



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

PDB ID : 2V50
Title : THE MISSING PART OF THE BACTERIAL MEXAB-OPRM SYSTEM:
STRUCTURAL DETERMINATION OF THE MULTIDRUG EXPORTER
MEXB
Authors : Sennhauser, G.; Bukowska, M.A.; Gruetter, M.G.
Deposited on : 2008-10-01
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
<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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

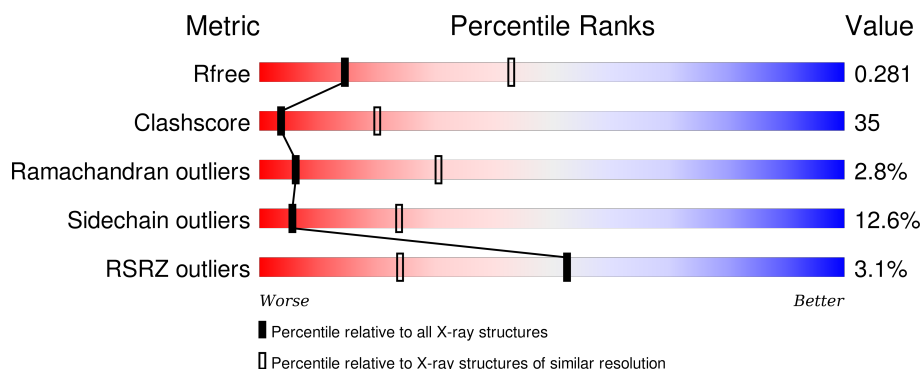
1 Overall quality at a glance

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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.

Mol	Chain	Length	Quality of chain
1	A	1052	<div> <div>37%</div> <div>46%</div> <div>12%</div> <div>• •</div> </div>
1	B	1052	<div> <div>2%</div> <div>46%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>
1	C	1052	<div> <div>4%</div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div>
1	D	1052	<div> <div>2%</div> <div>38%</div> <div>46%</div> <div>11%</div> <div>• 5%</div> </div>
1	E	1052	<div> <div>4%</div> <div>44%</div> <div>44%</div> <div>8%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1052	

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	LMT	B	2032	-	-	-	X
2	LMT	B	2033	-	-	-	X
2	LMT	E	2032	-	-	-	X
2	LMT	E	2033	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 46628 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 MULTIDRUG RESISTANCE PROTEIN MEXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1005	Total	C	N	O	S	6	0	0
			7634	4920	1265	1410	39			
1	B	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			
1	C	1030	Total	C	N	O	S	12	0	0
			7812	5027	1298	1447	40			
1	D	998	Total	C	N	O	S	0	0	0
			7582	4888	1255	1399	40			
1	E	1012	Total	C	N	O	S	0	0	0
			7696	4956	1279	1421	40			
1	F	1030	Total	C	N	O	S	0	0	0
			7812	5027	1298	1447	40			

There are 36 discrepancies between the modelled and reference sequences:

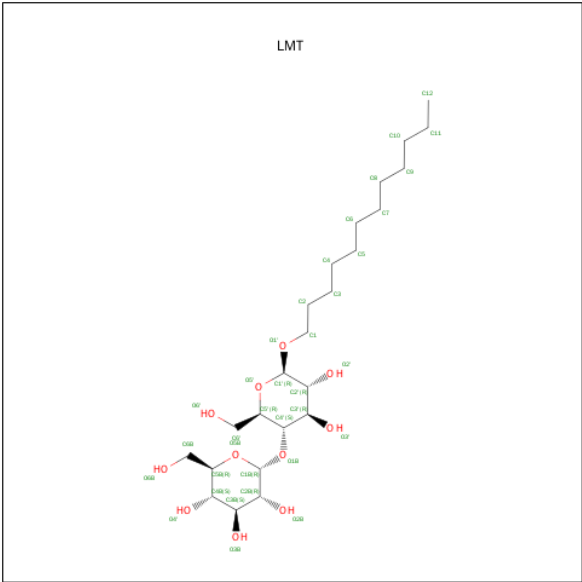
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	EXPRESSION TAG	UNP P52002
A	1048	HIS	-	EXPRESSION TAG	UNP P52002
A	1049	HIS	-	EXPRESSION TAG	UNP P52002
A	1050	HIS	-	EXPRESSION TAG	UNP P52002
A	1051	HIS	-	EXPRESSION TAG	UNP P52002
A	1052	HIS	-	EXPRESSION TAG	UNP P52002
B	1047	HIS	-	EXPRESSION TAG	UNP P52002
B	1048	HIS	-	EXPRESSION TAG	UNP P52002
B	1049	HIS	-	EXPRESSION TAG	UNP P52002
B	1050	HIS	-	EXPRESSION TAG	UNP P52002
B	1051	HIS	-	EXPRESSION TAG	UNP P52002
B	1052	HIS	-	EXPRESSION TAG	UNP P52002
C	1047	HIS	-	EXPRESSION TAG	UNP P52002
C	1048	HIS	-	EXPRESSION TAG	UNP P52002
C	1049	HIS	-	EXPRESSION TAG	UNP P52002
C	1050	HIS	-	EXPRESSION TAG	UNP P52002
C	1051	HIS	-	EXPRESSION TAG	UNP P52002

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1052	HIS	-	EXPRESSION TAG	UNP P52002
D	1047	HIS	-	EXPRESSION TAG	UNP P52002
D	1048	HIS	-	EXPRESSION TAG	UNP P52002
D	1049	HIS	-	EXPRESSION TAG	UNP P52002
D	1050	HIS	-	EXPRESSION TAG	UNP P52002
D	1051	HIS	-	EXPRESSION TAG	UNP P52002
D	1052	HIS	-	EXPRESSION TAG	UNP P52002
E	1047	HIS	-	EXPRESSION TAG	UNP P52002
E	1048	HIS	-	EXPRESSION TAG	UNP P52002
E	1049	HIS	-	EXPRESSION TAG	UNP P52002
E	1050	HIS	-	EXPRESSION TAG	UNP P52002
E	1051	HIS	-	EXPRESSION TAG	UNP P52002
E	1052	HIS	-	EXPRESSION TAG	UNP P52002
F	1047	HIS	-	EXPRESSION TAG	UNP P52002
F	1048	HIS	-	EXPRESSION TAG	UNP P52002
F	1049	HIS	-	EXPRESSION TAG	UNP P52002
F	1050	HIS	-	EXPRESSION TAG	UNP P52002
F	1051	HIS	-	EXPRESSION TAG	UNP P52002
F	1052	HIS	-	EXPRESSION TAG	UNP P52002

- Molecule 2 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		

Continued on next page...

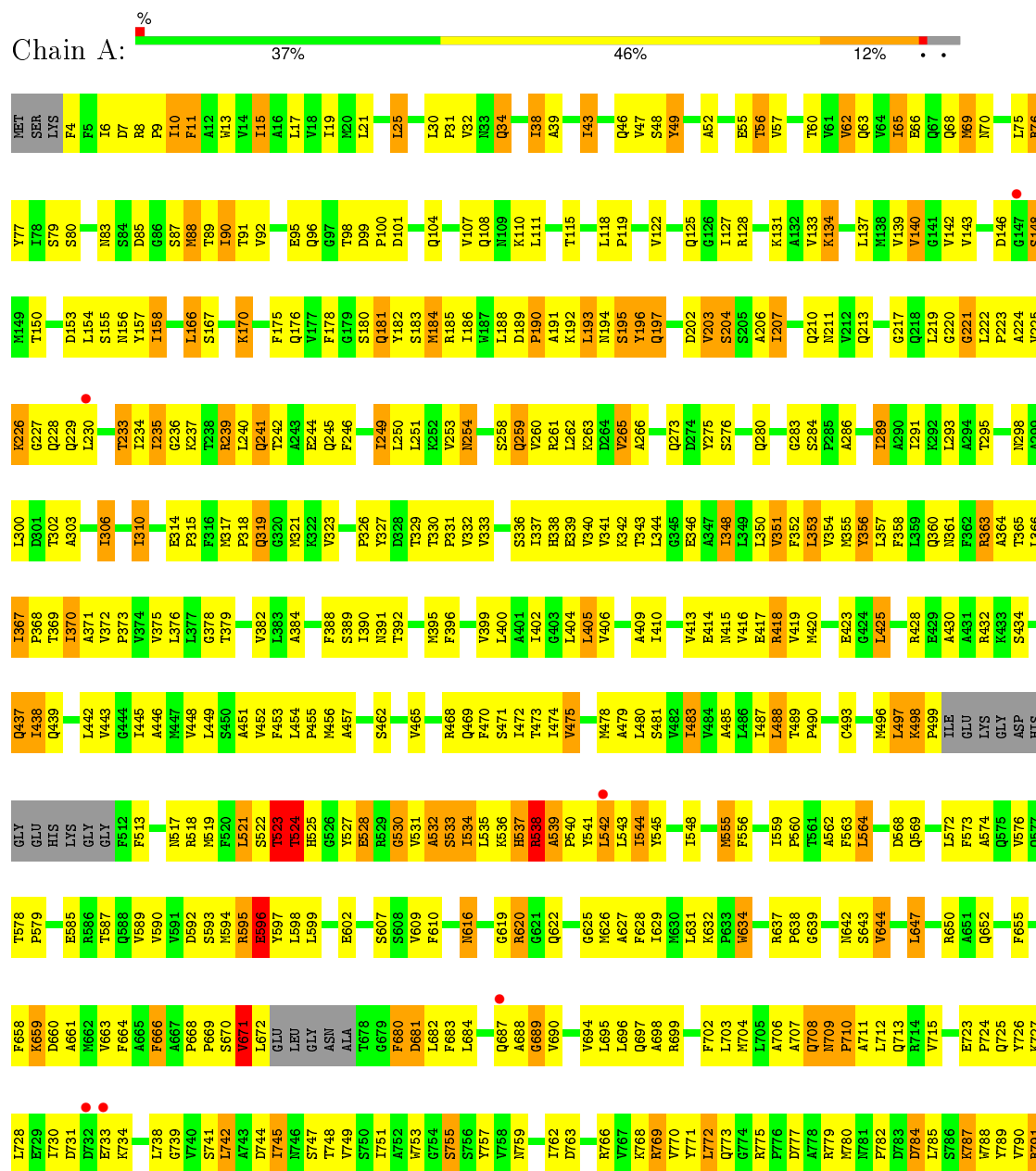
Continued from previous page...

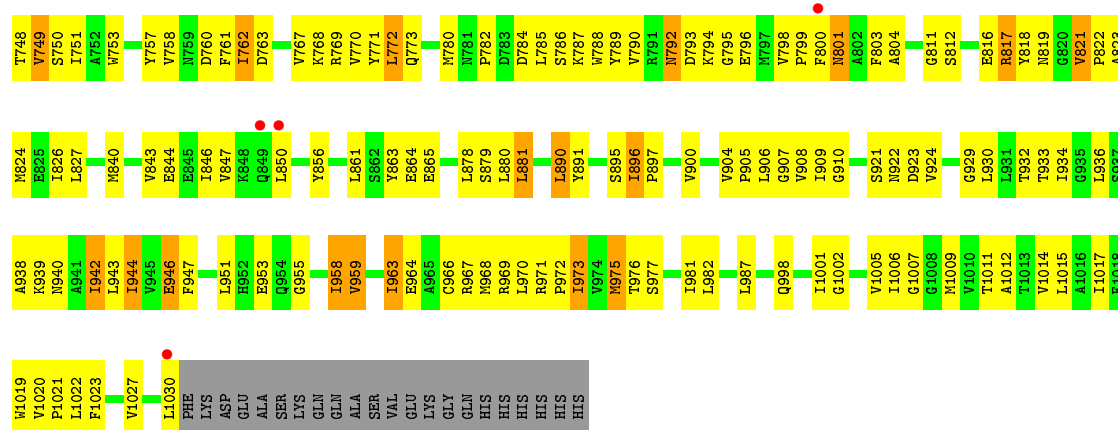
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

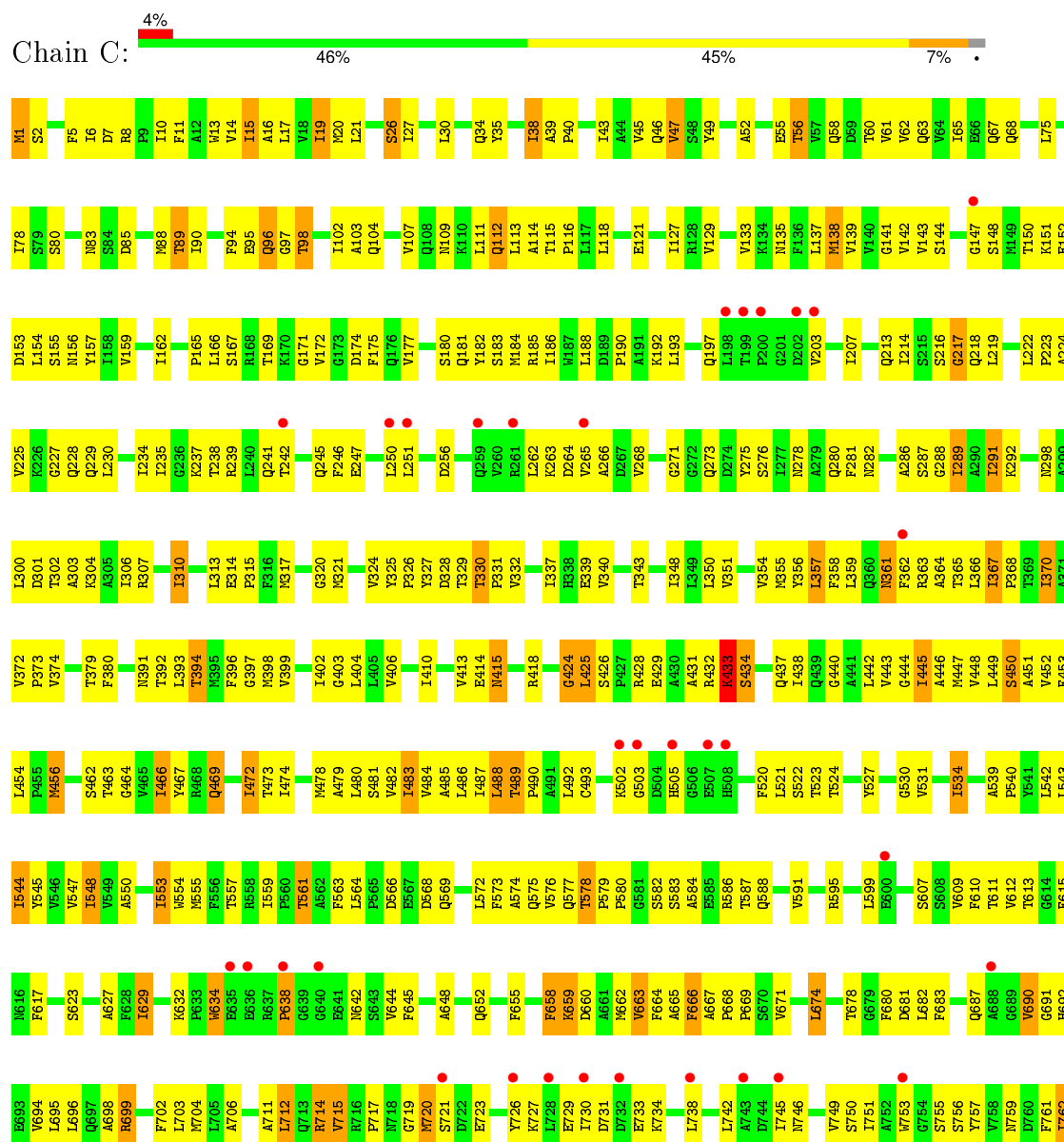
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

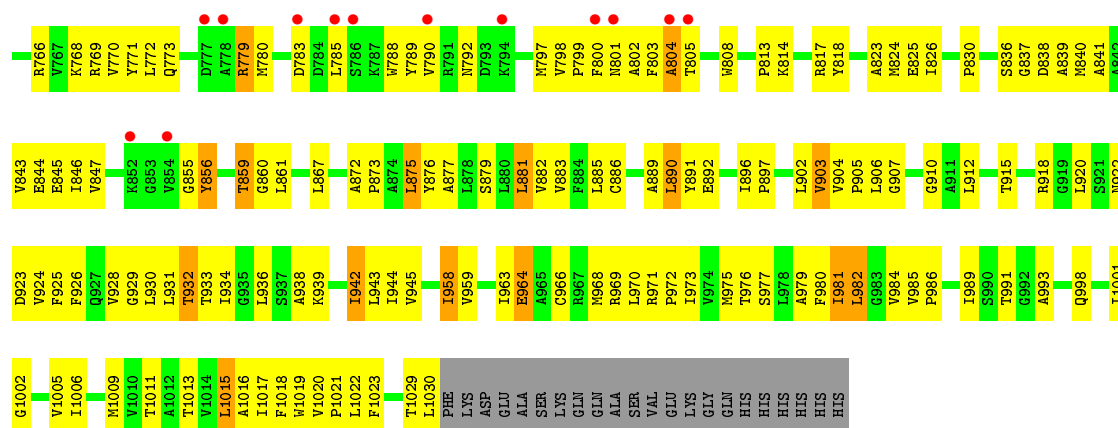
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB



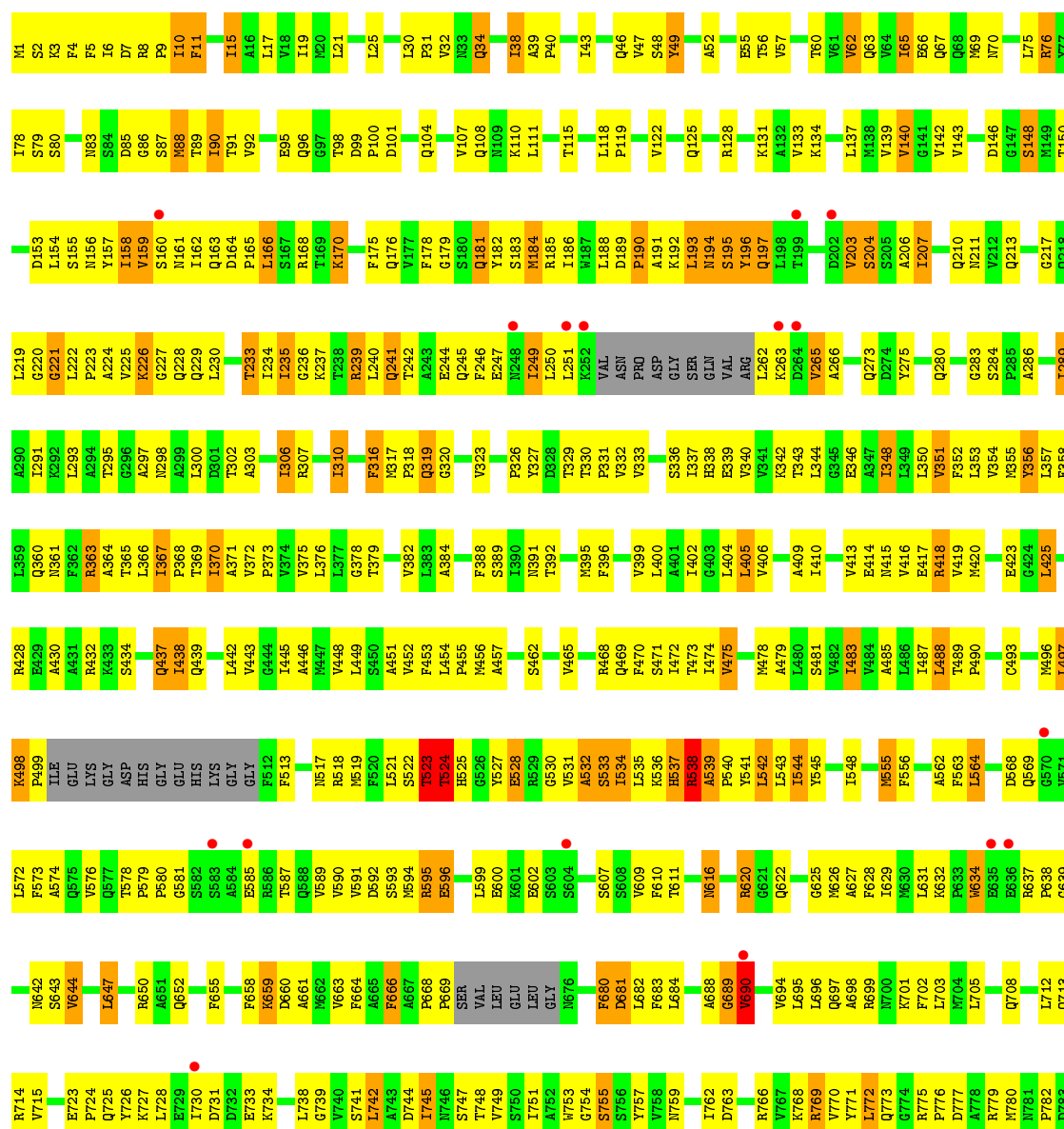


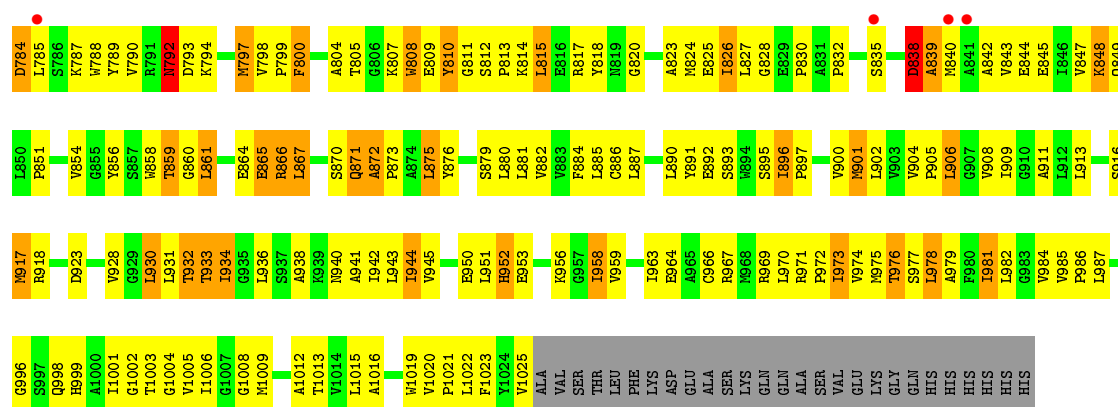
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

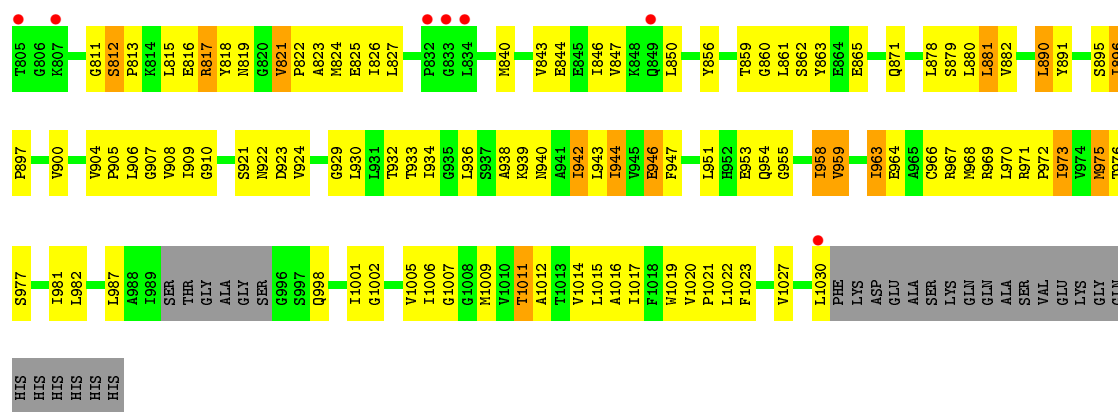




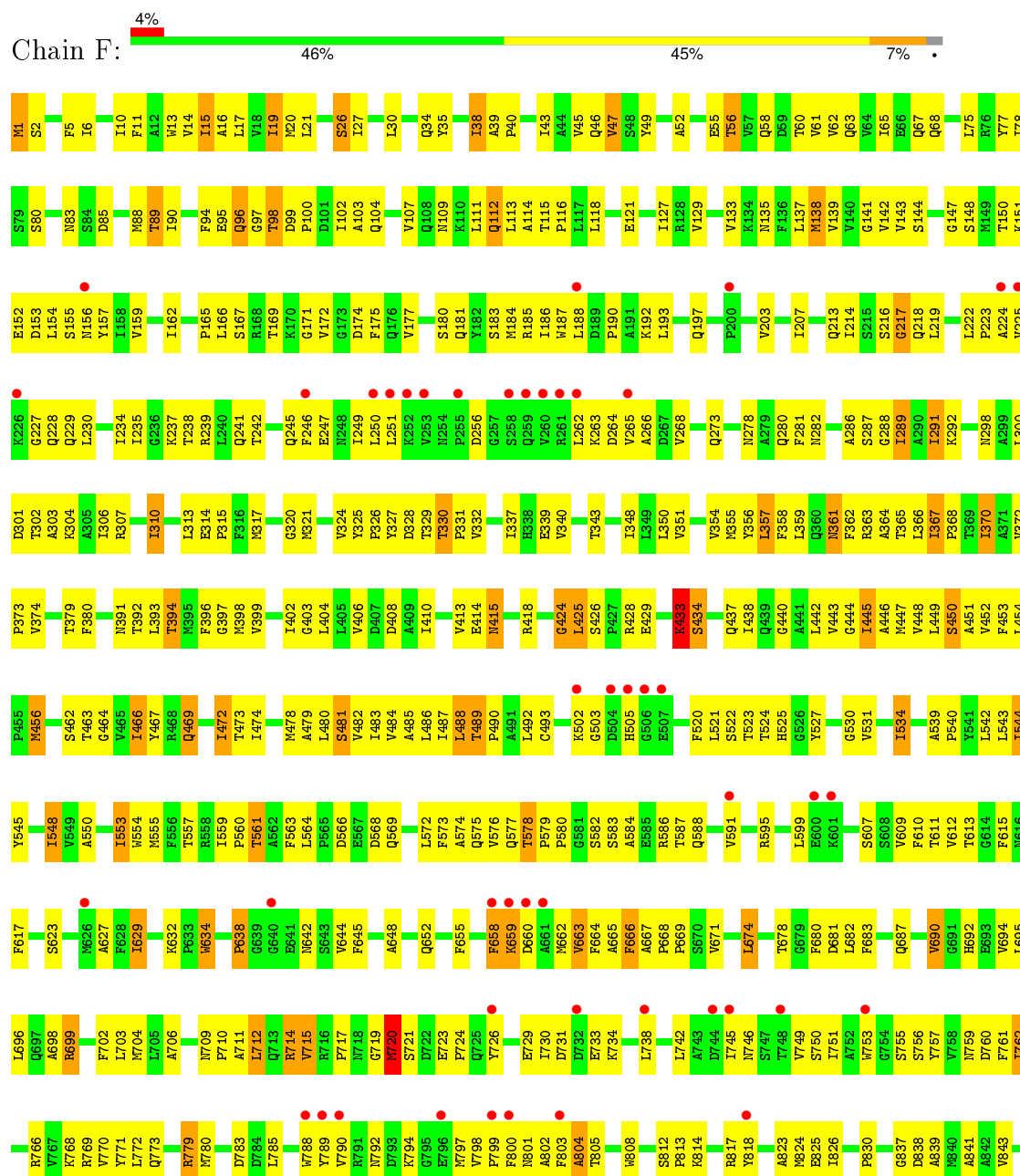
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB







● Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB



A1012	T932	I946
T1013	T933	I947
T1014	I934	
A1015	G935	G955
A1016	L936	Y956
T1017	S937	
F1018	A938	T959
W1019	K939	G960
P1020		
P1021	I942	L967
L1022	L943	
F1023	I944	A872
	V945	P873
	E946	A874
T1029		L875
L1030	I958	Y876
PHE	V959	A877
LVS		L878
ASP		S879
GLU	I963	A880
ALA	E964	L881
SER	A965	V882
LVS	G966	V883
GLN	G967	F884
GLN	M968	L885
ALA	R969	L886
SER	L970	
VAL	R971	C986
GLU	I972	
LVS	I973	A889
LVS		L890
GLY	T974	Y891
GLN	M975	E992
HIS	T976	
HIS	L977	I896
HIS	F978	P997
HIS	A979	
HIS	F980	L902
HIS	I981	V903
	L982	P904
	G983	P905
	V984	L906
	V985	G907
	P986	
		G910
	I989	A911
	S990	L912
	T991	
	G992	T915
	A993	
		L920
	Q998	S921
		N922
	I1001	D923
	I1002	V924
	G1005	F925
	V1005	F926
	I1006	Q927
		V928
	M1009	G929
	V1010	L930
	T1011	L931

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	125.05Å 134.58Å 151.02Å 86.99° 69.70° 88.16°	Depositor
Resolution (Å)	49.76 – 3.00 49.76 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.76-3.00) 95.2 (49.76-3.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 3.01Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.242 , 0.287 0.237 , 0.281	Depositor DCC
R_{free} test set	3536 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 66.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 176904 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	46628	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/7789	0.50	0/10588
1	B	0.30	0/7971	0.46	0/10833
1	C	0.27	0/7971	0.45	0/10833
1	D	0.30	0/7735	0.50	0/10510
1	E	0.29	0/7851	0.47	0/10666
1	F	0.28	0/7971	0.45	0/10833
All	All	0.29	0/47288	0.47	0/64263

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	7634	0	7765	689	0
1	B	7812	0	7944	541	0
1	C	7812	0	7944	509	0
1	D	7582	0	7716	665	0
1	E	7696	0	7832	528	0
1	F	7812	0	7944	509	0
2	A	35	0	46	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	105	0	138	17	0
2	D	35	0	46	5	0
2	E	105	0	138	22	0
All	All	46628	0	47513	3338	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 35.

