLY:C	2.27	1.02
1:B:157:THR:HB	2:B:502:NAD:H3D	1.37	1.02
1:D:407:LYS:CB	1:D:407:LYS:NZ	2.19	1.02
1:B:278:VAL:CG1	1:B:303:VAL:HB	1.88	1.02
1:C:425:LYS:HA	1:C:425:LYS:CE	1.87	1.02
1:D:10:ASP:HB3	1:D:13:LEU:HD22	1.40	1.02
1:D:126:MET:HE3	1:D:150:ARG:HB3	1.41	1.01
1:C:315:VAL:HG22	1:C:330:LYS:HG2	1.36	1.01
1:D:169:ASN:HB2	1:D:171:ILE:HD11	1.42	1.01
1:C:425:LYS:NZ	1:C:426:PRO:HD2	1.76	1.01
1:D:291:ASP:OD2	1:D:334:ARG:NH2	1.92	1.01
1:A:430:ARG:HA	1:B:430:ARG:HG2	1.43	1.01
1:D:279:ASP:HB3	1:D:282:LEU:HD11	1.40	1.00
1:C:419:PRO:CB	1:C:422:GLY:HA3	1.91	1.00
1:A:177:ILE:HG13	1:A:371:LEU:HD21	1.44	1.00
1:C:10:ASP:HB3	1:C:13:LEU:HD22	1.40	1.00
1:B:158:THR:CG2	1:B:301:PHE:HE2	1.74	1.00
1:A:153:SER:HB3	1:A:364:GLN:NE2	1.78	0.99
1:A:154:GLU:O	1:A:179:VAL:HB	1.62	0.99
1:A:277:CYS:CB	1:B:416:LEU:HD21	1.92	0.99
1:D:369:ILE:O	1:D:373:THR:HB	1.61	0.99
1:D:39:SER:O	1:D:42:LYS:HG2	1.61	0.99
1:B:425:LYS:CD	1:B:431:TYR:OH	2.09	0.99
1:A:81:PHE:O	1:A:102:LYS:HE3	1.63	0.98
1:B:91:ILE:HG22	1:B:98:VAL:CG2	1.93	0.98
1:D:386:PRO:HG2	1:D:389:LEU:CD1	1.92	0.98
1:A:299:GLY:O	1:A:343:LEU:CD1	2.11	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:HB	1:A:84:GLN:OE1	1.65	0.97
1:B:299:GLY:O	1:B:343:LEU:CD1	2.12	0.97
1:C:164:TYR:CZ	1:D:428:HIS:HE1	1.82	0.97
1:C:418:MET:SD	1:C:424:PHE:HB3	2.04	0.97
1:A:291:ASP:CG	1:A:334:ARG:HH21	1.66	0.97
1:B:419:PRO:CG	1:B:422:GLY:HA3	1.94	0.97
1:A:225:LYS:NZ	1:A:250:GLN:NE2	2.12	0.97
1:A:419:PRO:CB	1:A:422:GLY:CA	2.36	0.97
1:C:45:LYS:HD3	1:C:46:GLY:N	1.79	0.97
1:A:419:PRO:HG2	1:A:422:GLY:O	1.65	0.97
1:D:39:SER:O	1:D:42:LYS:NZ	1.99	0.96
1:D:425:LYS:HA	1:D:425:LYS:HE3	1.48	0.96
1:D:45:LYS:HD3	1:D:46:GLY:H	1.31	0.96
1:B:309:TRP:CE3	1:B:310:LEU:HD23	2.01	0.96
1:C:19:LYS:O	1:C:23:ILE:HG13	1.64	0.96
1:B:407:LYS:HB2	1:B:407:LYS:HZ3	1.30	0.95
1:C:244:GLU:OE2	1:D:425:LYS:CD	2.13	0.95
1:B:110:LEU:CD1	1:B:110:LEU:O	2.14	0.95
1:D:407:LYS:HZ3	1:D:407:LYS:CB	1.79	0.95
1:A:299:GLY:O	1:A:343:LEU:HD12	1.67	0.95
1:C:275:THR:HG22	1:C:277:CYS:H	1.32	0.95
1:D:65:THR:O	1:D:69:LEU:HD13	1.67	0.95
1:D:75:TRP:O	1:D:116:THR:HG21	1.67	0.95
1:B:275:THR:HG22	1:B:277:CYS:H	1.32	0.94
1:C:48:ARG:HD3	1:C:121:ASP:OD2	1.68	0.94
1:C:425:LYS:HZ2	1:C:426:PRO:HD3	1.32	0.94
1:A:387:LYS:HE2	1:A:391:GLU:OE2	1.68	0.94
1:D:134:LEU:O	1:D:134:LEU:HD22	1.67	0.94
1:C:315:VAL:CG2	1:C:330:LYS:HG2	1.97	0.94
1:C:419:PRO:HB2	1:C:422:GLY:H	1.12	0.94
1:D:419:PRO:HB2	1:D:422:GLY:CA	1.96	0.94
1:C:3:LYS:HG2	1:C:4:LEU:H	1.33	0.94
1:D:60:ALA:HB1	1:D:91:ILE:HD11	1.48	0.94
1:C:419:PRO:HG2	1:C:422:GLY:HA3	1.50	0.93
1:B:309:TRP:HE3	1:B:310:LEU:HD23	1.33	0.93
1:D:81:PHE:HE2	1:D:342:ARG:HD2	1.27	0.93
1:B:291:ASP:OD2	1:B:334:ARG:NH2	2.00	0.93
1:B:33:ARG:NH1	1:B:36:GLU:OE1	2.02	0.93
1:D:362:THR:O	1:D:366:MET:HG3	1.68	0.93
1:C:395:GLU:O	1:C:395:GLU:OE2	1.85	0.92
1:D:3:LYS:HE3	1:D:115:GLN:OE1	1.69	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:TYR:CZ	1:D:428:HIS:CE1	2.57	0.92
1:C:345:ASN:HD22	1:C:346:LEU:N	1.67	0.92
1:D:110:LEU:O	1:D:110:LEU:CD1	2.16	0.92
1:D:418:MET:CB	1:D:424:PHE:HB3	1.99	0.92
1:B:60:ALA:HB1	1:B:91:ILE:HD11	1.48	0.92
1:C:206:THR:HG21	1:C:294:ILE:HD13	1.51	0.92
1:C:425:LYS:HA	1:C:425:LYS:NZ	1.83	0.92
1:A:110:LEU:O	1:A:110:LEU:HD13	1.69	0.92
1:C:428:HIS:CE1	1:D:164:TYR:CZ	2.58	0.92
1:B:299:GLY:O	1:B:343:LEU:HD11	1.70	0.92
1:D:59:THR:O	1:D:63:ILE:HG13	1.70	0.92
1:B:410:GLU:OE2	1:B:414:GLN:OE1	1.89	0.91
1:C:312:GLU:HG2	1:C:313:ASN:ND2	1.86	0.91
1:C:419:PRO:CG	1:C:422:GLY:HA3	1.99	0.91
1:C:418:MET:SD	1:C:424:PHE:CB	2.58	0.91
1:C:425:LYS:HZ1	1:C:426:PRO:HD2	1.32	0.91
1:C:35:ARG:O	1:C:39:SER:OG	1.88	0.91
1:A:359:ASN:HD22	1:A:393:VAL:HG12	1.34	0.91
1:A:199:ILE:CD1	1:A:231:LEU:HD23	1.99	0.91
1:A:387:LYS:HZ1	1:A:425:LYS:CG	1.83	0.91
1:D:74:ARG:NH1	1:D:115:GLN:O	2.02	0.91
1:B:126:MET:HE3	1:B:150:ARG:HB3	1.50	0.91
1:D:126:MET:HE2	1:D:151:GLY:N	1.86	0.91
1:B:419:PRO:HG2	1:B:422:GLY:HA3	1.50	0.90
1:C:425:LYS:HZ2	1:C:425:LYS:HA	1.33	0.90
1:D:407:LYS:HB2	1:D:407:LYS:HZ2	1.29	0.90
1:C:273:THR:OG1	1:C:297:ASN:HB2	1.71	0.90
1:C:3:LYS:HG2	1:C:4:LEU:N	1.81	0.90
1:A:300:HIS:HA	1:A:343:LEU:HD11	1.52	0.90
1:C:387:LYS:NZ	1:C:426:PRO:O	2.05	0.90
1:A:3:LYS:HE2	1:A:74:ARG:HH12	1.35	0.90
1:B:156:THR:HG21	1:B:300:HIS:ND1	1.86	0.90
1:C:345:ASN:HD22	1:C:346:LEU:H	1.19	0.90
1:A:398:LEU:CD2	1:A:405:LEU:HD22	2.01	0.90
1:B:157:THR:CB	2:B:502:NAD:H52N	2.00	0.90
1:C:300:HIS:HB2	2:C:503:NAD:O2D	1.72	0.90
1:D:154:GLU:OE1	1:D:159:GLY:HA3	1.72	0.89
1:C:430:ARG:HH12	1:D:187:LYS:HE3	1.34	0.89
1:A:140:THR:OG1	1:A:141:LYS:HD2	1.73	0.89
1:C:27:GLU:C	1:C:29:PRO:HD3	1.91	0.89
1:D:418:MET:HG3	1:D:424:PHE:HD1	1.30	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:LYS:CD	1:D:46:GLY:H	1.84	0.89
1:B:110:LEU:HD13	1:B:110:LEU:O	1.73	0.89
1:D:223:VAL:HG12	1:D:274:THR:HB	1.55	0.89
1:C:117:LEU:CD2	1:C:138:ILE:HD11	2.03	0.88
1:C:126:MET:CE	1:C:150:ARG:HB3	2.04	0.88
1:D:7:LYS:HG2	1:D:101:TRP:CZ3	2.08	0.88
1:A:431:TYR:HE2	1:B:247:ASN:HD21	1.19	0.88
1:D:291:ASP:CG	1:D:334:ARG:HH21	1.76	0.88
1:A:275:THR:O	1:A:304:GLU:OE2	1.90	0.88
1:A:127:ILE:HG12	1:A:134:LEU:HD13	1.56	0.88
1:D:63:ILE:HD11	1:D:75:TRP:CD2	2.08	0.88
1:C:419:PRO:HB2	1:C:422:GLY:HA3	1.47	0.87
1:D:407:LYS:HZ3	1:D:407:LYS:HB2	1.06	0.87
1:A:408:LEU:O	1:A:420:ILE:HD12	1.73	0.87
1:C:424:PHE:O	1:C:426:PRO:HD3	1.74	0.87
1:B:129:ASP:OD2	1:B:135:THR:HG23	1.75	0.87
1:B:425:LYS:HD3	1:B:431:TYR:HH	1.32	0.87
1:B:292:ASP:OD2	1:B:326:ARG:NH2	2.08	0.87
1:A:225:LYS:HZ1	1:A:250:GLN:HE22	0.89	0.87
1:A:164:TYR:CD1	1:A:382:VAL:HG11	2.08	0.86
1:B:153:SER:HB3	1:B:364:GLN:NE2	1.90	0.86
1:D:53:LEU:HD11	1:D:155:GLU:HG3	1.57	0.86
1:B:110:LEU:CD1	1:B:110:LEU:C	2.43	0.86
1:B:359:ASN:HD22	1:B:393:VAL:HG12	1.40	0.86
1:C:386:PRO:HG2	1:C:389:LEU:HD12	1.55	0.86
1:C:425:LYS:NZ	1:C:426:PRO:HD3	1.88	0.86
1:D:126:MET:CE	1:D:151:GLY:N	2.38	0.86
1:B:169:ASN:CB	1:B:171:ILE:HD12	2.06	0.86
1:D:152:ILE:HB	1:D:176:ALA:HB2	1.58	0.86
1:A:431:TYR:HE2	1:B:247:ASN:ND2	1.73	0.85
1:B:317:LYS:HB2	1:B:327:TYR:CD2	2.11	0.85
1:D:373:THR:CG2	1:D:374:HIS:CE1	2.58	0.85
1:D:300:HIS:O	1:D:343:LEU:HD11	1.75	0.85
1:C:80:ILE:O	1:C:103:GLY:N	2.08	0.85
1:A:425:LYS:CA	1:A:425:LYS:HZ2	1.85	0.85
1:B:373:THR:HG22	1:B:374:HIS:CE1	2.11	0.85
1:A:430:ARG:HG2	1:B:430:ARG:HA	1.58	0.85
1:C:221:GLY:O	1:C:225:LYS:HG3	1.77	0.85
1:D:418:MET:HB2	1:D:419:PRO:CD	2.06	0.85
1:A:7:LYS:HG2	1:A:101:TRP:CZ3	2.12	0.85
1:A:91:ILE:CG2	1:A:98:VAL:HG22	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:LEU:CD2	1:D:405:LEU:HD22	2.07	0.85
1:B:339:ALA:O	1:B:342:ARG:HG3	1.77	0.84
1:C:55:MET:CE	1:C:59:THR:HB	2.07	0.84
1:A:419:PRO:CB	1:A:422:GLY:H	1.90	0.84
1:A:275:THR:HG23	2:A:501:NAD:C4A	2.07	0.84
1:D:275:THR:O	1:D:304:GLU:OE2	1.95	0.84
1:D:387:LYS:O	1:D:391:GLU:HG2	1.77	0.84
1:D:419:PRO:CB	1:D:422:GLY:CA	2.46	0.84
1:D:339:ALA:O	1:D:342:ARG:HG3	1.78	0.84
1:A:181:ASP:O	1:B:430:ARG:NH2	2.10	0.84
1:C:299:GLY:O	1:C:343:LEU:HD11	1.77	0.84
1:D:178:ASN:HD21	1:D:181:ASP:HB2	1.02	0.84
1:D:337:LEU:HD13	1:D:340:GLU:HA	1.60	0.84
1:A:424:PHE:O	1:A:426:PRO:CD	2.25	0.83
1:C:214:VAL:H	1:C:269:ASN:HD22	1.25	0.83
1:A:308:LYS:O	1:A:312:GLU:HG2	1.77	0.83
1:C:277:CYS:HB3	1:D:416:LEU:HD21	1.60	0.83
1:B:143:PRO:HA	1:B:146:LEU:CD2	2.08	0.83
1:B:300:HIS:HB2	2:B:502:NAD:O2D	1.78	0.83
1:B:425:LYS:CG	1:B:431:TYR:OH	2.27	0.83
1:A:419:PRO:HB2	1:A:422:GLY:CA	2.03	0.83
1:B:317:LYS:HD2	1:B:327:TYR:HE2	1.41	0.83
1:C:387:LYS:HE3	4:C:658:HOH:O	1.77	0.83
1:C:316:GLU:HG2	1:C:328:LEU:HB3	1.61	0.83
1:C:184:THR:HG23	1:C:390:ASP:OD2	1.77	0.83
1:D:126:MET:HE2	1:D:151:GLY:H	1.42	0.83
1:B:127:ILE:HG12	1:B:134:LEU:CD1	2.08	0.83
1:C:137:LEU:CD1	1:C:137:LEU:O	2.19	0.83
1:D:178:ASN:HD21	1:D:181:ASP:CG	1.81	0.83
1:A:387:LYS:NZ	1:A:425:LYS:CG	2.35	0.82
1:B:126:MET:HE1	1:B:151:GLY:N	1.94	0.82
1:B:21:LEU:HD21	1:B:60:ALA:HB3	1.59	0.82
1:D:320:ILE:HD12	1:D:320:ILE:N	1.94	0.82
1:C:299:GLY:O	1:C:343:LEU:HD12	1.79	0.82
1:C:27:GLU:O	1:C:29:PRO:CD	2.26	0.82
1:C:126:MET:HE3	1:C:150:ARG:HB3	1.61	0.82
1:C:419:PRO:CB	1:C:422:GLY:CA	2.55	0.82
1:A:225:LYS:HZ1	1:A:250:GLN:NE2	1.72	0.82
1:A:39:SER:O	1:A:42:LYS:NZ	2.12	0.82
1:D:110:LEU:O	1:D:110:LEU:HD13	1.75	0.81
1:D:214:VAL:H	1:D:269:ASN:HD22	1.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:VAL:HG22	1:B:209:MET:N	1.96	0.81
1:A:128:LEU:HD21	1:A:364:GLN:CG	2.10	0.81
1:D:54:HIS:HB3	1:D:82:SER:OG	1.79	0.81
1:D:105:THR:OG1	1:D:108:GLU:HG3	1.81	0.81
1:B:126:MET:CE	1:B:150:ARG:HB3	2.10	0.81
1:D:45:LYS:CD	1:D:46:GLY:N	2.43	0.81
1:C:275:THR:HG21	1:C:280:ILE:CD1	2.05	0.81
1:B:45:LYS:HD2	1:B:46:GLY:N	1.96	0.81
1:B:110:LEU:HD12	1:B:110:LEU:C	2.01	0.81
1:B:53:LEU:HG	1:B:130:ASP:HB2	1.63	0.81
1:D:292:ASP:OD2	1:D:326:ARG:NH2	2.12	0.81
1:A:143:PRO:HA	1:A:146:LEU:CD2	2.11	0.80
1:A:398:LEU:HD23	1:A:405:LEU:HD22	1.61	0.80
1:C:60:ALA:HB1	1:C:91:ILE:HD11	1.61	0.80
1:A:292:ASP:HA	1:A:334:ARG:O	1.79	0.80
1:A:425:LYS:HA	1:A:425:LYS:CE	2.10	0.80
1:D:418:MET:CG	1:D:424:PHE:CD1	2.61	0.80
1:A:317:LYS:HD2	1:A:327:TYR:CE2	2.17	0.80
1:C:177:ILE:HG13	1:C:371:LEU:CD2	2.03	0.80
1:D:46:GLY:O	1:D:372:TRP:CZ2	2.34	0.80
1:D:419:PRO:HG2	1:D:423:PRO:N	1.97	0.80
1:A:430:ARG:O	1:A:431:TYR:OXT	2.00	0.80
1:C:137:LEU:O	1:C:141:LYS:HB2	1.82	0.80
1:A:225:LYS:HZ2	1:A:250:GLN:HE22	1.28	0.80
1:C:430:ARG:HG2	1:D:430:ARG:HA	1.64	0.80
1:C:430:ARG:HH12	1:D:187:LYS:CE	1.93	0.79
1:B:308:LYS:HD2	1:B:308:LYS:H	1.47	0.79
1:D:186:SER:O	1:D:190:ASN:HB2	1.83	0.79
1:B:126:MET:CE	1:B:151:GLY:N	2.46	0.79
1:B:39:SER:O	1:B:42:LYS:NZ	2.15	0.79
1:C:425:LYS:CE	1:C:426:PRO:HD2	2.11	0.79
1:C:33:ARG:NH1	1:C:36:GLU:OE1	2.15	0.79
1:A:223:VAL:HG12	1:A:274:THR:HB	1.64	0.79
1:A:387:LYS:HZ3	1:A:425:LYS:HG3	1.44	0.79
1:A:126:MET:CE	1:A:151:GLY:N	2.45	0.79
1:A:299:GLY:O	1:A:343:LEU:HD11	1.82	0.79
1:C:110:LEU:O	1:C:110:LEU:CD1	2.30	0.79
1:D:398:LEU:HD23	1:D:405:LEU:HD22	1.64	0.79
2:C:503:NAD:C4N	3:C:603:ADN:H3'	2.12	0.79
1:D:154:GLU:CD	1:D:159:GLY:HA3	2.03	0.79
1:D:81:PHE:CE2	1:D:342:ARG:CD	2.62	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:THR:HG23	1:B:412:GLN:HE21	1.48	0.78
1:C:3:LYS:HE2	1:C:74:ARG:HH12	1.47	0.78
1:D:110:LEU:O	1:D:110:LEU:HD12	1.83	0.78
1:D:199:ILE:HD12	1:D:234:PHE:CE2	2.18	0.78
1:D:45:LYS:HD2	1:D:46:GLY:N	1.97	0.78
1:A:317:LYS:HG3	1:A:327:TYR:CE2	2.18	0.78
1:C:21:LEU:HD21	1:C:60:ALA:HB3	1.66	0.78
1:D:137:LEU:HD12	1:D:141:LYS:HB2	1.65	0.78
1:D:262:ASP:OD1	1:D:284:ARG:NH1	2.16	0.78
1:B:169:ASN:HB2	1:B:171:ILE:HD12	1.64	0.78
1:B:110:LEU:HD12	1:B:110:LEU:O	1.81	0.78
1:B:419:PRO:CG	1:B:422:GLY:CA	2.57	0.78
1:B:370:GLU:HB3	1:B:378:TYR:CE1	2.19	0.77
1:D:418:MET:HB3	1:D:424:PHE:HB3	1.64	0.77
1:D:317:LYS:HG3	1:D:327:TYR:CZ	2.20	0.77
1:B:178:ASN:ND2	1:B:181:ASP:HB2	2.00	0.77
1:C:415:TYR:CD2	1:D:278:VAL:HG22	2.19	0.77
1:A:359:ASN:ND2	1:A:393:VAL:HG12	1.99	0.77
1:C:425:LYS:CA	1:C:425:LYS:CE	2.63	0.77
1:D:424:PHE:O	1:D:426:PRO:HD3	1.83	0.77
