



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:39 pm BST

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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

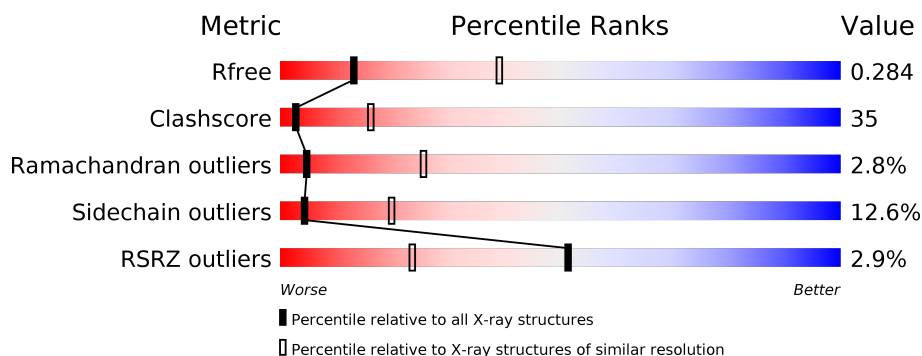
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>0%</div> <div> <div>37%</div> <div>46%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	1052	<div> <div>2%</div> <div> <div>46%</div> <div>44%</div> <div>8%</div> <div>•</div> </div> </div>
1	C	1052	<div> <div>4%</div> <div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div> </div>
1	D	1052	<div> <div>2%</div> <div> <div>38%</div> <div>46%</div> <div>11%</div> <div>• 5%</div> </div> </div>
1	E	1052	<div> <div>4%</div> <div> <div>44%</div> <div>44%</div> <div>8%</div> <div>•</div> </div> </div>
1	F	1052	<div> <div>4%</div> <div> <div>46%</div> <div>45%</div> <div>7%</div> <div>•</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	2033	-	-	-	X

2 Entry composition

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:

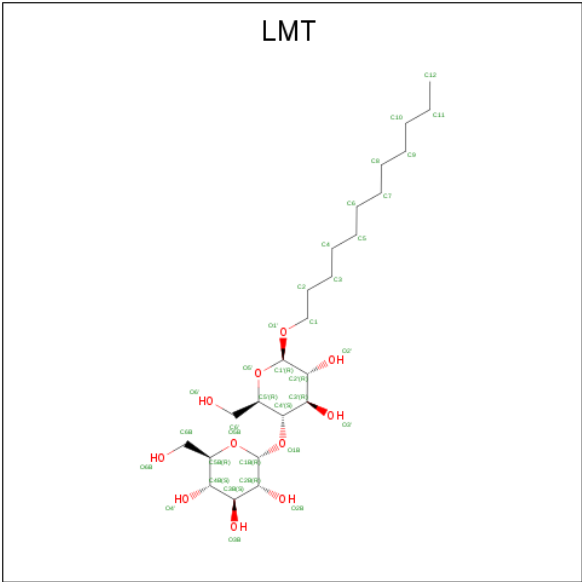
Chain	Residue	Modelled	Actual	Comment	Reference
A	1047	HIS	-	expression tag	UNP P52002
A	1048	HIS	-	expression tag	UNP P52002
A	1049	HIS	-	expression tag	UNP P52002
A	1050	HIS	-	expression tag	UNP P52002
A	1051	HIS	-	expression tag	UNP P52002
A	1052	HIS	-	expression tag	UNP P52002
B	1047	HIS	-	expression 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-MALTOSIDE (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...

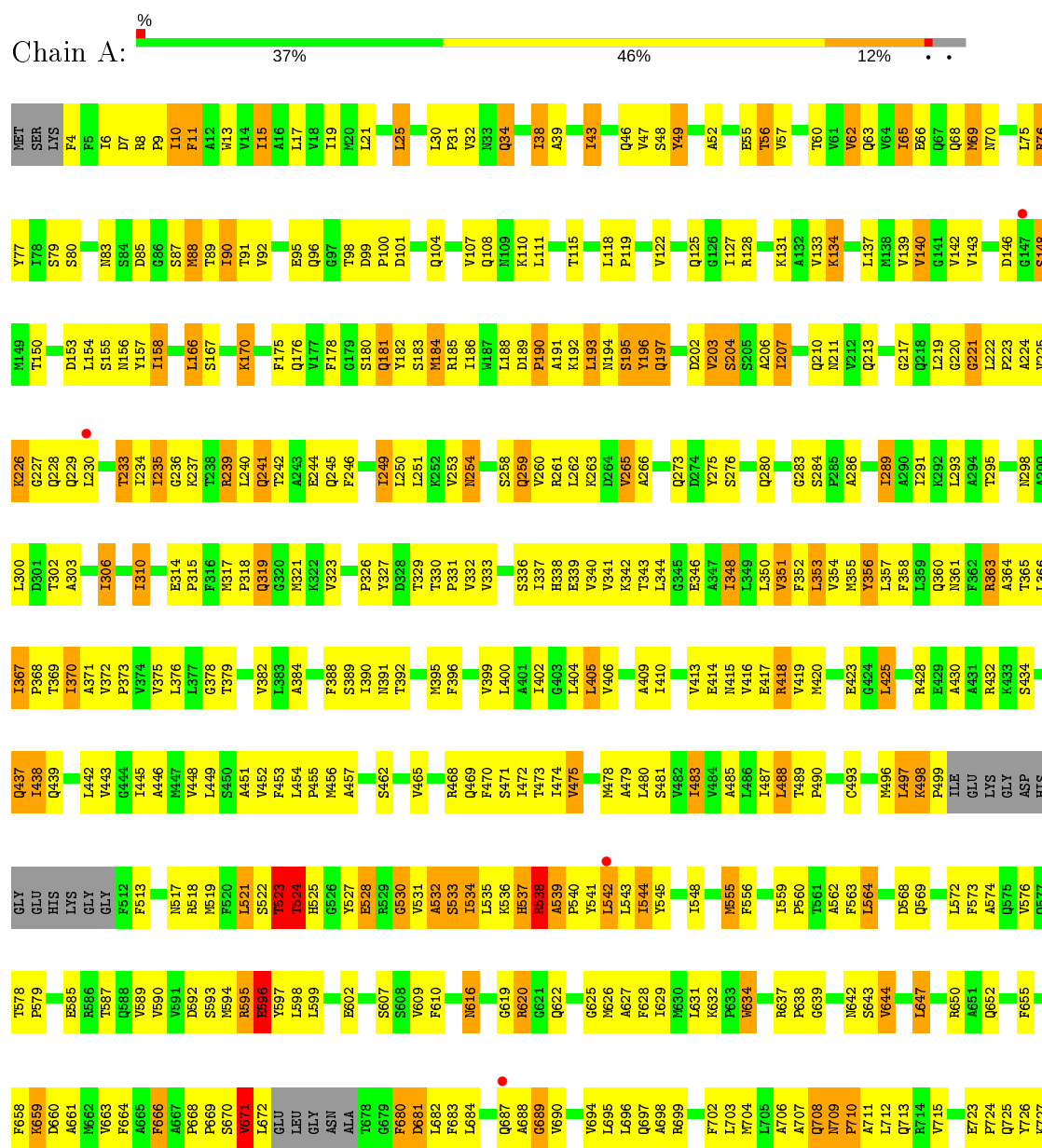
Continued from previous page...

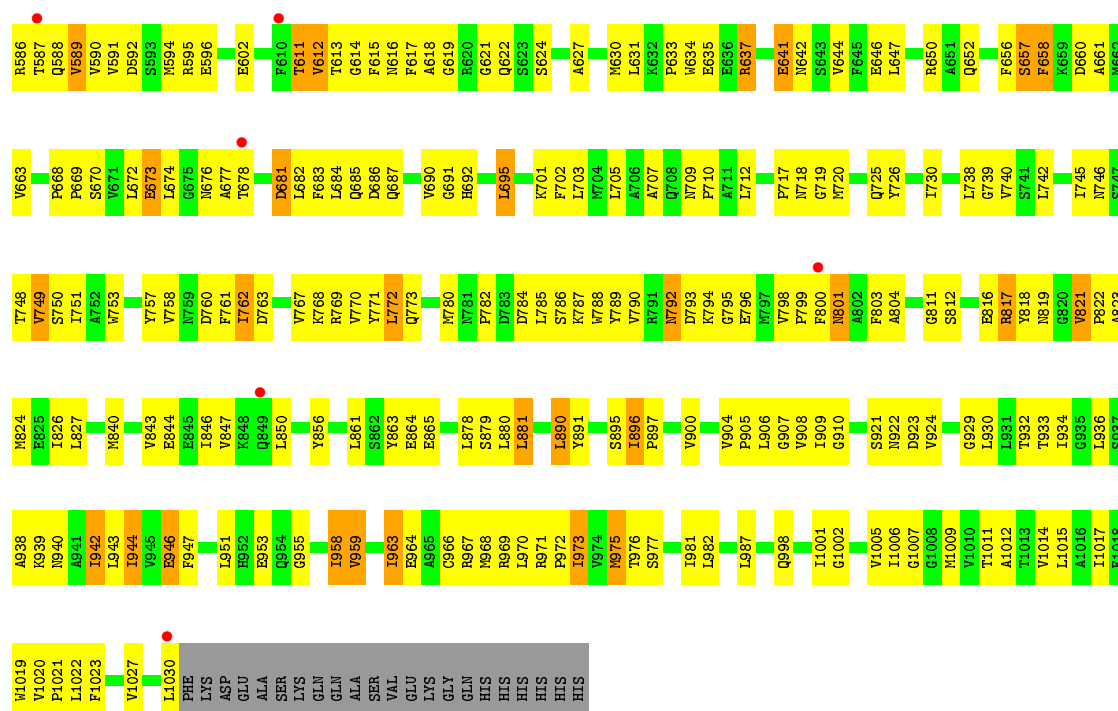
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		

3 Residue-property plots

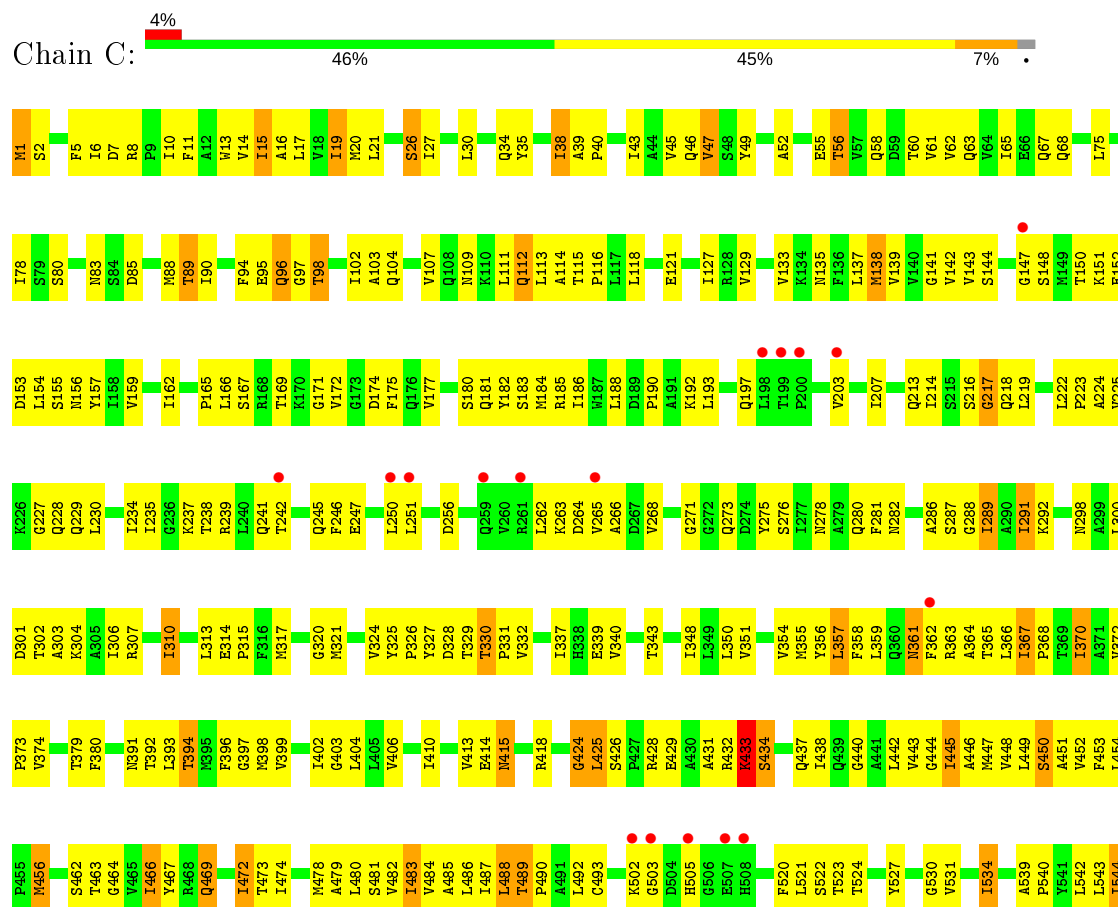
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

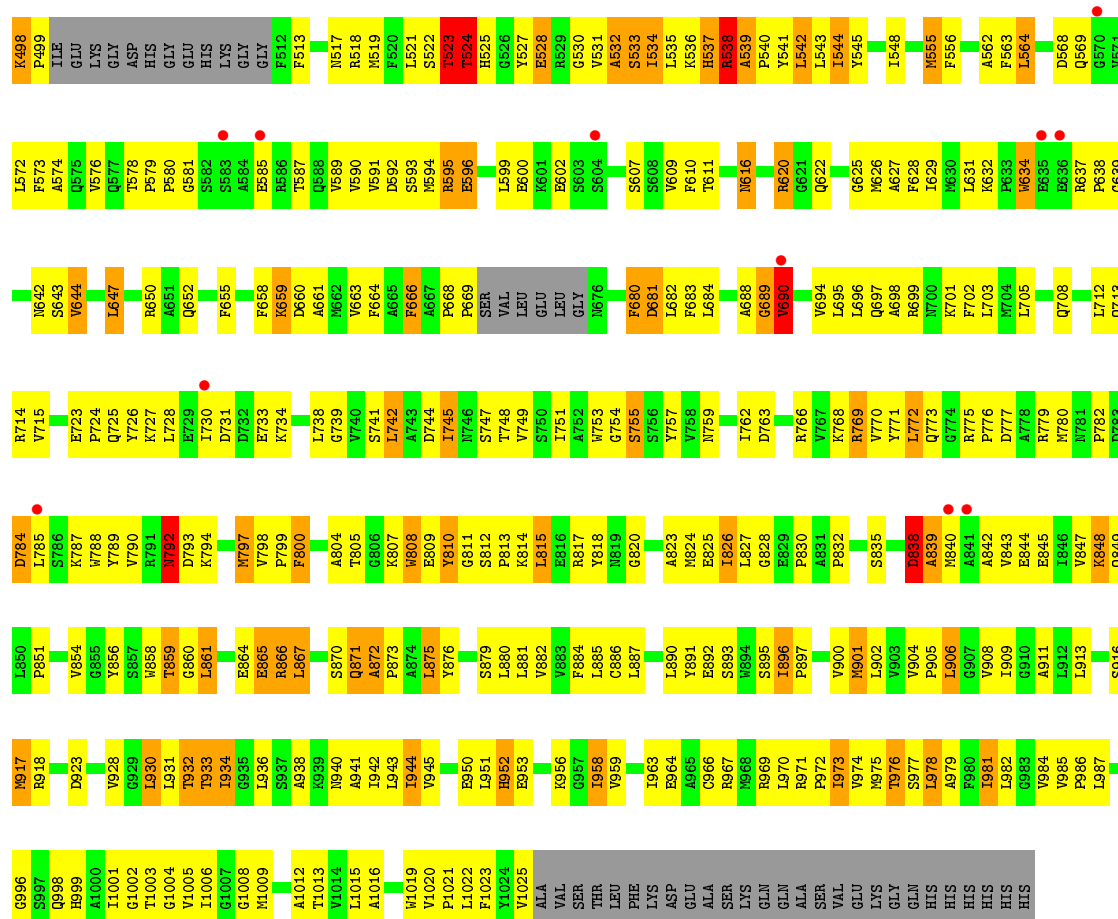




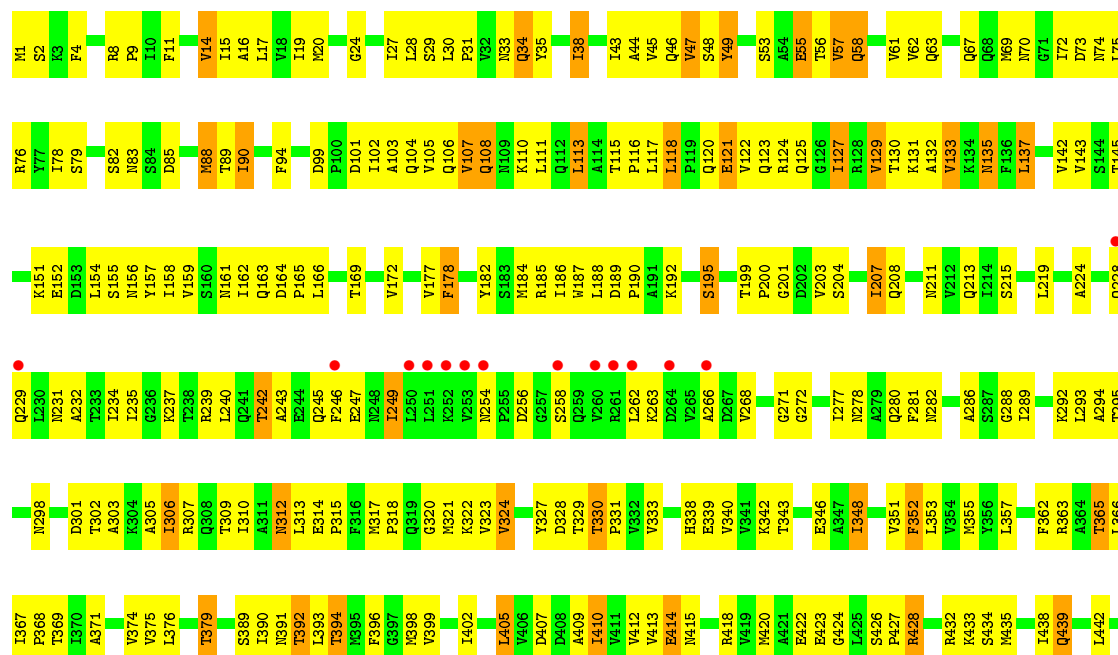
Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB

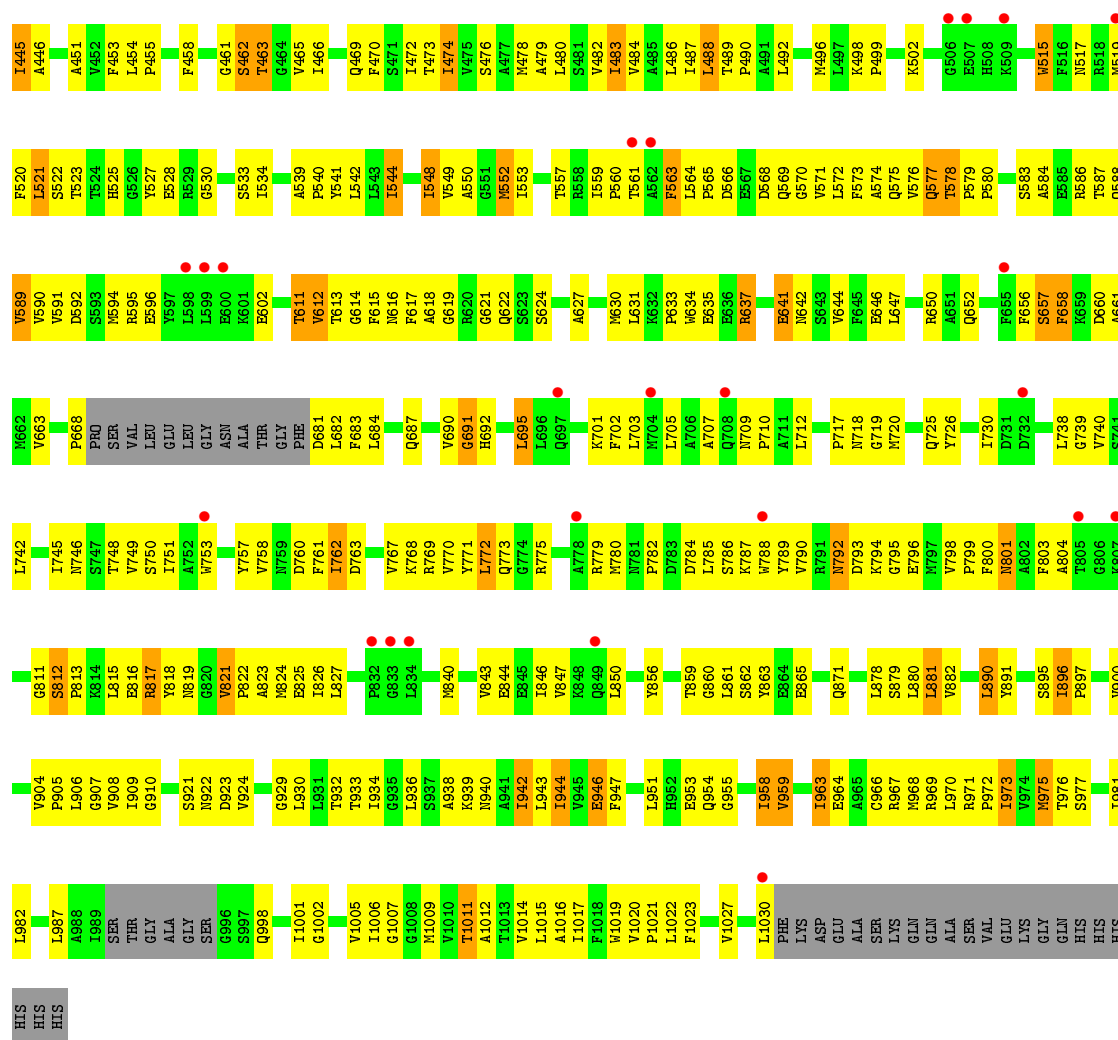




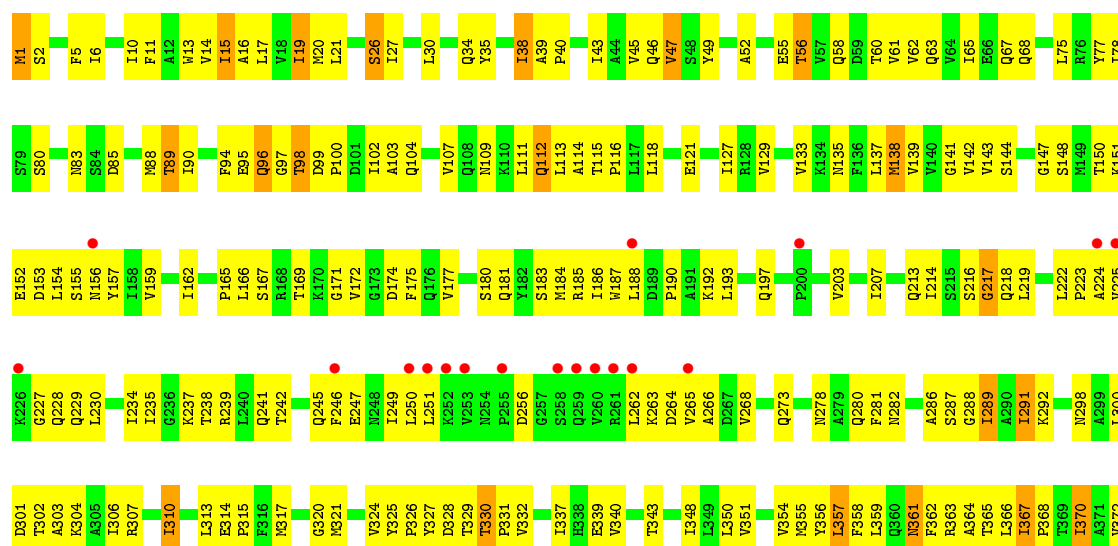


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB





• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXB



A1012	T1013	T932	I846	R766	L696	F617	Y545	P455	P373
V1014	I934	I933	V847	V767	Q897	S623	I548	M456	V374
A1016	I935	I934	G855	K768	R699	M626	V549	S462	T379
I1017	I936	I935	Y856	R769	F702	F628	A550	T463	F380
F1018	S937	I936	T859	V770	L703	I629	I553	G464	I831
I1019	A938	I937	G860	L772	M704	L705	M554	I466	T392
V1020	I939	I938	L867	Q773	A706	K632	F556	Y467	L393
F1021	I942	I941	A872	R779	M709	P633	T557	Q469	T394
P1022	I944	I943	P873	M780	P710	M634	I559	I472	M395
F1023	I945	I944	P873	D783	A711	P638	P560	T473	F396
T1029	I946	I945	A874	L785	L712	G639	T561	I474	G397
PHE	I958	I957	L875	D784	Q713	E640	A562	I474	M398
LYS	V959	I958	L876	L785	R714	E641	F563	I474	V999
ASP	I963	I962	A877	L785	R715	N642	L564	I474	I402
GLU	I964	I963	L878	L785	R716	S643	P565	I474	G403
ALA	E965	I964	L880	L785	P717	N644	D566	I474	L404
SER	A966	I965	L881	L785	P718	V644	E567	I474	L405
LYS	C966	I966	V882	L785	G719	F645	D568	I474	L406
GLN	R967	I967	V883	L785	M720	A648	I569	I474	D407
GLN	N968	I968	F884	L785	S721	Q652	I572	I474	D408
GLN	R969	I969	L885	L785	D722	Q652	F573	I474	A409
ALA	L970	I970	C886	L785	E723	F655	I574	I474	I410
SER	L971	I971	A889	L785	P724	F655	A574	I474	I411
VAL	R972	I972	V890	L785	Q725	F655	Q575	I474	V413
GLU	P973	I973	L890	L785	V726	F655	Q575	I474	E414
LYS	I974	I974	Y891	L785	F659	F659	Q575	I474	N415
GLY	N975	I975	E892	L785	D660	D660	Q575	I474	N415
GLN	T976	I976	I896	L785	E729	A661	Q575	I474	R418
HIS	S977	I977	P897	L785	I730	M662	P579	I474	G424
HIS	L978	I978	L896	L785	D731	A662	P580	I474	L425
HIS	A979	I979	P897	L785	D732	V663	S581	I474	S426
HIS	F980	I980	L902	L785	E733	F664	S582	I474	P427
HIS	I981	I981	V903	L785	K734	A665	S583	I474	R428
HIS	L982	I982	V904	L785	L738	F666	A584	I474	E429
G983	G983	I983	P905	L785	L742	A667	E585	I474	R433
V984	V984	I984	P813	L785	A743	P668	R586	I474	S434
V985	V985	I985	K814	L785	D744	P669	T587	I474	Q437
P986	P986	I986	G910	L785	I745	V671	Q588	I474	I438
I989	I989	I989	G911	L785	I746	L674	V591	I474	Q439
S990	S990	I990	L912	L785	S747	L674	R595	I474	G440
T991	T991	I991	T915	L785	T748	T678	I599	I474	A441
G992	G992	I992	T915	L785	V749	G679	L599	I474	L442
A993	A993	I993	E925	L785	S750	F680	E600	I474	V443
I998	I998	I998	I826	L785	I751	D681	R601	I474	G444
I1001	I1001	I1001	S921	L785	A752	L682	I601	I474	I445
G1002	G1002	I1002	P830	L785	W753	F683	S607	I474	A446
V1005	V1005	I1005	G837	L785	G754	Q687	S608	I474	A447
I1006	I1006	I1006	D838	L785	S755	Q687	V609	I474	M447
M1009	M1009	I1009	F925	L785	S756	V690	F610	I474	V448
V1010	V1010	I1010	A839	L785	Y757	V690	T611	I474	L449
T1011	T1011	I1011	Q927	L785	V758	G691	V612	I474	S450
			V928	L785	N759	H692	T613	I474	A451
			G929	L785	D760	E693	G614	I474	V452
			L930	L785	F761	V694	L543	I474	F453
			I931	L785	I762	L695	I616	I474	L454

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) 96.3 (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 0.241 , 0.284	Depositor DCC
R_{free} test set	3539 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 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:A:140:VAL:HG23	1:A:289:ILE:HG23	1.44	0.99
1:E:817:ARG:HG3	1:E:817:ARG:HH11	1.25	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:C:485:ALA:HA	1:C:489:THR:HG23	1.48	0.95
1:D:568:ASP:HB3	1:D:634:TRP:CZ3	2.00	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:C:577:GLN:HB3	1:C:662:MET:HB2	1.52	0.92
1:D:156:ASN:HD22	1:D:182:TYR:H	0.92	0.92
1:A:730:ILE:HD11	1:C:237:LYS:HD3	1.50	0.92
1:D:470:PHE:O	1:D:473:THR:HG22	1.70	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:PRO:HD2	1:A:321:MET:HE2	1.51	0.91
1:E:966:CYS:SG	1:E:1021:PRO:HG3	2.11	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:A:757:TYR:HE2	1:A:769:ARG:HB3	1.35	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: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:A:253:VAL:HG12	1:A:259:GLN:HB3	1.52	0.89
1:D:569:GLN:H	1:D:634:TRP:HH2	1.16	0.89
1:A:569:GLN:H	1:A:634:TRP:HH2	1.17	0.88
1:D:76:ARG:HG2	1:D:76:ARG:NH1	1.85	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: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:D:730:ILE:HD11	1:F:237:LYS:HD3	1.56	0.86
1:A:226:LYS:HD2	1:A:226:LYS:H	1.40	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: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:C:166:LEU:HD12	1:C:289:ILE:HD12	1.57	0.85
1:D:498:LYS:H	1:D:499:PRO:CD	1.88	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:A:706:ALA:HB2	1:A:846:ILE:HD13	1.59	0.84
1:B:247:GLU:HB3	1:B:263:LYS:HG2	1.57	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:B:520:PHE:HA	1:B:523:THR:HG22	1.61	0.83
1:F:166:LEU:HD12	1:F:289:ILE:HD12	1.60	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:A:540:PRO:O	1:A:544:ILE:HG22	1.79	0.82
1:B:568:ASP:HB3	1:B:634:TRP:HZ3	1.44	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:D:540:PRO:O	1:D:544:ILE:HG22	1.80	0.82
1:F:241:GLN:HG2	1:F:762:ILE:HG13	1.60	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:C:138:MET:HB2	1:C:328:ASP:HA	1.62	0.81
1:D:680:PHE:CE2	1:D:858:TRP:HZ3	1.96	0.81
1:A:808:TRP:CZ3	1:D:708:GLN:HB3	2.15	0.81
1:D:228:GLN:HE21	1:D:230:LEU:H	1.26	0.81
1:D:733:GLU:HG2	1:F:250:LEU:HD11	1.60	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:C:544:ILE:HG12	1:C:1019:TRP:HH2	1.44	0.81
1:D:699:ARG:NH2	1:D:824:MET:HG3	1.95	0.81
1:B:158:ILE:HD11	1:B:177:VAL:HG13	1.63	0.80
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.63	0.80
1:E:158:ILE:HD11	1:E:177:VAL:HG13	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:C:362:PHE:O	1:C:366:LEU:HB2	1.81	0.80
1:F:652:GLN:NE2	1:F:665:ALA:H	1.80	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:B:938:ALA:O	1:B:942:ILE:HG12	1.82	0.80
1:D:262:LEU:HD21	1:D:265:VAL:HB	1.64	0.80
1:E:213:GLN:HG3	1:E:239:ARG:HG3	1.62	0.80
1:F:544:ILE:HG12	1:F:1019:TRP:HH2	1.46	0.80
1:F:574:ALA:HB3	1:F:627:ALA:HB3	1.64	0.80
1:A:419:VAL:HG23	1:A:430:ALA:HB1	1.62	0.79
1:F:928:VAL:O	1:F:932:THR:HG22	1.82	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
2:A:2026:LMT:H6D	2:A:2026:LMT:H5B	1.62	0.79
1:E:938:ALA:O	1:E:942:ILE:HG12	1.82	0.79
1:C:652:GLN:NE2	1:C:665:ALA:H	1.79	0.79
2:E:2031:LMT:H6E	2:E:2031:LMT:H5B	1.65	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: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:D:634:TRP:H	1:D:634:TRP:HD1	1.31	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: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:76:ARG:HH11	1:D:76:ARG:CG	1.95	0.78
1:D:170:LYS:NZ	1:E:74:ASN:H	1.80	0.78
1:A:938:ALA:O	1:A:942:ILE:HG12	1.84	0.78
1:D:56:THR:HG22	1:F:213:GLN:HB3	1.65	0.78
1:A:800:PHE:HD2	1:A:804:ALA:HB2	1.48	0.78
1:B:158:ILE:HG22	1:B:162:ILE:HD11	1.64	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:E:969:ARG:O	1:E:972:PRO:HD2	1.84	0.78
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.48	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:D:234:ILE:HG22	1:E:726:TYR:HB3	1.65	0.77
1:E:367:ILE:HB	1:E:368:PRO:HD3	1.65	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:F:485:ALA:HA	1:F:489:THR:CG2	2.14	0.77
1:A:710:PRO:O	1:A:831:ALA:HB2	1.83	0.77
1:D:827:LEU:O	1:D:827:LEU:HD12	1.84	0.77
1:E:703:LEU:HD11	1:E:717:PRO:HG3	1.65	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:C:415:ASN:HD22	1:C:434:SER:HB3	1.49	0.76

