



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:02 am BST

PDB ID : 1RXT
Title : Crystal structure of human myristoyl-CoA:protein N-myristoyltransferase.
Authors : Yang, J.; Wang, Y.; Frey, G.; Abeles, R.H.; Petsko, G.A.; Ringe, D.
Deposited on : 2003-12-18
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

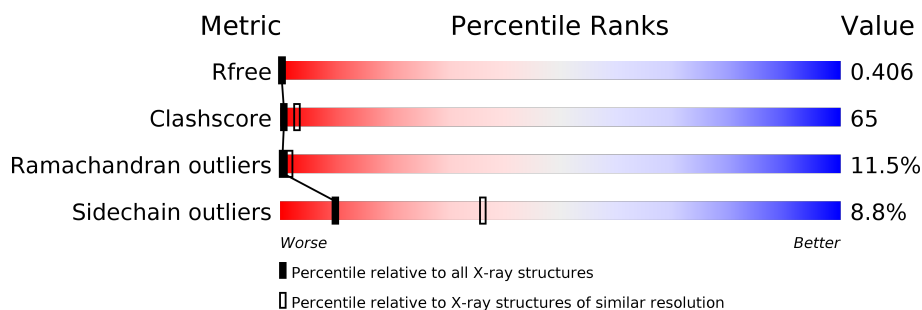
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	496	
1	B	496	
1	C	496	
1	D	496	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10420 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 Glycylpeptide N-tetradecanoyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2646	1724	439	471	12			
1	B	342	Total	C	N	O	S	0	0	0
			2640	1718	438	472	12			
1	C	325	Total	C	N	O	S	0	0	0
			2538	1652	424	450	12			
1	D	326	Total	C	N	O	S	0	0	0
			2523	1642	418	451	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	452	ILE	LEU	CONFLICT	UNP P30419
B	452	ILE	LEU	CONFLICT	UNP P30419
C	452	ILE	LEU	CONFLICT	UNP P30419
D	452	ILE	LEU	CONFLICT	UNP P30419

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Co	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		
4	B	13	Total	O	0	0
			13	13		
4	C	10	Total	O	0	0
			10	10		
4	D	16	Total	O	0	0
			16	16		



L380	N381	S382	D383	A384	L385	V386	L387	A388	K389	M390	K391	G392	F393		M397		D400	L401	M402	M403	M404	K405	T406	F407	L408	E409	K410	L411	K412	P413	G414	I415	G416	D417	G418	M419		Y423	L424	Y425		M432	G433	A447	E448	K449		I452	V453	L454	Q455									
V294	E295	E296	H297	F298	Y299	P300	Q301	E302	N303	I310	I311	D312	T313	F314	V315	V316		A319		E322	V323	T324	D325	F326	L327	S328	F329	Y330	T331	L332	P333	S334	T335	I336	M337	N338	H339	P340	T341	H342	K343	S344	L345	K346	A347	A348	Y349		Y352	N353	V354	H355	T356	T357	Q374	T375	P376	L377	D379	
P226	R227	K228	L229		V232	K233	F234	S235	H236	L237	S238	R239	M240	M241	T242	M243	Q244	R245	T246	M247	K248	L249	Y250	R251		T258		L261	R262	P263	M264	E265	T266	K267	D268	I269	P270	V271	V272	H273	Q274	L275	L276		Y279	L280	F281	Q282	F283	H284	L285	T286	P287	V288	M289	S290	Q291	E292	E293	
K164	M165	V166	E167	I168	N169	F170	L171	C172	V173	H174	K175	K176	L177	R178	S179	K180	R181	V182	A183	P184	V185	L186	I187	R188	E189	I190	T191	R192	R193	V194	H195	L196	E197	G198	I199	F200	Q201	A202	V203		G207	V208	V209	L210	P211	R212	P213	V214	G215	T216	C217	R218	Y219	W220	H221	R222	S223	L224	N225	
V104	E105	D106	D107	N108	M109	M110	F111	R112	F113	D114	Y115	S116	P117	E118	F119	L120	L121	W122	A123	L124	R125	P126	P127	G128	M129	L130	P131	Q132	W133	H134	C135	G136	V137	ARG	VAL	VAL	SER	SER	ARG	ARG	LYS	LEU	VAL	G147	F148	I149	S150	A151	I152	P153	A154	N155	I156	H157	I158	Y159	D160	T161	E162	R163
ASP	THR	GLN	PRO	VAL	PRO	LYS	LEU	GLY	GLU	VAL	VAL	ASN	THR	HIS	GLY	PRO	VAL	GLU	PRO	ASP	LYS	ASP	ASN	ILE	ARG	GLN	GLU	PRO	TYR	THR	LEU	PRO	GLN	GLY	PHE	THR	TRP	ASP	ALA	ALA	LEU	D85	L86	G87	D88	R89	G90	V91	L92	K93	E94	L95	Y96	T97	L98	L99	M100	E101	N102	Y103

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.63Å 116.42Å 90.36Å 90.00° 90.13° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.00) 96.5 (29.44-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.283 , 0.391 0.338 , 0.406	Depositor DCC
R_{free} test set	1412 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	45.2	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 121.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.43$	Xtriage
Estimated twinning fraction	0.380 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7162e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO, SO4

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	0.76	3/2718 (0.1%)	1.01	8/3715 (0.2%)
1	B	1.04	4/2712 (0.1%)	1.15	8/3709 (0.2%)
1	C	0.74	3/2605 (0.1%)	0.96	6/3551 (0.2%)
1	D	1.10	4/2592 (0.2%)	1.12	9/3542 (0.3%)
All	All	0.92	14/10627 (0.1%)	1.06	31/14517 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
1	D	0	3
All	All	0	13

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	LEU	C-N	-32.53	0.59	1.34
1	D	401	LEU	C-N	-32.37	0.59	1.34
1	B	401	LEU	C-N	-31.27	0.62	1.34
1	B	402	MET	C-N	28.57	1.99	1.34
1	D	302	GLU	C-N	-27.80	0.70	1.34
1	D	402	MET	C-N	27.64	1.97	1.34
1	B	302	GLU	C-N	-24.04	0.78	1.34
1	C	302	GLU	C-N	-22.49	0.82	1.34
1	C	401	LEU	C-N	-19.99	0.88	1.34
1	D	301	GLN	C-N	-15.88	0.97	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	301	GLN	C-N	-15.36	0.98	1.34
1	B	301	GLN	C-N	-14.99	0.99	1.34
1	A	301	GLN	C-N	-12.33	1.05	1.34
1	A	302	GLU	C-N	-8.16	1.15	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	301	GLN	O-C-N	-47.53	46.66	122.70
1	B	301	GLN	O-C-N	-44.79	51.04	122.70
1	C	301	GLN	O-C-N	-37.26	63.09	122.70
1	A	301	GLN	O-C-N	-29.43	75.62	122.70
1	B	401	LEU	O-C-N	-24.32	83.78	122.70
1	A	401	LEU	O-C-N	-23.70	84.78	122.70
1	D	402	MET	C-N-CA	-19.24	73.61	121.70
1	B	402	MET	C-N-CA	-19.14	73.85	121.70
1	A	302	GLU	O-C-N	-18.80	92.62	122.70
1	A	302	GLU	C-N-CA	16.06	161.84	121.70
1	C	401	LEU	O-C-N	-15.96	97.17	122.70
1	B	401	LEU	C-N-CA	14.60	158.20	121.70
1	A	302	GLU	CA-C-N	14.20	148.45	117.20
1	B	402	MET	O-C-N	13.52	144.33	122.70
1	C	302	GLU	O-C-N	-13.29	101.43	122.70
1	D	402	MET	O-C-N	13.05	143.58	122.70
1	D	401	LEU	O-C-N	-12.55	102.62	122.70
1	B	401	LEU	CA-C-N	11.55	142.60	117.20
1	C	302	GLU	C-N-CA	11.50	150.46	121.70
1	D	402	MET	CA-C-N	-10.64	93.79	117.20
1	B	402	MET	CA-C-N	-10.06	95.08	117.20
1	A	401	LEU	C-N-CA	9.36	145.10	121.70
1	A	301	GLN	CA-C-N	-8.97	97.46	117.20
1	C	302	GLU	CA-C-N	8.91	136.79	117.20
1	D	401	LEU	C-N-CA	7.64	140.81	121.70
1	A	401	LEU	CA-C-N	7.11	132.84	117.20
1	D	401	LEU	CA-C-N	6.61	131.74	117.20
1	D	302	GLU	C-N-CA	6.06	136.86	121.70
1	C	401	LEU	C-N-CA	5.83	136.28	121.70
1	B	302	GLU	C-N-CA	5.69	135.92	121.70
1	D	301	GLN	CA-C-N	5.37	129.01	117.20

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	301	GLN	Mainchain
1	A	401	LEU	Mainchain,Peptide
1	B	301	GLN	Mainchain
1	B	401	LEU	Mainchain,Peptide
1	C	301	GLN	Mainchain
1	C	302	GLU	Mainchain
1	C	401	LEU	Mainchain,Peptide
1	D	301	GLN	Mainchain
1	D	401	LEU	Mainchain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2646	0	2523	316	0
1	B	2640	0	2514	336	0
1	C	2538	0	2434	338	1
1	D	2523	0	2395	332	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	C	1	0	0	0	0
4	A	13	0	0	3	0
4	B	13	0	0	3	0
4	C	10	0	0	4	0
4	D	16	0	0	2	0
All	All	10420	0	9866	1322	1

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 65.