All (3338) 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:76:ARG:HH11	1:A:76:ARG:HG2	1.09	1.13
1:B:43:ILE:HG21	1:B:107:VAL:HG11	1.30	1.12
1:A:375:VAL:HG21	1:A:405:LEU:HG	1.33	1.11
1:C:699:ARG:HH11	1:C:699:ARG:HG3	1.09	1.10
1:F:699:ARG:HH11	1:F:699:ARG:HG3	1.08	1.09
1:D:76:ARG:HH11	1:D:76:ARG:HG2	1.11	1.08
1:E:43:ILE:HG21	1:E:107:VAL:HG11	1.32	1.07
1:E:882:VAL:HG11	2:E:2032:LMT:H101	1.38	1.05
1:D:375:VAL:HG21	1:D:405:LEU:HG	1.33	1.05
1:B:410:ILE:HD11	1:B:976:THR:HG22	1.43	1.01
1:B:817:ARG:HG3	1:B:817:ARG:HH11	1.23	1.00
1:E:817:ARG:HG3	1:E:817:ARG:HH11	1.25	0.99
1:A:140:VAL:HG23	1:A:289:ILE:HG23	1.44	0.99
1:D:140:VAL:HG23	1:D:289:ILE:HG23	1.43	0.98
1:E:162:ILE:HG22	1:E:313:LEU:HD13	1.45	0.98
1:D:251:LEU:HD11	1:D:262:LEU:HB2	1.45	0.98
1:E:410:ILE:HD11	1:E:976:THR:HG22	1.43	0.97
1:F:485:ALA:HA	1:F:489:THR:HG23	1.45	0.97
1:E:234:ILE:HG22	1:F:726:TYR:HB2	1.45	0.96
1:A:568:ASP:HB3	1:A:634:TRP:CZ3	2.01	0.96
1:B:162:ILE:HG22	1:B:313:LEU:HD13	1.47	0.96
1:D:568:ASP:HB3	1:D:634:TRP:CZ3	2.00	0.95
1:C:485:ALA:HA	1:C:489:THR:HG23	1.48	0.95
1:E:442:LEU:HD23	1:E:445:ILE:HD11	1.51	0.93
1:A:56:THR:O	1:A:60:THR:HB	1.69	0.93
1:F:577:GLN:HB3	1:F:662:MET:HB2	1.50	0.92
1:D:156:ASN:HD22	1:D:182:TYR:H	0.92	0.92
1:C:577:GLN:HB3	1:C:662:MET:HB2	1.52	0.92
1:D:470:PHE:O	1:D:473:THR:HG22	1.70	0.92
1:A:730:ILE:HD11	1:C:237:LYS:HD3	1.50	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:966:CYS:SG	1:E:1021:PRO:HG3	2.11	0.91
1:A:318:PRO:HD2	1:A:321:MET:HE2	1.51	0.91
1:E:878:LEU:HD13	2:E:2032:LMT:H31	1.52	0.91
1:A:360:GLN:HE22	1:A:517:ASN:HD21	1.18	0.91
1:B:966:CYS:SG	1:B:1021:PRO:HG3	2.11	0.91
1:D:56:THR:O	1:D:60:THR:HB	1.69	0.91
1:A:757:TYR:HE2	1:A:769:ARG:HB3	1.35	0.91
1:B:442:LEU:HD23	1:B:445:ILE:HD11	1.53	0.91
1:E:435:MET:O	1:E:439:GLN:HB2	1.71	0.90
1:B:527:TYR:CD2	1:B:970:LEU:HD12	2.07	0.90
1:E:527:TYR:CD2	1:E:970:LEU:HD12	2.06	0.90
2:B:2032:LMT:H5B	2:B:2032:LMT:H6D	1.53	0.89
1:B:435:MET:O	1:B:439:GLN:HB2	1.72	0.89
1:D:569:GLN:H	1:D:634:TRP:HH2	1.16	0.89
1:A:253:VAL:HG12	1:A:259:GLN:HB3	1.52	0.89
1:D:76:ARG:HG2	1:D:76:ARG:NH1	1.85	0.88
1:A:569:GLN:H	1:A:634:TRP:HH2	1.17	0.88
1:D:680:PHE:HD1	1:D:828:GLY:O	1.57	0.88
1:A:242:THR:HG22	1:A:245:GLN:HE21	1.39	0.88
1:A:966:CYS:SG	1:A:1021:PRO:HG3	2.14	0.88
1:D:226:LYS:H	1:D:226:LYS:HD2	1.39	0.87
1:D:156:ASN:ND2	1:D:182:TYR:H	1.73	0.87
2:A:2026:LMT:H82	2:A:2026:LMT:H122	1.54	0.87
1:E:900:VAL:HG11	1:E:942:ILE:HG23	1.55	0.87
1:A:470:PHE:O	1:A:473:THR:HG22	1.75	0.87
1:D:966:CYS:SG	1:D:1021:PRO:HG3	2.15	0.87
1:A:733:GLU:HG2	1:C:250:LEU:HD11	1.56	0.86
1:D:730:ILE:HD11	1:F:237:LYS:HD3	1.56	0.86
1:D:757:TYR:HE2	1:D:769:ARG:HB3	1.38	0.86
1:E:125:GLN:NE2	1:E:769:ARG:HH12	1.73	0.86
1:A:831:ALA:HB3	1:A:834:LEU:HD22	1.56	0.86
1:E:560:PRO:HB2	1:E:921:SER:HB3	1.57	0.86
1:A:226:LYS:HD2	1:A:226:LYS:H	1.40	0.86
1:B:900:VAL:HG11	1:B:942:ILE:HG23	1.55	0.86
1:A:76:ARG:NH1	1:A:76:ARG:HG2	1.82	0.86
1:B:560:PRO:HB2	1:B:921:SER:HB3	1.57	0.86
1:A:498:LYS:H	1:A:499:PRO:CD	1.89	0.85
1:D:360:GLN:HE22	1:D:517:ASN:HD21	1.19	0.85
1:C:699:ARG:NH1	1:C:699:ARG:HG3	1.90	0.85
1:F:936:LEU:HD13	1:F:1009:MET:HG2	1.58	0.85
1:F:38:ILE:HG13	1:F:38:ILE:O	1.75	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:699:ARG:NH1	1:F:699:ARG:HG3	1.89	0.85
1:D:731:ASP:HB3	1:D:734:LYS:HB2	1.58	0.85
1:D:498:LYS:H	1:D:499:PRO:CD	1.88	0.85
1:C:166:LEU:HD12	1:C:289:ILE:HD12	1.57	0.85
1:B:125:GLN:NE2	1:B:769:ARG:HH12	1.75	0.85
1:C:38:ILE:O	1:C:38:ILE:HG13	1.76	0.85
1:C:936:LEU:HD13	1:C:1009:MET:HG2	1.58	0.84
1:B:247:GLU:HB3	1:B:263:LYS:HG2	1.57	0.84
1:A:706:ALA:HB2	1:A:846:ILE:HD13	1.59	0.84
1:A:680:PHE:HD1	1:A:828:GLY:O	1.58	0.84
2:E:2033:LMT:H62	2:E:2033:LMT:H122	1.57	0.84
1:B:234:ILE:HG22	1:C:726:TYR:HB2	1.60	0.84
1:E:247:GLU:HB3	1:E:263:LYS:HG2	1.59	0.84
1:A:56:THR:HG22	1:C:213:GLN:HB3	1.57	0.84
1:F:699:ARG:HH11	1:F:699:ARG:CG	1.91	0.83
1:E:520:PHE:HA	1:E:523:THR:HG22	1.60	0.83
1:A:731:ASP:HB3	1:A:734:LYS:HB2	1.58	0.83
1:F:472:ILE:HD13	1:F:472:ILE:H	1.43	0.83
1:E:158:ILE:HG22	1:E:162:ILE:HD11	1.61	0.83
1:F:166:LEU:HD12	1:F:289:ILE:HD12	1.60	0.83
1:B:520:PHE:HA	1:B:523:THR:HG22	1.61	0.83
1:D:156:ASN:HD22	1:D:182:TYR:N	1.76	0.82
1:D:242:THR:HG22	1:D:245:GLN:HE21	1.41	0.82
1:B:568:ASP:HB3	1:B:634:TRP:HZ3	1.44	0.82
1:A:540:PRO:O	1:A:544:ILE:HG22	1.79	0.82
1:E:428:ARG:HB3	1:E:432:ARG:HH21	1.42	0.82
1:C:159:VAL:HG22	1:C:177:VAL:HG11	1.59	0.82
1:F:241:GLN:HG2	1:F:762:ILE:HG13	1.60	0.82
1:D:540:PRO:O	1:D:544:ILE:HG22	1.80	0.82
1:C:241:GLN:HG2	1:C:762:ILE:HG13	1.59	0.82
1:A:76:ARG:CG	1:A:76:ARG:HH11	1.92	0.82
1:D:680:PHE:CE2	1:D:858:TRP:HZ3	1.96	0.81
1:C:138:MET:HB2	1:C:328:ASP:HA	1.62	0.81
1:D:733:GLU:HG2	1:F:250:LEU:HD11	1.60	0.81
1:D:228:GLN:HE21	1:D:230:LEU:H	1.26	0.81
1:A:808:TRP:CZ3	1:D:708:GLN:HB3	2.15	0.81
1:B:687:GLN:HE22	1:B:821:VAL:HG21	1.45	0.81
1:E:568:ASP:HB3	1:E:634:TRP:HZ3	1.44	0.81
1:A:699:ARG:NH2	1:A:824:MET:HG3	1.94	0.81
1:B:428:ARG:HB3	1:B:432:ARG:HH21	1.46	0.81
1:A:228:GLN:HE21	1:A:230:LEU:H	1.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:699:ARG:NH2	1:D:824:MET:HG3	1.95	0.81
1:C:544:ILE:HG12	1:C:1019:TRP:HH2	1.44	0.81
1:B:158:ILE:HD11	1:B:177:VAL:HG13	1.63	0.80
1:E:158:ILE:HD11	1:E:177:VAL:HG13	1.63	0.80
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.63	0.80
1:F:159:VAL:HG22	1:F:177:VAL:HG11	1.62	0.80
1:B:969:ARG:O	1:B:972:PRO:HD2	1.81	0.80
1:F:46:GLN:HG2	1:F:89:THR:HB	1.63	0.80
1:F:652:GLN:NE2	1:F:665:ALA:H	1.80	0.80
1:C:362:PHE:O	1:C:366:LEU:HB2	1.81	0.80
1:F:138:MET:HB2	1:F:328:ASP:HA	1.62	0.80
1:E:472:ILE:HD11	2:E:2031:LMT:H61	1.63	0.80
1:F:362:PHE:O	1:F:366:LEU:HB2	1.81	0.80
1:D:262:LEU:HD21	1:D:265:VAL:HB	1.64	0.80
1:B:938:ALA:O	1:B:942:ILE:HG12	1.82	0.80
1:E:213:GLN:HG3	1:E:239:ARG:HG3	1.62	0.80
1:F:574:ALA:HB3	1:F:627:ALA:HB3	1.64	0.80
1:F:544:ILE:HG12	1:F:1019:TRP:HH2	1.46	0.80
1:F:928:VAL:O	1:F:932:THR:HG22	1.82	0.79
1:A:419:VAL:HG23	1:A:430:ALA:HB1	1.62	0.79
1:C:928:VAL:O	1:C:932:THR:HG22	1.81	0.79
1:B:213:GLN:HG3	1:B:239:ARG:HG3	1.62	0.79
1:C:574:ALA:HB3	1:C:627:ALA:HB3	1.62	0.79
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.47	0.79
1:B:534:ILE:HG22	1:B:1022:LEU:HD23	1.64	0.79
1:A:234:ILE:HG22	1:B:726:TYR:HB3	1.65	0.79
1:B:703:LEU:HD11	1:B:717:PRO:HG3	1.64	0.79
1:C:472:ILE:H	1:C:472:ILE:HD13	1.46	0.79
1:E:938:ALA:O	1:E:942:ILE:HG12	1.82	0.79
2:A:2026:LMT:H6D	2:A:2026:LMT:H5B	1.62	0.79
2:E:2031:LMT:H6E	2:E:2031:LMT:H5B	1.65	0.79
1:C:652:GLN:NE2	1:C:665:ALA:H	1.79	0.79
1:B:428:ARG:H	1:B:428:ARG:HD2	1.49	0.78
1:D:352:PHE:HD1	1:D:369:THR:HG21	1.47	0.78
1:F:43:ILE:HD13	1:F:104:GLN:HA	1.65	0.78
1:A:757:TYR:CE2	1:A:769:ARG:HB3	2.19	0.78
1:E:583:SER:O	1:E:587:THR:HG22	1.84	0.78
1:D:634:TRP:H	1:D:634:TRP:HD1	1.31	0.78
1:A:170:LYS:HA	1:A:170:LYS:HE3	1.63	0.78
1:A:170:LYS:NZ	1:B:74:ASN:H	1.81	0.78
1:E:534:ILE:HG22	1:E:1022:LEU:HD23	1.63	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:HH11	1:D:76:ARG:CG	1.95	0.78
1:C:46:GLN:HG2	1:C:89:THR:HB	1.63	0.78
1:D:170:LYS:HE3	1:D:170:LYS:HA	1.65	0.78
1:D:170:LYS:NZ	1:E:74:ASN:H	1.80	0.78
1:D:56:THR:HG22	1:F:213:GLN:HB3	1.65	0.78
1:A:938:ALA:O	1:A:942:ILE:HG12	1.84	0.78
1:B:158:ILE:HG22	1:B:162:ILE:HD11	1.64	0.78
1:A:800:PHE:HD2	1:A:804:ALA:HB2	1.48	0.78
1:E:969:ARG:O	1:E:972:PRO:HD2	1.84	0.78
2:B:2032:LMT:C5B	2:B:2032:LMT:H6D	2.13	0.78
1:D:800:PHE:HD2	1:D:804:ALA:HB2	1.47	0.78
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.48	0.77
1:D:234:ILE:HG22	1:E:726:TYR:HB3	1.65	0.77
1:B:20:MET:HE2	1:B:374:VAL:HG23	1.66	0.77
1:A:237:LYS:HD2	1:B:730:ILE:HD11	1.66	0.77
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.65	0.77
1:F:485:ALA:HA	1:F:489:THR:CG2	2.14	0.77
1:B:125:GLN:HE22	1:B:769:ARG:HH12	1.32	0.77
1:C:938:ALA:O	1:C:942:ILE:HG23	1.84	0.77
1:D:616:ASN:ND2	1:D:626:MET:HB3	2.00	0.77
1:A:710:PRO:O	1:A:831:ALA:HB2	1.83	0.77
1:E:703:LEU:HD11	1:E:717:PRO:HG3	1.65	0.77
1:D:827:LEU:HD12	1:D:827:LEU:O	1.84	0.77
1:E:45:VAL:HB	1:E:90:ILE:HG23	1.67	0.77
1:A:634:TRP:HD1	1:A:634:TRP:H	1.32	0.77
1:D:90:ILE:HD12	1:D:91:THR:N	2.00	0.77
1:A:534:ILE:O	1:A:538:ARG:HB3	1.85	0.76
1:B:583:SER:O	1:B:587:THR:HG22	1.85	0.76
1:C:43:ILE:HD13	1:C:104:GLN:HA	1.66	0.76
1:E:891:TYR:CG	1:E:896:ILE:HD11	2.20	0.76
1:A:453:PHE:CD2	1:A:474:ILE:HD11	2.21	0.76
1:E:125:GLN:HE22	1:E:769:ARG:HH12	1.31	0.76
1:F:415:ASN:HD22	1:F:434:SER:HB3	1.50	0.76
1:B:817:ARG:HG3	1:B:817:ARG:NH1	1.99	0.76
1:A:708:GLN:HG2	1:D:809:GLU:HB3	1.66	0.76
1:E:614:GLY:HA2	1:E:621:GLY:O	1.86	0.76
1:E:751:ILE:HG21	1:E:772:LEU:HD13	1.67	0.76
1:A:616:ASN:ND2	1:A:626:MET:HB3	2.01	0.76
1:B:789:TYR:CE2	1:B:799:PRO:HG3	2.21	0.76
1:D:938:ALA:O	1:D:942:ILE:HG12	1.85	0.76
1:F:980:PHE:CD2	1:F:1009:MET:HG3	2.21	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HD22	1:C:434:SER:HB3	1.49	0.76
1:D:237:LYS:HD2	1:E:730:ILE:HD11	1.67	0.75
1:E:789:TYR:CE2	1:E:799:PRO:HG3	2.21	0.75
1:D:419:VAL:HG23	1:D:430:ALA:HB1	1.66	0.75
1:D:534:ILE:O	1:D:538:ARG:HB3	1.86	0.75
1:B:753:TRP:HZ2	1:B:785:LEU:HA	1.51	0.75
1:A:578:THR:CG2	1:A:579:PRO:HD2	2.17	0.75
1:C:524:THR:HG22	1:C:970:LEU:HD12	1.68	0.75
1:A:90:ILE:HD12	1:A:91:THR:N	2.01	0.75
1:E:293:LEU:HD23	1:E:302:THR:HG21	1.67	0.75
1:C:485:ALA:HA	1:C:489:THR:CG2	2.16	0.75
1:A:156:ASN:HD21	1:A:768:LYS:HZ1	1.33	0.75
1:F:524:THR:HG22	1:F:970:LEU:HD12	1.68	0.75
1:E:428:ARG:HD2	1:E:428:ARG:H	1.51	0.75
1:E:964:GLU:O	1:E:968:MET:HG3	1.86	0.75
1:D:757:TYR:CE2	1:D:769:ARG:HB3	2.21	0.75
1:C:699:ARG:CG	1:C:699:ARG:HH11	1.93	0.75
1:D:453:PHE:CD2	1:D:474:ILE:HD11	2.21	0.75
1:B:190:PRO:HG3	1:B:788:TRP:CZ2	2.22	0.75
1:C:980:PHE:CD2	1:C:1009:MET:HG3	2.22	0.75
1:A:680:PHE:CE2	1:A:858:TRP:HZ3	2.04	0.75
1:B:278:ASN:HB2	1:B:613:THR:HG22	1.69	0.74
1:F:938:ALA:O	1:F:942:ILE:HG23	1.84	0.74
1:F:943:LEU:HD13	1:F:973:ILE:HG22	1.68	0.74
1:A:827:LEU:HD12	1:A:827:LEU:O	1.87	0.74
1:A:318:PRO:HD2	1:A:321:MET:CE	2.17	0.74
1:D:682:LEU:HD21	1:D:856:TYR:HB2	1.69	0.74
1:A:723:GLU:HG3	1:A:813:PRO:HG3	1.69	0.74
1:A:682:LEU:HD21	1:A:856:TYR:HB2	1.67	0.74
1:B:751:ILE:HG21	1:B:772:LEU:HD13	1.68	0.74
1:B:602:GLU:OE2	1:B:650:ARG:HD2	1.88	0.74
1:E:753:TRP:HZ2	1:E:785:LEU:HA	1.52	0.74
1:F:566:ASP:HB3	1:F:645:PHE:CZ	2.23	0.74
1:C:943:LEU:HD13	1:C:973:ILE:HG22	1.70	0.74
1:B:470:PHE:O	1:B:474:ILE:HG23	1.88	0.74
1:A:671:VAL:HG13	1:A:672:LEU:N	2.02	0.74
1:F:548:ILE:HD11	1:F:906:LEU:HD23	1.69	0.74
1:D:918:ARG:HH21	1:D:1003:THR:HB	1.52	0.74
1:B:614:GLY:HA2	1:B:621:GLY:O	1.86	0.74
1:F:578:THR:HG22	1:F:623:SER:HB2	1.70	0.74
1:B:293:LEU:HD23	1:B:302:THR:HG21	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:980:PHE:HD2	1:F:1009:MET:HG3	1.52	0.73
1:B:45:VAL:HB	1:B:90:ILE:HG23	1.68	0.73
1:C:544:ILE:HG12	1:C:1019:TRP:CH2	2.23	0.73
1:D:637:ARG:N	1:D:638:PRO:HD3	2.02	0.73
1:E:186:ILE:HD11	1:E:772:LEU:HG	1.69	0.73
1:E:470:PHE:O	1:E:474:ILE:HG23	1.88	0.73
1:F:563:PHE:O	1:F:923:ASP:HB2	1.89	0.73
1:C:980:PHE:HD2	1:C:1009:MET:HG3	1.52	0.73
1:C:434:SER:O	1:C:438:ILE:HG12	1.87	0.73
1:B:964:GLU:O	1:B:968:MET:HG3	1.88	0.73
1:A:637:ARG:N	1:A:638:PRO:HD3	2.03	0.73
1:A:259:GLN:H	1:A:259:GLN:HE21	1.36	0.73
1:D:498:LYS:H	1:D:499:PRO:HD2	1.53	0.73
1:A:527:TYR:O	1:A:531:VAL:HG23	1.87	0.73
1:A:448:VAL:HG22	1:A:886:CYS:HB3	1.70	0.73
1:E:681:ASP:HB3	1:E:827:LEU:HD13	1.69	0.73
1:E:58:GLN:O	1:E:63:GLN:HG3	1.88	0.73
1:A:723:GLU:CG	1:A:813:PRO:HG3	2.19	0.73
1:B:58:GLN:O	1:B:63:GLN:HG3	1.89	0.73
1:E:190:PRO:HG3	1:E:788:TRP:CZ2	2.24	0.73
1:D:405:LEU:HD22	1:D:406:VAL:N	2.03	0.73
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.52	0.73
1:D:319:GLN:H	1:D:319:GLN:CD	1.91	0.73
1:A:451:ALA:HB1	1:A:882:VAL:HG12	1.69	0.73
1:E:451:ALA:O	1:E:879:SER:HB2	1.88	0.73
1:F:184:MET:HB2	1:F:770:VAL:HG12	1.71	0.73
1:D:742:LEU:H	1:D:742:LEU:HD12	1.54	0.73
1:E:278:ASN:HB2	1:E:613:THR:HG22	1.70	0.73
1:D:451:ALA:HB1	1:D:882:VAL:HG12	1.71	0.73
1:E:78:ILE:HD11	1:E:90:ILE:HD11	1.71	0.72
1:F:434:SER:O	1:F:438:ILE:HG12	1.88	0.72
1:D:437:GLN:O	1:D:438:ILE:HG13	1.88	0.72
1:C:566:ASP:HB3	1:C:645:PHE:CZ	2.23	0.72
1:B:451:ALA:O	1:B:879:SER:HB2	1.89	0.72
1:D:574:ALA:HB3	1:D:627:ALA:HB3	1.71	0.72
1:D:680:PHE:CE2	1:D:858:TRP:CZ3	2.77	0.72
1:A:708:GLN:HG3	1:D:807:LYS:HE2	1.72	0.72
1:C:548:ILE:HD11	1:C:906:LEU:HD23	1.69	0.72
1:B:676:ASN:HD21	1:B:827:LEU:HD12	1.52	0.72
1:F:753:TRP:CZ2	1:F:785:LEU:HD23	2.24	0.72
1:C:563:PHE:O	1:C:923:ASP:HB2	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:THR:CG2	1:D:579:PRO:HD2	2.18	0.72
1:D:448:VAL:HG22	1:D:886:CYS:HB3	1.71	0.72
1:C:291:ILE:HD12	1:C:306:ILE:HD12	1.72	0.72
1:A:437:GLN:O	1:A:438:ILE:HG13	1.90	0.72
1:B:615:PHE:HE1	2:B:2033:LMT:H111	1.55	0.72
1:C:399:VAL:O	1:C:402:ILE:HG13	1.90	0.72
1:A:742:LEU:H	1:A:742:LEU:HD12	1.55	0.72
1:D:156:ASN:HA	1:D:181:GLN:HA	1.72	0.72
1:A:498:LYS:H	1:A:499:PRO:HD2	1.53	0.72
1:B:186:ILE:HD11	1:B:772:LEU:HG	1.70	0.72
1:B:229:GLN:HA	1:C:583:SER:HB3	1.72	0.72
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.71	0.72
1:E:940:ASN:O	1:E:944:ILE:HG23	1.90	0.72
1:C:133:VAL:HG12	1:C:135:ASN:H	1.55	0.72
1:B:78:ILE:HD11	1:B:90:ILE:HD11	1.70	0.71
1:A:189:ASP:O	1:A:193:LEU:HD23	1.90	0.71
1:A:273:GLN:CD	1:A:769:ARG:HD2	2.11	0.71
1:F:544:ILE:HG12	1:F:1019:TRP:CH2	2.24	0.71
2:B:2031:LMT:O5B	2:B:2031:LMT:H6E	1.91	0.71
1:A:405:LEU:HD22	1:A:406:VAL:N	2.06	0.71
1:C:138:MET:SD	1:C:291:ILE:HD11	2.30	0.71
1:D:233:THR:HG23	1:E:725:GLN:HG2	1.72	0.71
1:F:580:PRO:HB3	1:F:723:GLU:HG2	1.71	0.71
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.73	0.71
1:C:753:TRP:CZ2	1:C:785:LEU:HD23	2.25	0.71
1:C:184:MET:HB2	1:C:770:VAL:HG12	1.72	0.71
1:C:572:LEU:HD23	1:C:573:PHE:H	1.55	0.71
1:A:918:ARG:HH21	1:A:1003:THR:HB	1.53	0.71
1:C:364:ALA:O	1:C:367:ILE:HG12	1.91	0.71
1:D:273:GLN:CD	1:D:769:ARG:HD2	2.11	0.71
1:D:723:GLU:CG	1:D:813:PRO:HG3	2.21	0.71
1:B:847:VAL:HG11	1:B:856:TYR:CD1	2.26	0.71
1:B:891:TYR:CG	1:B:896:ILE:HD11	2.25	0.71
1:E:228:GLN:HG2	1:F:583:SER:HB2	1.73	0.71
1:B:940:ASN:O	1:B:944:ILE:HG23	1.91	0.71
1:E:414:GLU:HG2	1:E:972:PRO:HG3	1.73	0.71
1:F:291:ILE:HD12	1:F:306:ILE:HD12	1.73	0.71
1:E:847:VAL:HG11	1:E:856:TYR:CD1	2.26	0.71
1:D:213:GLN:HG3	1:E:56:THR:HG23	1.71	0.71
1:F:133:VAL:HG12	1:F:135:ASN:H	1.56	0.71
1:F:364:ALA:O	1:F:367:ILE:HG12	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:723:GLU:HG3	1:D:813:PRO:HG3	1.72	0.70
1:C:578:THR:HG22	1:C:623:SER:HB2	1.71	0.70
1:C:985:VAL:HG23	1:C:986:PRO:HD3	1.73	0.70
1:F:399:VAL:O	1:F:402:ILE:HG13	1.91	0.70
1:E:821:VAL:HG12	1:E:822:PRO:HD2	1.73	0.70
1:E:682:LEU:HD11	1:E:856:TYR:HB2	1.72	0.70
1:B:542:LEU:HG	1:B:1022:LEU:HD11	1.73	0.70
1:B:821:VAL:HG12	1:B:822:PRO:HD2	1.73	0.70
1:E:602:GLU:OE2	1:E:650:ARG:HD2	1.90	0.70
1:A:17:LEU:HD21	2:A:2026:LMT:H61	1.73	0.70
1:B:38:ILE:O	1:B:462:SER:HB3	1.92	0.70
1:A:671:VAL:HG13	1:A:672:LEU:H	1.57	0.70
1:A:532:ALA:O	1:A:534:ILE:N	2.25	0.70
1:A:535:LEU:CD2	1:A:959:VAL:HG13	2.21	0.70
1:B:215:SER:HB2	1:C:750:SER:HB2	1.73	0.70
1:A:233:THR:HG23	1:B:725:GLN:HG2	1.72	0.70
1:E:987:LEU:HD22	1:E:998:GLN:HB3	1.74	0.70
1:D:32:VAL:HG11	1:D:337:ILE:HD13	1.74	0.70
1:C:542:LEU:HD21	1:C:1022:LEU:HD21	1.72	0.70
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.73	0.70
1:E:142:VAL:HG11	1:E:158:ILE:HG21	1.74	0.70
1:C:364:ALA:HA	1:C:367:ILE:HD11	1.74	0.70
1:D:928:VAL:O	1:D:932:THR:HG23	1.91	0.70
1:D:17:LEU:HD21	2:D:2026:LMT:H52	1.74	0.70
1:F:364:ALA:HA	1:F:367:ILE:HD11	1.72	0.70
1:B:560:PRO:HB2	1:B:921:SER:CB	2.22	0.70
1:D:535:LEU:CD2	1:D:959:VAL:HG13	2.22	0.70
1:B:4:PHE:O	1:B:8:ARG:HG3	1.92	0.70
1:C:47:VAL:HB	1:C:127:ILE:HG23	1.74	0.70
1:F:572:LEU:HD23	1:F:573:PHE:H	1.57	0.70
1:C:580:PRO:HB3	1:C:723:GLU:HG2	1.72	0.70
1:D:203:VAL:HG12	1:D:207:ILE:HD11	1.74	0.69
1:F:542:LEU:HD21	1:F:1022:LEU:HD21	1.74	0.69
1:B:142:VAL:HG11	1:B:158:ILE:HG21	1.73	0.69
1:F:472:ILE:HD13	1:F:472:ILE:N	2.07	0.69
1:D:532:ALA:O	1:D:534:ILE:N	2.25	0.69
1:E:20:MET:HE2	1:E:374:VAL:HG23	1.72	0.69
1:B:987:LEU:HD22	1:B:998:GLN:HB3	1.74	0.69
1:A:680:PHE:CE2	1:A:858:TRP:CZ3	2.80	0.69
1:B:929:GLY:O	1:B:932:THR:HG22	1.92	0.69
1:F:47:VAL:HG12	1:F:88:MET:HE3	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:MET:HE3	1:F:224:ALA:HA	1.73	0.69
1:E:38:ILE:O	1:E:462:SER:HB3	1.93	0.69
1:A:32:VAL:HG11	1:A:337:ILE:HD13	1.75	0.69
1:A:928:VAL:O	1:A:932:THR:HG23	1.91	0.69
1:D:224:ALA:HB1	1:E:780:MET:HE1	1.73	0.69
2:B:2033:LMT:H122	2:B:2033:LMT:H62	1.73	0.69
1:A:574:ALA:HB3	1:A:627:ALA:HB3	1.75	0.69
1:B:402:ILE:HA	1:B:405:LEU:HB2	1.74	0.69
1:E:971:ARG:HB3	1:E:972:PRO:HD3	1.75	0.69
1:D:724:PRO:HA	1:D:810:TYR:HB2	1.75	0.69
1:A:545:TYR:HB2	1:A:1019:TRP:CZ3	2.28	0.69
1:D:684:LEU:O	1:D:823:ALA:HB1	1.93	0.69
1:F:910:GLY:HA3	1:F:1011:THR:CG2	2.23	0.69
1:D:904:VAL:HB	1:D:905:PRO:HD3	1.73	0.69
1:E:133:VAL:HG23	1:E:135:ASN:OD1	1.93	0.69
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.55	0.69
1:D:568:ASP:HB3	1:D:634:TRP:HZ3	1.54	0.69
1:E:560:PRO:HB2	1:E:921:SER:CB	2.21	0.69
1:C:910:GLY:HA3	1:C:1011:THR:CG2	2.22	0.69
1:E:4:PHE:O	1:E:8:ARG:HG3	1.92	0.69
1:E:402:ILE:HA	1:E:405:LEU:HB2	1.75	0.69
1:E:742:LEU:O	1:E:745:ILE:HG22	1.92	0.69
1:C:561:THR:HG23	1:C:837:GLY:HA3	1.75	0.69
2:E:2032:LMT:H5B	2:E:2032:LMT:H6D	1.75	0.69
1:D:680:PHE:HE2	1:D:858:TRP:CZ3	2.09	0.69
1:A:538:ARG:HA	1:A:541:TYR:HD1	1.57	0.69
1:C:520:PHE:HA	1:C:523:THR:HG22	1.75	0.69
1:D:194:ASN:ND2	1:D:797:MET:HG2	2.08	0.69
1:D:300:LEU:HD21	1:D:333:VAL:HB	1.74	0.69
1:F:47:VAL:HB	1:F:127:ILE:HG23	1.73	0.69
1:F:96:GLN:NE2	1:F:462:SER:HB3	2.07	0.69
1:A:634:TRP:N	1:A:634:TRP:CD1	2.62	0.68
1:D:527:TYR:O	1:D:531:VAL:HG23	1.93	0.68
1:E:158:ILE:HA	1:E:162:ILE:HG12	1.76	0.68
1:E:88:MET:HG2	1:E:89:THR:N	2.08	0.68
1:A:724:PRO:HA	1:A:810:TYR:HB2	1.73	0.68
1:B:414:GLU:HG2	1:B:972:PRO:HG3	1.74	0.68
1:D:634:TRP:CD1	1:D:634:TRP:N	2.61	0.68
1:E:428:ARG:CB	1:E:432:ARG:HH21	2.05	0.68
1:C:472:ILE:N	1:C:472:ILE:HD13	2.09	0.68
1:F:818:TYR:HH	1:F:825:GLU:HB2	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:830:PRO:HB3	1:F:839:ALA:HB2	1.74	0.68
1:C:830:PRO:HB3	1:C:839:ALA:HB2	1.73	0.68
1:E:817:ARG:HG3	1:E:817:ARG:NH1	2.01	0.68
1:E:442:LEU:CD2	1:E:445:ILE:HD11	2.22	0.68
1:C:1016:ALA:O	1:C:1020:VAL:HG23	1.94	0.68
1:F:966:CYS:SG	1:F:1021:PRO:HG3	2.34	0.68
1:F:985:VAL:HG23	1:F:986:PRO:HD3	1.74	0.68
1:F:138:MET:SD	1:F:291:ILE:HD11	2.33	0.68
1:D:538:ARG:HA	1:D:541:TYR:HD1	1.58	0.68
1:F:682:LEU:HD11	1:F:843:VAL:HG11	1.75	0.68
1:E:929:GLY:O	1:E:932:THR:HG22	1.92	0.68
1:A:280:GLN:HB2	1:A:284:SER:O	1.94	0.68
1:A:224:ALA:HB1	1:B:780:MET:HE1	1.76	0.68
2:A:2026:LMT:O2'	2:A:2026:LMT:H11	1.93	0.68
1:C:545:TYR:HB2	1:C:1019:TRP:CZ3	2.29	0.68
2:B:2031:LMT:H6E	2:B:2031:LMT:C5B	2.23	0.68
1:B:959:VAL:O	1:B:963:ILE:HG22	1.94	0.68
1:E:47:VAL:HG13	1:E:127:ILE:HA	1.75	0.68
1:D:545:TYR:HB2	1:D:1019:TRP:CZ3	2.28	0.68
1:E:637:ARG:HB2	1:E:642:ASN:HB3	1.76	0.68
1:A:47:VAL:HG22	1:A:48:SER:H	1.59	0.68
1:A:578:THR:HG23	1:A:579:PRO:HD2	1.76	0.67
1:B:742:LEU:O	1:B:745:ILE:HG22	1.94	0.67
1:F:561:THR:HG23	1:F:837:GLY:HA3	1.74	0.67
1:B:158:ILE:HA	1:B:162:ILE:HG12	1.75	0.67
1:F:1016:ALA:O	1:F:1020:VAL:HG23	1.94	0.67
1:B:228:GLN:HG2	1:C:583:SER:HB2	1.75	0.67
1:A:300:LEU:HD21	1:A:333:VAL:HB	1.76	0.67
1:A:254:ASN:ND2	1:A:258:SER:HB3	2.08	0.67
1:A:838:ASP:HA	1:A:842:ALA:HB3	1.77	0.67
1:A:569:GLN:NE2	1:A:670:SER:HA	2.09	0.67
1:A:904:VAL:HB	1:A:905:PRO:HD3	1.75	0.67
1:A:156:ASN:HD21	1:A:768:LYS:NZ	1.91	0.67
1:D:838:ASP:HA	1:D:842:ALA:HB3	1.76	0.67
1:A:376:LEU:O	1:A:379:THR:HG22	1.95	0.67
1:B:88:MET:HG2	1:B:89:THR:N	2.10	0.67
1:B:328:ASP:OD1	1:B:330:THR:HG23	1.95	0.67
1:B:35:TYR:CE1	1:B:392:THR:HG21	2.29	0.67
1:E:959:VAL:O	1:E:963:ILE:HG22	1.94	0.67
1:F:367:ILE:HG12	1:F:368:PRO:HD3	1.77	0.67
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:LEU:HB3	1:C:982:LEU:HD12	1.76	0.67
1:D:280:GLN:HB2	1:D:284:SER:O	1.94	0.67
1:E:125:GLN:HE22	1:E:769:ARG:NH1	1.92	0.67
1:F:520:PHE:HA	1:F:523:THR:HG22	1.75	0.67
1:E:169:THR:HG21	1:E:309:THR:OG1	1.95	0.67
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.59	0.67
1:F:545:TYR:HB2	1:F:1019:TRP:CZ3	2.30	0.67
1:E:186:ILE:HG22	1:E:268:VAL:HG22	1.77	0.67
1:C:554:TRP:O	1:C:557:THR:HG22	1.94	0.67
1:D:753:TRP:CZ3	1:D:779:ARG:HB3	2.29	0.67
1:B:602:GLU:HG3	1:B:650:ARG:NH1	2.10	0.67
1:D:523:THR:OG1	1:D:524:THR:N	2.28	0.67
1:A:808:TRP:O	1:D:705:LEU:HD22	1.95	0.67
1:D:189:ASP:O	1:D:193:LEU:HD23	1.95	0.66
1:E:542:LEU:HG	1:E:1022:LEU:HD11	1.75	0.66
1:B:712:LEU:HD21	1:B:843:VAL:HG23	1.78	0.66
1:C:682:LEU:HD11	1:C:843:VAL:HG11	1.76	0.66
1:E:35:TYR:CE1	1:E:392:THR:HG21	2.29	0.66
1:A:845:GLU:O	1:A:848:LYS:HB3	1.95	0.66
1:F:959:VAL:O	1:F:963:ILE:HG23	1.93	0.66
1:B:47:VAL:HG13	1:B:127:ILE:HA	1.75	0.66
1:F:350:LEU:HB3	1:F:982:LEU:HD12	1.76	0.66
1:A:791:ARG:HB2	1:A:797:MET:HE2	1.77	0.66
1:B:428:ARG:CB	1:B:432:ARG:HH21	2.08	0.66
1:F:554:TRP:O	1:F:557:THR:HG22	1.95	0.66
1:C:648:ALA:HB1	1:C:714:ARG:HH12	1.61	0.66
1:B:472:ILE:HD11	2:B:2031:LMT:H61	1.78	0.66
1:B:14:VAL:HG11	1:C:889:ALA:HB2	1.77	0.66
1:D:193:LEU:CD2	1:D:265:VAL:HG13	2.26	0.66
1:D:680:PHE:CD1	1:D:828:GLY:O	2.46	0.66
1:F:43:ILE:HD11	1:F:107:VAL:HB	1.78	0.66
1:D:892:GLU:C	1:F:10:ILE:HD11	2.16	0.66
1:C:218:GLN:HA	1:C:234:ILE:HG23	1.75	0.66
1:D:400:LEU:HD12	1:D:470:PHE:HZ	1.60	0.66
1:B:442:LEU:CD2	1:B:445:ILE:HD11	2.25	0.66
1:A:400:LEU:HD12	1:A:470:PHE:HZ	1.60	0.66
1:A:895:SER:C	1:A:897:PRO:HD2	2.16	0.66
1:C:96:GLN:NE2	1:C:462:SER:HB3	2.10	0.66
1:B:72:ILE:HD11	1:B:75:LEU:HD13	1.76	0.66
1:D:695:LEU:CD1	1:D:699:ARG:HH21	2.08	0.66
1:F:891:TYR:CB	1:F:896:ILE:HD11	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PHE:CE1	2:B:2033:LMT:H111	2.31	0.66
1:D:213:GLN:HE21	1:D:239:ARG:HG2	1.61	0.66
1:F:339:GLU:O	1:F:343:THR:HG22	1.95	0.66
2:D:2026:LMT:H6D	2:D:2026:LMT:O5B	1.96	0.66
1:A:710:PRO:HD3	1:D:807:LYS:HE3	1.77	0.66
1:A:810:TYR:OH	1:D:701:LYS:HG2	1.96	0.66
1:A:254:ASN:HD21	1:A:258:SER:HB3	1.60	0.66
1:F:372:VAL:HB	1:F:373:PRO:HD3	1.78	0.66
1:B:753:TRP:CZ2	1:B:785:LEU:HG	2.31	0.66
1:D:47:VAL:HG22	1:D:48:SER:H	1.61	0.66
1:A:810:TYR:CE2	1:D:701:LYS:HE3	2.31	0.66
1:C:367:ILE:HG12	1:C:368:PRO:HD3	1.78	0.65
1:D:723:GLU:O	1:D:810:TYR:HB2	1.97	0.65
1:F:447:MET:CE	1:F:886:CYS:HB3	2.26	0.65
1:B:637:ARG:HB2	1:B:642:ASN:HB3	1.77	0.65
1:E:712:LEU:HD21	1:E:843:VAL:HG23	1.77	0.65
1:C:15:ILE:O	1:C:19:ILE:HG23	1.96	0.65
1:A:753:TRP:CZ3	1:A:779:ARG:HB3	2.30	0.65
1:A:684:LEU:O	1:A:823:ALA:HB1	1.96	0.65
1:D:941:ALA:O	1:D:945:VAL:HG12	1.97	0.65
1:B:186:ILE:HG22	1:B:268:VAL:HG22	1.78	0.65
1:B:169:THR:HG21	1:B:309:THR:OG1	1.96	0.65
2:E:2033:LMT:H71	2:E:2033:LMT:H111	1.78	0.65
1:A:213:GLN:HE21	1:A:239:ARG:HG2	1.61	0.65
1:C:683:PHE:O	1:C:856:TYR:HA	1.97	0.65
1:D:563:PHE:O	1:D:564:LEU:HB2	1.96	0.65
1:A:563:PHE:O	1:A:564:LEU:HB2	1.97	0.65
1:A:808:TRP:CH2	1:D:708:GLN:HB3	2.31	0.65
1:F:80:SER:OG	1:F:817:ARG:HB2	1.96	0.65
1:C:80:SER:OG	1:C:817:ARG:HB2	1.96	0.65
1:C:247:GLU:HB3	1:C:263:LYS:HG2	1.79	0.65
1:E:328:ASP:OD1	1:E:330:THR:HG23	1.95	0.65
1:D:908:VAL:O	1:D:911:ALA:HB3	1.96	0.65
1:C:447:MET:CE	1:C:886:CYS:HB3	2.26	0.65
1:D:753:TRP:HZ3	1:D:779:ARG:HB3	1.62	0.65
1:A:134:LYS:HD3	1:A:672:LEU:HD12	1.78	0.65
1:C:488:LEU:HD13	1:C:492:LEU:HD11	1.77	0.65
1:C:1011:THR:O	1:C:1015:LEU:HB2	1.97	0.65
1:D:2:SER:O	1:D:6:ILE:HD12	1.96	0.65
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.78	0.65
1:C:445:ILE:HG22	1:C:939:LYS:HG2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:578:THR:HG23	1:D:579:PRO:HD2	1.78	0.65
1:D:845:GLU:O	1:D:848:LYS:HB3	1.97	0.65
1:C:444:GLY:O	1:C:448:VAL:HG23	1.97	0.65
1:A:695:LEU:CD1	1:A:699:ARG:HH21	2.09	0.65
1:F:683:PHE:O	1:F:856:TYR:HA	1.97	0.65
1:D:241:GLN:HG3	1:D:762:ILE:O	1.96	0.65
1:E:602:GLU:HG3	1:E:650:ARG:NH1	2.11	0.65
1:C:959:VAL:O	1:C:963:ILE:HG23	1.97	0.65
1:D:329:THR:O	1:D:332:VAL:HG12	1.97	0.65
1:B:125:GLN:HE22	1:B:769:ARG:NH1	1.94	0.64
1:C:966:CYS:SG	1:C:1021:PRO:HG3	2.36	0.64
1:F:648:ALA:HB1	1:F:714:ARG:HH12	1.63	0.64
1:B:718:ASN:HB2	1:B:827:LEU:HD23	1.79	0.64
1:A:302:THR:O	1:A:306:ILE:HG23	1.97	0.64
1:E:215:SER:HB2	1:F:750:SER:HB2	1.80	0.64
1:C:339:GLU:O	1:C:343:THR:HG22	1.96	0.64
1:B:391:ASN:HD22	1:B:393:LEU:H	1.45	0.64
1:D:996:GLY:N	1:D:999:HIS:HD2	1.95	0.64
1:A:969:ARG:O	1:A:973:ILE:HG12	1.97	0.64
1:E:757:TYR:CE1	1:E:769:ARG:HG3	2.32	0.64
1:B:478:MET:O	1:B:482:VAL:HG23	1.97	0.64
1:A:893:SER:OG	1:A:896:ILE:HG23	1.97	0.64
1:D:893:SER:OG	1:D:896:ILE:HG23	1.97	0.64
1:F:969:ARG:O	1:F:973:ILE:HG23	1.97	0.64
1:A:157:TYR:OH	1:A:317:MET:HG2	1.96	0.64
1:F:910:GLY:HA3	1:F:1011:THR:HG21	1.79	0.64
1:A:723:GLU:O	1:A:810:TYR:HB2	1.97	0.64
1:A:726:TYR:CZ	1:A:782:PRO:HB3	2.32	0.64
1:D:376:LEU:O	1:D:379:THR:HG22	1.97	0.64
1:D:302:THR:O	1:D:306:ILE:HG23	1.97	0.64
1:C:332:VAL:HG11	1:C:569:GLN:HG2	1.80	0.64
1:E:718:ASN:HB2	1:E:827:LEU:HD23	1.78	0.64
1:C:251:LEU:HD12	1:C:265:VAL:HG21	1.80	0.64
1:C:699:ARG:NE	1:C:824:MET:HG2	2.13	0.64
1:B:757:TYR:CE1	1:B:769:ARG:HG3	2.33	0.64
1:F:683:PHE:CE2	1:F:818:TYR:CZ	2.86	0.64
1:A:48:SER:O	1:A:125:GLN:HG2	1.98	0.64
1:A:43:ILE:HG21	1:A:107:VAL:HG11	1.80	0.64
1:F:488:LEU:HD13	1:F:492:LEU:HD11	1.79	0.64
1:F:472:ILE:CD1	1:F:472:ILE:H	2.11	0.64
1:C:910:GLY:HA3	1:C:1011:THR:HG21	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:818:TYR:HH	1:C:825:GLU:HB2	1.62	0.64
1:A:134:LYS:HD3	1:A:672:LEU:C	2.18	0.64
1:A:680:PHE:HE2	1:A:858:TRP:CZ3	2.14	0.64
1:E:753:TRP:CZ2	1:E:785:LEU:HG	2.32	0.64
1:D:48:SER:O	1:D:125:GLN:HG2	1.97	0.64
1:C:43:ILE:HD11	1:C:107:VAL:HB	1.78	0.64
1:A:342:LYS:O	1:A:346:GLU:HG3	1.97	0.64
1:E:72:ILE:HD11	1:E:75:LEU:HD13	1.80	0.64
1:A:241:GLN:HG3	1:A:762:ILE:O	1.97	0.64
1:E:104:GLN:NE2	1:E:131:LYS:HE2	2.12	0.64
1:A:669:PRO:HB2	1:A:671:VAL:HG12	1.79	0.64
1:C:891:TYR:CB	1:C:896:ILE:HD11	2.27	0.64
1:C:903:VAL:HG21	1:C:1020:VAL:HG22	1.80	0.64
1:D:780:MET:SD	1:F:228:GLN:HG3	2.37	0.64
1:F:818:TYR:OH	1:F:825:GLU:HB2	1.97	0.64
1:C:969:ARG:O	1:C:972:PRO:HD2	1.98	0.63
1:C:818:TYR:OH	1:C:825:GLU:HB2	1.98	0.63
1:D:602:GLU:HG3	1:D:647:LEU:HD21	1.80	0.63
1:B:971:ARG:HB3	1:B:972:PRO:HD3	1.78	0.63
1:F:896:ILE:HB	1:F:945:VAL:HG11	1.80	0.63
1:B:386:PHE:CE2	2:B:2031:LMT:H81	2.33	0.63
1:F:247:GLU:HB3	1:F:263:LYS:HG2	1.80	0.63
1:F:332:VAL:HG11	1:F:569:GLN:HG2	1.80	0.63
1:E:971:ARG:O	1:E:975:MET:HG2	1.98	0.63
1:A:941:ALA:O	1:A:945:VAL:HG12	1.97	0.63
1:E:895:SER:C	1:E:897:PRO:HD2	2.19	0.63
1:C:683:PHE:CE2	1:C:818:TYR:CZ	2.86	0.63
1:D:247:GLU:HA	1:D:262:LEU:O	1.98	0.63
1:F:213:GLN:HE21	1:F:239:ARG:HB2	1.64	0.63
1:A:523:THR:OG1	1:A:524:THR:N	2.28	0.63
1:D:895:SER:C	1:D:897:PRO:HD2	2.18	0.63
1:F:447:MET:HE3	1:F:886:CYS:HB3	1.80	0.63
1:B:164:ASP:HB2	1:C:67:GLN:NE2	2.12	0.63
1:E:14:VAL:HG11	1:F:889:ALA:HB2	1.81	0.63
1:F:361:ASN:O	1:F:365:THR:HG22	1.99	0.63
1:F:445:ILE:HG22	1:F:939:LYS:HG2	1.81	0.63
1:D:43:ILE:HG21	1:D:107:VAL:HG11	1.79	0.63
1:B:104:GLN:NE2	1:B:131:LYS:HE2	2.13	0.63
1:A:193:LEU:CD2	1:A:265:VAL:HG13	2.29	0.63
1:F:969:ARG:O	1:F:972:PRO:HD2	1.99	0.63
1:B:718:ASN:HB2	1:B:827:LEU:CD2	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:963:ILE:HG13	1:F:964:GLU:N	2.14	0.63
1:E:466:ILE:HD11	1:E:924:VAL:HG21	1.81	0.63
1:F:699:ARG:NE	1:F:824:MET:HG2	2.14	0.63
1:B:541:TYR:HA	1:B:544:ILE:HG23	1.80	0.63
1:F:218:GLN:HA	1:F:234:ILE:HG23	1.80	0.63
1:A:908:VAL:O	1:A:911:ALA:HB3	1.99	0.63
1:D:726:TYR:CZ	1:D:782:PRO:HB3	2.34	0.63
1:B:527:TYR:CE2	1:B:966:CYS:HB3	2.33	0.63
1:A:680:PHE:CD1	1:A:828:GLY:O	2.47	0.63
1:C:361:ASN:O	1:C:365:THR:HG22	1.99	0.63
1:E:229:GLN:HA	1:F:583:SER:HB3	1.80	0.63
1:F:15:ILE:O	1:F:19:ILE:HG23	1.99	0.63
1:D:528:GLU:OE2	1:D:967:ARG:CZ	2.47	0.62
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.81	0.62
1:A:188:LEU:HD23	1:A:266:ALA:HB2	1.81	0.62
1:D:342:LYS:O	1:D:346:GLU:HG3	1.99	0.62
1:A:319:GLN:H	1:A:319:GLN:CD	2.03	0.62
1:E:49:TYR:CE1	1:E:121:GLU:HG3	2.34	0.62
1:A:602:GLU:HG3	1:A:647:LEU:HD21	1.81	0.62
1:D:985:VAL:HA	1:D:1006:ILE:HD11	1.81	0.62
1:D:156:ASN:HD21	1:D:768:LYS:NZ	1.96	0.62
1:A:892:GLU:C	1:C:10:ILE:HD11	2.19	0.62
1:E:478:MET:O	1:E:482:VAL:HG23	1.99	0.62
1:E:541:TYR:HA	1:E:544:ILE:HG23	1.81	0.62
1:C:896:ILE:HB	1:C:945:VAL:HG11	1.81	0.62
1:F:359:LEU:HD12	1:F:365:THR:HA	1.81	0.62
1:F:1011:THR:O	1:F:1015:LEU:HB2	2.00	0.62
1:C:969:ARG:O	1:C:973:ILE:HG23	1.98	0.62
1:B:424:GLY:HA3	1:B:502:LYS:HG2	1.81	0.62
1:A:996:GLY:N	1:A:999:HIS:HD2	1.97	0.62
1:D:789:TYR:CE2	1:D:799:PRO:HG3	2.34	0.62
1:C:213:GLN:HE21	1:C:239:ARG:HB2	1.64	0.62
1:A:753:TRP:HZ3	1:A:779:ARG:HB3	1.63	0.62
1:E:520:PHE:HA	1:E:523:THR:CG2	2.29	0.62
1:A:417:GLU:HA	1:A:420:MET:HE3	1.80	0.62
1:C:472:ILE:H	1:C:472:ILE:CD1	2.13	0.62
1:C:43:ILE:HD11	1:C:107:VAL:CB	2.29	0.62
1:B:847:VAL:HG13	1:B:850:LEU:HD12	1.82	0.62
1:F:682:LEU:O	1:F:683:PHE:CD2	2.53	0.62
1:B:414:GLU:CD	1:B:972:PRO:HG3	2.20	0.62
1:E:527:TYR:CE2	1:E:966:CYS:HB3	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:MET:O	1:A:523:THR:HG23	1.99	0.62
1:F:903:VAL:HG21	1:F:1020:VAL:HG22	1.82	0.62
1:E:718:ASN:HB2	1:E:827:LEU:CD2	2.28	0.62
1:F:63:GLN:HE22	1:F:67:GLN:HE21	1.48	0.62
1:A:789:TYR:CE2	1:A:799:PRO:HG3	2.33	0.62
1:A:176:GLN:HE21	1:A:178:PHE:HE1	1.48	0.62
1:A:365:THR:O	1:A:369:THR:HG23	2.00	0.62
1:C:944:ILE:HG13	1:C:945:VAL:N	2.13	0.62
1:B:303:ALA:CB	1:B:330:THR:HG21	2.30	0.62
1:A:985:VAL:HA	1:A:1006:ILE:HD11	1.81	0.62
1:A:355:MET:HG3	1:A:365:THR:HG23	1.82	0.62
1:C:63:GLN:HE22	1:C:67:GLN:HE21	1.47	0.62
1:B:390:ILE:HA	1:B:394:THR:HG21	1.81	0.62
1:F:738:LEU:HD12	1:F:803:PHE:CZ	2.35	0.62
1:E:391:ASN:HD22	1:E:393:LEU:H	1.48	0.62
1:D:367:ILE:HD11	1:D:413:VAL:HG22	1.82	0.62
1:B:47:VAL:H	1:B:88:MET:HE2	1.65	0.62
1:E:745:ILE:O	1:E:748:THR:HG22	1.99	0.62
1:A:65:ILE:HD11	1:A:90:ILE:HG21	1.80	0.61
1:E:469:GLN:O	1:E:473:THR:HG22	2.00	0.61
1:C:572:LEU:HD23	1:C:573:PHE:N	2.15	0.61
1:E:303:ALA:CB	1:E:330:THR:HG21	2.30	0.61
1:B:49:TYR:CE1	1:B:121:GLU:HG3	2.34	0.61
1:D:906:LEU:HD23	1:D:906:LEU:H	1.64	0.61
1:C:742:LEU:HB3	1:C:746:ASN:HD21	1.64	0.61
1:B:410:ILE:CD1	1:B:976:THR:HG22	2.25	0.61
1:A:329:THR:O	1:A:332:VAL:HG12	1.98	0.61
1:D:535:LEU:HD23	1:D:959:VAL:HG13	1.82	0.61
1:F:47:VAL:HG12	1:F:88:MET:CE	2.30	0.61
1:F:738:LEU:HD12	1:F:803:PHE:HZ	1.64	0.61
1:B:616:ASN:HB3	1:B:618:ALA:H	1.64	0.61
1:F:742:LEU:HB3	1:F:746:ASN:HD21	1.65	0.61
1:A:183:SER:HB2	1:A:769:ARG:O	2.00	0.61
1:C:971:ARG:HB2	1:C:972:PRO:HD3	1.82	0.61
1:F:251:LEU:HD12	1:F:265:VAL:HG21	1.80	0.61
1:D:417:GLU:HA	1:D:420:MET:HE3	1.82	0.61
1:A:622:GLN:HE21	1:C:222:LEU:HG	1.66	0.61
1:F:281:PHE:CE2	1:F:324:VAL:HG11	2.35	0.61
1:E:424:GLY:HA3	1:E:502:LYS:HG2	1.81	0.61
1:D:2:SER:O	1:D:6:ILE:CD1	2.49	0.61
1:A:794:LYS:HD3	1:A:795:GLY:H	1.65	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HH12	1:A:432:ARG:HE	1.48	0.61
1:E:616:ASN:HB3	1:E:618:ALA:H	1.65	0.61
1:A:1016:ALA:O	1:A:1020:VAL:HG23	2.01	0.61
1:C:573:PHE:HE2	1:C:668:PRO:HG3	1.65	0.61
1:D:188:LEU:HD23	1:D:266:ALA:HB2	1.81	0.61
1:A:538:ARG:O	1:A:539:ALA:CB	2.49	0.61
1:A:528:GLU:OE2	1:A:967:ARG:CZ	2.48	0.61
1:C:544:ILE:O	1:C:548:ILE:HG23	2.01	0.61
1:F:652:GLN:HG3	1:F:714:ARG:HD2	1.82	0.61
1:C:10:ILE:HA	1:C:13:TRP:HB2	1.83	0.61
1:E:847:VAL:HG13	1:E:850:LEU:HD12	1.82	0.61
1:C:47:VAL:HG12	1:C:88:MET:CE	2.30	0.61
1:C:963:ILE:HG13	1:C:964:GLU:N	2.15	0.61
1:B:589:VAL:HA	1:B:592:ASP:HB2	1.82	0.61
1:D:428:ARG:HH12	1:D:432:ARG:HE	1.47	0.61
1:D:365:THR:O	1:D:369:THR:HG23	2.00	0.61
1:E:414:GLU:CG	1:E:972:PRO:HG3	2.31	0.61
1:D:156:ASN:HD21	1:D:768:LYS:HZ1	1.46	0.61
1:F:43:ILE:HD11	1:F:107:VAL:CB	2.31	0.61
1:D:337:ILE:HG13	1:D:338:HIS:N	2.16	0.61
1:B:958:ILE:N	1:B:958:ILE:HD13	2.15	0.61
1:D:280:GLN:HG2	1:D:595:ARG:HH21	1.65	0.61
1:C:910:GLY:H	1:C:1011:THR:HG21	1.66	0.61
1:C:359:LEU:HD12	1:C:365:THR:HA	1.82	0.61
1:B:453:PHE:CE2	1:B:474:ILE:HD11	2.35	0.61
1:A:451:ALA:HB1	1:A:882:VAL:CG1	2.29	0.61
1:E:958:ILE:N	1:E:958:ILE:HD13	2.16	0.61
1:C:738:LEU:HD12	1:C:803:PHE:HZ	1.65	0.61
1:A:780:MET:HE3	1:C:224:ALA:HA	1.82	0.61
1:D:749:VAL:HG13	1:D:753:TRP:HD1	1.66	0.61
1:A:538:ARG:CB	1:A:1022:LEU:HD21	2.30	0.61
1:C:445:ILE:CG2	1:C:939:LYS:HG2	2.30	0.61
1:E:38:ILE:HA	1:E:465:VAL:HG11	1.82	0.61
1:A:337:ILE:HG13	1:A:338:HIS:N	2.15	0.61
1:C:738:LEU:HD12	1:C:803:PHE:CZ	2.36	0.61
1:C:115:THR:HB	1:C:116:PRO:HD3	1.83	0.61
1:A:880:LEU:HD11	1:A:904:VAL:HG21	1.83	0.61
1:A:535:LEU:HD23	1:A:959:VAL:HG13	1.83	0.61
1:C:47:VAL:HG12	1:C:88:MET:HE3	1.82	0.61
1:D:780:MET:CE	1:F:224:ALA:HA	2.30	0.61
1:A:30:LEU:HD21	1:A:384:ALA:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:589:VAL:HA	1:E:592:ASP:HB2	1.81	0.61
1:A:119:PRO:O	1:A:122:VAL:HG12	2.01	0.61
1:A:367:ILE:HD11	1:A:413:VAL:HG22	1.82	0.60
1:A:569:GLN:N	1:A:634:TRP:CH2	2.69	0.60
1:D:1016:ALA:O	1:D:1020:VAL:HG23	2.01	0.60
1:C:652:GLN:HG3	1:C:714:ARG:HD2	1.83	0.60
1:A:896:ILE:N	1:A:897:PRO:HD2	2.16	0.60
1:B:469:GLN:O	1:B:473:THR:HG22	2.01	0.60
1:D:451:ALA:HB1	1:D:882:VAL:CG1	2.31	0.60
1:D:622:GLN:HE21	1:F:222:LEU:HG	1.66	0.60
1:B:895:SER:C	1:B:897:PRO:HD2	2.21	0.60
1:C:682:LEU:O	1:C:683:PHE:CD2	2.54	0.60
1:E:157:TYR:O	1:E:161:ASN:HB2	2.01	0.60
1:F:115:THR:HB	1:F:116:PRO:HD3	1.82	0.60
1:E:414:GLU:CD	1:E:972:PRO:HG3	2.21	0.60
1:C:166:LEU:O	1:C:169:THR:HG22	2.01	0.60
1:F:573:PHE:HE2	1:F:668:PRO:HG3	1.64	0.60
1:B:745:ILE:O	1:B:748:THR:HG22	2.01	0.60
1:A:83:ASN:ND2	1:A:620:ARG:HG2	2.16	0.60
1:C:111:LEU:C	1:C:113:LEU:H	2.04	0.60
1:D:569:GLN:N	1:D:634:TRP:CH2	2.68	0.60
1:A:13:TRP:NE1	2:A:2026:LMT:H11	2.16	0.60
1:A:537:HIS:O	1:A:538:ARG:O	2.19	0.60
1:D:538:ARG:CB	1:D:1022:LEU:HD21	2.30	0.60
1:D:538:ARG:O	1:D:539:ALA:CB	2.50	0.60
1:A:280:GLN:HG2	1:A:595:ARG:HH21	1.65	0.60
1:A:166:LEU:HG	1:A:291:ILE:HD11	1.84	0.60
1:E:115:THR:HB	1:E:116:PRO:HD3	1.82	0.60
1:A:521:LEU:HD13	1:A:521:LEU:O	2.01	0.60
1:E:1020:VAL:HB	1:E:1021:PRO:HD3	1.82	0.60
1:E:410:ILE:CD1	1:E:976:THR:HG22	2.25	0.60
1:A:749:VAL:HG13	1:A:753:TRP:HD1	1.67	0.60
1:E:47:VAL:H	1:E:88:MET:HE2	1.66	0.60
1:D:242:THR:HG22	1:D:245:GLN:NE2	2.16	0.60
1:D:30:LEU:HD21	1:D:384:ALA:HA	1.83	0.60
1:C:281:PHE:CE2	1:C:324:VAL:HG11	2.36	0.60
1:D:83:ASN:ND2	1:D:620:ARG:HG2	2.16	0.60
1:A:906:LEU:HD23	1:A:906:LEU:H	1.64	0.60
1:B:1020:VAL:HB	1:B:1021:PRO:HD3	1.82	0.60
1:B:414:GLU:CG	1:B:972:PRO:HG3	2.31	0.60
1:A:753:TRP:CZ2	1:A:785:LEU:HG	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:906:LEU:HD22	1:C:1015:LEU:HD12	1.83	0.60
1:A:791:ARG:HB2	1:A:797:MET:CE	2.30	0.60
1:A:875:LEU:C	1:A:875:LEU:HD12	2.21	0.60
1:A:706:ALA:CB	1:A:846:ILE:HD13	2.30	0.60
1:A:541:TYR:HA	1:A:544:ILE:CG2	2.32	0.60
1:F:907:GLY:HA2	1:F:1011:THR:HG23	1.83	0.60
1:F:910:GLY:H	1:F:1011:THR:HG21	1.65	0.60
1:D:880:LEU:HD11	1:D:904:VAL:HG21	1.84	0.60
1:F:683:PHE:CZ	1:F:818:TYR:CE2	2.90	0.60
1:D:472:ILE:HA	1:D:475:VAL:HG13	1.84	0.60
1:E:199:THR:HG23	1:E:200:PRO:HD2	1.83	0.60
1:F:358:PHE:CG	1:F:975:MET:HG2	2.36	0.60
1:A:7:ASP:O	1:A:9:PRO:HD3	2.01	0.60
1:E:156:ASN:HD21	1:E:768:LYS:NZ	2.00	0.60
1:A:569:GLN:CD	1:A:670:SER:HA	2.22	0.60
1:A:753:TRP:CZ2	1:A:785:LEU:HA	2.36	0.60
1:B:520:PHE:HA	1:B:523:THR:CG2	2.32	0.60
1:F:906:LEU:HD22	1:F:1015:LEU:HD12	1.82	0.60
1:D:780:MET:HE3	1:F:225:VAL:H	1.66	0.60
1:B:591:VAL:HA	1:B:594:MET:HG3	1.83	0.60
1:D:7:ASP:O	1:D:9:PRO:HD3	2.02	0.60
1:F:944:ILE:HG13	1:F:945:VAL:N	2.16	0.60
1:D:65:ILE:HD11	1:D:90:ILE:HG21	1.83	0.60
1:F:703:LEU:HA	1:F:706:ALA:HB3	1.83	0.60
1:F:444:GLY:O	1:F:448:VAL:HG23	2.00	0.60
1:B:966:CYS:SG	1:B:1021:PRO:CG	2.89	0.60
1:B:971:ARG:O	1:B:975:MET:HG2	2.02	0.60
1:D:537:HIS:O	1:D:538:ARG:O	2.19	0.60
1:D:372:VAL:HB	1:D:373:PRO:HD3	1.83	0.60
1:C:575:GLN:NE2	1:C:617:PHE:HB2	2.17	0.60
1:D:541:TYR:HA	1:D:544:ILE:CG2	2.32	0.60
1:C:907:GLY:HA2	1:C:1011:THR:HG23	1.84	0.60
1:F:544:ILE:O	1:F:548:ILE:HG23	2.01	0.60
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.84	0.60
1:E:390:ILE:HA	1:E:394:THR:HG21	1.83	0.60
1:F:162:ILE:C	1:F:165:PRO:HD2	2.21	0.60
1:F:10:ILE:HA	1:F:13:TRP:HB2	1.82	0.59
1:B:190:PRO:HG3	1:B:788:TRP:CE2	2.37	0.59
1:D:119:PRO:O	1:D:122:VAL:HG12	2.01	0.59
1:B:930:LEU:O	1:B:934:ILE:HG23	2.02	0.59
1:B:199:THR:HG23	1:B:200:PRO:HD2	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:CD2	2:D:2026:LMT:H81	2.32	0.59
1:B:878:LEU:HD13	2:B:2032:LMT:H31	1.84	0.59
1:B:371:ALA:O	1:B:375:VAL:HG23	2.02	0.59
1:B:115:THR:HB	1:B:116:PRO:HD3	1.84	0.59
1:A:242:THR:HG22	1:A:245:GLN:HG3	1.84	0.59
1:E:520:PHE:CA	1:E:523:THR:HG22	2.31	0.59
1:F:330:THR:HG22	1:F:331:PRO:HD3	1.84	0.59
1:E:453:PHE:CE2	1:E:474:ILE:HD11	2.36	0.59
1:F:184:MET:HE1	1:F:268:VAL:HG13	1.84	0.59
1:A:472:ILE:HA	1:A:475:VAL:HG13	1.84	0.59
1:D:519:MET:O	1:D:523:THR:HG23	2.03	0.59
1:B:187:TRP:HA	1:B:773:GLN:O	2.02	0.59
1:E:930:LEU:O	1:E:934:ILE:HG23	2.01	0.59
1:D:523:THR:O	1:D:525:HIS:N	2.35	0.59
1:D:616:ASN:HD22	1:D:626:MET:HB3	1.65	0.59
1:D:896:ILE:N	1:D:897:PRO:HD2	2.17	0.59
1:F:572:LEU:HD23	1:F:573:PHE:N	2.15	0.59
1:D:780:MET:HE3	1:F:225:VAL:N	2.17	0.59
1:B:669:PRO:HD2	1:B:672:LEU:HD12	1.83	0.59
1:C:162:ILE:C	1:C:165:PRO:HD2	2.22	0.59
1:D:150:THR:HG22	1:D:153:ASP:CG	2.23	0.59
1:A:748:THR:HG21	1:A:790:VAL:HG22	1.83	0.59
1:E:224:ALA:HB1	1:F:780:MET:SD	2.42	0.59
1:D:196:TYR:H	1:D:196:TYR:HD2	1.51	0.59
1:D:193:LEU:HD22	1:D:265:VAL:HG13	1.84	0.59
1:A:568:ASP:HB3	1:A:634:TRP:CH2	2.37	0.59
1:F:445:ILE:CG2	1:F:939:LYS:HG2	2.32	0.59
1:F:985:VAL:O	1:F:989:ILE:HG12	2.02	0.59
1:F:452:VAL:HG22	1:F:883:VAL:HG21	1.85	0.59
1:C:703:LEU:HA	1:C:706:ALA:HB3	1.84	0.59
1:A:402:ILE:HA	1:A:405:LEU:CD1	2.33	0.59
1:D:751:ILE:HG21	1:D:772:LEU:HD13	1.83	0.59
1:D:753:TRP:CZ2	1:D:785:LEU:HA	2.38	0.59
1:E:966:CYS:SG	1:E:1021:PRO:CG	2.90	0.59
1:A:273:GLN:NE2	1:A:769:ARG:HH11	2.01	0.59
1:E:156:ASN:HD22	1:E:182:TYR:N	2.00	0.59
1:A:150:THR:H	1:A:153:ASP:HB2	1.68	0.59
1:D:139:VAL:O	1:D:326:PRO:HD2	2.02	0.59
1:F:575:GLN:NE2	1:F:617:PHE:HB2	2.17	0.59
1:C:985:VAL:O	1:C:989:ILE:HG12	2.03	0.59
1:D:576:VAL:HG21	1:D:594:MET:HE1	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:VAL:HG21	1:B:591:VAL:HG22	1.83	0.59
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.84	0.59
1:B:156:ASN:HD21	1:B:768:LYS:NZ	2.00	0.59
1:D:699:ARG:CZ	1:D:824:MET:HG3	2.32	0.59
1:D:139:VAL:HG12	1:D:327:TYR:HB3	1.83	0.59
1:D:739:GLY:HA3	1:D:793:ASP:HB2	1.84	0.59
1:A:966:CYS:SG	1:A:1021:PRO:CG	2.90	0.58
1:A:699:ARG:CZ	1:A:824:MET:HG3	2.32	0.58
1:D:568:ASP:HB3	1:D:634:TRP:CH2	2.38	0.58
1:E:190:PRO:HG3	1:E:788:TRP:CE2	2.38	0.58
1:E:576:VAL:HG22	1:E:663:VAL:HG22	1.84	0.58
1:A:523:THR:O	1:A:525:HIS:N	2.36	0.58
1:A:170:LYS:HZ3	1:B:74:ASN:H	1.51	0.58
1:E:187:TRP:HA	1:E:773:GLN:O	2.02	0.58
1:C:186:ILE:HG22	1:C:268:VAL:HG22	1.85	0.58
1:B:38:ILE:HA	1:B:465:VAL:HG11	1.85	0.58
1:A:337:ILE:HG13	1:A:338:HIS:H	1.68	0.58
1:C:683:PHE:CZ	1:C:818:TYR:CE2	2.90	0.58
1:F:144:SER:HA	1:F:320:GLY:O	2.03	0.58
1:D:951:LEU:O	1:D:956:LYS:HB2	2.03	0.58
1:E:861:LEU:O	1:E:865:GLU:HG2	2.03	0.58
1:F:111:LEU:C	1:F:113:LEU:H	2.04	0.58
1:D:166:LEU:HG	1:D:291:ILE:HD11	1.85	0.58
1:D:355:MET:HG3	1:D:365:THR:HG23	1.83	0.58
1:D:183:SER:HB2	1:D:769:ARG:O	2.03	0.58
1:E:58:GLN:HA	1:E:62:VAL:HB	1.84	0.58
1:D:875:LEU:HD12	1:D:875:LEU:C	2.23	0.58
1:F:939:LYS:HZ1	1:F:976:THR:HG22	1.69	0.58
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.84	0.58
1:F:49:TYR:HE1	1:F:121:GLU:HG3	1.69	0.58
1:C:425:LEU:HD22	1:C:429:GLU:HB2	1.85	0.58
1:D:966:CYS:SG	1:D:1021:PRO:CG	2.91	0.58
1:D:283:GLY:HA2	1:D:595:ARG:HE	1.68	0.58
1:E:907:GLY:CA	1:E:1012:ALA:HB2	2.34	0.58
1:C:138:MET:HB2	1:C:327:TYR:O	2.04	0.58
1:A:616:ASN:HD22	1:A:626:MET:HB3	1.64	0.58
1:D:337:ILE:HG13	1:D:338:HIS:H	1.69	0.58
1:D:150:THR:H	1:D:153:ASP:HB2	1.68	0.58
1:C:141:GLY:HA2	1:C:288:GLY:HA3	1.86	0.58
1:B:520:PHE:CA	1:B:523:THR:HG22	2.33	0.58
1:B:58:GLN:HA	1:B:62:VAL:HB	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:VAL:HA	1:E:594:MET:HG3	1.84	0.58
1:C:109:ASN:HA	1:C:112:GLN:NE2	2.18	0.58
1:C:480:LEU:O	1:C:484:VAL:HG23	2.04	0.58
1:C:150:THR:HG22	1:C:153:ASP:OD2	2.03	0.58
1:C:242:THR:HG22	1:C:245:GLN:HG3	1.86	0.58
1:D:521:LEU:O	1:D:521:LEU:HD13	2.04	0.58
1:D:175:PHE:HB2	1:D:289:ILE:HD11	1.86	0.58
1:D:622:GLN:NE2	1:F:222:LEU:HG	2.18	0.58
1:A:576:VAL:HG21	1:A:594:MET:HE1	1.85	0.58
1:A:751:ILE:HG21	1:A:772:LEU:HD13	1.86	0.58
1:E:391:ASN:H	1:E:394:THR:CG2	2.16	0.58
1:C:49:TYR:HE1	1:C:121:GLU:HG3	1.69	0.58
1:A:483:ILE:HG13	1:A:487:ILE:HD13	1.86	0.58
1:C:452:VAL:HG22	1:C:883:VAL:HG21	1.86	0.58
1:D:242:THR:HG22	1:D:245:GLN:HG3	1.84	0.58
1:A:181:GLN:HG3	1:A:768:LYS:HZ3	1.68	0.58
1:A:203:VAL:O	1:A:206:ALA:N	2.32	0.58
1:E:115:THR:O	1:E:118:LEU:HB2	2.04	0.58
1:B:156:ASN:HD22	1:B:182:TYR:N	2.02	0.58
1:A:951:LEU:O	1:A:956:LYS:HB2	2.03	0.58
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.85	0.58
1:D:402:ILE:HA	1:D:405:LEU:CD1	2.33	0.58
1:E:910:GLY:H	1:E:1011:THR:HG21	1.69	0.58
1:D:57:VAL:HG13	1:D:88:MET:HB3	1.86	0.58
2:E:2032:LMT:H42	2:E:2032:LMT:H82	1.86	0.57
1:D:524:THR:HG22	1:D:970:LEU:HD12	1.86	0.57
1:B:188:LEU:HA	1:B:266:ALA:HB2	1.86	0.57
1:A:283:GLY:HA2	1:A:595:ARG:HE	1.69	0.57
1:C:757:TYR:CE1	1:C:769:ARG:HD3	2.39	0.57
1:C:190:PRO:HA	1:C:193:LEU:HD12	1.86	0.57
1:D:753:TRP:CZ2	1:D:785:LEU:HG	2.38	0.57
1:E:541:TYR:HA	1:E:544:ILE:CG2	2.35	0.57
1:A:242:THR:HG22	1:A:245:GLN:NE2	2.14	0.57
1:E:185:ARG:HD2	1:E:272:GLY:O	2.04	0.57
1:D:262:LEU:HD11	1:D:266:ALA:N	2.19	0.57
1:F:186:ILE:HG22	1:F:268:VAL:HG22	1.86	0.57
1:B:861:LEU:O	1:B:865:GLU:HG2	2.04	0.57
1:A:727:LYS:HD3	1:A:728:LEU:H	1.68	0.57
1:D:251:LEU:N	1:D:251:LEU:HD12	2.19	0.57
1:E:559:ILE:HD12	1:E:560:PRO:HD2	1.87	0.57
1:F:166:LEU:O	1:F:169:THR:HG22	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:SER:CB	1:F:90:ILE:HG22	2.34	0.57
1:B:94:PHE:CE2	1:B:103:ALA:HB1	2.40	0.57
1:B:317:MET:SD	1:B:321:MET:HE3	2.45	0.57
1:F:138:MET:HB2	1:F:327:TYR:O	2.03	0.57
1:E:151:LYS:HZ1	1:E:278:ASN:HB3	1.70	0.57
1:D:900:VAL:HG13	1:D:941:ALA:HB3	1.87	0.57
1:D:893:SER:N	1:F:10:ILE:HD11	2.19	0.57
1:C:80:SER:CB	1:C:90:ILE:HG22	2.34	0.57
1:F:150:THR:HG22	1:F:153:ASP:OD2	2.04	0.57
1:C:479:ALA:O	1:C:482:VAL:HG12	2.04	0.57
1:E:701:LYS:O	1:E:705:LEU:HB2	2.05	0.57
1:D:404:LEU:HD22	1:D:936:LEU:HD23	1.87	0.57
1:F:203:VAL:O	1:F:207:ILE:HG13	2.05	0.57
1:A:404:LEU:HD22	1:A:936:LEU:HD23	1.86	0.57
1:B:541:TYR:HA	1:B:544:ILE:CG2	2.34	0.57
1:B:907:GLY:CA	1:B:1012:ALA:HB2	2.35	0.57
1:C:932:THR:O	1:C:936:LEU:HG	2.03	0.57
1:C:939:LYS:HZ3	1:C:976:THR:HG21	1.70	0.57
1:F:393:LEU:CD1	1:F:466:ILE:HB	2.34	0.57
1:E:695:LEU:HD13	1:E:824:MET:HG3	1.85	0.57
1:A:367:ILE:HG12	1:A:368:PRO:HD3	1.86	0.57
1:B:910:GLY:H	1:B:1011:THR:HG21	1.69	0.57
1:A:157:TYR:CZ	1:A:317:MET:HG2	2.40	0.57
1:E:188:LEU:HA	1:E:266:ALA:HB2	1.86	0.57
1:B:958:ILE:HG12	1:B:959:VAL:N	2.20	0.57
1:C:478:MET:O	1:C:481:SER:HB3	2.05	0.57
1:C:181:GLN:OE1	1:C:766:ARG:NH1	2.37	0.57
1:B:155:SER:O	1:B:159:VAL:HG23	2.05	0.57
1:D:969:ARG:O	1:D:973:ILE:HG12	2.04	0.57
1:A:831:ALA:O	1:A:834:LEU:HB2	2.04	0.57
1:B:453:PHE:CD2	1:B:474:ILE:HD11	2.39	0.57
1:E:116:PRO:HA	1:E:123:GLN:HE22	1.69	0.57
1:F:141:GLY:HA2	1:F:288:GLY:HA3	1.87	0.57
1:D:350:LEU:O	1:D:354:VAL:HG23	2.05	0.57
1:B:185:ARG:HD2	1:B:272:GLY:O	2.04	0.57
1:A:524:THR:O	1:A:527:TYR:HB3	2.05	0.57
1:A:539:ALA:HB3	1:A:540:PRO:HD3	1.87	0.57
1:D:228:GLN:HE21	1:D:230:LEU:N	2.01	0.57
1:F:43:ILE:CD1	1:F:104:GLN:HA	2.35	0.57
1:C:393:LEU:CD1	1:C:466:ILE:HB	2.34	0.57
1:E:44:ALA:HB2	1:E:132:ALA:HB2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ILE:HD11	1:B:924:VAL:HG21	1.85	0.57
1:E:881:LEU:HD22	1:E:881:LEU:O	2.05	0.57
1:F:159:VAL:HG12	1:F:159:VAL:O	2.05	0.57
1:A:57:VAL:HG13	1:A:88:MET:HB3	1.86	0.57
1:E:577:GLN:OE1	1:E:720:MET:HG2	2.05	0.57
1:A:139:VAL:O	1:A:326:PRO:HD2	2.04	0.57
1:C:144:SER:HA	1:C:320:GLY:O	2.04	0.57
1:F:109:ASN:HA	1:F:112:GLN:NE2	2.20	0.57
1:A:659:LYS:HD2	1:A:660:ASP:N	2.20	0.57
1:B:115:THR:O	1:B:118:LEU:HB2	2.05	0.56
1:E:281:PHE:CZ	1:E:324:VAL:HG11	2.39	0.56
1:D:573:PHE:HB2	1:D:666:PHE:CE2	2.40	0.56
1:E:94:PHE:CE2	1:E:103:ALA:HB1	2.40	0.56
1:C:27:ILE:HD11	1:C:380:PHE:CD1	2.39	0.56
1:A:453:PHE:CE2	1:A:474:ILE:HD11	2.39	0.56
1:A:695:LEU:HD13	1:A:699:ARG:HH21	1.70	0.56
1:F:573:PHE:CE2	1:F:668:PRO:HG3	2.41	0.56
1:E:164:ASP:HB2	1:F:67:GLN:NE2	2.20	0.56
1:E:35:TYR:HE1	1:E:392:THR:HG21	1.70	0.56
1:A:298:ASN:O	1:A:302:THR:HG22	2.05	0.56
1:B:391:ASN:H	1:B:394:THR:CG2	2.16	0.56
1:D:176:GLN:HE21	1:D:178:PHE:HE1	1.52	0.56
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.40	0.56
1:D:818:TYR:HH	1:D:859:THR:HG1	1.51	0.56
1:A:175:PHE:HB2	1:A:289:ILE:HD11	1.86	0.56
1:E:313:LEU:O	1:E:317:MET:HG3	2.05	0.56
1:D:262:LEU:HD22	1:D:263:LYS:H	1.70	0.56
1:B:313:LEU:O	1:B:317:MET:HG3	2.05	0.56
1:D:332:VAL:HG21	1:D:569:GLN:HA	1.86	0.56
1:D:533:SER:O	1:D:536:LYS:HG3	2.06	0.56
1:B:363:ARG:HD3	1:B:496:MET:O	2.04	0.56
1:B:386:PHE:CZ	2:B:2031:LMT:H81	2.39	0.56
1:E:958:ILE:HG12	1:E:959:VAL:N	2.21	0.56
1:E:169:THR:O	1:E:172:VAL:HG23	2.05	0.56
1:F:58:GLN:HA	1:F:62:VAL:HB	1.87	0.56
1:D:996:GLY:H	1:D:999:HIS:HD2	1.54	0.56
1:D:162:ILE:HG23	1:D:166:LEU:CD2	2.36	0.56
1:C:60:THR:HG23	1:C:61:VAL:HG23	1.85	0.56
1:D:652:GLN:HE22	1:D:664:PHE:HD1	1.53	0.56
1:B:157:TYR:O	1:B:161:ASN:HB2	2.05	0.56
1:F:425:LEU:HD22	1:F:429:GLU:HB2	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:MET:SD	1:A:913:LEU:HD23	2.45	0.56
1:B:695:LEU:HD13	1:B:824:MET:HG3	1.86	0.56
1:F:896:ILE:HG12	1:F:897:PRO:HD3	1.87	0.56
1:F:910:GLY:N	1:F:1011:THR:HG21	2.20	0.56
1:C:358:PHE:CG	1:C:975:MET:HG2	2.40	0.56
1:A:98:THR:O	1:A:100:PRO:HD3	2.04	0.56
1:D:727:LYS:HD3	1:D:728:LEU:H	1.68	0.56
1:A:352:PHE:CD1	1:A:369:THR:HG21	2.37	0.56
1:A:193:LEU:HD22	1:A:265:VAL:HG13	1.86	0.56
1:A:317:MET:HE2	1:A:321:MET:HG3	1.88	0.56
1:F:910:GLY:CA	1:F:1011:THR:HG21	2.36	0.56
1:E:363:ARG:HD3	1:E:496:MET:O	2.05	0.56
1:F:971:ARG:HB2	1:F:972:PRO:HD3	1.86	0.56
1:D:1008:GLY:O	1:D:1012:ALA:HB2	2.06	0.56
1:D:339:GLU:O	1:D:343:THR:HG23	2.06	0.56
1:C:203:VAL:O	1:C:207:ILE:HG13	2.05	0.56
1:A:365:THR:O	1:A:368:PRO:HD2	2.06	0.56
1:E:871:GLN:HA	2:E:2032:LMT:O2B	2.06	0.56
1:A:332:VAL:HG21	1:A:569:GLN:HA	1.87	0.56
1:F:939:LYS:NZ	1:F:976:THR:CG2	2.69	0.56
1:B:231:ASN:HD21	1:C:584:ALA:H	1.54	0.56
1:D:343:THR:HG21	1:D:998:GLN:OE1	2.05	0.56
1:D:478:MET:O	1:D:481:SER:HB3	2.05	0.56
1:D:659:LYS:HD2	1:D:660:ASP:N	2.20	0.56
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.89	0.56
1:E:1015:LEU:O	1:E:1019:TRP:HD1	1.89	0.56
1:A:142:VAL:HG12	1:A:154:LEU:HD22	1.87	0.56
1:A:545:TYR:HB2	1:A:1019:TRP:HZ3	1.70	0.56
1:C:910:GLY:CA	1:C:1011:THR:HG21	2.35	0.56
1:D:453:PHE:CE2	1:D:474:ILE:HD11	2.41	0.56
1:D:203:VAL:O	1:D:206:ALA:N	2.31	0.56
1:F:559:ILE:HD11	1:F:922:ASN:HB2	1.86	0.56
1:C:396:PHE:CE2	1:C:998:GLN:HG2	2.41	0.56
1:F:779:ARG:HD2	1:F:779:ARG:O	2.06	0.56
1:A:478:MET:O	1:A:481:SER:HB3	2.06	0.56
1:F:190:PRO:HG3	1:F:788:TRP:CZ2	2.40	0.56
1:E:817:ARG:HD2	1:E:822:PRO:HA	1.88	0.56
1:D:524:THR:O	1:D:527:TYR:HB3	2.05	0.56
1:C:945:VAL:HG23	1:C:1020:VAL:HG12	1.88	0.56
1:C:910:GLY:N	1:C:1011:THR:HG21	2.20	0.56
1:E:371:ALA:O	1:E:375:VAL:HG23	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:THR:HG22	1:F:245:GLN:HG3	1.86	0.56
1:F:712:LEU:N	1:F:712:LEU:HD23	2.21	0.56
1:B:686:ASP:HB2	1:B:690:VAL:HG12	1.86	0.56
1:A:339:GLU:O	1:A:343:THR:HG23	2.05	0.56
1:D:225:VAL:HG12	1:E:780:MET:HE2	1.87	0.56
1:A:900:VAL:HG13	1:A:941:ALA:HB3	1.88	0.56
1:A:222:LEU:HD23	1:B:622:GLN:NE2	2.21	0.56
1:A:203:VAL:O	1:A:204:SER:C	2.44	0.56
1:A:622:GLN:NE2	1:C:222:LEU:HG	2.20	0.56
1:A:350:LEU:O	1:A:354:VAL:HG23	2.06	0.56
1:A:637:ARG:N	1:A:638:PRO:CD	2.69	0.56
1:D:637:ARG:N	1:D:638:PRO:CD	2.68	0.56
1:A:800:PHE:CD2	1:A:804:ALA:HB2	2.37	0.56
1:E:782:PRO:O	1:E:785:LEU:HB2	2.06	0.56
1:B:612:VAL:HG11	1:B:615:PHE:HD2	1.71	0.56
1:D:162:ILE:HG23	1:D:166:LEU:HD23	1.88	0.56
1:B:211:ASN:HD21	1:B:240:LEU:H	1.54	0.56
1:B:479:ALA:O	1:B:483:ILE:HG22	2.05	0.56
1:F:396:PHE:CE2	1:F:998:GLN:HG2	2.41	0.56
1:C:904:VAL:HB	1:C:905:PRO:HD3	1.88	0.56
1:D:367:ILE:HG12	1:D:368:PRO:HD3	1.86	0.55
1:E:445:ILE:HG22	1:E:942:ILE:HD12	1.89	0.55
1:C:330:THR:HG22	1:C:331:PRO:HD3	1.87	0.55
1:F:314:GLU:HA	1:F:317:MET:SD	2.47	0.55
1:A:884:PHE:HB2	1:A:901:MET:HE2	1.88	0.55
1:A:950:GLU:O	1:A:953:GLU:HG3	2.05	0.55
1:F:757:TYR:CE1	1:F:769:ARG:HD3	2.40	0.55
1:F:479:ALA:O	1:F:482:VAL:HG12	2.06	0.55
1:E:155:SER:O	1:E:159:VAL:HG23	2.06	0.55
1:E:454:LEU:HD11	2:E:2031:LMT:H101	1.88	0.55
1:F:367:ILE:CG2	1:F:492:LEU:HB3	2.36	0.55
1:A:695:LEU:CD1	1:A:699:ARG:NH2	2.69	0.55
1:C:573:PHE:CE2	1:C:668:PRO:HG3	2.40	0.55
1:A:150:THR:HG22	1:A:153:ASP:CG	2.26	0.55
1:C:638:PRO:HD2	1:C:642:ASN:ND2	2.22	0.55
1:D:1001:ILE:HG23	1:D:1002:GLY:N	2.20	0.55
1:B:936:LEU:HD12	1:B:1009:MET:HE3	1.88	0.55
1:C:559:ILE:HD11	1:C:922:ASN:HB2	1.89	0.55
1:A:196:TYR:H	1:A:196:TYR:HD2	1.52	0.55
1:A:590:VAL:HG11	1:A:661:ALA:HB3	1.88	0.55
1:D:363:ARG:O	1:D:367:ILE:HG22	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ILE:CG2	1:C:492:LEU:HB3	2.36	0.55
1:D:809:GLU:O	1:D:810:TYR:HB3	2.05	0.55
1:F:980:PHE:CE2	1:F:1005:VAL:HG13	2.42	0.55
1:C:896:ILE:HG12	1:C:897:PRO:HD3	1.86	0.55
1:B:782:PRO:O	1:B:785:LEU:HB2	2.06	0.55
1:E:453:PHE:CD2	1:E:474:ILE:HD11	2.40	0.55
1:A:726:TYR:CE1	1:A:782:PRO:HB3	2.42	0.55
1:D:298:ASN:O	1:D:302:THR:HG22	2.06	0.55
1:B:576:VAL:HG22	1:B:663:VAL:HG22	1.88	0.55
1:B:701:LYS:O	1:B:705:LEU:HB2	2.06	0.55
1:F:699:ARG:CG	1:F:699:ARG:NH1	2.60	0.55
1:D:352:PHE:CD1	1:D:369:THR:HG21	2.37	0.55
1:A:680:PHE:CD2	1:A:858:TRP:HZ3	2.25	0.55
1:C:43:ILE:HD11	1:C:107:VAL:CG2	2.37	0.55
1:F:80:SER:HB2	1:F:90:ILE:HG22	1.88	0.55
1:A:196:TYR:HD1	1:A:260:VAL:HG21	1.71	0.55
1:E:24:GLY:O	1:E:27:ILE:HG12	2.07	0.55
1:E:739:GLY:HA3	1:E:793:ASP:HB2	1.89	0.55
1:E:479:ALA:O	1:E:483:ILE:HG22	2.05	0.55
1:D:950:GLU:O	1:D:953:GLU:HG3	2.07	0.55
1:E:977:SER:O	1:E:981:ILE:HG23	2.07	0.55
1:A:524:THR:HG22	1:A:970:LEU:HD12	1.87	0.55
1:A:871:GLN:O	1:A:872:ALA:HB2	2.07	0.55
1:A:1001:ILE:HG23	1:A:1002:GLY:N	2.21	0.55
1:F:68:GLN:HG3	1:F:114:ALA:HB2	1.87	0.55
1:C:925:PHE:HD2	1:C:1001:ILE:HG23	1.71	0.55
1:D:1015:LEU:O	1:D:1019:TRP:HD1	1.90	0.55
1:D:695:LEU:CD1	1:D:699:ARG:NH2	2.69	0.55
1:B:682:LEU:HD11	1:B:856:TYR:HD2	1.72	0.55
1:F:818:TYR:HD1	1:F:823:ALA:HB3	1.70	0.55
1:C:80:SER:HB2	1:C:90:ILE:HG22	1.87	0.55
1:F:143:VAL:HG13	1:F:286:ALA:HB2	1.88	0.55
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.71	0.55
1:D:930:LEU:O	1:D:934:ILE:HG23	2.05	0.55
1:F:60:THR:HG23	1:F:61:VAL:HG23	1.87	0.55
1:D:539:ALA:HB3	1:D:540:PRO:HD3	1.88	0.55
1:A:228:GLN:HE21	1:A:230:LEU:N	2.02	0.55
1:E:612:VAL:HG11	1:E:615:PHE:HD2	1.71	0.55
1:C:402:ILE:HD12	1:C:403:GLY:N	2.22	0.55
1:B:35:TYR:HE1	1:B:392:THR:HG21	1.71	0.55
1:E:576:VAL:HG21	1:E:591:VAL:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HG23	1:B:245:GLN:HG3	1.88	0.55
1:E:936:LEU:HD12	1:E:1009:MET:HE3	1.88	0.55
1:D:690:VAL:HG22	1:D:694:VAL:CG2	2.36	0.55
1:A:363:ARG:O	1:A:367:ILE:HG22	2.06	0.55
1:E:458:PHE:HA	2:E:2031:LMT:H11	1.88	0.55
1:D:273:GLN:NE2	1:D:769:ARG:HH11	2.05	0.55
1:A:843:VAL:O	1:A:847:VAL:HG23	2.06	0.55
1:C:530:GLY:O	1:C:534:ILE:HG23	2.07	0.55
1:D:196:TYR:N	1:D:196:TYR:CD2	2.74	0.55
1:F:184:MET:HG3	1:F:246:PHE:CE1	2.42	0.55
1:D:578:THR:HG22	1:D:579:PRO:HD2	1.88	0.55
1:C:314:GLU:HA	1:C:317:MET:SD	2.47	0.55
1:E:552:MET:HG3	1:E:553:ILE:N	2.22	0.55
1:F:638:PRO:HD2	1:F:642:ASN:ND2	2.22	0.55
1:A:573:PHE:HB2	1:A:666:PHE:CE2	2.41	0.55
1:D:843:VAL:O	1:D:847:VAL:HG23	2.07	0.55
1:A:533:SER:O	1:A:536:LYS:HG3	2.07	0.55
1:D:203:VAL:O	1:D:204:SER:C	2.45	0.55
1:F:925:PHE:HD2	1:F:1001:ILE:HG23	1.72	0.55
1:D:851:PRO:O	1:D:854:VAL:HG12	2.07	0.55
1:C:712:LEU:HD23	1:C:712:LEU:N	2.21	0.55
1:D:498:LYS:N	1:D:499:PRO:CD	2.62	0.54
1:C:977:SER:O	1:C:981:ILE:HG12	2.06	0.54
1:D:47:VAL:HG22	1:D:48:SER:N	2.22	0.54
1:F:943:LEU:CD1	1:F:973:ILE:HG22	2.37	0.54
1:D:590:VAL:HG11	1:D:661:ALA:HB3	1.88	0.54
1:C:818:TYR:HD1	1:C:823:ALA:HB3	1.71	0.54
1:B:169:THR:O	1:B:172:VAL:HG23	2.06	0.54
1:A:186:ILE:HG13	1:A:262:LEU:HD21	1.89	0.54
1:C:575:GLN:NE2	1:C:666:PHE:HZ	2.05	0.54
1:E:549:VAL:O	1:E:552:MET:HG2	2.07	0.54
1:E:351:VAL:O	1:E:355:MET:HB2	2.07	0.54
1:B:739:GLY:HA3	1:B:793:ASP:HB2	1.89	0.54
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.89	0.54
1:D:161:ASN:O	1:D:165:PRO:HD2	2.08	0.54
1:D:725:GLN:HG3	1:D:811:GLY:H	1.73	0.54
1:E:48:SER:N	2:E:2033:LMT:O3B	2.40	0.54
1:D:807:LYS:HG3	1:D:808:TRP:H	1.72	0.54
1:B:559:ILE:HD12	1:B:560:PRO:HD2	1.89	0.54
1:F:932:THR:O	1:F:936:LEU:HG	2.06	0.54
1:A:902:LEU:HD23	1:A:1023:PHE:CE1	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:MET:HE3	1:C:225:VAL:H	1.73	0.54
1:F:190:PRO:HA	1:F:193:LEU:HD12	1.87	0.54
1:F:142:VAL:HG12	1:F:154:LEU:HD22	1.88	0.54
1:D:483:ILE:HG13	1:D:487:ILE:HD13	1.89	0.54
1:E:211:ASN:HD21	1:E:240:LEU:H	1.55	0.54
1:D:607:SER:HB2	1:D:632:LYS:HG2	1.88	0.54
1:A:375:VAL:CG2	1:A:405:LEU:HG	2.23	0.54
1:D:800:PHE:CD2	1:D:804:ALA:HB2	2.37	0.54
1:B:738:LEU:HD13	1:B:798:VAL:HG11	1.90	0.54
1:F:530:GLY:O	1:F:534:ILE:HG23	2.06	0.54
1:B:577:GLN:OE1	1:B:720:MET:HG2	2.07	0.54
1:F:575:GLN:NE2	1:F:666:PHE:HZ	2.05	0.54
1:C:68:GLN:HG3	1:C:114:ALA:HB2	1.89	0.54
1:E:203:VAL:O	1:E:207:ILE:HG12	2.07	0.54
1:E:683:PHE:CE2	1:E:825:GLU:HB2	2.42	0.54
1:A:409:ALA:O	1:A:413:VAL:HG23	2.06	0.54
1:C:980:PHE:CE2	1:C:1005:VAL:HG13	2.41	0.54
1:D:902:LEU:HD23	1:D:1023:PHE:CE1	2.42	0.54
1:F:945:VAL:HG23	1:F:1020:VAL:HG12	1.88	0.54
1:E:738:LEU:HD13	1:E:798:VAL:HG11	1.89	0.54
1:C:184:MET:HG3	1:C:246:PHE:CE1	2.42	0.54
1:D:197:GLN:HA	1:D:797:MET:SD	2.47	0.54
1:E:595:ARG:HG3	1:E:596:GLU:N	2.22	0.54
1:D:859:THR:HG23	1:D:860:GLY:N	2.22	0.54
1:D:100:PRO:HB3	1:D:295:THR:HG21	1.90	0.54
1:F:904:VAL:HB	1:F:905:PRO:HD3	1.89	0.54
1:A:1020:VAL:HB	1:A:1021:PRO:HD3	1.89	0.54
1:A:535:LEU:HD21	1:A:959:VAL:HG13	1.88	0.54
1:D:738:LEU:H	1:D:738:LEU:HD12	1.72	0.54
1:B:1023:PHE:O	1:B:1027:VAL:HG23	2.07	0.54
1:E:816:GLU:HB2	1:E:823:ALA:O	2.07	0.54
1:A:792:ASN:ND2	1:A:793:ASP:H	2.04	0.54
1:A:738:LEU:H	1:A:738:LEU:HD12	1.71	0.54
1:F:181:GLN:OE1	1:F:766:ARG:NH1	2.39	0.54
1:C:142:VAL:HG12	1:C:154:LEU:HD22	1.89	0.54
1:A:866:ARG:O	1:A:867:LEU:HG	2.06	0.54
1:A:652:GLN:HE22	1:A:664:PHE:HD1	1.54	0.54
1:E:43:ILE:HG12	1:E:104:GLN:HA	1.90	0.54
1:A:142:VAL:HB	1:A:158:ILE:HD11	1.89	0.54
1:B:445:ILE:HG22	1:B:942:ILE:HD12	1.88	0.54
1:D:1020:VAL:HB	1:D:1021:PRO:HD3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:O	1:A:420:MET:HB2	2.07	0.54
1:A:47:VAL:HG22	1:A:48:SER:N	2.23	0.54
1:B:11:PHE:CD1	1:C:889:ALA:HB1	2.42	0.54
1:E:305:ALA:C	1:E:307:ARG:H	2.10	0.54
1:F:281:PHE:O	1:F:282:ASN:HB2	2.08	0.54
1:C:190:PRO:HG3	1:C:788:TRP:CZ2	2.43	0.54
1:A:343:THR:HG21	1:A:998:GLN:OE1	2.06	0.54
1:E:242:THR:HG23	1:E:245:GLN:HG3	1.90	0.54
1:B:203:VAL:O	1:B:207:ILE:HG12	2.07	0.54
1:F:433:LYS:HD2	1:F:437:GLN:NE2	2.22	0.54
1:F:582:SER:HB3	1:F:586:ARG:HD3	1.89	0.54
1:B:43:ILE:HG12	1:B:104:GLN:HA	1.89	0.54
1:A:1015:LEU:O	1:A:1019:TRP:HD1	1.91	0.54
1:D:249:ILE:HG23	1:D:262:LEU:N	2.23	0.54
1:F:214:ILE:CG1	1:F:237:LYS:HB2	2.38	0.54
1:A:670:SER:O	1:A:671:VAL:HB	2.08	0.54
1:C:159:VAL:CG2	1:C:177:VAL:HG11	2.33	0.54
1:A:893:SER:N	1:C:10:ILE:HD11	2.23	0.54
1:D:830:PRO:HA	1:D:838:ASP:OD2	2.07	0.54
1:E:108:GLN:HB2	1:E:129:VAL:HG21	1.89	0.54
1:A:189:ASP:OD2	1:A:191:ALA:HB3	2.08	0.54
1:F:977:SER:O	1:F:981:ILE:HG12	2.08	0.54
1:E:293:LEU:CD2	1:E:302:THR:HG21	2.36	0.54
1:F:402:ILE:HD12	1:F:403:GLY:N	2.23	0.54
1:B:592:ASP:O	1:B:595:ARG:HG2	2.07	0.54
1:E:592:ASP:O	1:E:595:ARG:HG2	2.07	0.54
1:B:904:VAL:O	1:B:908:VAL:HG23	2.07	0.54
1:D:142:VAL:HG23	1:D:158:ILE:HD11	1.90	0.54
1:C:1029:THR:O	1:C:1030:LEU:HD23	2.08	0.54
1:F:729:GLU:HB2	1:F:805:THR:HG23	1.90	0.54
1:E:317:MET:SD	1:E:321:MET:HE3	2.48	0.54
2:A:2026:LMT:C8	2:A:2026:LMT:H122	2.33	0.54
1:A:531:VAL:O	1:A:532:ALA:O	2.26	0.54
1:F:683:PHE:CD2	1:F:818:TYR:CE1	2.97	0.54
1:E:800:PHE:HD2	1:E:804:ALA:HB2	1.73	0.54
1:E:657:SER:O	1:E:658:PHE:C	2.46	0.54
1:D:866:ARG:O	1:D:867:LEU:HG	2.06	0.54
1:D:535:LEU:HD21	1:D:959:VAL:HG13	1.90	0.53
1:E:891:TYR:CD2	1:E:896:ILE:HD11	2.42	0.53
1:D:712:LEU:HD21	1:D:842:ALA:CB	2.37	0.53
1:B:305:ALA:C	1:B:307:ARG:H	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:ARG:HG3	1:B:596:GLU:N	2.21	0.53
1:B:44:ALA:HB2	1:B:132:ALA:HB2	1.89	0.53
1:C:779:ARG:O	1:C:779:ARG:HD2	2.08	0.53
1:A:710:PRO:O	1:A:831:ALA:CB	2.55	0.53
1:F:896:ILE:HB	1:F:945:VAL:CG1	2.38	0.53
1:A:213:GLN:CG	1:B:56:THR:HG23	2.37	0.53
1:D:726:TYR:CE1	1:D:782:PRO:HB3	2.43	0.53
1:A:780:MET:CE	1:C:224:ALA:HA	2.37	0.53
1:C:143:VAL:HG13	1:C:286:ALA:HB2	1.88	0.53
1:B:904:VAL:HB	1:B:905:PRO:HD3	1.90	0.53
1:D:142:VAL:CG2	1:D:158:ILE:HD11	2.39	0.53
1:E:981:ILE:HG13	1:E:982:LEU:N	2.23	0.53
1:B:761:PHE:HE2	1:B:763:ASP:HB3	1.73	0.53
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.90	0.53
1:D:871:GLN:O	1:D:872:ALA:HB2	2.08	0.53
1:D:884:PHE:N	1:D:901:MET:HE1	2.23	0.53
1:B:657:SER:O	1:B:658:PHE:C	2.46	0.53
1:E:420:MET:HE1	1:E:499:PRO:HA	1.90	0.53
1:D:367:ILE:CD1	1:D:413:VAL:HG22	2.39	0.53
1:C:355:MET:SD	1:C:368:PRO:HB2	2.48	0.53
2:E:2033:LMT:C12	2:E:2033:LMT:H62	2.33	0.53
1:A:807:LYS:HG3	1:A:808:TRP:H	1.74	0.53
1:C:520:PHE:C	1:C:522:SER:H	2.11	0.53
1:D:62:VAL:O	1:D:65:ILE:HD13	2.08	0.53
1:D:416:VAL:HG12	1:D:420:MET:CE	2.38	0.53
1:A:930:LEU:O	1:A:934:ILE:HG23	2.08	0.53
1:B:240:LEU:HA	1:B:245:GLN:HE22	1.74	0.53
1:D:585:GLU:O	1:D:589:VAL:HG23	2.08	0.53
1:B:351:VAL:O	1:B:355:MET:HB2	2.09	0.53
1:C:446:ALA:O	1:C:450:SER:HB2	2.09	0.53
1:A:1008:GLY:O	1:A:1012:ALA:HB2	2.07	0.53
1:C:683:PHE:CD2	1:C:818:TYR:CE1	2.96	0.53
1:B:165:PRO:O	1:B:169:THR:HG23	2.09	0.53
1:E:391:ASN:H	1:E:394:THR:HG22	1.73	0.53
1:C:742:LEU:HB3	1:C:746:ASN:ND2	2.23	0.53
1:C:745:ILE:HG22	1:C:790:VAL:HG21	1.91	0.53
1:D:388:PHE:CE2	1:D:472:ILE:HG12	2.43	0.53
1:A:196:TYR:N	1:A:196:TYR:CD2	2.75	0.53
1:E:240:LEU:HA	1:E:245:GLN:HE22	1.74	0.53
1:D:98:THR:O	1:D:100:PRO:HD3	2.08	0.53
1:C:792:ASN:OD1	1:C:798:VAL:HG23	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:792:ASN:OD1	1:F:798:VAL:HG23	2.09	0.53
1:F:159:VAL:CG2	1:F:177:VAL:HG11	2.36	0.53
1:F:520:PHE:C	1:F:522:SER:H	2.12	0.53
1:E:151:LYS:NZ	1:E:278:ASN:HB3	2.24	0.53
1:C:43:ILE:HD11	1:C:107:VAL:HG21	1.89	0.53
1:B:62:VAL:CG2	1:B:88:MET:HG3	2.38	0.53
1:C:58:GLN:HA	1:C:62:VAL:HB	1.89	0.53
1:E:156:ASN:HD21	1:E:768:LYS:HZ3	1.55	0.53
1:F:393:LEU:HD13	1:F:466:ILE:HB	1.90	0.53
1:A:884:PHE:N	1:A:901:MET:HE1	2.23	0.53
1:F:433:LYS:HD2	1:F:437:GLN:HE21	1.74	0.53
1:C:582:SER:HB3	1:C:586:ARG:HD3	1.90	0.53
1:B:192:LYS:O	1:B:195:SER:HB3	2.08	0.53
1:D:365:THR:O	1:D:368:PRO:HD2	2.09	0.53
1:E:1014:VAL:O	1:E:1017:ILE:HG12	2.08	0.53
1:C:939:LYS:NZ	1:C:976:THR:CG2	2.71	0.53
1:A:578:THR:HG22	1:A:579:PRO:HD2	1.87	0.53
1:F:939:LYS:NZ	1:F:976:THR:HG22	2.23	0.53
1:B:676:ASN:ND2	1:B:827:LEU:HD12	2.20	0.53
1:E:843:VAL:O	1:E:847:VAL:HG23	2.08	0.53
1:C:45:VAL:HG22	1:C:129:VAL:HG22	1.90	0.53
1:D:131:LYS:O	1:D:295:THR:HG22	2.09	0.53
1:A:251:LEU:HD12	1:A:251:LEU:N	2.24	0.53
1:B:1014:VAL:O	1:B:1017:ILE:HG12	2.08	0.53
1:D:453:PHE:O	1:D:456:MET:HB2	2.08	0.53
1:B:392:THR:O	1:B:396:PHE:HD1	1.92	0.53
1:C:1001:ILE:HG13	1:C:1002:GLY:H	1.74	0.53
1:C:391:ASN:HB2	1:C:394:THR:H	1.74	0.53
1:B:143:VAL:HG12	1:B:286:ALA:CB	2.39	0.53
1:B:800:PHE:HD2	1:B:804:ALA:HB2	1.73	0.53
1:A:366:LEU:O	1:A:370:ILE:HG23	2.08	0.53
1:B:8:ARG:HB3	1:C:892:GLU:OE1	2.09	0.53
1:D:875:LEU:HD11	1:D:931:LEU:HD11	1.90	0.53
1:E:586:ARG:O	1:E:589:VAL:HG12	2.09	0.53
1:E:156:ASN:ND2	1:E:182:TYR:H	2.07	0.53
1:D:133:VAL:HG12	1:D:293:LEU:O	2.08	0.53
1:A:344:LEU:O	1:A:348:ILE:HG22	2.09	0.53
1:D:356:TYR:HE1	1:D:513:PHE:HZ	1.57	0.53
1:E:62:VAL:CG2	1:E:88:MET:HG3	2.38	0.53
1:A:532:ALA:HA	1:A:535:LEU:HB2	1.90	0.53
1:F:652:GLN:HG3	1:F:714:ARG:HH11	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:652:GLN:HG3	1:C:714:ARG:HH11	1.74	0.53
1:A:809:GLU:O	1:A:810:TYR:HB3	2.08	0.53
1:B:552:MET:HG3	1:B:553:ILE:N	2.23	0.53
1:D:366:LEU:O	1:D:370:ILE:HG23	2.09	0.53
1:E:761:PHE:HE2	1:E:763:ASP:HB3	1.73	0.53
1:E:953:GLU:C	1:E:955:GLY:H	2.12	0.53
1:F:1029:THR:O	1:F:1030:LEU:HD23	2.09	0.53
1:D:143:VAL:HG22	1:D:286:ALA:HB2	1.91	0.53
1:A:859:THR:HG23	1:A:860:GLY:N	2.23	0.53
1:B:817:ARG:HD2	1:B:822:PRO:HA	1.91	0.53
1:A:453:PHE:O	1:A:456:MET:HB2	2.09	0.53
1:C:939:LYS:HZ3	1:C:976:THR:CG2	2.22	0.53
1:F:742:LEU:HB3	1:F:746:ASN:ND2	2.24	0.53
1:D:690:VAL:HG22	1:D:694:VAL:HG21	1.90	0.53
1:F:326:PRO:HB3	1:F:610:PHE:HB2	1.90	0.53
1:B:24:GLY:O	1:B:27:ILE:HG12	2.09	0.53
1:C:539:ALA:N	1:C:540:PRO:HD2	2.24	0.53
1:D:753:TRP:HB2	1:F:217:GLY:H	1.74	0.52
1:E:944:ILE:HD11	1:E:1020:VAL:HG11	1.90	0.52
1:E:969:ARG:O	1:E:973:ILE:HG23	2.09	0.52
1:A:753:TRP:CB	1:C:217:GLY:H	2.21	0.52
1:B:435:MET:SD	1:B:438:ILE:HD11	2.50	0.52
1:D:723:GLU:HG2	1:D:813:PRO:HG3	1.91	0.52
1:B:530:GLY:O	1:B:534:ILE:HG13	2.10	0.52
1:C:43:ILE:CD1	1:C:104:GLN:HA	2.36	0.52
1:B:243:ALA:HB1	1:B:268:VAL:HG12	1.91	0.52
1:B:758:VAL:HG21	1:B:772:LEU:HB2	1.91	0.52
1:C:680:PHE:CE2	1:C:682:LEU:HD12	2.44	0.52
1:B:108:GLN:HB2	1:B:129:VAL:HG21	1.92	0.52
1:A:100:PRO:HB3	1:A:295:THR:HG21	1.90	0.52
1:D:358:PHE:CD2	1:D:975:MET:HB2	2.44	0.52
1:A:607:SER:HB2	1:A:632:LYS:HG2	1.91	0.52
1:F:568:ASP:CG	1:F:644:VAL:HG23	2.29	0.52
1:B:684:LEU:O	1:B:823:ALA:HB1	2.09	0.52
1:A:538:ARG:C	1:A:540:PRO:HD2	2.29	0.52
1:A:823:ALA:O	1:A:824:MET:HG2	2.09	0.52
1:F:944:ILE:HD11	1:F:1020:VAL:HB	1.92	0.52
1:A:416:VAL:HG11	1:A:497:LEU:HD23	1.91	0.52
1:E:530:GLY:O	1:E:534:ILE:HG13	2.09	0.52
1:C:939:LYS:NZ	1:C:976:THR:HG22	2.25	0.52
1:A:830:PRO:HA	1:A:838:ASP:OD2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:O	1:A:295:THR:HG22	2.09	0.52
1:C:303:ALA:O	1:C:307:ARG:HB2	2.09	0.52
1:E:794:LYS:HD3	1:E:795:GLY:N	2.24	0.52
1:A:851:PRO:O	1:A:854:VAL:HG12	2.09	0.52
1:A:485:ALA:O	1:A:490:PRO:HD3	2.08	0.52
1:B:53:SER:O	1:B:57:VAL:HG12	2.09	0.52
1:A:39:ALA:CB	1:A:672:LEU:HD11	2.40	0.52
1:A:875:LEU:HD11	1:A:931:LEU:HD11	1.91	0.52
1:C:896:ILE:HB	1:C:945:VAL:CG1	2.40	0.52
1:E:587:THR:HG21	1:E:622:GLN:O	2.09	0.52
1:C:225:VAL:O	1:C:228:GLN:HB2	2.10	0.52
1:F:773:GLN:HB3	1:F:779:ARG:HH12	1.74	0.52
1:A:449:LEU:HD12	1:A:478:MET:HG2	1.91	0.52
1:E:240:LEU:HA	1:E:245:GLN:NE2	2.24	0.52
1:D:210:GLN:HB2	1:D:249:ILE:HD12	1.91	0.52
1:F:355:MET:SD	1:F:368:PRO:HB2	2.49	0.52
1:A:709:ASN:O	1:A:711:ALA:N	2.43	0.52
1:A:680:PHE:CZ	1:A:843:VAL:HG21	2.45	0.52
1:D:538:ARG:C	1:D:540:PRO:HD2	2.30	0.52
1:D:696:LEU:HD13	1:D:699:ARG:NH1	2.25	0.52
1:F:225:VAL:O	1:F:228:GLN:HB2	2.09	0.52
1:A:943:LEU:HB3	1:A:969:ARG:NH1	2.24	0.52
1:E:904:VAL:HB	1:E:905:PRO:HD3	1.90	0.52
1:A:933:THR:OG1	1:A:1009:MET:HG2	2.09	0.52
1:B:977:SER:O	1:B:981:ILE:HG23	2.09	0.52
1:B:352:PHE:CD2	1:B:353:LEU:HD23	2.44	0.52
1:D:355:MET:HE2	1:D:410:ILE:HD11	1.91	0.52
1:E:435:MET:SD	1:E:438:ILE:HD11	2.49	0.52
1:D:545:TYR:HB2	1:D:1019:TRP:HZ3	1.70	0.52
1:C:943:LEU:CD1	1:C:973:ILE:HG22	2.39	0.52
1:E:165:PRO:O	1:E:169:THR:HG23	2.10	0.52
1:D:943:LEU:HB3	1:D:969:ARG:NH1	2.24	0.52
1:A:489:THR:HB	1:A:490:PRO:HD3	1.92	0.52
1:B:981:ILE:HG13	1:B:982:LEU:N	2.24	0.52
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.30	0.52
1:E:192:LYS:O	1:E:195:SER:HB3	2.10	0.52
1:A:358:PHE:CD2	1:A:975:MET:HB2	2.44	0.52
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.45	0.52
1:F:480:LEU:O	1:F:484:VAL:HG23	2.09	0.52
1:D:977:SER:O	1:D:981:ILE:HG23	2.09	0.52
1:C:433:LYS:HD2	1:C:437:GLN:NE2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:PHE:CD2	1:D:858:TRP:HZ3	2.26	0.52
1:D:531:VAL:O	1:D:532:ALA:O	2.28	0.52
1:A:416:VAL:HG12	1:A:420:MET:CE	2.39	0.52
1:E:243:ALA:HB1	1:E:268:VAL:HG12	1.91	0.52
1:B:891:TYR:CD2	1:B:896:ILE:HD11	2.45	0.52
1:F:609:VAL:HG22	1:F:629:ILE:HG23	1.92	0.52
1:F:680:PHE:CE2	1:F:682:LEU:HD12	2.44	0.52
1:A:996:GLY:H	1:A:999:HIS:HD2	1.58	0.52
1:F:358:PHE:CD1	1:F:975:MET:HG2	2.45	0.52
1:C:393:LEU:HD13	1:C:466:ILE:HB	1.92	0.52
1:B:816:GLU:HB2	1:B:823:ALA:O	2.09	0.52
1:D:688:ALA:O	1:D:689:GLY:C	2.48	0.52
1:C:607:SER:HB2	1:C:632:LYS:HG2	1.92	0.52
1:B:881:LEU:O	1:B:881:LEU:HD22	2.10	0.52
1:A:710:PRO:HD3	1:D:807:LYS:CE	2.39	0.52
1:B:125:GLN:NE2	1:B:769:ARG:NH1	2.53	0.52
1:C:902:LEU:HD13	1:C:1023:PHE:CD2	2.45	0.52
1:C:527:TYR:HD1	1:C:1018:PHE:CE2	2.28	0.52
1:F:939:LYS:HZ3	1:F:976:THR:HG21	1.73	0.52
1:B:293:LEU:CD2	1:B:302:THR:HG21	2.38	0.52
1:C:447:MET:HE3	1:C:886:CYS:HB3	1.91	0.52
1:B:549:VAL:O	1:B:552:MET:HG2	2.09	0.52
1:A:388:PHE:CE2	1:A:472:ILE:HG12	2.43	0.52
1:D:159:VAL:HA	1:D:163:GLN:HB2	1.90	0.52
1:E:348:ILE:HD12	1:E:369:THR:HG23	1.92	0.52
1:B:574:ALA:HB3	1:B:627:ALA:HB3	1.91	0.52
1:F:692:HIS:O	1:F:696:LEU:HB2	2.10	0.52
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.10	0.52
1:D:695:LEU:HD13	1:D:699:ARG:HH21	1.74	0.52
1:F:818:TYR:CD1	1:F:823:ALA:HB3	2.45	0.52
1:E:392:THR:O	1:E:396:PHE:HD1	1.93	0.52
1:D:449:LEU:HD12	1:D:478:MET:HG2	1.92	0.52
1:B:794:LYS:HD3	1:B:795:GLY:N	2.25	0.52
1:C:159:VAL:HG12	1:C:159:VAL:O	2.08	0.52
1:E:703:LEU:CD1	1:E:717:PRO:HG3	2.37	0.52
1:F:534:ILE:HD12	1:F:1022:LEU:HD12	1.92	0.52
1:D:933:THR:OG1	1:D:1009:MET:HG2	2.10	0.52
1:C:912:LEU:CD2	1:C:926:PHE:HZ	2.23	0.52
1:A:259:GLN:N	1:A:259:GLN:HE21	2.07	0.52
1:A:708:GLN:OE1	1:D:809:GLU:HA	2.10	0.52
1:D:823:ALA:O	1:D:824:MET:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:745:ILE:HG22	1:F:790:VAL:HG21	1.91	0.52
1:A:356:TYR:HE1	1:A:513:PHE:HZ	1.58	0.52
1:B:102:ILE:HD12	1:B:102:ILE:C	2.29	0.52
1:A:725:GLN:HG3	1:A:811:GLY:H	1.75	0.52
1:F:751:ILE:HB	1:F:756:SER:HB2	1.91	0.52
1:B:162:ILE:HG22	1:B:313:LEU:CD1	2.32	0.51
1:D:680:PHE:CZ	1:D:843:VAL:HG21	2.45	0.51
1:A:453:PHE:HE2	1:A:932:THR:HG22	1.74	0.51
1:E:46:GLN:HE22	2:E:2033:LMT:H42	1.74	0.51
2:E:2033:LMT:O6B	2:E:2033:LMT:H6E	2.10	0.51
1:D:593:SER:HB3	1:D:658:PHE:CZ	2.45	0.51
1:F:912:LEU:CD2	1:F:926:PHE:HZ	2.22	0.51
1:A:572:LEU:HB3	1:A:629:ILE:HB	1.92	0.51
1:C:773:GLN:HB3	1:C:779:ARG:HH12	1.74	0.51
1:E:574:ALA:HB3	1:E:627:ALA:HB3	1.92	0.51
1:C:687:GLN:NE2	1:C:855:GLY:HA3	2.25	0.51
1:D:485:ALA:O	1:D:490:PRO:HD3	2.10	0.51
1:A:812:SER:OG	1:A:815:LEU:HD13	2.10	0.51
1:B:348:ILE:HD12	1:B:369:THR:HG23	1.92	0.51
1:D:15:ILE:HD13	1:D:15:ILE:C	2.29	0.51
1:B:151:LYS:NZ	1:B:278:ASN:HB3	2.25	0.51
1:D:416:VAL:O	1:D:420:MET:HB2	2.10	0.51
1:C:188:LEU:HA	1:C:266:ALA:HB2	1.92	0.51
1:A:356:TYR:O	1:A:356:TYR:HD1	1.93	0.51
1:D:555:MET:SD	1:D:913:LEU:HD23	2.49	0.51
1:C:751:ILE:HB	1:C:756:SER:HB2	1.92	0.51
1:F:539:ALA:N	1:F:540:PRO:HD2	2.25	0.51
1:F:456:MET:HE3	1:F:931:LEU:HD12	1.92	0.51
1:D:409:ALA:O	1:D:413:VAL:HG23	2.11	0.51
1:F:214:ILE:HG12	1:F:237:LYS:HB2	1.92	0.51
1:D:242:THR:HG23	1:D:245:GLN:H	1.75	0.51
1:D:958:ILE:HD13	1:D:959:VAL:H	1.76	0.51
1:B:703:LEU:CD1	1:B:717:PRO:HG3	2.36	0.51
1:F:43:ILE:HD11	1:F:107:VAL:CG2	2.39	0.51
1:B:587:THR:HG21	1:B:622:GLN:O	2.10	0.51
1:A:594:MET:O	1:A:595:ARG:C	2.49	0.51
1:B:240:LEU:HA	1:B:245:GLN:NE2	2.25	0.51
1:B:420:MET:HE3	1:B:427:PRO:HA	1.92	0.51
1:D:439:GLN:O	1:D:443:VAL:HG23	2.10	0.51
1:E:517:ASN:O	1:E:521:LEU:HB2	2.10	0.51
1:E:143:VAL:HG12	1:E:286:ALA:CB	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE1	1:A:406:VAL:CG1	2.40	0.51
1:E:906:LEU:O	1:E:1011:THR:HG23	2.10	0.51
1:D:181:GLN:HG3	1:D:768:LYS:HZ3	1.74	0.51
1:A:242:THR:HG23	1:A:245:GLN:H	1.76	0.51
1:C:980:PHE:HE2	1:C:1005:VAL:HG13	1.75	0.51
1:C:109:ASN:HA	1:C:112:GLN:CD	2.30	0.51
1:A:485:ALA:HA	1:A:489:THR:OG1	2.10	0.51
1:A:977:SER:O	1:A:981:ILE:HG23	2.10	0.51
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.45	0.51
1:A:142:VAL:CG1	1:A:154:LEU:HD22	2.40	0.51
1:C:527:TYR:O	1:C:531:VAL:HG23	2.11	0.51
1:E:188:LEU:HD11	1:E:772:LEU:HD21	1.93	0.51
1:D:780:MET:HE3	1:F:224:ALA:CA	2.41	0.51
1:D:913:LEU:O	1:D:917:MET:HG2	2.11	0.51
1:E:102:ILE:C	1:E:102:ILE:HD12	2.31	0.51
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.92	0.51
1:A:688:ALA:O	1:A:689:GLY:C	2.48	0.51
1:F:227:GLY:O	1:F:229:GLN:HG3	2.11	0.51
1:D:749:VAL:HG13	1:D:753:TRP:CD1	2.46	0.51
1:D:812:SER:OG	1:D:815:LEU:HD13	2.10	0.51
1:E:428:ARG:CD	1:E:428:ARG:H	2.17	0.51
1:D:538:ARG:C	1:D:538:ARG:HE	2.13	0.51
1:E:1:MET:O	1:E:4:PHE:HB3	2.10	0.51
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.75	0.51
1:B:34:GLN:HG3	1:B:35:TYR:CD2	2.45	0.51
1:D:548:ILE:HG23	1:D:909:ILE:HD13	1.92	0.51
1:F:49:TYR:HE1	1:F:121:GLU:CG	2.23	0.51
1:A:196:TYR:CD1	1:A:260:VAL:HG11	2.45	0.51
1:F:391:ASN:HB2	1:F:394:THR:H	1.75	0.51
1:C:729:GLU:HB2	1:C:805:THR:HG23	1.91	0.51
1:A:367:ILE:CD1	1:A:413:VAL:HG22	2.40	0.51
1:B:415:ASN:ND2	1:B:434:SER:HB2	2.22	0.51
1:D:193:LEU:HD21	1:D:265:VAL:HG13	1.92	0.51
1:C:169:THR:HG23	1:C:172:VAL:HG21	1.92	0.51
1:C:977:SER:OG	1:C:1009:MET:HE1	2.11	0.51
1:C:891:TYR:CD1	1:C:896:ILE:HD11	2.46	0.51
1:C:944:ILE:HD11	1:C:1020:VAL:HB	1.93	0.51
1:F:527:TYR:HD1	1:F:1018:PHE:CE2	2.29	0.51
1:D:213:GLN:CG	1:E:56:THR:HG23	2.41	0.51
1:F:682:LEU:HD11	1:F:843:VAL:CG1	2.39	0.51
1:A:225:VAL:HG12	1:B:780:MET:HE2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:15:ILE:HG13	1:F:16:ALA:N	2.24	0.51
1:F:143:VAL:O	1:F:321:MET:HA	2.10	0.51
1:F:109:ASN:HA	1:F:112:GLN:CD	2.31	0.51
1:A:210:GLN:HB2	1:A:249:ILE:HD12	1.93	0.51
1:E:423:GLU:OE2	1:E:433:LYS:HE3	2.10	0.51
1:F:687:GLN:NE2	1:F:855:GLY:HA3	2.26	0.51
1:A:376:LEU:O	1:A:379:THR:CG2	2.59	0.51
1:D:156:ASN:ND2	1:D:768:LYS:NZ	2.58	0.51
1:A:273:GLN:NE2	1:A:769:ARG:HD2	2.25	0.51
1:B:367:ILE:HB	1:B:368:PRO:CD	2.38	0.51
1:A:62:VAL:O	1:A:65:ILE:HD13	2.10	0.51
1:C:609:VAL:HG22	1:C:629:ILE:HG23	1.91	0.51
1:F:247:GLU:HB3	1:F:263:LYS:HE2	1.93	0.51
1:A:780:MET:SD	1:C:228:GLN:HG3	2.51	0.51
1:C:49:TYR:HE1	1:C:121:GLU:CG	2.23	0.51
1:F:607:SER:HB2	1:F:632:LYS:HG2	1.93	0.51
1:A:15:ILE:C	1:A:15:ILE:HD13	2.31	0.51
1:A:704:MET:O	1:A:707:ALA:HB3	2.11	0.51
1:A:723:GLU:HG2	1:A:813:PRO:HG3	1.90	0.51
1:D:594:MET:O	1:D:595:ARG:C	2.49	0.51
1:C:680:PHE:HE2	1:C:682:LEU:HD12	1.76	0.51
1:C:80:SER:HA	1:C:90:ILE:HA	1.93	0.51
1:A:548:ILE:HG23	1:A:909:ILE:HD13	1.93	0.51
1:D:572:LEU:HB3	1:D:629:ILE:HB	1.92	0.51
1:F:1001:ILE:HG13	1:F:1002:GLY:H	1.76	0.51
1:F:446:ALA:O	1:F:450:SER:HB2	2.10	0.51
1:D:423:GLU:HB3	1:D:425:LEU:HD13	1.92	0.51
1:B:969:ARG:O	1:B:973:ILE:HG23	2.10	0.51
1:C:367:ILE:CG1	1:C:368:PRO:HD3	2.41	0.51
1:A:875:LEU:HD12	1:A:876:TYR:N	2.26	0.51
1:A:708:GLN:HE21	1:A:708:GLN:HA	1.76	0.51
1:B:1:MET:O	1:B:4:PHE:HB3	2.11	0.51
1:C:545:TYR:CD1	1:C:1023:PHE:HZ	2.30	0.51
1:C:891:TYR:CG	1:C:896:ILE:HD11	2.46	0.51
1:E:584:ALA:O	1:E:588:GLN:HB2	2.11	0.51
1:E:418:ARG:CZ	1:E:968:MET:HE3	2.41	0.51
1:D:428:ARG:HH12	1:D:432:ARG:NE	2.09	0.51
1:C:150:THR:HG23	1:C:152:GLU:H	1.76	0.51
1:C:456:MET:HE3	1:C:931:LEU:HD12	1.91	0.51
1:B:517:ASN:O	1:B:521:LEU:HB2	2.11	0.51
1:F:303:ALA:O	1:F:307:ARG:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:O	1:D:348:ILE:HG22	2.11	0.51
1:A:115:THR:HA	1:A:118:LEU:HD13	1.92	0.51
1:D:375:VAL:CG2	1:D:405:LEU:HG	2.24	0.50
1:F:980:PHE:HE2	1:F:1005:VAL:HG13	1.75	0.50
1:E:751:ILE:O	1:E:773:GLN:HA	2.11	0.50
1:E:11:PHE:CD1	1:F:889:ALA:HB1	2.46	0.50
1:A:909:ILE:C	1:A:911:ALA:H	2.14	0.50
1:B:586:ARG:O	1:B:589:VAL:HG12	2.10	0.50
1:F:150:THR:HG23	1:F:152:GLU:H	1.76	0.50
1:F:188:LEU:HA	1:F:266:ALA:HB2	1.92	0.50
1:A:930:LEU:O	1:A:933:THR:HG22	2.10	0.50
1:A:865:GLU:O	1:A:866:ARG:HB2	2.11	0.50
1:D:146:ASP:C	1:D:148:SER:H	2.14	0.50
1:B:906:LEU:O	1:B:1011:THR:HG23	2.11	0.50
1:A:753:TRP:CH2	1:A:785:LEU:HA	2.46	0.50
1:A:699:ARG:O	1:A:703:LEU:HD23	2.11	0.50
1:E:8:ARG:HB3	1:F:892:GLU:OE1	2.10	0.50
1:B:239:ARG:HD3	1:B:760:ASP:O	2.11	0.50
1:D:195:SER:C	1:D:197:GLN:H	2.15	0.50
1:A:655:PHE:HD2	1:A:658:PHE:HE2	1.60	0.50
1:C:247:GLU:HB3	1:C:263:LYS:HE2	1.94	0.50
1:C:143:VAL:O	1:C:321:MET:HA	2.11	0.50
1:C:466:ILE:O	1:C:469:GLN:HB2	2.11	0.50
1:F:142:VAL:CG1	1:F:154:LEU:HD22	2.41	0.50
1:D:884:PHE:HB2	1:D:901:MET:HE2	1.93	0.50
1:A:518:ARG:O	1:A:522:SER:N	2.41	0.50
1:C:872:ALA:HB1	1:C:876:TYR:CE1	2.45	0.50
1:B:681:ASP:OD1	1:B:681:ASP:C	2.48	0.50
1:E:312:ASN:HD22	1:E:312:ASN:N	2.09	0.50
1:A:6:ILE:HD12	1:A:6:ILE:H	1.75	0.50
1:E:882:VAL:HG13	2:E:2032:LMT:H121	1.92	0.50
1:D:753:TRP:CH2	1:D:785:LEU:HA	2.47	0.50
1:D:544:ILE:HG23	1:D:1019:TRP:HH2	1.76	0.50
1:E:758:VAL:HG21	1:E:772:LEU:HB2	1.92	0.50
1:A:156:ASN:ND2	1:A:182:TYR:H	2.09	0.50
1:C:973:ILE:HD11	1:C:1017:ILE:HG22	1.93	0.50
1:C:135:ASN:O	1:C:292:LYS:HG2	2.11	0.50
1:E:20:MET:CE	1:E:374:VAL:HG23	2.41	0.50
1:F:466:ILE:O	1:F:469:GLN:HB2	2.12	0.50
1:C:379:THR:HB	1:C:398:MET:HE3	1.93	0.50
1:F:27:ILE:HD11	1:F:380:PHE:CD1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:HE2	1:A:410:ILE:HD11	1.93	0.50
1:A:133:VAL:HG12	1:A:293:LEU:O	2.12	0.50
1:A:538:ARG:HG3	1:A:1022:LEU:CD2	2.42	0.50
1:B:584:ALA:O	1:B:588:GLN:HB2	2.11	0.50
1:C:534:ILE:HD12	1:C:1022:LEU:HD12	1.94	0.50
1:F:680:PHE:HE2	1:F:682:LEU:HD12	1.77	0.50
1:A:593:SER:HB3	1:A:658:PHE:CZ	2.46	0.50
1:F:478:MET:O	1:F:481:SER:HB3	2.10	0.50
1:A:562:ALA:O	1:A:923:ASP:HA	2.11	0.50
1:B:2:SER:HB3	1:B:486:LEU:O	2.11	0.50
1:D:751:ILE:CG2	1:D:772:LEU:HD13	2.42	0.50
1:D:785:LEU:HD11	1:F:219:LEU:HD21	1.93	0.50
1:C:214:ILE:CG1	1:C:237:LYS:HB2	2.41	0.50
1:A:498:LYS:N	1:A:499:PRO:CD	2.62	0.50
1:C:166:LEU:HA	1:C:169:THR:HG22	1.94	0.50
1:D:538:ARG:HG3	1:D:1022:LEU:CD2	2.42	0.50
1:B:367:ILE:HD13	1:B:496:MET:HE2	1.92	0.50
1:A:896:ILE:N	1:A:897:PRO:CD	2.74	0.50
1:E:896:ILE:N	1:E:897:PRO:CD	2.75	0.50
1:B:751:ILE:O	1:B:773:GLN:HA	2.11	0.50
1:D:655:PHE:HD2	1:D:658:PHE:HE2	1.59	0.50
1:D:909:ILE:C	1:D:911:ALA:H	2.14	0.50
1:C:711:ALA:HB3	1:C:712:LEU:HD23	1.94	0.50
1:D:210:GLN:NE2	1:D:249:ILE:HG13	2.26	0.50
1:A:637:ARG:O	1:A:642:ASN:HB2	2.12	0.50
1:D:273:GLN:NE2	1:D:769:ARG:HD2	2.27	0.50
1:D:724:PRO:CA	1:D:810:TYR:HB2	2.42	0.50
1:A:958:ILE:HD13	1:A:959:VAL:H	1.76	0.50
1:A:438:ILE:O	1:A:442:LEU:HD13	2.12	0.50
1:A:1003:THR:HG23	1:A:1004:GLY:N	2.27	0.50
1:B:528:GLU:HB3	1:B:963:ILE:HD11	1.94	0.50
1:D:576:VAL:HB	1:D:625:GLY:O	2.11	0.50
1:C:317:MET:HB3	1:C:321:MET:SD	2.51	0.50
1:A:913:LEU:O	1:A:917:MET:HG2	2.12	0.50
1:A:131:LYS:O	1:A:131:LYS:HG3	2.12	0.50
1:C:192:LYS:HD3	1:C:264:ASP:O	2.11	0.50
1:D:160:SER:O	1:D:766:ARG:NH1	2.45	0.50