1:D:129:ASP:OD2	1:D:135:THR:HG23	1.85	0.77
1:C:425:LYS:HZ1	1:C:426:PRO:CD	1.92	0.77
1:B:125:ASN:O	1:B:126:MET:HG2	1.85	0.76
1:A:373:THR:HG21	1:A:374:HIS:HE1	1.46	0.76
1:B:353:PRO:HB2	1:D:209:MET:HB2	1.68	0.76
1:D:169:ASN:HD22	1:D:171:ILE:CD1	1.98	0.76
1:B:48:ARG:HD2	1:B:119:PHE:HB2	1.67	0.76
1:B:273:THR:OG1	1:B:297:ASN:HA	1.84	0.76
1:C:428:HIS:HE1	1:D:164:TYR:CZ	2.02	0.76
1:D:363:ASN:ND2	1:D:393:VAL:HG21	2.01	0.76
1:B:299:GLY:O	1:B:343:LEU:HD12	1.85	0.76
1:C:7:LYS:HG2	1:C:101:TRP:CZ3	2.20	0.76
1:A:10:ASP:HB3	1:A:13:LEU:CD2	2.15	0.76
1:B:373:THR:HG22	1:B:374:HIS:ND1	2.00	0.76
1:C:153:SER:HB3	1:C:364:GLN:NE2	2.00	0.76
1:A:126:MET:HE3	1:A:150:ARG:CB	2.11	0.76
1:A:211:ALA:HB2	1:A:234:PHE:O	1.85	0.76
1:D:183:VAL:HG11	1:D:431:TYR:CD1	2.19	0.76
1:B:157:THR:HB	2:B:502:NAD:C3D	2.16	0.76
1:A:199:ILE:HD11	1:A:231:LEU:CD2	2.14	0.76
1:C:91:ILE:HG22	1:C:98:VAL:CG2	2.16	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:152:ILE:HB	1:D:176:ALA:CB	2.16	0.76
1:A:369:ILE:O	1:A:373:THR:HB	1.86	0.75
1:B:91:ILE:HG22	1:B:98:VAL:HG21	1.67	0.75
1:C:428:HIS:HE1	1:D:164:TYR:CE1	2.03	0.75
1:A:343:LEU:HD23	1:A:346:LEU:HD12	1.67	0.75
1:B:190:ASN:ND2	2:B:502:NAD:H5N	2.02	0.75
1:C:202:ILE:O	1:C:206:THR:OG1	2.04	0.75
1:D:160:VAL:HG21	1:D:178:ASN:OD1	1.86	0.75
1:A:237:ARG:NH2	1:A:267:GLU:OE2	2.18	0.75
1:A:430:ARG:NH1	1:B:187:LYS:HE3	2.02	0.75
1:A:419:PRO:CB	1:A:422:GLY:N	2.41	0.75
1:A:126:MET:HE2	1:A:151:GLY:N	2.02	0.75
1:A:275:THR:CG2	2:A:501:NAD:C5A	2.64	0.75
1:B:157:THR:OG1	2:B:502:NAD:H52N	1.86	0.75
1:C:164:TYR:CE1	1:D:428:HIS:HE1	2.05	0.75
1:B:81:PHE:O	1:B:102:LYS:HE3	1.87	0.75
1:B:407:LYS:HB2	1:B:407:LYS:NZ	1.99	0.75
1:C:275:THR:CG2	1:C:280:ILE:HD11	2.09	0.75
1:D:7:LYS:HG2	1:D:101:TRP:CH2	2.22	0.75
1:D:162:ASN:O	1:D:166:MET:HG3	1.87	0.75
1:D:3:LYS:CE	1:D:115:GLN:OE1	2.34	0.75
1:A:317:LYS:HD2	1:A:327:TYR:HE2	1.51	0.74
1:B:385:LEU:HG	1:B:386:PRO:HD2	1.69	0.74
1:D:53:LEU:HD11	1:D:155:GLU:CG	2.17	0.74
1:A:359:ASN:HD22	1:A:393:VAL:CG1	1.99	0.74
1:A:409:THR:H	1:A:412:GLN:HE21	1.34	0.74
1:B:74:ARG:HB3	1:B:116:THR:HB	1.68	0.74
1:B:223:VAL:HG12	1:B:274:THR:HB	1.70	0.74
1:B:408:LEU:O	1:B:420:ILE:HD12	1.86	0.74
1:A:373:THR:CG2	1:A:374:HIS:ND1	2.45	0.74
1:A:300:HIS:HB2	2:A:501:NAD:O2D	1.88	0.74
1:B:156:THR:O	1:B:160:VAL:HG23	1.88	0.74
1:A:153:SER:HB3	1:A:364:GLN:HE22	1.51	0.74
1:B:45:LYS:HD3	4:B:661:HOH:O	1.86	0.74
1:D:178:ASN:ND2	1:D:181:ASP:CB	2.24	0.74
1:D:379:PRO:HD2	1:D:383:HIS:NE2	2.03	0.74
1:A:186:SER:O	1:A:190:ASN:HB2	1.88	0.74
1:D:129:ASP:OD2	1:D:135:THR:CG2	2.36	0.74
1:B:302:ASP:O	1:B:302:ASP:OD1	2.05	0.74
1:B:409:THR:HG23	1:B:412:GLN:NE2	2.02	0.74
1:A:137:LEU:O	1:A:141:LYS:HB2	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:HG22	1:B:276:GLY:N	2.02	0.73
1:D:317:LYS:CG	1:D:327:TYR:CE2	2.69	0.73
1:B:385:LEU:HD23	1:B:389:LEU:HB2	1.70	0.73
1:C:182:SER:O	1:C:185:LYS:N	2.21	0.73
1:D:223:VAL:CG1	1:D:274:THR:HB	2.18	0.73
1:D:425:LYS:HE3	1:D:426:PRO:CD	2.18	0.73
1:D:425:LYS:HE3	1:D:426:PRO:HD2	1.70	0.73
1:D:113:ILE:HG21	1:D:137:LEU:HD23	1.69	0.73
1:A:125:ASN:ND2	1:A:372:TRP:CH2	2.56	0.73
1:A:125:ASN:ND2	1:A:372:TRP:CZ3	2.57	0.73
1:C:169:ASN:HB2	1:C:171:ILE:HD12	1.70	0.73
1:B:89:ALA:HB2	4:B:612:HOH:O	1.87	0.73
1:A:353:PRO:HB2	1:C:209:MET:HB2	1.71	0.73
1:C:425:LYS:HZ2	1:C:426:PRO:CD	1.93	0.73
1:B:193:GLY:O	1:B:197:SER:OG	2.05	0.73
1:C:363:ASN:ND2	1:C:393:VAL:HG21	2.03	0.73
1:D:419:PRO:HB2	1:D:422:GLY:HA3	1.57	0.73
1:B:370:GLU:HB3	1:B:378:TYR:HE1	1.52	0.73
1:B:419:PRO:HB2	1:B:422:GLY:H	1.53	0.73
1:B:91:ILE:CG2	1:B:98:VAL:CG2	2.67	0.73
1:D:143:PRO:HA	1:D:146:LEU:HD22	1.70	0.73
1:C:174:VAL:HG23	1:C:175:PRO:HD2	1.71	0.73
1:D:300:HIS:HB2	2:D:504:NAD:O2D	1.89	0.73
1:C:275:THR:CG2	1:C:277:CYS:H	2.00	0.73
1:A:425:LYS:HD3	1:A:431:TYR:CZ	2.22	0.72
1:C:10:ASP:HB3	1:C:13:LEU:CD2	2.18	0.72
1:C:160:VAL:HG12	1:C:164:TYR:CE2	2.23	0.72
1:A:209:MET:HB2	1:C:353:PRO:HB2	1.69	0.72
1:C:181:ASP:OD2	1:D:428:HIS:HB3	1.90	0.72
1:A:169:ASN:HB2	1:A:171:ILE:CD1	2.17	0.72
1:A:419:PRO:HB2	1:A:422:GLY:HA3	1.66	0.72
1:C:387:LYS:O	1:C:391:GLU:HG2	1.88	0.72
1:D:81:PHE:CD2	1:D:342:ARG:HD2	2.23	0.72
1:C:298:ILE:O	1:C:299:GLY:O	2.07	0.72
1:D:107:GLU:H	1:D:107:GLU:CD	1.90	0.72
1:D:320:ILE:CD1	1:D:320:ILE:N	2.52	0.72
1:A:127:ILE:HG12	1:A:134:LEU:CD1	2.19	0.72
1:A:275:THR:HG21	2:A:501:NAD:C5A	2.20	0.72
1:C:79:ASN:HB3	1:C:82:SER:HB3	1.71	0.72
1:C:164:TYR:OH	1:D:428:HIS:CE1	2.43	0.72
1:B:184:THR:HA	1:B:188:PHE:CD1	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:THR:HG21	1:D:300:HIS:ND1	2.05	0.72
1:D:232:ARG:HG3	1:D:256:TYR:HE1	1.52	0.72
1:C:221:GLY:O	1:C:225:LYS:CG	2.38	0.72
1:D:169:ASN:CB	1:D:171:ILE:HD12	2.14	0.72
1:D:27:GLU:O	1:D:29:PRO:HD3	1.89	0.72
1:B:153:SER:HB3	1:B:364:GLN:HE22	1.54	0.71
1:D:48:ARG:HD3	1:D:121:ASP:OD2	1.88	0.71
1:D:93:LYS:C	1:D:95:GLY:H	1.94	0.71
1:B:125:ASN:HA	1:B:148:GLY:O	1.90	0.71
1:C:279:ASP:HB3	1:C:282:LEU:HD11	1.71	0.71
1:C:418:MET:SD	1:C:424:PHE:HB2	2.29	0.71
1:C:430:ARG:HB2	1:C:430:ARG:CZ	2.18	0.71
1:C:431:TYR:HE2	1:D:247:ASN:ND2	1.88	0.71
1:D:418:MET:CG	1:D:424:PHE:HD1	2.01	0.71
1:B:21:LEU:O	1:B:25:GLU:HG3	1.91	0.71
1:C:425:LYS:HA	1:C:425:LYS:HE3	1.73	0.71
1:A:320:ILE:HD12	1:C:19:LYS:HD2	1.72	0.71
1:A:160:VAL:HG11	1:A:178:ASN:CG	2.11	0.71
1:A:28:MET:HB3	1:A:358:SER:HB2	1.70	0.71
1:C:334:ARG:HD3	1:C:334:ARG:N	2.05	0.71
1:D:418:MET:HB2	1:D:419:PRO:HD2	1.71	0.71
1:B:118:HIS:NE2	4:B:692:HOH:O	2.23	0.71
1:C:225:LYS:NZ	1:C:250:GLN:HE22	1.89	0.70
1:C:81:PHE:O	1:C:102:LYS:HE3	1.90	0.70
1:A:128:LEU:HD21	1:A:364:GLN:HG2	1.73	0.70
1:A:419:PRO:HD2	1:A:423:PRO:O	1.91	0.70
1:B:81:PHE:CE2	1:B:342:ARG:HD2	2.26	0.70
1:A:430:ARG:CA	1:B:430:ARG:HG2	2.20	0.70
1:C:419:PRO:CB	1:C:422:GLY:H	2.00	0.70
1:A:200:ASP:O	1:A:204:ARG:HG3	1.91	0.70
1:C:430:ARG:HH11	1:D:187:LYS:HE3	1.56	0.70
1:D:295:VAL:HG12	1:D:305:ILE:HD13	1.71	0.70
1:A:74:ARG:NH1	1:A:115:GLN:O	2.24	0.70
1:B:278:VAL:HG12	1:B:303:VAL:CB	2.12	0.70
1:B:419:PRO:CB	1:B:422:GLY:HA3	2.22	0.70
1:B:39:SER:O	1:B:42:LYS:HG2	1.91	0.70
1:D:374:HIS:N	1:D:375:PRO:CD	2.55	0.70
1:C:126:MET:CE	1:C:151:GLY:N	2.55	0.70
1:C:45:LYS:C	1:C:45:LYS:HD3	2.12	0.70
1:B:150:ARG:HD2	1:B:372:TRP:HA	1.74	0.70
1:C:25:GLU:HG2	1:C:32:MET:SD	2.31	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:LEU:CD2	1:B:405:LEU:HD13	2.22	0.70
1:B:81:PHE:HE2	1:B:342:ARG:HD2	1.56	0.70
1:C:425:LYS:HE3	1:C:425:LYS:CA	2.21	0.70
1:D:282:LEU:HD23	1:D:284:ARG:NH2	2.07	0.70
1:D:80:ILE:HG13	1:D:81:PHE:CE1	2.27	0.70
1:C:16:TRP:CD1	1:C:16:TRP:O	2.44	0.69
1:D:81:PHE:CD2	1:D:342:ARG:CD	2.74	0.69
1:D:419:PRO:CB	1:D:422:GLY:H	2.02	0.69
1:A:126:MET:HE1	1:A:151:GLY:N	2.07	0.69
1:A:3:LYS:CE	1:A:74:ARG:HH12	2.05	0.69
1:A:56:THR:HB	1:A:84:GLN:CD	2.11	0.69
1:D:169:ASN:CB	1:D:171:ILE:CD1	2.60	0.69
1:D:379:PRO:O	1:D:380:VAL:C	2.30	0.69
1:D:194:CYS:SG	1:D:223:VAL:HG22	2.31	0.69
1:A:408:LEU:O	1:A:420:ILE:CD1	2.40	0.69
1:B:273:THR:OG1	1:B:297:ASN:HB2	1.93	0.69
1:C:130:ASP:OD1	1:C:156:THR:HG22	1.93	0.69
1:C:291:ASP:OD2	1:C:334:ARG:NH2	2.24	0.69
1:B:214:VAL:H	1:B:269:ASN:HD22	1.39	0.69
1:C:117:LEU:HD22	1:C:138:ILE:HD11	1.75	0.69
1:D:425:LYS:CE	1:D:425:LYS:HA	2.15	0.69
1:D:99:PHE:O	1:D:100:ALA:HB2	1.91	0.69
1:C:5:PRO:O	1:C:6:TYR:HB3	1.92	0.69
1:B:128:LEU:HD11	1:B:364:GLN:HG3	1.75	0.69
1:D:214:VAL:N	1:D:269:ASN:HD22	1.90	0.69
1:B:178:ASN:HD21	1:B:181:ASP:CG	1.96	0.69
1:C:225:LYS:HZ3	1:C:250:GLN:NE2	1.90	0.69
1:C:277:CYS:HB3	1:D:416:LEU:CD2	2.21	0.69
1:B:210:ILE:HG21	1:B:234:PHE:CB	2.23	0.69
1:B:378:TYR:HB2	4:B:647:HOH:O	1.92	0.69
1:B:408:LEU:HD21	1:B:416:LEU:HD12	1.74	0.69
1:B:186:SER:O	1:B:190:ASN:HB2	1.93	0.69
1:A:7:LYS:CG	1:A:101:TRP:CZ3	2.75	0.68
1:C:128:LEU:HD21	1:C:364:GLN:HG2	1.75	0.68
1:A:295:VAL:HG12	1:A:305:ILE:HD13	1.75	0.68
1:C:28:MET:O	1:C:32:MET:HG2	1.91	0.68
1:A:199:ILE:HG21	1:A:234:PHE:HE2	1.58	0.68
1:B:385:LEU:CD2	1:B:389:LEU:HB2	2.21	0.68
1:C:48:ARG:HD3	1:C:121:ASP:CG	2.14	0.68
1:D:279:ASP:HB3	1:D:282:LEU:CD1	2.21	0.68
1:B:291:ASP:CG	1:B:334:ARG:HH21	1.96	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:VAL:O	4:B:634:HOH:O	2.10	0.68
1:D:300:HIS:O	1:D:343:LEU:CD1	2.41	0.68
1:A:126:MET:CE	1:A:150:ARG:CB	2.69	0.68
1:A:158:THR:HG21	1:A:301:PHE:CE2	2.29	0.68
1:C:39:SER:O	1:C:42:LYS:NZ	2.25	0.68
1:D:419:PRO:CB	1:D:422:GLY:N	2.54	0.68
1:C:273:THR:HG22	1:C:280:ILE:HG21	1.73	0.68
1:C:177:ILE:CD1	1:C:371:LEU:HD21	2.24	0.68
1:A:126:MET:HE2	1:A:151:GLY:H	1.57	0.68
1:A:425:LYS:HE2	1:A:429:TYR:CG	2.29	0.68
1:A:91:ILE:HG21	1:A:98:VAL:CG2	2.22	0.68
1:B:208:VAL:HG22	1:B:209:MET:H	1.56	0.68
1:D:74:ARG:HB3	1:D:116:THR:HB	1.76	0.68
1:A:393:VAL:O	1:A:397:HIS:ND1	2.27	0.68
1:C:137:LEU:CD1	1:C:141:LYS:HB2	2.24	0.68
1:C:312:GLU:CG	1:C:313:ASN:ND2	2.56	0.68
1:C:337:LEU:HD22	1:C:338:LEU:N	2.09	0.68
1:C:79:ASN:CB	1:C:82:SER:HB3	2.24	0.68
1:A:225:LYS:HZ2	1:A:250:GLN:NE2	1.86	0.68
1:B:345:ASN:O	1:B:349:ALA:HB3	1.93	0.68
1:C:200:ASP:O	1:C:204:ARG:HG3	1.94	0.68
1:A:153:SER:CB	1:A:364:GLN:NE2	2.57	0.67
1:A:430:ARG:HH12	1:B:187:LYS:CE	2.07	0.67
1:A:55:MET:CE	1:A:59:THR:HG22	2.23	0.67
1:B:369:ILE:O	1:B:373:THR:HB	1.94	0.67
1:B:6:TYR:CD1	1:B:6:TYR:C	2.66	0.67
1:C:382:VAL:O	1:C:382:VAL:HG22	1.93	0.67
1:C:94:ALA:HB3	1:C:96:ILE:CD1	2.23	0.67
1:A:3:LYS:HE2	1:A:74:ARG:NH1	2.09	0.67
1:B:372:TRP:O	1:B:372:TRP:CG	2.47	0.67
1:D:63:ILE:CD1	1:D:75:TRP:CD2	2.78	0.67
1:A:5:PRO:O	1:A:6:TYR:HB3	1.93	0.67
1:B:91:ILE:HG22	1:B:98:VAL:HG22	1.77	0.67
1:C:275:THR:O	1:C:304:GLU:OE2	2.12	0.67
1:B:157:THR:HG21	2:B:502:NAD:O1A	1.94	0.67
1:D:292:ASP:CG	1:D:326:ARG:HH21	1.98	0.67
1:C:137:LEU:HD11	1:C:142:HIS:CD2	2.29	0.67
1:D:200:ASP:O	1:D:204:ARG:HG3	1.95	0.67
1:D:158:THR:CG2	1:D:301:PHE:HE2	2.00	0.67
1:A:137:LEU:HD11	1:A:142:HIS:NE2	2.10	0.67
1:C:223:VAL:HG12	1:C:274:THR:HB	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:O	1:B:377:LYS:HB2	1.95	0.67
1:D:180:ASN:HA	1:D:185:LYS:HD2	1.76	0.67
1:D:150:ARG:HD2	1:D:372:TRP:HA	1.76	0.67
1:D:156:THR:HG21	1:D:300:HIS:HD1	1.57	0.67
1:A:361:PHE:O	1:A:365:VAL:HG23	1.95	0.66
1:B:169:ASN:HB3	1:B:171:ILE:CD1	2.25	0.66
1:A:24:ALA:O	1:A:27:GLU:N	2.23	0.66
1:B:169:ASN:HB3	1:B:171:ILE:HD12	1.77	0.66
1:B:385:LEU:HD21	1:B:389:LEU:CB	2.25	0.66
1:D:199:ILE:HD12	1:D:234:PHE:CD2	2.31	0.66
1:A:317:LYS:CG	1:A:327:TYR:CE2	2.77	0.66
1:C:225:LYS:NZ	1:C:250:GLN:NE2	2.43	0.66
1:A:430:ARG:NH1	1:B:187:LYS:CE	2.58	0.66
1:C:419:PRO:HG2	1:C:422:GLY:CA	2.23	0.66
1:C:430:ARG:HG2	1:D:430:ARG:CA	2.24	0.66
1:A:51:GLY:HA2	1:A:128:LEU:O	1.95	0.66
1:C:406:THR:CG2	1:C:407:LYS:N	2.57	0.66
1:B:119:PHE:N	1:B:119:PHE:CD1	2.63	0.66
1:D:137:LEU:O	1:D:141:LYS:HB2	1.96	0.66
1:B:326:ARG:HD2	1:D:23:ILE:HD13	1.77	0.66
1:D:419:PRO:CD	1:D:423:PRO:O	2.43	0.66
1:A:163:LEU:HD11	1:A:176:ALA:CB	2.25	0.66
1:D:75:TRP:O	1:D:116:THR:CG2	2.43	0.66
1:C:430:ARG:O	1:D:430:ARG:HB3	1.95	0.66
1:C:283:GLY:HA2	1:C:286:PHE:HD2	1.59	0.66
1:C:428:HIS:CE1	1:D:164:TYR:CE1	2.82	0.66