All (1322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLU:CA	1:B:303:ASN:N	1.95	1.29
1:D:302:GLU:CA	1:D:303:ASN:N	1.94	1.29
1:D:302:GLU:C	1:D:303:ASN:CA	2.03	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLU:O	1:C:303:ASN:N	1.61	1.26
1:D:302:GLU:O	1:D:303:ASN:N	1.68	1.25
1:B:302:GLU:C	1:B:303:ASN:CA	2.09	1.21
1:D:402:MET:C	1:D:403:GLU:CA	2.09	1.20
1:B:402:MET:C	1:B:403:GLU:HA	1.63	1.19
1:A:402:MET:C	1:A:403:GLU:CA	2.10	1.19
1:B:402:MET:C	1:B:403:GLU:CA	2.12	1.18
1:D:402:MET:C	1:D:403:GLU:HA	1.63	1.17
1:D:402:MET:C	1:D:403:GLU:N	1.97	1.17
1:B:222:ARG:HH21	1:B:250:TYR:HA	1.10	1.16
1:B:402:MET:C	1:B:403:GLU:N	1.99	1.14
1:A:222:ARG:HH21	1:A:250:TYR:HA	1.09	1.14
1:A:402:MET:C	1:A:403:GLU:N	2.01	1.14
1:B:302:GLU:O	1:B:303:ASN:N	1.80	1.14
1:A:402:MET:C	1:A:403:GLU:HA	1.68	1.13
1:C:181:ARG:HH11	1:C:181:ARG:HA	1.11	1.12
1:C:402:MET:C	1:C:403:GLU:HA	1.71	1.11
1:D:222:ARG:HH21	1:D:250:TYR:HA	1.12	1.11
1:C:402:MET:C	1:C:403:GLU:CA	2.20	1.10
1:A:228:LYS:HZ2	1:A:343:LYS:HE2	1.13	1.09
1:C:302:GLU:C	1:C:303:ASN:CA	2.21	1.07
1:C:302:GLU:CA	1:C:303:ASN:N	2.18	1.05
1:C:222:ARG:HH21	1:C:250:TYR:HA	1.14	1.05
1:B:156:ILE:HG21	1:B:203:VAL:HG21	1.38	1.04
1:C:402:MET:C	1:C:403:GLU:N	2.12	1.02
1:A:222:ARG:HG2	1:A:412:LYS:HB2	1.40	1.02
1:A:156:ILE:HG21	1:A:203:VAL:HG21	1.40	1.00
1:D:222:ARG:HG2	1:D:412:LYS:HB2	1.40	0.99
1:B:222:ARG:HG2	1:B:412:LYS:HB2	1.43	0.98
1:C:222:ARG:HG2	1:C:412:LYS:HB2	1.47	0.97
1:C:156:ILE:HG21	1:C:203:VAL:HG21	1.44	0.96
1:D:156:ILE:HG21	1:D:203:VAL:HG21	1.48	0.95
1:D:412:LYS:H	1:D:412:LYS:HD2	1.32	0.95
1:A:412:LYS:H	1:A:412:LYS:HD2	1.31	0.95
1:D:338:ASN:HD22	1:D:338:ASN:H	0.99	0.95
1:B:412:LYS:H	1:B:412:LYS:HD2	1.32	0.94
1:A:269:ILE:HB	1:A:270:PRO:HD3	1.50	0.92
1:D:331:THR:HG22	1:D:333:PRO:HD3	1.52	0.91
1:D:325:ASP:HB3	1:D:355:HIS:HA	1.49	0.91
1:B:269:ILE:HB	1:B:270:PRO:HD3	1.51	0.91
1:B:331:THR:HG22	1:B:333:PRO:HD3	1.53	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LYS:H	1:B:343:LYS:HD3	1.35	0.91
1:C:269:ILE:HB	1:C:270:PRO:HD3	1.53	0.90
1:A:325:ASP:HB3	1:A:355:HIS:HA	1.52	0.90
1:C:331:THR:HG22	1:C:333:PRO:HD3	1.51	0.90
1:A:222:ARG:NH2	1:A:250:TYR:HA	1.87	0.90
1:A:331:THR:HG22	1:A:333:PRO:HD3	1.52	0.90
1:D:338:ASN:H	1:D:338:ASN:ND2	1.70	0.90
1:B:325:ASP:HB3	1:B:355:HIS:HA	1.51	0.90
1:A:130:LEU:HB2	1:A:132:GLN:HE22	1.37	0.89
1:D:269:ILE:HD13	1:D:295:GLU:HG3	1.54	0.89
1:C:130:LEU:HB2	1:C:132:GLN:HE22	1.38	0.87
1:C:302:GLU:C	1:C:303:ASN:N	0.82	0.87
1:D:269:ILE:HB	1:D:270:PRO:HD3	1.53	0.87
1:C:412:LYS:H	1:C:412:LYS:HD2	1.37	0.86
1:C:325:ASP:HB3	1:C:355:HIS:HA	1.58	0.86
1:C:275:LEU:HD23	1:C:326:PHE:CE1	2.11	0.85
1:B:222:ARG:NH2	1:B:250:TYR:HA	1.92	0.84
1:B:302:GLU:C	1:B:303:ASN:N	0.78	0.83
1:D:283:PHE:HB2	1:D:286:THR:CG2	2.08	0.83
1:C:275:LEU:HD23	1:C:326:PHE:HE1	1.43	0.83
1:B:388:ALA:O	1:B:393:PHE:HB2	1.79	0.83
1:A:133:TRP:HZ3	1:A:153:PRO:HG3	1.42	0.83
1:D:130:LEU:HB2	1:D:132:GLN:HE22	1.41	0.83
1:A:404:ASN:HA	1:A:407:PHE:CE2	2.13	0.83
1:A:275:LEU:HD23	1:A:326:PHE:CE1	2.15	0.82
1:C:283:PHE:HB2	1:C:286:THR:CG2	2.10	0.82
1:B:229:LEU:HD22	1:B:234:PHE:HD2	1.44	0.82
1:D:133:TRP:HZ3	1:D:153:PRO:HG3	1.42	0.82
1:A:405:LYS:HA	1:A:408:LEU:HD12	1.60	0.82
1:B:130:LEU:HB2	1:B:132:GLN:HE22	1.43	0.82
1:C:130:LEU:CB	1:C:132:GLN:HE22	1.92	0.81
1:A:283:PHE:HB2	1:A:286:THR:CG2	2.10	0.81
1:A:122:TRP:CZ2	1:A:311:ILE:HG21	2.15	0.81
1:D:275:LEU:HD23	1:D:326:PHE:CE1	2.15	0.81
1:C:269:ILE:HD13	1:C:295:GLU:HG3	1.61	0.81
1:C:222:ARG:NH2	1:C:250:TYR:HA	1.95	0.81
1:A:130:LEU:CB	1:A:132:GLN:HE22	1.94	0.81
1:D:404:ASN:O	1:D:408:LEU:HG	1.80	0.81
1:C:343:LYS:HD2	1:C:343:LYS:H	1.44	0.81
1:C:267:LYS:H	1:C:267:LYS:HD3	1.44	0.80
1:D:130:LEU:CB	1:D:132:GLN:HE22	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TRP:HZ3	1:B:153:PRO:HG3	1.46	0.80
1:A:302:GLU:HA	1:A:302:GLU:OE1	1.81	0.80
1:B:336:ILE:HG12	1:B:337:MET:N	1.96	0.80
1:A:404:ASN:O	1:A:408:LEU:HG	1.82	0.80
1:C:315:VAL:HG22	1:C:324:THR:OG1	1.80	0.80
1:D:221:HIS:O	1:D:413:PHE:HA	1.82	0.80
1:D:181:ARG:HD3	1:D:184:PRO:HB2	1.61	0.79
1:A:229:LEU:HD22	1:A:234:PHE:HD2	1.47	0.79
1:B:404:ASN:O	1:B:408:LEU:HG	1.82	0.79
1:B:275:LEU:HD23	1:B:326:PHE:CE1	2.17	0.79
1:B:400:ASP:HB3	1:B:447:ALA:HB1	1.64	0.79
1:B:404:ASN:HA	1:B:407:PHE:CE2	2.17	0.79
1:C:404:ASN:O	1:C:408:LEU:HG	1.82	0.78
1:D:338:ASN:HD22	1:D:338:ASN:N	1.73	0.78
1:A:183:ALA:HA	1:A:186:LEU:HB3	1.65	0.78
1:A:222:ARG:HH21	1:A:250:TYR:CA	1.94	0.78
1:B:218:ARG:HG2	1:B:419:ASN:HB3	1.66	0.78
1:D:102:ASN:HB3	1:D:172:CYS:SG	2.24	0.78
1:B:275:LEU:HD23	1:B:326:PHE:HE1	1.48	0.78
1:D:404:ASN:HA	1:D:407:PHE:CE2	2.19	0.78
1:D:122:TRP:CZ2	1:D:311:ILE:HG21	2.19	0.77
1:A:122:TRP:NE1	1:A:311:ILE:HD13	2.00	0.77
1:B:122:TRP:CZ2	1:B:311:ILE:HG21	2.19	0.77
1:D:275:LEU:HD23	1:D:326:PHE:HE1	1.47	0.77
1:D:181:ARG:C	1:D:184:PRO:HD2	2.05	0.77
1:C:104:VAL:HG13	1:C:111:PHE:O	1.85	0.77
1:D:315:VAL:HG22	1:D:324:THR:OG1	1.83	0.77
1:D:137:VAL:HG12	1:D:137:VAL:O	1.83	0.76
1:C:122:TRP:CZ2	1:C:311:ILE:HG21	2.19	0.76
1:B:283:PHE:HB2	1:B:286:THR:CG2	2.16	0.76
1:A:218:ARG:HG2	1:A:419:ASN:HB3	1.67	0.76
1:B:269:ILE:HD13	1:B:295:GLU:HG3	1.68	0.76
1:C:401:LEU:O	1:C:402:MET:C	2.20	0.76
1:D:388:ALA:O	1:D:393:PHE:HB2	1.86	0.76
1:D:183:ALA:HA	1:D:186:LEU:HB3	1.67	0.76
1:B:412:LYS:N	1:B:412:LYS:HD2	2.01	0.76
1:D:222:ARG:NH2	1:D:250:TYR:HA	1.95	0.76
1:C:229:LEU:HD22	1:C:234:PHE:HD2	1.51	0.75
1:A:388:ALA:O	1:A:393:PHE:HB2	1.85	0.75
1:B:102:ASN:HD21	1:B:174:HIS:HA	1.51	0.75
1:B:267:LYS:HD3	1:B:267:LYS:H	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ILE:HD13	1:A:295:GLU:HG3	1.67	0.75
1:B:130:LEU:CB	1:B:132:GLN:HE22	1.98	0.75
1:D:412:LYS:N	1:D:412:LYS:HD2	2.02	0.75
1:A:228:LYS:NZ	1:A:343:LYS:HE2	1.98	0.75
1:D:173:VAL:HG23	1:D:174:HIS:H	1.51	0.75
1:D:302:GLU:C	1:D:303:ASN:N	0.70	0.75
1:D:218:ARG:HG2	1:D:419:ASN:HB3	1.68	0.75
1:B:222:ARG:HH21	1:B:250:TYR:CA	1.96	0.75
1:C:388:ALA:O	1:C:393:PHE:HB2	1.86	0.75
1:A:275:LEU:HD23	1:A:326:PHE:HE1	1.50	0.74
1:B:336:ILE:HB	1:B:344:SER:HA	1.68	0.74
1:C:404:ASN:HA	1:C:407:PHE:CE2	2.22	0.74
1:D:135:CYS:HB2	1:D:149:ILE:CG2	2.17	0.74
1:A:400:ASP:HB3	1:A:447:ALA:HB1	1.69	0.74
1:B:183:ALA:HA	1:B:186:LEU:HB3	1.68	0.74
1:A:267:LYS:H	1:A:267:LYS:HD3	1.52	0.74
1:A:232:VAL:HG22	1:A:233:LYS:H	1.53	0.74
1:C:405:LYS:HA	1:C:408:LEU:HD12	1.70	0.74
1:C:412:LYS:N	1:C:412:LYS:HD2	2.02	0.73
1:B:402:MET:O	1:B:403:GLU:HA	1.88	0.73
1:C:104:VAL:HG22	1:C:112:ARG:HA	1.70	0.73
1:A:315:VAL:HG22	1:A:324:THR:OG1	1.89	0.73
1:B:83:ALA:HB3	1:B:136:GLY:O	1.88	0.73
1:A:343:LYS:H	1:A:343:LYS:HD3	1.54	0.73
1:B:122:TRP:NE1	1:B:311:ILE:HD13	2.04	0.73
1:D:222:ARG:HH21	1:D:250:TYR:CA	1.98	0.73
1:A:412:LYS:N	1:A:412:LYS:HD2	2.03	0.73
1:C:222:ARG:HH21	1:C:250:TYR:CA	1.97	0.73
1:D:207:GLY:O	1:D:208:VAL:HG13	1.89	0.73
1:C:232:VAL:HG22	1:C:233:LYS:H	1.53	0.73
1:C:267:LYS:HD3	1:C:267:LYS:N	2.04	0.73
1:B:81:TRP:CZ2	1:B:140:VAL:HG22	2.24	0.73
1:B:202:ALA:HB3	1:B:425:TYR:CB	2.19	0.72
1:B:221:HIS:O	1:B:413:PHE:HA	1.89	0.72
1:C:149:ILE:HD13	1:C:171:LEU:HB2	1.70	0.72
1:D:232:VAL:HG22	1:D:233:LYS:H	1.54	0.72
1:A:267:LYS:N	1:A:267:LYS:HD3	2.05	0.72
1:C:221:HIS:O	1:C:413:PHE:HA	1.89	0.72
1:C:149:ILE:HD12	1:C:169:ASN:O	1.90	0.72
1:C:122:TRP:NE1	1:C:311:ILE:HD13	2.05	0.72
1:C:155:ASN:OD1	1:C:164:LYS:HG3	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD22	1:C:99:LEU:H	1.52	0.72
1:B:202:ALA:HB3	1:B:425:TYR:HB2	1.72	0.71
1:B:149:ILE:HD12	1:B:169:ASN:O	1.89	0.71
1:B:232:VAL:HG22	1:B:233:LYS:H	1.55	0.71
1:B:167:GLU:HB3	1:B:454:LEU:HD11	1.71	0.71
1:D:181:ARG:CD	1:D:184:PRO:HB2	2.20	0.71
1:B:405:LYS:HA	1:B:408:LEU:HD12	1.71	0.71
1:B:83:ALA:HB1	4:B:902:HOH:O	1.90	0.71
1:C:105:GLU:CD	1:C:207:GLY:HA3	2.11	0.71
1:D:343:LYS:HD3	1:D:344:SER:N	2.04	0.71
1:B:267:LYS:HD3	1:B:267:LYS:N	2.05	0.71
1:B:158:ILE:HD12	1:B:158:ILE:H	1.54	0.71
1:C:137:VAL:HB	1:C:147:GLY:N	2.05	0.71
1:A:149:ILE:HD12	1:A:169:ASN:O	1.91	0.71
1:C:202:ALA:HB3	1:C:425:TYR:CB	2.21	0.71
1:D:111:PHE:HZ	1:D:234:PHE:HA	1.52	0.71
1:D:400:ASP:HB3	1:D:447:ALA:HB1	1.73	0.71
1:D:402:MET:O	1:D:403:GLU:HA	1.92	0.70
1:C:400:ASP:HB3	1:C:447:ALA:HB1	1.73	0.70
1:B:315:VAL:HG22	1:B:324:THR:OG1	1.90	0.70
1:D:267:LYS:N	1:D:267:LYS:HD3	2.07	0.70
1:C:103:TYR:O	1:C:113:PHE:HB2	1.91	0.70
1:C:202:ALA:HB3	1:C:425:TYR:HB2	1.73	0.70
1:D:202:ALA:HB3	1:D:425:TYR:CB	2.22	0.70
1:C:135:CYS:HB2	1:C:149:ILE:HG22	1.72	0.70
1:C:302:GLU:OE1	1:C:302:GLU:HA	1.91	0.70
1:D:229:LEU:HD22	1:D:234:PHE:HD2	1.57	0.69
1:A:155:ASN:OD1	1:A:164:LYS:HG3	1.92	0.69
1:A:99:LEU:H	1:A:99:LEU:HD22	1.56	0.69
1:D:89:ARG:HA	1:D:89:ARG:CZ	2.22	0.69
1:D:149:ILE:HD13	1:D:171:LEU:HB2	1.72	0.69
1:A:102:ASN:HD21	1:A:174:HIS:HA	1.58	0.69
1:C:207:GLY:O	1:C:208:VAL:HG13	1.92	0.69
1:C:228:LYS:NZ	1:C:343:LYS:HB2	2.07	0.69
1:A:190:ILE:O	1:A:194:VAL:HG23	1.93	0.69
1:B:99:LEU:H	1:B:99:LEU:HD22	1.57	0.69
1:C:89:ARG:CZ	1:C:89:ARG:HA	2.23	0.68
1:D:155:ASN:OD1	1:D:164:LYS:HG3	1.93	0.68
1:A:221:HIS:O	1:A:413:PHE:HA	1.93	0.68
1:A:99:LEU:HD12	1:A:103:TYR:HB2	1.74	0.68
1:B:155:ASN:OD1	1:B:164:LYS:HG3	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LYS:HA	1:D:408:LEU:HD12	1.74	0.68
1:D:267:LYS:HD3	1:D:267:LYS:H	1.57	0.68
1:A:222:ARG:O	1:A:222:ARG:HD3	1.92	0.68
1:A:279:TYR:CD2	1:A:354:VAL:HG13	2.29	0.68
1:D:133:TRP:CZ3	1:D:153:PRO:HG3	2.28	0.68
1:A:228:LYS:HZ2	1:A:343:LYS:CE	1.99	0.68
1:D:107:ASP:HA	1:D:111:PHE:H	1.59	0.68
1:D:402:MET:CA	1:D:403:GLU:N	2.57	0.68
1:A:126:PRO:HB3	1:A:297:TRP:CZ2	2.30	0.67
1:B:149:ILE:HD13	1:B:171:LEU:HB2	1.75	0.67
1:C:412:LYS:H	1:C:412:LYS:CD	2.07	0.67
1:C:107:ASP:HA	1:C:111:PHE:H	1.59	0.67
1:C:292:GLU:O	1:C:295:GLU:HB3	1.94	0.67
1:D:154:ALA:HB2	1:D:167:GLU:HG3	1.75	0.67
1:D:122:TRP:NE1	1:D:311:ILE:HD13	2.10	0.67
1:A:224:LEU:HD22	1:A:389:LYS:HB2	1.76	0.66
1:D:222:ARG:HD3	1:D:222:ARG:O	1.94	0.66
1:D:301:GLN:HB3	1:D:310:ILE:HD12	1.77	0.66
1:A:311:ILE:HG22	1:A:330:TYR:CB	2.25	0.66
1:B:94:GLU:HB2	1:B:145:LEU:CD1	2.25	0.66
1:B:233:LYS:HA	1:B:236:HIS:HE1	1.60	0.66
1:B:412:LYS:H	1:B:412:LYS:CD	2.06	0.66
1:A:232:VAL:HG22	1:A:233:LYS:N	2.11	0.66
1:D:355:HIS:CG	1:D:377:LEU:HB3	2.30	0.66
1:C:311:ILE:HG22	1:C:330:TYR:CB	2.26	0.66
1:C:94:GLU:O	1:C:97:THR:HB	1.95	0.66
1:D:412:LYS:CD	1:D:412:LYS:H	2.06	0.66
1:B:79:PHE:HE1	1:B:140:VAL:HG23	1.61	0.66
1:A:114:ASP:HB2	1:A:335:THR:OG1	1.96	0.66
1:B:292:GLU:O	1:B:295:GLU:HB3	1.96	0.66
1:C:343:LYS:HD2	1:C:343:LYS:N	2.11	0.66
1:A:233:LYS:HA	1:A:236:HIS:HE1	1.61	0.65
1:D:94:GLU:O	1:D:97:THR:HB	1.96	0.65
1:C:218:ARG:HG2	1:C:419:ASN:HB3	1.76	0.65
1:D:185:VAL:HG13	1:D:188:ARG:HE	1.61	0.65
1:D:224:LEU:HD22	1:D:389:LYS:HB2	1.78	0.65
1:B:156:ILE:CG2	1:B:203:VAL:HG21	2.22	0.65
1:B:268:ASP:O	1:B:272:VAL:HG23	1.96	0.65
1:C:102:ASN:ND2	1:C:174:HIS:O	2.29	0.65
1:A:202:ALA:HB3	1:A:425:TYR:CB	2.27	0.65
1:B:280:LEU:HD21	1:B:287:PRO:HD2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ILE:HD13	1:D:295:GLU:CG	2.24	0.65
1:D:283:PHE:HB2	1:D:286:THR:HG23	1.78	0.65
1:D:292:GLU:O	1:D:295:GLU:HB3	1.96	0.65
1:A:263:PRO:HG3	1:A:314:PHE:CE2	2.31	0.65
1:C:181:ARG:NH1	1:C:181:ARG:HA	1.97	0.65
1:D:99:LEU:HD22	1:D:99:LEU:H	1.60	0.65
1:A:123:ALA:HA	1:A:297:TRP:CZ3	2.32	0.65
1:A:268:ASP:O	1:A:272:VAL:HG23	1.96	0.65
1:B:116:SER:HB3	1:B:119:PHE:HB2	1.79	0.65
1:C:222:ARG:O	1:C:222:ARG:HD3	1.95	0.65
1:C:355:HIS:NE2	1:C:377:LEU:HD22	2.11	0.65
1:D:126:PRO:HB3	1:D:297:TRP:CZ2	2.31	0.65
1:D:233:LYS:HA	1:D:236:HIS:HE1	1.60	0.65