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:VAL:HB	1:B:90:ILE:HG23	1.68	0.73
1:F:980:PHE:HD2	1:F:1009:MET:HG3	1.52	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:B:964:GLU:O	1:B:968:MET:HG3	1.88	0.73
1:C:434:SER:O	1:C:438:ILE:HG12	1.87	0.73
1:C:980:PHE:HD2	1:C:1009:MET:HG3	1.52	0.73
1:A:259:GLN:H	1:A:259:GLN:HE21	1.36	0.73
1:A:448:VAL:HG22	1:A:886:CYS:HB3	1.70	0.73
1:A:527:TYR:O	1:A:531:VAL:HG23	1.87	0.73
1:A:637:ARG:N	1:A:638:PRO:HD3	2.03	0.73
1:D:498:LYS:H	1:D:499:PRO:HD2	1.53	0.73
1:E:681:ASP:HB3	1:E:827:LEU:HD13	1.69	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:58:GLN:O	1:E:63:GLN:HG3	1.88	0.73
1:E:190:PRO:HG3	1:E:788:TRP:CZ2	2.24	0.73
1:D:319:GLN:H	1:D:319:GLN:CD	1.91	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:A:451:ALA:HB1	1:A:882:VAL:HG12	1.69	0.73
1:D:742:LEU:H	1:D:742:LEU:HD12	1.54	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:451:ALA:HB1	1:D:882:VAL:HG12	1.71	0.73
1:E:278:ASN:HB2	1:E:613:THR:HG22	1.70	0.73
1:B:451:ALA:O	1:B:879:SER:HB2	1.89	0.72
1:C:566:ASP:HB3	1:C:645:PHE:CZ	2.23	0.72
1:D:437:GLN:O	1:D:438:ILE:HG13	1.88	0.72
1:D:574:ALA:HB3	1:D:627:ALA:HB3	1.71	0.72
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:680:PHE:CE2	1:D:858:TRP:CZ3	2.77	0.72
1:B:676:ASN:HD21	1:B:827:LEU:HD12	1.52	0.72
1:C:548:ILE:HD11	1:C:906:LEU:HD23	1.69	0.72
1:A:708:GLN:HG3	1:D:807:LYS:HE2	1.72	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: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:291:ILE:HD12	1:C:306:ILE:HD12	1.72	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:A:213:GLN:HG3	1:B:56:THR:HG23	1.71	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:D:156:ASN:HA	1:D:181:GLN:HA	1.72	0.72
1:C:133:VAL:HG12	1:C:135:ASN:H	1.55	0.72
1:E:940:ASN:O	1:E:944:ILE:HG23	1.90	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
2:B:2031:LMT:O5B	2:B:2031:LMT:H6E	1.91	0.71
1:F:544:ILE:HG12	1:F:1019:TRP:CH2	2.24	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:572:LEU:HD23	1:C:573:PHE:H	1.55	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:A:918:ARG:HH21	1:A:1003:THR:HB	1.53	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: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: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:D:213:GLN:HG3	1:E:56:THR:HG23	1.71	0.71
1:E:847:VAL:HG11	1:E:856:TYR:CD1	2.26	0.71
1:E:414:GLU:HG2	1:E:972:PRO:HG3	1.73	0.71
1:F:133:VAL:HG12	1:F:135:ASN:H	1.56	0.71
1:F:291:ILE:HD12	1:F:306:ILE:HD12	1.73	0.71
1:C:578:THR:HG22	1:C:623:SER:HB2	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:985:VAL:HG23	1:C:986:PRO:HD3	1.73	0.70
1:D:723:GLU:HG3	1:D:813:PRO:HG3	1.72	0.70
1:F:364:ALA:O	1:F:367:ILE:HG12	1.91	0.70
1:F:399:VAL:O	1:F:402:ILE:HG13	1.91	0.70
1:E:682:LEU:HD11	1:E:856:TYR:HB2	1.72	0.70
1:E:821:VAL:HG12	1:E:822:PRO:HD2	1.73	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:233:THR:HG23	1:B:725:GLN:HG2	1.72	0.70
1:A:532:ALA:O	1:A:534:ILE:N	2.25	0.70
1:A:671:VAL:HG13	1:A:672:LEU:H	1.57	0.70
1:A:535:LEU:CD2	1:A:959:VAL:HG13	2.21	0.70
1:C:542:LEU:HD21	1:C:1022:LEU:HD21	1.72	0.70
1:B:215:SER:HB2	1:C:750:SER:HB2	1.73	0.70
1:D:32:VAL:HG11	1:D:337:ILE:HD13	1.74	0.70
1:E:987:LEU:HD22	1:E:998:GLN:HB3	1.74	0.70
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.73	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:E:142:VAL:HG11	1:E:158:ILE:HG21	1.74	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:4:PHE:O	1:B:8:ARG:HG3	1.92	0.70
1:B:560:PRO:HB2	1:B:921:SER:CB	2.22	0.70
1:C:47:VAL:HB	1:C:127:ILE:HG23	1.74	0.70
1:C:580:PRO:HB3	1:C:723:GLU:HG2	1.72	0.70
1:D:535:LEU:CD2	1:D:959:VAL:HG13	2.22	0.70
1:F:572:LEU:HD23	1:F:573:PHE:H	1.57	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:B:987:LEU:HD22	1:B:998:GLN:HB3	1.74	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:F:472:ILE:HD13	1:F:472:ILE:N	2.07	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:D:780:MET:HE3	1:F:224:ALA:HA	1.73	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:VAL:HG12	1:F:88:MET:HE3	1.74	0.69
1:A:32:VAL:HG11	1:A:337:ILE:HD13	1.75	0.69
1:E:38:ILE:O	1:E:462:SER:HB3	1.93	0.69
1:A:574:ALA:HB3	1:A:627:ALA:HB3	1.75	0.69
1:A:928:VAL:O	1:A:932:THR:HG23	1.91	0.69
2:B:2033:LMT:H122	2:B:2033:LMT:H62	1.73	0.69
1:B:402:ILE:HA	1:B:405:LEU:HB2	1.74	0.69
1:D:224:ALA:HB1	1:E:780:MET:HE1	1.73	0.69
1:A:545:TYR:HB2	1:A:1019:TRP:CZ3	2.28	0.69
1:D:724:PRO:HA	1:D:810:TYR:HB2	1.75	0.69
1:D:684:LEU:O	1:D:823:ALA:HB1	1.93	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:E:971:ARG:HB3	1:E:972:PRO:HD3	1.75	0.69
1:F:910:GLY:HA3	1:F:1011:THR:CG2	2.23	0.69
1:A:568:ASP:HB3	1:A:634:TRP:HZ3	1.55	0.69
1:C:910:GLY:HA3	1:C:1011:THR:CG2	2.22	0.69
1:D:568:ASP:HB3	1:D:634:TRP:HZ3	1.54	0.69
1:E:402:ILE:HA	1:E:405:LEU:HB2	1.75	0.69
1:C:561:THR:HG23	1:C:837:GLY:HA3	1.75	0.69
1:E:4:PHE:O	1:E:8:ARG:HG3	1.92	0.69
1:E:560:PRO:HB2	1:E:921:SER:CB	2.21	0.69
1:E:742:LEU:O	1:E:745:ILE:HG22	1.92	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:680:PHE:HE2	1:D:858:TRP:CZ3	2.09	0.69
1:D:194:ASN:ND2	1:D:797:MET:HG2	2.08	0.69
2:E:2032:LMT:H5B	2:E:2032:LMT:H6D	1.75	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:A:724:PRO:HA	1:A:810:TYR:HB2	1.73	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:B:414:GLU:HG2	1:B:972:PRO:HG3	1.74	0.68
1:C:472:ILE:N	1:C:472:ILE:HD13	2.09	0.68
1:C:830:PRO:HB3	1:C:839:ALA:HB2	1.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:818:TYR:HH	1:F:825:GLU:HB2	1.59	0.68
1:F:830:PRO:HB3	1:F:839:ALA:HB2	1.74	0.68
1:C:1016:ALA:O	1:C:1020:VAL:HG23	1.94	0.68
1:E:442:LEU:CD2	1:E:445:ILE:HD11	2.22	0.68
1:E:817:ARG:HG3	1:E:817:ARG:NH1	2.01	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:A:280:GLN:HB2	1:A:284:SER:O	1.94	0.68
1:D:538:ARG:HA	1:D:541:TYR:HD1	1.58	0.68
1:E:929:GLY:O	1:E:932:THR:HG22	1.92	0.68
1:F:138:MET:SD	1:F:291:ILE:HD11	2.33	0.68
1:F:682:LEU:HD11	1:F:843:VAL:HG11	1.75	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
2:B:2031:LMT:H6E	2:B:2031:LMT:C5B	2.23	0.68
1:C:545:TYR:HB2	1:C:1019:TRP:CZ3	2.29	0.68
1:B:959:VAL:O	1:B:963:ILE:HG22	1.94	0.68
1:A:47:VAL:HG22	1:A:48:SER:H	1.59	0.68
1:D:545:TYR:HB2	1:D:1019:TRP:CZ3	2.28	0.68
1:E:47:VAL:HG13	1:E:127:ILE:HA	1.75	0.68
1:E:637:ARG:HB2	1:E:642:ASN:HB3	1.76	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:A:254:ASN:ND2	1:A:258:SER:HB3	2.08	0.67
1:A:300:LEU:HD21	1:A:333:VAL:HB	1.76	0.67
1:A:838:ASP:HA	1:A:842:ALA:HB3	1.77	0.67
1:B:158:ILE:HA	1:B:162:ILE:HG12	1.75	0.67
1:B:228:GLN:HG2	1:C:583:SER:HB2	1.75	0.67
1:F:1016:ALA:O	1:F:1020:VAL:HG23	1.94	0.67
1:A:156:ASN:HD21	1:A:768:LYS:NZ	1.91	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: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: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:B:88:MET:HG2	1:B:89:THR:N	2.10	0.67
1:E:959:VAL:O	1:E:963:ILE:HG22	1.94	0.67
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.59	0.67
1:F:367:ILE:HG12	1:F:368:PRO:HD3	1.77	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:169:THR:HG21	1:E:309:THR:OG1	1.95	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:C:554:TRP:O	1:C:557:THR:HG22	1.94	0.67
1:E:186:ILE:HG22	1:E:268:VAL:HG22	1.77	0.67
1:F:545:TYR:HB2	1:F:1019:TRP:CZ3	2.30	0.67
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.59	0.67
1:B:602:GLU:HG3	1:B:650:ARG:NH1	2.10	0.67
1:D:753:TRP:CZ3	1:D:779:ARG:HB3	2.29	0.67
1:A:808:TRP:O	1:D:705:LEU:HD22	1.95	0.67
1:D:523:THR:OG1	1:D:524:THR:N	2.28	0.67
1:A:845:GLU:O	1:A:848:LYS:HB3	1.95	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: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:E:35:TYR:CE1	1:E:392:THR:HG21	2.29	0.66
1:F:959:VAL:O	1:F:963:ILE:HG23	1.93	0.66
1:A:791:ARG:HB2	1:A:797:MET:HE2	1.77	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: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:B:14:VAL:HG11	1:C:889:ALA:HB2	1.77	0.66
1:B:472:ILE:HD11	2:B:2031:LMT:H61	1.78	0.66
1:C:648:ALA:HB1	1:C:714:ARG:HH12	1.61	0.66
1:C:218:GLN:HA	1:C:234:ILE:HG23	1.75	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: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:B:442:LEU:CD2	1:B:445:ILE:HD11	2.25	0.66
1:C:96:GLN:NE2	1:C:462:SER:HB3	2.10	0.66
1:D:400:LEU:HD12	1:D:470:PHE:HZ	1.60	0.66
1:B:72:ILE:HD11	1:B:75:LEU:HD13	1.76	0.66
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:695:LEU:CD1	1:D:699:ARG:HH21	2.08	0.66
1:F:339:GLU:O	1:F:343:THR:HG22	1.95	0.66
1:F:891:TYR:CB	1:F:896:ILE:HD11	2.26	0.66
1:A:254:ASN:HD21	1:A:258:SER:HB3	1.60	0.66
2:D:2026:LMT:H6D	2:D:2026:LMT:O5B	1.96	0.66
1:A:810:TYR:OH	1:D:701:LYS:HG2	1.96	0.66
1:A:710:PRO:HD3	1:D:807:LYS:HE3	1.77	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:B:637:ARG:HB2	1:B:642:ASN:HB3	1.77	0.65
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:C:15:ILE:O	1:C:19:ILE:HG23	1.96	0.65
1:E:712:LEU:HD21	1:E:843:VAL:HG23	1.77	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: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
1:D:941:ALA:O	1:D:945:VAL:HG12	1.97	0.65
1:A:213:GLN:HE21	1:A:239:ARG:HG2	1.61	0.65
1:A:563:PHE:O	1:A:564:LEU:HB2	1.97	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
2:E:2033:LMT:H111	2:E:2033:LMT:H71	1.78	0.65
1:A:808:TRP:CH2	1:D:708:GLN:HB3	2.31	0.65
1:C:247:GLU:HB3	1:C:263:LYS:HG2	1.79	0.65
1:C:80:SER:OG	1:C:817:ARG:HB2	1.96	0.65
1:C:447:MET:CE	1:C:886:CYS:HB3	2.26	0.65
1:D:908:VAL:O	1:D:911:ALA:HB3	1.96	0.65
1:E:328:ASP:OD1	1:E:330:THR:HG23	1.95	0.65
1:F:80:SER:OG	1:F:817:ARG:HB2	1.96	0.65
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.78	0.65
1:A:134:LYS:HD3	1:A:672:LEU:HD12	1.78	0.65
1:C:1011:THR:O	1:C:1015:LEU:HB2	1.97	0.65
1:C:488:LEU:HD13	1:C:492:LEU:HD11	1.77	0.65
1:D:2:SER:O	1:D:6:ILE:HD12	1.96	0.65
1:D:753:TRP:HZ3	1:D:779:ARG:HB3	1.62	0.65
1:C:444:GLY:O	1:C:448:VAL:HG23	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HG22	1:C:939:LYS:HG2	1.78	0.65
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:A:695:LEU:CD1	1:A:699:ARG:HH21	2.09	0.65
1:D:241:GLN:HG3	1:D:762:ILE:O	1.96	0.65
1:F:683:PHE:O	1:F:856:TYR:HA	1.97	0.65
1:C:959:VAL:O	1:C:963:ILE:HG23	1.97	0.65
1:E:602:GLU:HG3	1:E:650:ARG:NH1	2.11	0.65
1:D:329:THR:O	1:D:332:VAL:HG12	1.97	0.65
1:A:302:THR:O	1:A:306:ILE:HG23	1.97	0.64
1:A:969:ARG:O	1:A:973:ILE:HG12	1.97	0.64
1:B:125:GLN:HE22	1:B:769:ARG:NH1	1.94	0.64
1:B:391:ASN:HD22	1:B:393:LEU:H	1.45	0.64
1:B:718:ASN:HB2	1:B:827:LEU:HD23	1.79	0.64
1:C:966:CYS:SG	1:C:1021:PRO:HG3	2.36	0.64
1:C:339:GLU:O	1:C:343:THR:HG22	1.96	0.64
1:D:996:GLY:N	1:D:999:HIS:HD2	1.95	0.64
1:F:648:ALA:HB1	1:F:714:ARG:HH12	1.63	0.64
1:E:215:SER:HB2	1:F:750:SER:HB2	1.80	0.64
1:B:478:MET:O	1:B:482:VAL:HG23	1.97	0.64
1:E:757:TYR:CE1	1:E:769:ARG:HG3	2.32	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: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:C:332:VAL:HG11	1:C:569:GLN:HG2	1.80	0.64
1:D:302:THR:O	1:D:306:ILE:HG23	1.97	0.64
1:D:376:LEU:O	1:D:379:THR:HG22	1.97	0.64
1:F:910:GLY:HA3	1:F:1011:THR:HG21	1.79	0.64
1:C:251:LEU:HD12	1:C:265:VAL:HG21	1.80	0.64
1:E:718:ASN:HB2	1:E:827:LEU:HD23	1.78	0.64
1:A:43:ILE:HG21	1:A:107:VAL:HG11	1.80	0.64
1:A:48:SER:O	1:A:125:GLN:HG2	1.98	0.64
1:B:757:TYR:CE1	1:B:769:ARG:HG3	2.33	0.64
1:C:699:ARG:NE	1:C:824:MET:HG2	2.13	0.64
1:F:683:PHE:CE2	1:F:818:TYR:CZ	2.86	0.64
1:C:818:TYR:HH	1:C:825:GLU:HB2	1.62	0.64
1:C:910:GLY:HA3	1:C:1011:THR:HG21	1.78	0.64
1:F:472:ILE:H	1:F:472:ILE:CD1	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:LEU:HD13	1:F:492:LEU:HD11	1.79	0.64
1:A:342:LYS:O	1:A:346:GLU:HG3	1.97	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:C:43:ILE:HD11	1:C:107:VAL:HB	1.78	0.64
1:D:48:SER:O	1:D:125:GLN:HG2	1.97	0.64
1:E:72:ILE:HD11	1:E:75:LEU:HD13	1.80	0.64
1:E:753:TRP:CZ2	1:E:785:LEU:HG	2.32	0.64
1:A:241:GLN:HG3	1:A:762:ILE:O	1.97	0.64
1:A:669:PRO:HB2	1:A:671:VAL:HG12	1.79	0.64
1:C:903:VAL:HG21	1:C:1020:VAL:HG22	1.80	0.64
1:C:891:TYR:CB	1:C:896:ILE:HD11	2.27	0.64
1:D:780:MET:SD	1:F:228:GLN:HG3	2.37	0.64
1:E:104:GLN:NE2	1:E:131:LYS:HE2	2.12	0.64
1:F:818:TYR:OH	1:F:825:GLU:HB2	1.97	0.64
1:C:818:TYR:OH	1:C:825:GLU:HB2	1.98	0.63
1:C:969:ARG:O	1:C:972:PRO:HD2	1.98	0.63
1:D:602:GLU:HG3	1:D:647:LEU:HD21	1.80	0.63
1:B:386:PHE:CE2	2:B:2031:LMT:H81	2.33	0.63
1:B:971:ARG:HB3	1:B:972:PRO:HD3	1.78	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:F:896:ILE:HB	1:F:945:VAL:HG11	1.80	0.63
1:A:941:ALA:O	1:A:945:VAL:HG12	1.97	0.63
1:C:683:PHE:CE2	1:C:818:TYR:CZ	2.86	0.63
1:E:895:SER:C	1:E:897:PRO:HD2	2.19	0.63
1:E:971:ARG:O	1:E:975:MET:HG2	1.98	0.63
1:A:523:THR:OG1	1:A:524:THR:N	2.28	0.63
1:B:164:ASP:HB2	1:C:67:GLN:NE2	2.12	0.63
1:D:247:GLU:HA	1:D:262:LEU:O	1.98	0.63
1:D:895:SER:C	1:D:897:PRO:HD2	2.18	0.63
1:E:14:VAL:HG11	1:F:889:ALA:HB2	1.81	0.63
1:F:213:GLN:HE21	1:F:239:ARG:HB2	1.64	0.63
1:F:447:MET:HE3	1:F:886:CYS:HB3	1.80	0.63
1:D:43:ILE:HG21	1:D:107:VAL:HG11	1.79	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:A:193:LEU:CD2	1:A:265:VAL:HG13	2.29	0.63
1:B:104:GLN:NE2	1:B:131:LYS:HE2	2.13	0.63
1:B:718:ASN:HB2	1:B:827:LEU:CD2	2.28	0.63
1:E:466:ILE:HD11	1:E:924:VAL:HG21	1.81	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:F:969:ARG:O	1:F:972:PRO:HD2	1.99	0.63
1:B:541:TYR:HA	1:B:544:ILE:HG23	1.80	0.63
1:F:699:ARG:NE	1:F:824:MET:HG2	2.14	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:F:218:GLN:HA	1:F:234:ILE:HG23	1.80	0.63
1:A:680:PHE:CD1	1:A:828:GLY:O	2.47	0.63
1:B:527:TYR:CE2	1:B:966:CYS:HB3	2.33	0.63
1:C:361:ASN:O	1:C:365:THR:HG22	1.99	0.63
1:F:15:ILE:O	1:F:19:ILE:HG23	1.99	0.63
1:E:229:GLN:HA	1:F:583:SER:HB3	1.80	0.63
1:A:188:LEU:HD23	1:A:266:ALA:HB2	1.81	0.62
1:A:319:GLN:H	1:A:319:GLN:CD	2.03	0.62
1:C:372:VAL:HB	1:C:373:PRO:HD3	1.81	0.62
1:D:342:LYS:O	1:D:346:GLU:HG3	1.99	0.62
1:D:528:GLU:OE2	1:D:967:ARG:CZ	2.47	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:E:49:TYR:CE1	1:E:121:GLU:HG3	2.34	0.62
1:A:892:GLU:C	1:C:10:ILE:HD11	2.19	0.62
1:D:156:ASN:HD21	1:D:768:LYS:NZ	1.96	0.62
1:E:478:MET:O	1:E:482:VAL:HG23	1.99	0.62
1:A:996:GLY:N	1:A:999:HIS:HD2	1.97	0.62
1:B:424:GLY:HA3	1:B:502:LYS:HG2	1.81	0.62
1:C:896:ILE:HB	1:C:945:VAL:HG11	1.81	0.62
1:C:969:ARG:O	1:C:973:ILE:HG23	1.98	0.62
1:D:789:TYR:CE2	1:D:799:PRO:HG3	2.34	0.62
1:E:541:TYR:HA	1:E:544:ILE:HG23	1.81	0.62
1:F:1011:THR:O	1:F:1015:LEU:HB2	2.00	0.62
1:F:359:LEU:HD12	1:F:365:THR:HA	1.81	0.62
1:A:417:GLU:HA	1:A:420:MET:HE3	1.80	0.62
1:A:753:TRP:HZ3	1:A:779:ARG:HB3	1.63	0.62
1:B:847:VAL:HG13	1:B:850:LEU:HD12	1.82	0.62
1:C:43:ILE:HD11	1:C:107:VAL:CB	2.29	0.62
1:C:213:GLN:HE21	1:C:239:ARG:HB2	1.64	0.62
1:C:472:ILE:H	1:C:472:ILE:CD1	2.13	0.62
1:E:520:PHE:HA	1:E:523:THR:CG2	2.29	0.62
1:F:682:LEU:O	1:F:683:PHE:CD2	2.53	0.62
1:A:176:GLN:HE21	1:A:178:PHE:HE1	1.48	0.62
1:A:519:MET:O	1:A:523:THR:HG23	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:TYR:CE2	1:A:799:PRO:HG3	2.33	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
1:E:718:ASN:HB2	1:E:827:LEU:CD2	2.28	0.62
1:F:903:VAL:HG21	1:F:1020:VAL:HG22	1.82	0.62
1:F:63:GLN:HE22	1:F:67:GLN:HE21	1.48	0.62
1:A:985:VAL:HA	1:A:1006:ILE:HD11	1.81	0.62
1:A:365:THR:O	1:A:369:THR:HG23	2.00	0.62
1:B:303:ALA:CB	1:B:330:THR:HG21	2.30	0.62
1:C:944:ILE:HG13	1:C:945:VAL:N	2.13	0.62
1:A:355:MET:HG3	1:A:365:THR:HG23	1.82	0.62
1:B:390:ILE:HA	1:B:394:THR:HG21	1.81	0.62
1:C:63:GLN:HE22	1:C:67:GLN:HE21	1.47	0.62
1:E:391:ASN:HD22	1:E:393:LEU:H	1.48	0.62
1:F:738:LEU:HD12	1:F:803:PHE:CZ	2.35	0.62
1:B:47:VAL:H	1:B:88:MET:HE2	1.65	0.62
1:D:367:ILE:HD11	1:D:413:VAL:HG22	1.82	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:B:49:TYR:CE1	1:B:121:GLU:HG3	2.34	0.61
1:C:572:LEU:HD23	1:C:573:PHE:N	2.15	0.61
1:C:742:LEU:HB3	1:C:746:ASN:HD21	1.64	0.61
1:D:906:LEU:HD23	1:D:906:LEU:H	1.64	0.61
1:E:303:ALA:CB	1:E:330:THR:HG21	2.30	0.61
1:E:469:GLN:O	1:E:473:THR:HG22	2.00	0.61
1:A:329:THR:O	1:A:332:VAL:HG12	1.98	0.61
1:B:616:ASN:HB3	1:B:618:ALA:H	1.64	0.61
1:B:410:ILE:CD1	1:B:976:THR:HG22	2.25	0.61
1:D:535:LEU:HD23	1:D:959:VAL:HG13	1.82	0.61
1:F:742:LEU:HB3	1:F:746:ASN:HD21	1.65	0.61
1:F:738:LEU:HD12	1:F:803:PHE:HZ	1.64	0.61
1:F:47:VAL:HG12	1:F:88:MET:CE	2.30	0.61
1:A:622:GLN:HE21	1:C:222:LEU:HG	1.66	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:D:417:GLU:HA	1:D:420:MET:HE3	1.82	0.61
1:E:424:GLY:HA3	1:E:502:LYS:HG2	1.81	0.61
1:F:251:LEU:HD12	1:F:265:VAL:HG21	1.80	0.61
1:F:281:PHE:CE2	1:F:324:VAL:HG11	2.35	0.61
1:A:428:ARG:HH12	1:A:432:ARG:HE	1.48	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:D:2:SER:O	1:D:6:ILE:CD1	2.49	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:A:528:GLU:OE2	1:A:967:ARG:CZ	2.48	0.61
1:A:538:ARG:O	1:A:539:ALA:CB	2.49	0.61
1:B:589:VAL:HA	1:B:592:ASP:HB2	1.82	0.61
1:C:10:ILE:HA	1:C:13:TRP:HB2	1.83	0.61
1:C:544:ILE:O	1:C:548:ILE:HG23	2.01	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:D:188:LEU:HD23	1:D:266:ALA:HB2	1.81	0.61
1:D:428:ARG:HH12	1:D:432:ARG:HE	1.47	0.61
1:E:847:VAL:HG13	1:E:850:LEU:HD12	1.82	0.61
1:F:652:GLN:HG3	1:F:714:ARG:HD2	1.82	0.61
1:B:958:ILE:N	1:B:958:ILE:HD13	2.15	0.61
1:D:337:ILE:HG13	1:D:338:HIS:N	2.16	0.61
1:D:365:THR:O	1:D:369:THR:HG23	2.00	0.61
1:D:280:GLN:HG2	1:D:595:ARG:HH21	1.65	0.61
1:D:156:ASN:HD21	1:D:768:LYS:HZ1	1.46	0.61
1:E:414:GLU:CG	1:E:972:PRO:HG3	2.31	0.61
1:F:43:ILE:HD11	1:F:107:VAL:CB	2.31	0.61
1:A:451:ALA:HB1	1:A:882:VAL:CG1	2.29	0.61
1:B:453:PHE:CE2	1:B:474:ILE:HD11	2.35	0.61
1:A:780:MET:HE3	1:C:224:ALA:HA	1.82	0.61
1:C:359:LEU:HD12	1:C:365:THR:HA	1.82	0.61
1:C:738:LEU:HD12	1:C:803:PHE:HZ	1.65	0.61
1:C:910:GLY:H	1:C:1011:THR:HG21	1.66	0.61
1:E:958:ILE:N	1:E:958:ILE:HD13	2.16	0.61
1:A:337:ILE:HG13	1:A:338:HIS:N	2.15	0.61
1:A:538:ARG:CB	1:A:1022:LEU:HD21	2.30	0.61
1:C:115:THR:HB	1:C:116:PRO:HD3	1.83	0.61
1:C:738:LEU:HD12	1:C:803:PHE:CZ	2.36	0.61
1:C:445:ILE:CG2	1:C:939:LYS:HG2	2.30	0.61
1:D:749:VAL:HG13	1:D:753:TRP:HD1	1.66	0.61
1:E:38:ILE:HA	1:E:465:VAL:HG11	1.82	0.61
1:A:119:PRO:O	1:A:122:VAL:HG12	2.01	0.61
1:A:30:LEU:HD21	1:A:384:ALA:HA	1.82	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