1:A:409:THR:N	1:A:412:GLN:HE21	1.93	0.66
1:A:129:ASP:OD2	1:A:135:THR:HG23	1.96	0.65
1:A:429:TYR:CD2	1:A:431:TYR:CZ	2.84	0.65
1:B:126:MET:HE1	1:B:151:GLY:CA	2.26	0.65
1:D:387:LYS:NZ	1:D:426:PRO:O	2.29	0.65
1:C:126:MET:CE	1:C:150:ARG:CB	2.73	0.65
1:C:185:LYS:C	1:C:185:LYS:HD3	2.16	0.65
1:D:79:ASN:HB3	1:D:82:SER:HB3	1.76	0.65
1:D:6:TYR:HE1	1:D:8:VAL:HG22	1.62	0.65
1:A:387:LYS:O	1:A:391:GLU:HG2	1.97	0.65
1:C:146:LEU:HG	1:C:173:LYS:HB2	1.79	0.65
1:D:126:MET:CE	1:D:150:ARG:HB3	2.22	0.65
1:B:286:PHE:CD2	1:B:310:LEU:HD21	2.31	0.65
1:A:277:CYS:HB2	1:B:416:LEU:HD21	1.76	0.65
1:A:320:ILE:N	1:A:320:ILE:HD13	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HA	1:B:425:LYS:NZ	2.11	0.65
1:C:415:TYR:CG	1:D:278:VAL:HG22	2.32	0.65
1:C:430:ARG:NH1	1:C:430:ARG:CB	2.60	0.65
1:A:278:VAL:HG12	1:A:303:VAL:HB	1.78	0.65
1:D:189:ASP:O	1:D:352:HIS:CE1	2.49	0.65
1:D:35:ARG:O	1:D:39:SER:OG	2.12	0.65
1:B:119:PHE:N	1:B:119:PHE:HD1	1.95	0.65
1:C:126:MET:HE1	1:C:151:GLY:N	2.12	0.65
1:C:259:THR:HA	1:D:404:LYS:HB2	1.78	0.65
1:D:124:LEU:HD21	1:D:149:ILE:HD11	1.77	0.65
1:D:91:ILE:HG22	1:D:98:VAL:CG2	2.27	0.65
1:A:429:TYR:HD2	1:A:431:TYR:CZ	2.15	0.65
1:C:110:LEU:CD1	1:C:110:LEU:C	2.65	0.65
1:C:91:ILE:HG23	1:C:96:ILE:HB	1.79	0.65
1:D:425:LYS:CA	1:D:425:LYS:HE3	2.23	0.65
1:D:46:GLY:O	1:D:372:TRP:HZ2	1.79	0.65
1:A:110:LEU:CD1	1:A:110:LEU:O	2.44	0.64
1:A:140:THR:OG1	1:A:141:LYS:CD	2.44	0.64
1:B:158:THR:HG22	1:B:159:GLY:N	2.10	0.64
1:C:169:ASN:HB2	1:C:171:ILE:CD1	2.27	0.64
1:B:3:LYS:HG2	1:B:4:LEU:H	1.62	0.64
1:B:273:THR:O	1:B:298:ILE:HG22	1.97	0.64
1:C:431:TYR:HE2	1:D:247:ASN:HD21	1.43	0.64
1:D:28:MET:O	1:D:32:MET:HG2	1.97	0.64
1:D:7:LYS:N	1:D:98:VAL:O	2.29	0.64
1:B:178:ASN:HD21	1:B:181:ASP:HB2	1.62	0.64
1:C:214:VAL:N	1:C:269:ASN:HD22	1.93	0.64
1:A:215:ALA:HB1	1:A:231:LEU:HD13	1.80	0.64
1:B:385:LEU:HD21	1:B:389:LEU:HB3	1.79	0.64
1:C:379:PRO:O	1:C:383:HIS:CE1	2.51	0.64
1:C:59:THR:O	1:C:63:ILE:HG13	1.98	0.64
1:A:430:ARG:HH12	1:B:187:LYS:HE2	1.61	0.64
1:A:275:THR:CG2	2:A:501:NAD:C4A	2.76	0.64
1:B:379:PRO:HD2	1:B:383:HIS:NE2	2.12	0.64
1:C:137:LEU:HD12	1:C:141:LYS:HB2	1.79	0.64
1:C:24:ALA:O	1:C:28:MET:HG3	1.98	0.64
1:B:7:LYS:HG2	1:B:101:TRP:CZ3	2.33	0.64
1:B:178:ASN:HD21	1:B:181:ASP:CB	2.10	0.64
1:C:186:SER:O	1:C:190:ASN:HB2	1.98	0.64
2:D:504:NAD:C4N	3:D:604:ADN:H3'	2.28	0.64
1:B:358:SER:HG	1:B:397:HIS:HE2	1.46	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ILE:HD12	1:D:234:PHE:HE2	1.63	0.64
1:A:110:LEU:O	1:A:114:GLU:HG2	1.97	0.64
1:C:134:LEU:HD22	1:C:138:ILE:HD12	1.78	0.64
1:D:63:ILE:HD11	1:D:75:TRP:CG	2.32	0.64
1:B:143:PRO:HA	1:B:146:LEU:HD22	1.79	0.63
1:B:129:ASP:HB3	1:B:154:GLU:OE2	1.97	0.63
1:C:410:GLU:OE2	1:C:414:GLN:OE1	2.14	0.63
1:C:425:LYS:CE	1:C:426:PRO:CD	2.75	0.63
1:A:142:HIS:HA	1:A:144:GLN:OE1	1.98	0.63
1:C:55:MET:HE2	1:C:59:THR:HB	1.80	0.63
1:A:196:GLU:HB3	1:C:203:LYS:NZ	2.13	0.63
1:C:177:ILE:CD1	1:C:371:LEU:CD2	2.75	0.63
1:D:430:ARG:O	1:D:431:TYR:HB2	1.96	0.63
1:A:184:THR:HA	1:A:188:PHE:CD1	2.34	0.63
1:C:169:ASN:O	1:C:171:ILE:HG13	1.98	0.63
1:D:169:ASN:HD22	1:D:171:ILE:HD13	1.63	0.63
1:D:373:THR:O	1:D:373:THR:CG2	2.46	0.63
1:D:48:ARG:HG3	1:D:48:ARG:HH11	1.62	0.63
1:A:379:PRO:HD2	1:A:383:HIS:NE2	2.13	0.63
1:B:317:LYS:O	1:B:317:LYS:HG2	1.98	0.63
1:C:183:VAL:C	1:C:185:LYS:H	2.02	0.63
1:A:164:TYR:CE1	1:A:382:VAL:HG21	2.34	0.63
1:A:27:GLU:C	1:A:29:PRO:HD3	2.20	0.63
1:A:49:ILE:HD13	1:A:66:LEU:HD13	1.80	0.63
1:B:308:LYS:CD	1:B:308:LYS:H	2.12	0.63
1:B:425:LYS:CE	1:B:425:LYS:HA	2.29	0.63
1:C:179:VAL:O	1:C:182:SER:HB2	1.99	0.63
1:C:39:SER:O	1:C:42:LYS:HG2	1.99	0.63
1:B:398:LEU:HD21	1:B:405:LEU:HD13	1.81	0.63
1:B:91:ILE:HG23	1:B:96:ILE:HB	1.81	0.63
1:C:361:PHE:O	1:C:365:VAL:HG23	1.99	0.63
1:D:169:ASN:CB	1:D:171:ILE:HD11	2.24	0.63
1:A:358:SER:O	1:A:362:THR:OG1	2.10	0.62
1:B:318:VAL:CG1	1:D:19:LYS:HE2	2.29	0.62
1:C:164:TYR:HH	1:D:428:HIS:CE1	2.17	0.62
1:C:198:LEU:C	1:C:198:LEU:HD12	2.19	0.62
1:C:275:THR:HG22	1:C:277:CYS:N	2.10	0.62
1:B:278:VAL:HG12	1:B:303:VAL:O	1.99	0.62
1:A:111:TRP:HA	1:A:114:GLU:HG3	1.81	0.62
1:A:246:ILE:O	1:A:250:GLN:HG3	1.98	0.62
1:A:420:ILE:O	1:A:420:ILE:HG13	1.90	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ASP:OD2	1:B:135:THR:CG2	2.47	0.62
1:C:398:LEU:HG	1:C:403:VAL:CG1	2.29	0.62
1:D:320:ILE:CD1	1:D:320:ILE:H	2.12	0.62
1:A:189:ASP:OD2	1:A:357:MET:HE1	1.99	0.62
1:B:263:GLU:O	1:B:266:LYS:HG3	1.99	0.62
1:B:223:VAL:CG1	1:B:274:THR:HB	2.29	0.62
1:C:312:GLU:HG2	1:C:313:ASN:HD22	1.59	0.62
1:D:58:GLU:O	1:D:361:PHE:HE2	1.81	0.62
1:A:107:GLU:H	1:A:107:GLU:CD	2.03	0.62
1:A:169:ASN:CB	1:A:171:ILE:HD12	2.22	0.62
1:A:430:ARG:O	1:B:430:ARG:HB3	1.99	0.62
1:C:171:ILE:HG23	4:C:714:HOH:O	1.98	0.62
1:D:183:VAL:CG1	1:D:431:TYR:CD1	2.82	0.62
1:A:7:LYS:HG2	1:A:101:TRP:CH2	2.35	0.62
1:C:160:VAL:CG1	1:C:164:TYR:CE2	2.83	0.62
1:D:321:LYS:HE3	1:D:324:VAL:HG21	1.81	0.62
1:A:275:THR:HG23	2:A:501:NAD:N9A	2.15	0.62
1:A:317:LYS:CD	1:A:327:TYR:CE2	2.83	0.62
1:A:425:LYS:HZ2	1:A:426:PRO:CD	2.13	0.62
1:B:53:LEU:HG	1:B:130:ASP:CB	2.29	0.62
1:B:16:TRP:CD1	1:B:16:TRP:O	2.52	0.62
1:C:395:GLU:C	1:C:395:GLU:OE2	2.37	0.62
1:B:300:HIS:HA	1:B:343:LEU:HD11	1.82	0.62
1:C:55:MET:H	1:C:77:SER:HB2	1.64	0.62
1:C:91:ILE:HG22	1:C:98:VAL:HG21	1.80	0.62
1:D:48:ARG:HD3	1:D:121:ASP:CG	2.20	0.62
1:B:179:VAL:O	1:B:182:SER:HB2	2.00	0.62
1:C:5:PRO:O	1:C:97:PRO:HB3	2.00	0.62
1:A:425:LYS:HE2	1:A:429:TYR:CD1	2.34	0.61
1:D:211:ALA:HB2	1:D:234:PHE:O	2.00	0.61
1:B:34:MET:O	1:B:69:LEU:HD11	2.00	0.61
1:B:91:ILE:CG2	1:B:98:VAL:HG22	2.29	0.61
1:C:174:VAL:HG23	1:C:175:PRO:CD	2.30	0.61
1:C:81:PHE:CE2	1:C:342:ARG:HD2	2.35	0.61
1:D:126:MET:HE1	1:D:151:GLY:N	2.16	0.61
1:A:189:ASP:OD1	1:A:352:HIS:CE1	2.53	0.61
1:A:408:LEU:HA	1:A:412:GLN:NE2	2.15	0.61
1:C:225:LYS:HZ3	1:C:250:GLN:HE22	1.47	0.61
1:D:57:VAL:H	1:D:84:GLN:NE2	1.98	0.61
1:A:425:LYS:CE	1:A:425:LYS:CA	2.78	0.61
1:B:198:LEU:HD11	1:B:202:ILE:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:PHE:CD1	1:D:119:PHE:N	2.69	0.61
1:A:199:ILE:HG21	1:A:234:PHE:CE2	2.35	0.61
1:B:419:PRO:HB2	1:B:422:GLY:N	2.15	0.61
1:C:180:ASN:HA	1:C:185:LYS:HD2	1.81	0.61
1:D:60:ALA:CB	1:D:91:ILE:HD11	2.26	0.61
2:A:501:NAD:C4N	3:A:601:ADN:H3'	2.30	0.61
1:B:210:ILE:HG21	1:B:234:PHE:HB2	1.83	0.61
1:B:130:ASP:OD2	1:B:155:GLU:HB3	2.00	0.61
1:B:208:VAL:CG2	1:B:209:MET:N	2.64	0.61
1:C:400:LYS:HG3	1:C:400:LYS:O	1.99	0.61
1:D:113:ILE:CG2	1:D:137:LEU:HD23	2.30	0.61
1:D:74:ARG:CD	1:D:116:THR:HA	2.30	0.61
1:D:137:LEU:HD13	1:D:141:LYS:HD3	1.83	0.61
1:A:150:ARG:HD2	1:A:372:TRP:HA	1.81	0.60
1:B:315:VAL:N	1:B:328:LEU:O	2.34	0.60
1:D:373:THR:C	1:D:374:HIS:ND1	2.54	0.60
1:B:101:TRP:O	1:B:104:GLU:HG2	2.02	0.60
1:B:275:THR:CG2	1:B:276:GLY:N	2.64	0.60
1:B:292:ASP:CG	1:B:326:ARG:HH21	2.03	0.60
1:B:57:VAL:H	1:B:84:GLN:NE2	1.99	0.60
1:B:210:ILE:CG2	1:B:234:PHE:HB3	2.32	0.60
1:C:14:ALA:HB2	1:C:89:ALA:O	2.02	0.60
1:D:317:LYS:HB2	1:D:327:TYR:CE2	2.37	0.60
1:A:109:TYR:OH	1:A:133:ASP:OD2	2.16	0.60
1:B:273:THR:OG1	1:B:297:ASN:CB	2.49	0.60
1:B:329:LEU:N	1:B:329:LEU:HD23	2.16	0.60
1:A:245:PRO:HD3	1:B:405:LEU:HD21	1.82	0.60
1:C:277:CYS:HB3	1:D:416:LEU:CG	2.32	0.60
1:C:419:PRO:CG	1:C:422:GLY:CA	2.79	0.60
1:A:164:TYR:CE1	1:A:382:VAL:CG2	2.84	0.60
1:C:126:MET:HE2	1:C:150:ARG:HB3	1.80	0.60
1:C:358:SER:HG	1:C:397:HIS:HE2	1.50	0.60
1:C:79:ASN:HB3	1:C:82:SER:CB	2.30	0.60
1:A:44:LEU:HB3	1:A:71:ALA:HB2	1.83	0.60
1:B:60:ALA:O	1:B:64:GLU:HG3	2.00	0.60
1:D:6:TYR:HB2	1:D:98:VAL:H	1.65	0.60
1:B:109:TYR:OH	1:B:133:ASP:OD2	2.14	0.60
1:C:398:LEU:HG	1:C:403:VAL:HG11	1.83	0.60
1:D:408:LEU:O	1:D:420:ILE:HD13	1.98	0.60
1:B:152:ILE:HB	1:B:176:ALA:HB2	1.84	0.60
1:C:137:LEU:CD1	1:C:137:LEU:C	2.51	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LYS:C	1:A:143:PRO:HD3	2.22	0.60
1:B:177:ILE:HG13	1:B:371:LEU:CD2	2.20	0.60
1:A:430:ARG:HB3	1:B:430:ARG:O	2.01	0.60
1:B:223:VAL:HG23	2:B:502:NAD:O2N	2.02	0.60
1:B:5:PRO:O	1:B:6:TYR:HB3	2.01	0.60
1:C:128:LEU:HD21	1:C:364:GLN:CG	2.31	0.60
1:C:125:ASN:HA	1:C:148:GLY:O	2.02	0.60
1:C:126:MET:HE2	1:C:151:GLY:N	2.16	0.60
1:C:47:ALA:HA	1:C:125:ASN:HD21	1.67	0.60
1:A:223:VAL:CG1	1:A:274:THR:HB	2.32	0.59
1:C:145:LEU:HD23	1:C:145:LEU:N	2.17	0.59
1:B:171:ILE:O	1:B:171:ILE:HG22	2.02	0.59
1:C:140:THR:OG1	1:C:141:LYS:HD2	2.01	0.59
1:C:237:ARG:NH2	1:C:267:GLU:OE2	2.35	0.59
1:D:337:LEU:CD1	1:D:340:GLU:HA	2.30	0.59
1:B:385:LEU:CD2	1:B:389:LEU:CB	2.80	0.59
1:A:374:HIS:N	1:A:375:PRO:CD	2.64	0.59
1:A:91:ILE:HG21	1:A:98:VAL:HG22	1.80	0.59
1:C:144:GLN:C	1:C:145:LEU:HD23	2.23	0.59
1:D:121:ASP:N	1:D:121:ASP:OD1	2.35	0.59
1:D:6:TYR:CE1	1:D:8:VAL:HG22	2.37	0.59
1:C:223:VAL:CG1	1:C:274:THR:HB	2.33	0.59
1:C:339:ALA:O	1:C:342:ARG:HG3	2.01	0.59
1:B:374:HIS:N	1:B:375:PRO:CD	2.66	0.59
1:D:81:PHE:CD2	1:D:342:ARG:HD3	2.38	0.59
1:A:425:LYS:CA	1:A:425:LYS:NZ	2.44	0.59
1:B:418:MET:HB2	1:B:424:PHE:HD1	1.68	0.59
1:A:386:PRO:HB2	1:A:389:LEU:HG	1.85	0.59
1:C:139:HIS:ND1	1:C:146:LEU:HD11	2.17	0.59
1:C:239:ILE:HG23	1:C:257:GLU:HG2	1.83	0.59
1:A:127:ILE:HD11	1:A:138:ILE:HD13	1.83	0.59
1:A:394:ALA:O	1:A:398:LEU:HD13	2.02	0.59
1:A:54:HIS:CE1	1:A:78:CYS:SG	2.96	0.59
1:B:157:THR:HB	2:B:502:NAD:H52N	1.82	0.59
1:B:309:TRP:CZ3	1:B:310:LEU:HD23	2.38	0.59
1:A:374:HIS:ND1	1:A:374:HIS:N	2.50	0.59
1:B:203:LYS:O	1:B:207:ASP:N	2.36	0.59
1:B:210:ILE:HG21	1:B:234:PHE:HB3	1.85	0.59
1:C:398:LEU:HD21	1:D:245:PRO:HA	1.85	0.59
1:D:406:THR:HG22	1:D:407:LYS:N	2.17	0.59
1:D:93:LYS:C	1:D:95:GLY:N	2.56	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:CD2	1:A:227:CYS:SG	2.91	0.58
1:A:199:ILE:CD1	1:A:231:LEU:CD2	2.79	0.58
1:A:244:GLU:OE2	1:B:425:LYS:HD2	2.03	0.58
1:B:91:ILE:CG2	1:B:98:VAL:HG21	2.31	0.58
1:A:356:VAL:HB	1:C:209:MET:SD	2.43	0.58
1:D:47:ALA:O	1:D:72:GLU:HB2	2.03	0.58
1:B:169:ASN:CB	1:B:171:ILE:CD1	2.80	0.58
1:B:58:GLU:O	1:B:361:PHE:HE2	1.86	0.58
1:A:320:ILE:HG13	1:C:23:ILE:HD11	1.84	0.58
1:C:277:CYS:CB	1:D:416:LEU:HG	2.33	0.58
1:D:322:PRO:O	1:D:323:GLN:HB2	2.03	0.58
1:D:328:LEU:HD22	4:D:675:HOH:O	2.03	0.58
1:B:209:MET:SD	1:D:353:PRO:HG2	2.43	0.58
1:A:189:ASP:OD1	1:A:352:HIS:HE1	1.86	0.58
1:B:418:MET:SD	1:B:424:PHE:HB3	2.43	0.58
1:D:119:PHE:HD1	1:D:119:PHE:N	2.01	0.58
1:D:306:ASP:OD1	1:D:308:LYS:HD2	2.03	0.58
1:D:48:ARG:HD2	1:D:119:PHE:HB2	1.85	0.58
1:D:48:ARG:HG3	1:D:48:ARG:NH1	2.17	0.58
1:A:157:THR:OG1	2:A:501:NAD:H52N	2.03	0.58
1:A:297:ASN:HB3	1:A:341:GLY:O	2.03	0.58
1:B:419:PRO:HB2	1:B:422:GLY:HA3	1.85	0.58
1:C:363:ASN:HD21	1:C:393:VAL:HG21	1.67	0.58
1:D:198:LEU:HG	1:D:199:ILE:N	2.18	0.58
1:D:374:HIS:HD2	1:D:377:LYS:NZ	2.00	0.58
1:B:19:LYS:O	1:B:23:ILE:HG13	2.04	0.58
1:B:410:GLU:O	1:B:414:GLN:HG3	2.04	0.58
1:B:425:LYS:HZ2	1:B:425:LYS:HA	1.66	0.58
1:A:373:THR:C	1:A:375:PRO:HD2	2.23	0.58
1:B:125:ASN:ND2	1:B:372:TRP:CZ3	2.71	0.58
1:B:292:ASP:HA	1:B:334:ARG:O	2.04	0.58
1:D:33:ARG:HD2	1:D:37:MET:SD	2.44	0.58
1:D:419:PRO:HD3	1:D:423:PRO:O	2.02	0.58