1:A:172:CYS:SG	1:A:173:VAL:N	2.71	0.65
1:C:279:TYR:CD2	1:C:354:VAL:HG13	2.32	0.65
1:A:433:GLY:H	1:A:449:LYS:HD3	1.62	0.64
1:A:116:SER:HB3	1:A:119:PHE:HB2	1.79	0.64
1:A:149:ILE:HD13	1:A:171:LEU:HB2	1.78	0.64
1:A:232:VAL:HG13	1:A:233:LYS:N	2.12	0.64
1:B:133:TRP:CZ3	1:B:153:PRO:HG3	2.32	0.64
1:B:220:TRP:HB3	1:B:413:PHE:HB3	1.80	0.64
1:D:232:VAL:HG22	1:D:233:LYS:N	2.12	0.64
1:A:133:TRP:CZ3	1:A:153:PRO:HG3	2.29	0.64
1:C:227:ARG:HB2	1:C:247:MET:HE3	1.79	0.64
1:A:192:ARG:O	1:A:196:LEU:HD13	1.97	0.64
1:A:174:HIS:HB3	1:A:177:LEU:CD1	2.28	0.64
1:C:183:ALA:HA	1:C:186:LEU:HB3	1.80	0.64
1:C:232:VAL:HG22	1:C:233:LYS:N	2.13	0.64
1:A:202:ALA:HB3	1:A:425:TYR:HB2	1.79	0.64
1:A:433:GLY:N	1:A:449:LYS:HD3	2.13	0.64
1:C:185:VAL:HG13	1:C:188:ARG:HE	1.62	0.64
1:D:149:ILE:HD12	1:D:169:ASN:O	1.97	0.64
1:D:202:ALA:HB3	1:D:425:TYR:HB2	1.79	0.64
1:A:412:LYS:H	1:A:412:LYS:CD	2.05	0.64
1:B:99:LEU:HD12	1:B:103:TYR:HB2	1.80	0.64
1:B:232:VAL:HG22	1:B:233:LYS:N	2.13	0.64
1:D:268:ASP:O	1:D:272:VAL:HG23	1.98	0.64
1:A:94:GLU:O	1:A:97:THR:HB	1.97	0.64
1:C:263:PRO:HG3	1:C:314:PHE:CE2	2.32	0.64
1:D:158:ILE:HG23	1:D:285:LEU:HD13	1.80	0.64
1:B:402:MET:CA	1:B:403:GLU:N	2.61	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:MET:SD	1:A:272:VAL:HG21	2.39	0.63
1:B:126:PRO:HB3	1:B:297:TRP:CZ2	2.33	0.63
1:B:355:HIS:CG	1:B:377:LEU:HB3	2.33	0.63
1:B:455:GLN:N	1:B:455:GLN:HE21	1.97	0.63
1:C:355:HIS:CG	1:C:377:LEU:HB3	2.34	0.63
1:C:225:ASN:OD1	1:C:228:LYS:HB2	1.98	0.63
1:D:135:CYS:HB2	1:D:149:ILE:HG23	1.80	0.63
1:A:266:THR:O	1:A:269:ILE:HG13	1.99	0.63
1:D:99:LEU:HD12	1:D:103:TYR:HB2	1.80	0.63
1:A:156:ILE:CG2	1:A:203:VAL:HG21	2.22	0.63
1:A:331:THR:HG1	1:A:393:PHE:HZ	1.47	0.63
1:C:116:SER:HB3	1:C:119:PHE:HB2	1.81	0.63
1:D:315:VAL:HG22	1:D:324:THR:HG1	1.62	0.63
1:D:152:ILE:HG13	1:D:167:GLU:HB2	1.80	0.63
1:D:183:ALA:O	1:D:187:ILE:HG13	1.99	0.63
1:B:158:ILE:HD13	1:B:159:TYR:H	1.63	0.63
1:B:264:MET:SD	1:B:272:VAL:HG21	2.39	0.63
1:C:269:ILE:HD13	1:C:295:GLU:CG	2.29	0.63
1:A:301:GLN:HB3	1:A:310:ILE:HD12	1.80	0.63
1:B:172:CYS:SG	1:B:173:VAL:N	2.72	0.63
1:C:102:ASN:O	1:C:104:VAL:N	2.32	0.63
1:A:355:HIS:NE2	1:A:377:LEU:HD22	2.14	0.62
1:B:279:TYR:CD2	1:B:354:VAL:HG13	2.34	0.62
1:B:102:ASN:O	1:B:104:VAL:N	2.32	0.62
1:B:301:GLN:HB3	1:B:310:ILE:HD12	1.81	0.62
1:D:381:MET:HG3	1:D:407:PHE:CE2	2.34	0.62
1:C:237:LEU:HD22	1:C:241:MET:O	1.98	0.62
1:D:263:PRO:HG3	1:D:314:PHE:CE2	2.34	0.62
1:A:154:ALA:HB2	1:A:167:GLU:HG3	1.80	0.62
1:B:123:ALA:HA	1:B:297:TRP:CZ3	2.33	0.62
1:B:283:PHE:HE2	1:B:402:MET:CB	2.13	0.62
1:C:381:MET:HG3	1:C:407:PHE:CE2	2.35	0.62
1:A:102:ASN:HB3	1:A:172:CYS:SG	2.39	0.62
1:D:242:THR:C	1:D:244:GLN:H	2.02	0.62
1:A:280:LEU:HG	1:A:286:THR:HB	1.82	0.62
1:A:377:LEU:HD23	1:A:377:LEU:H	1.64	0.62
1:C:283:PHE:HB2	1:C:286:THR:HG23	1.81	0.62
1:D:311:ILE:HG22	1:D:330:TYR:CB	2.29	0.62
1:D:383:ASP:O	1:D:387:LEU:HD23	2.00	0.62
1:C:232:VAL:HG13	1:C:233:LYS:N	2.14	0.62
1:B:110:MET:CB	1:B:337:MET:HG3	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:VAL:HG13	1:B:233:LYS:N	2.15	0.62
1:C:233:LYS:HA	1:C:236:HIS:HE1	1.64	0.62
1:D:264:MET:SD	1:D:272:VAL:HG21	2.40	0.62
1:A:104:VAL:HG12	1:A:106:ASP:H	1.65	0.61
1:B:123:ALA:HA	1:B:297:TRP:HZ3	1.65	0.61
1:C:314:PHE:HB2	1:C:327:LEU:HD11	1.81	0.61
1:C:355:HIS:CE1	1:C:377:LEU:HD22	2.35	0.61
1:D:218:ARG:HG2	1:D:419:ASN:CB	2.29	0.61
1:A:158:ILE:HD12	1:A:158:ILE:H	1.66	0.61
1:A:355:HIS:CG	1:A:377:LEU:HB3	2.35	0.61
1:C:228:LYS:HE3	1:C:343:LYS:HD3	1.80	0.61
1:C:325:ASP:OD1	1:C:356:THR:HG23	2.00	0.61
1:B:455:GLN:N	1:B:455:GLN:NE2	2.47	0.61
1:D:355:HIS:NE2	1:D:377:LEU:HD22	2.15	0.61
1:D:222:ARG:HD3	1:D:222:ARG:C	2.21	0.61
1:A:183:ALA:O	1:A:187:ILE:HG13	2.00	0.61
1:D:85:ASP:HA	1:D:91:VAL:HG11	1.81	0.61
1:A:242:THR:C	1:A:244:GLN:H	2.03	0.61
1:B:315:VAL:HG22	1:B:324:THR:HG1	1.64	0.61
1:B:314:PHE:O	1:B:327:LEU:HD13	2.00	0.61
1:C:154:ALA:HB2	1:C:167:GLU:HG3	1.81	0.61
1:D:232:VAL:HG13	1:D:233:LYS:N	2.16	0.61
1:C:152:ILE:HG13	1:C:167:GLU:HB2	1.83	0.61
1:D:311:ILE:HG22	1:D:330:TYR:HB3	1.83	0.61
1:A:292:GLU:O	1:A:295:GLU:HB3	2.00	0.61
1:B:154:ALA:HB2	1:B:167:GLU:HG3	1.81	0.61
1:D:116:SER:HB3	1:D:119:PHE:HB2	1.83	0.61
1:B:222:ARG:HD3	1:B:222:ARG:O	2.00	0.60
1:B:343:LYS:N	1:B:343:LYS:HD3	2.13	0.60
1:C:242:THR:C	1:C:244:GLN:H	2.04	0.60
1:C:158:ILE:H	1:C:158:ILE:HD12	1.66	0.60
1:C:287:PRO:HD3	1:C:452:ILE:HG12	1.83	0.60
1:C:220:TRP:HB3	1:C:413:PHE:HB3	1.83	0.60
1:C:268:ASP:O	1:C:272:VAL:HG23	2.01	0.60
1:A:174:HIS:HB3	1:A:177:LEU:HD12	1.84	0.60
1:B:135:CYS:HB2	1:B:149:ILE:CG2	2.31	0.60
1:B:313:THR:HA	1:B:327:LEU:O	2.01	0.60
1:C:311:ILE:HG22	1:C:330:TYR:HB3	1.82	0.60
1:D:291:GLN:O	1:D:295:GLU:HB2	2.01	0.60
1:A:355:HIS:CE1	1:A:377:LEU:HD22	2.36	0.60
1:A:92:LEU:O	1:A:95:LEU:HB3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:MET:SD	1:C:272:VAL:HG21	2.41	0.60
1:D:126:PRO:HB3	1:D:297:TRP:HZ2	1.65	0.60
1:A:455:GLN:HE21	1:A:455:GLN:N	1.99	0.60
1:B:283:PHE:HB3	1:B:449:LYS:O	2.01	0.60
1:D:128:GLY:O	1:D:153:PRO:HG2	2.02	0.60
1:A:146:VAL:HB	1:A:177:LEU:HD11	1.83	0.60
1:A:311:ILE:HG22	1:A:330:TYR:HB3	1.83	0.60
1:D:158:ILE:HA	1:D:284:HIS:O	2.02	0.60
1:D:158:ILE:HD12	1:D:158:ILE:H	1.67	0.60
1:B:242:THR:C	1:B:244:GLN:H	2.04	0.60
1:C:99:LEU:HD12	1:C:103:TYR:HB2	1.83	0.60
1:C:126:PRO:HG3	1:C:152:ILE:HB	1.84	0.60
1:C:323:VAL:HG23	4:C:993:HOH:O	2.02	0.60
1:D:181:ARG:O	1:D:184:PRO:HD2	2.02	0.60
1:A:222:ARG:HD3	1:A:222:ARG:C	2.22	0.60
1:A:123:ALA:HA	1:A:297:TRP:HZ3	1.66	0.60
1:D:315:VAL:HA	1:D:326:PHE:HB3	1.84	0.60
1:B:218:ARG:HG2	1:B:419:ASN:CB	2.32	0.59
1:D:197:GLU:O	1:D:197:GLU:HG2	2.01	0.59
1:B:266:THR:O	1:B:269:ILE:HG13	2.01	0.59
1:B:336:ILE:HG12	1:B:337:MET:H	1.67	0.59
1:C:301:GLN:HB3	1:C:310:ILE:HD12	1.84	0.59
1:C:313:THR:HA	1:C:327:LEU:O	2.03	0.59
1:C:402:MET:HA	1:C:448:GLU:HA	1.83	0.59
1:A:380:LEU:HD23	1:A:380:LEU:O	2.02	0.59
1:B:167:GLU:HA	1:B:203:VAL:O	2.02	0.59
1:B:207:GLY:O	1:B:208:VAL:HG13	2.02	0.59
1:C:315:VAL:HA	1:C:326:PHE:HB3	1.85	0.59
1:C:390:MET:SD	1:C:391:LYS:HG3	2.42	0.59
1:A:104:VAL:HG22	1:A:112:ARG:CB	2.32	0.59
1:A:126:PRO:HB3	1:A:297:TRP:HZ2	1.67	0.59
1:A:402:MET:CA	1:A:403:GLU:N	2.66	0.59
1:B:433:GLY:N	1:B:449:LYS:HD3	2.17	0.59
1:B:315:VAL:HA	1:B:326:PHE:HB3	1.85	0.59
1:C:409:GLU:C	1:C:411:LEU:H	2.05	0.59
1:B:81:TRP:CE2	1:B:140:VAL:HG22	2.38	0.59
1:C:355:HIS:CE1	1:C:377:LEU:HD13	2.37	0.59
1:A:409:GLU:C	1:A:411:LEU:H	2.06	0.59
1:C:203:VAL:HG13	4:C:997:HOH:O	2.01	0.59
1:C:385:LEU:HD11	1:C:411:LEU:HD21	1.84	0.59
1:C:433:GLY:N	1:C:449:LYS:HD3	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:TRP:CE2	1:A:311:ILE:HG21	2.38	0.58
1:A:169:ASN:HB2	4:A:907:HOH:O	2.01	0.58
1:A:269:ILE:HD13	1:A:295:GLU:CG	2.33	0.58
1:B:192:ARG:O	1:B:196:LEU:HD13	2.03	0.58
1:D:387:LEU:HA	1:D:390:MET:HG3	1.86	0.58
1:D:348:ALA:HB2	1:D:393:PHE:CD1	2.38	0.58
1:D:455:GLN:NE2	1:D:455:GLN:N	2.51	0.58
1:D:237:LEU:HD22	1:D:241:MET:O	2.03	0.58
1:A:218:ARG:HG2	1:A:419:ASN:CB	2.33	0.58
1:B:343:LYS:HG2	1:B:344:SER:H	1.68	0.58
1:C:315:VAL:HG22	1:C:324:THR:HG1	1.67	0.58
1:C:135:CYS:HB2	1:C:149:ILE:CG2	2.33	0.58
1:C:190:ILE:O	1:C:194:VAL:HG23	2.02	0.58
1:C:222:ARG:C	1:C:222:ARG:HD3	2.23	0.58
1:A:404:ASN:HA	1:A:407:PHE:HE2	1.66	0.58
1:D:324:THR:OG1	1:D:325:ASP:N	2.36	0.58
1:A:291:GLN:O	1:A:295:GLU:HB2	2.03	0.58
1:B:327:LEU:H	1:B:327:LEU:HD13	1.69	0.58
1:C:102:ASN:HB3	1:C:172:CYS:SG	2.42	0.58
1:B:197:GLU:HG2	1:B:197:GLU:O	2.04	0.58
1:D:377:LEU:HD23	1:D:377:LEU:H	1.69	0.58
1:A:280:LEU:HD21	1:A:287:PRO:HD2	1.86	0.58
1:B:311:ILE:HG22	1:B:330:TYR:CB	2.33	0.58
1:D:181:ARG:HH11	1:D:185:VAL:CG2	2.17	0.58
1:D:301:GLN:CB	1:D:310:ILE:HD12	2.33	0.58
1:B:102:ASN:ND2	1:B:174:HIS:HA	2.17	0.58
1:C:133:TRP:HZ3	1:C:153:PRO:HG3	1.67	0.58
1:C:122:TRP:CE2	1:C:311:ILE:HD13	2.38	0.58
1:A:99:LEU:N	1:A:99:LEU:HD22	2.19	0.57
1:B:158:ILE:CD1	1:B:159:TYR:H	2.17	0.57
1:C:380:LEU:HD23	1:C:380:LEU:O	2.04	0.57
1:B:222:ARG:C	1:B:222:ARG:HD3	2.25	0.57
1:C:138:ARG:H	1:C:147:GLY:N	2.01	0.57
1:B:302:GLU:CB	1:B:303:ASN:N	2.67	0.57
1:B:224:LEU:HD22	1:B:389:LYS:HB2	1.86	0.57
1:C:264:MET:HG3	1:C:268:ASP:HB2	1.87	0.57
1:C:341:THR:O	1:C:342:HIS:HB2	2.03	0.57
1:D:126:PRO:HG3	1:D:152:ILE:HB	1.85	0.57
1:D:239:ARG:N	1:D:239:ARG:HE	2.02	0.57
1:A:207:GLY:O	1:A:208:VAL:HG13	2.04	0.57
1:A:122:TRP:CE2	1:A:311:ILE:HD13	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:MET:HG3	1:B:407:PHE:CE2	2.39	0.57
1:C:149:ILE:HD11	1:C:168:ILE:HG22	1.86	0.57
1:D:302:GLU:O	1:D:303:ASN:CA	2.37	0.57
1:A:197:GLU:O	1:A:197:GLU:HG2	2.04	0.57
1:A:301:GLN:CB	1:A:310:ILE:HD12	2.34	0.57
1:A:315:VAL:HA	1:A:326:PHE:HB3	1.86	0.57
1:B:98:LEU:O	1:B:102:ASN:HB2	2.04	0.57
1:C:86:LEU:HA	1:C:92:LEU:HD23	1.87	0.57
1:D:409:GLU:C	1:D:411:LEU:H	2.07	0.57
1:C:194:VAL:CG1	1:C:199:ILE:HB	2.34	0.57
1:C:192:ARG:O	1:C:196:LEU:HD13	2.05	0.57
1:A:104:VAL:HG12	1:A:105:GLU:N	2.20	0.57
1:A:157:HIS:O	1:A:285:LEU:HA	2.04	0.57
1:A:224:LEU:HB3	1:A:389:LYS:HD3	1.86	0.57
1:A:313:THR:HA	1:A:327:LEU:O	2.04	0.57
1:A:402:MET:O	1:A:403:GLU:HA	2.05	0.57
1:D:148:PHE:CG	1:D:149:ILE:N	2.72	0.57
1:D:390:MET:SD	1:D:391:LYS:HG3	2.44	0.57
1:A:411:LEU:HD12	1:A:412:LYS:HD2	1.87	0.57
1:D:192:ARG:O	1:D:196:LEU:HD13	2.05	0.57
1:A:455:GLN:NE2	1:A:455:GLN:N	2.52	0.57
1:A:220:TRP:HB3	1:A:413:PHE:HB3	1.87	0.56
1:B:122:TRP:CE2	1:B:311:ILE:HD13	2.40	0.56
1:C:272:VAL:HG13	1:C:326:PHE:CZ	2.40	0.56
1:A:314:PHE:O	1:A:327:LEU:HD13	2.06	0.56
1:A:336:ILE:CG2	1:A:344:SER:HA	2.35	0.56
1:B:433:GLY:H	1:B:449:LYS:HD3	1.71	0.56
1:B:92:LEU:O	1:B:95:LEU:HB3	2.05	0.56
1:D:185:VAL:HA	1:D:188:ARG:HG2	1.87	0.56
1:D:313:THR:HA	1:D:327:LEU:O	2.05	0.56
1:B:377:LEU:H	1:B:377:LEU:HD23	1.71	0.56
1:C:148:PHE:CG	1:C:149:ILE:N	2.74	0.56
1:C:280:LEU:HG	1:C:286:THR:HB	1.87	0.56
1:D:280:LEU:HD21	1:D:287:PRO:HD2	1.86	0.56
1:D:225:ASN:OD1	1:D:228:LYS:HB2	2.05	0.56
1:A:355:HIS:CE1	1:A:377:LEU:HD13	2.41	0.56
1:A:167:GLU:HB3	1:A:454:LEU:HD11	1.88	0.56
1:B:409:GLU:C	1:B:411:LEU:H	2.07	0.56
1:C:383:ASP:O	1:C:387:LEU:HD23	2.04	0.56
1:B:157:HIS:O	1:B:285:LEU:HA	2.05	0.56
1:B:280:LEU:CD2	1:B:286:THR:HB	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:VAL:HA	1:C:188:ARG:HG2	1.88	0.56
1:C:227:ARG:HB2	1:C:247:MET:CE	2.34	0.56
1:C:126:PRO:HB3	1:C:297:TRP:CZ2	2.41	0.56
1:D:233:LYS:HA	1:D:236:HIS:CE1	2.39	0.56
1:A:138:ARG:HA	1:A:144:LYS:O	2.05	0.56
1:B:194:VAL:CG1	1:B:199:ILE:HB	2.36	0.56
1:B:239:ARG:CA	1:B:239:ARG:HE	2.19	0.56
1:C:377:LEU:H	1:C:377:LEU:HD23	1.71	0.56
1:D:355:HIS:CE1	1:D:377:LEU:HD22	2.41	0.56
1:D:283:PHE:HB3	1:D:449:LYS:O	2.05	0.56
1:A:158:ILE:HD13	1:A:159:TYR:H	1.71	0.56
1:C:348:ALA:HB2	1:C:393:PHE:CD1	2.41	0.56
1:C:455:GLN:N	1:C:455:GLN:NE2	2.53	0.56
1:D:269:ILE:CD1	1:D:295:GLU:HG3	2.33	0.56
1:A:158:ILE:CD1	1:A:159:TYR:H	2.18	0.56
1:A:102:ASN:ND2	1:A:174:HIS:HA	2.20	0.56
1:A:232:VAL:HG13	1:A:233:LYS:H	1.69	0.56
1:A:381:MET:HG3	1:A:407:PHE:CE2	2.41	0.56
1:B:158:ILE:H	1:B:158:ILE:CD1	2.14	0.56
1:B:291:GLN:O	1:B:295:GLU:HB2	2.06	0.56
1:B:99:LEU:N	1:B:99:LEU:HD22	2.21	0.56
1:B:185:VAL:HA	1:B:188:ARG:HG2	1.88	0.56
1:B:190:ILE:O	1:B:194:VAL:HG23	2.06	0.56
1:B:301:GLN:CB	1:B:310:ILE:HD12	2.36	0.56
1:C:123:ALA:O	1:C:152:ILE:HG21	2.06	0.56
1:D:258:THR:HG23	1:D:261:LEU:HB2	1.88	0.56
1:D:264:MET:HG3	1:D:268:ASP:HB2	1.88	0.56
1:B:287:PRO:HG3	1:B:352:TYR:OH	2.05	0.56
1:C:197:GLU:O	1:C:197:GLU:HG2	2.06	0.56
1:D:343:LYS:HD3	1:D:344:SER:HB3	1.88	0.56
1:B:145:LEU:O	1:B:145:LEU:HG	2.06	0.55