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:D:780:MET:CE	1:F:224:ALA:HA	2.30	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: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: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:C:652:GLN:HG3	1:C:714:ARG:HD2	1.83	0.60
1:D:1016:ALA:O	1:D:1020:VAL:HG23	2.01	0.60
1:D:451:ALA:HB1	1:D:882:VAL:CG1	2.31	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:D:622:GLN:HE21	1:F:222:LEU:HG	1.66	0.60
1:A:83:ASN:ND2	1:A:620:ARG:HG2	2.16	0.60
1:B:745:ILE:O	1:B:748:THR:HG22	2.01	0.60
1:C:111:LEU:C	1:C:113:LEU:H	2.04	0.60
1:C:166:LEU:O	1:C:169:THR:HG22	2.01	0.60
1:E:414:GLU:CD	1:E:972:PRO:HG3	2.21	0.60
1:F:573:PHE:HE2	1:F:668:PRO:HG3	1.64	0.60
1:A:13:TRP:NE1	2:A:2026:LMT:H11	2.16	0.60
1:A:166:LEU:HG	1:A:291:ILE:HD11	1.84	0.60
1:A:521:LEU:O	1:A:521:LEU:HD13	2.01	0.60
1:A:537:HIS:O	1:A:538:ARG:O	2.19	0.60
1:A:280:GLN:HG2	1:A:595:ARG:HH21	1.65	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:D:569:GLN:N	1:D:634:TRP:CH2	2.68	0.60
1:E:115:THR:HB	1:E:116:PRO:HD3	1.82	0.60
1:A:749:VAL:HG13	1:A:753:TRP:HD1	1.67	0.60
1:A:906:LEU:HD23	1:A:906:LEU:H	1.64	0.60
1:C:281:PHE:CE2	1:C:324:VAL:HG11	2.36	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:D:83:ASN:ND2	1:D:620:ARG:HG2	2.16	0.60
1:E:1020:VAL:HB	1:E:1021:PRO:HD3	1.82	0.60
1:E:47:VAL:H	1:E:88:MET:HE2	1.66	0.60
1:E:410:ILE:CD1	1:E:976:THR:HG22	2.25	0.60
1:A:753:TRP:CZ2	1:A:785:LEU:HG	2.36	0.60
1:A:791:ARG:HB2	1:A:797:MET:CE	2.30	0.60
1:B:1020:VAL:HB	1:B:1021:PRO:HD3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:GLU:CG	1:B:972:PRO:HG3	2.31	0.60
1:C:906:LEU:HD22	1:C:1015:LEU:HD12	1.83	0.60
1:A:541:TYR:HA	1:A:544:ILE:CG2	2.32	0.60
1:A:706:ALA:CB	1:A:846:ILE:HD13	2.30	0.60
1:A:875:LEU:C	1:A:875:LEU:HD12	2.21	0.60
1:A:7:ASP:O	1:A:9:PRO:HD3	2.01	0.60
1:D:472:ILE:HA	1:D:475:VAL:HG13	1.84	0.60
1:D:880:LEU:HD11	1:D:904:VAL:HG21	1.84	0.60
1:E:156:ASN:HD21	1:E:768:LYS:NZ	2.00	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:F:683:PHE:CZ	1:F:818:TYR:CE2	2.90	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: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:B:591:VAL:HA	1:B:594:MET:HG3	1.83	0.60
1:D:780:MET:HE3	1:F:225:VAL:H	1.66	0.60
1:D:7:ASP:O	1:D:9:PRO:HD3	2.02	0.60
1:F:906:LEU:HD22	1:F:1015:LEU:HD12	1.82	0.60
1:D:65:ILE:HD11	1:D:90:ILE:HG21	1.83	0.60
1:F:444:GLY:O	1:F:448:VAL:HG23	2.00	0.60
1:F:703:LEU:HA	1:F:706:ALA:HB3	1.83	0.60
1:F:944:ILE:HG13	1:F:945:VAL:N	2.16	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:C:575:GLN:NE2	1:C:617:PHE:HB2	2.17	0.60
1:D:372:VAL:HB	1:D:373:PRO:HD3	1.83	0.60
1:D:537:HIS:O	1:D:538:ARG:O	2.19	0.60
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.84	0.60
1:C:907:GLY:HA2	1:C:1011:THR:HG23	1.84	0.60
1:D:541:TYR:HA	1:D:544:ILE:CG2	2.32	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:544:ILE:O	1:F:548:ILE:HG23	2.01	0.60
1:B:199:THR:HG23	1:B:200:PRO:HD2	1.83	0.59
1:B:190:PRO:HG3	1:B:788:TRP:CE2	2.37	0.59
1:B:930:LEU:O	1:B:934:ILE:HG23	2.02	0.59
1:D:119:PRO:O	1:D:122:VAL:HG12	2.01	0.59
1:F:10:ILE:HA	1:F:13:TRP:HB2	1.82	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:HB	1:B:116:PRO:HD3	1.84	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:D:17:LEU:CD2	2:D:2026:LMT:H81	2.32	0.59
1:A:242:THR:HG22	1:A:245:GLN:HG3	1.84	0.59
1:A:472:ILE:HA	1:A:475:VAL:HG13	1.84	0.59
1:E:453:PHE:CE2	1:E:474:ILE:HD11	2.36	0.59
1:E:520:PHE:CA	1:E:523:THR:HG22	2.31	0.59
1:F:184:MET:HE1	1:F:268:VAL:HG13	1.84	0.59
1:F:330:THR:HG22	1:F:331:PRO:HD3	1.84	0.59
1:B:187:TRP:HA	1:B:773:GLN:O	2.02	0.59
1:D:519:MET:O	1:D:523:THR:HG23	2.03	0.59
1:E:930:LEU:O	1:E:934:ILE:HG23	2.01	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: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:780:MET:HE3	1:F:225:VAL:N	2.17	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:A:748:THR:HG21	1:A:790:VAL:HG22	1.83	0.59
1:D:196:TYR:H	1:D:196:TYR:HD2	1.51	0.59
1:E:224:ALA:HB1	1:F:780:MET:SD	2.42	0.59
1:A:568:ASP:HB3	1:A:634:TRP:CH2	2.37	0.59
1:C:703:LEU:HA	1:C:706:ALA:HB3	1.84	0.59
1:D:193:LEU:HD22	1:D:265:VAL:HG13	1.84	0.59
1:F:452:VAL:HG22	1:F:883:VAL:HG21	1.85	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:A:150:THR:H	1:A:153:ASP:HB2	1.68	0.59
1:A:402:ILE:HA	1:A:405:LEU:CD1	2.33	0.59
1:A:273:GLN:NE2	1:A:769:ARG:HH11	2.01	0.59
1:D:139:VAL:O	1:D:326:PRO:HD2	2.02	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:156:ASN:HD22	1:E:182:TYR:N	2.00	0.59
1:E:966:CYS:SG	1:E:1021:PRO:CG	2.90	0.59
1:F:575:GLN:NE2	1:F:617:PHE:HB2	2.17	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