1:A:53:LEU:HG	1:A:130:ASP:HB2	1.85	0.58
1:B:62:LEU:HB2	1:B:361:PHE:CD2	2.39	0.58
1:C:327:TYR:O	1:C:334:ARG:HA	2.04	0.58
1:D:345:ASN:O	1:D:349:ALA:HB3	2.04	0.58
1:B:306:ASP:OD2	1:B:309:TRP:HB2	2.03	0.58
1:C:142:HIS:HA	1:C:144:GLN:OE1	2.03	0.58
1:B:121:ASP:OD1	1:B:121:ASP:N	2.37	0.57
1:B:60:ALA:HB1	1:B:91:ILE:CD1	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:LYS:HE2	1:C:74:ARG:NH1	2.18	0.57
1:B:4:LEU:HD12	1:B:111:TRP:HZ2	1.69	0.57
1:B:48:ARG:HD2	1:B:119:PHE:CB	2.33	0.57
1:C:419:PRO:HD2	1:C:423:PRO:O	2.04	0.57
1:D:134:LEU:C	1:D:134:LEU:HD22	2.24	0.57
1:D:373:THR:O	1:D:374:HIS:ND1	2.37	0.57
1:D:63:ILE:HD11	1:D:75:TRP:CE2	2.38	0.57
1:A:164:TYR:CE1	1:A:382:VAL:HG11	2.39	0.57
1:C:176:ALA:O	1:C:382:VAL:HA	2.04	0.57
1:D:117:LEU:CD2	1:D:138:ILE:HD11	2.34	0.57
1:C:431:TYR:OXT	1:D:187:LYS:NZ	2.37	0.57
1:D:45:LYS:HD3	1:D:46:GLY:N	2.09	0.57
1:A:156:THR:OG1	2:A:501:NAD:H2D	2.04	0.57
1:A:162:ASN:O	1:A:166:MET:HG3	2.04	0.57
1:A:163:LEU:CD1	1:A:176:ALA:CB	2.82	0.57
1:B:181:ASP:CB	1:B:384:PHE:HE1	2.16	0.57
1:C:345:ASN:ND2	1:C:346:LEU:N	2.45	0.57
1:D:342:ARG:NH1	1:D:342:ARG:HG2	2.18	0.57
1:A:320:ILE:CD1	1:A:320:ILE:N	2.67	0.57
1:A:379:PRO:O	1:A:380:VAL:C	2.42	0.57
1:B:424:PHE:C	1:B:426:PRO:HD3	2.13	0.57
1:C:11:ILE:HA	1:C:89:ALA:HB1	1.87	0.57
1:C:183:VAL:O	1:C:185:LYS:N	2.38	0.57
1:C:353:PRO:O	1:C:356:VAL:HG12	2.05	0.57
1:C:424:PHE:O	1:C:426:PRO:CD	2.51	0.57
1:D:295:VAL:HG12	1:D:305:ILE:CD1	2.34	0.57
1:D:317:LYS:HB2	1:D:327:TYR:CD2	2.40	0.57
1:B:273:THR:OG1	1:B:297:ASN:CA	2.52	0.57
1:C:379:PRO:O	1:C:383:HIS:HE1	1.86	0.57
1:D:81:PHE:O	1:D:102:LYS:HE3	2.05	0.57
1:D:27:GLU:C	1:D:29:PRO:HD3	2.25	0.57
1:D:181:ASP:HB3	1:D:384:PHE:HE1	1.69	0.57
1:C:223:VAL:HG11	1:C:298:ILE:HG21	1.86	0.57
1:C:325:ASP:O	1:C:336:ILE:HA	2.05	0.57
1:D:91:ILE:CD1	1:D:91:ILE:N	2.68	0.57
1:B:393:VAL:O	1:B:397:HIS:ND1	2.37	0.57
1:B:79:ASN:HB3	1:B:82:SER:CB	2.35	0.57
1:C:140:THR:OG1	1:C:141:LYS:CD	2.53	0.57
1:D:300:HIS:C	1:D:343:LEU:HD11	2.25	0.57
1:A:163:LEU:CD1	1:A:176:ALA:HB3	2.35	0.57
1:B:201:GLY:HA2	1:B:349:ALA:HB2	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LYS:HG2	1:B:431:TYR:OH	2.05	0.57
1:C:45:LYS:CD	1:C:45:LYS:C	2.74	0.57
1:D:220:TYR:CD2	1:D:225:LYS:HE3	2.39	0.57
1:A:164:TYR:CE1	1:A:382:VAL:CG1	2.88	0.56
1:C:182:SER:O	1:C:183:VAL:C	2.42	0.56
1:B:359:ASN:ND2	1:B:393:VAL:HG12	2.17	0.56
1:D:240:ILE:O	1:D:258:VAL:HA	2.05	0.56
1:A:17:GLY:O	1:A:21:LEU:HG	2.05	0.56
1:A:27:GLU:O	1:A:29:PRO:HD3	2.05	0.56
1:A:55:MET:HE3	1:A:59:THR:HG22	1.86	0.56
1:B:127:ILE:HG23	1:B:134:LEU:HD12	1.85	0.56
1:B:208:VAL:CG2	1:B:209:MET:H	2.18	0.56
1:B:35:ARG:O	1:B:39:SER:OG	2.22	0.56
1:C:135:THR:HB	1:C:152:ILE:HD13	1.86	0.56
1:C:422:GLY:O	1:C:424:PHE:CE1	2.58	0.56
1:D:363:ASN:HD21	1:D:393:VAL:HG21	1.71	0.56
1:C:284:ARG:HG3	1:C:284:ARG:O	2.05	0.56
1:C:430:ARG:CB	1:C:430:ARG:CZ	2.84	0.56
1:C:55:MET:HG2	1:C:75:TRP:CD1	2.39	0.56
1:D:91:ILE:HG22	1:D:98:VAL:HG22	1.87	0.56
1:A:292:ASP:CA	1:A:334:ARG:O	2.52	0.56
1:A:406:THR:CG2	1:A:407:LYS:N	2.68	0.56
1:D:74:ARG:HD3	1:D:116:THR:HA	1.87	0.56
1:A:179:VAL:O	1:A:182:SER:HB2	2.05	0.56
1:B:33:ARG:HH11	1:B:36:GLU:CD	2.09	0.56
1:B:181:ASP:HB3	1:B:384:PHE:HE1	1.70	0.56
1:C:275:THR:HB	1:C:304:GLU:OE1	2.04	0.56
1:D:189:ASP:O	1:D:352:HIS:HE1	1.89	0.56
1:D:373:THR:O	1:D:373:THR:HG22	2.04	0.56
1:D:373:THR:CG2	1:D:374:HIS:HE1	2.16	0.56
1:A:373:THR:HG21	1:A:374:HIS:CE1	2.21	0.56
1:B:184:THR:HA	1:B:188:PHE:CE1	2.41	0.56
1:D:149:ILE:CG2	1:D:174:VAL:HG21	2.36	0.56
1:D:6:TYR:HD1	1:D:8:VAL:HG13	1.71	0.56
1:B:398:LEU:HD23	1:B:405:LEU:HD13	1.88	0.56
1:C:74:ARG:HB3	1:C:116:THR:HB	1.86	0.56
1:C:141:LYS:HB3	4:C:626:HOH:O	2.06	0.56
1:C:374:HIS:HD2	1:C:377:LYS:NZ	2.04	0.56
1:B:27:GLU:C	1:B:29:PRO:HD3	2.25	0.56
1:B:193:GLY:HA3	1:B:352:HIS:ND1	2.21	0.56
1:C:156:THR:OG1	1:C:157:THR:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:VAL:CG1	1:C:298:ILE:HG21	2.36	0.56
1:D:215:ALA:HB1	1:D:231:LEU:HD13	1.87	0.56
1:A:121:ASP:OD1	1:A:121:ASP:N	2.26	0.56
1:A:235:GLY:O	1:D:255:GLY:HA2	2.05	0.56
1:D:101:TRP:CE2	1:D:104:GLU:HG2	2.41	0.56
1:A:164:TYR:HD1	1:A:382:VAL:HG11	1.63	0.56
1:A:387:LYS:HZ3	1:A:425:LYS:C	2.09	0.56
1:B:418:MET:HB3	1:B:424:PHE:HB3	1.87	0.56
1:C:161:HIS:CE1	1:C:165:LYS:CE	2.89	0.56
1:C:355:PHE:CZ	1:C:401:LEU:HD21	2.40	0.56
1:C:430:ARG:O	1:C:431:TYR:OXT	2.24	0.56
1:D:406:THR:CG2	1:D:407:LYS:N	2.69	0.56
1:C:160:VAL:O	1:C:164:TYR:CD2	2.59	0.55
1:C:262:ASP:OD1	1:C:284:ARG:NH1	2.39	0.55
1:C:60:ALA:O	1:C:64:GLU:HG3	2.06	0.55
1:A:198:LEU:HD22	1:A:227:CYS:SG	2.45	0.55
1:A:315:VAL:N	1:A:328:LEU:O	2.39	0.55
1:C:406:THR:HG23	1:C:407:LYS:N	2.22	0.55
1:A:419:PRO:HG2	1:A:422:GLY:N	2.15	0.55
1:C:418:MET:HB2	1:C:419:PRO:CD	2.36	0.55
1:D:155:GLU:OE2	1:D:364:GLN:OE1	2.24	0.55
1:A:403:VAL:HG13	1:B:258:VAL:HB	1.89	0.55
1:B:33:ARG:HH11	1:B:36:GLU:CG	2.19	0.55
1:D:58:GLU:O	1:D:361:PHE:CE2	2.59	0.55
1:B:197:SER:HB2	1:B:345:ASN:HB2	1.88	0.55
1:B:48:ARG:HD3	1:B:121:ASP:OD1	2.06	0.55
1:A:110:LEU:C	1:A:110:LEU:CD1	2.75	0.55
1:A:425:LYS:NZ	1:A:426:PRO:HD2	2.22	0.55
1:B:130:ASP:OD2	1:B:155:GLU:CB	2.55	0.55
1:B:419:PRO:CD	1:B:423:PRO:O	2.54	0.55
1:D:320:ILE:HD11	1:D:326:ARG:HB2	1.88	0.55
1:D:409:THR:H	1:D:412:GLN:HE21	1.54	0.55
1:A:327:TYR:O	1:A:334:ARG:HA	2.07	0.55
1:C:344:VAL:HG13	1:C:345:ASN:N	2.20	0.55
1:C:53:LEU:O	1:C:54:HIS:C	2.45	0.55
1:A:418:MET:HB2	1:A:419:PRO:HD2	1.88	0.55
1:A:83:THR:HG21	1:A:101:TRP:HA	1.89	0.55
1:B:372:TRP:CD1	1:B:372:TRP:O	2.60	0.55
1:A:143:PRO:HA	1:A:146:LEU:HD23	1.86	0.55
1:A:300:HIS:HA	1:A:343:LEU:CD1	2.33	0.55
1:B:74:ARG:HD2	1:B:116:THR:HA	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:425:LYS:HD3	1:C:431:TYR:OH	2.06	0.55
1:A:57:VAL:O	1:A:60:ALA:HB3	2.07	0.55
1:C:316:GLU:HG2	1:C:328:LEU:CB	2.34	0.55
1:C:317:LYS:HD2	1:C:327:TYR:CE2	2.42	0.55
1:D:382:VAL:HG22	1:D:382:VAL:O	2.07	0.55
1:A:416:LEU:HD21	1:B:277:CYS:HB3	1.88	0.54
1:C:273:THR:HG1	1:C:297:ASN:HB2	1.69	0.54
1:C:298:ILE:C	1:C:299:GLY:O	2.43	0.54
1:C:81:PHE:HE2	1:C:342:ARG:HD2	1.72	0.54
1:D:142:HIS:CA	1:D:144:GLN:OE1	2.55	0.54
1:D:364:GLN:NE2	1:D:364:GLN:HA	2.21	0.54
1:D:56:THR:HA	1:D:84:GLN:HB2	1.89	0.54
1:A:164:TYR:CZ	1:B:428:HIS:CE1	2.96	0.54
1:B:45:LYS:C	1:B:45:LYS:HD2	2.24	0.54
1:C:126:MET:HE3	1:C:150:ARG:CB	2.33	0.54
1:B:254:GLU:HB3	1:B:256:TYR:CD2	2.42	0.54
1:A:228:ALA:HB1	1:A:256:TYR:CZ	2.42	0.54
1:B:342:ARG:O	1:B:343:LEU:C	2.46	0.54
1:C:282:LEU:N	1:C:285:HIS:ND1	2.48	0.54
1:C:302:ASP:O	1:C:303:VAL:HG13	2.07	0.54
1:D:425:LYS:CE	1:D:426:PRO:HD2	2.35	0.54
1:A:74:ARG:HD2	1:A:116:THR:HA	1.88	0.54
1:B:10:ASP:HB3	1:B:13:LEU:HD22	1.89	0.54
1:B:292:ASP:OD1	1:B:336:ILE:CD1	2.56	0.54
1:B:317:LYS:HB2	1:B:327:TYR:CE2	2.42	0.54
1:B:353:PRO:HG2	1:D:209:MET:SD	2.47	0.54
1:D:143:PRO:CA	1:D:146:LEU:HD22	2.38	0.54
1:D:188:PHE:O	1:D:192:TYR:HB2	2.08	0.54
1:B:382:VAL:HG22	1:B:382:VAL:O	2.07	0.54
1:C:305:ILE:O	1:C:307:VAL:HG23	2.07	0.54
1:A:45:LYS:HA	1:A:70:GLY:O	2.07	0.54
1:B:126:MET:HE2	1:B:151:GLY:N	2.23	0.54
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.21	0.54
1:D:419:PRO:HD2	1:D:424:PHE:CD1	2.43	0.54
1:A:277:CYS:HB2	1:B:416:LEU:CD2	2.38	0.54
1:C:295:VAL:HG12	1:C:305:ILE:HD13	1.90	0.54
1:B:425:LYS:HE2	1:B:429:TYR:CD1	2.42	0.54
1:D:321:LYS:HG2	1:D:324:VAL:CG2	2.38	0.54
1:C:186:SER:HB2	1:D:430:ARG:HH22	1.72	0.54
1:A:223:VAL:HB	2:A:501:NAD:O2N	2.07	0.53
1:A:232:ARG:HG3	1:A:238:VAL:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:TYR:HD2	1:A:431:TYR:CE1	2.26	0.53
1:B:137:LEU:O	1:B:141:LYS:HB2	2.09	0.53
1:B:419:PRO:HB2	1:B:422:GLY:CA	2.37	0.53
1:C:198:LEU:O	1:C:198:LEU:HD12	2.08	0.53
1:D:99:PHE:CZ	1:D:115:GLN:HB3	2.43	0.53
1:D:6:TYR:HB2	1:D:98:VAL:O	2.09	0.53
1:A:13:LEU:HB3	1:A:86:HIS:HA	1.91	0.53
1:A:188:PHE:O	1:A:192:TYR:HB2	2.07	0.53
1:A:342:ARG:O	1:A:343:LEU:C	2.46	0.53
1:A:48:ARG:HD3	1:A:121:ASP:CG	2.25	0.53
1:A:428:HIS:CE1	1:B:164:TYR:CZ	2.96	0.53
1:B:16:TRP:CD1	1:B:16:TRP:C	2.81	0.53
1:B:183:VAL:C	1:B:185:LYS:H	2.12	0.53
1:B:278:VAL:CG1	1:B:303:VAL:CB	2.75	0.53
1:C:139:HIS:CE1	1:C:146:LEU:HD11	2.44	0.53
1:D:221:GLY:O	1:D:225:LYS:CG	2.44	0.53
1:D:291:ASP:O	1:D:292:ASP:HB2	2.07	0.53
1:B:302:ASP:OD2	1:B:342:ARG:NH2	2.40	0.53
1:B:387:LYS:O	1:B:391:GLU:HG2	2.08	0.53
1:C:315:VAL:CG2	1:C:330:LYS:CG	2.79	0.53
1:D:137:LEU:HA	1:D:141:LYS:HD2	1.91	0.53
1:D:317:LYS:HG3	1:D:327:TYR:CD2	2.42	0.53
1:D:370:GLU:O	1:D:374:HIS:N	2.42	0.53
1:A:198:LEU:HD21	1:A:272:VAL:HG11	1.91	0.53
1:C:216:VAL:HB	1:C:271:PHE:CD2	2.44	0.53
1:C:374:HIS:N	1:C:375:PRO:CD	2.71	0.53
1:D:223:VAL:HG12	1:D:274:THR:CB	2.35	0.53
1:D:418:MET:HB2	1:D:419:PRO:HD3	1.90	0.53
1:D:54:HIS:CE1	1:D:78:CYS:SG	3.02	0.53
1:A:134:LEU:O	1:A:138:ILE:HD12	2.09	0.53
1:B:292:ASP:N	1:B:334:ARG:O	2.41	0.53
1:C:117:LEU:HD21	1:C:138:ILE:HD11	1.89	0.53
1:C:125:ASN:ND2	1:C:372:TRP:CH2	2.77	0.53
1:D:13:LEU:HB3	1:D:86:HIS:HA	1.90	0.53
1:D:206:THR:OG1	1:D:208:VAL:HG12	2.08	0.53
1:A:145:LEU:O	1:A:149:ILE:HD12	2.09	0.53
1:C:127:ILE:HG12	1:C:134:LEU:HD13	1.89	0.53
1:D:153:SER:HB3	1:D:364:GLN:NE2	2.24	0.53
1:D:418:MET:HB2	1:D:424:PHE:HD1	1.74	0.53
1:A:419:PRO:CD	1:A:423:PRO:O	2.57	0.53
1:D:101:TRP:NE1	1:D:104:GLU:HG2	2.24	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:LYS:O	1:D:207:ASP:N	2.37	0.53
1:D:203:LYS:NZ	1:D:208:VAL:O	2.39	0.53
1:A:387:LYS:O	1:A:391:GLU:CG	2.56	0.53
1:A:425:LYS:CG	1:A:431:TYR:OH	2.55	0.53
1:A:80:ILE:O	1:A:103:GLY:N	2.36	0.53
1:B:79:ASN:HB3	1:B:82:SER:HB3	1.90	0.53
1:C:206:THR:CG2	1:C:294:ILE:HD13	2.32	0.53
1:C:428:HIS:N	1:C:428:HIS:CD2	2.73	0.53
1:C:55:MET:HE3	1:C:59:THR:HB	1.87	0.53
1:C:91:ILE:CG2	1:C:98:VAL:CG2	2.87	0.53
1:D:10:ASP:O	1:D:13:LEU:HB2	2.09	0.53
1:D:142:HIS:HA	1:D:144:GLN:OE1	2.09	0.53
1:A:129:ASP:OD2	1:A:135:THR:CG2	2.56	0.52
1:A:137:LEU:HD12	1:A:141:LYS:HB2	1.91	0.52
1:B:110:LEU:C	1:B:110:LEU:HD13	2.23	0.52
1:B:120:LYS:C	1:B:122:GLY:H	2.12	0.52
1:B:13:LEU:HB3	1:B:86:HIS:HA	1.91	0.52
1:C:160:VAL:HG12	1:C:164:TYR:HE2	1.69	0.52
1:C:261:MET:O	1:C:261:MET:HG3	2.08	0.52
1:C:298:ILE:O	1:C:343:LEU:CD1	2.56	0.52
1:D:153:SER:HB3	1:D:364:GLN:HE22	1.74	0.52
1:D:44:LEU:O	1:D:47:ALA:CB	2.58	0.52
1:A:53:LEU:HG	1:A:130:ASP:CB	2.39	0.52
1:B:430:ARG:O	1:B:431:TYR:OXT	2.28	0.52
1:B:157:THR:CG2	2:B:502:NAD:H52N	2.39	0.52
1:B:44:LEU:CB	1:B:71:ALA:HB2	2.39	0.52
1:A:228:ALA:O	1:A:232:ARG:HB2	2.09	0.52
1:A:321:LYS:HE3	1:A:324:VAL:HG21	1.91	0.52
1:A:431:TYR:CE2	1:B:247:ASN:ND2	2.63	0.52
1:B:48:ARG:HD3	1:B:121:ASP:CG	2.29	0.52
1:D:225:LYS:NZ	1:D:250:GLN:HE22	2.06	0.52
1:D:418:MET:HB2	1:D:424:PHE:HB3	1.85	0.52
1:A:419:PRO:HG3	1:A:422:GLY:CA	2.01	0.52
1:B:125:ASN:ND2	1:B:372:TRP:CH2	2.77	0.52
1:B:79:ASN:HB3	1:B:82:SER:OG	2.09	0.52
1:C:158:THR:HG21	1:C:301:PHE:CE2	2.45	0.52
1:C:185:LYS:O	1:C:185:LYS:HD3	2.10	0.52
1:C:161:HIS:CE1	1:C:165:LYS:HE3	2.45	0.52
1:D:374:HIS:N	1:D:375:PRO:HD2	2.23	0.52
1:A:110:LEU:C	1:A:110:LEU:HD13	2.25	0.52