1:C:183:SER:OG	1:C:273:GLN:HG3	2.12	0.50
1:B:1030:LEU:O	1:B:1030:LEU:HD22	2.12	0.50
1:E:16:ALA:HB2	1:E:488:LEU:HG	1.93	0.50
1:D:637:ARG:HB2	1:D:642:ASN:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:489:THR:OG1	1:E:490:PRO:HD3	2.12	0.50
1:B:569:GLN:O	1:B:571:VAL:N	2.44	0.50
1:B:418:ARG:CZ	1:B:968:MET:HE3	2.42	0.50
1:E:38:ILE:HG13	1:E:462:SER:HB2	1.94	0.50
1:F:192:LYS:HD3	1:F:264:ASP:O	2.12	0.50
1:F:872:ALA:HB1	1:F:876:TYR:CE1	2.47	0.50
1:A:235:ILE:HD13	1:A:235:ILE:H	1.76	0.50
1:B:944:ILE:HD11	1:B:1020:VAL:HG11	1.92	0.50
1:D:262:LEU:HD22	1:D:263:LYS:N	2.26	0.50
1:F:367:ILE:CG1	1:F:368:PRO:HD3	2.41	0.50
1:E:219:LEU:HD12	1:F:726:TYR:CE1	2.46	0.50
1:A:637:ARG:HB2	1:A:642:ASN:HB3	1.93	0.50
1:C:281:PHE:O	1:C:282:ASN:HB2	2.11	0.50
1:F:188:LEU:HD21	1:F:203:VAL:HG11	1.94	0.50
1:D:573:PHE:HB2	1:D:666:PHE:CD2	2.47	0.50
1:A:739:GLY:HA3	1:A:793:ASP:HB2	1.94	0.50
1:B:102:ILE:O	1:B:105:VAL:HG12	2.12	0.50
1:B:423:GLU:OE2	1:B:433:LYS:HE3	2.11	0.50
1:E:515:TRP:CZ2	1:E:519:MET:HG3	2.47	0.50
1:A:585:GLU:O	1:A:589:VAL:HG23	2.10	0.50
1:B:235:ILE:HG13	1:B:235:ILE:O	2.11	0.50
1:F:891:TYR:CG	1:F:896:ILE:HD11	2.47	0.50
1:A:156:ASN:HD22	1:A:182:TYR:H	1.59	0.50
1:E:371:ALA:O	1:E:374:VAL:HG12	2.12	0.50
1:F:65:ILE:CD1	1:F:90:ILE:HG12	2.42	0.50
1:D:865:GLU:O	1:D:866:ARG:HB2	2.12	0.50
1:B:352:PHE:HD1	1:B:365:THR:HG23	1.77	0.50
1:B:224:ALA:HB1	1:C:780:MET:SD	2.51	0.50
1:F:658:PHE:O	1:F:659:LYS:C	2.50	0.50
1:E:235:ILE:O	1:E:235:ILE:HG13	2.12	0.50
1:E:46:GLN:HE22	2:E:2033:LMT:C4	2.25	0.49
1:F:166:LEU:HD21	1:F:310:ILE:HG23	1.93	0.49
1:F:891:TYR:CD1	1:F:896:ILE:HD11	2.47	0.49
1:C:939:LYS:HZ1	1:C:976:THR:HG22	1.77	0.49
1:B:896:ILE:N	1:B:897:PRO:CD	2.75	0.49
1:A:195:SER:C	1:A:197:GLN:H	2.14	0.49
1:F:317:MET:HB3	1:F:321:MET:SD	2.52	0.49
1:A:449:LEU:HD13	1:A:449:LEU:O	2.12	0.49
1:A:818:TYR:O	1:A:820:GLY:N	2.45	0.49
1:F:139:VAL:O	1:F:326:PRO:HD2	2.11	0.49
1:F:612:VAL:HG11	1:F:615:PHE:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:LEU:HD21	2:D:2026:LMT:H81	1.92	0.49
1:A:175:PHE:CD1	1:A:289:ILE:HD11	2.47	0.49
1:F:977:SER:OG	1:F:1009:MET:HE1	2.12	0.49
1:D:222:LEU:HD23	1:E:622:GLN:NE2	2.26	0.49
1:B:188:LEU:HD11	1:B:772:LEU:HD21	1.94	0.49
1:F:80:SER:HA	1:F:90:ILE:HA	1.94	0.49
1:B:391:ASN:H	1:B:394:THR:HG22	1.75	0.49
1:B:616:ASN:CG	1:B:624:SER:HB2	2.33	0.49
1:E:553:ILE:O	1:E:557:THR:HG23	2.12	0.49
1:B:156:ASN:ND2	1:B:182:TYR:H	2.10	0.49
1:D:131:LYS:O	1:D:131:LYS:HG3	2.11	0.49
1:D:356:TYR:HE1	1:D:513:PHE:CZ	2.30	0.49
1:B:343:THR:HA	1:B:346:GLU:HG2	1.94	0.49
1:E:786:SER:HB2	1:E:801:ASN:OD1	2.12	0.49
1:D:155:SER:OG	1:D:179:GLY:HA3	2.11	0.49
1:A:766:ARG:NE	1:B:67:GLN:NE2	2.60	0.49
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.93	0.49
1:E:47:VAL:H	1:E:88:MET:CE	2.25	0.49
1:A:708:GLN:NE2	1:A:708:GLN:HA	2.27	0.49
1:C:453:PHE:CE2	1:C:474:ILE:HD12	2.47	0.49
1:F:902:LEU:HD13	1:F:1023:PHE:CD2	2.47	0.49
1:D:875:LEU:CD1	1:D:931:LEU:HD11	2.43	0.49
1:F:186:ILE:HG13	1:F:772:LEU:HD23	1.95	0.49
1:C:186:ILE:HG13	1:C:772:LEU:HD23	1.94	0.49
1:F:135:ASN:O	1:F:292:LYS:HG2	2.12	0.49
1:C:818:TYR:CD1	1:C:823:ALA:HB3	2.46	0.49
1:B:185:ARG:NH2	1:B:771:TYR:HB3	2.27	0.49
1:F:757:TYR:CD1	1:F:769:ARG:HD3	2.48	0.49
1:C:695:LEU:CD1	1:C:699:ARG:HH22	2.25	0.49
1:C:692:HIS:O	1:C:696:LEU:HB2	2.11	0.49
1:D:355:MET:HE1	1:D:406:VAL:CG1	2.42	0.49
1:A:749:VAL:HG13	1:A:753:TRP:CD1	2.46	0.49
1:A:498:LYS:H	1:A:499:PRO:HD3	1.75	0.49
1:A:170:LYS:CA	1:A:170:LYS:HE3	2.37	0.49
1:D:875:LEU:HD12	1:D:876:TYR:N	2.27	0.49
1:A:576:VAL:HB	1:A:625:GLY:O	2.13	0.49
1:D:996:GLY:N	1:D:999:HIS:CD2	2.78	0.49
1:C:757:TYR:CD1	1:C:769:ARG:HD3	2.47	0.49
1:C:358:PHE:CD1	1:C:975:MET:HG2	2.48	0.49
1:C:139:VAL:O	1:C:326:PRO:HD2	2.12	0.49
1:C:433:LYS:HD2	1:C:437:GLN:HE21	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:PHE:CD2	1:E:353:LEU:HD23	2.48	0.49
1:D:562:ALA:O	1:D:923:ASP:HA	2.12	0.49
1:E:53:SER:O	1:E:57:VAL:HG12	2.12	0.49
1:B:246:PHE:O	1:B:249:ILE:HD11	2.12	0.49
1:A:439:GLN:O	1:A:443:VAL:HG23	2.11	0.49
1:D:753:TRP:CB	1:F:217:GLY:H	2.25	0.49
1:B:158:ILE:CG2	1:B:162:ILE:HD11	2.39	0.49
1:A:730:ILE:CD1	1:A:745:ILE:HD11	2.43	0.49
1:A:535:LEU:CD2	1:A:963:ILE:HD11	2.42	0.49
1:B:428:ARG:H	1:B:428:ARG:CD	2.16	0.49
1:C:903:VAL:CG2	1:C:1020:VAL:HG22	2.43	0.49
1:D:170:LYS:CA	1:D:170:LYS:HE3	2.40	0.49
1:D:896:ILE:N	1:D:897:PRO:CD	2.75	0.49
1:D:453:PHE:HE2	1:D:932:THR:HG22	1.77	0.49
1:C:682:LEU:HD11	1:C:843:VAL:CG1	2.41	0.49
1:C:65:ILE:CD1	1:C:90:ILE:HG12	2.42	0.49
1:E:904:VAL:O	1:E:908:VAL:HG23	2.12	0.49
1:B:104:GLN:HE21	1:B:131:LYS:HE2	1.77	0.49
1:A:730:ILE:HD12	1:A:745:ILE:HD11	1.93	0.49
1:D:518:ARG:O	1:D:522:SER:HB3	2.12	0.49
1:D:217:GLY:O	1:D:234:ILE:HG12	2.12	0.49
1:D:194:ASN:HD22	1:D:797:MET:HG2	1.77	0.49
1:E:616:ASN:CG	1:E:624:SER:HB2	2.33	0.49
1:F:711:ALA:HB3	1:F:712:LEU:HD23	1.94	0.49
1:F:154:LEU:O	1:F:157:TYR:HB3	2.13	0.49
1:F:872:ALA:HB3	1:F:873:PRO:HD3	1.94	0.49
1:E:352:PHE:HD1	1:E:365:THR:HG23	1.78	0.49
1:C:658:PHE:O	1:C:659:LYS:C	2.50	0.49
1:F:183:SER:OG	1:F:273:GLN:HG3	2.13	0.49
1:C:227:GLY:O	1:C:229:GLN:HG3	2.13	0.49
1:E:1023:PHE:O	1:E:1027:VAL:HG23	2.13	0.49
1:B:944:ILE:HG22	1:B:969:ARG:HG3	1.95	0.49
1:A:544:ILE:HG23	1:A:1019:TRP:HH2	1.78	0.49
1:E:239:ARG:HD3	1:E:760:ASP:O	2.12	0.49
1:E:578:THR:HG21	1:E:587:THR:HB	1.95	0.49
1:D:170:LYS:HZ3	1:E:74:ASN:H	1.56	0.49
1:C:969:ARG:C	1:C:972:PRO:HD2	2.33	0.49
1:F:143:VAL:HG23	1:F:324:VAL:HG21	1.95	0.49
1:A:780:MET:HE3	1:C:225:VAL:N	2.28	0.49
1:B:953:GLU:C	1:B:955:GLY:H	2.16	0.49
1:B:445:ILE:HG22	1:B:942:ILE:CD1	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:ALA:HA	1:D:535:LEU:HB2	1.94	0.49
1:A:696:LEU:HD13	1:A:699:ARG:NH1	2.28	0.49
1:D:699:ARG:O	1:D:703:LEU:HD23	2.13	0.49
1:F:759:ASN:H	1:F:770:VAL:HG22	1.77	0.49
1:F:443:VAL:O	1:F:447:MET:HB2	2.12	0.49
1:B:515:TRP:CZ2	1:B:519:MET:HG3	2.48	0.49
1:E:76:ARG:HD3	1:E:863:TYR:CE2	2.48	0.49
1:E:426:SER:HB2	1:E:427:PRO:HD2	1.94	0.49
1:C:695:LEU:HD13	1:C:699:ARG:HH12	1.78	0.49
1:D:724:PRO:HA	1:D:810:TYR:CB	2.43	0.49
1:E:367:ILE:HD13	1:E:496:MET:HE2	1.95	0.49
1:C:759:ASN:H	1:C:770:VAL:HG22	1.78	0.49
1:C:985:VAL:CG2	1:C:986:PRO:HD3	2.43	0.49
1:E:1001:ILE:HG13	1:E:1002:GLY:N	2.27	0.49
1:A:840:MET:HA	1:A:844:GLU:HB2	1.94	0.49
1:C:143:VAL:HG23	1:C:324:VAL:HG21	1.94	0.49
1:A:146:ASP:C	1:A:148:SER:H	2.14	0.49
1:B:635:GLU:H	1:B:635:GLU:CD	2.16	0.49
1:E:973:ILE:HD11	1:E:1017:ILE:CG2	2.43	0.49
1:E:445:ILE:HG22	1:E:942:ILE:CD1	2.43	0.49
1:A:538:ARG:C	1:A:538:ARG:HE	2.17	0.49
1:A:952:HIS:CE1	1:A:958:ILE:HG22	2.48	0.49
1:E:571:VAL:HG23	1:E:668:PRO:HG2	1.95	0.49
1:C:438:ILE:C	1:C:440:GLY:H	2.16	0.49
1:A:235:ILE:N	1:A:235:ILE:HD13	2.28	0.49
1:B:786:SER:HB2	1:B:801:ASN:OD1	2.13	0.49
1:B:312:ASN:N	1:B:312:ASN:HD22	2.11	0.49
1:E:1030:LEU:O	1:E:1030:LEU:HD22	2.12	0.49
1:A:193:LEU:HD21	1:A:265:VAL:HG13	1.94	0.48
1:E:4:PHE:CZ	1:E:8:ARG:HD2	2.47	0.48
1:B:753:TRP:CH2	1:B:785:LEU:HG	2.48	0.48
1:B:843:VAL:O	1:B:847:VAL:HG23	2.13	0.48
1:C:188:LEU:HD21	1:C:203:VAL:HG11	1.94	0.48
1:D:449:LEU:O	1:D:449:LEU:HD13	2.13	0.48
1:D:698:ALA:HB2	1:D:851:PRO:HG2	1.93	0.48
1:D:489:THR:HB	1:D:490:PRO:HD3	1.94	0.48
1:E:102:ILE:O	1:E:105:VAL:HG12	2.13	0.48
1:D:316:PHE:CG	1:E:687:GLN:HB2	2.47	0.48
1:F:576:VAL:HG22	1:F:663:VAL:HG12	1.95	0.48
1:F:690:VAL:HG11	1:F:694:VAL:HG11	1.95	0.48
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:ILE:O	1:D:442:LEU:HD13	2.12	0.48
1:C:973:ILE:CD1	1:C:1017:ILE:HG22	2.43	0.48
1:A:428:ARG:HH12	1:A:432:ARG:NE	2.10	0.48
1:A:85:ASP:OD2	1:A:620:ARG:HG3	2.13	0.48
1:E:156:ASN:ND2	1:E:182:TYR:N	2.60	0.48
1:B:904:VAL:HG22	1:B:934:ILE:HD12	1.95	0.48
1:A:143:VAL:HG22	1:A:286:ALA:HB2	1.95	0.48
1:E:234:ILE:HG22	1:F:726:TYR:CB	2.31	0.48
1:C:924:VAL:O	1:C:928:VAL:HG23	2.13	0.48
1:A:418:ARG:HD3	1:A:419:VAL:N	2.28	0.48
1:D:80:SER:HA	1:D:90:ILE:HA	1.94	0.48
1:D:418:ARG:HD3	1:D:419:VAL:N	2.28	0.48
1:B:1001:ILE:HG13	1:B:1002:GLY:N	2.28	0.48
1:F:45:VAL:HG22	1:F:129:VAL:HG22	1.95	0.48
1:C:886:CYS:O	1:C:890:LEU:HB2	2.14	0.48
1:D:115:THR:HA	1:D:118:LEU:HD13	1.95	0.48
1:F:185:ARG:HH11	1:F:771:TYR:CB	2.26	0.48
1:B:565:PRO:HG3	1:B:923:ASP:HB3	1.95	0.48
1:B:104:GLN:O	1:B:107:VAL:HG12	2.13	0.48
1:B:69:MET:HE3	1:B:107:VAL:HG22	1.95	0.48
1:D:367:ILE:HG12	1:D:368:PRO:CD	2.43	0.48
1:D:175:PHE:CD1	1:D:289:ILE:HD11	2.48	0.48
1:A:416:VAL:HG12	1:A:420:MET:HE2	1.95	0.48
1:F:969:ARG:C	1:F:972:PRO:HD2	2.34	0.48
1:E:528:GLU:HB3	1:E:963:ILE:HD11	1.95	0.48
1:C:579:PRO:HG3	1:C:660:ASP:CG	2.34	0.48
1:D:713:GLN:OE1	1:D:832:PRO:HD3	2.14	0.48
1:F:695:LEU:CD1	1:F:699:ARG:HH22	2.27	0.48
1:B:318:PRO:HD2	1:B:321:MET:HG3	1.95	0.48
1:A:753:TRP:HB2	1:C:217:GLY:H	1.78	0.48
1:C:214:ILE:HG12	1:C:237:LYS:HB2	1.96	0.48
1:F:924:VAL:O	1:F:928:VAL:HG23	2.13	0.48
1:F:527:TYR:O	1:F:531:VAL:HG23	2.14	0.48
1:D:1003:THR:HG23	1:D:1004:GLY:N	2.29	0.48
1:A:751:ILE:CG2	1:A:772:LEU:HD13	2.44	0.48
1:D:416:VAL:HG12	1:D:420:MET:HE2	1.95	0.48
1:F:314:GLU:N	1:F:315:PRO:CD	2.76	0.48
1:B:936:LEU:HD12	1:B:1009:MET:CE	2.43	0.48
1:A:573:PHE:HB2	1:A:666:PHE:CD2	2.48	0.48
1:C:154:LEU:O	1:C:157:TYR:HB3	2.14	0.48
1:D:34:GLN:O	1:D:392:THR:HG23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:PHE:O	1:E:249:ILE:HD11	2.13	0.48
1:E:635:GLU:CD	1:E:635:GLU:H	2.16	0.48
1:C:166:LEU:HD21	1:C:310:ILE:HG23	1.94	0.48
1:F:166:LEU:HA	1:F:169:THR:HG22	1.95	0.48
1:D:57:VAL:CG1	1:D:88:MET:HB3	2.43	0.48
1:A:838:ASP:O	1:A:839:ALA:C	2.51	0.48
1:D:845:GLU:OE2	1:D:845:GLU:HA	2.13	0.48
1:D:416:VAL:HG11	1:D:497:LEU:HD23	1.96	0.48
1:E:108:GLN:O	1:E:111:LEU:HB3	2.12	0.48
1:A:916:SER:O	1:A:917:MET:C	2.52	0.48
1:C:142:VAL:CG1	1:C:154:LEU:HD22	2.43	0.48
1:D:316:PHE:CE2	1:E:687:GLN:HG3	2.48	0.48
1:E:104:GLN:HE21	1:E:131:LYS:HE2	1.79	0.48
1:E:162:ILE:HG22	1:E:313:LEU:CD1	2.31	0.48
1:F:545:TYR:CD1	1:F:1023:PHE:HZ	2.31	0.48
1:F:43:ILE:HD11	1:F:107:VAL:HG21	1.93	0.48
1:A:826:ILE:HD12	1:A:827:LEU:N	2.27	0.48
1:B:577:GLN:HG3	1:B:616:ASN:HD21	1.78	0.48
1:F:442:LEU:HD12	1:F:486:LEU:HD21	1.96	0.48
1:B:575:GLN:HE21	1:B:617:PHE:HB2	1.78	0.48
1:B:944:ILE:HG22	1:B:969:ARG:CG	2.44	0.48
1:D:262:LEU:HD11	1:D:266:ALA:H	1.79	0.48
1:B:435:MET:CE	1:B:490:PRO:HG3	2.44	0.48
1:A:944:ILE:HD11	1:A:1020:VAL:HB	1.95	0.48
2:A:2026:LMT:H82	2:A:2026:LMT:C12	2.37	0.48
1:D:944:ILE:HD11	1:D:1020:VAL:HB	1.96	0.48
1:D:498:LYS:H	1:D:499:PRO:HD3	1.73	0.48
1:B:571:VAL:HG23	1:B:668:PRO:HG2	1.96	0.48
1:E:571:VAL:HG12	1:E:630:MET:SD	2.54	0.48
1:F:1020:VAL:N	1:F:1021:PRO:CD	2.77	0.48
1:B:742:LEU:HA	1:B:745:ILE:HG22	1.96	0.48
1:D:7:ASP:C	1:D:9:PRO:HD3	2.34	0.48
1:C:162:ILE:O	1:C:165:PRO:HD2	2.14	0.48
1:D:162:ILE:CG2	1:D:166:LEU:HD23	2.44	0.48
1:B:572:LEU:HD23	1:B:573:PHE:N	2.29	0.48
1:B:707:ALA:C	1:B:709:ASN:H	2.17	0.48
1:C:156:ASN:OD1	1:C:180:SER:O	2.32	0.48
1:D:96:GLN:HA	1:D:96:GLN:NE2	2.29	0.48
1:E:944:ILE:HD11	1:E:1020:VAL:CG1	2.43	0.48
1:F:169:THR:HG23	1:F:172:VAL:HG21	1.95	0.48
1:A:808:TRP:CE3	1:D:708:GLN:HB3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLY:O	1:A:234:ILE:HG12	2.14	0.48
1:B:156:ASN:ND2	1:B:182:TYR:N	2.62	0.48
1:D:940:ASN:HB3	1:D:973:ILE:HG22	1.96	0.48
1:D:356:TYR:O	1:D:356:TYR:HD1	1.96	0.48
1:A:356:TYR:HE1	1:A:513:PHE:CZ	2.31	0.48
1:D:766:ARG:NE	1:E:67:GLN:NE2	2.62	0.48
1:C:690:VAL:HG11	1:C:694:VAL:HG11	1.95	0.48
1:B:571:VAL:HG12	1:B:630:MET:SD	2.53	0.48
1:D:535:LEU:HD22	1:D:963:ILE:HD11	1.94	0.48
1:F:973:ILE:HD11	1:F:1017:ILE:HG22	1.95	0.48
1:A:724:PRO:CA	1:A:810:TYR:HB2	2.40	0.48
1:E:742:LEU:HA	1:E:745:ILE:HG22	1.95	0.48
1:E:618:ALA:O	1:E:719:GLY:HA2	2.14	0.48
1:F:242:THR:HG22	1:F:245:GLN:OE1	2.14	0.48
1:D:741:SER:OG	1:D:744:ASP:HB2	2.14	0.48
1:A:984:VAL:HG21	1:A:1005:VAL:HG11	1.96	0.48
1:E:817:ARG:CG	1:E:817:ARG:NH1	2.72	0.47
1:D:730:ILE:CD1	1:D:745:ILE:HD11	2.45	0.47
1:D:730:ILE:HD12	1:D:745:ILE:HD11	1.94	0.47
1:B:578:THR:HG21	1:B:587:THR:HB	1.95	0.47
1:D:682:LEU:HD23	1:D:683:PHE:N	2.29	0.47
1:A:57:VAL:CG1	1:A:88:MET:HB3	2.43	0.47
1:D:838:ASP:O	1:D:839:ALA:C	2.52	0.47
1:D:376:LEU:O	1:D:379:THR:CG2	2.61	0.47
1:E:550:ALA:O	1:E:553:ILE:HG12	2.13	0.47
1:B:156:ASN:HD21	1:B:768:LYS:HZ3	1.61	0.47
1:E:185:ARG:NH2	1:E:771:TYR:HB3	2.28	0.47
1:F:190:PRO:HG3	1:F:788:TRP:CE2	2.48	0.47
1:D:916:SER:O	1:D:917:MET:C	2.51	0.47
1:F:379:THR:HB	1:F:398:MET:HE3	1.94	0.47
1:C:612:VAL:HG11	1:C:615:PHE:HB3	1.95	0.47
1:A:46:GLN:HG2	1:A:89:THR:HG23	1.96	0.47
1:B:43:ILE:CG2	1:B:107:VAL:HG11	2.20	0.47
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.61	0.47
1:E:821:VAL:HG12	1:E:822:PRO:CD	2.44	0.47
1:D:745:ILE:O	1:D:749:VAL:HG23	2.14	0.47
1:D:637:ARG:O	1:D:642:ASN:HB2	2.13	0.47
1:A:13:TRP:CG	2:A:2026:LMT:H22	2.49	0.47
1:A:876:TYR:O	1:A:880:LEU:HD23	2.13	0.47
1:A:875:LEU:CD1	1:A:931:LEU:HD11	2.42	0.47
1:F:648:ALA:HB1	1:F:714:ARG:NH1	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:363:ARG:NE	1:E:498:LYS:HE3	2.29	0.47
1:E:929:GLY:HA2	1:E:932:THR:HG22	1.97	0.47
1:C:15:ILE:HG13	1:C:16:ALA:N	2.27	0.47
1:A:940:ASN:HB3	1:A:973:ILE:HG22	1.95	0.47
1:A:996:GLY:N	1:A:999:HIS:CD2	2.81	0.47
1:E:907:GLY:HA3	1:E:1012:ALA:HB2	1.95	0.47
1:C:190:PRO:HG3	1:C:788:TRP:CE2	2.49	0.47
1:B:281:PHE:O	1:B:282:ASN:HB2	2.14	0.47
1:D:818:TYR:O	1:D:820:GLY:N	2.46	0.47
1:E:953:GLU:C	1:E:955:GLY:N	2.67	0.47
1:D:395:MET:O	1:D:399:VAL:HG12	2.14	0.47
1:E:343:THR:HA	1:E:346:GLU:HG2	1.95	0.47
1:F:695:LEU:HD13	1:F:699:ARG:HH12	1.78	0.47
1:E:520:PHE:O	1:E:523:THR:HG22	2.14	0.47
1:B:4:PHE:CZ	1:B:8:ARG:HD2	2.50	0.47
1:E:578:THR:CG2	1:E:587:THR:HB	2.45	0.47
1:F:723:GLU:HG3	1:F:813:PRO:HG3	1.96	0.47
1:D:840:MET:HA	1:D:844:GLU:HB2	1.95	0.47
1:E:199:THR:HG22	1:E:201:GLY:H	1.79	0.47
1:A:210:GLN:NE2	1:A:249:ILE:HG13	2.29	0.47
1:E:362:PHE:O	1:E:365:THR:HB	2.13	0.47
1:F:404:LEU:HD13	1:F:449:LEU:HD13	1.96	0.47
1:C:185:ARG:HH11	1:C:771:TYR:CB	2.27	0.47
1:C:34:GLN:O	1:C:392:THR:HG22	2.14	0.47
1:E:339:GLU:HG2	1:E:342:LYS:NZ	2.29	0.47
1:E:158:ILE:HG22	1:E:162:ILE:CD1	2.39	0.47
1:A:535:LEU:HD22	1:A:963:ILE:HD11	1.95	0.47
1:D:535:LEU:CD2	1:D:963:ILE:HD11	2.44	0.47
1:F:903:VAL:CG2	1:F:1020:VAL:HG22	2.43	0.47
1:A:219:LEU:C	1:A:221:GLY:H	2.18	0.47
1:E:578:THR:OG1	1:E:579:PRO:HD2	2.14	0.47
1:B:371:ALA:O	1:B:374:VAL:HG12	2.14	0.47
1:F:939:LYS:HZ3	1:F:976:THR:CG2	2.27	0.47
1:D:6:ILE:H	1:D:6:ILE:HD12	1.79	0.47
1:D:150:THR:N	1:D:153:ASP:HB2	2.29	0.47
1:C:452:VAL:HG22	1:C:883:VAL:CG2	2.44	0.47
1:D:354:VAL:HG11	1:D:979:ALA:HA	1.97	0.47
1:F:456:MET:HB2	1:F:467:TYR:HB3	1.97	0.47
1:D:4:PHE:CZ	1:D:8:ARG:HD2	2.49	0.47
1:E:563:PHE:CD2	1:E:564:LEU:HD22	2.48	0.47
1:F:587:THR:O	1:F:591:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:984:VAL:HG21	1:D:1005:VAL:HG11	1.96	0.47
1:B:907:GLY:HA2	1:B:1012:ALA:HB2	1.97	0.47
1:D:190:PRO:C	1:D:192:LYS:H	2.18	0.47
1:A:400:LEU:HD12	1:A:470:PHE:CZ	2.47	0.47
1:C:966:CYS:O	1:C:970:LEU:HB2	2.15	0.47
1:B:20:MET:CE	1:B:374:VAL:HG23	2.40	0.47
1:D:891:TYR:CG	1:D:896:ILE:HD11	2.49	0.47
1:A:156:ASN:ND2	1:A:768:LYS:NZ	2.61	0.47
1:B:108:GLN:O	1:B:111:LEU:HB3	2.13	0.47
1:C:242:THR:HG22	1:C:245:GLN:OE1	2.15	0.47
1:E:281:PHE:O	1:E:282:ASN:HB2	2.14	0.47
1:B:480:LEU:O	1:B:483:ILE:HG23	2.14	0.47
1:E:936:LEU:HD12	1:E:1009:MET:CE	2.44	0.47
1:A:465:VAL:O	1:A:469:GLN:HG2	2.15	0.47
1:D:705:LEU:HD13	1:D:849:GLN:OE1	2.13	0.47
1:C:544:ILE:HD11	1:C:1019:TRP:HZ2	1.79	0.47
1:F:544:ILE:HD11	1:F:1019:TRP:HZ2	1.80	0.47
1:B:426:SER:HB2	1:B:427:PRO:HD2	1.97	0.47
1:B:563:PHE:CD2	1:B:564:LEU:HD22	2.49	0.47
1:A:314:GLU:N	1:A:315:PRO:CD	2.77	0.47
1:E:572:LEU:HD23	1:E:573:PHE:N	2.29	0.47
1:F:579:PRO:HG3	1:F:660:ASP:CG	2.34	0.47
1:D:982:LEU:HD23	1:D:982:LEU:O	2.15	0.47
1:D:10:ILE:O	1:D:10:ILE:HG13	2.13	0.47
1:A:406:VAL:O	1:A:410:ILE:HG12	2.15	0.47
1:B:944:ILE:HD11	1:B:1020:VAL:CG1	2.44	0.47
1:B:527:TYR:CG	1:B:970:LEU:HD12	2.50	0.47
1:B:318:PRO:O	1:B:321:MET:HB2	2.15	0.47
1:D:763:ASP:HB3	1:D:768:LYS:HE3	1.97	0.47
1:A:775:ARG:O	1:A:779:ARG:HG2	2.15	0.47
1:A:190:PRO:HA	1:A:193:LEU:HB2	1.97	0.47
1:B:445:ILE:HD12	1:B:939:LYS:HG3	1.97	0.47
1:B:568:ASP:O	1:B:569:GLN:C	2.53	0.47
1:A:958:ILE:HG12	1:A:959:VAL:N	2.29	0.47
1:F:438:ILE:C	1:F:440:GLY:H	2.18	0.47
1:E:298:ASN:O	1:E:302:THR:HG22	2.15	0.47
1:A:763:ASP:HB3	1:A:768:LYS:HE3	1.96	0.47
1:D:876:TYR:O	1:D:880:LEU:HD23	2.15	0.47
1:F:354:VAL:CG2	1:F:982:LEU:HG	2.45	0.47
1:B:72:ILE:CD1	1:B:75:LEU:HD13	2.42	0.47
1:C:314:GLU:N	1:C:315:PRO:CD	2.77	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASP:OD2	1:D:620:ARG:HG3	2.15	0.47
1:E:476:SER:O	1:E:480:LEU:HB2	2.15	0.47
1:E:684:LEU:O	1:E:823:ALA:HA	2.15	0.47
1:A:698:ALA:HB2	1:A:851:PRO:HG2	1.95	0.47
1:D:485:ALA:HA	1:D:489:THR:OG1	2.14	0.47
1:C:872:ALA:HB3	1:C:873:PRO:HD3	1.96	0.47
1:D:396:PHE:HA	1:D:399:VAL:CG1	2.44	0.47
1:C:587:THR:O	1:C:591:VAL:HG23	2.14	0.47
1:D:227:GLY:O	1:D:229:GLN:HG3	2.15	0.47
1:A:99:ASP:OD2	1:A:101:ASP:HB2	2.15	0.47
1:B:76:ARG:HD3	1:B:863:TYR:CE2	2.49	0.47
1:C:406:VAL:HG13	1:C:410:ILE:HG23	1.95	0.47
1:A:687:GLN:NE2	1:A:821:VAL:HG21	2.30	0.47
1:A:396:PHE:HA	1:A:399:VAL:CG1	2.44	0.47
1:E:158:ILE:CG2	1:E:162:ILE:HD11	2.37	0.47
1:C:169:THR:HG23	1:C:172:VAL:CG2	2.45	0.47
1:B:47:VAL:H	1:B:88:MET:CE	2.26	0.47
1:B:896:ILE:N	1:B:897:PRO:HD2	2.30	0.47
1:C:723:GLU:HG3	1:C:813:PRO:HG3	1.96	0.47
1:E:376:LEU:O	1:E:379:THR:HG22	2.15	0.47
1:A:839:ALA:O	1:A:844:GLU:HB2	2.15	0.47
1:E:34:GLN:CB	1:E:333:VAL:HG22	2.45	0.47
1:C:443:VAL:O	1:C:447:MET:HB2	2.15	0.47
1:A:7:ASP:C	1:A:9:PRO:HD3	2.36	0.47
1:F:162:ILE:O	1:F:165:PRO:HD2	2.15	0.47
1:B:158:ILE:HG22	1:B:162:ILE:CD1	2.41	0.47
1:A:419:VAL:CG2	1:A:430:ALA:HB1	2.42	0.47
1:C:648:ALA:HB1	1:C:714:ARG:NH1	2.27	0.47
1:D:456:MET:HE1	1:D:928:VAL:HA	1.97	0.47
1:E:34:GLN:HG3	1:E:35:TYR:CD2	2.49	0.47
1:A:563:PHE:CZ	1:A:564:LEU:HD23	2.49	0.47
1:E:577:GLN:HG3	1:E:616:ASN:HD21	1.79	0.47
1:D:465:VAL:O	1:D:469:GLN:HG2	2.15	0.47
1:F:34:GLN:O	1:F:392:THR:HG22	2.15	0.47
1:C:26:SER:O	1:C:30:LEU:HG	2.15	0.47
1:E:318:PRO:O	1:E:321:MET:HB2	2.14	0.47
1:E:540:PRO:O	1:E:544:ILE:HG22	2.15	0.47
1:E:412:VAL:HG11	1:E:489:THR:OG1	2.15	0.47
1:D:807:LYS:HG3	1:D:808:TRP:N	2.30	0.47
1:D:524:THR:CG2	1:D:970:LEU:HD12	2.45	0.47
1:D:952:HIS:CE1	1:D:958:ILE:HG22	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:ARG:NE	1:B:498:LYS:HE3	2.30	0.47
1:F:155:SER:O	1:F:159:VAL:HG23	2.14	0.47
1:B:179:GLY:HA2	2:B:2033:LMT:O3'	2.15	0.47
1:B:38:ILE:HG13	1:B:462:SER:HB2	1.96	0.47
1:B:215:SER:HB2	1:C:750:SER:CB	2.44	0.47
1:B:618:ALA:O	1:B:719:GLY:HA2	2.15	0.47
1:A:370:ILE:HD11	1:A:488:LEU:CD1	2.45	0.47
1:C:463:THR:HG23	1:C:464:GLY:N	2.30	0.47
1:C:859:THR:HG23	1:C:860:GLY:N	2.30	0.47
1:A:741:SER:OG	1:A:744:ASP:HB2	2.15	0.47
1:D:235:ILE:HD13	1:D:235:ILE:H	1.80	0.47
1:D:235:ILE:HD13	1:D:235:ILE:N	2.30	0.47
1:D:371:ALA:O	1:D:375:VAL:HG22	2.14	0.46
1:D:219:LEU:C	1:D:221:GLY:H	2.18	0.46
1:A:655:PHE:CD2	1:A:663:VAL:HG11	2.49	0.46
1:B:389:SER:O	1:B:394:THR:HG21	2.15	0.46
1:B:550:ALA:O	1:B:553:ILE:HG12	2.14	0.46
1:F:452:VAL:HG22	1:F:883:VAL:CG2	2.44	0.46
1:D:930:LEU:O	1:D:933:THR:HG22	2.14	0.46
1:F:922:ASN:OD1	1:F:926:PHE:HD2	1.98	0.46
1:C:922:ASN:OD1	1:C:926:PHE:HD2	1.98	0.46
1:E:207:ILE:H	1:E:207:ILE:HG12	1.61	0.46
1:D:15:ILE:O	1:D:19:ILE:HG13	2.15	0.46
1:F:540:PRO:O	1:F:543:LEU:HB2	2.15	0.46
1:E:565:PRO:HG3	1:E:923:ASP:HB3	1.96	0.46
1:B:817:ARG:NH1	1:B:817:ARG:CG	2.71	0.46
1:D:190:PRO:HA	1:D:193:LEU:HB2	1.97	0.46
1:F:453:PHE:CE2	1:F:474:ILE:HD12	2.50	0.46
1:A:731:ASP:CB	1:A:734:LYS:HB2	2.37	0.46
1:C:749:VAL:O	1:C:753:TRP:HD1	1.98	0.46
1:D:655:PHE:CD2	1:D:663:VAL:HG11	2.50	0.46
1:A:943:LEU:HB3	1:A:969:ARG:HH11	1.80	0.46
1:D:493:CYS:HA	1:D:497:LEU:HD22	1.97	0.46
1:B:553:ILE:O	1:B:557:THR:HG23	2.15	0.46
1:D:158:ILE:HG22	1:D:159:VAL:N	2.29	0.46
1:F:150:THR:H	1:F:153:ASP:HB2	1.80	0.46
1:A:354:VAL:HG11	1:A:979:ALA:HA	1.96	0.46
1:A:11:PHE:O	1:A:15:ILE:HG22	2.15	0.46
1:B:702:PHE:CE2	1:B:826:ILE:HD12	2.50	0.46
1:A:96:GLN:NE2	1:A:96:GLN:HA	2.31	0.46
1:A:363:ARG:NH1	1:A:496:MET:O	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HG12	1:A:368:PRO:CD	2.44	0.46
1:A:371:ALA:O	1:A:375:VAL:HG22	2.14	0.46
1:D:251:LEU:HD13	1:D:262:LEU:HD23	1.97	0.46
1:E:578:THR:HA	1:E:661:ALA:HA	1.98	0.46
1:E:681:ASP:OD1	1:E:859:THR:HG23	2.16	0.46
1:F:985:VAL:N	1:F:986:PRO:CD	2.78	0.46
1:D:839:ALA:O	1:D:844:GLU:HB2	2.15	0.46
1:F:886:CYS:O	1:F:890:LEU:HB2	2.16	0.46
1:A:186:ILE:HG22	1:A:772:LEU:HD23	1.97	0.46
1:A:794:LYS:HA	1:A:794:LYS:HD3	1.66	0.46
1:F:425:LEU:HD23	1:F:426:SER:H	1.81	0.46
1:B:207:ILE:H	1:B:207:ILE:HG12	1.61	0.46
1:E:702:PHE:CE2	1:E:826:ILE:HD12	2.50	0.46
1:D:355:MET:CE	1:D:410:ILE:HD11	2.45	0.46
1:A:456:MET:HE1	1:A:928:VAL:HA	1.96	0.46
1:A:525:HIS:O	1:A:528:GLU:HB2	2.15	0.46
1:E:753:TRP:CH2	1:E:785:LEU:HG	2.50	0.46
1:E:45:VAL:HB	1:E:90:ILE:CG2	2.41	0.46
1:D:437:GLN:C	1:D:438:ILE:HG13	2.35	0.46
1:A:810:TYR:CD2	1:A:810:TYR:O	2.69	0.46
1:E:907:GLY:HA2	1:E:1012:ALA:HB2	1.96	0.46
1:D:573:PHE:CB	1:D:666:PHE:HE2	2.29	0.46
1:B:762:ILE:HG22	1:B:767:VAL:HG22	1.97	0.46
1:F:171:GLY:HA3	1:F:302:THR:OG1	2.14	0.46
1:E:575:GLN:HE21	1:E:617:PHE:HB2	1.81	0.46
1:A:982:LEU:HD23	1:A:982:LEU:O	2.16	0.46
1:B:907:GLY:HA3	1:B:1012:ALA:HB2	1.96	0.46
1:E:318:PRO:HD2	1:E:321:MET:HG3	1.97	0.46
1:B:317:MET:HE1	1:B:323:VAL:HG23	1.98	0.46
1:D:958:ILE:HG12	1:D:959:VAL:N	2.30	0.46
1:C:527:TYR:CE2	1:C:966:CYS:HB3	2.51	0.46
1:F:527:TYR:CE2	1:F:966:CYS:HB3	2.51	0.46
1:A:682:LEU:HD23	1:A:683:PHE:N	2.30	0.46
1:F:749:VAL:O	1:F:753:TRP:HD1	1.98	0.46
1:F:753:TRP:CZ2	1:F:785:LEU:HA	2.51	0.46
1:E:725:GLN:OE1	1:E:811:GLY:HA3	2.16	0.46
1:A:845:GLU:HA	1:A:845:GLU:OE2	2.15	0.46
1:E:389:SER:O	1:E:394:THR:HG21	2.16	0.46
1:E:480:LEU:O	1:E:483:ILE:HG23	2.15	0.46
1:D:303:ALA:HB2	1:D:330:THR:HG21	1.98	0.46
1:B:339:GLU:HG2	1:B:342:LYS:NZ	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:VAL:CG2	1:E:122:VAL:HG21	2.46	0.46
1:A:4:PHE:CZ	1:A:8:ARG:HD2	2.51	0.46
1:A:70:ASN:ND2	1:C:175:PHE:CE1	2.83	0.46
1:B:692:HIS:C	1:B:692:HIS:CD2	2.89	0.46
1:B:687:GLN:NE2	1:B:821:VAL:HG21	2.23	0.46
1:D:188:LEU:HG	1:D:772:LEU:HD21	1.96	0.46
1:A:56:THR:CG2	1:C:213:GLN:HB3	2.37	0.46
1:B:578:THR:CG2	1:B:587:THR:HB	2.45	0.46
1:F:973:ILE:CD1	1:F:1017:ILE:HG22	2.45	0.46
1:A:724:PRO:HA	1:A:810:TYR:CB	2.41	0.46
1:A:682:LEU:CD2	1:A:856:TYR:HB2	2.41	0.46
1:B:137:LEU:HD21	1:B:302:THR:HG23	1.97	0.46
1:C:184:MET:CE	1:C:268:VAL:HG13	2.46	0.46
1:F:595:ARG:O	1:F:599:LEU:N	2.48	0.46
1:D:792:ASN:CG	1:D:793:ASP:H	2.17	0.46
1:C:242:THR:CG2	1:C:245:GLN:HG3	2.45	0.46
1:F:242:THR:CG2	1:F:245:GLN:HG3	2.45	0.46
1:A:227:GLY:O	1:A:229:GLN:HG3	2.15	0.46
1:A:275:TYR:CD1	1:C:223:PRO:HG3	2.50	0.46
1:B:1006:ILE:HG13	1:B:1007:GLY:N	2.29	0.46
1:D:190:PRO:HG3	1:D:788:TRP:CE2	2.51	0.46
1:E:944:ILE:HG22	1:E:969:ARG:CG	2.46	0.46
1:E:590:VAL:HG11	1:E:661:ALA:CB	2.45	0.46
1:C:985:VAL:N	1:C:986:PRO:CD	2.79	0.46
1:E:399:VAL:O	1:E:402:ILE:HG12	2.16	0.46
1:E:958:ILE:HG12	1:E:959:VAL:H	1.81	0.46
1:F:58:GLN:O	1:F:63:GLN:HB2	2.15	0.46
1:D:378:GLY:O	1:D:382:VAL:HG23	2.16	0.46
1:C:575:GLN:HE21	1:C:666:PHE:HZ	1.63	0.46
1:A:395:MET:O	1:A:399:VAL:HG12	2.16	0.46
1:C:576:VAL:HG22	1:C:663:VAL:HG12	1.97	0.46
1:F:397:GLY:HA3	1:F:473:THR:HG21	1.97	0.46
1:E:15:ILE:O	1:E:19:ILE:HG23	2.16	0.46
1:B:540:PRO:O	1:B:544:ILE:HG22	2.15	0.46
1:F:216:SER:HB2	1:F:234:ILE:HG13	1.97	0.46
1:E:1014:VAL:HG12	1:E:1015:LEU:HD12	1.98	0.46
1:E:942:ILE:O	1:E:946:GLU:HB2	2.16	0.46
1:B:376:LEU:O	1:B:379:THR:HG22	2.15	0.46
1:B:590:VAL:HG11	1:B:661:ALA:CB	2.46	0.46
1:D:452:VAL:HG11	1:D:931:LEU:O	2.16	0.46
1:F:184:MET:CE	1:F:268:VAL:HG13	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:683:PHE:CE1	1:F:818:TYR:CD2	3.04	0.46
1:A:225:VAL:H	1:B:780:MET:HE1	1.81	0.46
1:E:958:ILE:N	1:E:958:ILE:CD1	2.79	0.46
1:A:202:ASP:OD1	1:A:791:ARG:NH2	2.44	0.46
1:A:85:ASP:HB3	1:A:87:SER:OG	2.16	0.46
1:D:1009:MET:O	1:D:1013:THR:HG23	2.16	0.46
1:E:800:PHE:CD2	1:E:804:ALA:HB2	2.50	0.46
1:F:655:PHE:HB3	1:F:663:VAL:HG23	1.97	0.46
1:D:1022:LEU:HA	1:D:1022:LEU:HD23	1.77	0.46
1:D:228:GLN:NE2	1:D:230:LEU:H	2.04	0.46
2:B:2033:LMT:O6B	2:B:2033:LMT:H6E	2.16	0.46
1:D:891:TYR:OH	1:D:945:VAL:HG13	2.15	0.46
1:D:434:SER:O	1:D:437:GLN:HG2	2.16	0.46
1:D:197:GLN:HB3	1:D:797:MET:SD	2.56	0.46
1:D:840:MET:HA	1:D:844:GLU:CB	2.46	0.46
1:E:904:VAL:HG22	1:E:934:ILE:HD12	1.96	0.46
1:A:150:THR:N	1:A:153:ASP:HB2	2.30	0.46
1:D:158:ILE:HD13	1:D:162:ILE:HD12	1.97	0.46
1:C:150:THR:H	1:C:153:ASP:HB2	1.80	0.46
1:B:800:PHE:CD2	1:B:804:ALA:HB2	2.51	0.46
1:C:540:PRO:O	1:C:543:LEU:HB2	2.16	0.46
1:C:612:VAL:CG1	1:C:615:PHE:HB3	2.46	0.46
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.16	0.46
1:E:1006:ILE:HG13	1:E:1007:GLY:N	2.30	0.46
1:E:2:SER:HB3	1:E:486:LEU:O	2.15	0.46
1:B:15:ILE:O	1:B:19:ILE:HG23	2.16	0.46
1:C:695:LEU:HD13	1:C:699:ARG:HH22	1.81	0.46
1:D:128:ARG:NH2	1:D:175:PHE:CE2	2.84	0.46
1:D:189:ASP:OD2	1:D:191:ALA:HB3	2.16	0.46
1:D:784:ASP:O	1:D:787:LYS:HB3	2.17	0.46
1:E:942:ILE:HG12	1:E:942:ILE:H	1.50	0.46
1:E:125:GLN:HG3	2:E:2033:LMT:O4'	2.16	0.46
1:A:541:TYR:C	1:A:543:LEU:H	2.20	0.46
1:C:472:ILE:N	1:C:472:ILE:CD1	2.77	0.46
1:A:891:TYR:CG	1:A:896:ILE:HD11	2.51	0.46
1:B:740:VAL:HG23	1:B:792:ASN:ND2	2.31	0.46
1:C:982:LEU:O	1:C:985:VAL:HG22	2.16	0.46
1:A:592:ASP:O	1:A:595:ARG:HB2	2.16	0.46
1:A:254:ASN:HD21	1:A:258:SER:CB	2.26	0.46
1:D:472:ILE:C	1:D:472:ILE:HD12	2.36	0.46
1:D:943:LEU:HB3	1:D:969:ARG:HH11	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:550:ALA:HA	1:C:553:ILE:CG1	2.46	0.46
1:A:559:ILE:HA	1:A:560:PRO:HD3	1.78	0.46
1:F:490:PRO:O	1:F:493:CYS:HB2	2.16	0.46
1:E:458:PHE:CE2	2:E:2032:LMT:H52	2.51	0.45
1:D:189:ASP:C	1:D:193:LEU:HD23	2.36	0.45
1:D:249:ILE:H	1:D:262:LEU:N	2.14	0.45
1:D:748:THR:HG21	1:D:790:VAL:HG22	1.97	0.45
1:A:157:TYR:O	1:A:158:ILE:C	2.55	0.45
1:E:133:VAL:O	1:E:292:LYS:HE2	2.16	0.45
1:A:840:MET:HA	1:A:844:GLU:CB	2.46	0.45
1:C:683:PHE:CZ	1:C:818:TYR:CZ	3.05	0.45
1:B:619:GLY:HA3	1:B:720:MET:SD	2.56	0.45
1:D:157:TYR:CZ	1:D:317:MET:HG3	2.51	0.45
1:F:766:ARG:O	1:F:768:LYS:HG3	2.16	0.45
1:A:518:ARG:O	1:A:522:SER:HB3	2.16	0.45
1:E:362:PHE:O	1:E:366:LEU:HD23	2.16	0.45
1:E:55:GLU:C	1:E:57:VAL:H	2.19	0.45
1:B:709:ASN:HA	1:B:710:PRO:HD3	1.81	0.45
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.97	0.45
1:E:178:PHE:HE2	1:E:277:ILE:HD12	1.81	0.45
1:F:95:GLU:O	1:F:97:GLY:N	2.47	0.45
1:A:713:GLN:OE1	1:A:832:PRO:HD3	2.16	0.45
1:F:915:THR:HG23	1:F:920:LEU:HB2	1.98	0.45
1:D:361:ASN:HB3	1:D:364:ALA:HB3	1.98	0.45
1:B:972:PRO:O	1:B:976:THR:HG23	2.16	0.45
1:E:541:TYR:O	1:E:544:ILE:HG23	2.16	0.45
1:A:568:ASP:CB	1:A:634:TRP:CZ3	2.89	0.45
1:A:189:ASP:C	1:A:193:LEU:HD23	2.36	0.45
1:A:540:PRO:O	1:A:543:LEU:HG	2.17	0.45
1:A:958:ILE:HG13	1:A:1025:VAL:HG13	1.98	0.45
1:F:527:TYR:CD2	1:F:970:LEU:HG	2.51	0.45
1:A:891:TYR:OH	1:A:942:ILE:HA	2.16	0.45
1:B:578:THR:OG1	1:B:579:PRO:HD2	2.15	0.45
1:A:80:SER:OG	1:A:817:ARG:HB2	2.16	0.45
1:B:676:ASN:HD21	1:B:827:LEU:CD1	2.23	0.45
1:D:578:THR:OG1	1:D:587:THR:HG22	2.16	0.45
1:C:753:TRP:CZ2	1:C:785:LEU:HA	2.51	0.45
1:E:231:ASN:HD21	1:F:584:ALA:H	1.64	0.45
1:F:572:LEU:HB3	1:F:629:ILE:HD12	1.97	0.45
1:F:985:VAL:CG2	1:F:986:PRO:HD3	2.44	0.45
1:B:958:ILE:H	1:B:958:ILE:HD13	1.80	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:HG3	1:C:462:SER:N	2.31	0.45
1:D:85:ASP:HB3	1:D:87:SER:OG	2.17	0.45
1:E:705:LEU:O	1:E:705:LEU:HD23	2.17	0.45
1:F:550:ALA:HA	1:F:553:ILE:CG1	2.45	0.45
1:F:695:LEU:HD13	1:F:699:ARG:HH22	1.81	0.45
1:B:973:ILE:HD11	1:B:1017:ILE:CG2	2.46	0.45
1:B:541:TYR:O	1:B:1019:TRP:HZ3	1.98	0.45
1:D:186:ILE:HG22	1:D:186:ILE:O	2.16	0.45
1:E:972:PRO:O	1:E:976:THR:HG23	2.17	0.45
1:E:442:LEU:O	1:E:445:ILE:HG12	2.16	0.45
1:F:169:THR:HG23	1:F:172:VAL:CG2	2.46	0.45
1:C:291:ILE:CD1	1:C:306:ILE:HD12	2.44	0.45
1:D:65:ILE:HD13	1:D:66:GLU:N	2.31	0.45
1:E:137:LEU:HD21	1:E:302:THR:HG23	1.98	0.45
1:F:683:PHE:CZ	1:F:818:TYR:CZ	3.05	0.45
1:C:90:ILE:O	1:C:90:ILE:HD12	2.17	0.45
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.99	0.45
1:D:792:ASN:HB2	1:D:798:VAL:HG23	1.99	0.45
1:B:521:LEU:O	1:B:525:HIS:ND1	2.49	0.45
1:C:442:LEU:HD12	1:C:486:LEU:HD21	1.96	0.45
1:F:731:ASP:C	1:F:733:GLU:H	2.19	0.45
1:A:34:GLN:O	1:A:392:THR:HG23	2.16	0.45
1:D:363:ARG:NH1	1:D:496:MET:O	2.49	0.45
1:A:133:VAL:HG22	1:A:672:LEU:HD13	1.99	0.45
1:C:328:ASP:O	1:C:331:PRO:HD2	2.17	0.45
1:A:437:GLN:C	1:A:438:ILE:HG13	2.37	0.45
1:E:579:PRO:HD3	1:E:660:ASP:O	2.17	0.45
1:A:887:LEU:HD21	1:A:942:ILE:CD1	2.47	0.45
1:C:10:ILE:O	1:C:14:VAL:HG23	2.17	0.45
1:B:792:ASN:HB2	1:B:796:GLU:O	2.16	0.45
1:B:45:VAL:HB	1:B:90:ILE:CG2	2.43	0.45
1:C:456:MET:CE	1:C:931:LEU:HD12	2.47	0.45
1:C:428:ARG:HB2	1:C:428:ARG:CZ	2.46	0.45
1:A:710:PRO:HD3	1:D:807:LYS:NZ	2.32	0.45
1:F:169:THR:CG2	1:F:306:ILE:HG22	2.47	0.45
1:D:541:TYR:C	1:D:543:LEU:H	2.19	0.45
1:F:1015:LEU:O	1:F:1019:TRP:HD1	1.99	0.45
1:D:80:SER:OG	1:D:817:ARG:HB2	2.16	0.45
1:E:896:ILE:N	1:E:897:PRO:HD2	2.30	0.45
1:B:399:VAL:O	1:B:402:ILE:HG12	2.17	0.45
1:F:96:GLN:HG3	1:F:462:SER:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:PHE:CZ	1:D:564:LEU:HD23	2.52	0.45
1:D:43:ILE:HG12	1:D:104:GLN:HA	1.99	0.45
1:B:362:PHE:O	1:B:365:THR:HB	2.15	0.45
1:B:420:MET:HE1	1:B:499:PRO:HA	1.99	0.45
1:A:15:ILE:O	1:A:19:ILE:HG13	2.16	0.45
1:C:175:PHE:CD2	1:C:175:PHE:C	2.89	0.45
1:F:418:ARG:NH1	1:F:968:MET:HB3	2.32	0.45
1:C:503:GLY:C	1:C:505:HIS:H	2.20	0.45
1:E:709:ASN:OD1	1:E:710:PRO:HD2	2.17	0.45
1:A:355:MET:CE	1:A:410:ILE:HD11	2.46	0.45
1:B:548:ILE:HG12	1:B:548:ILE:H	1.65	0.45
1:A:157:TYR:CD2	1:A:321:MET:HE3	2.51	0.45
1:D:273:GLN:HG3	1:D:771:TYR:HE1	1.81	0.45
1:F:981:ILE:HG22	1:F:1006:ILE:HB	1.99	0.45
1:E:568:ASP:O	1:E:569:GLN:C	2.54	0.45
1:F:966:CYS:O	1:F:970:LEU:HB2	2.15	0.45
1:E:418:ARG:HG2	1:E:418:ARG:HH11	1.82	0.45
1:C:58:GLN:O	1:C:63:GLN:HB2	2.16	0.45
1:B:390:ILE:HG23	1:B:395:MET:SD	2.56	0.45
1:A:738:LEU:HD12	1:A:738:LEU:N	2.31	0.45
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.99	0.45
1:C:397:GLY:HA3	1:C:473:THR:HG21	1.99	0.45
1:E:652:GLN:O	1:E:656:PHE:HB2	2.16	0.45
1:F:351:VAL:HG22	1:F:979:ALA:O	2.17	0.45
1:F:726:TYR:CZ	1:F:808:TRP:CZ3	3.05	0.45
1:D:181:GLN:HG3	1:D:768:LYS:NZ	2.32	0.45
1:A:273:GLN:HG3	1:A:771:TYR:HE1	1.81	0.45
1:A:702:PHE:HZ	1:A:843:VAL:HG13	1.81	0.45
1:D:528:GLU:OE2	1:D:967:ARG:NE	2.49	0.45
1:D:538:ARG:O	1:D:539:ALA:HB3	2.17	0.45
1:C:1020:VAL:N	1:C:1021:PRO:CD	2.80	0.45
1:F:575:GLN:HE21	1:F:666:PHE:HZ	1.63	0.45
1:C:550:ALA:HA	1:C:553:ILE:HG12	1.98	0.45
1:C:1:MET:O	1:C:2:SER:C	2.54	0.45
1:E:232:ALA:HB1	1:F:724:PRO:O	2.16	0.45
1:C:351:VAL:HG22	1:C:979:ALA:O	2.17	0.45
1:D:186:ILE:HG22	1:D:772:LEU:HD23	1.97	0.45
1:D:775:ARG:O	1:D:779:ARG:HG2	2.16	0.45
1:F:219:LEU:HG	1:F:234:ILE:HG22	1.99	0.45
1:A:273:GLN:NE2	1:A:769:ARG:NH1	2.65	0.45
1:A:711:ALA:HA	1:A:834:LEU:HD23	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:O	1:A:539:ALA:HB3	2.16	0.45
1:A:545:TYR:CD1	1:A:1023:PHE:HZ	2.35	0.45
1:D:958:ILE:HG13	1:D:1025:VAL:HG13	1.99	0.45
1:D:518:ARG:O	1:D:522:SER:N	2.43	0.45
1:D:525:HIS:O	1:D:528:GLU:HB2	2.16	0.45
1:B:8:ARG:N	1:B:9:PRO:HD3	2.31	0.45
1:C:354:VAL:CG2	1:C:982:LEU:HG	2.46	0.45
1:B:705:LEU:O	1:B:705:LEU:HD23	2.17	0.45
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.17	0.45
1:A:971:ARG:HB3	1:A:972:PRO:HD3	1.99	0.45
1:D:1:MET:O	1:D:5:PHE:HD1	2.00	0.45
1:C:280:GLN:NE2	1:C:588:GLN:HE22	2.15	0.45
1:C:418:ARG:NH1	1:C:968:MET:HB3	2.31	0.45
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.99	0.45
1:F:2:SER:O	1:F:6:ILE:HG13	2.16	0.45
1:D:405:LEU:C	1:D:405:LEU:HD22	2.37	0.45
1:B:1014:VAL:HG12	1:B:1015:LEU:HD12	1.98	0.45
1:D:224:ALA:CB	1:E:780:MET:HE1	2.46	0.45
1:B:428:ARG:N	1:B:428:ARG:HD2	2.26	0.45
1:C:1015:LEU:O	1:C:1019:TRP:HD1	1.99	0.45
1:A:891:TYR:OH	1:A:945:VAL:HG13	2.16	0.45
1:D:219:LEU:HD11	1:E:726:TYR:CD2	2.52	0.45
1:D:826:ILE:HD12	1:D:827:LEU:N	2.31	0.45
1:F:683:PHE:CE1	1:F:818:TYR:CE2	3.05	0.45
1:B:958:ILE:N	1:B:958:ILE:CD1	2.79	0.45
1:C:216:SER:HB2	1:C:234:ILE:HG13	1.99	0.45
1:F:313:LEU:O	1:F:317:MET:HG3	2.17	0.45
1:C:282:ASN:HD22	1:C:599:LEU:HD11	1.82	0.45
1:D:971:ARG:HB3	1:D:972:PRO:HD3	1.99	0.45
1:C:61:VAL:HG22	1:C:118:LEU:HD22	1.98	0.45
1:F:798:VAL:HA	1:F:799:PRO:HD3	1.81	0.45
1:F:550:ALA:HA	1:F:553:ILE:HG12	1.99	0.45
1:E:30:LEU:HA	1:E:31:PRO:HD2	1.68	0.45
1:D:99:ASP:OD2	1:D:101:ASP:HB2	2.16	0.45
1:E:120:GLN:O	1:E:124:ARG:HG3	2.17	0.45
1:F:428:ARG:CZ	1:F:428:ARG:HB2	2.47	0.45
1:E:944:ILE:HG22	1:E:969:ARG:HG3	1.98	0.45
1:A:190:PRO:HG3	1:A:788:TRP:CE2	2.52	0.45
1:A:530:GLY:O	1:A:531:VAL:C	2.56	0.45
1:E:327:TYR:HD1	1:E:571:VAL:HG11	1.82	0.45
1:E:568:ASP:O	1:E:634:TRP:CH2	2.70	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLU:O	1:A:418:ARG:HG3	2.17	0.45
1:B:798:VAL:HA	1:B:799:PRO:HD3	1.82	0.45
1:A:80:SER:HA	1:A:90:ILE:HA	1.97	0.45
1:B:188:LEU:HD23	1:B:266:ALA:HB2	1.99	0.45
1:D:789:TYR:HE2	1:D:799:PRO:HG3	1.81	0.45
1:C:595:ARG:O	1:C:599:LEU:HB2	2.16	0.45
1:A:936:LEU:HD12	1:A:1009:MET:CE	2.46	0.45
1:D:154:LEU:HD12	1:D:286:ALA:HA	1.99	0.45
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.52	0.45
1:E:818:TYR:O	1:E:819:ASN:HB2	2.17	0.45
1:F:859:THR:HG23	1:F:860:GLY:N	2.32	0.45
1:B:969:ARG:C	1:B:972:PRO:HD2	2.38	0.44
1:B:821:VAL:HG12	1:B:822:PRO:CD	2.43	0.44
1:E:527:TYR:CG	1:E:970:LEU:HD12	2.50	0.44
1:A:303:ALA:HB2	1:A:330:THR:HG21	1.99	0.44
1:A:668:PRO:HA	1:A:669:PRO:HD3	1.74	0.44
1:D:568:ASP:CB	1:D:634:TRP:CZ3	2.89	0.44
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.82	0.44
1:D:234:ILE:HA	1:E:726:TYR:O	2.17	0.44
1:B:725:GLN:OE1	1:B:811:GLY:HA3	2.17	0.44
1:F:984:VAL:C	1:F:986:PRO:HD2	2.38	0.44
1:B:958:ILE:H	1:B:958:ILE:CD1	2.30	0.44
1:C:219:LEU:HG	1:C:234:ILE:HG22	1.98	0.44
1:F:45:VAL:HB	1:F:90:ILE:HG13	1.98	0.44
1:C:569:GLN:HA	1:C:634:TRP:HH2	1.82	0.44
1:F:19:ILE:HD11	1:F:374:VAL:HG12	1.98	0.44
1:A:794:LYS:O	1:A:796:GLU:N	2.50	0.44
1:C:595:ARG:O	1:C:599:LEU:N	2.48	0.44
1:D:738:LEU:N	1:D:738:LEU:HD12	2.31	0.44
1:D:358:PHE:CG	1:D:975:MET:HB2	2.52	0.44
1:D:11:PHE:O	1:D:15:ILE:HG22	2.17	0.44
1:F:26:SER:O	1:F:30:LEU:HG	2.16	0.44
1:F:406:VAL:HG13	1:F:410:ILE:HG23	1.98	0.44
1:A:452:VAL:HG11	1:A:931:LEU:O	2.17	0.44
1:D:185:ARG:NH1	1:D:771:TYR:HB3	2.33	0.44
1:F:453:PHE:HZ	1:F:932:THR:HB	1.82	0.44
1:A:528:GLU:OE2	1:A:967:ARG:NE	2.50	0.44
1:D:228:GLN:OE1	1:E:780:MET:HB3	2.17	0.44
1:A:703:LEU:O	1:A:707:ALA:HB2	2.16	0.44
1:A:47:VAL:HG12	1:A:88:MET:HG3	1.99	0.44
1:C:683:PHE:CE1	1:C:818:TYR:CD2	3.05	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:LYS:HD3	1:A:795:GLY:N	2.31	0.44
1:B:476:SER:O	1:B:480:LEU:HB2	2.17	0.44
1:A:573:PHE:CB	1:A:666:PHE:HE2	2.29	0.44
1:B:953:GLU:C	1:B:955:GLY:N	2.69	0.44
1:F:463:THR:HG23	1:F:464:GLY:N	2.32	0.44
1:C:95:GLU:O	1:C:97:GLY:N	2.49	0.44
1:E:409:ALA:O	1:E:413:VAL:HG23	2.17	0.44
1:F:280:GLN:NE2	1:F:588:GLN:HE22	2.16	0.44
1:C:731:ASP:C	1:C:733:GLU:H	2.19	0.44
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.73	0.44
1:E:69:MET:HE3	1:E:107:VAL:HG22	2.00	0.44
1:B:541:TYR:O	1:B:544:ILE:HG23	2.17	0.44
1:E:435:MET:CE	1:E:490:PRO:HG3	2.47	0.44
1:D:702:PHE:HZ	1:D:843:VAL:HG13	1.82	0.44
1:A:807:LYS:HG3	1:A:808:TRP:N	2.32	0.44
1:C:527:TYR:CD2	1:C:970:LEU:HG	2.52	0.44
1:E:792:ASN:HB2	1:E:796:GLU:O	2.16	0.44
1:B:461:GLY:O	1:B:465:VAL:HG23	2.17	0.44
1:E:748:THR:HG21	1:E:790:VAL:HG22	2.00	0.44
1:F:569:GLN:HA	1:F:634:TRP:HH2	1.82	0.44
1:B:199:THR:HG22	1:B:201:GLY:H	1.81	0.44
1:F:61:VAL:HG22	1:F:118:LEU:HD22	1.99	0.44
1:B:362:PHE:O	1:B:366:LEU:HD23	2.17	0.44
1:F:612:VAL:CG1	1:F:615:PHE:HB3	2.47	0.44
1:E:707:ALA:C	1:E:709:ASN:H	2.19	0.44
1:E:631:LEU:CD1	1:E:644:VAL:HG22	2.47	0.44
1:B:133:VAL:O	1:B:292:LYS:HE2	2.16	0.44
1:C:490:PRO:O	1:C:493:CYS:HB2	2.16	0.44
1:D:262:LEU:HD13	1:D:262:LEU:C	2.37	0.44
1:E:541:TYR:O	1:E:1019:TRP:HZ3	1.99	0.44
1:C:306:ILE:O	1:C:306:ILE:HG13	2.17	0.44
1:A:434:SER:O	1:A:437:GLN:HG2	2.18	0.44
1:A:493:CYS:HA	1:A:497:LEU:HD22	1.99	0.44
1:E:188:LEU:HD23	1:E:266:ALA:HB2	1.98	0.44
1:B:528:GLU:CD	1:B:967:ARG:HG3	2.38	0.44
1:E:72:ILE:CD1	1:E:75:LEU:HD13	2.46	0.44
1:C:370:ILE:O	1:C:373:PRO:HD2	2.18	0.44
1:F:111:LEU:C	1:F:113:LEU:N	2.71	0.44
1:B:55:GLU:C	1:B:57:VAL:H	2.20	0.44
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.17	0.44
1:B:709:ASN:OD1	1:B:710:PRO:HD2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HG12	1:B:135:ASN:OD1	2.18	0.44
1:B:61:VAL:CG2	1:B:122:VAL:HG21	2.47	0.44
1:E:338:HIS:C	1:E:340:VAL:H	2.20	0.44
1:D:363:ARG:NH2	2:D:2026:LMT:O3B	2.49	0.44
1:E:559:ILE:CD1	1:E:560:PRO:HD2	2.48	0.44
1:B:568:ASP:O	1:B:634:TRP:CH2	2.70	0.44
1:F:652:GLN:HG3	1:F:714:ARG:NH1	2.32	0.44
1:C:652:GLN:HG3	1:C:714:ARG:NH1	2.31	0.44
1:A:887:LEU:HD23	1:A:887:LEU:HA	1.78	0.44
1:D:891:TYR:OH	1:D:942:ILE:HA	2.18	0.44
1:D:414:GLU:O	1:D:418:ARG:HG3	2.17	0.44
1:A:810:TYR:CZ	1:D:701:LYS:HG2	2.53	0.44
1:F:982:LEU:O	1:F:985:VAL:HG22	2.18	0.44
1:A:738:LEU:HD22	1:A:798:VAL:HG11	1.99	0.44
1:D:861:LEU:O	1:D:865:GLU:HB2	2.18	0.44
1:A:146:ASP:C	1:A:148:SER:N	2.71	0.44
1:F:503:GLY:C	1:F:505:HIS:H	2.21	0.44
1:C:278:ASN:HB2	1:C:613:THR:CG2	2.48	0.44
1:C:404:LEU:HD13	1:C:449:LEU:HD13	1.98	0.44
1:A:10:ILE:HG13	1:A:10:ILE:O	2.17	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.80	0.44
1:B:314:GLU:N	1:B:315:PRO:CD	2.80	0.44
2:B:2033:LMT:H111	2:B:2033:LMT:H71	1.98	0.44
1:B:418:ARG:O	1:B:422:GLU:HG3	2.17	0.44
1:F:186:ILE:CG2	1:F:268:VAL:HG22	2.48	0.44
1:C:186:ILE:CG2	1:C:268:VAL:HG22	2.46	0.44
1:A:333:VAL:O	1:A:337:ILE:HG12	2.17	0.44
1:F:65:ILE:HD11	1:F:90:ILE:HG12	2.00	0.44
1:D:157:TYR:O	1:D:158:ILE:C	2.55	0.44
1:B:189:ASP:HB3	1:B:192:LYS:HB3	1.99	0.44
1:B:223:PRO:HG3	1:C:275:TYR:CD2	2.53	0.44
1:D:668:PRO:HA	1:D:669:PRO:HD3	1.75	0.44
1:D:631:LEU:HD22	1:D:644:VAL:HG23	2.00	0.44
1:F:720:MET:SD	1:F:720:MET:N	2.81	0.44
1:D:747:SER:O	1:D:751:ILE:HG13	2.17	0.44
1:E:544:ILE:O	1:E:548:ILE:HG12	2.17	0.44
1:B:438:ILE:O	1:B:439:GLN:C	2.56	0.44
1:C:453:PHE:HZ	1:C:932:THR:HB	1.83	0.44
1:D:219:LEU:HG	1:D:234:ILE:HG23	1.99	0.44
1:C:572:LEU:HB3	1:C:629:ILE:HD12	2.00	0.44
1:C:45:VAL:HB	1:C:90:ILE:HG13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:282:ASN:HD22	1:F:599:LEU:HD11	1.83	0.44
1:A:166:LEU:HA	1:A:166:LEU:HD13	1.78	0.44
1:A:572:LEU:HD12	1:A:666:PHE:O	2.17	0.44
1:B:133:VAL:CG1	1:B:135:ASN:OD1	2.66	0.44
1:D:38:ILE:HD13	1:D:38:ILE:H	1.83	0.44
1:C:39:ALA:HA	1:C:40:PRO:HD3	1.78	0.44
1:D:974:VAL:O	1:D:978:LEU:HB2	2.17	0.44
1:D:357:LEU:HD22	1:D:357:LEU:O	2.18	0.44
1:E:692:HIS:CD2	1:E:692:HIS:C	2.90	0.44
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.58	0.44
1:E:142:VAL:HG12	1:E:288:GLY:HA2	1.99	0.44
1:E:414:GLU:HG3	1:E:415:ASN:N	2.33	0.44
1:B:412:VAL:HG11	1:B:489:THR:OG1	2.18	0.44
1:F:138:MET:O	1:F:291:ILE:HG12	2.18	0.44
1:A:228:GLN:NE2	1:A:230:LEU:H	2.06	0.44
1:B:492:LEU:O	1:B:496:MET:HG3	2.18	0.44
1:B:578:THR:HA	1:B:661:ALA:HA	1.99	0.44
1:F:408:ASP:OD1	1:F:445:ILE:HD11	2.18	0.44
1:F:783:ASP:C	1:F:785:LEU:H	2.19	0.44
1:B:958:ILE:HG12	1:B:959:VAL:H	1.81	0.44
1:B:748:THR:HG21	1:B:790:VAL:HG22	2.00	0.44
1:D:655:PHE:HD2	1:D:658:PHE:CE2	2.36	0.44
1:C:19:ILE:HD11	1:C:374:VAL:HG12	1.98	0.44
1:D:3:LYS:HA	1:D:6:ILE:HD13	2.00	0.44
1:B:577:GLN:HG3	1:B:616:ASN:ND2	2.32	0.44
1:E:577:GLN:HG3	1:E:616:ASN:ND2	2.33	0.44
1:D:738:LEU:HD22	1:D:798:VAL:HG11	1.98	0.44
1:F:755:SER:HB3	1:F:773:GLN:HE21	1.83	0.44
1:E:189:ASP:HB3	1:E:192:LYS:HB3	1.98	0.44
1:F:709:ASN:HA	1:F:710:PRO:HD3	1.72	0.44
1:A:108:GLN:HA	1:A:111:LEU:HB3	2.00	0.44
1:B:652:GLN:O	1:B:656:PHE:HB2	2.17	0.44
1:A:534:ILE:HD11	1:A:1022:LEU:HG	2.00	0.44
1:C:155:SER:O	1:C:159:VAL:HG23	2.18	0.44
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.99	0.44
1:E:740:VAL:HG23	1:E:792:ASN:ND2	2.32	0.44
1:C:783:ASP:C	1:C:785:LEU:H	2.20	0.44
1:C:683:PHE:CE1	1:C:818:TYR:CE2	3.05	0.44
1:F:281:PHE:CZ	1:F:324:VAL:HG11	2.53	0.44
1:A:1009:MET:O	1:A:1013:THR:HG23	2.17	0.44
1:A:984:VAL:HG13	1:A:987:LEU:HD12	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ILE:HD12	1:C:103:ALA:N	2.33	0.44
1:E:943:LEU:O	1:E:947:PHE:HD1	2.01	0.44
1:A:355:MET:HE1	1:A:406:VAL:HG11	2.00	0.43
1:A:332:VAL:HG23	1:A:634:TRP:HZ2	1.83	0.43
1:B:942:ILE:O	1:B:946:GLU:HB2	2.17	0.43
1:C:726:TYR:CZ	1:C:808:TRP:CZ3	3.05	0.43
1:A:237:LYS:HD3	1:B:746:ASN:HD21	1.82	0.43
1:D:887:LEU:HD21	1:D:942:ILE:CD1	2.47	0.43
1:F:682:LEU:O	1:F:683:PHE:HD2	2.01	0.43
1:E:528:GLU:CD	1:E:967:ARG:HG3	2.39	0.43
1:C:425:LEU:HD23	1:C:426:SER:H	1.82	0.43
1:B:240:LEU:HD22	1:B:245:GLN:HE21	1.83	0.43
1:D:872:ALA:N	1:D:873:PRO:CD	2.81	0.43
1:C:418:ARG:CZ	1:C:968:MET:HB3	2.48	0.43
1:F:156:ASN:OD1	1:F:180:SER:O	2.36	0.43
1:D:39:ALA:HA	1:D:40:PRO:HD3	1.89	0.43
1:D:46:GLN:HG2	1:D:89:THR:HG23	1.98	0.43
1:C:197:GLN:HA	1:C:797:MET:SD	2.58	0.43
1:A:631:LEU:HD22	1:A:644:VAL:HG23	1.99	0.43
2:E:2032:LMT:H1B	2:E:2032:LMT:O3'	2.19	0.43
1:A:175:PHE:HD1	1:A:289:ILE:HD11	1.84	0.43
1:A:190:PRO:C	1:A:192:LYS:H	2.21	0.43
1:A:745:ILE:O	1:A:749:VAL:HG23	2.17	0.43
1:B:442:LEU:O	1:B:445:ILE:HG12	2.18	0.43
1:C:973:ILE:HG13	1:C:973:ILE:O	2.18	0.43
1:F:578:THR:CG2	1:F:623:SER:HB2	2.46	0.43
1:B:293:LEU:HD13	1:B:294:ALA:O	2.18	0.43
1:D:712:LEU:HD21	1:D:842:ALA:HB1	1.99	0.43
1:B:34:GLN:CB	1:B:333:VAL:HG22	2.48	0.43
1:C:15:ILE:HD13	1:C:487:ILE:HD12	2.00	0.43
1:D:909:ILE:C	1:D:911:ALA:N	2.72	0.43
1:E:215:SER:HB2	1:F:750:SER:CB	2.47	0.43
1:B:391:ASN:ND2	1:B:394:THR:H	2.16	0.43
1:D:859:THR:CG2	1:D:860:GLY:N	2.80	0.43
1:A:872:ALA:N	1:A:873:PRO:CD	2.82	0.43
1:A:861:LEU:O	1:A:865:GLU:HB2	2.18	0.43
1:F:424:GLY:HA3	1:F:502:LYS:HG3	2.00	0.43
1:C:300:LEU:O	1:C:304:LYS:HG3	2.18	0.43
1:B:338:HIS:C	1:B:340:VAL:H	2.21	0.43
1:F:734:LYS:HD3	1:F:802:ALA:O	2.18	0.43
1:E:104:GLN:O	1:E:107:VAL:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:HG3	1:B:415:ASN:N	2.33	0.43
1:A:541:TYR:HA	1:A:544:ILE:HG23	1.99	0.43
1:D:530:GLY:O	1:D:534:ILE:HG22	2.18	0.43
1:D:540:PRO:O	1:D:543:LEU:HG	2.19	0.43
1:C:762:ILE:H	1:C:762:ILE:HG12	1.51	0.43
1:A:181:GLN:HG3	1:A:768:LYS:NZ	2.33	0.43
1:B:712:LEU:HD21	1:B:843:VAL:CG2	2.48	0.43
1:D:207:ILE:H	1:D:207:ILE:HG12	1.47	0.43
1:A:254:ASN:N	1:A:254:ASN:ND2	2.64	0.43
1:F:958:ILE:HD13	1:F:959:VAL:H	1.84	0.43
1:D:379:THR:HA	1:D:382:VAL:HG23	2.00	0.43
1:C:313:LEU:O	1:C:317:MET:HG3	2.18	0.43
1:B:182:TYR:HB2	1:B:768:LYS:HZ3	1.82	0.43
1:B:575:GLN:NE2	1:B:617:PHE:HB2	2.34	0.43
1:F:1:MET:O	1:F:2:SER:C	2.57	0.43
1:E:690:VAL:O	1:E:691:GLY:O	2.36	0.43
1:A:25:LEU:HA	1:A:25:LEU:HD12	1.86	0.43
1:B:544:ILE:O	1:B:548:ILE:HG12	2.18	0.43
1:E:410:ILE:HD11	1:E:976:THR:CG2	2.32	0.43
1:B:520:PHE:O	1:B:523:THR:HG22	2.18	0.43
1:A:219:LEU:HD11	1:B:726:TYR:CD2	2.54	0.43
1:A:234:ILE:HA	1:B:726:TYR:O	2.18	0.43
1:C:438:ILE:O	1:C:440:GLY:N	2.51	0.43
1:E:418:ARG:O	1:E:422:GLU:HG3	2.18	0.43
1:E:375:VAL:O	1:E:379:THR:HB	2.19	0.43
1:D:780:MET:HB3	1:F:228:GLN:HE21	1.82	0.43
1:E:958:ILE:CD1	1:E:958:ILE:H	2.30	0.43
1:F:595:ARG:O	1:F:599:LEU:HB2	2.17	0.43
1:B:552:MET:HE3	1:B:908:VAL:HB	2.00	0.43
1:E:240:LEU:HD22	1:E:245:GLN:HE21	1.84	0.43
1:E:951:LEU:C	1:E:953:GLU:N	2.71	0.43
1:A:358:PHE:CG	1:A:975:MET:HB2	2.53	0.43
1:B:105:VAL:CG1	1:B:106:GLN:N	2.81	0.43
1:C:687:GLN:CD	1:C:855:GLY:HA3	2.39	0.43
1:A:784:ASP:O	1:A:787:LYS:HB3	2.18	0.43
1:C:838:ASP:O	1:C:841:ALA:HB3	2.18	0.43
1:B:254:ASN:HB2	1:B:258:SER:OG	2.18	0.43
1:F:99:ASP:O	1:F:102:ILE:HG13	2.18	0.43
1:D:190:PRO:HG2	1:D:787:LYS:HG2	2.01	0.43
1:F:219:LEU:HG	1:F:234:ILE:CG2	2.48	0.43
1:D:810:TYR:O	1:D:810:TYR:CD2	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:SER:O	1:D:537:HIS:N	2.31	0.43
1:B:753:TRP:CZ2	1:B:785:LEU:HA	2.42	0.43
1:B:579:PRO:HD3	1:B:660:ASP:O	2.19	0.43
1:A:32:VAL:HG22	1:A:390:ILE:HB	2.00	0.43
1:D:592:ASP:O	1:D:595:ARG:HB2	2.18	0.43
1:C:65:ILE:HD11	1:C:90:ILE:HG12	2.00	0.43
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.00	0.43
1:D:572:LEU:HD12	1:D:666:PHE:O	2.18	0.43
1:A:131:LYS:NZ	1:B:73:ASP:OD2	2.52	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE1	2.53	0.43
1:D:316:PHE:CD2	1:E:687:GLN:HG3	2.54	0.43
1:B:145:THR:HB	1:B:320:GLY:HA2	1.99	0.43
1:E:145:THR:HB	1:E:320:GLY:HA2	2.01	0.43
1:C:83:ASN:OD1	1:C:814:LYS:HG2	2.18	0.43
1:A:881:LEU:HD12	1:A:881:LEU:O	2.19	0.43
1:D:189:ASP:HB2	1:D:775:ARG:HD3	2.01	0.43
1:F:368:PRO:HG3	1:F:413:VAL:HG21	2.01	0.43
1:E:125:GLN:NE2	1:E:769:ARG:NH1	2.51	0.43
1:B:757:TYR:CZ	1:B:769:ARG:HG3	2.53	0.43
1:B:219:LEU:HD12	1:C:726:TYR:CE1	2.54	0.43
1:D:242:THR:CG2	1:D:245:GLN:HG3	2.49	0.43
1:C:891:TYR:O	1:C:892:GLU:C	2.57	0.43
1:A:219:LEU:HG	1:A:234:ILE:HG23	2.00	0.43
1:C:1013:THR:O	1:C:1017:ILE:HG12	2.19	0.43
1:B:987:LEU:HD13	1:B:1001:ILE:HD11	2.00	0.43
1:A:594:MET:HG3	1:A:655:PHE:CZ	2.54	0.43
1:D:594:MET:HG3	1:D:655:PHE:CZ	2.53	0.43
1:C:219:LEU:HG	1:C:234:ILE:CG2	2.49	0.43
1:C:447:MET:HE1	1:C:886:CYS:HB3	1.98	0.43
1:D:310:ILE:HD13	1:D:323:VAL:HG11	2.01	0.43
1:E:619:GLY:HA3	1:E:720:MET:SD	2.59	0.43
1:B:818:TYR:O	1:B:819:ASN:HB2	2.19	0.43
1:B:702:PHE:CE2	1:B:826:ILE:CD1	3.02	0.43
1:D:49:TYR:CD1	1:D:52:ALA:HB2	2.53	0.43
1:C:451:ALA:HB1	1:C:882:VAL:HG12	2.00	0.43
1:D:650:ARG:HB2	1:D:650:ARG:HH11	1.84	0.43
1:E:1016:ALA:O	1:E:1020:VAL:HG23	2.18	0.43
1:E:412:VAL:HG13	1:E:435:MET:CE	2.49	0.43
1:D:616:ASN:HD22	1:D:616:ASN:HA	1.63	0.43
1:B:151:LYS:HD2	1:B:151:LYS:H	1.83	0.43
1:F:10:ILE:O	1:F:14:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.99	0.43
1:B:470:PHE:O	1:B:473:THR:HG22	2.19	0.43
1:E:712:LEU:HD21	1:E:843:VAL:CG2	2.47	0.43
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.54	0.43
1:E:552:MET:HE3	1:E:908:VAL:HB	2.00	0.43
1:E:204:SER:O	1:E:207:ILE:HG12	2.19	0.43
1:D:370:ILE:HD11	1:D:488:LEU:CD1	2.47	0.43
1:E:105:VAL:HG13	1:E:106:GLN:N	2.34	0.43
1:D:330:THR:N	1:D:331:PRO:CD	2.82	0.43
1:A:70:ASN:HB2	1:C:167:SER:HB2	2.00	0.43
1:D:31:PRO:HG2	1:D:389:SER:HB3	2.01	0.43
1:B:178:PHE:HE2	1:B:277:ILE:HD12	1.83	0.43
1:E:254:ASN:HB2	1:E:258:SER:OG	2.19	0.43
1:D:454:LEU:HD23	1:D:454:LEU:HA	1.74	0.43
1:F:930:LEU:HA	1:F:930:LEU:HD23	1.90	0.43
1:A:189:ASP:HB2	1:A:775:ARG:HD3	2.01	0.43
1:E:757:TYR:CZ	1:E:769:ARG:HG3	2.53	0.43
1:B:391:ASN:ND2	1:B:393:LEU:H	2.13	0.43
1:E:108:GLN:HG2	1:F:112:GLN:OE1	2.18	0.43
1:F:555:MET:O	1:F:559:ILE:HG23	2.19	0.43
1:D:146:ASP:C	1:D:148:SER:N	2.71	0.43
1:E:515:TRP:CH2	1:E:519:MET:HG3	2.54	0.43
1:E:79:SER:HB2	1:E:818:TYR:HD1	1.84	0.43
1:F:102:ILE:HD12	1:F:103:ALA:N	2.33	0.43
1:D:318:PRO:O	1:D:320:GLY:N	2.51	0.43
1:E:317:MET:HE1	1:E:323:VAL:HG23	2.00	0.43
1:E:415:ASN:ND2	1:E:434:SER:HB2	2.26	0.43
1:D:731:ASP:CB	1:D:734:LYS:HB2	2.38	0.43
1:C:563:PHE:CD2	1:C:564:LEU:HG	2.54	0.43
1:B:228:GLN:HE21	1:B:231:ASN:HD21	1.67	0.43
1:C:184:MET:HE1	1:C:268:VAL:HG13	2.01	0.43
1:B:682:LEU:HD11	1:B:856:TYR:CD2	2.53	0.43
1:E:958:ILE:HD13	1:E:958:ILE:H	1.80	0.43
1:F:958:ILE:N	1:F:958:ILE:HD13	2.34	0.43
1:F:90:ILE:O	1:F:90:ILE:HD12	2.18	0.43
1:E:330:THR:N	1:E:331:PRO:CD	2.81	0.43
1:C:958:ILE:HD13	1:C:959:VAL:H	1.84	0.43
1:D:306:ILE:O	1:D:310:ILE:HG23	2.18	0.43
1:A:188:LEU:HG	1:A:772:LEU:HD21	2.00	0.43
1:F:321:MET:HB3	1:F:321:MET:HE2	1.90	0.43
1:D:184:MET:HG2	1:D:246:PHE:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:VAL:HG22	1:E:322:LYS:O	2.19	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:F:99:ASP:HA	1:F:100:PRO:HD3	1.92	0.43
1:B:120:GLN:O	1:B:124:ARG:HG3	2.19	0.43
1:E:184:MET:HB2	1:E:770:VAL:HG22	2.01	0.43
1:D:755:SER:HA	1:D:773:GLN:HG3	2.01	0.43
1:D:108:GLN:HA	1:D:111:LEU:HB3	1.99	0.43
1:C:695:LEU:O	1:C:698:ALA:HB3	2.19	0.43
1:F:695:LEU:O	1:F:698:ALA:HB3	2.19	0.43
1:B:410:ILE:HD11	1:B:976:THR:CG2	2.31	0.43
1:A:128:ARG:NH2	1:A:175:PHE:CE2	2.87	0.43
1:B:158:ILE:O	1:B:163:GLN:HB2	2.19	0.43
1:B:142:VAL:HG12	1:B:288:GLY:HA2	2.00	0.43
1:D:332:VAL:HG23	1:D:634:TRP:HZ2	1.83	0.43
1:D:400:LEU:HD12	1:D:470:PHE:CZ	2.47	0.43
1:C:929:GLY:HA2	1:C:932:THR:CG2	2.49	0.43
1:A:1022:LEU:HA	1:A:1022:LEU:HD23	1.76	0.43
1:A:545:TYR:CE1	1:A:1023:PHE:HZ	2.37	0.43
1:E:8:ARG:N	1:E:9:PRO:HD3	2.34	0.43
1:D:683:PHE:CZ	1:D:825:GLU:HB2	2.54	0.43
1:E:470:PHE:O	1:E:473:THR:HG22	2.18	0.43
1:E:987:LEU:HD13	1:E:1001:ILE:HD11	2.01	0.43
1:A:655:PHE:HD2	1:A:658:PHE:CE2	2.36	0.43
1:B:303:ALA:O	1:B:307:ARG:HB2	2.19	0.43
1:B:164:ASP:HB3	1:B:165:PRO:HD3	2.01	0.43
1:F:111:LEU:O	1:F:113:LEU:N	2.51	0.43
1:C:150:THR:HG22	1:C:153:ASP:CG	2.39	0.43
1:B:79:SER:HB2	1:B:818:TYR:HD1	1.83	0.43
1:E:105:VAL:CG1	1:E:106:GLN:N	2.81	0.43
1:C:671:VAL:O	1:C:674:LEU:HB2	2.19	0.43
1:F:300:LEU:O	1:F:304:LYS:HG3	2.19	0.43
1:E:46:GLN:HA	1:E:88:MET:HE3	2.01	0.42
1:A:711:ALA:HA	1:A:834:LEU:CD2	2.49	0.42
1:A:523:THR:O	1:A:524:THR:C	2.57	0.42
1:C:903:VAL:O	1:C:906:LEU:HB2	2.18	0.42
1:E:762:ILE:HG22	1:E:767:VAL:HG22	2.00	0.42
1:E:726:TYR:HE2	1:E:785:LEU:CD1	2.32	0.42
2:B:2033:LMT:H62	2:B:2033:LMT:C12	2.46	0.42
1:D:682:LEU:CD2	1:D:856:TYR:HB2	2.44	0.42
1:A:682:LEU:HD21	1:A:856:TYR:HD1	1.84	0.42
1:E:228:GLN:HE21	1:E:231:ASN:HD21	1.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:776:PRO:O	1:D:780:MET:HG2	2.19	0.42
1:D:936:LEU:HD12	1:D:1009:MET:CE	2.48	0.42
1:D:818:TYR:OH	1:D:859:THR:OG1	2.28	0.42
1:B:352:PHE:CD1	1:B:365:THR:CG2	3.02	0.42
1:E:521:LEU:O	1:E:525:HIS:ND1	2.50	0.42
1:C:456:MET:HB2	1:C:467:TYR:HB3	2.00	0.42
1:B:515:TRP:CH2	1:B:519:MET:HG3	2.54	0.42
1:A:76:ARG:HD3	1:A:95:GLU:OE1	2.19	0.42
1:B:541:TYR:O	1:B:1019:TRP:CZ3	2.72	0.42
1:A:634:TRP:O	1:A:638:PRO:HG3	2.19	0.42
1:B:314:GLU:HA	1:B:317:MET:HE2	2.01	0.42
1:E:445:ILE:HD12	1:E:939:LYS:HG3	2.00	0.42
1:D:530:GLY:O	1:D:531:VAL:C	2.57	0.42
1:E:569:GLN:O	1:E:571:VAL:N	2.45	0.42
1:A:695:LEU:HD13	1:A:699:ARG:NH2	2.34	0.42
1:F:438:ILE:O	1:F:440:GLY:N	2.53	0.42
1:D:453:PHE:CG	1:D:474:ILE:HD11	2.54	0.42
1:C:667:ALA:HA	1:C:668:PRO:HD3	1.84	0.42
1:E:375:VAL:HG22	1:E:484:VAL:HG21	2.01	0.42
1:F:803:PHE:O	1:F:804:ALA:HB2	2.19	0.42
1:A:794:LYS:CD	1:A:795:GLY:H	2.29	0.42
1:C:324:VAL:HG12	1:C:325:TYR:N	2.34	0.42
1:D:969:ARG:O	1:D:972:PRO:HD2	2.19	0.42
1:F:757:TYR:OH	1:F:760:ASP:OD1	2.33	0.42
1:A:1001:ILE:CG2	1:A:1002:GLY:N	2.82	0.42
1:C:712:LEU:HD12	1:C:715:VAL:HG21	2.00	0.42
1:B:204:SER:O	1:B:207:ILE:HG12	2.19	0.42
1:A:818:TYR:HH	1:A:859:THR:HG1	1.51	0.42
1:B:105:VAL:HG13	1:B:106:GLN:N	2.33	0.42
1:F:687:GLN:CD	1:F:855:GLY:HA3	2.39	0.42
1:F:185:ARG:HD3	1:F:771:TYR:HB2	2.01	0.42
1:B:840:MET:O	1:B:844:GLU:HG3	2.19	0.42
1:E:280:GLN:HB2	1:E:611:THR:HG23	2.00	0.42
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.89	0.42
1:B:412:VAL:HG13	1:B:435:MET:CE	2.49	0.42
2:E:2033:LMT:C7	2:E:2033:LMT:H111	2.48	0.42
1:F:291:ILE:CD1	1:F:306:ILE:HD12	2.45	0.42
1:A:532:ALA:O	1:A:533:SER:C	2.58	0.42
1:C:545:TYR:CE1	1:C:1023:PHE:HZ	2.37	0.42
1:F:903:VAL:O	1:F:906:LEU:HB2	2.19	0.42
1:E:738:LEU:C	1:E:792:ASN:HD21	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:CZ	1:A:825:GLU:HB2	2.54	0.42
1:E:681:ASP:CB	1:E:827:LEU:HD13	2.44	0.42
1:F:184:MET:H	1:F:761:PHE:HE1	1.67	0.42
1:B:228:GLN:NE2	1:B:231:ASN:HD21	2.17	0.42
1:A:655:PHE:CG	1:A:663:VAL:HG11	2.55	0.42
1:E:172:VAL:HG22	1:E:306:ILE:CG2	2.49	0.42
1:C:755:SER:HB3	1:C:773:GLN:HE21	1.83	0.42
1:E:352:PHE:CD1	1:E:365:THR:CG2	3.03	0.42
1:A:694:VAL:O	1:A:697:GLN:HB3	2.20	0.42
1:B:631:LEU:CD1	1:B:644:VAL:HG22	2.49	0.42
1:D:110:LYS:HD2	1:D:110:LYS:HA	1.85	0.42
1:C:734:LYS:HD3	1:C:802:ALA:O	2.18	0.42
1:E:909:ILE:HG13	1:E:910:GLY:N	2.34	0.42
1:D:568:ASP:O	1:D:569:GLN:HB2	2.20	0.42
1:B:942:ILE:H	1:B:942:ILE:HG12	1.50	0.42
1:A:944:ILE:HD11	1:A:1020:VAL:CG1	2.50	0.42
1:D:815:LEU:HA	1:D:815:LEU:HD12	1.89	0.42
1:B:568:ASP:HB3	1:B:634:TRP:CZ3	2.37	0.42
1:A:532:ALA:O	1:A:535:LEU:N	2.36	0.42
1:E:151:LYS:HD2	1:E:151:LYS:H	1.84	0.42
1:E:753:TRP:CZ2	1:E:785:LEU:HA	2.42	0.42
1:B:298:ASN:O	1:B:302:THR:HG22	2.17	0.42
1:B:62:VAL:HG23	1:B:88:MET:HG3	1.99	0.42
1:E:461:GLY:O	1:E:465:VAL:HG23	2.19	0.42
1:B:172:VAL:HG22	1:B:306:ILE:CG2	2.50	0.42
1:D:168:ARG:HD3	1:E:75:LEU:HD21	2.02	0.42
1:A:909:ILE:C	1:A:911:ALA:N	2.72	0.42
1:E:446:ALA:HB2	1:E:482:VAL:HG21	2.01	0.42
1:C:803:PHE:O	1:C:804:ALA:HB2	2.19	0.42
1:E:592:ASP:CG	1:E:595:ARG:HH12	2.23	0.42
1:A:906:LEU:N	1:A:906:LEU:HD23	2.33	0.42
1:D:154:LEU:CD1	1:D:286:ALA:HA	2.48	0.42
1:E:515:TRP:O	1:E:519:MET:HG2	2.19	0.42
1:E:55:GLU:HG2	1:E:815:LEU:HD11	2.01	0.42
1:C:690:VAL:HB	1:C:691:GLY:H	1.64	0.42
1:B:409:ALA:O	1:B:413:VAL:HG23	2.19	0.42
1:F:83:ASN:OD1	1:F:814:LYS:HG2	2.20	0.42
1:E:840:MET:O	1:E:844:GLU:HG3	2.19	0.42
1:C:424:GLY:HA3	1:C:502:LYS:HG3	2.01	0.42
1:B:30:LEU:HD23	1:B:31:PRO:HD2	2.02	0.42
1:D:610:PHE:HB3	1:D:628:PHE:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.78	0.42
1:A:568:ASP:O	1:A:569:GLN:HB2	2.19	0.42
1:A:185:ARG:NH1	1:A:771:TYR:HB3	2.34	0.42
2:B:2032:LMT:H101	2:B:2032:LMT:H72	1.74	0.42
1:A:453:PHE:CG	1:A:474:ILE:HD11	2.54	0.42
1:E:89:THR:HG21	2:E:2033:LMT:H82	2.02	0.42
1:B:726:TYR:HE2	1:B:785:LEU:CD1	2.32	0.42
1:D:223:PRO:O	1:E:779:ARG:NH2	2.52	0.42
1:B:376:LEU:HD22	1:B:398:MET:HE2	2.02	0.42
1:F:1013:THR:O	1:F:1017:ILE:HG12	2.20	0.42
1:D:682:LEU:HD21	1:D:856:TYR:HD1	1.84	0.42
1:F:578:THR:HG22	1:F:623:SER:CB	2.46	0.42
1:F:563:PHE:CD2	1:F:564:LEU:HG	2.55	0.42
1:B:890:LEU:HD13	1:B:891:TYR:CE2	2.54	0.42
1:B:929:GLY:HA2	1:B:932:THR:HG22	2.02	0.42
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.42
1:C:5:PHE:CD1	1:C:487:ILE:HG23	2.55	0.42
1:D:100:PRO:HB3	1:D:295:THR:CG2	2.49	0.42
1:A:859:THR:CG2	1:A:860:GLY:N	2.81	0.42
1:A:167:SER:O	1:B:70:ASN:HB2	2.19	0.42
1:E:812:SER:HA	1:E:813:PRO:HD3	1.73	0.42
1:E:314:GLU:N	1:E:315:PRO:CD	2.82	0.42
1:B:370:ILE:O	1:B:373:PRO:HD2	2.20	0.42
1:F:695:LEU:HD12	1:F:696:LEU:N	2.34	0.42
1:C:1005:VAL:HG12	1:C:1006:ILE:N	2.35	0.42
1:F:306:ILE:HG13	1:F:306:ILE:O	2.19	0.42
1:D:958:ILE:N	1:D:958:ILE:HD13	2.35	0.42
1:F:891:TYR:O	1:F:892:GLU:C	2.58	0.42
1:A:578:THR:OG1	1:A:587:THR:HG22	2.19	0.42
1:B:1001:ILE:O	1:B:1005:VAL:HG23	2.19	0.42
1:E:303:ALA:O	1:E:307:ARG:HB2	2.19	0.42
1:A:306:ILE:O	1:A:310:ILE:HG23	2.20	0.42
1:D:164:ASP:HB2	1:D:165:PRO:HD3	2.01	0.42
1:B:564:LEU:HD21	1:B:670:SER:HB3	2.01	0.42
1:E:30:LEU:HD23	1:E:31:PRO:HD2	2.02	0.42
1:D:70:ASN:ND2	1:F:175:PHE:CE1	2.87	0.42
1:A:49:TYR:CD1	1:A:52:ALA:HB2	2.55	0.42
1:C:17:LEU:HD23	1:C:20:MET:CE	2.49	0.42
1:A:755:SER:HA	1:A:773:GLN:HG3	2.00	0.42
1:A:405:LEU:C	1:A:405:LEU:HD22	2.39	0.42
1:C:695:LEU:HD12	1:C:696:LEU:N	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:981:ILE:HG22	1:C:1006:ILE:HB	2.00	0.42
1:B:367:ILE:HG12	1:B:367:ILE:H	1.63	0.42
1:E:455:PRO:HG2	1:E:879:SER:HB3	2.02	0.42
1:B:56:THR:O	1:B:56:THR:HG22	2.20	0.42
1:C:667:ALA:O	1:C:678:THR:HG22	2.19	0.42
1:C:958:ILE:HD13	1:C:958:ILE:N	2.35	0.42
1:A:747:SER:O	1:A:751:ILE:HG13	2.20	0.42
1:E:391:ASN:ND2	1:E:393:LEU:H	2.16	0.42
1:E:237:LYS:NZ	1:F:742:LEU:HD22	2.35	0.42
1:E:616:ASN:ND2	1:E:624:SER:HB2	2.35	0.42
1:F:456:MET:CE	1:F:931:LEU:HD12	2.49	0.42
1:C:94:PHE:HB3	1:C:98:THR:HG21	2.02	0.42
1:C:789:TYR:HE2	1:C:799:PRO:HG3	1.85	0.42
1:A:885:LEU:HA	1:A:885:LEU:HD12	1.77	0.42
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.82	0.42
1:C:698:ALA:O	1:C:702:PHE:HB2	2.19	0.42
1:B:1011:THR:O	1:B:1015:LEU:HB2	2.20	0.42
1:D:745:ILE:HA	1:D:748:THR:HG22	2.02	0.42
1:E:910:GLY:HA3	1:E:1011:THR:CG2	2.50	0.42
1:C:368:PRO:HG3	1:C:413:VAL:HG21	2.00	0.42
1:D:523:THR:O	1:D:524:THR:C	2.56	0.42
1:C:138:MET:O	1:C:291:ILE:HG12	2.20	0.42
1:A:415:ASN:HA	1:A:418:ARG:HD2	2.01	0.42
1:A:887:LEU:CD2	1:A:942:ILE:HD12	2.50	0.42
1:B:278:ASN:O	1:B:612:VAL:HA	2.19	0.42
1:A:65:ILE:HD13	1:A:66:GLU:N	2.34	0.42
1:D:456:MET:CE	1:D:931:LEU:HD12	2.49	0.42
1:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.42
1:A:186:ILE:O	1:A:186:ILE:HG22	2.18	0.42
1:C:555:MET:O	1:C:559:ILE:HG23	2.19	0.42
1:A:681:ASP:OD1	1:A:859:THR:HG22	2.20	0.42
1:D:984:VAL:HG13	1:D:987:LEU:HD12	2.00	0.42
1:E:702:PHE:CE2	1:E:826:ILE:CD1	3.03	0.42
1:D:137:LEU:HD11	1:D:330:THR:HG23	2.02	0.42
1:A:974:VAL:O	1:A:978:LEU:HB2	2.20	0.42
1:D:336:SER:O	1:D:340:VAL:HG23	2.19	0.42
1:C:861:LEU:HD23	1:C:861:LEU:O	2.20	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD12	1.88	0.42
1:B:944:ILE:HD11	1:B:1020:VAL:HB	2.02	0.42
1:D:188:LEU:HG	1:D:772:LEU:CD2	2.50	0.42
1:D:753:TRP:HZ3	1:D:779:ARG:CB	2.29	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:GLN:H	1:D:181:GLN:HE21	1.67	0.42
1:A:456:MET:CE	1:A:931:LEU:HD12	2.50	0.42
1:B:559:ILE:CD1	1:B:560:PRO:HD2	2.49	0.42
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.42
1:A:530:GLY:O	1:A:534:ILE:HG22	2.19	0.42
1:D:541:TYR:HA	1:D:544:ILE:HG23	2.00	0.42
1:D:542:LEU:HD12	1:D:1022:LEU:HD13	2.02	0.42
1:A:616:ASN:N	1:A:619:GLY:O	2.50	0.42
1:C:133:VAL:HG12	1:C:135:ASN:N	2.31	0.42
1:C:843:VAL:O	1:C:847:VAL:HG23	2.20	0.42
1:A:197:GLN:CB	1:A:797:MET:HE3	2.50	0.42
1:F:150:THR:HG22	1:F:153:ASP:CG	2.40	0.42
1:E:204:SER:O	1:E:208:GLN:HG3	2.20	0.42
1:A:356:TYR:C	1:A:356:TYR:CD1	2.93	0.42
1:F:418:ARG:CZ	1:F:968:MET:HB3	2.49	0.42
1:D:70:ASN:HB2	1:F:167:SER:HB2	2.01	0.42
1:A:910:GLY:HA3	1:A:1011:THR:HG21	2.02	0.42
1:B:48:SER:O	1:B:50:PRO:HD3	2.20	0.42
1:F:698:ALA:O	1:F:702:PHE:HB2	2.20	0.42
1:A:242:THR:CG2	1:A:245:GLN:HG3	2.48	0.42
1:A:13:TRP:CE2	2:A:2026:LMT:C1	3.03	0.42
1:D:944:ILE:HD11	1:D:1020:VAL:CG1	2.50	0.42
1:B:375:VAL:O	1:B:379:THR:HB	2.20	0.42
1:E:367:ILE:HB	1:E:368:PRO:CD	2.40	0.42
1:B:587:THR:HG23	1:B:588:GLN:N	2.35	0.42
1:A:90:ILE:C	1:A:90:ILE:HD12	2.39	0.42
1:C:749:VAL:HG22	1:C:800:PHE:HZ	1.85	0.42
1:E:228:GLN:NE2	1:E:231:ASN:HD21	2.17	0.42
1:C:984:VAL:C	1:C:986:PRO:HD2	2.40	0.42
1:A:88:MET:C	1:A:88:MET:SD	2.98	0.42
1:E:303:ALA:HB2	1:E:330:THR:HG21	2.01	0.42
1:B:616:ASN:ND2	1:B:624:SER:HB2	2.35	0.42
1:C:111:LEU:C	1:C:113:LEU:N	2.71	0.42
1:A:936:LEU:HD12	1:A:1009:MET:HE1	2.01	0.42
1:A:341:VAL:O	1:A:344:LEU:HB2	2.20	0.42
1:D:976:THR:CG2	1:D:977:SER:N	2.83	0.42
1:E:352:PHE:CD2	1:E:352:PHE:C	2.93	0.42
1:D:396:PHE:HA	1:D:399:VAL:HG12	2.02	0.42
1:F:34:GLN:HG2	1:F:35:TYR:CD1	2.55	0.42
1:A:275:TYR:CG	1:C:223:PRO:HG3	2.55	0.42
1:B:222:LEU:HD12	1:C:276:SER:HA	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:ASN:HB2	1:F:613:THR:CG2	2.50	0.42
1:A:261:ARG:CZ	1:A:263:LYS:HZ3	2.33	0.42
1:F:671:VAL:O	1:F:674:LEU:HB2	2.20	0.42
1:D:175:PHE:HD1	1:D:289:ILE:HD11	1.84	0.41
1:F:488:LEU:HD22	1:F:492:LEU:HG	2.02	0.41
1:A:253:VAL:HG12	1:A:259:GLN:CB	2.37	0.41
1:F:520:PHE:O	1:F:524:THR:HG23	2.20	0.41
1:D:47:VAL:HG12	1:D:88:MET:HG3	2.00	0.41
1:F:1013:THR:O	1:F:1017:ILE:HG23	2.20	0.41
1:B:418:ARG:CZ	1:B:968:MET:CE	2.97	0.41
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.01	0.41
1:B:592:ASP:CG	1:B:595:ARG:HH12	2.23	0.41
1:E:199:THR:HG22	1:E:201:GLY:N	2.35	0.41
1:E:182:TYR:HD2	1:E:271:GLY:O	2.03	0.41
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.83	0.41
1:F:712:LEU:HD12	1:F:715:VAL:HG21	2.02	0.41
1:A:354:VAL:HG11	1:A:979:ALA:CA	2.50	0.41
1:A:866:ARG:HA	1:A:866:ARG:HD2	1.78	0.41
1:A:356:TYR:O	1:A:356:TYR:CD1	2.72	0.41
1:B:943:LEU:O	1:B:947:PHE:HD1	2.02	0.41
1:E:746:ASN:O	1:E:749:VAL:HG12	2.19	0.41
1:F:39:ALA:HA	1:F:40:PRO:HD3	1.78	0.41
1:B:280:GLN:HB2	1:B:611:THR:HG23	2.02	0.41
1:D:881:LEU:O	1:D:881:LEU:HD12	2.20	0.41
1:E:1011:THR:O	1:E:1015:LEU:HB2	2.21	0.41
1:E:944:ILE:HD11	1:E:1020:VAL:HB	2.02	0.41
1:D:634:TRP:O	1:D:638:PRO:HG3	2.20	0.41
1:A:453:PHE:CE2	1:A:932:THR:HG22	2.54	0.41
1:F:652:GLN:HE22	1:F:664:PHE:HB3	1.86	0.41
1:B:534:ILE:CG2	1:B:1022:LEU:HD23	2.44	0.41
1:C:652:GLN:HE22	1:C:664:PHE:HB3	1.85	0.41
1:E:587:THR:HG23	1:E:588:GLN:N	2.35	0.41
1:B:278:ASN:HB2	1:B:588:GLN:HE21	1.85	0.41
1:E:890:LEU:HD13	1:E:891:TYR:CE2	2.55	0.41
1:F:184:MET:HB3	1:F:184:MET:HE2	1.88	0.41
1:F:749:VAL:HG22	1:F:800:PHE:HZ	1.84	0.41
1:F:667:ALA:HA	1:F:668:PRO:HD3	1.83	0.41
1:B:958:ILE:CG1	1:B:959:VAL:N	2.82	0.41
1:A:789:TYR:HE2	1:A:799:PRO:HG3	1.81	0.41
1:B:237:LYS:NZ	1:C:742:LEU:HD22	2.35	0.41
1:F:324:VAL:HG12	1:F:325:TYR:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:ILE:HA	1:F:560:PRO:HD3	1.87	0.41
1:A:864:GLU:C	1:A:866:ARG:H	2.24	0.41
1:D:866:ARG:HD2	1:D:866:ARG:HA	1.78	0.41
1:B:685:GLN:HE22	1:B:818:TYR:HD2	1.66	0.41
1:F:197:GLN:HA	1:F:797:MET:SD	2.60	0.41
1:F:838:ASP:O	1:F:841:ALA:HB3	2.20	0.41
1:E:860:GLY:C	1:E:862:SER:N	2.74	0.41
1:A:378:GLY:O	1:A:382:VAL:HG23	2.20	0.41
1:C:75:LEU:C	1:C:75:LEU:HD23	2.40	0.41
1:A:355:MET:HE2	1:A:355:MET:HB3	1.90	0.41
1:F:214:ILE:HG13	1:F:237:LYS:HB2	2.03	0.41
1:A:753:TRP:HZ3	1:A:779:ARG:CB	2.28	0.41
1:A:470:PHE:CE2	1:A:928:VAL:HG13	2.56	0.41
1:A:524:THR:CG2	1:A:970:LEU:HD12	2.48	0.41
1:D:545:TYR:CD1	1:D:1023:PHE:HZ	2.38	0.41
1:D:519:MET:O	1:D:522:SER:OG	2.26	0.41
1:F:896:ILE:N	1:F:897:PRO:CD	2.83	0.41
1:E:278:ASN:HB2	1:E:588:GLN:HE21	1.86	0.41
1:D:90:ILE:HD12	1:D:90:ILE:C	2.39	0.41
1:E:186:ILE:CG2	1:E:268:VAL:HG22	2.48	0.41
1:A:578:THR:CG2	1:A:579:PRO:CD	2.94	0.41
1:C:90:ILE:C	1:C:90:ILE:HD12	2.41	0.41
1:A:472:ILE:HD12	1:A:472:ILE:C	2.41	0.41
1:B:108:GLN:HG2	1:C:112:GLN:OE1	2.20	0.41
1:E:44:ALA:CB	1:E:132:ALA:HB2	2.50	0.41
1:F:56:THR:O	1:F:60:THR:HG22	2.21	0.41
1:F:181:GLN:HB3	1:F:181:GLN:HE21	1.67	0.41
1:B:204:SER:O	1:B:208:GLN:HG3	2.19	0.41
1:E:521:LEU:HD22	1:E:525:HIS:CE1	2.56	0.41
1:B:951:LEU:C	1:B:953:GLU:N	2.73	0.41
1:B:563:PHE:O	1:B:923:ASP:HA	2.20	0.41
1:E:702:PHE:CD2	1:E:826:ILE:HD12	2.55	0.41
1:B:673:GLU:O	1:B:674:LEU:C	2.59	0.41
1:C:930:LEU:HA	1:C:930:LEU:HD23	1.86	0.41
1:B:784:ASP:HA	1:B:787:LYS:HE3	2.02	0.41
1:A:155:SER:OG	1:A:180:SER:N	2.54	0.41
1:F:451:ALA:HB1	1:F:882:VAL:HG12	2.02	0.41
1:C:357:LEU:O	1:C:357:LEU:HD22	2.20	0.41
1:D:76:ARG:HD3	1:D:95:GLU:OE1	2.21	0.41
1:F:367:ILE:HG22	1:F:492:LEU:HB3	2.01	0.41
1:C:367:ILE:HG22	1:C:492:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:438:ILE:O	1:E:439:GLN:C	2.58	0.41
1:E:239:ARG:HD2	1:E:762:ILE:HG23	2.03	0.41
1:D:887:LEU:CD2	1:D:942:ILE:HD12	2.50	0.41
1:F:445:ILE:N	1:F:942:ILE:HD11	2.35	0.41
1:C:971:ARG:CB	1:C:972:PRO:HD3	2.50	0.41
1:B:88:MET:HE2	1:B:88:MET:HB3	1.90	0.41
1:F:812:SER:HA	1:F:813:PRO:HD3	1.92	0.41
1:B:843:VAL:HA	1:B:846:ILE:HG12	2.03	0.41
1:D:333:VAL:O	1:D:337:ILE:HG12	2.20	0.41
1:F:683:PHE:CG	1:F:818:TYR:CE1	3.09	0.41
1:D:283:GLY:HA2	1:D:595:ARG:NE	2.35	0.41
1:E:616:ASN:HB2	1:E:619:GLY:O	2.20	0.41
1:D:694:VAL:O	1:D:697:GLN:HB3	2.21	0.41
1:D:479:ALA:O	1:D:483:ILE:HG22	2.20	0.41
1:B:154:LEU:CD1	1:B:286:ALA:HA	2.51	0.41
1:D:445:ILE:HG13	1:D:446:ALA:N	2.36	0.41
1:B:184:MET:HB2	1:B:770:VAL:HG22	2.01	0.41
1:F:357:LEU:O	1:F:357:LEU:HD22	2.20	0.41
1:D:406:VAL:O	1:D:410:ILE:HG12	2.19	0.41
1:B:910:GLY:HA3	1:B:1011:THR:CG2	2.50	0.41
1:B:909:ILE:HG13	1:B:910:GLY:N	2.36	0.41
1:F:330:THR:N	1:F:331:PRO:CD	2.84	0.41
1:E:534:ILE:CG2	1:E:1022:LEU:HD23	2.42	0.41
1:B:746:ASN:O	1:B:749:VAL:HG12	2.21	0.41
1:B:738:LEU:C	1:B:792:ASN:HD21	2.24	0.41
1:D:896:ILE:HD12	1:D:945:VAL:CG2	2.50	0.41
1:F:742:LEU:HD23	1:F:745:ILE:HD11	2.02	0.41
1:D:681:ASP:OD1	1:D:859:THR:HG22	2.20	0.41
1:A:336:SER:O	1:A:340:VAL:HG23	2.21	0.41
1:A:38:ILE:H	1:A:38:ILE:HD13	1.85	0.41
1:F:454:LEU:HA	1:F:454:LEU:HD23	1.60	0.41
1:E:454:LEU:HA	1:E:454:LEU:HD23	1.83	0.41
1:B:907:GLY:HA2	1:B:1011:THR:HG23	2.02	0.41
1:F:363:ARG:O	1:F:367:ILE:HD13	2.21	0.41
1:A:1015:LEU:O	1:A:1019:TRP:CD1	2.73	0.41
1:A:542:LEU:HD12	1:A:1022:LEU:HD13	2.02	0.41
1:F:652:GLN:OE1	1:F:652:GLN:HA	2.19	0.41
1:A:896:ILE:HD12	1:A:945:VAL:CG2	2.50	0.41
1:D:88:MET:SD	1:D:90:ILE:HG22	2.61	0.41
1:C:1013:THR:O	1:C:1017:ILE:HG23	2.20	0.41
1:C:668:PRO:HA	1:C:669:PRO:HD3	1.75	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:843:VAL:HA	1:E:846:ILE:HG12	2.02	0.41
1:F:534:ILE:HD11	1:F:1022:LEU:HB2	2.02	0.41
1:A:985:VAL:O	1:A:989:ILE:HG12	2.20	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD2	1.86	0.41
1:C:766:ARG:O	1:C:768:LYS:HG3	2.20	0.41
1:F:789:TYR:CE2	1:F:799:PRO:HG3	2.56	0.41
1:D:38:ILE:HB	1:D:462:SER:OG	2.20	0.41
1:D:275:TYR:CG	1:F:223:PRO:HG3	2.55	0.41
1:E:784:ASP:HA	1:E:787:LYS:HE3	2.01	0.41
1:A:357:LEU:HD22	1:A:357:LEU:O	2.21	0.41
1:B:527:TYR:CZ	1:B:966:CYS:HB3	2.56	0.41
1:F:929:GLY:HA2	1:F:932:THR:CG2	2.50	0.41
1:C:896:ILE:N	1:C:897:PRO:CD	2.84	0.41
1:F:522:SER:O	1:F:525:HIS:HB2	2.21	0.41
1:D:222:LEU:HA	1:D:223:PRO:C	2.41	0.41
1:E:278:ASN:O	1:E:612:VAL:HA	2.21	0.41
1:D:655:PHE:CG	1:D:663:VAL:HG11	2.55	0.41
1:C:150:THR:OG1	1:C:151:LYS:N	2.54	0.41
1:A:479:ALA:O	1:A:483:ILE:HG22	2.21	0.41
1:D:973:ILE:H	1:D:973:ILE:HG12	1.67	0.41
1:B:463:THR:O	1:B:466:ILE:HG12	2.20	0.41
1:A:100:PRO:HB3	1:A:295:THR:CG2	2.51	0.41
1:B:143:VAL:HG22	1:B:322:LYS:O	2.21	0.41
1:C:7:ASP:C	1:C:8:ARG:HG3	2.41	0.41
1:F:17:LEU:HD23	1:F:20:MET:CE	2.50	0.41
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.41
1:B:527:TYR:HE2	1:B:966:CYS:HB3	1.83	0.41
1:F:489:THR:HA	1:F:492:LEU:HD12	2.03	0.41
1:A:332:VAL:HG23	1:A:634:TRP:CZ2	2.56	0.41
1:A:745:ILE:HA	1:A:748:THR:HG22	2.03	0.41
1:A:699:ARG:NH2	1:A:824:MET:CG	2.77	0.41
1:C:520:PHE:O	1:C:524:THR:HG23	2.21	0.41
1:F:545:TYR:CE1	1:F:1023:PHE:HZ	2.39	0.41
1:C:652:GLN:HA	1:C:652:GLN:OE1	2.20	0.41
1:F:184:MET:CB	1:F:770:VAL:HG12	2.46	0.41
1:C:184:MET:H	1:C:761:PHE:HE1	1.67	0.41
1:E:641:GLU:O	1:E:650:ARG:NH2	2.54	0.41
1:F:843:VAL:O	1:F:847:VAL:HG23	2.21	0.41
1:A:224:ALA:CB	1:B:780:MET:HE1	2.49	0.41
1:E:164:ASP:HB3	1:E:165:PRO:HD3	2.03	0.41
1:A:780:MET:HB3	1:C:228:GLN:HE21	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:TRP:O	1:F:266:ALA:HB1	2.21	0.41
1:D:864:GLU:C	1:D:866:ARG:H	2.24	0.41
1:A:6:ILE:HD12	1:A:6:ILE:N	2.36	0.41
1:B:515:TRP:O	1:B:519:MET:HG2	2.20	0.41
1:C:553:ILE:HG12	1:C:553:ILE:H	1.73	0.41
1:D:631:LEU:CD2	1:D:644:VAL:HG23	2.51	0.41
1:C:789:TYR:CE2	1:C:799:PRO:HG3	2.56	0.41
1:C:930:LEU:O	1:C:933:THR:HB	2.20	0.41
1:A:445:ILE:HG13	1:A:446:ALA:N	2.34	0.41
1:C:881:LEU:O	1:C:885:LEU:HG	2.21	0.41
1:A:457:ALA:O	1:A:468:ARG:HD3	2.20	0.41
1:F:5:PHE:CD1	1:F:487:ILE:HG23	2.56	0.41
1:F:881:LEU:O	1:F:885:LEU:HG	2.20	0.41
1:A:650:ARG:HH11	1:A:650:ARG:HB2	1.86	0.41
1:D:355:MET:HE1	1:D:406:VAL:HG11	2.02	0.41
1:E:910:GLY:N	1:E:1011:THR:HG21	2.35	0.41
1:E:541:TYR:O	1:E:1019:TRP:CZ3	2.73	0.41
1:E:527:TYR:CZ	1:E:966:CYS:HB3	2.55	0.41
1:A:137:LEU:HD11	1:A:330:THR:HG23	2.02	0.41
1:C:489:THR:HA	1:C:492:LEU:HD12	2.03	0.41
2:A:2026:LMT:C8	2:A:2026:LMT:C12	2.98	0.41
1:B:757:TYR:CE1	1:B:769:ARG:CG	3.03	0.41
1:C:726:TYR:HB3	1:C:727:LYS:H	1.70	0.41
1:A:902:LEU:HD23	1:A:1023:PHE:CD1	2.56	0.41
1:A:958:ILE:HD13	1:A:958:ILE:N	2.36	0.41
1:D:902:LEU:HD23	1:D:1023:PHE:CD1	2.56	0.41
1:F:362:PHE:HA	1:F:365:THR:HG22	2.03	0.41
1:A:437:GLN:HE21	1:A:437:GLN:HB3	1.65	0.41
1:C:652:GLN:HE22	1:C:664:PHE:CB	2.34	0.41
1:D:220:GLY:O	1:D:221:GLY:C	2.59	0.41
1:A:616:ASN:HA	1:A:616:ASN:HD22	1.65	0.41
1:E:293:LEU:HD13	1:E:294:ALA:O	2.20	0.41
1:B:455:PRO:HG2	1:B:879:SER:HB3	2.02	0.41
1:D:587:THR:HG21	1:D:622:GLN:O	2.21	0.41
1:B:683:PHE:O	1:B:856:TYR:HA	2.21	0.41
1:A:233:THR:CG2	1:B:725:GLN:HG2	2.47	0.41
1:E:374:VAL:CG1	1:E:375:VAL:N	2.84	0.41
1:A:712:LEU:CD2	1:A:838:ASP:HB3	2.51	0.41
1:C:683:PHE:CG	1:C:818:TYR:CE1	3.08	0.41
1:C:845:GLU:C	1:C:847:VAL:H	2.24	0.41
1:F:370:ILE:O	1:F:373:PRO:HD2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:ILE:HG13	1:D:307:ARG:N	2.36	0.41
1:F:150:THR:OG1	1:F:151:LYS:N	2.54	0.41
1:D:930:LEU:HD23	1:D:930:LEU:HA	1.84	0.41
1:A:295:THR:HG23	1:A:295:THR:O	2.20	0.41
1:F:789:TYR:HE2	1:F:799:PRO:HG3	1.84	0.41
1:D:356:TYR:CD1	1:D:356:TYR:C	2.94	0.41
1:B:685:GLN:HB3	1:B:823:ALA:HB2	2.03	0.41
1:E:143:VAL:HG12	1:E:286:ALA:HB2	2.03	0.41
1:A:766:ARG:HE	1:B:67:GLN:NE2	2.19	0.41
1:F:690:VAL:HG12	1:F:694:VAL:HG21	2.03	0.41
1:E:563:PHE:O	1:E:923:ASP:HA	2.21	0.41
1:B:222:LEU:HA	1:B:223:PRO:C	2.40	0.41
1:D:457:ALA:O	1:D:468:ARG:HD3	2.21	0.41
1:B:99:ASP:OD2	1:B:101:ASP:HB2	2.21	0.41
1:C:915:THR:HG23	1:C:920:LEU:HB2	2.01	0.41
1:A:879:SER:O	1:A:883:VAL:HG23	2.20	0.41
1:D:591:VAL:HG11	1:D:611:THR:CG2	2.51	0.41
1:C:918:ARG:O	1:C:918:ARG:HG2	2.21	0.41
1:A:76:ARG:HB3	1:A:77:TYR:H	1.71	0.41
1:B:910:GLY:HA3	1:B:1007:GLY:O	2.21	0.41
1:D:192:LYS:O	1:D:193:LEU:C	2.59	0.41
1:E:47:VAL:HG22	1:E:127:ILE:HG23	2.03	0.41
1:D:812:SER:HA	1:D:813:PRO:HD3	1.80	0.41
1:D:527:TYR:O	1:D:531:VAL:N	2.45	0.41
1:C:548:ILE:HD11	1:C:906:LEU:CD2	2.47	0.41
1:C:445:ILE:N	1:C:942:ILE:HD11	2.36	0.41
1:A:578:THR:HG22	1:A:579:PRO:CD	2.50	0.41
1:D:579:PRO:HD3	1:D:661:ALA:HA	2.03	0.41
1:A:1003:THR:CG2	1:A:1004:GLY:N	2.84	0.41
1:E:1001:ILE:HG13	1:E:1002:GLY:H	1.85	0.41
1:D:376:LEU:HA	1:D:379:THR:HG22	2.03	0.41
1:A:69:MET:HE1	1:A:107:VAL:HG13	2.04	0.41
1:C:111:LEU:O	1:C:113:LEU:N	2.53	0.41
1:A:728:LEU:HA	1:A:728:LEU:HD23	1.83	0.41
1:B:483:ILE:O	1:B:487:ILE:HD13	2.21	0.41
1:D:1001:ILE:CG2	1:D:1002:GLY:N	2.82	0.41
1:F:52:ALA:HB1	1:F:56:THR:CG2	2.51	0.41
1:C:579:PRO:HG3	1:C:660:ASP:OD2	2.21	0.41
1:A:631:LEU:CD2	1:A:644:VAL:HG23	2.51	0.41
1:A:38:ILE:HB	1:A:462:SER:OG	2.21	0.41
1:C:52:ALA:HB1	1:C:56:THR:CG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:LEU:HD22	1:C:492:LEU:HG	2.03	0.40
1:A:192:LYS:O	1:A:193:LEU:C	2.58	0.40
1:A:220:GLY:O	1:A:221:GLY:C	2.59	0.40
1:E:775:ARG:O	1:E:779:ARG:HG2	2.21	0.40
1:E:798:VAL:HA	1:E:799:PRO:HD3	1.82	0.40
1:D:438:ILE:O	1:D:438:ILE:HD12	2.21	0.40
1:F:667:ALA:O	1:F:678:THR:HG22	2.20	0.40
1:E:958:ILE:CG1	1:E:959:VAL:N	2.83	0.40
1:A:43:ILE:HG12	1:A:104:GLN:HA	2.03	0.40
1:C:742:LEU:HD23	1:C:745:ILE:HD11	2.02	0.40
1:B:616:ASN:HB2	1:B:619:GLY:O	2.21	0.40
1:E:116:PRO:HA	1:E:123:GLN:NE2	2.35	0.40
1:B:936:LEU:HA	1:B:936:LEU:HD23	1.93	0.40
1:F:1001:ILE:HG13	1:F:1002:GLY:N	2.36	0.40
1:D:295:THR:HG23	1:D:295:THR:O	2.21	0.40
1:C:690:VAL:HG12	1:C:694:VAL:HG21	2.02	0.40
1:D:455:PRO:HG2	1:D:879:SER:HA	2.03	0.40
1:A:127:ILE:O	1:B:113:LEU:HG	2.21	0.40
1:C:836:SER:O	1:C:840:MET:HG3	2.21	0.40
1:A:375:VAL:O	1:A:379:THR:HG22	2.22	0.40
1:D:351:VAL:O	1:D:355:MET:HG2	2.22	0.40
1:D:787:LYS:HE2	1:D:787:LYS:HB2	1.84	0.40
1:E:969:ARG:C	1:E:972:PRO:HD2	2.39	0.40
1:F:138:MET:CB	1:F:328:ASP:HA	2.43	0.40
1:E:492:LEU:O	1:E:496:MET:HG3	2.21	0.40
2:B:2033:LMT:O5B	2:B:2033:LMT:H5'	2.21	0.40
1:E:929:GLY:C	1:E:932:THR:HG22	2.42	0.40
1:A:310:ILE:HD13	1:A:323:VAL:HG11	2.03	0.40
1:D:354:VAL:HG11	1:D:979:ALA:CA	2.51	0.40
1:D:609:VAL:HG13	1:D:629:ILE:HD13	2.02	0.40
1:D:131:LYS:NZ	1:E:73:ASP:OD2	2.51	0.40
1:A:792:ASN:HD22	1:A:793:ASP:H	1.68	0.40
1:B:143:VAL:HG12	1:B:286:ALA:HB2	2.02	0.40
1:D:293:LEU:HD21	1:D:297:ALA:HB3	2.04	0.40
1:E:575:GLN:NE2	1:E:617:PHE:HB2	2.36	0.40
1:F:94:PHE:HB3	1:F:98:THR:HG21	2.02	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	0.40
1:E:43:ILE:CG2	1:E:107:VAL:HG11	2.23	0.40
1:C:363:ARG:O	1:C:367:ILE:HD13	2.22	0.40
1:D:273:GLN:NE2	1:D:769:ARG:NH1	2.67	0.40
1:E:428:ARG:N	1:E:428:ARG:HD2	2.27	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ILE:C	1:A:438:ILE:HD12	2.41	0.40
1:A:62:VAL:HG12	1:A:63:GLN:N	2.36	0.40
1:B:641:GLU:O	1:B:650:ARG:NH2	2.54	0.40
1:D:563:PHE:O	1:D:563:PHE:CD2	2.74	0.40
1:F:90:ILE:C	1:F:90:ILE:HD12	2.42	0.40
1:E:463:THR:O	1:E:466:ILE:HG12	2.21	0.40
1:A:188:LEU:HG	1:A:772:LEU:CD2	2.51	0.40
1:B:199:THR:HG22	1:B:201:GLY:N	2.37	0.40
1:A:609:VAL:HG13	1:A:629:ILE:HD13	2.03	0.40
1:E:154:LEU:CD1	1:E:286:ALA:HA	2.51	0.40
1:C:2:SER:O	1:C:6:ILE:HG13	2.21	0.40
1:E:690:VAL:HG13	1:E:690:VAL:O	2.20	0.40
1:C:431:ALA:O	1:C:432:ARG:C	2.59	0.40
1:C:182:TYR:HD2	1:C:271:GLY:O	2.04	0.40
1:B:256:ASP:OD1	1:B:256:ASP:N	2.54	0.40
1:E:85:ASP:OD1	1:E:85:ASP:N	2.50	0.40
1:D:600:GLU:HA	1:D:600:GLU:OE1	2.21	0.40
1:A:137:LEU:HD22	1:A:293:LEU:HD12	2.04	0.40
1:D:763:ASP:CB	1:D:768:LYS:HD2	2.52	0.40
1:E:88:MET:HB3	1:E:88:MET:HE2	1.89	0.40
1:D:581:GLY:N	1:D:723:GLU:OE1	2.54	0.40
1:C:544:ILE:O	1:C:547:VAL:HB	2.20	0.40
1:C:907:GLY:HA2	1:C:1011:THR:CG2	2.50	0.40
1:A:415:ASN:O	1:A:416:VAL:C	2.59	0.40
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.02	0.40
1:D:78:ILE:HG13	1:D:90:ILE:HD11	2.02	0.40
1:D:701:LYS:HB3	1:D:701:LYS:HE2	1.91	0.40
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.37	0.40
1:E:1001:ILE:O	1:E:1005:VAL:HG23	2.20	0.40
1:E:376:LEU:HD22	1:E:398:MET:HE3	2.03	0.40
1:C:479:ALA:O	1:C:483:ILE:HG23	2.22	0.40
1:F:792:ASN:C	1:F:794:LYS:H	2.24	0.40
1:B:352:PHE:HD1	1:B:365:THR:CG2	2.34	0.40
1:C:185:ARG:HD3	1:C:771:TYR:HB2	2.03	0.40
1:D:49:TYR:O	1:D:86:GLY:HA3	2.22	0.40
1:D:63:GLN:O	1:D:67:GLN:HG3	2.21	0.40
1:A:924:VAL:HG23	1:A:925:PHE:N	2.36	0.40
1:A:68:GLN:O	1:A:110:LYS:HG3	2.21	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.22	0.40
1:E:158:ILE:O	1:E:163:GLN:HB2	2.22	0.40
1:B:162:ILE:O	1:B:166:LEU:HB2	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:528:GLU:OE2	1:D:967:ARG:NH2	2.55	0.40
1:C:362:PHE:HA	1:C:365:THR:HG22	2.04	0.40
1:C:939:LYS:HB3	1:C:939:LYS:HE3	1.90	0.40
1:C:438:ILE:C	1:C:440:GLY:N	2.75	0.40
1:D:415:ASN:HA	1:D:418:ARG:HD2	2.02	0.40
1:F:939:LYS:NZ	1:F:976:THR:HG21	2.33	0.40
1:F:753:TRP:HZ2	1:F:785:LEU:HA	1.86	0.40
1:D:579:PRO:HA	1:D:580:PRO:HD3	1.94	0.40
1:B:890:LEU:CD1	1:B:891:TYR:CE2	3.05	0.40
1:F:668:PRO:HA	1:F:669:PRO:HD3	1.75	0.40
1:D:985:VAL:N	1:D:986:PRO:CD	2.85	0.40
1:A:780:MET:HE3	1:C:224:ALA:CA	2.51	0.40
1:B:864:GLU:O	1:B:865:GLU:C	2.60	0.40
1:F:757:TYR:HE1	1:F:769:ARG:CG	2.35	0.40
1:B:44:ALA:CB	1:B:132:ALA:HB2	2.52	0.40
1:B:352:PHE:CD2	1:B:352:PHE:C	2.95	0.40
1:D:713:GLN:O	1:D:714:ARG:HB2	2.22	0.40
1:A:396:PHE:HA	1:A:399:VAL:HG12	2.03	0.40
1:B:702:PHE:CD2	1:B:826:ILE:HD12	2.56	0.40
1:D:754:GLY:O	1:D:755:SER:O	2.39	0.40
1:F:175:PHE:CD2	1:F:175:PHE:C	2.94	0.40
1:A:455:PRO:HG2	1:A:879:SER:HA	2.02	0.40
1:C:840:MET:O	1:C:844:GLU:HG3	2.22	0.40
1:E:99:ASP:OD2	1:E:101:ASP:HB2	2.21	0.40
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.56	0.40
1:A:596:GLU:O	1:A:597:TYR:C	2.60	0.40
1:A:353:LEU:HA	1:A:353:LEU:HD13	1.86	0.40
1:F:75:LEU:HD23	1:F:75:LEU:C	2.41	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	999/1052 (95%)	830 (83%)	123 (12%)	46 (5%)	3	18
1	B	1028/1052 (98%)	863 (84%)	147 (14%)	18 (2%)	11	45
1	C	1028/1052 (98%)	859 (84%)	143 (14%)	26 (2%)	7	34
1	D	990/1052 (94%)	820 (83%)	132 (13%)	38 (4%)	4	22
1	E	1006/1052 (96%)	847 (84%)	141 (14%)	18 (2%)	11	45
1	F	1028/1052 (98%)	866 (84%)	136 (13%)	26 (2%)	7	34
All	All	6079/6312 (96%)	5085 (84%)	822 (14%)	172 (3%)	6	30