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: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
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:D:699:ARG:CZ	1:D:824:MET:HG3	2.32	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:337:ILE:HG13	1:A:338:HIS:H	1.68	0.58
1:A:523:THR:O	1:A:525:HIS:N	2.36	0.58
1:B:38:ILE:HA	1:B:465:VAL:HG11	1.85	0.58
1:A:170:LYS:HZ3	1:B:74:ASN:H	1.51	0.58
1:C:186:ILE:HG22	1:C:268:VAL:HG22	1.85	0.58
1:C:683:PHE:CZ	1:C:818:TYR:CE2	2.90	0.58
1:D:166:LEU:HG	1:D:291:ILE:HD11	1.85	0.58
1:D:951:LEU:O	1:D:956:LYS:HB2	2.03	0.58
1:E:187:TRP:HA	1:E:773:GLN:O	2.02	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:F:144:SER:HA	1:F:320:GLY:O	2.03	0.58
1:C:425:LEU:HD22	1:C:429:GLU:HB2	1.85	0.58
1:D:355:MET:HG3	1:D:365:THR:HG23	1.83	0.58
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.84	0.58
1:D:183:SER:HB2	1:D:769:ARG:O	2.03	0.58
1:D:875:LEU:HD12	1:D:875:LEU:C	2.23	0.58
1:E:58:GLN:HA	1:E:62:VAL:HB	1.84	0.58
1:F:49:TYR:HE1	1:F:121:GLU:HG3	1.69	0.58
1:F:939:LYS:HZ1	1:F:976:THR:HG22	1.69	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:A:616:ASN:HD22	1:A:626:MET:HB3	1.64	0.58
1:C:141:GLY:HA2	1:C:288:GLY:HA3	1.86	0.58
1:C:138:MET:HB2	1:C:327:TYR:O	2.04	0.58
1:D:150:THR:H	1:D:153:ASP:HB2	1.68	0.58
1:D:337:ILE:HG13	1:D:338:HIS:H	1.69	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:C:109:ASN:HA	1:C:112:GLN:NE2	2.18	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:C:480:LEU:O	1:C:484:VAL:HG23	2.04	0.58
1:D:521:LEU:O	1:D:521:LEU:HD13	2.04	0.58
1:E:591:VAL:HA	1:E:594:MET:HG3	1.84	0.58
1:A:483:ILE:HG13	1:A:487:ILE:HD13	1.86	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:C:452:VAL:HG22	1:C:883:VAL:HG21	1.86	0.58
1:C:49:TYR:HE1	1:C:121:GLU:HG3	1.69	0.58
1:D:175:PHE:HB2	1:D:289:ILE:HD11	1.86	0.58
1:E:391:ASN:H	1:E:394:THR:CG2	2.16	0.58
1:D:622:GLN:NE2	1:F:222:LEU:HG	2.18	0.58
1:A:203:VAL:O	1:A:206:ALA:N	2.32	0.58
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.85	0.58
1:A:181:GLN:HG3	1:A:768:LYS:HZ3	1.68	0.58
1:A:951:LEU:O	1:A:956:LYS:HB2	2.03	0.58
1:B:156:ASN:HD22	1:B:182:TYR:N	2.02	0.58
1:D:242:THR:HG22	1:D:245:GLN:HG3	1.84	0.58
1:E:115:THR:O	1:E:118:LEU:HB2	2.04	0.58
1:D:402:ILE:HA	1:D:405:LEU:CD1	2.33	0.58
1:D:57:VAL:HG13	1:D:88:MET:HB3	1.86	0.58
1:E:910:GLY:H	1:E:1011:THR:HG21	1.69	0.58
1:A:283:GLY:HA2	1:A:595:ARG:HE	1.69	0.57
1:B:188:LEU:HA	1:B:266:ALA:HB2	1.86	0.57
1:C:190:PRO:HA	1:C:193:LEU:HD12	1.86	0.57
1:C:757:TYR:CE1	1:C:769:ARG:HD3	2.39	0.57
1:D:524:THR:HG22	1:D:970:LEU:HD12	1.86	0.57
2:E:2032:LMT:H42	2:E:2032:LMT:H82	1.86	0.57
1:A:242:THR:HG22	1:A:245:GLN:NE2	2.14	0.57
1:D:753:TRP:CZ2	1:D:785:LEU:HG	2.38	0.57
1:E:185:ARG:HD2	1:E:272:GLY:O	2.04	0.57
1:E:541:TYR:HA	1:E:544:ILE:CG2	2.35	0.57
1:A:727:LYS:HD3	1:A:728:LEU:H	1.68	0.57
1:B:861:LEU:O	1:B:865:GLU:HG2	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:94:PHE:CE2	1:B:103:ALA:HB1	2.40	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LEU:O	1:F:169:THR:HG22	2.05	0.57
1:F:80:SER:CB	1:F:90:ILE:HG22	2.34	0.57
1:A:404:LEU:HD22	1:A:936:LEU:HD23	1.86	0.57
1:B:317:MET:SD	1:B:321:MET:HE3	2.45	0.57
1:C:479:ALA:O	1:C:482:VAL:HG12	2.04	0.57
1:C:80:SER:CB	1:C:90:ILE:HG22	2.34	0.57
1:D:404:LEU:HD22	1:D:936:LEU:HD23	1.87	0.57
1:D:900:VAL:HG13	1:D:941:ALA:HB3	1.87	0.57
1:E:151:LYS:HZ1	1:E:278:ASN:HB3	1.70	0.57
1:E:701:LYS:O	1:E:705:LEU:HB2	2.05	0.57
1:D:893:SER:N	1:F:10:ILE:HD11	2.19	0.57
1:F:150:THR:HG22	1:F:153:ASP:OD2	2.04	0.57
1:F:203:VAL:O	1:F:207:ILE:HG13	2.05	0.57
1:F:138:MET:HB2	1:F:327:TYR:O	2.03	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:E:695:LEU:HD13	1:E:824:MET:HG3	1.85	0.57
1:F:393:LEU:CD1	1:F:466:ILE:HB	2.34	0.57
1:A:157:TYR:CZ	1:A:317:MET:HG2	2.40	0.57
1:A:367:ILE:HG12	1:A:368:PRO:HD3	1.86	0.57
1:B:155:SER:O	1:B:159:VAL:HG23	2.05	0.57
1:B:910:GLY:H	1:B:1011:THR:HG21	1.69	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:D:969:ARG:O	1:D:973:ILE:HG12	2.04	0.57
1:E:188:LEU:HA	1:E:266:ALA:HB2	1.86	0.57
1:A:831:ALA:O	1:A:834:LEU:HB2	2.04	0.57
1:B:185:ARG:HD2	1:B:272:GLY:O	2.04	0.57
1:B:453:PHE:CD2	1:B:474:ILE:HD11	2.39	0.57
1:D:350:LEU:O	1:D:354:VAL:HG23	2.05	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: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:B:466:ILE:HD11	1:B:924:VAL:HG21	1.85	0.57
1:C:393:LEU:CD1	1:C:466:ILE:HB	2.34	0.57
1:D:228:GLN:HE21	1:D:230:LEU:N	2.01	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:E:881:LEU:HD22	1:E:881:LEU:O	2.05	0.57
1:F:43:ILE:CD1	1:F:104:GLN:HA	2.35	0.57
1:A:139:VAL:O	1:A:326:PRO:HD2	2.04	0.57
1:A:659:LYS:HD2	1:A:660:ASP:N	2.20	0.57
1:A:57:VAL:HG13	1:A:88:MET:HB3	1.86	0.57
1:C:144:SER:HA	1:C:320:GLY:O	2.04	0.57
1:E:577:GLN:OE1	1:E:720:MET:HG2	2.05	0.57
1:F:109:ASN:HA	1:F:112:GLN:NE2	2.20	0.57
1:F:159:VAL:HG12	1:F:159:VAL:O	2.05	0.57
1:B:115:THR:O	1:B:118:LEU:HB2	2.05	0.56
1:C:27:ILE:HD11	1:C:380:PHE:CD1	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:E:281:PHE:CZ	1:E:324:VAL:HG11	2.39	0.56
1:A:298:ASN:O	1:A:302:THR:HG22	2.05	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:B:281:PHE:CZ	1:B:324:VAL:HG11	2.40	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:D:818:TYR:HH	1:D:859:THR:HG1	1.51	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:F:573:PHE:CE2	1:F:668:PRO:HG3	2.41	0.56
1:B:157:TYR:O	1:B:161:ASN:HB2	2.05	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:C:60:THR:HG23	1:C:61:VAL:HG23	1.85	0.56
1:D:162:ILE:HG23	1:D:166:LEU:CD2	2.36	0.56
1:D:332:VAL:HG21	1:D:569:GLN:HA	1.86	0.56
1:D:652:GLN:HE22	1:D:664:PHE:HD1	1.53	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:A:175:PHE:HB2	1:A:289:ILE:HD11	1.86	0.56
1:A:555:MET:SD	1:A:913:LEU:HD23	2.45	0.56
1:B:313:LEU:O	1:B:317:MET:HG3	2.05	0.56
1:B:695:LEU:HD13	1:B:824:MET:HG3	1.86	0.56
1:D:262:LEU:HD22	1:D:263:LYS:H	1.70	0.56
1:D:533:SER:O	1:D:536:LYS:HG3	2.06	0.56
1:D:996:GLY:H	1:D:999:HIS:HD2	1.54	0.56
1:E:313:LEU:O	1:E:317:MET:HG3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:958:ILE:HG12	1:E:959:VAL:N	2.21	0.56
1:F:425:LEU:HD22	1:F:429:GLU:HB2	1.87	0.56
1:A:98:THR:O	1:A:100:PRO:HD3	2.04	0.56
1:C:358:PHE:CG	1:C:975:MET:HG2	2.40	0.56
1:D:727:LYS:HD3	1:D:728:LEU:H	1.68	0.56
1:F:910:GLY:N	1:F:1011:THR:HG21	2.20	0.56
1:F:896:ILE:HG12	1:F:897:PRO:HD3	1.87	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:A:352:PHE:CD1	1:A:369:THR:HG21	2.37	0.56
1:C:203:VAL:O	1:C:207:ILE:HG13	2.05	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:E:363:ARG:HD3	1:E:496:MET:O	2.05	0.56
1:F:910:GLY:CA	1:F:1011:THR:HG21	2.36	0.56
1:F:971:ARG:HB2	1:F:972:PRO:HD3	1.86	0.56
1:A:365:THR:O	1:A:368:PRO:HD2	2.06	0.56
1:A:332:VAL:HG21	1:A:569:GLN:HA	1.87	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:E:871:GLN:HA	2:E:2032:LMT:O2B	2.06	0.56
1:F:939:LYS:NZ	1:F:976:THR:CG2	2.69	0.56
1:A:142:VAL:HG12	1:A:154:LEU:HD22	1.87	0.56
1:A:478:MET:O	1:A:481:SER:HB3	2.06	0.56
1:A:545:TYR:HB2	1:A:1019:TRP:HZ3	1.70	0.56
1:B:1015:LEU:O	1:B:1019:TRP:HD1	1.89	0.56
1:C:910:GLY:CA	1:C:1011:THR:HG21	2.35	0.56
1:C:396:PHE:CE2	1:C:998:GLN:HG2	2.41	0.56
1:D:203:VAL:O	1:D:206:ALA:N	2.31	0.56
1:D:453:PHE:CE2	1:D:474:ILE:HD11	2.41	0.56
1:E:1015:LEU:O	1:E:1019:TRP:HD1	1.89	0.56
1:F:190:PRO:HG3	1:F:788:TRP:CZ2	2.40	0.56
1:F:779:ARG:HD2	1:F:779:ARG:O	2.06	0.56
1:F:559:ILE:HD11	1:F:922:ASN:HB2	1.86	0.56
1:A:339:GLU:O	1:A:343:THR:HG23	2.05	0.56
1:B:686:ASP:HB2	1:B:690:VAL:HG12	1.86	0.56
1:C:910:GLY:N	1:C:1011:THR:HG21	2.20	0.56
1:C:945:VAL:HG23	1:C:1020:VAL:HG12	1.88	0.56
1:D:524:THR:O	1:D:527:TYR:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:ALA:O	1:E:375:VAL:HG23	2.04	0.56
1:E:817:ARG:HD2	1:E:822:PRO:HA	1.88	0.56
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:A:203:VAL:O	1:A:204:SER:C	2.44	0.56
1:A:350:LEU:O	1:A:354:VAL:HG23	2.06	0.56
1:A:622:GLN:NE2	1:C:222:LEU:HG	2.20	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:D:225:VAL:HG12	1:E:780:MET:HE2	1.87	0.56
1:A:637:ARG:N	1:A:638:PRO:CD	2.69	0.56
1:A:800:PHE:CD2	1:A:804:ALA:HB2	2.37	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:B:612:VAL:HG11	1:B:615:PHE:HD2	1.71	0.56
1:C:904:VAL:HB	1:C:905:PRO:HD3	1.88	0.56
1:D:162:ILE:HG23	1:D:166:LEU:HD23	1.88	0.56
1:D:637:ARG:N	1:D:638:PRO:CD	2.68	0.56
1:E:782:PRO:O	1:E:785:LEU:HB2	2.06	0.56
1:F:396:PHE:CE2	1:F:998:GLN:HG2	2.41	0.56
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:C:330:THR:HG22	1:C:331:PRO:HD3	1.87	0.55
1:D:367:ILE:HG12	1:D:368:PRO:HD3	1.86	0.55
1:E:155:SER:O	1:E:159:VAL:HG23	2.06	0.55
1:E:445:ILE:HG22	1:E:942:ILE:HD12	1.89	0.55
1:F:314:GLU:HA	1:F:317:MET:SD	2.47	0.55
1:F:479:ALA:O	1:F:482:VAL:HG12	2.06	0.55
1:F:757:TYR:CE1	1:F:769:ARG:HD3	2.40	0.55
1:A:150:THR:HG22	1:A:153:ASP:CG	2.26	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:A:695:LEU:CD1	1:A:699:ARG:NH2	2.69	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:C:573:PHE:CE2	1:C:668:PRO:HG3	2.40	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: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:726:TYR:CE1	1:A:782:PRO:HB3	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:782:PRO:O	1:B:785:LEU:HB2	2.06	0.55
1:C:367:ILE:CG2	1:C:492:LEU:HB3	2.36	0.55
1:C:896:ILE:HG12	1:C:897:PRO:HD3	1.86	0.55
1:D:298:ASN:O	1:D:302:THR:HG22	2.06	0.55
1:D:363:ARG:O	1:D:367:ILE:HG22	2.06	0.55
1:D:809:GLU:O	1:D:810:TYR:HB3	2.05	0.55
1:E:453:PHE:CD2	1:E:474:ILE:HD11	2.40	0.55
1:F:980:PHE:CE2	1:F:1005:VAL:HG13	2.42	0.55
1:A:196:TYR:HD1	1:A:260:VAL:HG21	1.71	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:D:352:PHE:CD1	1:D:369:THR:HG21	2.37	0.55
1:D:950:GLU:O	1:D:953:GLU:HG3	2.07	0.55
1:E:24:GLY:O	1:E:27:ILE:HG12	2.07	0.55
1:E:479:ALA:O	1:E:483:ILE:HG22	2.05	0.55
1:E:739:GLY:HA3	1:E:793:ASP:HB2	1.89	0.55
1:E:977:SER:O	1:E:981:ILE:HG23	2.07	0.55
1:F:699:ARG:CG	1:F:699:ARG:NH1	2.60	0.55
1:F:80:SER:HB2	1:F:90:ILE:HG22	1.88	0.55
1:A:1001:ILE:HG23	1:A:1002:GLY:N	2.21	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:C:925:PHE:HD2	1:C:1001:ILE:HG23	1.71	0.55
1:F:68:GLN:HG3	1:F:114:ALA:HB2	1.87	0.55
1:B:116:PRO:HA	1:B:123:GLN:HE22	1.71	0.55
1:B:682:LEU:HD11	1:B:856:TYR:HD2	1.72	0.55
1:C:80:SER:HB2	1:C:90:ILE:HG22	1.87	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:D:930:LEU:O	1:D:934:ILE:HG23	2.05	0.55
1:F:143:VAL:HG13	1:F:286:ALA:HB2	1.88	0.55
1:F:60:THR:HG23	1:F:61:VAL:HG23	1.87	0.55
1:F:818:TYR:HD1	1:F:823:ALA:HB3	1.70	0.55
1:A:228:GLN:HE21	1:A:230:LEU:N	2.02	0.55
1:B:242:THR:HG23	1:B:245:GLN:HG3	1.88	0.55
1:B:35:TYR:HE1	1:B:392:THR:HG21	1.71	0.55
1:C:402:ILE:HD12	1:C:403:GLY:N	2.22	0.55
1:D:539:ALA:HB3	1:D:540:PRO:HD3	1.88	0.55
1:D:690:VAL:HG22	1:D:694:VAL:CG2	2.36	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:936:LEU:HD12	1:E:1009:MET:HE3	1.88	0.55
1:E:576:VAL:HG21	1:E:591:VAL:HG22	1.88	0.55
1:E:612:VAL:HG11	1:E:615:PHE:HD2	1.71	0.55
1:A:363:ARG:O	1:A:367:ILE:HG22	2.06	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:D:273:GLN:NE2	1:D:769:ARG:HH11	2.05	0.55
1:E:458:PHE:HA	2:E:2031:LMT:H11	1.88	0.55
1:A:573:PHE:HB2	1:A:666:PHE:CE2	2.41	0.55
1:C:314:GLU:HA	1:C:317:MET:SD	2.47	0.55
1:D:578:THR:HG22	1:D:579:PRO:HD2	1.88	0.55
1:E:552:MET:HG3	1:E:553:ILE:N	2.22	0.55
1:F:184:MET:HG3	1:F:246:PHE:CE1	2.42	0.55
1:F:638:PRO:HD2	1:F:642:ASN:ND2	2.22	0.55
1:A:533:SER:O	1:A:536:LYS:HG3	2.07	0.55
1:C:712:LEU:HD23	1:C:712:LEU:N	2.21	0.55
1:D:203:VAL:O	1:D:204:SER:C	2.45	0.55
1:D:843:VAL:O	1:D:847:VAL:HG23	2.07	0.55
1:D:851:PRO:O	1:D:854:VAL:HG12	2.07	0.55
1:F:925:PHE:HD2	1:F:1001:ILE:HG23	1.72	0.55
1:A:186:ILE:HG13	1:A:262:LEU:HD21	1.89	0.54
1:B:169:THR:O	1:B:172:VAL:HG23	2.06	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:C:575:GLN:NE2	1:C:666:PHE:HZ	2.05	0.54
1:C:818:TYR:HD1	1:C:823:ALA:HB3	1.71	0.54
1:C:977:SER:O	1:C:981:ILE:HG12	2.06	0.54
1:D:161:ASN:O	1:D:165:PRO:HD2	2.08	0.54
1:D:47:VAL:HG22	1:D:48:SER:N	2.22	0.54
1:D:498:LYS:N	1:D:499:PRO:CD	2.62	0.54
1:D:590:VAL:HG11	1:D:661:ALA:HB3	1.88	0.54
1:D:725:GLN:HG3	1:D:811:GLY:H	1.73	0.54
1:E:351:VAL:O	1:E:355:MET:HB2	2.07	0.54
1:E:549:VAL:O	1:E:552:MET:HG2	2.07	0.54
1:F:943:LEU:CD1	1:F:973:ILE:HG22	2.37	0.54
1:A:902:LEU:HD23	1:A:1023:PHE:CE1	2.42	0.54
1:B:559:ILE:HD12	1:B:560:PRO:HD2	1.89	0.54
1:A:780:MET:HE3	1:C:225:VAL:H	1.73	0.54
1:D:483:ILE:HG13	1:D:487:ILE:HD13	1.89	0.54
1:D:607:SER:HB2	1:D:632:LYS:HG2	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:807:LYS:HG3	1:D:808:TRP:H	1.72	0.54
1:E:48:SER:N	2:E:2033:LMT:O3B	2.40	0.54
1:E:211:ASN:HD21	1:E:240:LEU:H	1.55	0.54
1:F:142:VAL:HG12	1:F:154:LEU:HD22	1.88	0.54
1:F:190:PRO:HA	1:F:193:LEU:HD12	1.87	0.54
1:F:932:THR:O	1:F:936:LEU:HG	2.06	0.54
1:A:375:VAL:CG2	1:A:405:LEU:HG	2.23	0.54
1:B:577:GLN:OE1	1:B:720:MET:HG2	2.07	0.54
1:B:738:LEU:HD13	1:B:798:VAL:HG11	1.90	0.54
1:C:68:GLN:HG3	1:C:114:ALA:HB2	1.89	0.54
1:D:800:PHE:CD2	1:D:804:ALA:HB2	2.37	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:F:530:GLY:O	1:F:534:ILE:HG23	2.06	0.54
1:F:575:GLN:NE2	1:F:666:PHE:HZ	2.05	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:C:184:MET:HG3	1:C:246:PHE:CE1	2.42	0.54
1:D:902:LEU:HD23	1:D:1023:PHE:CE1	2.42	0.54
1:D:197:GLN:HA	1:D:797:MET:SD	2.47	0.54
1:D:100:PRO:HB3	1:D:295:THR:HG21	1.90	0.54
1:D:859:THR:HG23	1:D:860:GLY:N	2.22	0.54
1:E:595:ARG:HG3	1:E:596:GLU:N	2.22	0.54
1:E:738:LEU:HD13	1:E:798:VAL:HG11	1.89	0.54
1:F:945:VAL:HG23	1:F:1020:VAL:HG12	1.88	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:652:GLN:HE22	1:A:664:PHE:HD1	1.54	0.54
1:A:738:LEU:HD12	1:A:738:LEU:H	1.71	0.54
1:A:792:ASN:ND2	1:A:793:ASP:H	2.04	0.54
1:A:866:ARG:O	1:A:867:LEU:HG	2.06	0.54
1:A:535:LEU:HD21	1:A:959:VAL:HG13	1.88	0.54
1:B:1023:PHE:O	1:B:1027:VAL:HG23	2.07	0.54
1:C:142:VAL:HG12	1:C:154:LEU:HD22	1.89	0.54
1:D:738:LEU:H	1:D:738:LEU:HD12	1.72	0.54
1:E:816:GLU:HB2	1:E:823:ALA:O	2.07	0.54
1:F:181:GLN:OE1	1:F:766:ARG:NH1	2.39	0.54
1:A:142:VAL:HB	1:A:158:ILE:HD11	1.89	0.54
1:A:343:THR:HG21	1:A:998:GLN:OE1	2.06	0.54
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:O	1:B:207:ILE:HG12	2.07	0.54
1:B:445:ILE:HG22	1:B:942:ILE:HD12	1.88	0.54
1:C:190:PRO:HG3	1:C:788:TRP:CZ2	2.43	0.54
1:B:11:PHE:CD1	1:C:889:ALA:HB1	2.42	0.54
1:D:1020:VAL:HB	1:D:1021:PRO:HD3	1.88	0.54
1:E:43:ILE:HG12	1:E:104:GLN:HA	1.90	0.54
1:E:242:THR:HG23	1:E:245:GLN:HG3	1.90	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: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:A:1015:LEU:O	1:A:1019:TRP:HD1	1.91	0.54
1:B:43:ILE:HG12	1:B:104:GLN:HA	1.89	0.54
1:A:670:SER:O	1:A:671:VAL:HB	2.08	0.54
1:A:893:SER:N	1:C:10:ILE:HD11	2.23	0.54
1:C:159:VAL:CG2	1:C:177:VAL:HG11	2.33	0.54
1:D:249:ILE:HG23	1:D:262:LEU:N	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:F:214:ILE:CG1	1:F:237:LYS:HB2	2.38	0.54
1:A:189:ASP:OD2	1:A:191:ALA:HB3	2.08	0.54
1:B:592:ASP:O	1:B:595:ARG:HG2	2.07	0.54
1:B:904:VAL:O	1:B:908:VAL:HG23	2.07	0.54
1:C:1029:THR:O	1:C:1030:LEU:HD23	2.08	0.54
1:D:142:VAL:HG23	1:D:158:ILE:HD11	1.90	0.54
1:E:293:LEU:CD2	1:E:302:THR:HG21	2.36	0.54
1:E:592:ASP:O	1:E:595:ARG:HG2	2.07	0.54
1:F:402:ILE:HD12	1:F:403:GLY:N	2.23	0.54
1:F:729:GLU:HB2	1:F:805:THR:HG23	1.90	0.54
1:F:977:SER:O	1:F:981:ILE:HG12	2.08	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:D:866:ARG:O	1:D:867:LEU:HG	2.06	0.54
1:E:317:MET:SD	1:E:321:MET:HE3	2.48	0.54
1:E:657:SER:O	1:E:658:PHE:C	2.46	0.54
1:E:800:PHE:HD2	1:E:804:ALA:HB2	1.73	0.54
1:F:683:PHE:CD2	1:F:818:TYR:CE1	2.97	0.54
1:B:305:ALA:C	1:B:307:ARG:H	2.10	0.53
1:B:44:ALA:HB2	1:B:132:ALA:HB2	1.89	0.53
1:B:595:ARG:HG3	1:B:596:GLU:N	2.21	0.53
1:C:779:ARG:O	1:C:779:ARG:HD2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:LEU:HD21	1:D:842:ALA:CB	2.37	0.53
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:A:213:GLN:CG	1:B:56:THR:HG23	2.37	0.53
1:A:423:GLU:HB3	1:A:425:LEU:HD13	1.90	0.53
1:A:710:PRO:O	1:A:831:ALA:CB	2.55	0.53
1:B:657:SER:O	1:B:658:PHE:C	2.46	0.53
1:B:761:PHE:HE2	1:B:763:ASP:HB3	1.73	0.53
1:B:904:VAL:HB	1:B:905:PRO:HD3	1.90	0.53
1:C:143:VAL:HG13	1:C:286:ALA:HB2	1.88	0.53
1:A:780:MET:CE	1:C:224:ALA:HA	2.37	0.53