1:B:311:ILE:HG22	1:B:330:TYR:HB3	1.88	0.55
1:B:383:ASP:O	1:B:387:LEU:HD23	2.07	0.55
1:C:301:GLN:CB	1:C:310:ILE:HD12	2.36	0.55
1:A:139:VAL:O	1:A:141:SER:N	2.39	0.55
1:D:115:TYR:CE2	1:D:170:PHE:HE2	2.22	0.55
1:D:280:LEU:HG	1:D:286:THR:HB	1.88	0.55
1:A:287:PRO:HD3	1:A:452:ILE:HG12	1.88	0.55
1:B:148:PHE:CG	1:B:149:ILE:N	2.74	0.55
1:B:336:ILE:CG1	1:B:337:MET:N	2.69	0.55
1:B:89:ARG:CZ	1:B:89:ARG:HA	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD21	1:C:287:PRO:HD2	1.88	0.55
1:C:314:PHE:O	1:C:327:LEU:HD13	2.05	0.55
1:D:181:ARG:NE	1:D:184:PRO:HB2	2.22	0.55
1:A:327:LEU:HD13	1:A:327:LEU:H	1.72	0.55
1:B:280:LEU:HD21	1:B:286:THR:HB	1.88	0.55
1:A:233:LYS:HA	1:A:236:HIS:CE1	2.40	0.55
1:A:159:TYR:C	1:A:161:THR:H	2.09	0.55
1:A:302:GLU:CA	1:A:302:GLU:OE1	2.54	0.55
1:B:237:LEU:HD22	1:B:241:MET:O	2.07	0.55
1:C:324:THR:HG1	1:C:325:ASP:N	2.05	0.55
1:D:227:ARG:HB2	1:D:247:MET:HE3	1.87	0.55
1:B:94:GLU:O	1:B:97:THR:HB	2.07	0.55
1:D:180:LYS:O	1:D:181:ARG:HB2	2.05	0.55
1:A:336:ILE:HG23	1:A:344:SER:HA	1.87	0.55
1:A:411:LEU:O	1:A:413:PHE:N	2.40	0.55
1:D:433:GLY:N	1:D:449:LYS:HD3	2.21	0.55
1:B:173:VAL:HG11	1:B:179:SER:OG	2.07	0.55
1:C:158:ILE:HA	1:C:284:HIS:O	2.06	0.55
1:A:171:LEU:CD1	1:A:186:LEU:HD12	2.37	0.55
1:A:91:VAL:O	1:A:94:GLU:HG2	2.07	0.55
1:C:291:GLN:O	1:C:295:GLU:HB2	2.06	0.55
1:A:123:ALA:O	1:A:152:ILE:HG21	2.07	0.54
1:A:315:VAL:HG22	1:A:324:THR:HG1	1.72	0.54
1:D:280:LEU:HD12	1:D:283:PHE:CD1	2.41	0.54
1:A:375:THR:HG23	4:A:908:HOH:O	2.06	0.54
1:B:218:ARG:HB3	1:B:218:ARG:NH1	2.23	0.54
1:B:228:LYS:HZ2	1:B:343:LYS:HE3	1.72	0.54
1:C:179:SER:O	1:C:180:LYS:C	2.44	0.54
1:C:183:ALA:O	1:C:187:ILE:HG13	2.08	0.54
1:C:327:LEU:HD13	1:C:327:LEU:H	1.72	0.54
1:B:227:ARG:HB2	1:B:247:MET:HE3	1.89	0.54
1:C:98:LEU:O	1:C:102:ASN:HB2	2.08	0.54
1:D:292:GLU:HA	1:D:295:GLU:OE2	2.08	0.54
1:B:355:HIS:NE2	1:B:377:LEU:HD22	2.23	0.54
1:B:91:VAL:O	1:B:94:GLU:HG2	2.08	0.54
1:C:104:VAL:HG22	1:C:112:ARG:CA	2.36	0.54
1:D:194:VAL:CG1	1:D:199:ILE:HB	2.37	0.54
1:D:411:LEU:O	1:D:413:PHE:N	2.39	0.54
1:B:159:TYR:C	1:B:161:THR:H	2.10	0.54
1:B:233:LYS:HA	1:B:236:HIS:CE1	2.42	0.54
1:A:218:ARG:NH1	1:A:218:ARG:HB3	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ARG:NH1	1:A:412:LYS:HD3	2.23	0.54
1:B:258:THR:HG23	1:B:261:LEU:HB2	1.90	0.54
1:C:159:TYR:C	1:C:161:THR:H	2.10	0.54
1:C:239:ARG:HE	1:C:239:ARG:CA	2.21	0.54
1:D:224:LEU:HB3	1:D:389:LYS:HD3	1.90	0.54
1:A:270:PRO:O	1:A:274:GLN:HG2	2.08	0.54
1:A:327:LEU:O	1:A:327:LEU:HD22	2.08	0.54
1:A:343:LYS:H	1:A:343:LYS:CD	2.21	0.54
1:B:183:ALA:HB3	1:B:184:PRO:HD3	1.90	0.54
1:B:280:LEU:HG	1:B:286:THR:HB	1.88	0.54
1:C:402:MET:O	1:C:403:GLU:HA	2.07	0.54
1:D:239:ARG:CA	1:D:239:ARG:HE	2.20	0.54
1:D:279:TYR:CD2	1:D:354:VAL:HG13	2.42	0.54
1:A:239:ARG:HE	1:A:239:ARG:HA	1.73	0.54
1:B:232:VAL:HG13	1:B:233:LYS:H	1.71	0.54
1:C:237:LEU:O	1:C:237:LEU:HD12	2.08	0.54
1:C:280:LEU:HD12	1:C:283:PHE:CD1	2.42	0.54
1:C:130:LEU:HB3	1:C:132:GLN:HE22	1.73	0.54
1:C:115:TYR:CE2	1:C:170:PHE:HE2	2.26	0.54
1:C:224:LEU:HD22	1:C:389:LYS:HB2	1.89	0.54
1:A:225:ASN:OD1	1:A:228:LYS:HB2	2.08	0.54
1:A:287:PRO:HG3	1:A:352:TYR:OH	2.08	0.54
1:C:174:HIS:ND1	1:C:175:LYS:N	2.56	0.54
1:C:400:ASP:O	1:C:401:LEU:HB2	2.08	0.54
1:D:122:TRP:HE1	1:D:311:ILE:HD13	1.72	0.54
1:A:89:ARG:CZ	1:A:89:ARG:HA	2.38	0.53
1:B:227:ARG:HB2	1:B:247:MET:CE	2.38	0.53
1:D:159:TYR:C	1:D:161:THR:H	2.09	0.53
1:A:194:VAL:CG1	1:A:199:ILE:HB	2.38	0.53
1:A:283:PHE:HB3	1:A:449:LYS:O	2.08	0.53
1:A:122:TRP:HE1	1:A:311:ILE:HD13	1.72	0.53
1:A:349:TYR:HD1	1:A:349:TYR:H	1.56	0.53
1:B:183:ALA:O	1:B:187:ILE:HG13	2.09	0.53
1:D:194:VAL:C	1:D:196:LEU:H	2.12	0.53
1:B:81:TRP:HZ2	1:B:140:VAL:HG13	1.74	0.53
1:C:156:ILE:CG2	1:C:203:VAL:HG21	2.30	0.53
1:A:139:VAL:HB	1:A:144:LYS:HD2	1.90	0.53
1:A:149:ILE:HD11	1:A:168:ILE:HG22	1.91	0.53
1:C:194:VAL:C	1:C:196:LEU:H	2.12	0.53
1:A:194:VAL:C	1:A:196:LEU:H	2.12	0.53
1:B:121:LEU:HD12	1:B:121:LEU:H	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TRP:CE2	1:B:311:ILE:HG21	2.43	0.53
1:C:386:VAL:O	1:C:390:MET:HB3	2.08	0.53
1:D:220:TRP:HB3	1:D:413:PHE:HB3	1.91	0.53
1:A:126:PRO:HG3	1:A:152:ILE:HB	1.91	0.53
1:C:218:ARG:NH1	1:C:218:ARG:HB3	2.24	0.53
1:C:455:GLN:N	1:C:455:GLN:HE21	2.07	0.53
1:A:102:ASN:HD21	1:A:174:HIS:CA	2.21	0.53
1:B:269:ILE:HD13	1:B:295:GLU:CG	2.36	0.53
1:B:270:PRO:O	1:B:274:GLN:HG2	2.09	0.53
1:C:232:VAL:HG13	1:C:233:LYS:H	1.72	0.53
1:B:169:ASN:HB2	4:B:906:HOH:O	2.09	0.53
1:B:239:ARG:HE	1:B:239:ARG:HA	1.72	0.53
1:D:102:ASN:O	1:D:104:VAL:N	2.42	0.53
1:B:183:ALA:O	1:B:187:ILE:N	2.42	0.53
1:C:327:LEU:HD22	1:C:327:LEU:C	2.29	0.53
1:A:239:ARG:HE	1:A:239:ARG:CA	2.22	0.53
1:A:283:PHE:HB2	1:A:286:THR:HG23	1.90	0.53
1:B:94:GLU:HB2	1:B:145:LEU:HD13	1.91	0.53
1:C:151:ALA:HA	1:C:168:ILE:HA	1.91	0.53
1:C:194:VAL:HG12	1:C:199:ILE:HB	1.90	0.53
1:C:283:PHE:HB3	1:C:449:LYS:O	2.09	0.53
1:C:327:LEU:HD22	1:C:327:LEU:O	2.09	0.53
1:C:381:MET:HG3	1:C:407:PHE:CZ	2.44	0.53
1:D:130:LEU:HB3	1:D:132:GLN:HE22	1.72	0.53
1:D:232:VAL:HG13	1:D:233:LYS:H	1.72	0.53
1:D:269:ILE:CB	1:D:270:PRO:HD3	2.34	0.53
1:D:287:PRO:HD3	1:D:452:ILE:HG12	1.90	0.53
1:D:400:ASP:O	1:D:401:LEU:HB2	2.09	0.53
1:B:181:ARG:HA	1:B:181:ARG:NE	2.24	0.52
1:C:104:VAL:HG22	1:C:112:ARG:CB	2.39	0.52
1:D:227:ARG:HB2	1:D:247:MET:CE	2.39	0.52
1:B:269:ILE:CB	1:B:270:PRO:HD3	2.33	0.52
1:D:86:LEU:HA	1:D:92:LEU:HD23	1.91	0.52
1:A:198:GLY:O	1:A:200:PHE:HD1	1.92	0.52
1:A:269:ILE:HB	1:A:270:PRO:CD	2.33	0.52
1:C:128:GLY:O	1:C:153:PRO:HG2	2.09	0.52
1:C:324:THR:OG1	1:C:325:ASP:N	2.42	0.52
1:A:148:PHE:CG	1:A:149:ILE:N	2.78	0.52
1:C:233:LYS:HA	1:C:236:HIS:CE1	2.43	0.52
1:D:124:LEU:HD21	1:D:170:PHE:CD1	2.44	0.52
1:A:194:VAL:HG12	1:A:199:ILE:HB	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:TYR:CG	1:A:354:VAL:HG13	2.44	0.52
1:B:194:VAL:C	1:B:196:LEU:H	2.13	0.52
1:C:182:VAL:CG2	1:C:183:ALA:N	2.72	0.52
1:C:220:TRP:CZ3	1:C:409:GLU:HG2	2.44	0.52
1:A:258:THR:HG23	1:A:261:LEU:HB2	1.90	0.52
1:A:280:LEU:HD12	1:A:283:PHE:CD1	2.45	0.52
1:B:349:TYR:HD1	1:B:349:TYR:H	1.56	0.52
1:B:355:HIS:CE1	1:B:377:LEU:HD13	2.45	0.52
1:C:239:ARG:HE	1:C:239:ARG:N	2.07	0.52
1:C:279:TYR:CG	1:C:354:VAL:HG13	2.45	0.52
1:D:340:PRO:O	1:D:341:THR:HB	2.09	0.52
1:D:404:ASN:HA	1:D:407:PHE:HE2	1.71	0.52
1:D:455:GLN:HE21	1:D:455:GLN:N	2.08	0.52
1:A:185:VAL:HA	1:A:188:ARG:HG2	1.92	0.52
1:A:387:LEU:HA	1:A:390:MET:HG3	1.91	0.52
1:D:221:HIS:ND1	1:D:397:ASN:ND2	2.58	0.52
1:A:279:TYR:CD1	1:A:354:VAL:HG22	2.44	0.52
1:B:102:ASN:HD21	1:B:174:HIS:CA	2.22	0.52
1:B:263:PRO:HG3	1:B:314:PHE:CE2	2.44	0.52
1:C:301:GLN:O	1:C:303:ASN:N	2.43	0.52
1:A:324:THR:OG1	1:A:325:ASP:N	2.42	0.52
1:B:324:THR:OG1	1:B:325:ASP:N	2.42	0.52
1:B:99:LEU:CD2	1:B:99:LEU:H	2.23	0.52
1:C:175:LYS:O	1:C:176:LYS:HB2	2.10	0.52
1:C:218:ARG:HG2	1:C:419:ASN:CB	2.40	0.52
1:C:266:THR:O	1:C:269:ILE:HG13	2.10	0.52
1:A:102:ASN:O	1:A:104:VAL:N	2.43	0.52
1:A:128:GLY:O	1:A:153:PRO:HG2	2.10	0.52
1:A:182:VAL:HG12	1:A:183:ALA:N	2.24	0.52
1:C:258:THR:HG23	1:C:261:LEU:HB2	1.91	0.52
1:C:97:THR:HG21	4:C:999:HOH:O	2.09	0.52
1:B:123:ALA:O	1:B:152:ILE:HG21	2.09	0.51
1:B:228:LYS:HE3	1:B:343:LYS:HE3	1.91	0.51
1:B:185:VAL:HG13	1:B:188:ARG:HE	1.74	0.51
1:B:411:LEU:O	1:B:413:PHE:N	2.42	0.51
1:B:287:PRO:HD3	1:B:452:ILE:HG12	1.92	0.51
1:D:108:ASP:N	1:D:111:PHE:HD2	2.08	0.51
1:D:325:ASP:OD1	1:D:356:THR:HG23	2.10	0.51
1:B:322:GLU:O	1:B:323:VAL:C	2.49	0.51
1:A:102:ASN:O	1:A:104:VAL:HG23	2.10	0.51
1:A:390:MET:SD	1:A:391:LYS:HG3	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LYS:CE	1:B:343:LYS:HE3	2.40	0.51
1:C:113:PHE:HB3	1:C:115:TYR:CE1	2.45	0.51
1:D:98:LEU:O	1:D:102:ASN:HB2	2.09	0.51
1:D:172:CYS:SG	1:D:173:VAL:N	2.83	0.51
1:D:183:ALA:O	1:D:187:ILE:N	2.43	0.51
1:D:355:HIS:HB3	1:D:380:LEU:HD13	1.92	0.51
1:A:221:HIS:CE1	1:A:234:PHE:HZ	2.29	0.51
1:C:158:ILE:CD1	1:C:159:TYR:H	2.23	0.51
1:C:85:ASP:N	1:C:91:VAL:HG11	2.25	0.51
1:D:433:GLY:H	1:D:449:LYS:HD3	1.76	0.51
1:A:225:ASN:N	1:A:226:PRO:HD3	2.26	0.51
1:C:99:LEU:HD22	1:C:99:LEU:N	2.22	0.51
1:C:264:MET:HG3	1:C:268:ASP:CB	2.41	0.51
1:D:218:ARG:HB3	1:D:218:ARG:NH1	2.26	0.51
1:D:225:ASN:N	1:D:226:PRO:HD3	2.25	0.51
1:B:336:ILE:HD12	1:B:343:LYS:O	2.11	0.51
1:C:407:PHE:HA	1:C:410:LYS:CG	2.41	0.51
1:D:237:LEU:O	1:D:237:LEU:HD12	2.10	0.51
1:A:185:VAL:HG13	1:A:188:ARG:HE	1.76	0.51
1:B:283:PHE:HB2	1:B:286:THR:HG23	1.91	0.51
1:B:449:LYS:HD2	1:B:449:LYS:N	2.26	0.51
1:C:138:ARG:N	1:C:147:GLY:N	2.59	0.51
1:A:98:LEU:O	1:A:102:ASN:HB2	2.11	0.50
1:B:172:CYS:O	1:B:173:VAL:HG13	2.10	0.50
1:C:293:GLU:C	1:C:295:GLU:H	2.13	0.50
1:C:122:TRP:CZ2	1:C:297:TRP:HE3	2.28	0.50
1:C:452:ILE:HG22	1:C:454:LEU:HB2	1.93	0.50
1:D:135:CYS:HB2	1:D:149:ILE:HG22	1.93	0.50
1:D:233:LYS:HB3	4:D:459:HOH:O	2.10	0.50
1:A:272:VAL:HG13	1:A:326:PHE:CZ	2.46	0.50
1:B:381:MET:HG3	1:B:407:PHE:CD2	2.46	0.50
1:C:224:LEU:HB3	1:C:389:LYS:HD3	1.92	0.50
1:D:190:ILE:O	1:D:194:VAL:HG23	2.11	0.50
1:A:139:VAL:HB	1:A:144:LYS:HB2	1.93	0.50
1:A:237:LEU:HD22	1:A:241:MET:O	2.10	0.50
1:B:228:LYS:HZ2	1:B:343:LYS:CE	2.24	0.50
1:B:258:THR:HG23	1:B:258:THR:O	2.12	0.50
1:C:381:MET:O	1:C:384:ALA:HB3	2.11	0.50
1:A:183:ALA:O	1:A:187:ILE:N	2.43	0.50
1:A:241:MET:HE1	1:A:246:THR:HA	1.93	0.50
1:A:99:LEU:CD2	1:A:99:LEU:H	2.23	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:HIS:CE1	1:B:377:LEU:HD22	2.47	0.50
1:C:266:THR:HA	1:C:299:TYR:HE2	1.77	0.50
1:C:349:TYR:H	1:C:349:TYR:HD1	1.59	0.50
1:C:433:GLY:H	1:C:449:LYS:HD3	1.75	0.50
1:C:94:GLU:HA	4:C:999:HOH:O	2.12	0.50
1:D:258:THR:HG22	1:D:383:ASP:OD1	2.11	0.50
1:D:293:GLU:C	1:D:295:GLU:H	2.14	0.50
1:D:110:MET:O	1:D:337:MET:HB2	2.12	0.50
1:A:221:HIS:O	1:A:412:LYS:O	2.30	0.50
1:A:316:VAL:HG12	1:A:316:VAL:O	2.11	0.50
1:B:120:LEU:HB3	1:B:124:LEU:HD12	1.93	0.50
1:B:171:LEU:CD1	1:B:186:LEU:HD12	2.42	0.50
1:B:194:VAL:HG12	1:B:199:ILE:HB	1.92	0.50
1:C:114:ASP:HB2	1:C:335:THR:OG1	2.12	0.50
1:C:157:HIS:O	1:C:285:LEU:HA	2.11	0.50
1:D:202:ALA:HB3	1:D:425:TYR:HB3	1.93	0.50
1:A:348:ALA:HB2	1:A:393:PHE:CD1	2.47	0.50
1:B:280:LEU:CG	1:B:286:THR:HB	2.42	0.50
1:D:157:HIS:O	1:D:285:LEU:HA	2.12	0.50
1:A:183:ALA:HA	1:A:186:LEU:CB	2.39	0.50
1:A:416:GLY:O	1:A:417:ASP:C	2.51	0.50
1:C:228:LYS:HZ2	1:C:343:LYS:HB2	1.76	0.50
1:D:221:HIS:CE1	1:D:234:PHE:HZ	2.30	0.50
1:B:202:ALA:HB3	1:B:425:TYR:HB3	1.94	0.50
1:C:225:ASN:N	1:C:226:PRO:HD3	2.27	0.50
1:D:122:TRP:CE2	1:D:311:ILE:HG21	2.47	0.50
1:D:270:PRO:HG3	1:D:291:GLN:CD	2.33	0.50
1:D:347:ALA:HB1	1:D:349:TYR:CE1	2.46	0.50
1:D:355:HIS:CE1	1:D:377:LEU:HD13	2.47	0.50
1:D:283:PHE:HE2	1:D:402:MET:CB	2.25	0.50
1:A:264:MET:HG3	1:A:268:ASP:HB2	1.94	0.50
1:A:322:GLU:O	1:A:323:VAL:C	2.50	0.50
1:B:142:SER:O	1:B:144:LYS:N	2.45	0.50
1:D:151:ALA:HA	1:D:168:ILE:HA	1.93	0.50
1:B:279:TYR:CG	1:B:354:VAL:HG13	2.46	0.49
1:C:106:ASP:C	1:C:111:PHE:HB2	2.32	0.49
1:C:347:ALA:HB1	1:C:349:TYR:CE1	2.47	0.49
1:A:183:ALA:N	1:A:184:PRO:CD	2.76	0.49
1:B:355:HIS:HB3	1:B:380:LEU:HD13	1.93	0.49
1:A:218:ARG:HB3	1:A:218:ARG:HH11	1.77	0.49
1:B:380:LEU:O	1:B:380:LEU:HD23	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:LEU:O	1:C:95:LEU:HB3	2.12	0.49
1:D:158:ILE:CD1	1:D:158:ILE:H	2.25	0.49
1:A:85:ASP:O	1:A:86:LEU:CB	2.60	0.49
1:B:158:ILE:HG21	1:B:424:LEU:HD11	1.95	0.49
1:B:225:ASN:OD1	1:B:228:LYS:HB2	2.12	0.49
1:A:167:GLU:HA	1:A:203:VAL:O	2.13	0.49
1:B:182:VAL:HG12	1:B:183:ALA:N	2.26	0.49
1:B:454:LEU:C	1:B:455:GLN:HE21	2.15	0.49
1:B:209:VAL:O	1:B:210:LEU:HD12	2.13	0.49
1:B:213:PRO:HA	1:B:423:TYR:CD2	2.48	0.49