All (172) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	VAL
1	A	134	LYS
1	A	203	VAL
1	A	204	SER
1	A	498	LYS
1	A	524	THR
1	A	532	ALA
1	A	533	SER
1	A	538	ARG
1	A	539	ALA
1	A	671	VAL
1	A	755	SER
1	A	866	ARG
1	A	872	ALA
1	A	917	MET
1	C	96	GLN
1	C	690	VAL
1	C	779	ARG
1	C	801	ASN
1	D	134	LYS
1	D	203	VAL
1	D	204	SER
1	D	498	LYS
1	D	524	THR
1	D	532	ALA
1	D	533	SER
1	D	538	ARG
1	D	539	ALA
1	D	866	ARG
1	D	872	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	917	MET
1	E	691	GLY
1	F	96	GLN
1	F	690	VAL
1	F	779	ARG
1	F	801	ASN
1	A	158	ILE
1	A	221	GLY
1	A	471	SER
1	A	523	THR
1	A	689	GLY
1	A	795	GLY
1	A	835	SER
1	B	439	GLN
1	B	563	PHE
1	B	657	SER
1	B	658	PHE
1	B	691	GLY
1	C	112	GLN
1	C	720	MET
1	C	721	SER
1	D	62	VAL
1	D	221	GLY
1	D	471	SER
1	D	523	THR
1	D	689	GLY
1	D	755	SER
1	D	835	SER
1	E	28	LEU
1	E	439	GLN
1	E	563	PHE
1	E	657	SER
1	E	658	PHE
1	F	112	GLN
1	F	217	GLY
1	F	720	MET
1	F	721	SER
1	A	542	LEU
1	A	595	ARG
1	A	596	GLU
1	A	710	PRO
1	A	870	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	28	LEU
1	B	137	LEU
1	B	570	GLY
1	C	217	GLY
1	C	424	GLY
1	C	717	PRO
1	C	875	LEU
1	D	148	SER
1	D	158	ILE
1	D	319	GLN
1	D	542	LEU
1	D	595	ARG
1	D	596	GLU
1	D	792	ASN
1	D	870	SER
1	E	137	LEU
1	E	570	GLY
1	F	717	PRO
1	F	875	LEU
1	F	877	ALA
1	A	148	SER
1	A	564	LEU
1	A	639	GLY
1	A	690	VAL
1	A	787	LYS
1	A	819	ASN
1	A	839	ALA
1	A	865	GLU
1	B	306	ILE
1	B	677	ALA
1	B	750	SER
1	C	147	GLY
1	C	256	ASP
1	C	361	ASN
1	C	521	LEU
1	C	877	ALA
1	C	993	ALA
1	D	564	LEU
1	D	639	GLY
1	D	838	ASP
1	D	839	ALA
1	D	865	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	29	SER
1	E	306	ILE
1	E	750	SER
1	F	147	GLY
1	F	256	ASP
1	F	361	ASN
1	F	424	GLY
1	F	521	LEU
1	F	993	ALA
1	A	276	SER
1	A	319	GLN
1	A	838	ASP
1	A	867	LEU
1	B	29	SER
1	B	57	VAL
1	B	195	SER
1	B	339	GLU
1	B	633	PRO
1	C	433	LYS
1	C	658	PHE
1	C	659	LYS
1	D	159	VAL
1	D	690	VAL
1	D	867	LEU
1	E	195	SER
1	E	633	PRO
1	F	433	LYS
1	F	658	PHE
1	F	659	LYS
1	B	310	ILE
1	C	804	ALA
1	E	57	VAL
1	E	310	ILE
1	E	954	GLN
1	F	804	ALA
1	A	438	ILE
1	A	530	GLY
1	C	638	PRO
1	C	719	GLY
1	D	438	ILE
1	F	719	GLY
1	D	715	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	638	PRO
1	F	846	ILE
1	A	919	GLY
1	C	310	ILE
1	C	715	VAL
1	C	846	ILE
1	F	310	ILE
1	A	236	GLY
1	A	715	VAL
1	A	989	ILE
1	B	539	ALA
1	D	236	GLY
1	E	539	ALA
1	E	580	PRO
1	A	873	PRO
1	F	715	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	823/860 (96%)	697 (85%)	126 (15%)	3	16
1	B	841/860 (98%)	736 (88%)	105 (12%)	6	24
1	C	841/860 (98%)	755 (90%)	86 (10%)	9	33
1	D	816/860 (95%)	695 (85%)	121 (15%)	4	17
1	E	829/860 (96%)	727 (88%)	102 (12%)	6	25
1	F	841/860 (98%)	751 (89%)	90 (11%)	8	31
All	All	4991/5160 (97%)	4361 (87%)	630 (13%)	5	24