1:D:142:VAL:CG2	1:D:158:ILE:HD11	2.39	0.53
1:D:726:TYR:CE1	1:D:782:PRO:HB3	2.43	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:E:420:MET:HE1	1:E:499:PRO:HA	1.90	0.53
1:E:981:ILE:HG13	1:E:982:LEU:N	2.23	0.53
1:F:896:ILE:HB	1:F:945:VAL:CG1	2.38	0.53
1:A:1008:GLY:O	1:A:1012:ALA:HB2	2.07	0.53
1:A:807:LYS:HG3	1:A:808:TRP:H	1.74	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:B:351:VAL:O	1:B:355:MET:HB2	2.09	0.53
1:C:355:MET:SD	1:C:368:PRO:HB2	2.48	0.53
1:C:446:ALA:O	1:C:450:SER:HB2	2.09	0.53
1:C:520:PHE:C	1:C:522:SER:H	2.11	0.53
1:D:367:ILE:CD1	1:D:413:VAL:HG22	2.39	0.53
1:D:416:VAL:HG12	1:D:420:MET:CE	2.38	0.53
1:D:585:GLU:O	1:D:589:VAL:HG23	2.08	0.53
1:D:62:VAL:O	1:D:65:ILE:HD13	2.08	0.53
2:E:2033:LMT:C12	2:E:2033:LMT:H62	2.33	0.53
1:A:196:TYR:N	1:A:196:TYR:CD2	2.75	0.53
1:B:165:PRO:O	1:B:169:THR:HG23	2.09	0.53
1:C:683:PHE:CD2	1:C:818:TYR:CE1	2.96	0.53
1:C:745:ILE:HG22	1:C:790:VAL:HG21	1.91	0.53
1:C:742:LEU:HB3	1:C:746:ASN:ND2	2.23	0.53
1:C:792:ASN:OD1	1:C:798:VAL:HG23	2.08	0.53
1:D:98:THR:O	1:D:100:PRO:HD3	2.08	0.53
1:D:388:PHE:CE2	1:D:472:ILE:HG12	2.43	0.53
1:E:240:LEU:HA	1:E:245:GLN:HE22	1.74	0.53
1:E:391:ASN:H	1:E:394:THR:HG22	1.73	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:A:884:PHE:N	1:A:901:MET:HE1	2.23	0.53
1:B:192:LYS:O	1:B:195:SER:HB3	2.08	0.53
1:B:62:VAL:CG2	1:B:88:MET:HG3	2.38	0.53
1:C:43:ILE:HD11	1:C:107:VAL:HG21	1.89	0.53
1:C:582:SER:HB3	1:C:586:ARG:HD3	1.90	0.53
1:C:58:GLN:HA	1:C:62:VAL:HB	1.89	0.53
1:E:151:LYS:NZ	1:E:278:ASN:HB3	2.24	0.53
1:E:156:ASN:HD21	1:E:768:LYS:HZ3	1.55	0.53
1:F:159:VAL:CG2	1:F:177:VAL:HG11	2.36	0.53
1:F:433:LYS:HD2	1:F:437:GLN:HE21	1.74	0.53
1:F:393:LEU:HD13	1:F:466:ILE:HB	1.90	0.53
1:F:520:PHE:C	1:F:522:SER:H	2.12	0.53
1:A:251:LEU:HD12	1:A:251:LEU:N	2.24	0.53
1:A:578:THR:HG22	1:A:579:PRO:HD2	1.87	0.53
1:B:676:ASN:ND2	1:B:827:LEU:HD12	2.20	0.53
1:C:45:VAL:HG22	1:C:129:VAL:HG22	1.90	0.53
1:C:939:LYS:NZ	1:C:976:THR:CG2	2.71	0.53
1:D:131:LYS:O	1:D:295:THR:HG22	2.09	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:E:843:VAL:O	1:E:847:VAL:HG23	2.08	0.53
1:F:939:LYS:NZ	1:F:976:THR:HG22	2.23	0.53
1:A:366:LEU:O	1:A:370:ILE:HG23	2.08	0.53
1:B:1014:VAL:O	1:B:1017:ILE:HG12	2.08	0.53
1:B:143:VAL:HG12	1:B:286:ALA:CB	2.39	0.53
1:B:392:THR:O	1:B:396:PHE:HD1	1.92	0.53
1:B:800:PHE:HD2	1:B:804:ALA:HB2	1.73	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:D:453:PHE:O	1:D:456:MET:HB2	2.08	0.53
1:A:344:LEU:O	1:A:348:ILE:HG22	2.09	0.53
1:B:8:ARG:HB3	1:C:892:GLU:OE1	2.09	0.53
1:D:133:VAL:HG12	1:D:293:LEU:O	2.08	0.53
1:D:356:TYR:HE1	1:D:513:PHE:HZ	1.57	0.53
1:D:875:LEU:HD11	1:D:931:LEU:HD11	1.90	0.53
1:E:156:ASN:ND2	1:E:182:TYR:H	2.07	0.53
1:E:586:ARG:O	1:E:589:VAL:HG12	2.09	0.53
1:A:532:ALA:HA	1:A:535:LEU:HB2	1.90	0.53
1:A:809:GLU:O	1:A:810:TYR:HB3	2.08	0.53
1:A:859:THR:HG23	1:A:860:GLY:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:MET:HG3	1:B:553:ILE:N	2.23	0.53
1:C:652:GLN:HG3	1:C:714:ARG:HH11	1.74	0.53
1:D:143:VAL:HG22	1:D:286:ALA:HB2	1.91	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:62:VAL:CG2	1:E:88:MET:HG3	2.38	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:F:652:GLN:HG3	1:F:714:ARG:HH11	1.74	0.53
1:A:453:PHE:O	1:A:456:MET:HB2	2.09	0.53
1:B:24:GLY:O	1:B:27:ILE:HG12	2.09	0.53
1:B:817:ARG:HD2	1:B:822:PRO:HA	1.91	0.53
1:C:539:ALA:N	1:C:540:PRO:HD2	2.24	0.53
1:C:939:LYS:HZ3	1:C:976:THR:CG2	2.22	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:F:742:LEU:HB3	1:F:746:ASN:ND2	2.24	0.53
1:A:100:PRO:HB3	1:A:295:THR:HG21	1.90	0.52
1:A:607:SER:HB2	1:A:632:LYS:HG2	1.91	0.52
1:A:753:TRP:CB	1:C:217:GLY:H	2.21	0.52
1:B:108:GLN:HB2	1:B:129:VAL:HG21	1.92	0.52
1:B:243:ALA:HB1	1:B:268:VAL:HG12	1.91	0.52
1:B:435:MET:SD	1:B:438:ILE:HD11	2.50	0.52
1:B:530:GLY:O	1:B:534:ILE:HG13	2.10	0.52
1:B:758:VAL:HG21	1:B:772:LEU:HB2	1.91	0.52
1:B:684:LEU:O	1:B:823:ALA:HB1	2.09	0.52
1:C:43:ILE:CD1	1:C:104:GLN:HA	2.36	0.52
1:C:680:PHE:CE2	1:C:682:LEU:HD12	2.44	0.52
1:D:358:PHE:CD2	1:D:975:MET:HB2	2.44	0.52
1:D:723:GLU:HG2	1:D:813:PRO:HG3	1.91	0.52
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:F:568:ASP:CG	1:F:644:VAL:HG23	2.29	0.52
1:A:131:LYS:O	1:A:295:THR:HG22	2.09	0.52
1:A:416:VAL:HG11	1:A:497:LEU:HD23	1.91	0.52
1:A:485:ALA:O	1:A:490:PRO:HD3	2.08	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:A:830:PRO:HA	1:A:838:ASP:OD2	2.08	0.52
1:A:851:PRO:O	1:A:854:VAL:HG12	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:SER:O	1:B:57:VAL:HG12	2.09	0.52
1:C:303:ALA:O	1:C:307:ARG:HB2	2.09	0.52
1:C:939:LYS:NZ	1:C:976:THR:HG22	2.25	0.52
1:E:530:GLY:O	1:E:534:ILE:HG13	2.09	0.52
1:E:794:LYS:HD3	1:E:795:GLY:N	2.24	0.52
1:F:944:ILE:HD11	1:F:1020:VAL:HB	1.92	0.52
1:A:39:ALA:CB	1:A:672:LEU:HD11	2.40	0.52
1:A:449:LEU:HD12	1:A:478:MET:HG2	1.91	0.52
1:A:875:LEU:HD11	1:A:931:LEU:HD11	1.91	0.52
1:C:225:VAL:O	1:C:228:GLN:HB2	2.10	0.52
1:C:896:ILE:HB	1:C:945:VAL:CG1	2.40	0.52
1:E:240:LEU:HA	1:E:245:GLN:NE2	2.24	0.52
1:E:587:THR:HG21	1:E:622:GLN:O	2.09	0.52
1:F:773:GLN:HB3	1:F:779:ARG:HH12	1.74	0.52
1:A:680:PHE:CZ	1:A:843:VAL:HG21	2.45	0.52
1:A:709:ASN:O	1:A:711:ALA:N	2.43	0.52
1:A:933:THR:OG1	1:A:1009:MET:HG2	2.09	0.52
1:A:943:LEU:HB3	1:A:969:ARG:NH1	2.24	0.52
1:B:352:PHE:CD2	1:B:353:LEU:HD23	2.44	0.52
1:B:977:SER:O	1:B:981:ILE:HG23	2.09	0.52
1:D:210:GLN:HB2	1:D:249:ILE:HD12	1.91	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:E:904:VAL:HB	1:E:905:PRO:HD3	1.90	0.52
1:F:225:VAL:O	1:F:228:GLN:HB2	2.09	0.52
1:F:355:MET:SD	1:F:368:PRO:HB2	2.49	0.52
1:A:358:PHE:CD2	1:A:975:MET:HB2	2.44	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:433:LYS:HD2	1:C:437:GLN:NE2	2.24	0.52
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.30	0.52
1:C:943:LEU:CD1	1:C:973:ILE:HG22	2.39	0.52
1:D:545:TYR:HB2	1:D:1019:TRP:HZ3	1.70	0.52
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.45	0.52
1:D:355:MET:HE2	1:D:410:ILE:HD11	1.91	0.52
1:D:943:LEU:HB3	1:D:969:ARG:NH1	2.24	0.52
1:D:977:SER:O	1:D:981:ILE:HG23	2.09	0.52
1:E:165:PRO:O	1:E:169:THR:HG23	2.10	0.52
1:E:192:LYS:O	1:E:195:SER:HB3	2.10	0.52
1:E:435:MET:SD	1:E:438:ILE:HD11	2.49	0.52
1:F:480:LEU:O	1:F:484:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:HG12	1:A:420:MET:CE	2.39	0.52
1:A:996:GLY:H	1:A:999:HIS:HD2	1.58	0.52
1:B:816:GLU:HB2	1:B:823:ALA:O	2.09	0.52
1:B:881:LEU:O	1:B:881:LEU:HD22	2.10	0.52
1:B:891:TYR:CD2	1:B:896:ILE:HD11	2.45	0.52
1:C:393:LEU:HD13	1:C:466:ILE:HB	1.92	0.52
1:C:607:SER:HB2	1:C:632:LYS:HG2	1.92	0.52
1:D:531:VAL:O	1:D:532:ALA:O	2.28	0.52
1:D:688:ALA:O	1:D:689:GLY:C	2.48	0.52
1:D:680:PHE:CD2	1:D:858:TRP:HZ3	2.26	0.52
1:E:243:ALA:HB1	1:E:268:VAL:HG12	1.91	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:F:358:PHE:CD1	1:F:975:MET:HG2	2.45	0.52
1:A:388:PHE:CE2	1:A:472:ILE:HG12	2.43	0.52
1:B:125:GLN:NE2	1:B:769:ARG:NH1	2.53	0.52
1:B:293:LEU:CD2	1:B:302:THR:HG21	2.38	0.52
1:B:549:VAL:O	1:B:552:MET:HG2	2.09	0.52
1:B:574:ALA:HB3	1:B:627:ALA:HB3	1.91	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:C:447:MET:HE3	1:C:886:CYS:HB3	1.91	0.52
1:D:159:VAL:HA	1:D:163:GLN:HB2	1.90	0.52
1:A:710:PRO:HD3	1:D:807:LYS:CE	2.39	0.52
1:E:348:ILE:HD12	1:E:369:THR:HG23	1.92	0.52
1:F:939:LYS:HZ3	1:F:976:THR:HG21	1.73	0.52
1:B:489:THR:OG1	1:B:490:PRO:HD3	2.10	0.52
1:B:794:LYS:HD3	1:B:795:GLY:N	2.25	0.52
1:D:449:LEU:HD12	1:D:478:MET:HG2	1.92	0.52
1:D:695:LEU:HD13	1:D:699:ARG:HH21	1.74	0.52
1:E:392:THR:O	1:E:396:PHE:HD1	1.93	0.52
1:F:692:HIS:O	1:F:696:LEU:HB2	2.10	0.52
1:F:818:TYR:CD1	1:F:823:ALA:HB3	2.45	0.52
1:C:159:VAL:O	1:C:159:VAL:HG12	2.08	0.52
1:C:912:LEU:CD2	1:C:926:PHE:HZ	2.23	0.52
1:D:933:THR:OG1	1:D:1009:MET:HG2	2.10	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:A:259:GLN:N	1:A:259:GLN:HE21	2.07	0.52
1:A:356:TYR:HE1	1:A:513:PHE:HZ	1.58	0.52
1:A:708:GLN:OE1	1:D:809:GLU:HA	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLN:HG3	1:A:811:GLY:H	1.75	0.52
1:B:102:ILE:HD12	1:B:102:ILE:C	2.29	0.52
1:D:823:ALA:O	1:D:824:MET:HG2	2.10	0.52
1:F:751:ILE:HB	1:F:756:SER:HB2	1.91	0.52
1:F:745:ILE:HG22	1:F:790:VAL:HG21	1.91	0.52
1:A:453:PHE:HE2	1:A:932:THR:HG22	1.74	0.51
1:A:572:LEU:HB3	1:A:629:ILE:HB	1.92	0.51
1:A:812:SER:OG	1:A:815:LEU:HD13	2.10	0.51
1:B:162:ILE:HG22	1:B:313:LEU:CD1	2.32	0.51
1:B:348:ILE:HD12	1:B:369:THR:HG23	1.92	0.51
1:C:687:GLN:NE2	1:C:855:GLY:HA3	2.25	0.51
1:C:773:GLN:HB3	1:C:779:ARG:HH12	1.74	0.51
1:D:15:ILE:HD13	1:D:15:ILE:C	2.29	0.51
1:D:485:ALA:O	1:D:490:PRO:HD3	2.10	0.51
1:D:593:SER:HB3	1:D:658:PHE:CZ	2.45	0.51
1:D:680:PHE:CZ	1:D:843:VAL:HG21	2.45	0.51
1:E:46:GLN:HE22	2:E:2033:LMT:H42	1.74	0.51
2:E:2033:LMT:H6E	2:E:2033:LMT:O6B	2.10	0.51
1:E:574:ALA:HB3	1:E:627:ALA:HB3	1.92	0.51
1:F:912:LEU:CD2	1:F:926:PHE:HZ	2.22	0.51
1:A:356:TYR:O	1:A:356:TYR:HD1	1.93	0.51
1:B:151:LYS:NZ	1:B:278:ASN:HB3	2.25	0.51
1:C:188:LEU:HA	1:C:266:ALA:HB2	1.92	0.51
1:C:751:ILE:HB	1:C:756:SER:HB2	1.92	0.51
1:D:416:VAL:O	1:D:420:MET:HB2	2.10	0.51
1:D:555:MET:SD	1:D:913:LEU:HD23	2.49	0.51
1:F:456:MET:HE3	1:F:931:LEU:HD12	1.92	0.51
1:F:539:ALA:N	1:F:540:PRO:HD2	2.25	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:B:587:THR:HG21	1:B:622:GLN:O	2.10	0.51
1:B:703:LEU:CD1	1:B:717:PRO:HG3	2.36	0.51
1:D:242:THR:HG23	1:D:245:GLN:H	1.75	0.51
1:D:409:ALA:O	1:D:413:VAL:HG23	2.11	0.51
1:D:439:GLN:O	1:D:443:VAL:HG23	2.10	0.51
1:D:958:ILE:HD13	1:D:959:VAL:H	1.76	0.51
1:E:143:VAL:HG12	1:E:286:ALA:CB	2.40	0.51
1:E:517:ASN:O	1:E:521:LEU:HB2	2.10	0.51
1:F:43:ILE:HD11	1:F:107:VAL:CG2	2.39	0.51
1:F:214:ILE:HG12	1:F:237:LYS:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.45	0.51
1:A:242:THR:HG23	1:A:245:GLN:H	1.76	0.51
1:A:355:MET:HE1	1:A:406:VAL:CG1	2.40	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:C:109:ASN:HA	1:C:112:GLN:CD	2.30	0.51
1:C:980:PHE:HE2	1:C:1005:VAL:HG13	1.75	0.51
1:D:181:GLN:HG3	1:D:768:LYS:HZ3	1.74	0.51
1:E:906:LEU:O	1:E:1011:THR:HG23	2.10	0.51
1:A:142:VAL:CG1	1:A:154:LEU:HD22	2.40	0.51
1:A:688:ALA:O	1:A:689:GLY:C	2.48	0.51
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.92	0.51
1:C:527:TYR:O	1:C:531:VAL:HG23	2.11	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:E:188:LEU:HD11	1:E:772:LEU:HD21	1.93	0.51
1:F:227:GLY:O	1:F:229:GLN:HG3	2.11	0.51
1:A:196:TYR:CD1	1:A:260:VAL:HG11	2.45	0.51
1:B:34:GLN:HG3	1:B:35:TYR:CD2	2.45	0.51
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.75	0.51
1:C:729:GLU:HB2	1:C:805:THR:HG23	1.91	0.51
1:D:538:ARG:C	1:D:538:ARG:HE	2.13	0.51
1:D:548:ILE:HG23	1:D:909:ILE:HD13	1.92	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:E:1:MET:O	1:E:4:PHE:HB3	2.10	0.51
1:F:391:ASN:HB2	1:F:394:THR:H	1.75	0.51
1:F:49:TYR:HE1	1:F:121:GLU:CG	2.23	0.51
1:A:225:VAL:HG12	1:B:780:MET:HE2	1.93	0.51
1:A:210:GLN:HB2	1:A:249:ILE:HD12	1.93	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:C:944:ILE:HD11	1:C:1020:VAL:HB	1.93	0.51
1:C:169:THR:HG23	1:C:172:VAL:HG21	1.92	0.51
1:C:891:TYR:CD1	1:C:896:ILE:HD11	2.46	0.51
1:C:977:SER:OG	1:C:1009:MET:HE1	2.11	0.51
1:D:193:LEU:HD21	1:D:265:VAL:HG13	1.92	0.51
1:D:213:GLN:CG	1:E:56:THR:HG23	2.41	0.51
1:E:423:GLU:OE2	1:E:433:LYS:HE3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:TYR:HD1	1:F:1018:PHE:CE2	2.29	0.51
1:F:109:ASN:HA	1:F:112:GLN:CD	2.31	0.51
1:F:143:VAL:O	1:F:321:MET:HA	2.10	0.51
1:F:15:ILE:HG13	1:F:16:ALA:N	2.24	0.51
1:F:687:GLN:NE2	1:F:855:GLY:HA3	2.26	0.51
1:F:682:LEU:HD11	1:F:843:VAL:CG1	2.39	0.51
1:A:15:ILE:C	1:A:15:ILE:HD13	2.31	0.51
1:A:376:LEU:O	1:A:379:THR:CG2	2.59	0.51
1:A:62:VAL:O	1:A:65:ILE:HD13	2.10	0.51
1:A:273:GLN:NE2	1:A:769:ARG:HD2	2.25	0.51
1:A:780:MET:SD	1:C:228:GLN:HG3	2.51	0.51
1:B:367:ILE:HB	1:B:368:PRO:CD	2.38	0.51
1:C:49:TYR:HE1	1:C:121:GLU:CG	2.23	0.51
1:C:609:VAL:HG22	1:C:629:ILE:HG23	1.91	0.51
1:D:156:ASN:ND2	1:D:768:LYS:NZ	2.58	0.51
1:F:247:GLU:HB3	1:F:263:LYS:HE2	1.93	0.51
1:F:607:SER:HB2	1:F:632:LYS:HG2	1.93	0.51
1:A:548:ILE:HG23	1:A:909:ILE:HD13	1.93	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: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:D:423:GLU:HB3	1:D:425:LEU:HD13	1.92	0.51
1:D:594:MET:O	1:D:595:ARG:C	2.49	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:A:115:THR:HA	1:A:118:LEU:HD13	1.92	0.51
1:A:708:GLN:HE21	1:A:708:GLN:HA	1.76	0.51
1:A:875:LEU:HD12	1:A:876:TYR:N	2.26	0.51
1:B:1:MET:O	1:B:4:PHE:HB3	2.11	0.51
1:B:517:ASN:O	1:B:521:LEU:HB2	2.11	0.51
1:B:969:ARG:O	1:B:973:ILE:HG23	2.10	0.51
1:C:545:TYR:CD1	1:C:1023:PHE:HZ	2.30	0.51
1:C:150:THR:HG23	1:C:152:GLU:H	1.76	0.51
1:C:367:ILE:CG1	1:C:368:PRO:HD3	2.41	0.51
1:C:891:TYR:CG	1:C:896:ILE:HD11	2.46	0.51
1:C:456:MET:HE3	1:C:931:LEU:HD12	1.91	0.51
1:D:344:LEU:O	1:D:348:ILE:HG22	2.11	0.51
1:D:428:ARG:HH12	1:D:432:ARG:NE	2.09	0.51
1:E:584:ALA:O	1:E:588:GLN:HB2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:ARG:CZ	1:E:968:MET:HE3	2.41	0.51
1:F:303:ALA:O	1:F:307:ARG:HB2	2.11	0.51
1:A:865:GLU:O	1:A:866:ARG:HB2	2.11	0.50
1:A:909:ILE:C	1:A:911:ALA:H	2.14	0.50
1:A:930:LEU:O	1:A:933:THR:HG22	2.10	0.50
1:B:586:ARG:O	1:B:589:VAL:HG12	2.10	0.50
1:D:146:ASP:C	1:D:148:SER:H	2.14	0.50
1:D:375:VAL:CG2	1:D:405:LEU:HG	2.24	0.50
1:E:751:ILE:O	1:E:773:GLN:HA	2.11	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:E:11:PHE:CD1	1:F:889:ALA:HB1	2.46	0.50
1:F:980:PHE:HE2	1:F:1005:VAL:HG13	1.75	0.50
1:A:518:ARG:O	1:A:522:SER:N	2.41	0.50
1:A:655:PHE:HD2	1:A:658:PHE:HE2	1.60	0.50
1:A:699:ARG:O	1:A:703:LEU:HD23	2.11	0.50
1:A:6:ILE:HD12	1:A:6:ILE:H	1.75	0.50
1:A:753:TRP:CH2	1:A:785:LEU:HA	2.46	0.50
1:B:906:LEU:O	1:B:1011:THR:HG23	2.11	0.50
1:B:239:ARG:HD3	1:B:760:ASP:O	2.11	0.50
1:B:681:ASP:OD1	1:B:681:ASP:C	2.48	0.50
1:C:143:VAL:O	1:C:321:MET:HA	2.11	0.50
1:C:247:GLU:HB3	1:C:263:LYS:HE2	1.94	0.50
1:C:466:ILE:O	1:C:469:GLN:HB2	2.11	0.50
1:C:872:ALA:HB1	1:C:876:TYR:CE1	2.45	0.50
1:D:195:SER:C	1:D:197:GLN:H	2.15	0.50
1:D:884:PHE:HB2	1:D:901:MET:HE2	1.93	0.50
1:E:312:ASN:HD22	1:E:312:ASN:N	2.09	0.50
1:F:142:VAL:CG1	1:F:154:LEU:HD22	2.41	0.50
1:E:8:ARG:HB3	1:F:892:GLU:OE1	2.10	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:C:379:THR:HB	1:C:398:MET:HE3	1.93	0.50
1:D:544:ILE:HG23	1:D:1019:TRP:HH2	1.76	0.50
1:D:753:TRP:CH2	1:D:785:LEU:HA	2.47	0.50
1:E:20:MET:CE	1:E:374:VAL:HG23	2.41	0.50
1:E:758:VAL:HG21	1:E:772:LEU:HB2	1.92	0.50
1:E:882:VAL:HG13	2:E:2032:LMT:H121	1.92	0.50
1:F:27:ILE:HD11	1:F:380:PHE:CD1	2.45	0.50
1:F:466:ILE:O	1:F:469:GLN:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:ARG:HG3	1:A:1022:LEU:CD2	2.42	0.50
1:A:133:VAL:HG12	1:A:293:LEU:O	2.12	0.50
1:A:355:MET:HE2	1:A:410:ILE:HD11	1.93	0.50
1:A:562:ALA:O	1:A:923:ASP:HA	2.11	0.50
1:A:593:SER:HB3	1:A:658:PHE:CZ	2.46	0.50
1:B:2:SER:HB3	1:B:486:LEU:O	2.11	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:478:MET:O	1:F:481:SER:HB3	2.10	0.50
1:F:680:PHE:HE2	1:F:682:LEU:HD12	1.77	0.50
1:A:498:LYS:N	1:A:499:PRO:CD	2.62	0.50
1:A:896:ILE:N	1:A:897:PRO:CD	2.74	0.50
1:B:367:ILE:HD13	1:B:496:MET:HE2	1.92	0.50
1:B:751:ILE:O	1:B:773:GLN:HA	2.11	0.50
1:C:166:LEU:HA	1:C:169:THR:HG22	1.94	0.50
1:C:214:ILE:CG1	1:C:237:LYS:HB2	2.41	0.50
1:C:711:ALA:HB3	1:C:712:LEU:HD23	1.94	0.50
1:D:538:ARG:HG3	1:D:1022:LEU:CD2	2.42	0.50
1:D:655:PHE:HD2	1:D:658:PHE:HE2	1.59	0.50
1:D:751:ILE:CG2	1:D:772:LEU:HD13	2.42	0.50
1:D:909:ILE:C	1:D:911:ALA:H	2.14	0.50
1:E:896:ILE:N	1:E:897:PRO:CD	2.75	0.50
1:D:785:LEU:HD11	1:F:219:LEU:HD21	1.93	0.50
1:A:1003:THR:HG23	1:A:1004:GLY:N	2.27	0.50
1:A:131:LYS:O	1:A:131:LYS:HG3	2.12	0.50
1:A:438:ILE:O	1:A:442:LEU:HD13	2.12	0.50
1:A:637:ARG:O	1:A:642:ASN:HB2	2.12	0.50
1:A:913:LEU:O	1:A:917:MET:HG2	2.12	0.50
1:A:958:ILE:HD13	1:A:959:VAL:H	1.76	0.50
1:B:1030:LEU:O	1:B:1030:LEU:HD22	2.12	0.50
1:B:528:GLU:HB3	1:B:963:ILE:HD11	1.94	0.50
1:C:192:LYS:HD3	1:C:264:ASP:O	2.11	0.50
1:C:183:SER:OG	1:C:273:GLN:HG3	2.12	0.50
1:C:317:MET:HB3	1:C:321:MET:SD	2.51	0.50
1:D:160:SER:O	1:D:766:ARG:NH1	2.45	0.50
1:D:210:GLN:NE2	1:D:249:ILE:HG13	2.26	0.50
1:D:576:VAL:HB	1:D:625:GLY:O	2.11	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:E:16:ALA:HB2	1:E:488:LEU:HG	1.93	0.50
1:A:235:ILE:HD13	1:A:235:ILE:H	1.76	0.50