1:B:152:ILE:HB	1:B:176:ALA:CB	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:O	1:B:207:ASP:HB2	2.09	0.52
1:B:199:ILE:HD12	1:B:234:PHE:HD2	1.73	0.52
1:B:6:TYR:HB2	1:B:98:VAL:H	1.74	0.52
1:C:223:VAL:HG23	2:C:503:NAD:O2N	2.08	0.52
1:C:373:THR:C	1:C:375:PRO:HD2	2.30	0.52
1:B:127:ILE:HG12	1:B:134:LEU:HD11	1.92	0.52
1:B:371:LEU:HD13	1:B:378:TYR:CD1	2.45	0.52
1:C:247:ASN:HD21	1:D:431:TYR:HE2	1.58	0.52
1:D:137:LEU:CD1	1:D:141:LYS:HD3	2.40	0.52
1:D:143:PRO:O	1:D:146:LEU:HD22	2.10	0.52
1:B:110:LEU:CD1	1:B:114:GLU:CG	2.88	0.52
1:C:428:HIS:O	1:C:429:TYR:C	2.46	0.52
1:D:177:ILE:HG13	1:D:371:LEU:HD21	1.91	0.52
1:A:190:ASN:ND2	2:A:501:NAD:O1N	2.42	0.52
1:B:60:ALA:CB	1:B:91:ILE:HD11	2.32	0.52
1:C:325:ASP:O	1:C:337:LEU:N	2.39	0.52
1:A:177:ILE:HG13	1:A:371:LEU:CD2	2.30	0.52
1:B:3:LYS:HG2	1:B:4:LEU:N	2.24	0.52
1:B:80:ILE:HD11	1:B:342:ARG:NH1	2.25	0.52
1:C:333:HIS:C	1:C:334:ARG:HD3	2.30	0.52
1:C:387:LYS:HG3	4:C:658:HOH:O	2.08	0.52
1:D:163:LEU:CD1	1:D:176:ALA:HB3	2.40	0.52
1:D:5:PRO:O	1:D:6:TYR:HB3	2.10	0.52
1:D:91:ILE:HG22	1:D:98:VAL:HG21	1.92	0.52
1:B:110:LEU:HD12	1:B:114:GLU:CG	2.40	0.51
1:B:240:ILE:O	1:B:258:VAL:HA	2.09	0.51
1:D:318:VAL:CG1	1:D:319:ASN:N	2.73	0.51
1:B:209:MET:HB2	1:D:353:PRO:HB2	1.92	0.51
1:D:55:MET:HE2	1:D:59:THR:HB	1.92	0.51
1:A:157:THR:HB	2:A:501:NAD:C5D	2.40	0.51
1:A:6:TYR:HB2	1:A:98:VAL:H	1.76	0.51
1:C:156:THR:HG21	1:C:300:HIS:ND1	2.24	0.51
1:D:141:LYS:C	1:D:143:PRO:HD3	2.31	0.51
1:D:275:THR:HG22	1:D:277:CYS:H	1.76	0.51
1:D:398:LEU:HD21	1:D:405:LEU:HD22	1.91	0.51
1:A:239:ILE:HG12	1:A:257:GLU:HG2	1.92	0.51
1:B:177:ILE:CG1	1:B:371:LEU:HD21	2.21	0.51
1:B:275:THR:HG23	2:B:502:NAD:C8A	2.40	0.51
1:C:201:GLY:HA2	1:C:349:ALA:HB2	1.92	0.51
1:C:352:HIS:HB3	1:C:356:VAL:HG11	1.92	0.51
1:A:134:LEU:HD22	1:A:138:ILE:HD12	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:NZ	1:A:425:LYS:O	2.34	0.51
1:B:53:LEU:HD11	1:B:155:GLU:CG	2.41	0.51
1:C:197:SER:HB2	1:C:345:ASN:HB2	1.92	0.51
1:C:430:ARG:NH1	1:D:187:LYS:CE	2.49	0.51
1:A:143:PRO:HA	1:A:146:LEU:HD22	1.91	0.51
1:A:419:PRO:C	1:A:421:ASN:N	2.62	0.51
1:B:39:SER:O	1:B:42:LYS:CG	2.59	0.51
1:B:58:GLU:O	1:B:361:PHE:CE2	2.63	0.51
1:C:3:LYS:HE3	1:C:115:GLN:OE1	2.11	0.51
1:C:430:ARG:HH11	1:C:430:ARG:HB3	1.74	0.51
1:D:418:MET:CB	1:D:424:PHE:HD1	2.24	0.51
1:D:54:HIS:O	1:D:56:THR:HG23	2.11	0.51
1:C:105:THR:OG1	1:C:108:GLU:HG3	2.09	0.51
1:C:418:MET:CB	1:C:424:PHE:HB3	2.40	0.51
1:D:193:GLY:HA3	1:D:352:HIS:ND1	2.25	0.51
1:D:68:ALA:C	1:D:70:GLY:H	2.12	0.51
1:B:292:ASP:CA	1:B:334:ARG:O	2.58	0.51
1:B:419:PRO:HG2	1:B:423:PRO:N	2.23	0.51
1:C:425:LYS:HE3	1:C:426:PRO:CD	2.41	0.51
1:C:55:MET:HG2	1:C:75:TRP:HD1	1.74	0.51
1:C:195:ARG:CD	1:C:229:GLN:OE1	2.59	0.51
1:C:298:ILE:O	1:C:343:LEU:HD11	2.10	0.51
1:C:425:LYS:CG	1:C:431:TYR:OH	2.59	0.51
1:A:150:ARG:CZ	1:A:372:TRP:CZ3	2.94	0.51
1:B:57:VAL:O	1:B:61:VAL:HG23	2.11	0.51
1:C:130:ASP:HA	1:C:155:GLU:HB2	1.93	0.51
1:C:161:HIS:CE1	1:C:165:LYS:HE2	2.46	0.51
1:C:91:ILE:CG2	1:C:98:VAL:HG21	2.40	0.51
1:D:154:GLU:O	1:D:179:VAL:HB	2.11	0.51
1:D:308:LYS:HD2	1:D:308:LYS:H	1.74	0.51
1:D:91:ILE:N	1:D:91:ILE:HD13	2.25	0.51
1:A:54:HIS:CE1	1:A:346:LEU:HD13	2.46	0.50
1:A:181:ASP:CB	1:A:384:PHE:HE1	2.24	0.50
1:C:308:LYS:H	1:C:308:LYS:HD2	1.76	0.50
1:C:41:SER:O	1:C:42:LYS:C	2.49	0.50
1:D:141:LYS:O	1:D:143:PRO:HD3	2.11	0.50
1:D:342:ARG:HH11	1:D:342:ARG:HG2	1.75	0.50
1:D:386:PRO:O	1:D:387:LYS:C	2.50	0.50
1:B:48:ARG:HD2	1:B:119:PHE:CG	2.46	0.50
1:B:198:LEU:HG	1:B:199:ILE:N	2.26	0.50
1:C:57:VAL:H	1:C:84:GLN:NE2	2.09	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:O	1:B:122:GLY:N	2.45	0.50
1:B:167:MET:C	1:B:169:ASN:H	2.15	0.50
1:B:178:ASN:CG	1:B:181:ASP:HB2	2.31	0.50
1:C:302:ASP:O	1:C:303:VAL:CG1	2.59	0.50
1:B:283:GLY:HA3	1:B:309:TRP:CE2	2.46	0.50
1:B:320:ILE:O	1:B:321:LYS:HB3	2.11	0.50
1:C:7:LYS:N	1:C:98:VAL:O	2.39	0.50
1:D:208:VAL:HG22	1:D:209:MET:N	2.27	0.50
1:A:194:CYS:SG	1:A:223:VAL:HG22	2.52	0.50
1:B:126:MET:HE1	1:B:151:GLY:HA3	1.93	0.50
1:C:317:LYS:HB2	1:C:327:TYR:CD2	2.46	0.50
1:D:16:TRP:CD1	1:D:16:TRP:O	2.65	0.50
1:A:398:LEU:HD21	1:A:405:LEU:HD22	1.88	0.50
1:B:54:HIS:HB3	1:B:82:SER:OG	2.12	0.50
1:C:298:ILE:O	1:C:299:GLY:C	2.49	0.50
1:D:134:LEU:O	1:D:134:LEU:CD2	2.52	0.50
1:D:310:LEU:HD13	1:D:327:TYR:CD1	2.46	0.50
1:D:379:PRO:O	1:D:380:VAL:O	2.29	0.50
1:A:282:LEU:O	1:A:285:HIS:HB2	2.11	0.50
1:A:428:HIS:HB3	1:B:384:PHE:HZ	1.76	0.50
1:B:3:LYS:CE	1:B:115:GLN:OE1	2.60	0.50
1:C:317:LYS:HD2	1:C:327:TYR:HE2	1.77	0.50
1:D:3:LYS:HA	4:D:663:HOH:O	2.10	0.50
2:B:502:NAD:C4N	3:B:602:ADN:H3'	2.42	0.50
1:D:273:THR:O	1:D:298:ILE:HG22	2.12	0.50
1:A:429:TYR:CD2	1:A:431:TYR:CE2	2.99	0.49
1:C:130:ASP:HB2	1:C:155:GLU:HB2	1.93	0.49
1:C:321:LYS:HB2	1:C:322:PRO:HD2	1.93	0.49
1:C:345:ASN:O	1:C:349:ALA:HB3	2.12	0.49
1:D:164:TYR:CE1	1:D:382:VAL:HG21	2.47	0.49
1:D:358:SER:OG	1:D:397:HIS:NE2	2.38	0.49
1:A:326:ARG:HG3	1:A:336:ILE:HG13	1.94	0.49
1:A:430:ARG:HB2	1:A:430:ARG:NH1	2.26	0.49
1:B:110:LEU:CD1	1:B:114:GLU:HG2	2.42	0.49
1:B:283:GLY:HA2	1:B:286:PHE:HD2	1.77	0.49
1:B:410:GLU:OE2	1:B:414:GLN:CD	2.49	0.49
1:C:393:VAL:O	1:C:397:HIS:ND1	2.45	0.49
1:C:425:LYS:C	1:C:425:LYS:HE3	2.32	0.49
1:D:185:LYS:C	1:D:185:LYS:HD3	2.33	0.49
1:A:157:THR:CB	2:A:501:NAD:C5D	2.89	0.49
1:A:321:LYS:O	1:A:322:PRO:C	2.49	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HB2	1:A:430:ARG:CZ	2.42	0.49
1:B:74:ARG:CD	1:B:116:THR:HA	2.42	0.49
1:B:53:LEU:O	1:B:54:HIS:C	2.50	0.49
1:C:178:ASN:ND2	1:C:181:ASP:HB2	2.26	0.49
1:C:215:ALA:HA	1:C:270:ILE:O	2.13	0.49
1:D:184:THR:HA	1:D:188:PHE:CD1	2.48	0.49
1:A:250:GLN:O	1:A:251:ALA:C	2.50	0.49
1:A:157:THR:CB	2:A:501:NAD:H51N	2.42	0.49
1:B:53:LEU:HD11	1:B:155:GLU:HG2	1.94	0.49
1:B:57:VAL:HG23	1:B:87:ALA:HB2	1.95	0.49
1:B:5:PRO:O	1:B:97:PRO:HB3	2.12	0.49
1:C:334:ARG:N	1:C:334:ARG:CD	2.74	0.49
1:D:418:MET:HE3	1:D:418:MET:N	2.27	0.49
1:B:193:GLY:HA3	1:B:352:HIS:CE1	2.47	0.49
1:C:162:ASN:O	1:C:165:LYS:HB2	2.12	0.49
1:C:21:LEU:CD2	1:C:60:ALA:HB3	2.38	0.49
1:B:130:ASP:OD1	1:B:300:HIS:HE1	1.95	0.49
1:B:412:GLN:O	1:B:415:TYR:HB3	2.13	0.49
1:C:143:PRO:HA	1:C:146:LEU:HD22	1.94	0.49
1:C:161:HIS:HE1	1:C:165:LYS:HE2	1.77	0.49
1:C:88:ALA:C	1:C:90:ALA:H	2.16	0.49
1:D:254:GLU:OE1	1:D:254:GLU:HA	2.12	0.49
1:A:163:LEU:HD13	1:A:176:ALA:HB3	1.94	0.49
1:B:275:THR:HG22	1:B:277:CYS:N	2.15	0.49
1:C:74:ARG:NH1	1:C:115:GLN:O	2.43	0.49
1:C:124:LEU:HD23	1:C:124:LEU:H	1.77	0.49
1:C:430:ARG:NH1	1:C:430:ARG:HB2	2.26	0.49
1:D:117:LEU:HD21	1:D:138:ILE:HD11	1.94	0.49
1:D:183:VAL:HG11	1:D:431:TYR:CE1	2.47	0.49
1:D:99:PHE:O	1:D:100:ALA:CB	2.58	0.49
1:A:278:VAL:HG22	1:B:415:TYR:CG	2.47	0.49
1:C:195:ARG:HD2	1:C:229:GLN:OE1	2.13	0.49
1:D:169:ASN:ND2	1:D:171:ILE:CD1	2.72	0.49
1:A:418:MET:HB2	1:A:424:PHE:HD1	1.78	0.49
1:B:292:ASP:OD1	1:B:336:ILE:HD11	2.13	0.49
1:C:198:LEU:HG	1:C:199:ILE:N	2.26	0.49
1:C:96:ILE:H	1:C:96:ILE:HD12	1.77	0.49
1:D:370:GLU:HB3	1:D:378:TYR:CE1	2.48	0.49
1:D:418:MET:CG	1:D:424:PHE:HB3	2.43	0.49
1:A:322:PRO:O	1:A:324:VAL:HG23	2.13	0.49
1:A:55:MET:HE3	1:A:59:THR:CG2	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:HA	1:A:148:GLY:O	2.13	0.48
1:B:175:PRO:HB3	1:B:379:PRO:O	2.13	0.48
1:B:197:SER:OG	1:B:352:HIS:CD2	2.66	0.48
1:B:387:LYS:NZ	1:B:426:PRO:O	2.45	0.48
1:D:232:ARG:HG3	1:D:256:TYR:CE1	2.42	0.48
1:A:275:THR:HG21	2:A:501:NAD:C6A	2.43	0.48
1:B:206:THR:OG1	1:B:208:VAL:HG12	2.13	0.48
1:C:43:PRO:HG2	1:C:369:ILE:HD11	1.95	0.48
1:D:129:ASP:OD2	1:D:135:THR:HG22	2.12	0.48
1:B:398:LEU:HD21	1:B:405:LEU:CD1	2.44	0.48
1:C:110:LEU:HD13	1:C:110:LEU:C	2.11	0.48
1:D:414:GLN:O	1:D:415:TYR:C	2.51	0.48
1:A:52:CYS:HB3	1:A:129:ASP:OD1	2.13	0.48
1:C:206:THR:O	1:C:207:ASP:HB2	2.13	0.48
1:D:179:VAL:HG11	1:D:364:GLN:OE1	2.13	0.48
1:D:74:ARG:HD2	1:D:116:THR:HA	1.95	0.48
1:A:91:ILE:HG23	1:A:96:ILE:HB	1.94	0.48
1:B:286:PHE:CG	1:B:310:LEU:HD21	2.48	0.48
1:B:413:ALA:HB1	1:B:418:MET:O	2.13	0.48
1:C:344:VAL:CG1	1:C:345:ASN:N	2.77	0.48
1:C:181:ASP:OD2	1:D:428:HIS:CB	2.61	0.48
1:D:44:LEU:O	1:D:47:ALA:HB3	2.14	0.48
1:D:48:ARG:HD2	1:D:119:PHE:CG	2.49	0.48
1:A:150:ARG:NH2	1:A:372:TRP:CZ3	2.82	0.48
1:A:302:ASP:HB3	1:A:342:ARG:HG2	1.96	0.48
1:A:177:ILE:CG1	1:A:371:LEU:HD21	2.29	0.48
1:C:150:ARG:NH2	4:C:638:HOH:O	2.39	0.48
1:D:386:PRO:O	1:D:389:LEU:N	2.46	0.48
1:D:52:CYS:HB2	1:D:134:LEU:HB2	1.95	0.48
1:A:212:GLY:HA2	1:D:252:ALA:O	2.13	0.48
1:A:33:ARG:HG3	1:A:37:MET:SD	2.54	0.48
1:C:7:LYS:HG2	1:C:101:TRP:CH2	2.48	0.48
1:C:297:ASN:OD1	1:C:304:GLU:HG3	2.13	0.48
1:D:15:ALA:HB2	4:D:660:HOH:O	2.14	0.48
1:A:154:GLU:HG3	1:A:160:VAL:HG23	1.94	0.48
1:A:206:THR:O	1:A:207:ASP:HB2	2.13	0.48
1:C:161:HIS:CE1	1:D:416:LEU:O	2.67	0.48
1:C:191:LEU:HD12	1:C:226:GLY:CA	2.43	0.48
1:D:246:ILE:HG22	1:D:247:ASN:N	2.29	0.48
1:D:317:LYS:CB	1:D:327:TYR:CE2	2.96	0.48
1:D:41:SER:O	1:D:42:LYS:C	2.52	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASP:HB2	1:B:107:GLU:OE1	2.13	0.48
1:B:359:ASN:HD22	1:B:393:VAL:CG1	2.20	0.48
1:C:43:PRO:CG	1:C:369:ILE:HD11	2.44	0.48
1:D:215:ALA:CB	1:D:231:LEU:HD13	2.43	0.48
1:C:406:THR:HG22	1:D:243:ILE:HG22	1.95	0.48
1:D:342:ARG:CG	1:D:342:ARG:HH11	2.26	0.48
1:D:418:MET:HE2	1:D:418:MET:HB3	1.73	0.48
1:A:418:MET:HB3	1:A:424:PHE:HB3	1.95	0.48
1:A:6:TYR:CD1	1:A:6:TYR:C	2.87	0.48
1:B:240:ILE:O	1:B:258:VAL:HG13	2.14	0.48
1:C:178:ASN:CG	1:C:181:ASP:HB2	2.33	0.48
1:A:196:GLU:HB3	1:C:203:LYS:HZ2	1.78	0.48
1:C:274:THR:HA	1:C:298:ILE:HG22	1.96	0.48
1:C:91:ILE:CG2	1:C:96:ILE:HB	2.42	0.48
1:D:379:PRO:HD2	1:D:383:HIS:CE1	2.49	0.48
1:A:379:PRO:O	1:A:383:HIS:HE1	1.97	0.47
1:A:21:LEU:HD23	1:A:57:VAL:HG13	1.96	0.47
1:A:55:MET:CE	1:A:59:THR:CG2	2.90	0.47
1:B:110:LEU:HD11	1:B:114:GLU:CD	2.34	0.47
1:B:158:THR:CG2	1:B:159:GLY:N	2.76	0.47
1:C:26:ASN:ND2	1:C:26:ASN:O	2.47	0.47
1:D:228:ALA:O	1:D:232:ARG:HB2	2.13	0.47
1:A:142:HIS:N	1:A:143:PRO:HD3	2.29	0.47
1:A:54:HIS:CG	1:A:346:LEU:HD13	2.49	0.47
1:C:130:ASP:CB	1:C:155:GLU:HB2	2.45	0.47
1:C:28:MET:SD	1:C:31:LEU:HD12	2.54	0.47
1:A:3:LYS:CE	1:A:74:ARG:NH1	2.72	0.47
1:B:127:ILE:HG12	1:B:134:LEU:HD12	1.92	0.47
1:C:126:MET:HE2	1:C:151:GLY:H	1.78	0.47
1:D:327:TYR:O	1:D:334:ARG:HA	2.14	0.47
1:D:197:SER:HB2	1:D:345:ASN:HB2	1.96	0.47
1:A:196:GLU:HB3	1:C:203:LYS:HZ1	1.76	0.47
1:A:429:TYR:CE2	1:A:431:TYR:CE2	3.02	0.47
1:B:153:SER:CB	1:B:364:GLN:NE2	2.72	0.47
1:B:419:PRO:O	1:B:420:ILE:C	2.51	0.47
1:C:183:VAL:C	1:C:185:LYS:N	2.67	0.47
1:A:83:THR:HG21	1:A:101:TRP:CA	2.45	0.47
1:B:100:ALA:O	1:B:101:TRP:HB3	2.14	0.47
1:C:223:VAL:HG11	1:C:298:ILE:CG2	2.45	0.47
1:C:82:SER:HA	1:C:346:LEU:O	2.14	0.47
1:C:6:TYR:HB2	1:C:98:VAL:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:HA	1:A:146:LEU:HD21	1.97	0.47
1:A:154:GLU:HG3	1:A:160:VAL:CG2	2.44	0.47
1:A:198:LEU:HD23	1:A:227:CYS:CB	2.45	0.47
1:C:352:HIS:HB3	1:C:356:VAL:CG1	2.45	0.47
1:C:94:ALA:CB	1:C:96:ILE:CD1	2.91	0.47
1:A:165:LYS:O	1:A:166:MET:C	2.51	0.47
1:B:167:MET:C	1:B:169:ASN:N	2.68	0.47