1:B:85:ASP:O	1:B:86:LEU:CB	2.60	0.49
1:C:316:VAL:HG12	1:C:316:VAL:O	2.11	0.49
1:C:402:MET:CA	1:C:403:GLU:N	2.75	0.49
1:D:316:VAL:O	1:D:316:VAL:HG12	2.13	0.49
1:D:407:PHE:HA	1:D:410:LYS:CG	2.43	0.49
1:A:158:ILE:HG23	1:A:285:LEU:HD13	1.95	0.49
1:B:113:PHE:O	1:B:115:TYR:CD1	2.66	0.49
1:B:174:HIS:CG	1:B:175:LYS:N	2.80	0.49
1:C:107:ASP:C	1:C:109:ASN:H	2.16	0.49
1:C:166:VAL:HB	1:C:199:ILE:HG21	1.95	0.49
1:D:149:ILE:HD11	1:D:168:ILE:HG22	1.93	0.49
1:D:158:ILE:CD1	1:D:159:TYR:H	2.25	0.49
1:D:279:TYR:CG	1:D:354:VAL:HG13	2.47	0.49
1:A:280:LEU:CG	1:A:286:THR:HB	2.42	0.49
1:C:158:ILE:HD13	1:C:159:TYR:H	1.78	0.49
1:C:270:PRO:HG3	1:C:291:GLN:CD	2.33	0.49
1:C:397:ASN:N	1:C:397:ASN:HD22	2.09	0.49
1:C:92:LEU:O	1:C:92:LEU:HD13	2.12	0.49
1:D:181:ARG:HH11	1:D:185:VAL:HG22	1.76	0.49
1:D:355:HIS:HE1	1:D:403:GLU:HG3	1.78	0.49
1:B:87:GLY:HA3	1:B:125:ARG:NH2	2.28	0.49
1:B:209:VAL:HG12	1:B:210:LEU:N	2.28	0.49
1:B:237:LEU:O	1:B:237:LEU:HD12	2.12	0.49
1:B:293:GLU:C	1:B:295:GLU:H	2.16	0.49
1:B:301:GLN:O	1:B:303:ASN:N	2.46	0.49
1:C:269:ILE:HB	1:C:270:PRO:CD	2.36	0.49
1:D:266:THR:HA	1:D:299:TYR:HE2	1.78	0.49
1:D:327:LEU:HD13	1:D:327:LEU:H	1.78	0.49
1:D:381:MET:HG3	1:D:407:PHE:CZ	2.48	0.49
1:A:383:ASP:O	1:A:387:LEU:HD23	2.12	0.49
1:B:224:LEU:HB3	1:B:389:LYS:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:HG12	1:D:210:LEU:N	2.28	0.49
1:D:449:LYS:N	1:D:449:LYS:HD2	2.28	0.49
1:D:92:LEU:O	1:D:95:LEU:HB3	2.13	0.49
1:A:397:ASN:HD22	1:A:397:ASN:N	2.10	0.48
1:B:122:TRP:HE1	1:B:311:ILE:HD13	1.77	0.48
1:C:223:SER:OG	1:C:229:LEU:HD12	2.13	0.48
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.78	0.48
1:C:287:PRO:HD3	1:C:452:ILE:HA	1.95	0.48
1:B:145:LEU:N	1:B:145:LEU:HD23	2.28	0.48
1:B:198:GLY:O	1:B:200:PHE:HD1	1.97	0.48
1:B:343:LYS:H	1:B:343:LYS:CD	2.06	0.48
1:C:322:GLU:O	1:C:323:VAL:C	2.52	0.48
1:C:411:LEU:O	1:C:413:PHE:N	2.44	0.48
1:A:121:LEU:HD12	1:A:121:LEU:H	1.78	0.48
1:A:293:GLU:C	1:A:295:GLU:H	2.15	0.48
1:D:381:MET:HG3	1:D:407:PHE:CD2	2.48	0.48
1:A:327:LEU:HD22	1:A:327:LEU:C	2.32	0.48
1:A:120:LEU:HB3	1:A:124:LEU:HD12	1.96	0.48
1:A:158:ILE:HA	1:A:284:HIS:O	2.14	0.48
1:A:124:LEU:HD21	1:A:170:PHE:CD1	2.48	0.48
1:A:402:MET:HA	1:A:448:GLU:HA	1.94	0.48
1:C:287:PRO:HG3	1:C:352:TYR:OH	2.14	0.48
1:D:280:LEU:HD12	1:D:283:PHE:CE1	2.48	0.48
1:D:97:THR:HG21	4:D:469:HOH:O	2.12	0.48
1:A:325:ASP:OD1	1:A:356:THR:HG23	2.13	0.48
1:B:269:ILE:HB	1:B:270:PRO:CD	2.34	0.48
1:C:404:ASN:HA	1:C:407:PHE:HE2	1.77	0.48
1:C:178:ARG:O	1:C:181:ARG:CZ	2.62	0.48
1:D:179:SER:OG	1:D:182:VAL:HB	2.13	0.48
1:D:302:GLU:O	1:D:303:ASN:HA	2.12	0.48
1:D:322:GLU:O	1:D:323:VAL:C	2.51	0.48
1:D:92:LEU:HD13	1:D:92:LEU:O	2.14	0.48
1:A:158:ILE:CD1	1:A:158:ILE:H	2.24	0.48
1:A:223:SER:HB2	1:A:226:PRO:HG3	1.96	0.48
1:B:221:HIS:CE1	1:B:234:PHE:HZ	2.32	0.48
1:B:225:ASN:N	1:B:226:PRO:HD3	2.27	0.48
1:B:327:LEU:C	1:B:327:LEU:HD22	2.34	0.48
1:B:88:ASP:OD2	1:B:89:ARG:N	2.47	0.48
1:B:95:LEU:O	1:B:98:LEU:HB3	2.13	0.48
1:C:449:LYS:N	1:C:449:LYS:HD2	2.29	0.48
1:B:247:MET:O	1:B:248:LYS:C	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ILE:HG23	1:C:285:LEU:HD13	1.96	0.48
1:C:221:HIS:O	1:C:412:LYS:O	2.32	0.48
1:D:123:ALA:O	1:D:152:ILE:HG21	2.14	0.48
1:D:137:VAL:CG1	1:D:137:VAL:O	2.56	0.48
1:D:237:LEU:O	1:D:238:SER:O	2.31	0.48
1:A:209:VAL:HG12	1:A:210:LEU:N	2.28	0.48
1:B:327:LEU:O	1:B:327:LEU:HD22	2.14	0.48
1:B:355:HIS:HE1	1:B:403:GLU:HG3	1.79	0.48
1:D:338:ASN:N	1:D:338:ASN:ND2	2.42	0.48
1:A:174:HIS:CG	1:A:175:LYS:N	2.82	0.47
1:A:397:ASN:N	1:A:397:ASN:ND2	2.62	0.47
1:A:454:LEU:C	1:A:455:GLN:HE21	2.17	0.47
1:B:404:ASN:HA	1:B:407:PHE:HE2	1.76	0.47
1:C:174:HIS:O	1:C:175:LYS:HB2	2.14	0.47
1:B:126:PRO:HB3	1:B:297:TRP:HZ2	1.76	0.47
1:C:302:GLU:O	1:C:303:ASN:CA	2.49	0.47
1:C:221:HIS:ND1	1:C:397:ASN:ND2	2.62	0.47
1:D:114:ASP:HB2	1:D:335:THR:OG1	2.13	0.47
1:D:301:GLN:O	1:D:303:ASN:N	2.47	0.47
1:A:158:ILE:HG21	1:A:424:LEU:HD11	1.97	0.47
1:B:115:TYR:CE2	1:B:170:PHE:HE2	2.32	0.47
1:B:222:ARG:NH1	1:B:412:LYS:HD3	2.29	0.47
1:A:237:LEU:O	1:A:237:LEU:HD12	2.15	0.47
1:B:347:ALA:HB1	1:B:349:TYR:CE1	2.49	0.47
1:B:87:GLY:HA3	4:B:905:HOH:O	2.13	0.47
1:C:99:LEU:CD2	1:C:99:LEU:H	2.23	0.47
1:A:324:THR:HG1	1:A:325:ASP:N	2.12	0.47
1:B:266:THR:HA	1:B:299:TYR:HE2	1.79	0.47
1:B:348:ALA:HB2	1:B:393:PHE:CD1	2.50	0.47
1:B:411:LEU:HD12	1:B:412:LYS:HD2	1.96	0.47
1:C:218:ARG:HH11	1:C:218:ARG:HB3	1.79	0.47
1:D:173:VAL:HG23	1:D:174:HIS:N	2.24	0.47
1:D:349:TYR:H	1:D:349:TYR:HD1	1.61	0.47
1:D:352:TYR:CE2	1:D:453:VAL:HB	2.49	0.47
1:A:347:ALA:HB1	1:A:349:TYR:CE1	2.49	0.47
1:B:149:ILE:HD11	1:B:168:ILE:HG22	1.96	0.47
1:B:316:VAL:HG12	1:B:316:VAL:O	2.14	0.47
1:C:183:ALA:HA	1:C:186:LEU:CB	2.45	0.47
1:C:385:LEU:CD1	1:C:411:LEU:HD21	2.45	0.47
1:B:166:VAL:HB	1:B:199:ILE:HG21	1.96	0.47
1:C:182:VAL:HG23	1:C:183:ALA:N	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:HE	1:C:239:ARG:HA	1.80	0.47
1:D:287:PRO:HG3	1:D:352:TYR:OH	2.15	0.47
1:A:229:LEU:CB	1:A:235:SER:HB3	2.45	0.47
1:A:227:ARG:HB2	1:A:247:MET:HE3	1.97	0.47
1:A:122:TRP:HE1	1:A:297:TRP:HA	1.79	0.47
1:C:111:PHE:HZ	1:C:234:PHE:HD1	1.63	0.47
1:C:396:PHE:C	1:C:397:ASN:HD22	2.18	0.47
1:C:397:ASN:ND2	1:C:397:ASN:N	2.63	0.47
1:D:347:ALA:HB1	1:D:349:TYR:HE1	1.79	0.47
1:B:355:HIS:O	1:B:356:THR:O	2.33	0.47
1:B:221:HIS:O	1:B:412:LYS:O	2.33	0.47
1:C:355:HIS:HE1	1:C:403:GLU:HG3	1.78	0.47
1:D:122:TRP:CZ2	1:D:297:TRP:HE3	2.33	0.47
1:A:209:VAL:O	1:A:210:LEU:HD12	2.15	0.47
1:B:280:LEU:HD12	1:B:283:PHE:CD1	2.50	0.47
1:C:123:ALA:HA	1:C:297:TRP:CZ3	2.50	0.47
1:C:91:VAL:O	1:C:94:GLU:HG2	2.14	0.47
1:B:181:ARG:CZ	1:B:181:ARG:HA	2.45	0.46
1:B:264:MET:HG3	1:B:268:ASP:HB2	1.97	0.46
1:B:122:TRP:CZ2	1:B:297:TRP:HE3	2.32	0.46
1:C:279:TYR:CD1	1:C:354:VAL:HG22	2.49	0.46
1:A:213:PRO:HA	1:A:423:TYR:CD2	2.51	0.46
1:A:280:LEU:HG	1:A:286:THR:CB	2.45	0.46
1:B:325:ASP:OD1	1:B:356:THR:HG23	2.16	0.46
1:B:258:THR:HG22	1:B:383:ASP:OD1	2.15	0.46
1:B:452:ILE:HG22	1:B:454:LEU:HB2	1.97	0.46
1:C:183:ALA:HB3	1:C:184:PRO:HD3	1.97	0.46
1:D:213:PRO:HA	1:D:423:TYR:CD2	2.50	0.46
1:D:452:ILE:HG22	1:D:454:LEU:HB2	1.97	0.46
1:D:91:VAL:O	1:D:94:GLU:HG2	2.16	0.46
1:A:401:LEU:C	1:A:401:LEU:HD23	2.35	0.46
1:D:177:LEU:O	1:D:178:ARG:C	2.54	0.46
1:D:105:GLU:OE2	1:D:207:GLY:HA3	2.14	0.46
1:D:330:TYR:CD1	1:D:330:TYR:O	2.68	0.46
1:D:401:LEU:HD23	1:D:402:MET:N	2.30	0.46
1:A:377:LEU:H	1:A:377:LEU:CD2	2.26	0.46
1:A:355:HIS:HB3	1:A:380:LEU:HD13	1.97	0.46
1:A:449:LYS:N	1:A:449:LYS:HD2	2.31	0.46
1:B:179:SER:CB	1:B:182:VAL:HB	2.45	0.46
1:B:229:LEU:HB3	1:B:235:SER:HB3	1.97	0.46
1:B:287:PRO:HD3	1:B:452:ILE:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:THR:HG21	1:C:427:TRP:CH2	2.50	0.46
1:C:279:TYR:O	1:C:282:GLN:HG2	2.15	0.46
1:C:293:GLU:C	1:C:295:GLU:N	2.68	0.46
1:C:126:PRO:HB3	1:C:297:TRP:HZ2	1.79	0.46
1:C:406:THR:O	1:C:410:LYS:HG2	2.16	0.46
1:A:104:VAL:CG1	1:A:105:GLU:N	2.78	0.46
1:C:416:GLY:O	1:C:417:ASP:C	2.54	0.46
1:D:102:ASN:ND2	1:D:174:HIS:O	2.48	0.46
1:D:269:ILE:HB	1:D:270:PRO:CD	2.36	0.46
1:D:406:THR:O	1:D:410:LYS:HG2	2.16	0.46
1:D:385:LEU:HD11	1:D:411:LEU:HD21	1.97	0.46
1:B:151:ALA:HA	1:B:168:ILE:HA	1.98	0.46
1:A:287:PRO:HD3	1:A:452:ILE:HA	1.98	0.46
1:A:352:TYR:CE2	1:A:453:VAL:HB	2.51	0.46
1:C:181:ARG:N	1:C:181:ARG:HD2	2.29	0.46
1:C:329:PHE:CD1	1:C:329:PHE:O	2.69	0.46
1:D:107:ASP:N	1:D:111:PHE:HB2	2.31	0.46
1:D:314:PHE:O	1:D:327:LEU:HD13	2.15	0.46
1:D:88:ASP:OD2	1:D:89:ARG:N	2.49	0.46
1:B:116:SER:HB3	1:B:119:PHE:CB	2.46	0.46
1:B:327:LEU:N	1:B:327:LEU:HD13	2.30	0.46
1:C:228:LYS:HZ1	1:C:343:LYS:HB2	1.80	0.46
1:D:293:GLU:C	1:D:295:GLU:N	2.68	0.46
1:A:289:MET:HB3	1:A:293:GLU:HB2	1.97	0.46
1:A:400:ASP:O	1:A:401:LEU:HB2	2.16	0.46
1:B:158:ILE:N	1:B:158:ILE:HD12	2.23	0.46
1:D:181:ARG:HD3	1:D:181:ARG:O	2.15	0.46
1:D:239:ARG:HE	1:D:239:ARG:HA	1.81	0.46
1:D:380:LEU:HD23	1:D:380:LEU:O	2.16	0.46
1:A:145:LEU:HB3	4:A:906:HOH:O	2.16	0.46
1:A:229:LEU:HB3	1:A:235:SER:HB3	1.97	0.46
1:D:314:PHE:HB2	1:D:327:LEU:HD11	1.98	0.46
1:D:355:HIS:O	1:D:356:THR:O	2.34	0.46
1:A:266:THR:HA	1:A:299:TYR:HE2	1.81	0.45
1:C:292:GLU:HA	1:C:295:GLU:OE2	2.16	0.45
1:D:111:PHE:CZ	1:D:234:PHE:HA	2.43	0.45
1:D:287:PRO:HD3	1:D:452:ILE:HA	1.98	0.45
1:B:128:GLY:O	1:B:153:PRO:HG2	2.16	0.45
1:C:106:ASP:CB	1:C:111:PHE:HB2	2.46	0.45
1:C:258:THR:HG22	1:C:383:ASP:OD1	2.16	0.45
1:C:269:ILE:CB	1:C:270:PRO:HD3	2.36	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:VAL:HG12	1:D:294:VAL:CG1	2.47	0.45
1:D:292:GLU:HA	1:D:295:GLU:HB3	1.98	0.45
1:D:327:LEU:C	1:D:327:LEU:HD22	2.36	0.45
1:D:381:MET:HB3	1:D:381:MET:HE2	1.90	0.45
1:D:416:GLY:O	1:D:417:ASP:C	2.54	0.45
1:D:454:LEU:C	1:D:455:GLN:HE21	2.19	0.45
1:A:87:GLY:HA3	1:A:125:ARG:NH2	2.32	0.45
1:B:402:MET:HA	1:B:448:GLU:HA	1.98	0.45
1:C:111:PHE:CZ	1:C:234:PHE:HD1	2.34	0.45
1:D:158:ILE:HD13	1:D:159:TYR:H	1.81	0.45
1:D:166:VAL:HB	1:D:199:ILE:HG21	1.98	0.45
1:B:158:ILE:HG23	1:B:285:LEU:HD13	1.97	0.45
1:C:269:ILE:CD1	1:C:295:GLU:HG3	2.39	0.45
1:C:401:LEU:HD23	1:C:401:LEU:C	2.37	0.45
1:C:213:PRO:HA	1:C:423:TYR:CD2	2.52	0.45
1:A:151:ALA:HA	1:A:168:ILE:HA	1.99	0.45
1:B:347:ALA:HB1	1:B:349:TYR:HE1	1.81	0.45
1:A:385:LEU:HD11	1:A:411:LEU:HD21	1.98	0.45
1:B:221:HIS:ND1	1:B:397:ASN:ND2	2.65	0.45
1:B:96:TYR:CD1	1:B:96:TYR:C	2.90	0.45
1:C:221:HIS:CE1	1:C:234:PHE:HZ	2.35	0.45
1:C:454:LEU:C	1:C:455:GLN:HE21	2.19	0.45
1:D:183:ALA:HA	1:D:186:LEU:CB	2.43	0.45
1:D:123:ALA:HA	1:D:297:TRP:CZ3	2.52	0.45
1:B:280:LEU:HG	1:B:286:THR:CB	2.46	0.45
1:D:264:MET:HG3	1:D:268:ASP:CB	2.45	0.45
1:A:115:TYR:CE2	1:A:170:PHE:HE2	2.35	0.45
1:A:293:GLU:C	1:A:295:GLU:N	2.70	0.45
1:B:276:LEU:HD21	1:B:289:MET:HE3	1.99	0.45
1:B:401:LEU:C	1:B:401:LEU:HD23	2.37	0.45
1:B:79:PHE:HE1	1:B:140:VAL:CG2	2.30	0.45
1:C:275:LEU:HD23	1:C:326:PHE:CD1	2.52	0.45
1:D:247:MET:O	1:D:248:LYS:C	2.55	0.45
1:D:289:MET:HB3	1:D:293:GLU:HB2	1.98	0.45
1:D:99:LEU:HD22	1:D:99:LEU:N	2.28	0.45
1:C:172:CYS:SG	1:C:173:VAL:N	2.90	0.45
1:D:291:GLN:HG2	1:D:291:GLN:O	2.17	0.45
1:A:269:ILE:HD13	1:A:295:GLU:CD	2.36	0.44
1:B:264:MET:HG3	1:B:268:ASP:CB	2.46	0.44
1:B:327:LEU:HB3	1:B:380:LEU:CD2	2.47	0.44
1:B:355:HIS:HB3	1:B:380:LEU:CD1	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LEU:HB3	1:C:124:LEU:HD12	1.99	0.44
1:C:183:ALA:O	1:C:187:ILE:N	2.43	0.44
1:C:280:LEU:HD12	1:C:283:PHE:CE1	2.52	0.44
1:A:227:ARG:HB2	1:A:247:MET:CE	2.47	0.44
1:B:239:ARG:N	1:B:239:ARG:HE	2.15	0.44
1:B:349:TYR:N	1:B:349:TYR:CD1	2.86	0.44
1:D:194:VAL:HG12	1:D:199:ILE:O	2.17	0.44
1:D:276:LEU:HD21	1:D:289:MET:HE3	1.99	0.44
1:D:327:LEU:HA	1:D:353:ASN:OD1	2.17	0.44
1:D:377:LEU:H	1:D:377:LEU:CD2	2.30	0.44
1:A:180:LYS:O	1:A:184:PRO:HG2	2.16	0.44
1:A:347:ALA:HB1	1:A:349:TYR:HE1	1.82	0.44
1:C:113:PHE:HB3	1:C:115:TYR:HE1	1.82	0.44
1:C:122:TRP:CE2	1:C:311:ILE:HG21	2.50	0.44
1:A:275:LEU:HD23	1:A:326:PHE:CD1	2.52	0.44
1:A:221:HIS:ND1	1:A:397:ASN:ND2	2.65	0.44
1:A:96:TYR:C	1:A:96:TYR:CD1	2.91	0.44
1:B:289:MET:HB3	1:B:293:GLU:HB2	1.98	0.44
1:B:270:PRO:HG3	1:B:291:GLN:CD	2.38	0.44
1:B:386:VAL:O	1:B:390:MET:HB3	2.17	0.44
1:C:178:ARG:O	1:C:181:ARG:NH1	2.50	0.44
1:C:337:MET:O	1:C:337:MET:HG3	2.17	0.44
1:D:269:ILE:HD13	1:D:295:GLU:CD	2.36	0.44
1:D:376:PRO:O	1:D:379:ASP:OD1	2.34	0.44
1:B:150:SER:O	1:B:151:ALA:HB2	2.18	0.44
1:B:218:ARG:HB3	1:B:218:ARG:HH11	1.80	0.44
1:B:397:ASN:ND2	1:B:397:ASN:N	2.65	0.44
1:C:291:GLN:O	1:C:291:GLN:HG2	2.18	0.44
1:A:407:PHE:HA	1:A:410:LYS:CG	2.48	0.44
1:B:169:ASN:HA	1:B:169:ASN:HD22	1.61	0.44