All (630) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	11	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	LEU
1	A	25	LEU
1	A	34	GLN
1	A	38	ILE
1	A	43	ILE
1	A	49	TYR
1	A	55	GLU
1	A	56	THR
1	A	65	ILE
1	A	69	MET
1	A	75	LEU
1	A	76	ARG
1	A	79	SER
1	A	88	MET
1	A	90	ILE
1	A	92	VAL
1	A	140	VAL
1	A	166	LEU
1	A	170	LYS
1	A	181	GLN
1	A	184	MET
1	A	190	PRO
1	A	193	LEU
1	A	194	ASN
1	A	195	SER
1	A	196	TYR
1	A	197	GLN
1	A	207	ILE
1	A	226	LYS
1	A	233	THR
1	A	235	ILE
1	A	239	ARG
1	A	241	GLN
1	A	244	GLU
1	A	249	ILE
1	A	250	LEU
1	A	254	ASN
1	A	259	GLN
1	A	265	VAL
1	A	289	ILE
1	A	306	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	310	ILE
1	A	348	ILE
1	A	351	VAL
1	A	353	LEU
1	A	356	TYR
1	A	363	ARG
1	A	367	ILE
1	A	370	ILE
1	A	391	ASN
1	A	405	LEU
1	A	418	ARG
1	A	425	LEU
1	A	437	GLN
1	A	475	VAL
1	A	483	ILE
1	A	488	LEU
1	A	497	LEU
1	A	521	LEU
1	A	523	THR
1	A	524	THR
1	A	528	GLU
1	A	534	ILE
1	A	537	HIS
1	A	538	ARG
1	A	544	ILE
1	A	555	MET
1	A	556	PHE
1	A	596	GLU
1	A	599	LEU
1	A	616	ASN
1	A	620	ARG
1	A	634	TRP
1	A	643	SER
1	A	644	VAL
1	A	647	LEU
1	A	659	LYS
1	A	666	PHE
1	A	671	VAL
1	A	680	PHE
1	A	681	ASP
1	A	708	GLN
1	A	709	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	742	LEU
1	A	745	ILE
1	A	759	ASN
1	A	769	ARG
1	A	770	VAL
1	A	772	LEU
1	A	777	ASP
1	A	784	ASP
1	A	791	ARG
1	A	792	ASN
1	A	794	LYS
1	A	800	PHE
1	A	808	TRP
1	A	810	TYR
1	A	814	LYS
1	A	815	LEU
1	A	821	VAL
1	A	826	ILE
1	A	838	ASP
1	A	848	LYS
1	A	859	THR
1	A	861	LEU
1	A	871	GLN
1	A	875	LEU
1	A	885	LEU
1	A	890	LEU
1	A	896	ILE
1	A	901	MET
1	A	906	LEU
1	A	932	THR
1	A	933	THR
1	A	934	ILE
1	A	944	ILE
1	A	952	HIS
1	A	958	ILE
1	A	964	GLU
1	A	973	ILE
1	A	976	THR
1	A	978	LEU
1	A	981	ILE
1	B	14	VAL
1	B	17	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	33	ASN
1	B	34	GLN
1	B	38	ILE
1	B	47	VAL
1	B	49	TYR
1	B	55	GLU
1	B	58	GLN
1	B	70	ASN
1	B	82	SER
1	B	83	ASN
1	B	88	MET
1	B	90	ILE
1	B	107	VAL
1	B	108	GLN
1	B	110	LYS
1	B	113	LEU
1	B	117	LEU
1	B	118	LEU
1	B	121	GLU
1	B	127	ILE
1	B	129	VAL
1	B	130	THR
1	B	135	ASN
1	B	152	GLU
1	B	166	LEU
1	B	178	PHE
1	B	205	SER
1	B	207	ILE
1	B	242	THR
1	B	249	ILE
1	B	256	ASP
1	B	262	LEU
1	B	289	ILE
1	B	295	THR
1	B	301	ASP
1	B	312	ASN
1	B	324	VAL
1	B	329	THR
1	B	330	THR
1	B	348	ILE
1	B	352	PHE
1	B	357	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	365	THR
1	B	379	THR
1	B	392	THR
1	B	394	THR
1	B	405	LEU
1	B	407	ASP
1	B	410	ILE
1	B	414	GLU
1	B	428	ARG
1	B	445	ILE
1	B	462	SER
1	B	463	THR
1	B	474	ILE
1	B	483	ILE
1	B	487	ILE
1	B	488	LEU
1	B	515	TRP
1	B	521	LEU
1	B	522	SER
1	B	533	SER
1	B	544	ILE
1	B	548	ILE
1	B	552	MET
1	B	561	THR
1	B	566	ASP
1	B	577	GLN
1	B	578	THR
1	B	589	VAL
1	B	611	THR
1	B	612	VAL
1	B	637	ARG
1	B	641	GLU
1	B	646	GLU
1	B	647	LEU
1	B	673	GLU
1	B	678	THR
1	B	681	ASP
1	B	695	LEU
1	B	749	VAL
1	B	762	ILE
1	B	772	LEU
1	B	792	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	801	ASN
1	B	803	PHE
1	B	812	SER
1	B	817	ARG
1	B	821	VAL
1	B	880	LEU
1	B	881	LEU
1	B	890	LEU
1	B	896	ILE
1	B	922	ASN
1	B	933	THR
1	B	942	ILE
1	B	944	ILE
1	B	946	GLU
1	B	958	ILE
1	B	959	VAL
1	B	963	ILE
1	B	973	ILE
1	B	975	MET
1	C	1	MET
1	C	11	PHE
1	C	15	ILE
1	C	19	ILE
1	C	21	LEU
1	C	26	SER
1	C	38	ILE
1	C	47	VAL
1	C	55	GLU
1	C	56	THR
1	C	78	ILE
1	C	85	ASP
1	C	89	THR
1	C	98	THR
1	C	137	LEU
1	C	138	MET
1	C	148	SER
1	C	174	ASP
1	C	230	LEU
1	C	235	ILE
1	C	238	THR
1	C	262	LEU
1	C	287	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	289	ILE
1	C	291	ILE
1	C	329	THR
1	C	330	THR
1	C	337	ILE
1	C	340	VAL
1	C	348	ILE
1	C	357	LEU
1	C	367	ILE
1	C	370	ILE
1	C	394	THR
1	C	414	GLU
1	C	415	ASN
1	C	425	LEU
1	C	433	LYS
1	C	434	SER
1	C	445	ILE
1	C	450	SER
1	C	456	MET
1	C	466	ILE
1	C	469	GLN
1	C	472	ILE
1	C	483	ILE
1	C	488	LEU
1	C	489	THR
1	C	534	ILE
1	C	544	ILE
1	C	548	ILE
1	C	553	ILE
1	C	561	THR
1	C	578	THR
1	C	611	THR
1	C	629	ILE
1	C	634	TRP
1	C	663	VAL
1	C	666	PHE
1	C	674	LEU
1	C	681	ASP
1	C	699	ARG
1	C	704	MET
1	C	712	LEU
1	C	714	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	720	MET
1	C	730	ILE
1	C	762	ILE
1	C	826	ILE
1	C	856	TYR
1	C	859	THR
1	C	867	LEU
1	C	875	LEU
1	C	879	SER
1	C	881	LEU
1	C	890	LEU
1	C	903	VAL
1	C	932	THR
1	C	934	ILE
1	C	942	ILE
1	C	958	ILE
1	C	964	GLU
1	C	981	ILE
1	C	982	LEU
1	C	991	THR
1	C	1015	LEU
1	D	10	ILE
1	D	11	PHE
1	D	15	ILE
1	D	21	LEU
1	D	25	LEU
1	D	34	GLN
1	D	38	ILE
1	D	49	TYR
1	D	55	GLU
1	D	65	ILE
1	D	69	MET
1	D	75	LEU
1	D	76	ARG
1	D	79	SER
1	D	88	MET
1	D	90	ILE
1	D	92	VAL
1	D	140	VAL
1	D	166	LEU
1	D	170	LYS
1	D	181	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	184	MET
1	D	190	PRO
1	D	193	LEU
1	D	194	ASN
1	D	195	SER
1	D	196	TYR
1	D	197	GLN
1	D	207	ILE
1	D	226	LYS
1	D	233	THR
1	D	235	ILE
1	D	239	ARG
1	D	241	GLN
1	D	244	GLU
1	D	249	ILE
1	D	250	LEU
1	D	265	VAL
1	D	289	ILE
1	D	306	ILE
1	D	310	ILE
1	D	316	PHE
1	D	348	ILE
1	D	351	VAL
1	D	353	LEU
1	D	356	TYR
1	D	363	ARG
1	D	367	ILE
1	D	370	ILE
1	D	391	ASN
1	D	405	LEU
1	D	418	ARG
1	D	425	LEU
1	D	437	GLN
1	D	475	VAL
1	D	483	ILE
1	D	488	LEU
1	D	497	LEU
1	D	523	THR
1	D	524	THR
1	D	528	GLU
1	D	534	ILE
1	D	537	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	538	ARG
1	D	544	ILE
1	D	555	MET
1	D	556	PHE
1	D	596	GLU
1	D	599	LEU
1	D	616	ASN
1	D	620	ARG
1	D	634	TRP
1	D	643	SER
1	D	644	VAL
1	D	647	LEU
1	D	659	LYS
1	D	666	PHE
1	D	680	PHE
1	D	681	ASP
1	D	690	VAL
1	D	742	LEU
1	D	745	ILE
1	D	759	ASN
1	D	769	ARG
1	D	770	VAL
1	D	772	LEU
1	D	777	ASP
1	D	784	ASP
1	D	792	ASN
1	D	794	LYS
1	D	797	MET
1	D	800	PHE
1	D	805	THR
1	D	808	TRP
1	D	810	TYR
1	D	814	LYS
1	D	815	LEU
1	D	826	ILE
1	D	838	ASP
1	D	848	LYS
1	D	859	THR
1	D	861	LEU
1	D	871	GLN
1	D	875	LEU
1	D	885	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	890	LEU
1	D	896	ILE
1	D	901	MET
1	D	906	LEU
1	D	930	LEU
1	D	932	THR
1	D	933	THR
1	D	934	ILE
1	D	944	ILE
1	D	952	HIS
1	D	958	ILE
1	D	964	GLU
1	D	973	ILE
1	D	976	THR
1	D	978	LEU
1	D	981	ILE
1	E	14	VAL
1	E	17	LEU
1	E	33	ASN
1	E	34	GLN
1	E	38	ILE
1	E	47	VAL
1	E	49	TYR
1	E	55	GLU
1	E	58	GLN
1	E	70	ASN
1	E	82	SER
1	E	83	ASN
1	E	88	MET
1	E	90	ILE
1	E	107	VAL
1	E	108	GLN
1	E	110	LYS
1	E	113	LEU
1	E	117	LEU
1	E	118	LEU
1	E	121	GLU
1	E	127	ILE
1	E	129	VAL
1	E	130	THR
1	E	133	VAL
1	E	135	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	152	GLU
1	E	166	LEU
1	E	178	PHE
1	E	207	ILE
1	E	242	THR
1	E	249	ILE
1	E	256	ASP
1	E	262	LEU
1	E	289	ILE
1	E	295	THR
1	E	301	ASP
1	E	312	ASN
1	E	324	VAL
1	E	329	THR
1	E	330	THR
1	E	348	ILE
1	E	352	PHE
1	E	357	LEU
1	E	365	THR
1	E	379	THR
1	E	392	THR
1	E	394	THR
1	E	405	LEU
1	E	407	ASP
1	E	410	ILE
1	E	414	GLU
1	E	428	ARG
1	E	445	ILE
1	E	462	SER
1	E	463	THR
1	E	474	ILE
1	E	483	ILE
1	E	487	ILE
1	E	488	LEU
1	E	515	TRP
1	E	521	LEU
1	E	522	SER
1	E	533	SER
1	E	544	ILE
1	E	548	ILE
1	E	552	MET
1	E	561	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	566	ASP
1	E	577	GLN
1	E	578	THR
1	E	589	VAL
1	E	611	THR
1	E	612	VAL
1	E	637	ARG
1	E	641	GLU
1	E	646	GLU
1	E	647	LEU
1	E	695	LEU
1	E	762	ILE
1	E	772	LEU
1	E	792	ASN
1	E	801	ASN
1	E	803	PHE
1	E	812	SER
1	E	817	ARG
1	E	821	VAL
1	E	880	LEU
1	E	881	LEU
1	E	890	LEU
1	E	896	ILE
1	E	922	ASN
1	E	933	THR
1	E	942	ILE
1	E	944	ILE
1	E	946	GLU
1	E	958	ILE
1	E	959	VAL
1	E	963	ILE
1	E	973	ILE
1	E	975	MET
1	E	1011	THR
1	F	1	MET
1	F	11	PHE
1	F	15	ILE
1	F	19	ILE
1	F	21	LEU
1	F	26	SER
1	F	38	ILE
1	F	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	55	GLU
1	F	56	THR
1	F	77	TYR
1	F	78	ILE
1	F	85	ASP
1	F	89	THR
1	F	98	THR
1	F	137	LEU
1	F	138	MET
1	F	148	SER
1	F	174	ASP
1	F	230	LEU
1	F	235	ILE
1	F	238	THR
1	F	249	ILE
1	F	262	LEU
1	F	287	SER
1	F	289	ILE
1	F	291	ILE
1	F	329	THR
1	F	330	THR
1	F	337	ILE
1	F	340	VAL
1	F	348	ILE
1	F	357	LEU
1	F	367	ILE
1	F	370	ILE
1	F	394	THR
1	F	414	GLU
1	F	415	ASN
1	F	425	LEU
1	F	433	LYS
1	F	434	SER
1	F	445	ILE
1	F	450	SER
1	F	456	MET
1	F	466	ILE
1	F	469	GLN
1	F	472	ILE
1	F	481	SER
1	F	483	ILE
1	F	488	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	489	THR
1	F	534	ILE
1	F	544	ILE
1	F	548	ILE
1	F	553	ILE
1	F	561	THR
1	F	578	THR
1	F	611	THR
1	F	629	ILE
1	F	634	TRP
1	F	663	VAL
1	F	666	PHE
1	F	674	LEU
1	F	681	ASP
1	F	699	ARG
1	F	704	MET
1	F	712	LEU
1	F	714	ARG
1	F	720	MET
1	F	730	ILE
1	F	762	ILE
1	F	826	ILE
1	F	856	TYR
1	F	859	THR
1	F	867	LEU
1	F	875	LEU
1	F	879	SER
1	F	881	LEU
1	F	890	LEU
1	F	903	VAL
1	F	932	THR
1	F	934	ILE
1	F	942	ILE
1	F	946	GLU
1	F	958	ILE
1	F	964	GLU
1	F	981	ILE
1	F	982	LEU
1	F	991	THR
1	F	1015	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (158) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	34	GLN
1	A	68	GLN
1	A	83	ASN
1	A	96	GLN
1	A	156	ASN
1	A	181	GLN
1	A	194	ASN
1	A	213	GLN
1	A	228	GLN
1	A	245	GLN
1	A	254	ASN
1	A	259	GLN
1	A	273	GLN
1	A	308	GLN
1	A	360	GLN
1	A	437	GLN
1	A	569	GLN
1	A	575	GLN
1	A	577	GLN
1	A	616	ASN
1	A	642	ASN
1	A	654	HIS
1	A	700	ASN
1	A	709	ASN
1	A	725	GLN
1	A	792	ASN
1	A	819	ASN
1	A	871	GLN
1	A	922	ASN
1	A	952	HIS
1	B	33	ASN
1	B	34	GLN
1	B	46	GLN
1	B	67	GLN
1	B	104	GLN
1	B	108	GLN
1	B	125	GLN
1	B	156	ASN
1	B	161	ASN
1	B	163	GLN
1	B	176	GLN
1	B	181	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	211	ASN
1	B	228	GLN
1	B	231	ASN
1	B	245	GLN
1	B	278	ASN
1	B	308	GLN
1	B	312	ASN
1	B	391	ASN
1	B	415	ASN
1	B	575	GLN
1	B	588	GLN
1	B	652	GLN
1	B	676	ASN
1	B	685	GLN
1	B	687	GLN
1	B	692	HIS
1	B	759	ASN
1	B	773	GLN
1	B	792	ASN
1	B	922	ASN
1	C	34	GLN
1	C	67	GLN
1	C	125	GLN
1	C	280	GLN
1	C	282	ASN
1	C	319	GLN
1	C	391	ASN
1	C	415	ASN
1	C	437	GLN
1	C	439	GLN
1	C	469	GLN
1	C	508	HIS
1	C	652	GLN
1	C	713	GLN
1	C	759	ASN
1	D	33	ASN
1	D	34	GLN
1	D	68	GLN
1	D	83	ASN
1	D	96	GLN
1	D	108	GLN
1	D	156	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	163	GLN
1	D	181	GLN
1	D	194	ASN
1	D	213	GLN
1	D	228	GLN
1	D	231	ASN
1	D	245	GLN
1	D	273	GLN
1	D	308	GLN
1	D	360	GLN
1	D	437	GLN
1	D	575	GLN
1	D	577	GLN
1	D	616	ASN
1	D	622	GLN
1	D	642	ASN
1	D	652	GLN
1	D	654	HIS
1	D	697	GLN
1	D	700	ASN
1	D	708	GLN
1	D	725	GLN
1	D	792	ASN
1	D	819	ASN
1	D	871	GLN
1	D	922	ASN
1	D	952	HIS
1	E	33	ASN
1	E	34	GLN
1	E	46	GLN
1	E	67	GLN
1	E	104	GLN
1	E	108	GLN
1	E	125	GLN
1	E	156	ASN
1	E	161	ASN
1	E	163	GLN
1	E	176	GLN
1	E	181	GLN
1	E	211	ASN
1	E	228	GLN
1	E	231	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	245	GLN
1	E	278	ASN
1	E	308	GLN
1	E	312	ASN
1	E	391	ASN
1	E	415	ASN
1	E	575	GLN
1	E	588	GLN
1	E	652	GLN
1	E	685	GLN
1	E	692	HIS
1	E	759	ASN
1	E	773	GLN
1	E	792	ASN
1	E	922	ASN
1	F	34	GLN
1	F	67	GLN
1	F	125	GLN
1	F	280	GLN
1	F	282	ASN
1	F	319	GLN
1	F	391	ASN
1	F	415	ASN
1	F	437	GLN
1	F	439	GLN
1	F	469	GLN
1	F	508	HIS
1	F	517	ASN
1	F	652	GLN
1	F	713	GLN
1	F	759	ASN