1:C:96:ILE:N	1:C:96:ILE:HD12	2.30	0.47
1:D:58:GLU:C	1:D:361:PHE:HE2	2.18	0.47
1:A:163:LEU:HD11	1:A:176:ALA:HB1	1.95	0.47
1:A:198:LEU:HD23	1:A:227:CYS:HB3	1.97	0.47
1:B:110:LEU:O	1:B:114:GLU:HG2	2.14	0.47
1:B:137:LEU:HD12	1:B:141:LYS:HB2	1.96	0.47
1:B:418:MET:CB	1:B:424:PHE:HD1	2.27	0.47
1:B:44:LEU:HB3	1:B:71:ALA:HB2	1.95	0.47
1:B:6:TYR:C	1:B:6:TYR:HD1	2.18	0.47
1:C:418:MET:HB2	1:C:419:PRO:HD2	1.96	0.47
1:D:110:LEU:O	1:D:114:GLU:CG	2.63	0.47
1:B:286:PHE:CD2	1:B:310:LEU:CD2	2.97	0.47
1:A:249:LEU:CD1	1:B:401:LEU:HD12	2.45	0.47
1:B:62:LEU:CD1	1:B:365:VAL:HG23	2.45	0.47
1:C:406:THR:HG23	1:C:407:LYS:H	1.80	0.47
1:D:48:ARG:HD2	1:D:119:PHE:CB	2.43	0.47
1:D:172:LEU:HD23	1:D:172:LEU:HA	1.75	0.47
1:D:21:LEU:CD2	1:D:57:VAL:HG13	2.26	0.47
1:A:11:ILE:HA	1:A:89:ALA:HB1	1.96	0.47
1:A:247:ASN:O	1:A:250:GLN:HB2	2.15	0.47
1:B:375:PRO:O	1:B:378:TYR:N	2.41	0.47
1:B:55:MET:HE3	1:B:59:THR:CG2	2.45	0.47
1:C:214:VAL:H	1:C:269:ASN:ND2	2.02	0.47
1:C:386:PRO:O	1:C:389:LEU:N	2.47	0.47
1:D:192:TYR:O	1:D:193:GLY:C	2.52	0.47
1:D:210:ILE:HG21	1:D:234:PHE:HB2	1.96	0.47
1:D:309:TRP:HE3	1:D:310:LEU:HD23	1.80	0.47
1:A:285:HIS:O	1:A:288:GLN:N	2.46	0.47
1:B:199:ILE:HG21	1:B:234:PHE:CE2	2.50	0.47
1:B:282:LEU:O	1:B:285:HIS:HB2	2.15	0.47
1:D:193:GLY:HA3	1:D:352:HIS:CE1	2.50	0.47
1:A:203:LYS:O	1:A:207:ASP:N	2.45	0.46
1:A:238:VAL:HB	1:A:256:TYR:CE1	2.50	0.46
1:A:430:ARG:HG2	1:B:430:ARG:CA	2.37	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ARG:HH11	1:B:187:LYS:HE3	1.79	0.46
1:B:62:LEU:CD1	1:B:365:VAL:CG2	2.93	0.46
1:C:16:TRP:HD1	1:C:16:TRP:O	1.97	0.46
1:D:143:PRO:O	1:D:146:LEU:HB2	2.14	0.46
1:D:149:ILE:HG22	1:D:149:ILE:O	2.15	0.46
1:D:300:HIS:HB2	2:D:504:NAD:HO2N	1.77	0.46
1:A:130:ASP:HB2	1:A:155:GLU:HB2	1.97	0.46
1:A:310:LEU:HD13	1:A:327:TYR:CD1	2.50	0.46
1:A:60:ALA:HB1	1:A:91:ILE:HD11	1.96	0.46
1:B:278:VAL:HA	1:B:303:VAL:O	2.15	0.46
1:B:81:PHE:CE2	1:B:342:ARG:CD	2.98	0.46
1:C:153:SER:HB3	1:C:364:GLN:HE22	1.74	0.46
1:B:111:TRP:HA	1:B:114:GLU:HG3	1.97	0.46
1:C:10:ASP:O	1:C:12:GLY:N	2.48	0.46
1:A:81:PHE:O	1:A:102:LYS:HG3	2.15	0.46
1:A:345:ASN:O	1:A:349:ALA:HB3	2.15	0.46
1:D:318:VAL:HG12	1:D:319:ASN:N	2.30	0.46
1:D:300:HIS:HA	1:D:343:LEU:HD11	1.98	0.46
1:A:54:HIS:CD2	1:A:346:LEU:HD13	2.51	0.46
1:A:352:HIS:N	3:A:601:ADN:HN61	2.13	0.46
1:B:167:MET:SD	1:B:381:GLY:HA2	2.56	0.46
1:B:281:ILE:O	1:B:281:ILE:HG22	2.16	0.46
1:B:283:GLY:HA2	1:B:286:PHE:CD2	2.50	0.46
1:C:141:LYS:HG2	4:C:626:HOH:O	2.16	0.46
1:C:409:THR:HG23	1:C:412:GLN:HE21	1.80	0.46
1:A:283:GLY:HA2	1:A:286:PHE:HD2	1.80	0.46
1:B:130:ASP:HA	1:B:155:GLU:HB2	1.98	0.46
1:B:157:THR:HG21	2:B:502:NAD:H52N	1.97	0.46
1:B:228:ALA:O	1:B:232:ARG:HB2	2.16	0.46
1:B:361:PHE:O	1:B:365:VAL:HG23	2.16	0.46
1:B:373:THR:HG22	1:B:373:THR:O	2.15	0.46
1:B:373:THR:CG2	1:B:374:HIS:CE1	2.92	0.46
1:D:160:VAL:CG1	1:D:164:TYR:HE2	2.29	0.46
1:D:220:TYR:CE2	1:D:225:LYS:HE3	2.50	0.46
1:A:171:ILE:O	1:A:171:ILE:HG22	2.16	0.46
1:A:273:THR:CG2	1:A:281:ILE:HD12	2.46	0.46
1:A:317:LYS:HG3	1:A:327:TYR:CD2	2.50	0.46
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.73	0.46
1:B:198:LEU:HD22	1:B:227:CYS:HB3	1.98	0.46
1:B:391:GLU:HG2	1:B:391:GLU:H	1.45	0.46
1:B:80:ILE:HD11	1:B:342:ARG:CD	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:LEU:HD13	1:C:340:GLU:HA	1.97	0.46
1:D:54:HIS:HA	1:D:77:SER:OG	2.15	0.46
1:A:198:LEU:HD23	1:A:227:CYS:SG	2.55	0.46
1:A:374:HIS:N	1:A:375:PRO:HD2	2.31	0.46
1:A:422:GLY:O	1:A:424:PHE:CE1	2.69	0.46
1:A:278:VAL:HG22	1:B:415:TYR:CD2	2.51	0.46
1:C:11:ILE:CD1	1:C:92:ALA:HB3	2.45	0.46
1:C:16:TRP:CD1	1:C:16:TRP:C	2.88	0.46
1:C:182:SER:HB3	1:C:185:LYS:HB2	1.97	0.46
1:C:252:ALA:C	1:C:254:GLU:H	2.19	0.46
1:C:49:ILE:HD12	1:C:66:LEU:HD13	1.98	0.46
1:C:94:ALA:HB3	1:C:96:ILE:HD13	1.95	0.46
1:D:13:LEU:HA	1:D:13:LEU:HD12	1.80	0.46
1:D:182:SER:O	1:D:185:LYS:N	2.44	0.46
1:C:277:CYS:HB3	1:D:416:LEU:HG	1.97	0.46
1:D:38:TYR:O	1:D:43:PRO:HD2	2.15	0.46
1:D:6:TYR:HE1	1:D:8:VAL:CG2	2.28	0.46
1:A:6:TYR:OH	1:A:11:ILE:HD13	2.15	0.46
1:B:190:ASN:ND2	2:B:502:NAD:C5N	2.77	0.46
1:B:273:THR:HB	1:B:304:GLU:OE1	2.16	0.46
1:B:309:TRP:CZ3	1:B:310:LEU:CD2	2.98	0.46
1:B:317:LYS:HE3	4:B:632:HOH:O	2.16	0.46
1:C:133:ASP:O	1:C:137:LEU:HB3	2.16	0.46
1:D:275:THR:O	1:D:304:GLU:CD	2.52	0.46
1:D:60:ALA:O	1:D:64:GLU:HG3	2.16	0.46
2:B:502:NAD:H51N	2:B:502:NAD:O1A	2.15	0.46
1:C:163:LEU:HD13	1:C:176:ALA:CB	2.46	0.46
1:D:386:PRO:HG2	1:D:389:LEU:HD11	1.91	0.46
1:D:101:TRP:CD1	1:D:104:GLU:HG2	2.51	0.45
1:A:120:LYS:HE3	4:A:698:HOH:O	2.16	0.45
1:A:244:GLU:CD	1:B:425:LYS:HD2	2.37	0.45
1:A:127:ILE:CG1	1:A:134:LEU:HD13	2.36	0.45
1:A:152:ILE:CG2	1:A:153:SER:N	2.79	0.45
1:A:215:ALA:O	1:A:238:VAL:HA	2.16	0.45
1:B:167:MET:O	1:B:169:ASN:N	2.49	0.45
1:B:186:SER:HA	1:B:190:ASN:OD1	2.17	0.45
1:A:320:ILE:HA	1:C:19:LYS:HD2	1.98	0.45
1:C:428:HIS:ND1	1:D:164:TYR:CZ	2.83	0.45
1:D:331:ASN:C	1:D:331:ASN:OD1	2.53	0.45
1:C:277:CYS:HB2	1:D:416:LEU:HG	1.97	0.45
1:D:418:MET:CB	1:D:419:PRO:CD	2.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:VAL:HB	2:D:504:NAD:O2N	2.16	0.45
1:B:35:ARG:NH2	1:B:64:GLU:HB2	2.31	0.45
1:C:181:ASP:HB3	1:C:384:PHE:HE1	1.82	0.45
1:D:160:VAL:O	1:D:164:TYR:CD2	2.70	0.45
1:D:352:HIS:HB2	1:D:357:MET:SD	2.57	0.45
1:D:425:LYS:HE2	1:D:429:TYR:CD1	2.52	0.45
1:D:69:LEU:N	1:D:69:LEU:HD12	2.32	0.45
1:A:7:LYS:HA	4:A:672:HOH:O	2.16	0.45
1:B:321:LYS:HB2	1:B:322:PRO:HD2	1.99	0.45
1:C:282:LEU:O	1:C:285:HIS:HB2	2.16	0.45
1:D:160:VAL:CG1	1:D:164:TYR:CE2	3.00	0.45
1:D:172:LEU:HD22	1:D:174:VAL:H	1.82	0.45
1:D:401:LEU:O	1:D:402:ASN:CB	2.63	0.45
1:A:344:VAL:HG13	1:A:345:ASN:N	2.32	0.45
1:A:379:PRO:O	1:A:383:HIS:CE1	2.69	0.45
1:A:410:GLU:OE2	1:A:414:GLN:CG	2.47	0.45
1:B:199:ILE:HD12	1:B:234:PHE:CD2	2.51	0.45
1:B:320:ILE:N	1:B:320:ILE:HD13	2.31	0.45
1:C:21:LEU:HD21	1:C:60:ALA:CB	2.43	0.45
1:C:198:LEU:HD22	1:C:227:CYS:SG	2.57	0.45
1:C:386:PRO:HG2	1:C:389:LEU:CD1	2.38	0.45
1:D:275:THR:HG23	2:D:504:NAD:C8A	2.47	0.45
1:D:418:MET:HB2	1:D:424:PHE:CD1	2.52	0.45
1:D:419:PRO:HD2	1:D:424:PHE:HD1	1.80	0.45
1:A:302:ASP:CG	1:A:302:ASP:O	2.52	0.45
1:B:386:PRO:HG2	1:B:389:LEU:HG	1.98	0.45
1:B:51:GLY:HA2	1:B:128:LEU:O	2.16	0.45
1:D:146:LEU:HG	1:D:173:LYS:HB2	1.99	0.45
1:D:194:CYS:C	1:D:196:GLU:H	2.20	0.45
1:D:370:GLU:HB3	1:D:378:TYR:HE1	1.81	0.45
1:A:130:ASP:CB	1:A:155:GLU:HB2	2.47	0.45
1:A:224:GLY:HA2	1:A:274:THR:HG21	1.98	0.45
1:A:248:ALA:CB	1:B:405:LEU:HD11	2.47	0.45
1:A:57:VAL:H	1:A:84:GLN:NE2	2.15	0.45
1:A:44:LEU:CB	1:A:71:ALA:HB2	2.46	0.45
1:B:16:TRP:O	1:B:16:TRP:HD1	1.95	0.45
1:B:55:MET:HE2	1:B:59:THR:HB	1.98	0.45
1:C:121:ASP:OD1	1:C:121:ASP:N	2.39	0.45
1:C:91:ILE:HG22	1:C:98:VAL:HG22	1.97	0.45
1:C:428:HIS:CE1	1:D:164:TYR:OH	2.70	0.45
1:D:17:GLY:O	1:D:18:ARG:C	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:CD1	1:D:61:VAL:HG12	2.47	0.45
1:D:352:HIS:HB3	1:D:356:VAL:CG1	2.47	0.45
1:D:407:LYS:CB	1:D:407:LYS:HZ2	2.02	0.45
1:A:337:LEU:HD23	1:A:337:LEU:HA	1.70	0.45
1:A:352:HIS:H	3:A:601:ADN:HN61	1.65	0.45
1:A:373:THR:C	1:A:374:HIS:ND1	2.70	0.45
1:B:207:ASP:OD1	1:D:204:ARG:NH2	2.43	0.45
1:B:55:MET:HG2	1:B:75:TRP:CD1	2.51	0.45
1:C:110:LEU:CD1	1:C:114:GLU:CG	2.94	0.45
1:D:138:ILE:HG22	1:D:146:LEU:HD13	1.98	0.45
1:D:38:TYR:HB3	1:D:43:PRO:HG3	1.97	0.45
1:A:128:LEU:HD21	1:A:364:GLN:CD	2.37	0.44
1:A:174:VAL:HG23	1:A:175:PRO:HD2	1.99	0.44
1:A:180:ASN:HA	1:A:185:LYS:HD2	1.98	0.44
1:A:252:ALA:C	1:A:254:GLU:H	2.21	0.44
1:B:327:TYR:O	1:B:334:ARG:HA	2.17	0.44
1:C:387:LYS:HE2	1:C:391:GLU:OE2	2.17	0.44
1:D:185:LYS:O	1:D:189:ASP:HB3	2.17	0.44
1:D:285:HIS:O	1:D:286:PHE:C	2.55	0.44
1:D:352:HIS:HB3	1:D:356:VAL:HG11	1.98	0.44
1:A:275:THR:CG2	2:A:501:NAD:C8A	2.96	0.44
1:A:387:LYS:CE	1:A:425:LYS:HG3	2.39	0.44
1:B:143:PRO:HA	1:B:146:LEU:HD21	1.96	0.44
1:B:170:GLY:O	1:B:173:LYS:NZ	2.50	0.44
1:B:7:LYS:N	1:B:98:VAL:O	2.38	0.44
1:C:319:ASN:ND2	1:C:321:LYS:O	2.44	0.44
1:D:200:ASP:CG	1:D:204:ARG:HE	2.19	0.44
1:D:69:LEU:N	1:D:69:LEU:CD1	2.80	0.44
1:B:214:VAL:H	1:B:269:ASN:ND2	2.11	0.44
1:B:54:HIS:CE1	1:B:346:LEU:HD13	2.52	0.44
1:B:364:GLN:HA	1:B:364:GLN:NE2	2.32	0.44
1:C:126:MET:CE	1:C:150:ARG:HG2	2.46	0.44
1:A:55:MET:HG2	1:A:75:TRP:CD1	2.52	0.44
1:B:317:LYS:HB2	1:B:327:TYR:HD2	1.76	0.44
1:B:325:ASP:O	1:B:336:ILE:HA	2.17	0.44
1:B:373:THR:CG2	1:B:373:THR:O	2.65	0.44
1:B:48:ARG:HB3	1:B:119:PHE:CE2	2.53	0.44
1:C:406:THR:HG22	1:C:407:LYS:N	2.32	0.44
1:D:53:LEU:HG	1:D:130:ASP:OD2	2.17	0.44
1:D:160:VAL:HG13	1:D:164:TYR:CE2	2.52	0.44
1:D:326:ARG:HG3	1:D:336:ILE:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:THR:HG21	1:B:300:HIS:CE1	2.50	0.44
1:B:165:LYS:HG2	4:B:639:HOH:O	2.17	0.44
1:B:305:ILE:O	1:B:307:VAL:HG23	2.16	0.44
1:C:425:LYS:CD	1:C:431:TYR:OH	2.65	0.44
1:C:431:TYR:C	1:D:187:LYS:NZ	2.71	0.44
1:D:127:ILE:HG12	1:D:134:LEU:HD13	1.98	0.44
1:A:99:PHE:CD1	1:A:115:GLN:HG3	2.53	0.44
1:C:126:MET:HE3	1:C:150:ARG:HG2	1.98	0.44
1:C:154:GLU:O	1:C:179:VAL:HB	2.16	0.44
1:C:6:TYR:C	1:C:6:TYR:CD1	2.91	0.44
1:D:7:LYS:CG	1:D:101:TRP:CZ3	2.93	0.44
1:D:134:LEU:CD2	1:D:134:LEU:C	2.86	0.44
1:D:239:ILE:HG23	1:D:257:GLU:HG2	1.98	0.44
1:B:275:THR:CG2	1:B:276:GLY:H	2.29	0.44
1:B:48:ARG:HH11	1:B:48:ARG:HG3	1.82	0.44
1:C:7:LYS:CG	1:C:101:TRP:CZ3	2.98	0.44
1:C:249:LEU:HD12	1:D:401:LEU:HD12	2.00	0.44
1:D:54:HIS:HB3	1:D:82:SER:CB	2.47	0.44
1:A:395:GLU:OE2	1:A:395:GLU:O	2.36	0.44
1:A:406:THR:HG22	1:A:407:LYS:N	2.32	0.44
1:B:189:ASP:O	1:B:352:HIS:CE1	2.71	0.44
1:B:156:THR:OG1	2:B:502:NAD:H2D	2.18	0.44
1:B:35:ARG:HE	1:B:65:THR:HA	1.82	0.44
1:C:150:ARG:HD2	1:C:372:TRP:HA	1.99	0.44
1:C:130:ASP:OD1	1:C:156:THR:CG2	2.62	0.44
1:C:273:THR:OG1	1:C:297:ASN:CB	2.54	0.44
1:C:321:LYS:HE3	1:C:324:VAL:HG21	1.99	0.44
1:D:361:PHE:HA	1:D:364:GLN:HB2	1.99	0.44
1:A:302:ASP:O	1:A:302:ASP:OD1	2.36	0.44
1:A:181:ASP:HB3	1:A:384:PHE:HE1	1.83	0.44
1:A:398:LEU:CD2	1:A:405:LEU:CD2	2.88	0.44
1:A:401:LEU:O	1:A:402:ASN:CB	2.66	0.44
1:B:120:LYS:C	1:B:122:GLY:N	2.71	0.44
1:C:124:LEU:HD23	1:C:124:LEU:N	2.33	0.44
1:A:142:HIS:CA	1:A:144:GLN:OE1	2.66	0.43
1:A:263:GLU:OE2	1:A:266:LYS:NZ	2.46	0.43
1:B:246:ILE:O	1:B:250:GLN:HG3	2.17	0.43
1:B:425:LYS:HZ1	1:B:426:PRO:HD2	1.82	0.43
1:C:389:LEU:O	1:C:392:ALA:HB3	2.17	0.43
1:C:409:THR:H	1:C:412:GLN:HE21	1.65	0.43
1:B:317:LYS:CG	1:B:317:LYS:O	2.67	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:HG22	1:B:336:ILE:O	2.17	0.43
1:C:228:ALA:HB1	1:C:256:TYR:CE1	2.53	0.43
1:C:362:THR:O	1:C:366:MET:HG3	2.18	0.43
1:C:425:LYS:HE3	1:C:426:PRO:HD2	1.95	0.43
1:D:35:ARG:C	1:D:37:MET:H	2.20	0.43
1:A:174:VAL:HG23	1:A:175:PRO:N	2.33	0.43
1:A:240:ILE:O	1:A:258:VAL:HA	2.18	0.43
1:B:137:LEU:HD12	1:B:137:LEU:O	2.18	0.43
1:B:291:ASP:OD1	1:B:292:ASP:N	2.52	0.43
1:C:48:ARG:HD2	1:C:119:PHE:CG	2.53	0.43
1:C:244:GLU:OE2	1:D:425:LYS:CG	2.67	0.43
1:C:306:ASP:OD1	1:C:308:LYS:HD2	2.17	0.43
1:C:320:ILE:CD1	1:C:320:ILE:N	2.81	0.43
1:D:420:ILE:HG13	1:D:421:ASN:OD1	2.18	0.43