1:C:122:TRP:HE1	1:C:311:ILE:HD13	1.81	0.44
1:D:214:VAL:HG21	1:D:424:LEU:HG	2.00	0.44
1:D:292:GLU:C	1:D:295:GLU:HB3	2.37	0.44
1:A:129:TRP:O	1:A:130:LEU:HD23	2.18	0.44
1:A:220:TRP:CZ3	1:A:409:GLU:HG2	2.52	0.44
1:B:124:LEU:HD21	1:B:170:PHE:CD1	2.53	0.44
1:B:330:TYR:O	1:B:330:TYR:CD1	2.71	0.44
1:B:377:LEU:H	1:B:377:LEU:CD2	2.31	0.44
1:C:107:ASP:C	1:C:109:ASN:N	2.71	0.44
1:D:121:LEU:HD12	1:D:121:LEU:H	1.83	0.44
1:A:171:LEU:HD13	1:A:186:LEU:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:THR:O	1:A:195:HIS:ND1	2.51	0.44
1:B:314:PHE:HB2	1:B:327:LEU:HD11	1.98	0.44
1:B:400:ASP:O	1:B:401:LEU:HB2	2.17	0.44
1:C:107:ASP:OD2	1:C:110:MET:N	2.51	0.44
1:C:269:ILE:HD13	1:C:295:GLU:CD	2.38	0.44
1:D:191:THR:O	1:D:195:HIS:ND1	2.51	0.44
1:D:242:THR:C	1:D:244:GLN:N	2.70	0.44
1:D:402:MET:HA	1:D:448:GLU:HA	1.99	0.44
1:D:402:MET:N	1:D:403:GLU:N	2.66	0.44
1:D:99:LEU:H	1:D:99:LEU:CD2	2.29	0.44
1:A:237:LEU:O	1:A:238:SER:O	2.36	0.44
1:A:314:PHE:HB2	1:A:327:LEU:HD11	1.98	0.44
1:B:216:THR:HG22	1:B:216:THR:O	2.18	0.44
1:B:416:GLY:O	1:B:417:ASP:C	2.56	0.44
1:B:86:LEU:HA	1:B:92:LEU:HD23	1.99	0.44
1:D:118:GLU:O	1:D:119:PHE:C	2.55	0.44
1:D:245:ARG:HG3	1:D:245:ARG:HH11	1.82	0.44
1:D:280:LEU:HG	1:D:286:THR:CB	2.48	0.44
1:A:232:VAL:HG13	1:A:234:PHE:H	1.83	0.43
1:B:139:VAL:C	1:B:141:SER:H	2.21	0.43
1:C:194:VAL:O	1:C:196:LEU:N	2.51	0.43
1:C:280:LEU:HG	1:C:286:THR:CB	2.47	0.43
1:D:113:PHE:CE2	1:D:332:LEU:HD22	2.53	0.43
1:A:245:ARG:HG3	1:A:245:ARG:HH11	1.83	0.43
1:A:336:ILE:HB	1:A:337:MET:H	1.47	0.43
1:B:92:LEU:HD13	1:B:92:LEU:O	2.17	0.43
1:C:198:GLY:O	1:C:200:PHE:HD1	2.01	0.43
1:C:381:MET:HG3	1:C:407:PHE:CD2	2.53	0.43
1:A:223:SER:CB	1:A:226:PRO:HG3	2.48	0.43
1:B:293:GLU:C	1:B:295:GLU:N	2.71	0.43
1:C:214:VAL:HG21	1:C:424:LEU:HG	2.00	0.43
1:D:220:TRP:CZ3	1:D:409:GLU:HG2	2.53	0.43
1:D:213:PRO:HB3	1:D:423:TYR:CE2	2.54	0.43
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.83	0.43
1:B:272:VAL:HG13	1:B:326:PHE:CZ	2.53	0.43
1:D:103:TYR:O	1:D:113:PHE:CB	2.66	0.43
1:D:135:CYS:O	1:D:148:PHE:HA	2.18	0.43
1:D:270:PRO:HA	1:D:273:HIS:HB3	2.00	0.43
1:A:242:THR:C	1:A:244:GLN:N	2.70	0.43
1:A:88:ASP:OD2	1:A:89:ARG:N	2.51	0.43
1:B:181:ARG:HH12	1:B:184:PRO:HB2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD21	1:C:170:PHE:CD1	2.54	0.43
1:C:237:LEU:O	1:C:238:SER:O	2.36	0.43
1:C:88:ASP:OD2	1:C:89:ARG:N	2.51	0.43
1:D:181:ARG:CZ	1:D:184:PRO:HB2	2.47	0.43
1:D:232:VAL:O	1:D:233:LYS:HD3	2.19	0.43
1:B:79:PHE:CZ	1:B:139:VAL:HA	2.53	0.43
1:C:242:THR:C	1:C:244:GLN:N	2.71	0.43
1:D:294:VAL:HG12	1:D:294:VAL:O	2.19	0.43
1:D:337:MET:O	1:D:338:ASN:C	2.57	0.43
1:A:280:LEU:CD2	1:A:286:THR:HB	2.49	0.43
1:B:109:ASN:ND2	1:B:110:MET:H	2.16	0.43
1:B:119:PHE:O	1:B:122:TRP:HB3	2.18	0.43
1:A:118:GLU:OE1	1:A:310:ILE:HD13	2.19	0.43
1:A:329:PHE:O	1:A:329:PHE:CD1	2.71	0.43
1:A:355:HIS:HE1	1:A:403:GLU:HG3	1.82	0.43
1:A:452:ILE:HG22	1:A:454:LEU:HB2	2.00	0.43
1:C:343:LYS:H	1:C:343:LYS:CD	2.22	0.43
1:C:411:LEU:HD12	1:C:412:LYS:HD2	2.01	0.43
1:D:179:SER:HA	1:D:182:VAL:CG2	2.48	0.43
1:A:216:THR:HG22	1:A:216:THR:O	2.19	0.43
1:B:158:ILE:HA	1:B:284:HIS:O	2.19	0.43
1:B:402:MET:N	1:B:403:GLU:N	2.67	0.43
1:C:294:VAL:HG12	1:C:294:VAL:O	2.19	0.43
1:D:397:ASN:N	1:D:397:ASN:HD22	2.15	0.43
1:A:113:PHE:HB3	1:A:115:TYR:CE1	2.54	0.43
1:A:247:MET:O	1:A:248:LYS:C	2.56	0.43
1:B:79:PHE:HZ	1:B:139:VAL:HA	1.83	0.43
1:B:232:VAL:HG13	1:B:234:PHE:H	1.84	0.43
1:B:292:GLU:HA	1:B:295:GLU:OE2	2.19	0.43
1:C:292:GLU:C	1:C:295:GLU:HB3	2.39	0.43
1:C:452:ILE:CG2	1:C:454:LEU:HB2	2.49	0.43
1:A:194:VAL:C	1:A:196:LEU:N	2.73	0.42
1:B:130:LEU:HB3	1:B:132:GLN:HE22	1.80	0.42
1:C:194:VAL:C	1:C:196:LEU:N	2.72	0.42
1:C:262:ARG:NH2	1:C:317:GLU:HB2	2.34	0.42
1:D:96:TYR:CD1	1:D:96:TYR:C	2.93	0.42
1:A:294:VAL:O	1:A:294:VAL:HG12	2.19	0.42
1:A:381:MET:HG3	1:A:407:PHE:CZ	2.55	0.42
1:A:396:PHE:C	1:A:397:ASN:HD22	2.22	0.42
1:C:376:PRO:O	1:C:379:ASP:OD1	2.37	0.42
1:D:123:ALA:HA	1:D:297:TRP:HZ3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:HIS:HB3	1:A:380:LEU:CD1	2.49	0.42
1:B:267:LYS:H	1:B:267:LYS:CD	2.24	0.42
1:B:332:LEU:N	1:B:333:PRO:HD3	2.35	0.42
1:C:116:SER:HB3	1:C:119:PHE:CB	2.49	0.42
1:C:122:TRP:HE1	1:C:297:TRP:HA	1.84	0.42
1:C:347:ALA:HB1	1:C:349:TYR:HE1	1.81	0.42
1:C:409:GLU:C	1:C:411:LEU:N	2.73	0.42
1:D:327:LEU:HB3	1:D:380:LEU:CD2	2.49	0.42
1:A:194:VAL:O	1:A:196:LEU:N	2.53	0.42
1:A:258:THR:HG23	1:A:258:THR:O	2.19	0.42
1:A:86:LEU:HA	1:A:92:LEU:HD23	2.01	0.42
1:B:242:THR:C	1:B:244:GLN:N	2.70	0.42
1:B:161:THR:HG21	1:B:427:TRP:CH2	2.54	0.42
1:C:109:ASN:O	1:C:110:MET:CB	2.67	0.42
1:C:155:ASN:HA	1:C:164:LYS:HA	2.01	0.42
1:D:343:LYS:HD3	1:D:343:LYS:C	2.40	0.42
1:A:116:SER:HB3	1:A:119:PHE:CB	2.48	0.42
1:A:232:VAL:CG2	1:A:233:LYS:H	2.22	0.42
1:B:397:ASN:N	1:B:397:ASN:HD22	2.16	0.42
1:B:407:PHE:HA	1:B:410:LYS:CG	2.50	0.42
1:C:123:ALA:HA	1:C:297:TRP:HZ3	1.84	0.42
1:D:181:ARG:NH1	1:D:185:VAL:HG22	2.33	0.42
1:A:110:MET:CB	1:A:337:MET:HG3	2.50	0.42
1:A:174:HIS:HB3	1:A:177:LEU:HG	2.02	0.42
1:A:330:TYR:CD1	1:A:330:TYR:O	2.72	0.42
1:B:220:TRP:CZ3	1:B:409:GLU:HG2	2.54	0.42
1:B:232:VAL:O	1:B:233:LYS:HD3	2.20	0.42
1:C:209:VAL:HG12	1:C:210:LEU:N	2.34	0.42
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.85	0.42
1:C:229:LEU:CB	1:C:235:SER:HB3	2.50	0.42
1:C:280:LEU:CG	1:C:286:THR:HB	2.49	0.42
1:D:119:PHE:O	1:D:122:TRP:HB3	2.19	0.42
1:D:232:VAL:HG13	1:D:234:PHE:H	1.85	0.42
1:D:279:TYR:O	1:D:282:GLN:HG2	2.19	0.42
1:A:139:VAL:O	1:A:140:VAL:C	2.57	0.42
1:A:279:TYR:C	1:A:281:LYS:N	2.73	0.42
1:B:348:ALA:HB3	1:B:395:VAL:O	2.20	0.42
1:C:245:ARG:NH1	1:C:245:ARG:HG3	2.35	0.42
1:D:280:LEU:CD2	1:D:286:THR:HB	2.50	0.42
1:D:272:VAL:HG13	1:D:326:PHE:CZ	2.54	0.42
1:B:139:VAL:HG12	1:B:141:SER:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:O	1:B:238:SER:O	2.36	0.42
1:B:336:ILE:CG1	1:B:337:MET:H	2.29	0.42
1:C:287:PRO:HD3	1:C:452:ILE:CG1	2.50	0.42
1:D:174:HIS:CG	1:D:175:LYS:N	2.87	0.42
1:D:324:THR:HG1	1:D:325:ASP:N	2.17	0.42
1:B:102:ASN:HB3	1:B:172:CYS:SG	2.59	0.42
1:B:229:LEU:CB	1:B:235:SER:HB3	2.49	0.42
1:B:427:TRP:HD1	1:B:429:CYS:HG	1.64	0.42
1:D:266:THR:O	1:D:269:ILE:HG13	2.20	0.42
1:D:329:PHE:HB2	1:D:349:TYR:O	2.19	0.42
1:A:83:ALA:HB3	1:A:136:GLY:CA	2.50	0.42
1:A:301:GLN:O	1:A:303:ASN:N	2.45	0.42
1:B:381:MET:HB3	1:B:381:MET:HE2	1.85	0.42
1:C:169:ASN:HD22	1:C:169:ASN:HA	1.56	0.42
1:D:179:SER:CB	1:D:182:VAL:HB	2.50	0.42
1:D:397:ASN:ND2	1:D:397:ASN:N	2.68	0.42
1:A:264:MET:HG3	1:A:268:ASP:CB	2.50	0.41
1:A:353:ASN:ND2	1:A:381:MET:SD	2.92	0.41
1:A:381:MET:HG3	1:A:407:PHE:CD2	2.54	0.41
1:B:213:PRO:HB3	1:B:423:TYR:CE2	2.55	0.41
1:B:399:LEU:HD12	1:B:399:LEU:N	2.35	0.41
1:C:158:ILE:H	1:C:158:ILE:CD1	2.26	0.41
1:C:327:LEU:N	1:C:327:LEU:HD13	2.34	0.41
1:D:207:GLY:O	1:D:208:VAL:CG1	2.65	0.41
1:D:243:MET:O	1:D:247:MET:HE2	2.20	0.41
1:D:270:PRO:O	1:D:274:GLN:HG2	2.20	0.41
1:A:425:TYR:CD2	1:A:426:ASN:ND2	2.89	0.41
1:C:267:LYS:H	1:C:267:LYS:CD	2.17	0.41
1:D:149:ILE:HA	1:D:170:PHE:O	2.20	0.41
1:D:275:LEU:HD23	1:D:326:PHE:CD1	2.53	0.41
1:A:139:VAL:C	1:A:141:SER:N	2.73	0.41
1:A:311:ILE:HA	1:A:330:TYR:HA	2.02	0.41
1:C:315:VAL:HG22	1:C:316:VAL:H	1.85	0.41
1:A:375:THR:HA	1:A:376:PRO:HD3	1.97	0.41
1:B:232:VAL:CG2	1:B:233:LYS:N	2.80	0.41
1:B:279:TYR:C	1:B:281:LYS:N	2.72	0.41
1:C:292:GLU:HA	1:C:295:GLU:HB3	2.02	0.41
1:D:280:LEU:CG	1:D:286:THR:HB	2.49	0.41
1:A:292:GLU:HA	1:A:295:GLU:OE2	2.20	0.41
1:C:202:ALA:HB3	1:C:425:TYR:HB3	1.99	0.41
1:C:221:HIS:ND1	1:C:395:VAL:HG21	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:C	1:A:411:LEU:N	2.74	0.41
1:C:138:ARG:O	1:C:138:ARG:HG3	2.21	0.41
1:C:250:TYR:CE2	1:C:412:LYS:HB3	2.55	0.41
1:C:385:LEU:HD11	1:C:411:LEU:CD2	2.51	0.41
1:D:411:LEU:HD12	1:D:412:LYS:HD2	2.01	0.41
1:B:352:TYR:CE2	1:B:453:VAL:HB	2.56	0.41
1:C:289:MET:HB3	1:C:293:GLU:HB2	2.02	0.41
1:C:96:TYR:CD1	1:C:96:TYR:C	2.93	0.41
1:D:116:SER:HA	1:D:117:PRO:HD3	1.96	0.41
1:A:130:LEU:HA	1:A:131:PRO:HD3	1.84	0.41
1:A:122:TRP:CZ2	1:A:297:TRP:HE3	2.39	0.41
1:A:221:HIS:ND1	1:A:395:VAL:HG21	2.35	0.41
1:A:400:ASP:CB	1:A:447:ALA:HB1	2.43	0.41
1:B:174:HIS:HB3	1:B:177:LEU:HG	2.03	0.41
1:B:198:GLY:HA2	1:B:200:PHE:HE1	1.85	0.41
1:B:327:LEU:HB3	1:B:380:LEU:HD23	2.01	0.41
1:C:116:SER:HA	1:C:117:PRO:HD3	1.95	0.41
1:D:199:ILE:O	1:D:199:ILE:HG22	2.20	0.41
1:D:280:LEU:HG	1:D:286:THR:CG2	2.51	0.41
1:B:159:TYR:C	1:B:161:THR:N	2.74	0.41
1:C:149:ILE:HA	1:C:170:PHE:O	2.21	0.41
1:C:198:GLY:HA2	1:C:200:PHE:HE1	1.86	0.41
1:C:232:VAL:HG13	1:C:234:PHE:H	1.86	0.41
1:C:401:LEU:O	1:C:403:GLU:N	2.54	0.41
1:D:258:THR:O	1:D:258:THR:HG23	2.20	0.41
1:D:221:HIS:O	1:D:412:LYS:O	2.39	0.41
1:D:452:ILE:CG2	1:D:454:LEU:HB2	2.51	0.41
1:A:118:GLU:HA	1:A:121:LEU:HD13	2.01	0.41
1:A:327:LEU:HD13	1:A:327:LEU:N	2.34	0.41
1:B:177:LEU:O	1:B:177:LEU:HD12	2.20	0.41
1:C:183:ALA:N	1:C:184:PRO:CD	2.83	0.41
1:C:330:TYR:O	1:C:330:TYR:CD1	2.73	0.41
1:C:344:SER:O	1:C:345:LEU:HB2	2.20	0.41
1:A:327:LEU:HB3	1:A:380:LEU:CD2	2.51	0.41
1:A:336:ILE:O	1:A:337:MET:HG2	2.21	0.41
1:A:402:MET:C	1:A:403:GLU:C	2.75	0.41
1:B:395:VAL:HG13	1:B:397:ASN:HD21	1.85	0.41
1:B:283:PHE:CE2	1:B:402:MET:CB	3.00	0.41
1:C:138:ARG:HB3	1:C:177:LEU:HD11	2.02	0.41
1:C:177:LEU:O	1:C:178:ARG:CB	2.68	0.41
1:C:232:VAL:CG2	1:C:233:LYS:H	2.23	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:HIS:O	1:C:356:THR:O	2.39	0.41
1:D:432:MET:CB	1:D:449:LYS:HD3	2.51	0.41
1:A:159:TYR:C	1:A:161:THR:N	2.74	0.40
1:A:381:MET:HB3	1:A:381:MET:HE2	1.85	0.40
1:B:185:VAL:HA	1:B:188:ARG:CG	2.50	0.40
1:B:275:LEU:HD21	1:B:324:THR:O	2.20	0.40
1:B:292:GLU:HA	1:B:295:GLU:HB3	2.03	0.40
1:C:199:ILE:HG22	1:C:199:ILE:O	2.20	0.40
1:C:280:LEU:CD2	1:C:286:THR:HB	2.51	0.40
1:C:318:ASN:ND2	1:C:319:ALA:H	2.18	0.40
1:D:102:ASN:CB	1:D:172:CYS:SG	3.03	0.40
1:D:194:VAL:C	1:D:196:LEU:N	2.73	0.40
1:D:194:VAL:HG12	1:D:199:ILE:HB	2.02	0.40
1:D:198:GLY:O	1:D:200:PHE:HD1	2.05	0.40
1:D:299:TYR:HA	1:D:300:PRO:HD3	1.88	0.40
1:A:232:VAL:O	1:A:233:LYS:HD3	2.20	0.40
1:B:152:ILE:HA	1:B:153:PRO:HD3	1.85	0.40
1:B:156:ILE:HG22	1:B:452:ILE:HD11	2.02	0.40
1:B:291:GLN:HG2	1:B:291:GLN:O	2.21	0.40
1:B:294:VAL:O	1:B:294:VAL:HG12	2.21	0.40
1:B:114:ASP:HB2	1:B:335:THR:OG1	2.21	0.40
1:B:341:THR:HG22	1:B:341:THR:O	2.20	0.40
1:C:152:ILE:HA	1:C:153:PRO:HD3	1.85	0.40
1:C:211:PRO:O	1:C:213:PRO:HD3	2.21	0.40
1:D:159:TYR:C	1:D:161:THR:N	2.74	0.40
1:D:181:ARG:HH11	1:D:185:VAL:HG23	1.83	0.40
1:A:222:ARG:CZ	1:A:412:LYS:HD3	2.52	0.40
1:A:335:THR:HG22	1:A:336:ILE:N	2.36	0.40
1:A:217:CYS:HB3	1:A:400:ASP:HB2	2.03	0.40
1:B:171:LEU:HD13	1:B:186:LEU:HD12	2.02	0.40
1:B:311:ILE:HA	1:B:330:TYR:HA	2.04	0.40
1:C:249:LEU:C	1:C:251:ARG:H	2.24	0.40
1:D:120:LEU:HB3	1:D:124:LEU:HD12	2.03	0.40
1:D:198:GLY:HA2	1:D:200:PHE:HE1	1.85	0.40
1:D:249:LEU:C	1:D:251:ARG:H	2.24	0.40
1:D:315:VAL:HG22	1:D:316:VAL:H	1.86	0.40
1:A:181:ARG:NH1	1:A:184:PRO:HG2	2.36	0.40
1:B:96:TYR:O	1:B:100:ASN:HB2	2.22	0.40
1:B:199:ILE:O	1:B:199:ILE:HG22	2.21	0.40
1:C:316:VAL:N	1:C:324:THR:OG1	2.50	0.40
1:D:155:ASN:HA	1:D:164:LYS:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:CYS:SG	1:D:190:ILE:HB	2.61	0.40
1:D:222:ARG:NH1	1:D:412:LYS:HD3	2.36	0.40
1:B:292:GLU:C	1:B:295:GLU:HB3	2.41	0.40
1:C:118:GLU:O	1:C:119:PHE:C	2.58	0.40
1:D:311:ILE:HA	1:D:330:TYR:HA	2.04	0.40
1:D:349:TYR:N	1:D:349:TYR:CD1	2.90	0.40
1:D:375:THR:HA	1:D:376:PRO:HD3	1.97	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:LEU:O	1:D:196:LEU:O[1_655]	2.17	0.03