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:CD1	1:A:289:ILE:HD11	2.47	0.49
1:B:156:ASN:ND2	1:B:182:TYR:H	2.10	0.49
1:B:343:THR:HA	1:B:346:GLU:HG2	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:A:766:ARG:NE	1:B:67:GLN:NE2	2.60	0.49
1:B:188:LEU:HD11	1:B:772:LEU:HD21	1.94	0.49
1:D:131:LYS:O	1:D:131:LYS:HG3	2.11	0.49
1:D:155:SER:OG	1:D:179:GLY:HA3	2.11	0.49
1:D:17:LEU:HD21	2:D:2026:LMT:H81	1.92	0.49
1:D:356:TYR:HE1	1:D:513:PHE:CZ	2.30	0.49
1:E:553:ILE:O	1:E:557:THR:HG23	2.12	0.49
1:D:222:LEU:HD23	1:E:622:GLN:NE2	2.26	0.49
1:E:786:SER:HB2	1:E:801:ASN:OD1	2.12	0.49
1:F:80:SER:HA	1:F:90:ILE:HA	1.94	0.49
1:F:977:SER:OG	1:F:1009:MET:HE1	2.12	0.49
1:A:708:GLN:NE2	1:A:708:GLN:HA	2.27	0.49
1:B:185:ARG:NH2	1:B:771:TYR:HB3	2.27	0.49
1:C:186:ILE:HG13	1:C:772:LEU:HD23	1.94	0.49
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.93	0.49
1:C:453:PHE:CE2	1:C:474:ILE:HD12	2.47	0.49
1:C:818:TYR:CD1	1:C:823:ALA:HB3	2.46	0.49
1:D:875:LEU:CD1	1:D:931:LEU:HD11	2.43	0.49
1:E:47:VAL:H	1:E:88:MET:CE	2.25	0.49
1:F:902:LEU:HD13	1:F:1023:PHE:CD2	2.47	0.49
1:F:186:ILE:HG13	1:F:772:LEU:HD23	1.95	0.49
1:F:135:ASN:O	1:F:292:LYS:HG2	2.12	0.49
1:F:757:TYR:CD1	1:F:769:ARG:HD3	2.48	0.49
1:A:170:LYS:CA	1:A:170:LYS:HE3	2.37	0.49
1:A:439:GLN:O	1:A:443:VAL:HG23	2.11	0.49
1:A:498:LYS:H	1:A:499:PRO:HD3	1.75	0.49
1:A:576:VAL:HB	1:A:625:GLY:O	2.13	0.49
1:A:749:VAL:HG13	1:A:753:TRP:CD1	2.46	0.49
1:B:246:PHE:O	1:B:249:ILE:HD11	2.12	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
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: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:D:355:MET:HE1	1:D:406:VAL:CG1	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:875:LEU:HD12	1:D:876:TYR:N	2.27	0.49
1:D:562:ALA:O	1:D:923:ASP:HA	2.12	0.49
1:D:996:GLY:N	1:D:999:HIS:CD2	2.78	0.49
1:E:352:PHE:CD2	1:E:353:LEU:HD23	2.48	0.49
1:E:53:SER:O	1:E:57:VAL:HG12	2.12	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:158:ILE:CG2	1:B:162:ILE:HD11	2.39	0.49
1:B:428:ARG:H	1:B:428:ARG:CD	2.16	0.49
1:C:682:LEU:HD11	1:C:843:VAL:CG1	2.41	0.49
1:C:903:VAL:CG2	1:C:1020:VAL:HG22	2.43	0.49
1:C:65:ILE:CD1	1:C:90:ILE:HG12	2.42	0.49
1:D:170:LYS:CA	1:D:170:LYS:HE3	2.40	0.49
1:D:453:PHE:HE2	1:D:932:THR:HG22	1.77	0.49
1:D:753:TRP:CB	1:F:217:GLY:H	2.25	0.49
1:D:896:ILE:N	1:D:897:PRO:CD	2.75	0.49
1:E:904:VAL:O	1:E:908:VAL:HG23	2.12	0.49
1:A:730:ILE:HD12	1:A:745:ILE:HD11	1.93	0.49
1:B:104:GLN:HE21	1:B:131:LYS:HE2	1.77	0.49
1:C:227:GLY:O	1:C:229:GLN:HG3	2.13	0.49
1:C:658:PHE:O	1:C:659:LYS:C	2.50	0.49
1:D:217:GLY:O	1:D:234:ILE:HG12	2.12	0.49
1:D:518:ARG:O	1:D:522:SER:HB3	2.12	0.49
1:D:194:ASN:HD22	1:D:797:MET:HG2	1.77	0.49
1:E:1023:PHE:O	1:E:1027:VAL:HG23	2.13	0.49
1:E:352:PHE:HD1	1:E:365:THR:HG23	1.78	0.49
1:E:616:ASN:CG	1:E:624:SER:HB2	2.33	0.49
1:F:154:LEU:O	1:F:157:TYR:HB3	2.13	0.49
1:F:183:SER:OG	1:F:273:GLN:HG3	2.13	0.49
1:F:711:ALA:HB3	1:F:712:LEU:HD23	1.94	0.49
1:F:872:ALA:HB3	1:F:873:PRO:HD3	1.94	0.49
1:A:544:ILE:HG23	1:A:1019:TRP:HH2	1.78	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:944:ILE:HG22	1:B:969:ARG:HG3	1.95	0.49
1:C:969:ARG:C	1:C:972:PRO:HD2	2.33	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:F:143:VAL:HG23	1:F:324:VAL:HG21	1.95	0.49
1:A:696:LEU:HD13	1:A:699:ARG:NH1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HG22	1:B:942:ILE:CD1	2.43	0.49
1:B:515:TRP:CZ2	1:B:519:MET:HG3	2.48	0.49
1:D:532:ALA:HA	1:D:535:LEU:HB2	1.94	0.49
1:D:699:ARG:O	1:D:703:LEU:HD23	2.13	0.49
1:E:426:SER:HB2	1:E:427:PRO:HD2	1.94	0.49
1:E:76:ARG:HD3	1:E:863:TYR:CE2	2.48	0.49
1:F:443:VAL:O	1:F:447:MET:HB2	2.12	0.49
1:F:759:ASN:H	1:F:770:VAL:HG22	1.77	0.49
1:A:146:ASP:C	1:A:148:SER:H	2.14	0.49
1:A:840:MET:HA	1:A:844:GLU:HB2	1.94	0.49
1:B:635:GLU:H	1:B:635:GLU:CD	2.16	0.49
1:C:143:VAL:HG23	1:C:324:VAL:HG21	1.94	0.49
1:C:695:LEU:HD13	1:C:699:ARG:HH12	1.78	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:D:724:PRO:HA	1:D:810:TYR:CB	2.43	0.49
1:E:1001:ILE:HG13	1:E:1002:GLY:N	2.27	0.49
1:E:367:ILE:HD13	1:E:496:MET:HE2	1.95	0.49
1:A:235:ILE:N	1:A:235:ILE:HD13	2.28	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:B:312:ASN:N	1:B:312:ASN:HD22	2.11	0.49
1:B:786:SER:HB2	1:B:801:ASN:OD1	2.13	0.49
1:C:438:ILE:C	1:C:440:GLY:H	2.16	0.49
1:E:973:ILE:HD11	1:E:1017:ILE:CG2	2.43	0.49
1:E:1030:LEU:O	1:E:1030:LEU:HD22	2.12	0.49
1:E:445:ILE:HG22	1:E:942:ILE:CD1	2.43	0.49
1:E:571:VAL:HG23	1:E:668:PRO:HG2	1.95	0.49
1:A:193:LEU:HD21	1:A:265:VAL:HG13	1.94	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:316:PHE:CG	1:E:687:GLN:HB2	2.47	0.48
1:D:449:LEU:O	1:D:449:LEU:HD13	2.13	0.48
1:D:489:THR:HB	1:D:490:PRO:HD3	1.94	0.48
1:D:698:ALA:HB2	1:D:851:PRO:HG2	1.93	0.48
1:E:102:ILE:O	1:E:105:VAL:HG12	2.13	0.48
1:E:4:PHE:CZ	1:E:8:ARG:HD2	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:A:143:VAL:HG22	1:A:286:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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:B:904:VAL:HG22	1:B:934:ILE:HD12	1.95	0.48
1:C:973:ILE:CD1	1:C:1017:ILE:HG22	2.43	0.48
1:D:438:ILE:O	1:D:442:LEU:HD13	2.12	0.48
1:E:156:ASN:ND2	1:E:182:TYR:N	2.60	0.48
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.95	0.48
1:A:418:ARG:HD3	1:A:419:VAL:N	2.28	0.48
1:B:1001:ILE:HG13	1:B:1002:GLY:N	2.28	0.48
1:B:565:PRO:HG3	1:B:923:ASP:HB3	1.95	0.48
1:C:886:CYS:O	1:C:890:LEU:HB2	2.14	0.48
1:C:924:VAL:O	1:C:928:VAL:HG23	2.13	0.48
1:D:115:THR:HA	1:D:118:LEU:HD13	1.95	0.48
1:D:418:ARG:HD3	1:D:419:VAL:N	2.28	0.48
1:D:80:SER:HA	1:D:90:ILE:HA	1.94	0.48
1:E:234:ILE:HG22	1:F:726:TYR:CB	2.31	0.48
1:F:185:ARG:HH11	1:F:771:TYR:CB	2.26	0.48
1:F:45:VAL:HG22	1:F:129:VAL:HG22	1.95	0.48
1:A:416:VAL:HG12	1:A:420:MET:HE2	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:C:579:PRO:HG3	1:C:660:ASP:CG	2.34	0.48
1:D:175:PHE:CD1	1:D:289:ILE:HD11	2.48	0.48
1:D:367:ILE:HG12	1:D:368:PRO:CD	2.43	0.48
1:D:713:GLN:OE1	1:D:832:PRO:HD3	2.14	0.48
1:E:528:GLU:HB3	1:E:963:ILE:HD11	1.95	0.48
1:F:969:ARG:C	1:F:972:PRO:HD2	2.34	0.48
1:A:573:PHE:HB2	1:A:666:PHE:CD2	2.48	0.48
1:A:753:TRP:HB2	1:C:217:GLY:H	1.78	0.48
1:A:751:ILE:CG2	1:A:772:LEU:HD13	2.44	0.48
1:B:936:LEU:HD12	1:B:1009:MET:CE	2.43	0.48
1:B:318:PRO:HD2	1:B:321:MET:HG3	1.95	0.48
1:C:154:LEU:O	1:C:157:TYR:HB3	2.14	0.48
1:C:214:ILE:HG12	1:C:237:LYS:HB2	1.96	0.48
1:D:1003:THR:HG23	1:D:1004:GLY:N	2.29	0.48
1:D:34:GLN:O	1:D:392:THR:HG23	2.13	0.48
1:D:416:VAL:HG12	1:D:420:MET:HE2	1.95	0.48
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:F:314:GLU:N	1:F:315:PRO:CD	2.76	0.48
1:F:527:TYR:O	1:F:531:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:695:LEU:CD1	1:F:699:ARG:HH22	2.27	0.48
1:F:924:VAL:O	1:F:928:VAL:HG23	2.13	0.48
1:A:838:ASP:O	1:A:839:ALA:C	2.51	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:C:166:LEU:HD21	1:C:310:ILE:HG23	1.94	0.48
1:D:416:VAL:HG11	1:D:497:LEU:HD23	1.96	0.48
1:D:57:VAL:CG1	1:D:88:MET:HB3	2.43	0.48
1:D:845:GLU:OE2	1:D:845:GLU:HA	2.13	0.48
1:E:108:GLN:O	1:E:111:LEU:HB3	2.12	0.48
1:D:316:PHE:CE2	1:E:687:GLN:HG3	2.48	0.48
1:F:166:LEU:HA	1:F:169:THR:HG22	1.95	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:B:575:GLN:HE21	1:B:617:PHE:HB2	1.78	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:F:442:LEU:HD12	1:F:486:LEU:HD21	1.96	0.48
2:A:2026:LMT:H82	2:A:2026:LMT:C12	2.37	0.48
1:A:944:ILE:HD11	1:A:1020:VAL:HB	1.95	0.48
1:B:435:MET:CE	1:B:490:PRO:HG3	2.44	0.48
1:B:571:VAL:HG23	1:B:668:PRO:HG2	1.96	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:B:742:LEU:HA	1:B:745:ILE:HG22	1.96	0.48
1:B:944:ILE:HG22	1:B:969:ARG:CG	2.44	0.48
1:C:162:ILE:O	1:C:165:PRO:HD2	2.14	0.48
1:C:156:ASN:OD1	1:C:180:SER:O	2.32	0.48
1:D:162:ILE:CG2	1:D:166:LEU:HD23	2.44	0.48
1:D:262:LEU:HD11	1:D:266:ALA:H	1.79	0.48
1:D:498:LYS:H	1:D:499:PRO:HD3	1.73	0.48
1:D:944:ILE:HD11	1:D:1020:VAL:HB	1.96	0.48
1:D:96:GLN:HA	1:D:96:GLN:NE2	2.29	0.48
1:D:7:ASP:C	1:D:9:PRO:HD3	2.34	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:A:217:GLY:O	1:A:234:ILE:HG12	2.14	0.48
1:A:356:TYR:HE1	1:A:513:PHE:CZ	2.31	0.48
1:B:156:ASN:ND2	1:B:182:TYR:N	2.62	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:690:VAL:HG11	1:C:694:VAL:HG11	1.95	0.48
1:D:356:TYR:O	1:D:356:TYR:HD1	1.96	0.48
1:A:808:TRP:CE3	1:D:708:GLN:HB3	2.49	0.48
1:D:940:ASN:HB3	1:D:973:ILE:HG22	1.96	0.48
1:D:766:ARG:NE	1:E:67:GLN:NE2	2.62	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:984:VAL:HG21	1:A:1005:VAL:HG11	1.96	0.48
1:A:724:PRO:CA	1:A:810:TYR:HB2	2.40	0.48
1:B:571:VAL:HG12	1:B:630:MET:SD	2.53	0.48
1:D:741:SER:OG	1:D:744:ASP:HB2	2.14	0.48
1:D:535:LEU:HD22	1:D:963:ILE:HD11	1.94	0.48
1:E:618:ALA:O	1:E:719:GLY:HA2	2.14	0.48
1:E:742:LEU:HA	1:E:745:ILE:HG22	1.95	0.48
1:F:973:ILE:HD11	1:F:1017:ILE:HG22	1.95	0.48
1:F:242:THR:HG22	1:F:245:GLN:OE1	2.14	0.48
1:A:46:GLN:HG2	1:A:89:THR:HG23	1.96	0.47
1:A:57:VAL:CG1	1:A:88:MET:HB3	2.43	0.47
1:B:156:ASN:HD21	1:B:768:LYS:HZ3	1.61	0.47
1:B:578:THR:HG21	1:B:587:THR:HB	1.95	0.47
1:C:612:VAL:HG11	1:C:615:PHE:HB3	1.95	0.47
1:D:376:LEU:O	1:D:379:THR:CG2	2.61	0.47
1:D:682:LEU:HD23	1:D:683:PHE:N	2.29	0.47
1:D:730:ILE:HD12	1:D:745:ILE:HD11	1.94	0.47
1:D:730:ILE:CD1	1:D:745:ILE:HD11	2.45	0.47
1:D:838:ASP:O	1:D:839:ALA:C	2.52	0.47
1:D:916:SER:O	1:D:917:MET:C	2.51	0.47
1:E:185:ARG:NH2	1:E:771:TYR:HB3	2.28	0.47
1:E:550:ALA:O	1:E:553:ILE:HG12	2.13	0.47
1:E:817:ARG:CG	1:E:817:ARG:NH1	2.72	0.47
1:F:190:PRO:HG3	1:F:788:TRP:CE2	2.48	0.47
1:F:379:THR:HB	1:F:398:MET:HE3	1.94	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: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:B:43:ILE:CG2	1:B:107:VAL:HG11	2.20	0.47
1:B:281:PHE:O	1:B:282:ASN:HB2	2.14	0.47
1:C:15:ILE:HG13	1:C:16:ALA:N	2.27	0.47
1:C:190:PRO:HG3	1:C:788:TRP:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ARG:CG	1:C:699:ARG:NH1	2.61	0.47
1:D:395:MET:O	1:D:399:VAL:HG12	2.14	0.47
1:D:637:ARG:O	1:D:642:ASN:HB2	2.13	0.47
1:D:745:ILE:O	1:D:749:VAL:HG23	2.14	0.47
1:D:818:TYR:O	1:D:820:GLY:N	2.46	0.47
1:E:343:THR:HA	1:E:346:GLU:HG2	1.95	0.47
1:E:363:ARG:NE	1:E:498:LYS:HE3	2.29	0.47
1:E:821:VAL:HG12	1:E:822:PRO:CD	2.44	0.47
1:E:907:GLY:HA3	1:E:1012:ALA:HB2	1.95	0.47
1:E:929:GLY:HA2	1:E:932:THR:HG22	1.97	0.47
1:E:953:GLU:C	1:E:955:GLY:N	2.67	0.47
1:F:648:ALA:HB1	1:F:714:ARG:NH1	2.28	0.47
1:A:210:GLN:NE2	1:A:249:ILE:HG13	2.29	0.47
1:B:4:PHE:CZ	1:B:8:ARG:HD2	2.50	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: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:E:339:GLU:HG2	1:E:342:LYS:NZ	2.29	0.47
1:E:362:PHE:O	1:E:365:THR:HB	2.13	0.47
1:E:520:PHE:O	1:E:523:THR:HG22	2.14	0.47
1:E:578:THR:CG2	1:E:587:THR:HB	2.45	0.47
1:F:404:LEU:HD13	1:F:449:LEU:HD13	1.96	0.47
1:F:695:LEU:HD13	1:F:699:ARG:HH12	1.78	0.47
1:F:723:GLU:HG3	1:F:813:PRO:HG3	1.96	0.47
1:A:219:LEU:C	1:A:221:GLY:H	2.18	0.47
1:A:535:LEU:HD22	1:A:963:ILE:HD11	1.95	0.47
1:B:371:ALA:O	1:B:374:VAL:HG12	2.14	0.47
1:C:452:VAL:HG22	1:C:883:VAL:CG2	2.44	0.47
1:D:984:VAL:HG21	1:D:1005:VAL:HG11	1.96	0.47
1:D:150:THR:N	1:D:153:ASP:HB2	2.29	0.47
1:D:6:ILE:H	1:D:6:ILE:HD12	1.79	0.47
1:D:4:PHE:CZ	1:D:8:ARG:HD2	2.49	0.47
1:D:535:LEU:CD2	1:D:963:ILE:HD11	2.44	0.47
1:D:354:VAL:HG11	1:D:979:ALA:HA	1.97	0.47
1:E:158:ILE:HG22	1:E:162:ILE:CD1	2.39	0.47
1:E:563:PHE:CD2	1:E:564:LEU:HD22	2.48	0.47
1:E:578:THR:OG1	1:E:579:PRO:HD2	2.14	0.47
1:F:456:MET:HB2	1:F:467:TYR:HB3	1.97	0.47
1:F:587:THR:O	1:F:591:VAL:HG23	2.14	0.47
1:F:903:VAL:CG2	1:F:1020:VAL:HG22	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:939:LYS:HZ3	1:F:976:THR:CG2	2.27	0.47
1:A:400:LEU:HD12	1:A:470:PHE:CZ	2.47	0.47
1:A:465:VAL:O	1:A:469:GLN:HG2	2.15	0.47
1:A:156:ASN:ND2	1:A:768:LYS:NZ	2.61	0.47
1:B:907:GLY:HA2	1:B:1012:ALA:HB2	1.97	0.47
1:B:108:GLN:O	1:B:111:LEU:HB3	2.13	0.47
1:B:20:MET:CE	1:B:374:VAL:HG23	2.40	0.47
1:B:480:LEU:O	1:B:483:ILE:HG23	2.14	0.47
1:C:242:THR:HG22	1:C:245:GLN:OE1	2.15	0.47
1:C:966:CYS:O	1:C:970:LEU:HB2	2.15	0.47
1:D:190:PRO:C	1:D:192:LYS:H	2.18	0.47
1:D:891:TYR:CG	1:D:896:ILE:HD11	2.49	0.47
1:E:936:LEU:HD12	1:E:1009:MET:CE	2.44	0.47
1:E:281:PHE:O	1:E:282:ASN:HB2	2.14	0.47
1:A:314:GLU:N	1:A:315:PRO:CD	2.77	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:C:544:ILE:HD11	1:C:1019:TRP:HZ2	1.79	0.47
1:D:10:ILE:O	1:D:10:ILE:HG13	2.13	0.47
1:D:705:LEU:HD13	1:D:849:GLN:OE1	2.13	0.47
1:D:982:LEU:HD23	1:D:982:LEU:O	2.15	0.47
1:E:572:LEU:HD23	1:E:573:PHE:N	2.29	0.47
1:F:544:ILE:HD11	1:F:1019:TRP:HZ2	1.80	0.47
1:F:579:PRO:HG3	1:F:660:ASP:CG	2.34	0.47
1:A:406:VAL:O	1:A:410:ILE:HG12	2.15	0.47
1:A:775:ARG:O	1:A:779:ARG:HG2	2.15	0.47
1:A:698:ALA:HB2	1:A:851:PRO:HG2	1.95	0.47
1:B:318:PRO:O	1:B:321:MET:HB2	2.15	0.47
1:B:72:ILE:CD1	1:B:75:LEU:HD13	2.42	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:D:763:ASP:HB3	1:D:768:LYS:HE3	1.97	0.47
1:D:876:TYR:O	1:D:880:LEU:HD23	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:F:438:ILE:C	1:F:440:GLY:H	2.18	0.47
1:A:99:ASP:OD2	1:A:101:ASP:HB2	2.15	0.47
1:A:190:PRO:HA	1:A:193:LEU:HB2	1.97	0.47
1:A:396:PHE:HA	1:A:399:VAL:CG1	2.44	0.47
1:A:763:ASP:HB3	1:A:768:LYS:HE3	1.96	0.47
1:A:687:GLN:NE2	1:A:821:VAL:HG21	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:ILE:HG12	1:A:959:VAL:N	2.29	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:B:76:ARG:HD3	1:B:863:TYR:CE2	2.49	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:C:314:GLU:N	1:C:315:PRO:CD	2.77	0.47
1:C:406:VAL:HG13	1:C:410:ILE:HG23	1.95	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:D:485:ALA:HA	1:D:489:THR:OG1	2.14	0.47
1:D:85:ASP:OD2	1:D:620:ARG:HG3	2.15	0.47
1:E:298:ASN:O	1:E:302:THR:HG22	2.15	0.47
1:F:354:VAL:CG2	1:F:982:LEU:HG	2.45	0.47
1:A:839:ALA:O	1:A:844:GLU:HB2	2.15	0.47
1:A:7:ASP:C	1:A:9:PRO:HD3	2.36	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:169:THR:HG23	1:C:172:VAL:CG2	2.45	0.47
1:C:443:VAL:O	1:C:447:MET:HB2	2.15	0.47
1:C:723:GLU:HG3	1:C:813:PRO:HG3	1.96	0.47
1:E:158:ILE:CG2	1:E:162:ILE:HD11	2.37	0.47
1:E:34:GLN:CB	1:E:333:VAL:HG22	2.45	0.47
1:E:376:LEU:O	1:E:379:THR:HG22	2.15	0.47
1:F:162:ILE:O	1:F:165:PRO:HD2	2.15	0.47
1:A:419:VAL:CG2	1:A:430:ALA:HB1	2.42	0.47
1:A:563:PHE:CZ	1:A:564:LEU:HD23	2.49	0.47
1:B:158:ILE:HG22	1:B:162:ILE:CD1	2.41	0.47
1:C:26:SER:O	1:C:30:LEU:HG	2.15	0.47
1:C:648:ALA:HB1	1:C:714:ARG:NH1	2.27	0.47
1:D:465:VAL:O	1:D:469:GLN:HG2	2.15	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:E:577:GLN:HG3	1:E:616:ASN:HD21	1.79	0.47
1:F:34:GLN:O	1:F:392:THR:HG22	2.15	0.47
1:A:370:ILE:HD11	1:A:488:LEU:CD1	2.45	0.47
1:A:741:SER:OG	1:A:744:ASP:HB2	2.15	0.47
1:B:179:GLY:HA2	2:B:2033:LMT:O3'	2.15	0.47
1:B:215:SER:HB2	1:C:750:SER:CB	2.44	0.47
1:B:38:ILE:HG13	1:B:462:SER:HB2	1.96	0.47
1:B:363:ARG:NE	1:B:498:LYS:HE3	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:ALA:O	1:B:719:GLY:HA2	2.15	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: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:524:THR:CG2	1:D:970:LEU:HD12	2.45	0.47
1:D:807:LYS:HG3	1:D:808:TRP:N	2.30	0.47
1:D:952:HIS:CE1	1:D:958:ILE:HG22	2.50	0.47
1:E:318:PRO:O	1:E:321:MET:HB2	2.14	0.47
1:E:412:VAL:HG11	1:E:489:THR:OG1	2.15	0.47
1:E:540:PRO:O	1:E:544:ILE:HG22	2.15	0.47
1:F:155:SER:O	1:F:159:VAL:HG23	2.14	0.47