1:A:181:ASP:OD2	1:B:428:HIS:HB3	2.18	0.43
1:A:185:LYS:O	1:A:189:ASP:N	2.44	0.43
1:A:240:ILE:CD1	1:A:256:TYR:CG	3.02	0.43
1:A:419:PRO:CG	1:A:422:GLY:N	2.66	0.43
1:B:352:HIS:HB3	1:B:356:VAL:HG11	1.99	0.43
1:B:3:LYS:HE3	1:B:115:GLN:OE1	2.19	0.43
1:B:387:LYS:NZ	1:B:425:LYS:HG3	2.34	0.43
1:C:43:PRO:CG	1:C:369:ILE:CD1	2.97	0.43
1:C:242:GLU:OE1	2:C:503:NAD:H1B	2.17	0.43
1:C:94:ALA:HB3	1:C:96:ILE:HD12	1.97	0.43
1:D:240:ILE:HD12	1:D:256:TYR:HB3	2.00	0.43
1:D:93:LYS:O	1:D:95:GLY:N	2.51	0.43
1:A:126:MET:CE	1:A:150:ARG:C	2.87	0.43
1:A:154:GLU:HB3	1:A:160:VAL:HG22	2.01	0.43
1:A:320:ILE:H	1:A:320:ILE:HD13	1.83	0.43
1:B:126:MET:HE2	1:B:150:ARG:HB3	1.99	0.43
1:B:185:LYS:HD3	1:B:189:ASP:HB3	2.00	0.43
1:C:418:MET:HB2	1:C:424:PHE:HD1	1.83	0.43
1:B:53:LEU:HD12	1:B:128:LEU:CD2	2.49	0.43
1:C:419:PRO:CD	1:C:423:PRO:O	2.67	0.43
1:C:428:HIS:HB3	1:D:384:PHE:HZ	1.84	0.43
1:D:62:LEU:HB2	1:D:361:PHE:CD2	2.54	0.43
1:A:283:GLY:HA2	1:A:286:PHE:CD2	2.54	0.43
1:A:223:VAL:CB	2:A:501:NAD:O2N	2.67	0.43
1:B:113:ILE:CG2	1:B:134:LEU:HD23	2.47	0.43
1:B:35:ARG:C	1:B:37:MET:H	2.21	0.43
1:C:53:LEU:HG	1:C:130:ASP:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:ARG:NH1	1:D:36:GLU:OE1	2.52	0.43
1:A:244:GLU:HA	1:A:245:PRO:HD2	1.79	0.43
1:A:93:LYS:C	1:A:95:GLY:H	2.22	0.43
1:C:387:LYS:CG	1:C:391:GLU:OE2	2.66	0.43
1:D:197:SER:OG	1:D:352:HIS:CD2	2.71	0.43
1:D:281:ILE:O	1:D:281:ILE:HG22	2.18	0.43
1:A:271:PHE:CE1	1:A:289:MET:SD	3.12	0.43
1:A:82:SER:HA	1:A:346:LEU:O	2.19	0.43
1:A:428:HIS:HE1	1:B:164:TYR:CZ	2.37	0.43
1:B:407:LYS:CB	1:B:407:LYS:NZ	2.63	0.43
1:B:69:LEU:HD23	1:B:369:ILE:HD11	1.99	0.43
1:C:285:HIS:O	1:C:289:MET:HG3	2.18	0.43
1:C:302:ASP:C	1:C:303:VAL:HG13	2.38	0.43
1:B:374:HIS:N	1:B:375:PRO:HD2	2.34	0.43
1:B:419:PRO:HD2	1:B:423:PRO:O	2.18	0.43
1:C:135:THR:O	1:C:139:HIS:HB2	2.19	0.43
1:C:221:GLY:O	1:C:225:LYS:HG2	2.18	0.43
1:C:419:PRO:HG2	1:C:422:GLY:C	2.38	0.43
1:C:13:LEU:HB3	1:C:86:HIS:HA	1.99	0.43
1:D:113:ILE:HG21	1:D:137:LEU:CD2	2.45	0.43
1:C:431:TYR:CE2	1:D:247:ASN:ND2	2.78	0.43
1:A:373:THR:C	1:A:375:PRO:CD	2.88	0.42
1:A:419:PRO:C	1:A:421:ASN:H	2.22	0.42
1:A:3:LYS:NZ	1:A:74:ARG:NH1	2.67	0.42
1:A:91:ILE:O	1:A:96:ILE:HB	2.19	0.42
1:B:206:THR:HG21	1:B:294:ILE:HD13	2.01	0.42
1:B:91:ILE:CG2	1:B:96:ILE:HB	2.49	0.42
1:C:10:ASP:C	1:C:12:GLY:H	2.23	0.42
1:C:188:PHE:O	1:C:192:TYR:HB2	2.20	0.42
1:C:297:ASN:ND2	1:C:341:GLY:O	2.52	0.42
1:C:362:THR:HG21	1:C:393:VAL:HG13	2.02	0.42
1:D:110:LEU:O	1:D:114:GLU:HG2	2.19	0.42
1:D:425:LYS:NZ	1:D:429:TYR:CD1	2.86	0.42
1:D:157:THR:HB	2:D:504:NAD:H3D	2.01	0.42
1:A:21:LEU:HD22	1:A:60:ALA:HB3	2.01	0.42
1:A:275:THR:CG2	2:A:501:NAD:N7A	2.82	0.42
1:B:328:LEU:HD13	1:B:334:ARG:HD3	2.02	0.42
1:C:125:ASN:C	1:C:125:ASN:OD1	2.57	0.42
1:C:404:LYS:HB2	1:D:259:THR:HA	2.00	0.42
1:C:4:LEU:HA	1:C:5:PRO:HD3	1.91	0.42
1:D:225:LYS:HZ3	1:D:250:GLN:HE22	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:THR:HG22	1:D:84:GLN:N	2.34	0.42
1:A:223:VAL:HG12	1:A:274:THR:CB	2.41	0.42
1:A:295:VAL:HG12	1:A:305:ILE:CD1	2.44	0.42
1:B:178:ASN:OD1	1:B:178:ASN:C	2.56	0.42
1:B:31:LEU:HD21	1:B:361:PHE:HB3	2.00	0.42
1:C:298:ILE:HG13	2:C:503:NAD:N7N	2.34	0.42
1:C:373:THR:C	1:C:375:PRO:CD	2.88	0.42
1:C:391:GLU:H	1:C:391:GLU:HG2	1.34	0.42
1:C:415:TYR:CG	1:D:278:VAL:CG2	3.01	0.42
1:D:189:ASP:OD1	1:D:189:ASP:C	2.58	0.42
1:D:309:TRP:CE3	1:D:310:LEU:HD23	2.53	0.42
1:A:178:ASN:HD21	1:A:181:ASP:CG	2.23	0.42
1:A:419:PRO:C	1:A:422:GLY:H	2.22	0.42
1:C:223:VAL:CG2	2:C:503:NAD:O2N	2.67	0.42
1:C:62:LEU:HB2	1:C:361:PHE:CD2	2.54	0.42
1:D:84:GLN:O	1:D:87:ALA:HB3	2.19	0.42
1:A:7:LYS:HG3	1:A:101:TRP:CZ3	2.53	0.42
1:B:4:LEU:HD12	1:B:111:TRP:CZ2	2.51	0.42
1:C:91:ILE:HA	1:C:91:ILE:HD12	1.75	0.42
1:D:160:VAL:CG1	1:D:160:VAL:O	2.68	0.42
1:A:54:HIS:O	1:A:56:THR:HG23	2.19	0.42
1:B:369:ILE:O	1:B:369:ILE:CG2	2.67	0.42
1:C:126:MET:HE3	1:C:150:ARG:CG	2.50	0.42
1:C:247:ASN:HA	1:C:250:GLN:HE21	1.84	0.42
1:C:283:GLY:O	1:C:287:GLU:HG3	2.19	0.42
1:C:418:MET:CB	1:C:419:PRO:CD	2.96	0.42
1:C:60:ALA:CB	1:C:91:ILE:HD11	2.42	0.42
1:D:321:LYS:HG2	1:D:324:VAL:HG23	2.00	0.42
1:D:387:LYS:HE2	1:D:425:LYS:HG3	2.01	0.42
1:A:328:LEU:CD1	1:A:332:GLY:O	2.68	0.42
1:A:370:GLU:HB3	1:A:378:TYR:CE1	2.54	0.42
1:B:143:PRO:O	1:B:146:LEU:HD23	2.20	0.42
1:B:214:VAL:HB	1:B:268:GLY:HA2	2.00	0.42
1:C:240:ILE:O	1:C:258:VAL:HA	2.20	0.42
1:C:343:LEU:HA	1:C:343:LEU:HD12	1.85	0.42
1:A:210:ILE:CG2	1:A:234:PHE:HB2	2.50	0.42
1:A:408:LEU:HA	1:A:408:LEU:HD12	1.81	0.42
1:B:130:ASP:CB	1:B:155:GLU:HB2	2.50	0.42
1:B:298:ILE:C	1:B:299:GLY:O	2.57	0.42
1:C:163:LEU:CD1	1:C:176:ALA:CB	2.98	0.42
1:C:180:ASN:HA	1:C:185:LYS:CD	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:ARG:NH1	1:D:342:ARG:CG	2.81	0.42
1:A:369:ILE:O	1:A:373:THR:CB	2.63	0.42
1:B:418:MET:SD	1:B:424:PHE:CB	3.06	0.42
1:A:187:LYS:NZ	1:B:431:TYR:C	2.73	0.42
1:C:160:VAL:CG1	1:C:164:TYR:HE2	2.30	0.42
1:C:216:VAL:HG21	1:C:271:PHE:CE2	2.55	0.42
1:D:297:ASN:ND2	1:D:301:PHE:O	2.52	0.42
1:D:422:GLY:O	1:D:424:PHE:CE1	2.73	0.42
1:A:126:MET:HE2	1:A:150:ARG:HB3	1.93	0.42
1:A:38:TYR:HB3	1:A:43:PRO:HD3	2.00	0.42
1:D:142:HIS:C	1:D:144:GLN:OE1	2.58	0.42
1:D:225:LYS:NZ	1:D:250:GLN:NE2	2.67	0.42
1:D:386:PRO:O	1:D:388:LYS:N	2.53	0.42
1:D:53:LEU:HD11	1:D:155:GLU:HG2	2.00	0.42
1:D:80:ILE:HG13	1:D:81:PHE:CD1	2.55	0.42
1:A:124:LEU:H	1:A:124:LEU:HD23	1.84	0.41
1:A:418:MET:CB	1:A:424:PHE:HB3	2.50	0.41
1:B:134:LEU:O	1:B:134:LEU:HD22	2.19	0.41
1:B:164:TYR:CE1	1:B:382:VAL:CG2	3.03	0.41
1:B:418:MET:CB	1:B:419:PRO:CD	2.98	0.41
1:C:110:LEU:O	1:C:114:GLU:HG3	2.20	0.41
1:C:208:VAL:HG22	1:C:209:MET:N	2.35	0.41
1:A:23:ILE:HD11	1:C:320:ILE:HG12	2.02	0.41
1:D:91:ILE:H	1:D:91:ILE:HD13	1.85	0.41
1:A:157:THR:HG21	2:A:501:NAD:H51N	2.00	0.41
1:A:157:THR:HG21	2:A:501:NAD:O1A	2.20	0.41
1:A:307:VAL:H	1:A:308:LYS:HZ2	1.67	0.41
1:C:130:ASP:CA	1:C:155:GLU:HB2	2.49	0.41
1:C:190:ASN:ND2	2:C:503:NAD:O1N	2.53	0.41
1:C:251:ALA:O	1:C:256:TYR:HB2	2.21	0.41
1:C:291:ASP:OD1	1:C:334:ARG:NE	2.47	0.41
1:C:305:ILE:O	1:C:307:VAL:N	2.53	0.41
1:A:209:MET:SD	1:C:356:VAL:HB	2.60	0.41
1:C:57:VAL:HA	1:C:87:ALA:HB1	2.01	0.41
1:D:126:MET:CE	1:D:150:ARG:C	2.88	0.41
1:D:156:THR:OG1	2:D:504:NAD:H2D	2.19	0.41
1:D:240:ILE:CD1	1:D:256:TYR:CG	3.03	0.41
1:A:285:HIS:O	1:A:286:PHE:C	2.58	0.41
1:B:275:THR:HG22	1:B:276:GLY:H	1.83	0.41
1:B:55:MET:CE	1:B:59:THR:CG2	2.98	0.41
1:C:35:ARG:C	1:C:37:MET:H	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ALA:C	1:D:70:GLY:N	2.73	0.41
1:D:73:VAL:CG1	1:D:75:TRP:HE3	2.33	0.41
1:A:144:GLN:HG3	1:A:144:GLN:H	1.51	0.41
1:A:150:ARG:NH2	1:A:372:TRP:CH2	2.88	0.41
1:A:2:ASP:O	1:A:3:LYS:O	2.38	0.41
1:A:408:LEU:HG	1:A:412:GLN:CB	2.51	0.41
1:B:339:ALA:O	1:B:342:ARG:CG	2.58	0.41
1:C:275:THR:CG2	1:C:276:GLY:N	2.83	0.41
1:A:132:GLY:O	1:A:136:ASN:HB3	2.20	0.41
1:A:157:THR:CB	2:A:501:NAD:H52N	2.51	0.41
1:B:286:PHE:HD2	1:B:309:TRP:CE3	2.38	0.41
1:B:33:ARG:HD2	1:B:33:ARG:O	2.20	0.41
1:C:139:HIS:HA	1:C:146:LEU:HD21	2.02	0.41
1:C:172:LEU:HD23	1:C:172:LEU:HA	1.91	0.41
1:A:164:TYR:CZ	1:B:428:HIS:HE1	2.38	0.41
1:A:418:MET:HB2	1:A:419:PRO:CD	2.51	0.41
1:A:53:LEU:HD11	1:A:155:GLU:HG2	2.02	0.41
1:B:126:MET:CE	1:B:150:ARG:C	2.89	0.41
1:B:126:MET:HE2	1:B:151:GLY:H	1.85	0.41
1:B:62:LEU:HD12	1:B:365:VAL:CG2	2.50	0.41
1:A:127:ILE:HG22	1:A:127:ILE:O	2.21	0.41
1:A:385:LEU:O	1:A:386:PRO:C	2.59	0.41
1:A:47:ALA:HB2	1:A:372:TRP:CE2	2.56	0.41
1:A:157:THR:HB	2:A:501:NAD:H51N	2.01	0.41
1:B:143:PRO:CA	1:B:146:LEU:CD2	2.89	0.41
1:B:279:ASP:HA	1:B:282:LEU:HD11	2.01	0.41
1:B:419:PRO:CB	1:B:422:GLY:CA	2.89	0.41
1:B:255:GLY:HA2	1:C:235:GLY:O	2.21	0.41
1:D:99:PHE:CE1	1:D:115:GLN:HB3	2.56	0.41
1:D:129:ASP:HB3	1:D:154:GLU:OE2	2.19	0.41
1:B:320:ILE:HG13	1:D:23:ILE:HD11	2.03	0.41
1:D:31:LEU:HD13	1:D:61:VAL:HG12	2.02	0.41
1:D:410:GLU:OE2	1:D:414:GLN:OE1	2.39	0.41
1:D:418:MET:SD	1:D:424:PHE:CB	3.09	0.41
1:B:352:HIS:HB3	1:B:356:VAL:CG1	2.51	0.41
1:C:38:TYR:HB3	1:C:43:PRO:HD3	2.03	0.41
1:C:48:ARG:HD2	1:C:119:PHE:HB2	2.03	0.41
1:D:247:ASN:H	1:D:247:ASN:HD22	1.69	0.41
1:D:312:GLU:O	1:D:312:GLU:CG	2.68	0.41
1:D:175:PRO:HD3	1:D:380:VAL:HA	2.03	0.41
1:D:74:ARG:HB3	1:D:116:THR:CB	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:CD2	1:A:60:ALA:HB3	2.50	0.41
1:B:183:VAL:O	1:B:185:LYS:N	2.54	0.41
1:B:353:PRO:O	1:B:356:VAL:HG12	2.21	0.41
1:B:83:THR:HG22	1:B:84:GLN:N	2.35	0.41
1:C:83:THR:HG22	1:C:84:GLN:N	2.36	0.41
1:D:275:THR:HG23	2:D:504:NAD:C5A	2.51	0.41
1:A:31:LEU:HD21	1:A:361:PHE:HB3	2.03	0.41
1:A:33:ARG:HA	1:A:36:GLU:HG2	2.02	0.41
1:A:6:TYR:HB3	1:A:97:PRO:HA	2.02	0.41
1:B:111:TRP:O	1:B:115:GLN:HG2	2.21	0.41
1:B:48:ARG:HB3	1:B:119:PHE:CD2	2.56	0.41
1:C:10:ASP:C	1:C:12:GLY:N	2.72	0.41
1:C:141:LYS:CG	4:C:626:HOH:O	2.68	0.41
1:C:156:THR:HG21	1:C:300:HIS:CE1	2.56	0.41
1:D:105:THR:HB	1:D:107:GLU:OE2	2.20	0.41
1:D:202:ILE:HG22	1:D:203:LYS:N	2.36	0.41
1:D:361:PHE:O	1:D:365:VAL:HG23	2.21	0.41
1:D:408:LEU:HA	1:D:408:LEU:HD12	1.81	0.41
2:D:504:NAD:H52N	2:D:504:NAD:H6N	2.02	0.41
1:A:156:THR:O	1:A:160:VAL:HG23	2.21	0.41
1:A:40:ALA:HB3	4:A:701:HOH:O	2.20	0.41
1:B:156:THR:HB	3:B:602:ADN:H5'1	2.03	0.41
1:B:45:LYS:HD2	1:B:46:GLY:H	1.83	0.41
1:C:189:ASP:C	1:C:189:ASP:OD1	2.59	0.41
1:D:420:ILE:CG1	1:D:421:ASN:OD1	2.69	0.41
1:D:6:TYR:CB	1:D:98:VAL:H	2.32	0.41
1:A:130:ASP:HA	1:A:155:GLU:HB2	2.03	0.40
1:A:154:GLU:CG	1:A:160:VAL:HG22	2.51	0.40
1:B:171:ILE:O	1:B:171:ILE:CG2	2.67	0.40
1:B:198:LEU:HD22	1:B:227:CYS:SG	2.60	0.40
1:B:6:TYR:HB3	1:B:97:PRO:HA	2.01	0.40
1:C:152:ILE:HG13	1:C:174:VAL:CG2	2.51	0.40
1:D:389:LEU:O	1:D:392:ALA:HB3	2.20	0.40
1:A:100:ALA:O	1:A:101:TRP:HE3	2.04	0.40
1:A:240:ILE:HD12	1:A:256:TYR:HB3	2.04	0.40
1:B:271:PHE:CE1	1:B:289:MET:HG2	2.56	0.40
1:B:72:GLU:O	1:B:73:VAL:HG23	2.21	0.40
1:C:408:LEU:O	1:C:420:ILE:HD12	2.22	0.40
1:C:48:ARG:HD2	1:C:119:PHE:CB	2.51	0.40
1:D:428:HIS:CD2	1:D:428:HIS:N	2.89	0.40
1:D:48:ARG:CG	1:D:48:ARG:HH11	2.32	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:PHE:HB2	4:B:621:HOH:O	2.20	0.40
1:C:334:ARG:C	1:C:335:ILE:HG12	2.42	0.40
1:C:425:LYS:HG3	1:C:431:TYR:OH	2.22	0.40
1:D:240:ILE:HD12	1:D:256:TYR:CG	2.55	0.40
1:D:321:LYS:HG2	1:D:324:VAL:HG21	2.04	0.40
1:D:38:TYR:O	1:D:43:PRO:CD	2.70	0.40
1:D:419:PRO:C	1:D:421:ASN:N	2.71	0.40
1:D:54:HIS:CE1	1:D:78:CYS:HG	2.40	0.40
1:A:259:THR:HB	1:A:260:THR:H	1.67	0.40
1:A:425:LYS:HZ2	1:A:426:PRO:HD3	1.87	0.40
1:B:199:ILE:O	1:B:203:LYS:HB2	2.22	0.40
1:B:239:ILE:HG23	1:B:257:GLU:HG2	2.03	0.40
1:B:387:LYS:HZ1	1:B:425:LYS:HG3	1.87	0.40
1:B:389:LEU:O	1:B:393:VAL:HG23	2.21	0.40
1:C:30:GLY:O	1:C:33:ARG:HB3	2.21	0.40
1:C:38:TYR:HB3	1:C:43:PRO:CD	2.50	0.40
1:C:184:THR:CG2	1:C:390:ASP:OD2	2.59	0.40
1:D:113:ILE:CG2	1:D:137:LEU:CD2	2.98	0.40
1:D:285:HIS:O	1:D:287:GLU:N	2.54	0.40
1:A:277:CYS:HA	1:B:415:TYR:HE2	1.87	0.40
1:A:372:TRP:O	1:A:372:TRP:CG	2.75	0.40
1:B:214:VAL:CG1	1:B:239:ILE:HD12	2.51	0.40