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	338/496 (68%)	224 (66%)	80 (24%)	34 (10%)	0	2
1	B	340/496 (68%)	226 (66%)	73 (22%)	41 (12%)	0	1
1	C	317/496 (64%)	212 (67%)	65 (20%)	40 (13%)	0	1
1	D	322/496 (65%)	213 (66%)	73 (23%)	36 (11%)	0	2
All	All	1317/1984 (66%)	875 (66%)	291 (22%)	151 (12%)	0	2

All (151) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	SER
1	A	151	ALA
1	A	232	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	238	SER
1	A	239	ARG
1	A	337	MET
1	A	344	SER
1	A	356	THR
1	A	408	LEU
1	A	412	LYS
1	B	86	LEU
1	B	109	ASN
1	B	110	MET
1	B	112	ARG
1	B	113	PHE
1	B	143	ARG
1	B	145	LEU
1	B	151	ALA
1	B	182	VAL
1	B	232	VAL
1	B	238	SER
1	B	239	ARG
1	B	356	THR
1	B	408	LEU
1	B	412	LYS
1	C	109	ASN
1	C	175	LYS
1	C	178	ARG
1	C	179	SER
1	C	232	VAL
1	C	238	SER
1	C	239	ARG
1	C	344	SER
1	C	345	LEU
1	C	356	THR
1	C	412	LYS
1	D	107	ASP
1	D	178	ARG
1	D	181	ARG
1	D	232	VAL
1	D	238	SER
1	D	239	ARG
1	D	338	ASN
1	D	344	SER
1	D	356	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	412	LYS
1	A	86	LEU
1	A	103	TYR
1	A	140	VAL
1	A	176	LYS
1	A	195	HIS
1	A	222	ARG
1	A	323	VAL
1	B	103	TYR
1	B	147	GLY
1	B	174	HIS
1	B	175	LYS
1	B	176	LYS
1	B	178	ARG
1	B	181	ARG
1	B	323	VAL
1	B	338	ASN
1	B	344	SER
1	C	103	TYR
1	C	110	MET
1	C	137	VAL
1	C	149	ILE
1	C	151	ALA
1	C	176	LYS
1	C	195	HIS
1	C	401	LEU
1	C	408	LEU
1	D	103	TYR
1	D	109	ASN
1	D	149	ILE
1	D	151	ALA
1	D	175	LYS
1	D	323	VAL
1	D	343	LYS
1	D	408	LEU
1	A	109	ASN
1	A	159	TYR
1	A	174	HIS
1	A	211	PRO
1	A	340	PRO
1	A	401	LEU
1	B	149	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	159	TYR
1	B	195	HIS
1	B	211	PRO
1	B	222	ARG
1	B	401	LEU
1	C	135	CYS
1	C	159	TYR
1	C	173	VAL
1	C	216	THR
1	C	222	ARG
1	C	323	VAL
1	D	92	LEU
1	D	135	CYS
1	D	159	TYR
1	D	195	HIS
1	D	222	ARG
1	D	345	LEU
1	A	149	ILE
1	A	175	LYS
1	A	243	MET
1	A	336	ILE
1	B	80	THR
1	B	243	MET
1	B	454	LEU
1	C	174	HIS
1	C	211	PRO
1	C	250	TYR
1	C	281	LYS
1	C	319	ALA
1	C	414	GLY
1	D	91	VAL
1	D	176	LYS
1	D	211	PRO
1	D	243	MET
1	D	250	TYR
1	D	401	LEU
1	A	143	ARG
1	A	160	ASP
1	A	414	GLY
1	B	142	SER
1	B	414	GLY
1	C	92	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	208	VAL
1	C	243	MET
1	C	342	HIS
1	C	405	LYS
1	C	406	THR
1	D	319	ALA
1	D	414	GLY
1	A	91	VAL
1	A	250	TYR
1	B	319	ALA
1	B	406	THR
1	B	415	ILE
1	C	91	VAL
1	D	208	VAL
1	D	216	THR
1	D	415	ILE
1	A	208	VAL
1	B	91	VAL
1	B	208	VAL
1	D	173	VAL
1	A	415	ILE
1	C	415	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	272/443 (61%)	247 (91%)	25 (9%)	9	34
1	B	271/443 (61%)	247 (91%)	24 (9%)	9	35
1	C	263/443 (59%)	240 (91%)	23 (9%)	10	37
1	D	259/443 (58%)	237 (92%)	22 (8%)	10	38
All	All	1065/1772 (60%)	971 (91%)	94 (9%)	10	36