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	LMT	A	2026	-	36,36,36	0.56	0	47,47,47	1.54	7 (14%)
2	LMT	B	2031	-	36,36,36	0.95	2 (5%)	47,47,47	1.43	9 (19%)
2	LMT	B	2032	-	36,36,36	0.73	1 (2%)	47,47,47	2.01	9 (19%)
2	LMT	B	2033	-	36,36,36	1.15	3 (8%)	47,47,47	3.58	19 (40%)
2	LMT	D	2026	-	36,36,36	0.70	1 (2%)	47,47,47	1.85	8 (17%)
2	LMT	E	2031	-	36,36,36	0.86	1 (2%)	47,47,47	1.82	9 (19%)
2	LMT	E	2032	-	36,36,36	0.60	1 (2%)	47,47,47	1.42	5 (10%)
2	LMT	E	2033	-	36,36,36	1.07	3 (8%)	47,47,47	3.49	19 (40%)

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	LMT	A	2026	-	-	1/21/61/61	0/2/2/2
2	LMT	B	2031	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2033	-	-	1/21/61/61	0/2/2/2
2	LMT	D	2026	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2031	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	E	2033	-	-	1/21/61/61	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2033	LMT	O5'-C5'	2.05	1.49	1.44
2	B	2033	LMT	O5'-C5'	2.06	1.49	1.44
2	B	2031	LMT	O1B-C1B	2.06	1.47	1.41
2	E	2033	LMT	O1B-C1B	2.16	1.47	1.41
2	E	2032	LMT	O1'-C1'	2.32	1.44	1.40
2	D	2026	LMT	O1'-C1'	2.33	1.44	1.40
2	B	2033	LMT	C4'-C5'	2.43	1.59	1.52
2	E	2031	LMT	O1'-C1'	3.02	1.45	1.40
2	B	2031	LMT	O1'-C1'	3.26	1.46	1.40
2	B	2032	LMT	O1'-C1'	3.51	1.46	1.40
2	E	2033	LMT	O1'-C1'	3.60	1.46	1.40
2	B	2033	LMT	O1'-C1'	4.08	1.47	1.40