1:C:152:ILE:HG13	1:C:174:VAL:HG22	2.04	0.40
1:C:223:VAL:O	1:C:227:CYS:SG	2.79	0.40
1:D:31:LEU:HD23	1:D:31:LEU:HA	1.68	0.40
1:D:391:GLU:HG2	1:D:391:GLU:H	1.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	428/431 (99%)	367 (86%)	50 (12%)	11 (3%)	6	21
1	B	428/431 (99%)	373 (87%)	43 (10%)	12 (3%)	6	19
1	C	428/431 (99%)	374 (87%)	42 (10%)	12 (3%)	6	19
1	D	428/431 (99%)	358 (84%)	57 (13%)	13 (3%)	5	17
All	All	1712/1724 (99%)	1472 (86%)	192 (11%)	48 (3%)	6	19

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	425	LYS
1	B	425	LYS
1	C	184	THR
1	D	415	TYR
1	A	6	TYR
1	A	333	HIS
1	B	121	ASP
1	B	184	THR
1	B	265	CYS
1	C	3	LYS
1	C	6	TYR
1	C	183	VAL
1	C	299	GLY
1	C	303	VAL
1	D	380	VAL
1	A	85	ASP
1	A	424	PHE
1	B	6	TYR
1	D	55	MET
1	D	100	ALA
1	D	123	PRO
1	A	181	ASP
1	A	322	PRO
1	A	380	VAL
1	B	101	TRP
1	B	168	ALA
1	B	181	ASP
1	B	415	TYR
1	B	424	PHE
1	C	28	MET
1	C	181	ASP
1	C	424	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	6	TYR
1	D	424	PHE
1	A	253	MET
1	C	429	TYR
1	D	54	HIS
1	D	83	THR
1	D	181	ASP
1	D	195	ARG
1	D	386	PRO
1	A	386	PRO
1	C	11	ILE
1	B	303	VAL
1	C	425	LYS
1	B	322	PRO
1	D	246	ILE

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	353/353 (100%)	282 (80%)	71 (20%)	1	4
1	B	353/353 (100%)	271 (77%)	82 (23%)	1	2
1	C	353/353 (100%)	269 (76%)	84 (24%)	1	2
1	D	353/353 (100%)	281 (80%)	72 (20%)	1	4
All	All	1412/1412 (100%)	1103 (78%)	309 (22%)	1	3

All (309) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	A	13	LEU
1	A	26	ASN
1	A	53	LEU
1	A	55	MET
1	A	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	79	ASN
1	A	93	LYS
1	A	110	LEU
1	A	114	GLU
1	A	121	ASP
1	A	128	LEU
1	A	134	LEU
1	A	135	THR
1	A	136	ASN
1	A	139	HIS
1	A	144	GLN
1	A	146	LEU
1	A	153	SER
1	A	155	GLU
1	A	158	THR
1	A	163	LEU
1	A	165	LYS
1	A	172	LEU
1	A	174	VAL
1	A	177	ILE
1	A	182	SER
1	A	186	SER
1	A	187	LYS
1	A	198	LEU
1	A	232	ARG
1	A	242	GLU
1	A	257	GLU
1	A	263	GLU
1	A	267	GLU
1	A	275	THR
1	A	277	CYS
1	A	282	LEU
1	A	284	ARG
1	A	298	ILE
1	A	308	LYS
1	A	316	GLU
1	A	320	ILE
1	A	334	ARG
1	A	337	LEU
1	A	342	ARG
1	A	354	SER
1	A	356	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	357	MET
1	A	358	SER
1	A	360	SER
1	A	374	HIS
1	A	376	ASP
1	A	382	VAL
1	A	385	LEU
1	A	387	LYS
1	A	388	LYS
1	A	391	GLU
1	A	395	GLU
1	A	400	LYS
1	A	405	LEU
1	A	407	LYS
1	A	408	LEU
1	A	410	GLU
1	A	411	LYS
1	A	418	MET
1	A	420	ILE
1	A	424	PHE
1	A	425	LYS
1	A	427	ASP
1	A	429	TYR
1	B	3	LYS
1	B	6	TYR
1	B	13	LEU
1	B	26	ASN
1	B	39	SER
1	B	45	LYS
1	B	52	CYS
1	B	53	LEU
1	B	55	MET
1	B	86	HIS
1	B	91	ILE
1	B	93	LYS
1	B	104	GLU
1	B	107	GLU
1	B	110	LEU
1	B	114	GLU
1	B	116	THR
1	B	119	PHE
1	B	121	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	134	LEU
1	B	135	THR
1	B	136	ASN
1	B	137	LEU
1	B	144	GLN
1	B	146	LEU
1	B	153	SER
1	B	154	GLU
1	B	155	GLU
1	B	157	THR
1	B	158	THR
1	B	165	LYS
1	B	172	LEU
1	B	174	VAL
1	B	177	ILE
1	B	182	SER
1	B	186	SER
1	B	196	GLU
1	B	197	SER
1	B	198	LEU
1	B	199	ILE
1	B	209	MET
1	B	232	ARG
1	B	234	PHE
1	B	240	ILE
1	B	242	GLU
1	B	254	GLU
1	B	257	GLU
1	B	266	LYS
1	B	267	GLU
1	B	274	THR
1	B	277	CYS
1	B	278	VAL
1	B	282	LEU
1	B	284	ARG
1	B	297	ASN
1	B	308	LYS
1	B	317	LYS
1	B	320	ILE
1	B	334	ARG
1	B	337	LEU
1	B	357	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	358	SER
1	B	371	LEU
1	B	376	ASP
1	B	377	LYS
1	B	382	VAL
1	B	385	LEU
1	B	388	LYS
1	B	390	ASP
1	B	391	GLU
1	B	395	GLU
1	B	405	LEU
1	B	407	LYS
1	B	408	LEU
1	B	411	LYS
1	B	418	MET
1	B	420	ILE
1	B	423	PRO
1	B	424	PHE
1	B	425	LYS
1	B	427	ASP
1	B	429	TYR
1	C	2	ASP
1	C	3	LYS
1	C	13	LEU
1	C	26	ASN
1	C	39	SER
1	C	45	LYS
1	C	49	ILE
1	C	52	CYS
1	C	53	LEU
1	C	55	MET
1	C	57	VAL
1	C	69	LEU
1	C	79	ASN
1	C	86	HIS
1	C	91	ILE
1	C	93	LYS
1	C	98	VAL
1	C	102	LYS
1	C	106	ASP
1	C	110	LEU
1	C	121	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	134	LEU
1	C	135	THR
1	C	136	ASN
1	C	137	LEU
1	C	139	HIS
1	C	144	GLN
1	C	146	LEU
1	C	147	SER
1	C	150	ARG
1	C	154	GLU
1	C	155	GLU
1	C	156	THR
1	C	158	THR
1	C	172	LEU
1	C	174	VAL
1	C	182	SER
1	C	189	ASP
1	C	196	GLU
1	C	198	LEU
1	C	209	MET
1	C	225	LYS
1	C	232	ARG
1	C	240	ILE
1	C	242	GLU
1	C	267	GLU
1	C	274	THR
1	C	277	CYS
1	C	279	ASP
1	C	282	LEU
1	C	297	ASN
1	C	298	ILE
1	C	308	LYS
1	C	320	ILE
1	C	334	ARG
1	C	337	LEU
1	C	342	ARG
1	C	343	LEU
1	C	345	ASN
1	C	346	LEU
1	C	357	MET
1	C	358	SER
1	C	359	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	374	HIS
1	C	376	ASP
1	C	377	LYS
1	C	382	VAL
1	C	385	LEU
1	C	388	LYS
1	C	391	GLU
1	C	398	LEU
1	C	400	LYS
1	C	405	LEU
1	C	406	THR
1	C	407	LYS
1	C	408	LEU
1	C	411	LYS
1	C	418	MET
1	C	420	ILE
1	C	424	PHE
1	C	425	LYS
1	C	427	ASP
1	C	429	TYR
1	C	430	ARG
1	D	2	ASP
1	D	3	LYS
1	D	13	LEU
1	D	23	ILE
1	D	26	ASN
1	D	39	SER
1	D	52	CYS
1	D	53	LEU
1	D	55	MET
1	D	74	ARG
1	D	76	SER
1	D	80	ILE
1	D	86	HIS
1	D	91	ILE
1	D	93	LYS
1	D	98	VAL
1	D	106	ASP
1	D	110	LEU
1	D	114	GLU
1	D	119	PHE
1	D	134	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	135	THR
1	D	136	ASN
1	D	137	LEU
1	D	139	HIS
1	D	141	LYS
1	D	144	GLN
1	D	146	LEU
1	D	149	ILE
1	D	154	GLU
1	D	158	THR
1	D	163	LEU
1	D	169	ASN
1	D	172	LEU
1	D	174	VAL
1	D	182	SER
1	D	186	SER
1	D	213	LYS
1	D	232	ARG
1	D	254	GLU
1	D	267	GLU
1	D	277	CYS
1	D	278	VAL
1	D	281	ILE
1	D	282	LEU
1	D	298	ILE
1	D	308	LYS
1	D	320	ILE
1	D	321	LYS
1	D	334	ARG
1	D	336	ILE
1	D	337	LEU
1	D	342	ARG
1	D	357	MET
1	D	358	SER
1	D	364	GLN
1	D	371	LEU
1	D	374	HIS
1	D	377	LYS
1	D	382	VAL
1	D	388	LYS
1	D	391	GLU
1	D	395	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	405	LEU
1	D	407	LYS
1	D	408	LEU
1	D	418	MET
1	D	420	ILE
1	D	424	PHE
1	D	425	LYS
1	D	427	ASP
1	D	429	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	84	GLN
1	A	161	HIS
1	A	247	ASN
1	A	250	GLN
1	A	269	ASN
1	A	313	ASN
1	A	319	ASN
1	A	323	GLN
1	A	352	HIS
1	A	359	ASN
1	A	364	GLN
1	A	383	HIS
1	A	402	ASN
1	A	412	GLN
1	A	414	GLN
1	A	428	HIS
1	B	26	ASN
1	B	84	GLN
1	B	250	GLN
1	B	269	ASN
1	B	300	HIS
1	B	352	HIS
1	B	359	ASN
1	B	364	GLN
1	B	368	GLN
1	B	402	ASN
1	B	412	GLN
1	B	414	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	428	HIS
1	C	26	ASN
1	C	84	GLN
1	C	161	HIS
1	C	178	ASN
1	C	247	ASN
1	C	250	GLN
1	C	269	ASN
1	C	300	HIS
1	C	313	ASN
1	C	323	GLN
1	C	345	ASN
1	C	352	HIS
1	C	364	GLN
1	C	374	HIS
1	C	383	HIS
1	C	412	GLN
1	C	414	GLN
1	C	428	HIS
1	D	26	ASN
1	D	84	GLN
1	D	169	ASN
1	D	178	ASN
1	D	247	ASN
1	D	250	GLN
1	D	269	ASN
1	D	313	ASN
1	D	352	HIS
1	D	359	ASN
1	D	364	GLN
1	D	368	GLN
1	D	374	HIS
1	D	402	ASN
1	D	412	GLN
1	D	414	GLN
1	D	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 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	NAD	A	501	-	41,48,48	1.37	4 (9%)	43,73,73	2.40	11 (25%)
3	ADN	A	601	-	18,21,21	0.88	1 (5%)	17,31,31	2.18	4 (23%)
2	NAD	B	502	-	41,48,48	1.33	4 (9%)	43,73,73	1.60	7 (16%)
3	ADN	B	602	-	18,21,21	0.83	1 (5%)	17,31,31	2.50	7 (41%)
2	NAD	C	503	-	41,48,48	1.12	3 (7%)	43,73,73	1.86	7 (16%)
3	ADN	C	603	-	18,21,21	0.78	1 (5%)	17,31,31	2.36	7 (41%)
2	NAD	D	504	-	41,48,48	1.00	3 (7%)	43,73,73	1.92	8 (18%)
3	ADN	D	604	-	18,21,21	0.85	0	17,31,31	2.46	4 (23%)

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	NAD	A	501	-	-	0/22/62/62	0/5/5/5
3	ADN	A	601	-	-	0/2/22/22	0/3/3/3
2	NAD	B	502	-	-	0/22/62/62	0/5/5/5
3	ADN	B	602	-	-	0/2/22/22	0/3/3/3
2	NAD	C	503	-	-	0/22/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADN	C	603	-	-	0/2/22/22	0/3/3/3
2	NAD	D	504	-	-	0/22/62/62	0/5/5/5
3	ADN	D	604	-	-	0/2/22/22	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	NAD	C5A-N7A	-2.11	1.32	1.39
2	A	501	NAD	C5A-N7A	-2.06	1.32	1.39
3	C	603	ADN	C5-N7	-2.06	1.32	1.39
3	B	602	ADN	C5-N7	-2.04	1.32	1.39
2	D	504	NAD	C5A-N7A	-2.02	1.32	1.39
3	A	601	ADN	C5-N7	-2.02	1.32	1.39
2	A	501	NAD	C6N-N1N	2.08	1.40	1.35
2	C	503	NAD	O4D-C1D	2.12	1.44	1.41
2	D	504	NAD	O4D-C1D	2.22	1.44	1.41
2	D	504	NAD	C3N-C7N	2.55	1.54	1.50
2	B	502	NAD	C3N-C7N	2.74	1.54	1.50
2	A	501	NAD	C3N-C7N	3.32	1.55	1.50
2	C	503	NAD	C3N-C7N	3.41	1.55	1.50
2	C	503	NAD	O4B-C1B	3.59	1.46	1.41
2	B	502	NAD	O4D-C1D	4.34	1.47	1.41
2	B	502	NAD	O4B-C1B	4.93	1.48	1.41
2	A	501	NAD	O4B-C1B	5.94	1.49	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	ADN	N3-C2-N1	-6.70	123.03	128.86
3	D	604	ADN	N3-C2-N1	-6.53	123.17	128.86
3	B	602	ADN	N3-C2-N1	-6.11	123.53	128.86
2	C	503	NAD	N3A-C2A-N1A	-5.96	123.67	128.86
3	B	602	ADN	C4'-O4'-C1'	-5.87	103.52	109.77
2	D	504	NAD	N3A-C2A-N1A	-5.86	123.75	128.86
2	B	502	NAD	N3A-C2A-N1A	-5.84	123.78	128.86
3	A	601	ADN	N3-C2-N1	-5.64	123.95	128.86
3	A	601	ADN	C4'-O4'-C1'	-4.62	104.85	109.77
2	A	501	NAD	N3A-C2A-N1A	-4.57	124.88	128.86
2	A	501	NAD	C4B-O4B-C1B	-4.48	105.00	109.77
2	D	504	NAD	O4D-C4D-C3D	-4.15	96.92	105.17
3	D	604	ADN	O4'-C4'-C3'	-4.02	97.17	105.17
3	C	603	ADN	O2'-C2'-C3'	-3.99	99.04	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAD	O4D-C4D-C3D	-3.96	97.29	105.17
3	D	604	ADN	O2'-C2'-C3'	-3.45	100.79	111.83
2	C	503	NAD	O2D-C2D-C3D	-3.32	101.21	111.83
2	A	501	NAD	O3D-C3D-C2D	-3.09	101.95	111.83
2	C	503	NAD	O7N-C7N-N7N	-3.00	118.32	122.58
2	B	502	NAD	O2D-C2D-C3D	-2.79	102.89	111.83
3	C	603	ADN	C4'-O4'-C1'	-2.38	107.23	109.77
2	D	504	NAD	O2D-C2D-C3D	-2.31	104.42	111.83
3	C	603	ADN	O4'-C4'-C3'	-2.29	100.61	105.17
3	C	603	ADN	C5-C6-N1	-2.29	112.77	119.70
2	A	501	NAD	O4D-C4D-C5D	-2.26	101.77	109.40
2	A	501	NAD	C5B-C4B-C3B	-2.15	107.11	115.29
3	B	602	ADN	C5-C6-N1	-2.12	113.29	119.70
2	B	502	NAD	C4N-C3N-C7N	-2.10	115.49	121.07
2	D	504	NAD	O3D-C3D-C4D	-2.10	104.97	111.09
2	A	501	NAD	C4N-C3N-C7N	-2.07	115.56	121.07
3	A	601	ADN	O2'-C2'-C3'	-2.06	105.23	111.83
3	B	602	ADN	O2'-C2'-C3'	-2.01	105.39	111.83
2	D	504	NAD	C2N-C3N-C7N	2.00	125.16	119.34
2	B	502	NAD	C2N-C3N-C7N	2.06	125.32	119.34
3	A	601	ADN	O4'-C4'-C5'	2.07	113.59	109.16
3	B	602	ADN	C5-C6-N6	2.07	124.70	120.47
3	C	603	ADN	C5-C6-N6	2.14	124.84	120.47
2	B	502	NAD	O5D-PN-O1N	2.16	117.97	109.25
2	C	503	NAD	C5A-C6A-N6A	2.26	125.07	120.47
3	B	602	ADN	C2-N1-C6	2.28	122.75	118.77
2	A	501	NAD	C3N-C7N-N7N	2.34	120.44	117.77
2	B	502	NAD	C5A-C6A-N6A	2.34	125.25	120.47
2	A	501	NAD	C2N-C3N-C7N	2.37	126.23	119.34
2	C	503	NAD	C3N-C2N-N1N	2.38	122.83	120.43
3	B	602	ADN	C4-C5-N7	2.39	111.72	109.41
2	A	501	NAD	O4B-C4B-C3B	2.45	110.03	105.17
2	D	504	NAD	C4A-C5A-N7A	2.46	111.79	109.41
3	C	603	ADN	C2-N1-C6	2.49	123.13	118.77
2	D	504	NAD	C4B-O4B-C1B	2.51	112.44	109.77
3	D	604	ADN	C4-C5-N7	2.53	111.86	109.41
2	B	502	NAD	C4D-O4D-C1D	3.61	113.61	109.77
2	C	503	NAD	C4D-O4D-C1D	4.12	114.15	109.77
2	C	503	NAD	O7N-C7N-C3N	5.27	125.79	119.62
2	D	504	NAD	C4D-O4D-C1D	6.57	116.76	109.77
2	A	501	NAD	C4D-O4D-C1D	10.24	120.67	109.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	NAD	22	0
3	A	601	ADN	3	0
2	B	502	NAD	16	0
3	B	602	ADN	2	0
2	C	503	NAD	7	0
3	C	603	ADN	1	0
2	D	504	NAD	9	0
3	D	604	ADN	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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.