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	PHE
1	A	89	ARG
1	A	92	LEU
1	A	96	TYR
1	A	101	GLU
1	A	105	GLU
1	A	134	HIS
1	A	158	ILE
1	A	162	GLU
1	A	169	ASN
1	A	210	LEU
1	A	211	PRO
1	A	222	ARG
1	A	237	LEU
1	A	239	ARG
1	A	247	MET
1	A	267	LYS
1	A	302	GLU
1	A	325	ASP
1	A	327	LEU
1	A	343	LYS
1	A	390	MET
1	A	403	GLU
1	A	449	LYS
1	A	455	GLN
1	B	79	PHE
1	B	89	ARG
1	B	92	LEU
1	B	96	TYR
1	B	101	GLU
1	B	113	PHE
1	B	134	HIS
1	B	158	ILE
1	B	162	GLU
1	B	169	ASN
1	B	210	LEU
1	B	211	PRO
1	B	222	ARG
1	B	237	LEU
1	B	239	ARG
1	B	247	MET
1	B	267	LYS
1	B	325	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	LEU
1	B	343	LYS
1	B	390	MET
1	B	403	GLU
1	B	449	LYS
1	B	455	GLN
1	C	89	ARG
1	C	92	LEU
1	C	101	GLU
1	C	134	HIS
1	C	158	ILE
1	C	162	GLU
1	C	169	ASN
1	C	173	VAL
1	C	177	LEU
1	C	181	ARG
1	C	210	LEU
1	C	222	ARG
1	C	237	LEU
1	C	239	ARG
1	C	247	MET
1	C	267	LYS
1	C	302	GLU
1	C	325	ASP
1	C	327	LEU
1	C	390	MET
1	C	403	GLU
1	C	449	LYS
1	C	455	GLN
1	D	89	ARG
1	D	92	LEU
1	D	96	TYR
1	D	101	GLU
1	D	113	PHE
1	D	134	HIS
1	D	158	ILE
1	D	162	GLU
1	D	169	ASN
1	D	211	PRO
1	D	222	ARG
1	D	237	LEU
1	D	239	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	247	MET
1	D	267	LYS
1	D	325	ASP
1	D	327	LEU
1	D	338	ASN
1	D	390	MET
1	D	403	GLU
1	D	449	LYS
1	D	455	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	169	ASN
1	A	236	HIS
1	A	244	GLN
1	A	397	ASN
1	A	426	ASN
1	A	455	GLN
1	B	102	ASN
1	B	132	GLN
1	B	169	ASN
1	B	236	HIS
1	B	244	GLN
1	B	273	HIS
1	B	397	ASN
1	B	426	ASN
1	B	455	GLN
1	C	132	GLN
1	C	169	ASN
1	C	236	HIS
1	C	244	GLN
1	C	273	HIS
1	C	338	ASN
1	C	397	ASN
1	C	426	ASN
1	C	455	GLN
1	D	132	GLN
1	D	169	ASN
1	D	236	HIS
1	D	244	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	338	ASN
1	D	397	ASN
1	D	426	ASN
1	D	455	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	SO4	A	903	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	C	904	-	4,4,4	0.27	0	6,6,6	0.05	0
2	SO4	B	901	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	A	902	-	4,4,4	0.27	0	6,6,6	0.04	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	4
1	A	4
1	D	4
1	C	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	402:MET	C	403:GLU	N	2.12
1	A	402:MET	C	403:GLU	N	2.01
1	B	402:MET	C	403:GLU	N	1.99
1	D	402:MET	C	403:GLU	N	1.97
1	A	302:GLU	C	303:ASN	N	1.15
1	A	301:GLN	C	302:GLU	N	1.05
1	B	301:GLN	C	302:GLU	N	0.99
1	C	301:GLN	C	302:GLU	N	0.98
1	D	301:GLN	C	302:GLU	N	0.97
1	C	401:LEU	C	402:MET	N	0.88
1	C	302:GLU	C	303:ASN	N	0.82
1	B	302:GLU	C	303:ASN	N	0.78
1	D	302:GLU	C	303:ASN	N	0.70
1	B	401:LEU	C	402:MET	N	0.62
1	A	401:LEU	C	402:MET	N	0.59
1	D	401:LEU	C	402:MET	N	0.59

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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