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2033	LMT	C1B-O1B-C4'	-9.52	93.14	118.01
2	E	2033	LMT	C1B-O1B-C4'	-9.16	94.06	118.01
2	B	2033	LMT	C3'-C4'-C5'	-7.97	92.81	110.84
2	E	2033	LMT	C3'-C4'-C5'	-7.91	92.95	110.84
2	B	2032	LMT	C1-O1'-C1'	-7.22	101.33	113.94
2	E	2031	LMT	C1-O1'-C1'	-6.38	102.78	113.94
2	E	2032	LMT	C1-O1'-C1'	-6.14	103.21	113.94
2	B	2032	LMT	C3'-C4'-C5'	-5.68	98.00	110.84
2	B	2033	LMT	O1B-C4'-C3'	-4.59	95.33	107.17
2	D	2026	LMT	O1'-C1-C2	-4.23	93.06	109.88
2	D	2026	LMT	O5'-C5'-C6'	-4.23	95.67	106.36
2	B	2032	LMT	C6B-C5B-C4B	-4.03	103.08	113.02
2	E	2033	LMT	C4B-C3B-C2B	-3.72	103.85	110.79
2	E	2033	LMT	O1B-C4'-C3'	-3.66	97.73	107.17
2	E	2031	LMT	C6'-C5'-C4'	-3.54	102.94	113.25
2	B	2033	LMT	C3B-C4B-C5B	-3.49	104.11	110.20
2	B	2033	LMT	C4B-C3B-C2B	-3.48	104.29	110.79
2	E	2033	LMT	C3B-C4B-C5B	-3.44	104.19	110.20
2	D	2026	LMT	O5'-C1'-C2'	-3.35	103.40	110.28
2	B	2031	LMT	C3'-C4'-C5'	-3.34	103.29	110.84
2	E	2032	LMT	O1B-C1B-O5B	-3.30	102.32	110.68
2	E	2033	LMT	C1B-O5B-C5B	-3.25	107.44	113.75
2	D	2026	LMT	O5'-C1'-O1'	-3.19	102.36	110.05
2	E	2031	LMT	O1B-C1B-O5B	-3.08	102.87	110.68
2	B	2033	LMT	C1B-O5B-C5B	-3.06	107.80	113.75
2	B	2033	LMT	O5'-C1'-C2'	-2.99	104.15	110.28
2	A	2026	LMT	O5'-C5'-C6'	-2.92	98.99	106.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2026	LMT	O5'-C1'-O1'	-2.88	103.12	110.05
2	B	2033	LMT	C6B-C5B-C4B	-2.80	106.10	113.02
2	E	2033	LMT	C6B-C5B-C4B	-2.79	106.14	113.02
2	A	2026	LMT	O1B-C1B-O5B	-2.71	103.83	110.68
2	A	2026	LMT	C6'-C5'-C4'	-2.70	105.38	113.25
2	B	2031	LMT	C1-O1'-C1'	-2.65	109.31	113.94
2	E	2033	LMT	O5'-C1'-C2'	-2.61	104.92	110.28
2	B	2032	LMT	O1B-C1B-C2B	-2.50	102.02	108.10
2	E	2032	LMT	C1'-O5'-C5'	-2.50	108.90	113.75
2	E	2031	LMT	C1B-O1B-C4'	-2.33	111.92	118.01
2	B	2031	LMT	C4B-C3B-C2B	-2.28	106.54	110.79
2	B	2033	LMT	O2B-C2B-C3B	-2.22	105.34	110.34
2	B	2031	LMT	O5B-C1B-C2B	-2.21	105.74	110.28
2	D	2026	LMT	C6B-C5B-C4B	-2.19	107.61	113.02
2	B	2031	LMT	C1B-O1B-C4'	-2.16	112.35	118.01
2	E	2032	LMT	C9-C8-C7	-2.07	103.84	114.53
2	E	2033	LMT	O2B-C2B-C3B	-2.02	105.78	110.34
2	D	2026	LMT	C6'-C5'-C4'	2.02	119.11	113.25
2	A	2026	LMT	O1B-C1B-C2B	2.08	113.17	108.10
2	B	2031	LMT	C1B-C2B-C3B	2.18	114.27	109.97
2	B	2032	LMT	C1B-O5B-C5B	2.22	118.06	113.75
2	B	2032	LMT	C1B-C2B-C3B	2.49	114.89	109.97
2	E	2031	LMT	O1B-C1B-C2B	2.55	114.30	108.10
2	E	2033	LMT	O5B-C5B-C4B	2.75	114.85	109.68
2	E	2033	LMT	C2'-C3'-C4'	2.87	115.91	109.60
2	B	2031	LMT	O1B-C1B-O5B	2.89	118.01	110.68
2	E	2031	LMT	O1B-C4'-C3'	2.91	114.69	107.17
2	B	2032	LMT	O1'-C1'-C2'	2.96	111.78	108.04
2	B	2033	LMT	O5B-C5B-C4B	3.00	115.31	109.68
2	B	2031	LMT	O5'-C1'-O1'	3.07	117.44	110.05
2	B	2031	LMT	O1B-C4'-C5'	3.07	117.39	109.32
2	B	2033	LMT	C2'-C3'-C4'	3.08	116.36	109.60
2	A	2026	LMT	O1B-C4'-C3'	3.21	115.45	107.17
2	B	2032	LMT	O5'-C1'-O1'	3.24	117.85	110.05
2	E	2032	LMT	O1'-C1'-C2'	3.26	112.16	108.04
2	E	2031	LMT	O1'-C1-C2	3.48	123.72	109.88
2	D	2026	LMT	O1B-C4'-C5'	3.57	118.71	109.32
2	B	2032	LMT	O1B-C1B-O5B	3.60	119.78	110.68
2	B	2033	LMT	O1'-C1-C2	3.70	124.58	109.88
2	B	2033	LMT	O2B-C2B-C1B	3.82	118.39	110.02
2	B	2033	LMT	O5'-C1'-O1'	3.91	119.46	110.05
2	E	2033	LMT	O5'-C1'-O1'	4.04	119.78	110.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2033	LMT	O2B-C2B-C1B	4.07	118.93	110.02
2	E	2031	LMT	O5B-C5B-C6B	4.18	116.91	106.36
2	E	2033	LMT	O1'-C1'-C2'	4.23	113.38	108.04
2	B	2033	LMT	O1B-C1B-O5B	4.36	121.71	110.68
2	E	2031	LMT	O1'-C1'-C2'	4.52	113.75	108.04
2	E	2033	LMT	O1B-C1B-O5B	4.56	122.23	110.68
2	E	2033	LMT	O1'-C1-C2	4.65	128.37	109.88
2	E	2033	LMT	O1B-C4'-C5'	5.01	122.48	109.32
2	B	2033	LMT	O1'-C1'-C2'	5.03	114.39	108.04
2	B	2033	LMT	O1B-C4'-C5'	5.13	122.81	109.32
2	A	2026	LMT	O1'-C1'-C2'	5.15	114.54	108.04
2	B	2033	LMT	O5'-C5'-C4'	6.08	122.58	109.75
2	E	2033	LMT	O5'-C5'-C4'	6.09	122.62	109.75
2	D	2026	LMT	O1'-C1'-C2'	7.17	117.10	108.04
2	E	2033	LMT	C1-O1'-C1'	12.89	136.47	113.94
2	B	2033	LMT	C1-O1'-C1'	13.57	137.65	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2026	LMT	C1-O1'-C1'-O5'
2	E	2033	LMT	C1-O1'-C1'-O5'
2	B	2033	LMT	C1-O1'-C1'-O5'

There are no ring outliers.

8 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2026	LMT	10	0
2	B	2031	LMT	5	0
2	B	2032	LMT	4	0
2	B	2033	LMT	8	0
2	D	2026	LMT	5	0
2	E	2031	LMT	4	0
2	E	2032	LMT	8	0
2	E	2033	LMT	10	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 ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1004/1052 (95%)	-0.23	10 (0%)	84 60	54, 91, 132, 178	0
1	B	1030/1052 (97%)	-0.11	26 (2%)	61 30	53, 91, 143, 188	0
1	C	1028/1052 (97%)	-0.04	46 (4%)	37 15	58, 101, 178, 238	0
1	D	998/1052 (94%)	-0.26	20 (2%)	68 39	58, 91, 134, 179	0
1	E	1012/1052 (96%)	-0.13	43 (4%)	40 16	55, 93, 143, 189	0
1	F	1030/1052 (97%)	-0.06	47 (4%)	36 14	59, 100, 177, 238	0
All	All	6102/6312 (96%)	-0.14	192 (3%)	52 24	53, 94, 153, 238	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	803	PHE	7.8
1	E	260	VAL	6.8
1	C	778	ALA	6.2
1	E	251	LEU	6.1
1	F	753	TRP	5.6
1	F	660	ASP	5.4
1	C	503	GLY	5.3
1	A	841	ALA	4.9
1	F	640	GLY	4.8
1	D	585	GLU	4.8
1	C	783	ASP	4.8
1	C	505	HIS	4.7
1	D	252	LYS	4.6
1	F	745	ILE	4.4
1	F	744	ASP	4.4
1	F	659	LYS	4.4
1	E	506	GLY	4.3
1	E	834	LEU	4.3
1	B	140	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203	VAL	4.2
1	E	833	GLY	4.1
1	F	251	LEU	4.1
1	C	638	PRO	4.0
1	E	252	LYS	4.0
1	B	162	ILE	4.0
1	C	790	VAL	4.0
1	E	732	ASP	3.9
1	D	841	ALA	3.9
1	B	678	THR	3.9
1	C	753	TRP	3.9
1	C	636	GLU	3.9
1	F	658	PHE	3.8
1	F	506	GLY	3.8
1	D	199	THR	3.7
1	A	955	GLY	3.7
1	E	229	GLN	3.6
1	B	251	LEU	3.6
1	D	785	LEU	3.6
1	E	250	LEU	3.6
1	D	635	GLU	3.6
1	C	721	SER	3.6
1	C	738	LEU	3.6
1	E	246	PHE	3.5
1	F	600	GLU	3.5
1	F	507	GLU	3.5
1	B	224	ALA	3.5
1	E	253	VAL	3.4
1	F	502	LYS	3.4
1	E	261	ARG	3.4
1	C	688	ALA	3.4
1	C	745	ILE	3.4
1	F	790	VAL	3.3
1	E	507	GLU	3.3
1	A	230	LEU	3.3
1	A	868	SER	3.3
1	C	805	THR	3.3
1	B	237	LYS	3.2
1	E	600	GLU	3.2
1	C	507	GLU	3.2
1	D	570	GLY	3.2
1	E	1030	LEU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	3.2
1	E	807	LYS	3.2
1	C	199	THR	3.1
1	C	785	LEU	3.1
1	F	255	PRO	3.1
1	E	598	LEU	3.1
1	F	800	PHE	3.1
1	D	636	GLU	3.1
1	F	225	VAL	3.0
1	C	800	PHE	3.0
1	F	732	ASP	3.0
1	C	732	ASP	3.0
1	C	200	PRO	2.9
1	C	786	SER	2.9
1	F	250	LEU	2.9
1	E	262	LEU	2.9
1	C	147	GLY	2.9
1	D	202	ASP	2.9
1	C	198	LEU	2.9
1	D	840	MET	2.9
1	E	753	TRP	2.9
1	C	265	VAL	2.9
1	F	261	ARG	2.8
1	E	228	GLN	2.8
1	F	748	THR	2.8
1	F	601	LYS	2.8
1	A	147	GLY	2.8
1	E	655	PHE	2.8
1	C	794	LYS	2.7
1	F	591	VAL	2.7
1	D	264	ASP	2.7
1	F	726	TYR	2.7
1	B	360	GLN	2.7
1	D	251	LEU	2.7
1	F	789	TYR	2.7
1	E	561	THR	2.7
1	B	498	LYS	2.7
1	A	732	ASP	2.7
1	A	542	LEU	2.7
1	B	289	ILE	2.7
1	C	259	GLN	2.7
1	F	260	VAL	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	599	LEU	2.7
1	B	322	LYS	2.7
1	B	610	PHE	2.7
1	E	562	ALA	2.6
1	E	704	MET	2.6
1	A	687	GLN	2.6
1	C	362	PHE	2.6
1	C	502	LYS	2.6
1	B	225	VAL	2.6
1	C	250	LEU	2.6
1	F	799	PRO	2.6
1	B	362	PHE	2.6
1	F	259	GLN	2.6
1	A	839	ALA	2.6
1	E	258	SER	2.5
1	E	708	GLN	2.5
1	C	261	ARG	2.5
1	F	252	LYS	2.5
1	F	796	GLU	2.5
1	C	777	ASP	2.5
1	F	738	LEU	2.5
1	C	635	GLU	2.5
1	E	519	MET	2.4
1	B	1030	LEU	2.4
1	F	224	ALA	2.4
1	D	248	ASN	2.4
1	D	730	ILE	2.4
1	E	788	TRP	2.4
1	F	788	TRP	2.4
1	E	805	THR	2.4
1	F	156	ASN	2.4
1	F	200	PRO	2.4
1	C	508	HIS	2.4
1	F	258	SER	2.4
1	C	726	TYR	2.4
1	C	854	VAL	2.4
1	C	600	GLU	2.4
1	F	265	VAL	2.4
1	C	730	ILE	2.3
1	F	504	ASP	2.3
1	B	581	GLY	2.3
1	C	242	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	505	HIS	2.3
1	A	733	GLU	2.3
1	F	661	ALA	2.3
1	E	264	ASP	2.3
1	C	728	LEU	2.3
1	F	246	PHE	2.3
1	C	804	ALA	2.3
1	D	690	VAL	2.3
1	E	509	LYS	2.3
1	F	626	MET	2.2
1	B	587	THR	2.2
1	D	604	SER	2.2
1	C	251	LEU	2.2
1	E	832	PRO	2.2
1	B	250	LEU	2.2
1	D	583	SER	2.2
1	B	260	VAL	2.2
1	B	849	GLN	2.2
1	E	849	GLN	2.2
1	B	263	LYS	2.2
1	D	263	LYS	2.2
1	F	226	LYS	2.2
1	E	266	ALA	2.2
1	C	852	LYS	2.2
1	F	262	LEU	2.2
1	F	253	VAL	2.2
1	B	800	PHE	2.1
1	C	640	GLY	2.1
1	C	801	ASN	2.1
1	E	254	ASN	2.1
1	B	660	ASP	2.1
1	E	778	ALA	2.1
1	F	188	LEU	2.1
1	E	697	GLN	2.1
1	D	160	SER	2.1
1	D	835	SER	2.1
1	E	706	ALA	2.1
1	C	743	ALA	2.1
1	C	202	ASP	2.0
1	E	651	ALA	2.0
1	F	818	TYR	2.0
1	B	850	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	256	ASP	2.0
1	B	258	SER	2.0
1	E	538	ARG	2.0
1	E	663	VAL	2.0
1	E	513	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	LMT	B	2033	35/35	0.72	0.42	3.49	100,155,176,183	0
2	LMT	E	2033	35/35	0.76	0.33	2.43	111,146,174,179	0
2	LMT	B	2032	35/35	0.93	0.25	2.22	52,70,157,169	0
2	LMT	E	2032	35/35	0.93	0.23	2.19	66,90,115,128	0
2	LMT	E	2031	35/35	0.85	0.23	1.97	72,95,121,130	0
2	LMT	A	2026	35/35	0.90	0.21	0.66	80,110,145,173	0
2	LMT	B	2031	35/35	0.90	0.19	0.05	59,82,109,114	0
2	LMT	D	2026	35/35	0.91	0.16	-1.02	75,113,140,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.