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:C:922:ASN:OD1	1:C:926:PHE:HD2	1.98	0.46
1:D:15:ILE:O	1:D:19:ILE:HG13	2.15	0.46
1:D:219:LEU:C	1:D:221:GLY:H	2.18	0.46
1:D:371:ALA:O	1:D:375:VAL:HG22	2.14	0.46
1:D:930:LEU:O	1:D:933:THR:HG22	2.14	0.46
1:E:207:ILE:H	1:E:207:ILE:HG12	1.61	0.46
1:E:565:PRO:HG3	1:E:923:ASP:HB3	1.96	0.46
1:F:452:VAL:HG22	1:F:883:VAL:CG2	2.44	0.46
1:F:540:PRO:O	1:F:543:LEU:HB2	2.15	0.46
1:F:922:ASN:OD1	1:F:926:PHE:HD2	1.98	0.46
1:A:11:PHE:O	1:A:15:ILE:HG22	2.15	0.46
1:A:731:ASP:CB	1:A:734:LYS:HB2	2.37	0.46
1:A:943:LEU:HB3	1:A:969:ARG:HH11	1.80	0.46
1:A:96:GLN:NE2	1:A:96:GLN:HA	2.31	0.46
1:A:354:VAL:HG11	1:A:979:ALA:HA	1.96	0.46
1:B:553:ILE:O	1:B:557:THR:HG23	2.15	0.46
1:B:702:PHE:CE2	1:B:826:ILE:HD12	2.50	0.46
1:B:817:ARG:NH1	1:B:817:ARG:CG	2.71	0.46
1:C:749:VAL:O	1:C:753:TRP:HD1	1.98	0.46
1:D:158:ILE:HG22	1:D:159:VAL:N	2.29	0.46
1:D:190:PRO:HA	1:D:193:LEU:HB2	1.97	0.46
1:D:493:CYS:HA	1:D:497:LEU:HD22	1.97	0.46
1:D:655:PHE:CD2	1:D:663:VAL:HG11	2.50	0.46
1:F:150:THR:H	1:F:153:ASP:HB2	1.80	0.46
1:F:453:PHE:CE2	1:F:474:ILE:HD12	2.50	0.46
1:A:186:ILE:HG22	1:A:772:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:NH1	1:A:496:MET:O	2.49	0.46
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:A:794:LYS:HA	1:A:794:LYS:HD3	1.66	0.46
1:B:207:ILE:H	1:B:207:ILE:HG12	1.61	0.46
1:D:251:LEU:HD13	1:D:262:LEU:HD23	1.97	0.46
1:D:839:ALA:O	1:D:844:GLU:HB2	2.15	0.46
1:E:578:THR:HA	1:E:661:ALA:HA	1.98	0.46
1:E:702:PHE:CE2	1:E:826:ILE:HD12	2.50	0.46
1:E:681:ASP:OD1	1:E:859:THR:HG23	2.16	0.46
1:F:425:LEU:HD23	1:F:426:SER:H	1.81	0.46
1:F:886:CYS:O	1:F:890:LEU:HB2	2.16	0.46
1:F:985:VAL:N	1:F:986:PRO:CD	2.78	0.46
1:A:525:HIS:O	1:A:528:GLU:HB2	2.15	0.46
1:A:810:TYR:CD2	1:A:810:TYR:O	2.69	0.46
1:A:456:MET:HE1	1:A:928:VAL:HA	1.96	0.46
1:A:982:LEU:HD23	1:A:982:LEU:O	2.16	0.46
1:B:762:ILE:HG22	1:B:767:VAL:HG22	1.97	0.46
1:D:355:MET:CE	1:D:410:ILE:HD11	2.45	0.46
1:D:437:GLN:C	1:D:438:ILE:HG13	2.35	0.46
1:D:573:PHE:CB	1:D:666:PHE:HE2	2.29	0.46
1:E:907:GLY:HA2	1:E:1012:ALA:HB2	1.96	0.46
1:E:45:VAL:HB	1:E:90:ILE:CG2	2.41	0.46
1:E:575:GLN:HE21	1:E:617:PHE:HB2	1.81	0.46
1:E:753:TRP:CH2	1:E:785:LEU:HG	2.50	0.46
1:F:171:GLY:HA3	1:F:302:THR:OG1	2.14	0.46
1:A:682:LEU:HD23	1:A:683:PHE:N	2.30	0.46
1:A:845:GLU:HA	1:A:845:GLU:OE2	2.15	0.46
1:A:4:PHE:CZ	1:A:8:ARG:HD2	2.51	0.46
1:B:317:MET:HE1	1:B:323:VAL:HG23	1.98	0.46
1:B:339:GLU:HG2	1:B:342:LYS:NZ	2.30	0.46
1:B:692:HIS:C	1:B:692:HIS:CD2	2.89	0.46
1:B:907:GLY:HA3	1:B:1012:ALA:HB2	1.96	0.46
1:A:70:ASN:ND2	1:C:175:PHE:CE1	2.83	0.46
1:C:527:TYR:CE2	1:C:966:CYS:HB3	2.51	0.46
1:D:303:ALA:HB2	1:D:330:THR:HG21	1.98	0.46
1:D:958:ILE:HG12	1:D:959:VAL:N	2.30	0.46
1:E:61:VAL:CG2	1:E:122:VAL:HG21	2.46	0.46
1:E:318:PRO:HD2	1:E:321:MET:HG3	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:725:GLN:OE1	1:E:811:GLY:HA3	2.16	0.46
1:F:527:TYR:CE2	1:F:966:CYS:HB3	2.51	0.46
1:F:753:TRP:CZ2	1:F:785:LEU:HA	2.51	0.46
1:F:749:VAL:O	1:F:753:TRP:HD1	1.98	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: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:B:578:THR:CG2	1:B:587:THR:HB	2.45	0.46
1:B:687:GLN:NE2	1:B:821:VAL:HG21	2.23	0.46
1:A:56:THR:CG2	1:C:213:GLN:HB3	2.37	0.46
1:C:242:THR:CG2	1:C:245:GLN:HG3	2.45	0.46
1:C:184:MET:CE	1:C:268:VAL:HG13	2.46	0.46
1:D:188:LEU:HG	1:D:772:LEU:HD21	1.96	0.46
1:D:792:ASN:CG	1:D:793:ASP:H	2.17	0.46
1:F:242:THR:CG2	1:F:245:GLN:HG3	2.45	0.46
1:F:595:ARG:O	1:F:599:LEU:N	2.48	0.46
1:F:973:ILE:CD1	1:F:1017:ILE:HG22	2.45	0.46
1:A:395:MET:O	1:A:399:VAL:HG12	2.16	0.46
1:B:1006:ILE:HG13	1:B:1007:GLY:N	2.29	0.46
1:C:576:VAL:HG22	1:C:663:VAL:HG12	1.97	0.46
1:C:575:GLN:HE21	1:C:666:PHE:HZ	1.63	0.46
1:C:985:VAL:N	1:C:986:PRO:CD	2.79	0.46
1:D:190:PRO:HG3	1:D:788:TRP:CE2	2.51	0.46
1:D:378:GLY:O	1:D:382:VAL:HG23	2.16	0.46
1:E:15:ILE:O	1:E:19:ILE:HG23	2.16	0.46
1:E:399:VAL:O	1:E:402:ILE:HG12	2.16	0.46
1:E:590:VAL:HG11	1:E:661:ALA:CB	2.45	0.46
1:E:958:ILE:HG12	1:E:959:VAL:H	1.81	0.46
1:E:944:ILE:HG22	1:E:969:ARG:CG	2.46	0.46
1:F:397:GLY:HA3	1:F:473:THR:HG21	1.97	0.46
1:F:58:GLN:O	1:F:63:GLN:HB2	2.15	0.46
1:A:202:ASP:OD1	1:A:791:ARG:NH2	2.44	0.46
1:A:225:VAL:H	1:B:780:MET:HE1	1.81	0.46
1:A:85:ASP:HB3	1:A:87:SER:OG	2.16	0.46
1:B:376:LEU:O	1:B:379:THR:HG22	2.15	0.46
1:B:540:PRO:O	1:B:544:ILE:HG22	2.15	0.46
1:B:590:VAL:HG11	1:B:661:ALA:CB	2.46	0.46
1:D:1009:MET:O	1:D:1013:THR:HG23	2.16	0.46
1:D:452:VAL:HG11	1:D:931:LEU:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1014:VAL:HG12	1:E:1015:LEU:HD12	1.98	0.46
1:E:800:PHE:CD2	1:E:804:ALA:HB2	2.50	0.46
1:E:942:ILE:O	1:E:946:GLU:HB2	2.16	0.46
1:E:958:ILE:N	1:E:958:ILE:CD1	2.79	0.46
1:F:216:SER:HB2	1:F:234:ILE:HG13	1.97	0.46
1:F:184:MET:CE	1:F:268:VAL:HG13	2.45	0.46
1:F:655:PHE:HB3	1:F:663:VAL:HG23	1.97	0.46
1:F:683:PHE:CE1	1:F:818:TYR:CD2	3.04	0.46
1:A:150:THR:N	1:A:153:ASP:HB2	2.30	0.46
1:B:15:ILE:O	1:B:19:ILE:HG23	2.16	0.46
2:B:2033:LMT:O6B	2:B:2033:LMT:H6E	2.16	0.46
1:B:800:PHE:CD2	1:B:804:ALA:HB2	2.51	0.46
1:C:150:THR:H	1:C:153:ASP:HB2	1.80	0.46
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.16	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:D:1022:LEU:HA	1:D:1022:LEU:HD23	1.77	0.46
1:D:158:ILE:HD13	1:D:162:ILE:HD12	1.97	0.46
1:D:197:GLN:HB3	1:D:797:MET:SD	2.56	0.46
1:D:228:GLN:NE2	1:D:230:LEU:H	2.04	0.46
1:D:434:SER:O	1:D:437:GLN:HG2	2.16	0.46
1:D:840:MET:HA	1:D:844:GLU:CB	2.46	0.46
1:D:891:TYR:OH	1:D:945:VAL:HG13	2.15	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:E:904:VAL:HG22	1:E:934:ILE:HD12	1.96	0.46
1:A:254:ASN:HD21	1:A:258:SER:CB	2.26	0.46
1:A:541:TYR:C	1:A:543:LEU:H	2.20	0.46
1:A:559:ILE:HA	1:A:560:PRO:HD3	1.78	0.46
1:A:592:ASP:O	1:A:595:ARG:HB2	2.16	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:472:ILE:N	1:C:472:ILE:CD1	2.77	0.46
1:C:550:ALA:HA	1:C:553:ILE:CG1	2.46	0.46
1:C:695:LEU:HD13	1:C:699:ARG:HH22	1.81	0.46
1:C:982:LEU:O	1:C:985:VAL:HG22	2.16	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:472:ILE:C	1:D:472:ILE:HD12	2.36	0.46
1:D:784:ASP:O	1:D:787:LYS:HB3	2.17	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:E:125:GLN:HG3	2:E:2033:LMT:O4'	2.16	0.46
1:E:942:ILE:HG12	1:E:942:ILE:H	1.50	0.46
1:F:490:PRO:O	1:F:493:CYS:HB2	2.16	0.46
1:A:157:TYR:O	1:A:158:ILE:C	2.55	0.45
1:A:518:ARG:O	1:A:522:SER:HB3	2.16	0.45
1:A:713:GLN:OE1	1:A:832:PRO:HD3	2.16	0.45
1:A:840:MET:HA	1:A:844:GLU:CB	2.46	0.45
1:B:619:GLY:HA3	1:B:720:MET:SD	2.56	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:C:683:PHE:CZ	1:C:818:TYR:CZ	3.05	0.45
1:D:157:TYR:CZ	1:D:317:MET:HG3	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:361:ASN:HB3	1:D:364:ALA:HB3	1.98	0.45
1:D:748:THR:HG21	1:D:790:VAL:HG22	1.97	0.45
1:E:133:VAL:O	1:E:292:LYS:HE2	2.16	0.45
1:E:178:PHE:HE2	1:E:277:ILE:HD12	1.81	0.45
1:E:458:PHE:CE2	2:E:2032:LMT:H52	2.51	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:F:766:ARG:O	1:F:768:LYS:HG3	2.16	0.45
1:F:915:THR:HG23	1:F:920:LEU:HB2	1.98	0.45
1:F:95:GLU:O	1:F:97:GLY:N	2.47	0.45
1:A:958:ILE:HG13	1:A:1025:VAL:HG13	1.98	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:568:ASP:CB	1:A:634:TRP:CZ3	2.89	0.45
1:A:80:SER:OG	1:A:817:ARG:HB2	2.16	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:B:676:ASN:HD21	1:B:827:LEU:CD1	2.23	0.45
1:B:958:ILE:H	1:B:958:ILE:HD13	1.80	0.45
1:B:972:PRO:O	1:B:976:THR:HG23	2.16	0.45
1:C:96:GLN:HG3	1:C:462:SER:N	2.31	0.45
1:C:753:TRP:CZ2	1:C:785:LEU:HA	2.51	0.45
1:D:578:THR:OG1	1:D:587:THR:HG22	2.16	0.45
1:D:85:ASP:HB3	1:D:87:SER:OG	2.17	0.45
1:E:231:ASN:HD21	1:F:584:ALA:H	1.64	0.45
1:E:541:TYR:O	1:E:544:ILE:HG23	2.16	0.45
1:E:705:LEU:O	1:E:705:LEU:HD23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:TYR:CD2	1:F:970:LEU:HG	2.51	0.45
1:F:550:ALA:HA	1:F:553:ILE:CG1	2.45	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:A:34:GLN:O	1:A:392:THR:HG23	2.16	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:B:446:ALA:HB2	1:B:482:VAL:HG21	1.99	0.45
1:B:521:LEU:O	1:B:525:HIS:ND1	2.49	0.45
1:C:291:ILE:CD1	1:C:306:ILE:HD12	2.44	0.45
1:C:442:LEU:HD12	1:C:486:LEU:HD21	1.96	0.45
1:C:90:ILE:O	1:C:90:ILE:HD12	2.17	0.45
1:D:186:ILE:HG22	1:D:186:ILE:O	2.16	0.45
1:D:65:ILE:HD13	1:D:66:GLU:N	2.31	0.45
1:D:792:ASN:HB2	1:D:798:VAL:HG23	1.99	0.45
1:E:137:LEU:HD21	1:E:302:THR:HG23	1.98	0.45
1:E:442:LEU:O	1:E:445:ILE:HG12	2.16	0.45
1:E:972:PRO:O	1:E:976:THR:HG23	2.17	0.45
1:F:169:THR:HG23	1:F:172:VAL:CG2	2.46	0.45
1:F:695:LEU:HD13	1:F:699:ARG:HH22	1.81	0.45
1:F:731:ASP:C	1:F:733:GLU:H	2.19	0.45
1:F:683:PHE:CZ	1:F:818:TYR:CZ	3.05	0.45
1:A:133:VAL:HG22	1:A:672:LEU:HD13	1.99	0.45
1:A:437:GLN:C	1:A:438:ILE:HG13	2.37	0.45
1:A:887:LEU:HD21	1:A:942:ILE:CD1	2.47	0.45
1:B:45:VAL:HB	1:B:90:ILE:CG2	2.43	0.45
1:B:792:ASN:HB2	1:B:796:GLU:O	2.16	0.45
1:C:10:ILE:O	1:C:14:VAL:HG23	2.17	0.45
1:C:328:ASP:O	1:C:331:PRO:HD2	2.17	0.45
1:C:428:ARG:HB2	1:C:428:ARG:CZ	2.46	0.45
1:C:456:MET:CE	1:C:931:LEU:HD12	2.47	0.45
1:D:363:ARG:NH1	1:D:496:MET:O	2.49	0.45
1:E:579:PRO:HD3	1:E:660:ASP:O	2.17	0.45
1:A:15:ILE:O	1:A:19:ILE:HG13	2.16	0.45
1:A:710:PRO:HD3	1:D:807:LYS:NZ	2.32	0.45
1:B:362:PHE:O	1:B:365:THR:HB	2.15	0.45
1:B:399:VAL:O	1:B:402:ILE:HG12	2.17	0.45
1:B:420:MET:HE1	1:B:499:PRO:HA	1.99	0.45
1:C:175:PHE:CD2	1:C:175:PHE:C	2.89	0.45
1:C:503:GLY:C	1:C:505:HIS:H	2.20	0.45
1:D:43:ILE:HG12	1:D:104:GLN:HA	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:541:TYR:C	1:D:543:LEU:H	2.19	0.45
1:D:563:PHE:CZ	1:D:564:LEU:HD23	2.52	0.45
1:D:80:SER:OG	1:D:817:ARG:HB2	2.16	0.45
1:E:709:ASN:OD1	1:E:710:PRO:HD2	2.17	0.45
1:E:896:ILE:N	1:E:897:PRO:HD2	2.30	0.45
1:F:1015:LEU:O	1:F:1019:TRP:HD1	1.99	0.45
1:F:169:THR:CG2	1:F:306:ILE:HG22	2.47	0.45
1:F:96:GLN:HG3	1:F:462:SER:N	2.31	0.45
1:F:418:ARG:NH1	1:F:968:MET:HB3	2.32	0.45
1:A:157:TYR:CD2	1:A:321:MET:HE3	2.51	0.45
1:A:355:MET:CE	1:A:410:ILE:HD11	2.46	0.45
1:A:738:LEU:HD12	1:A:738:LEU:N	2.31	0.45
1:B:390:ILE:HG23	1:B:395:MET:SD	2.56	0.45
1:B:548:ILE:HG12	1:B:548:ILE:H	1.65	0.45
1:C:397:GLY:HA3	1:C:473:THR:HG21	1.99	0.45
1:C:58:GLN:O	1:C:63:GLN:HB2	2.16	0.45
1:D:273:GLN:HG3	1:D:771:TYR:HE1	1.81	0.45
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.99	0.45
1:E:418:ARG:HH11	1:E:418:ARG:HG2	1.82	0.45
1:E:568:ASP:O	1:E:569:GLN:C	2.54	0.45
1:E:652:GLN:O	1:E:656:PHE:HB2	2.16	0.45
1:F:981:ILE:HG22	1:F:1006:ILE:HB	1.99	0.45
1:F:966:CYS:O	1:F:970:LEU:HB2	2.15	0.45
1:F:351:VAL:HG22	1:F:979:ALA:O	2.17	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:C:1020:VAL:N	1:C:1021:PRO:CD	2.80	0.45
1:C:1:MET:O	1:C:2:SER:C	2.54	0.45
1:C:550:ALA:HA	1:C:553:ILE:HG12	1.98	0.45
1:C:351:VAL:HG22	1:C:979:ALA:O	2.17	0.45
1:D:181:GLN:HG3	1:D:768:LYS:NZ	2.32	0.45
1:D:538:ARG:O	1:D:539:ALA:HB3	2.17	0.45
1:D:528:GLU:OE2	1:D:967:ARG:NE	2.49	0.45
1:E:232:ALA:HB1	1:F:724:PRO:O	2.16	0.45
1:F:575:GLN:HE21	1:F:666:PHE:HZ	1.63	0.45
1:F:726:TYR:CZ	1:F:808:TRP:CZ3	3.05	0.45
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.17	0.45
1:A:273:GLN:NE2	1:A:769:ARG:NH1	2.65	0.45
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.99	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ALA:HA	1:A:834:LEU:HD23	1.97	0.45
1:A:971:ARG:HB3	1:A:972:PRO:HD3	1.99	0.45
1:B:705:LEU:O	1:B:705:LEU:HD23	2.17	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: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:D:958:ILE:HG13	1:D:1025:VAL:HG13	1.99	0.45
1:D:186:ILE:HG22	1:D:772:LEU:HD23	1.97	0.45
1:D:1:MET:O	1:D:5:PHE:HD1	2.00	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: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:F:2:SER:O	1:F:6:ILE:HG13	2.16	0.45
1:A:891:TYR:OH	1:A:945:VAL:HG13	2.16	0.45
1:B:1014:VAL:HG12	1:B:1015:LEU:HD12	1.98	0.45
1:B:428:ARG:N	1:B:428:ARG:HD2	2.26	0.45
1:B:958:ILE:N	1:B:958:ILE:CD1	2.79	0.45
1:C:1015:LEU:O	1:C:1019:TRP:HD1	1.99	0.45
1:C:216:SER:HB2	1:C:234:ILE:HG13	1.99	0.45
1:C:282:ASN:HD22	1:C:599:LEU:HD11	1.82	0.45
1:C:61:VAL:HG22	1:C:118:LEU:HD22	1.98	0.45
1:D:99:ASP:OD2	1:D:101:ASP:HB2	2.16	0.45
1:D:219:LEU:HD11	1:E:726:TYR:CD2	2.52	0.45
1:D:405:LEU:C	1:D:405:LEU:HD22	2.37	0.45
1:D:826:ILE:HD12	1:D:827:LEU:N	2.31	0.45
1:D:971:ARG:HB3	1:D:972:PRO:HD3	1.99	0.45
1:E:120:GLN:O	1:E:124:ARG:HG3	2.17	0.45
1:E:30:LEU:HA	1:E:31:PRO:HD2	1.68	0.45
1:D:224:ALA:CB	1:E:780:MET:HE1	2.46	0.45
1:F:313:LEU:O	1:F:317:MET:HG3	2.17	0.45
1:F:428:ARG:CZ	1:F:428:ARG:HB2	2.47	0.45
1:F:550:ALA:HA	1:F:553:ILE:HG12	1.99	0.45
1:F:683:PHE:CE1	1:F:818:TYR:CE2	3.05	0.45
1:F:798:VAL:HA	1:F:799:PRO:HD3	1.81	0.45
1:A:936:LEU:HD12	1:A:1009:MET:CE	2.46	0.45
1:A:190:PRO:HG3	1:A:788:TRP:CE2	2.52	0.45
1:A:414:GLU:O	1:A:418:ARG:HG3	2.17	0.45
1:A:530:GLY:O	1:A:531:VAL:C	2.56	0.45
1:A:80:SER:HA	1:A:90:ILE:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:HD23	1:B:266:ALA:HB2	1.99	0.45
1:B:798:VAL:HA	1:B:799:PRO:HD3	1.82	0.45
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.52	0.45
1:C:595:ARG:O	1:C:599:LEU:HB2	2.16	0.45
1:D:154:LEU:HD12	1:D:286:ALA:HA	1.99	0.45
1:D:789:TYR:HE2	1:D:799:PRO:HG3	1.81	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
1:E:818:TYR:O	1:E:819:ASN:HB2	2.17	0.45
1:E:944:ILE:HG22	1:E:969:ARG:HG3	1.98	0.45
1:F:859:THR:HG23	1:F:860:GLY:N	2.32	0.45
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:A:794:LYS:O	1:A:796:GLU:N	2.50	0.44
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.82	0.44
1:B:725:GLN:OE1	1:B:811:GLY:HA3	2.17	0.44
1:B:821:VAL:HG12	1:B:822:PRO:CD	2.43	0.44
1:B:958:ILE:H	1:B:958:ILE:CD1	2.30	0.44
1:B:969:ARG:C	1:B:972:PRO:HD2	2.38	0.44
1:C:219:LEU:HG	1:C:234:ILE:HG22	1.98	0.44
1:C:595:ARG:O	1:C:599:LEU:N	2.48	0.44
1:C:569:GLN:HA	1:C:634:TRP:HH2	1.82	0.44
1:D:11:PHE:O	1:D:15:ILE:HG22	2.17	0.44
1:D:234:ILE:HA	1:E:726:TYR:O	2.17	0.44
1:D:358:PHE:CG	1:D:975:MET:HB2	2.52	0.44
1:D:568:ASP:CB	1:D:634:TRP:CZ3	2.89	0.44
1:D:738:LEU:N	1:D:738:LEU:HD12	2.31	0.44
1:E:527:TYR:CG	1:E:970:LEU:HD12	2.50	0.44
1:F:19:ILE:HD11	1:F:374:VAL:HG12	1.98	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:F:45:VAL:HB	1:F:90:ILE:HG13	1.98	0.44
1:F:984:VAL:C	1:F:986:PRO:HD2	2.38	0.44
1:A:452:VAL:HG11	1:A:931:LEU:O	2.17	0.44
1:A:454:LEU:HD23	1:A:454:LEU:HA	1.73	0.44
1:A:47:VAL:HG12	1:A:88:MET:HG3	1.99	0.44
1:A:528:GLU:OE2	1:A:967:ARG:NE	2.50	0.44
1:A:573:PHE:CB	1:A:666:PHE:HE2	2.29	0.44
1:A:703:LEU:O	1:A:707:ALA:HB2	2.16	0.44
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:GLU:C	1:B:955:GLY:N	2.69	0.44
1:C:683:PHE:CE1	1:C:818:TYR:CD2	3.05	0.44
1:C:731:ASP:C	1:C:733:GLU:H	2.19	0.44
1:C:95:GLU:O	1:C:97:GLY:N	2.49	0.44
1:D:228:GLN:OE1	1:E:780:MET:HB3	2.17	0.44
1:D:185:ARG:NH1	1:D:771:TYR:HB3	2.33	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:F:463:THR:HG23	1:F:464:GLY:N	2.32	0.44
1:F:453:PHE:HZ	1:F:932:THR:HB	1.82	0.44
1:A:807:LYS:HG3	1:A:808:TRP:N	2.32	0.44
1:B:133:VAL:O	1:B:292:LYS:HE2	2.16	0.44
1:B:199:THR:HG22	1:B:201:GLY:H	1.81	0.44
1:B:362:PHE:O	1:B:366:LEU:HD23	2.17	0.44
1:B:461:GLY:O	1:B:465:VAL:HG23	2.17	0.44
1:B:541:TYR:O	1:B:544:ILE:HG23	2.17	0.44
1:C:490:PRO:O	1:C:493:CYS:HB2	2.16	0.44
1:C:527:TYR:CD2	1:C:970:LEU:HG	2.52	0.44
1:D:702:PHE:HZ	1:D:843:VAL:HG13	1.82	0.44
1:E:435:MET:CE	1:E:490:PRO:HG3	2.47	0.44
1:E:631:LEU:CD1	1:E:644:VAL:HG22	2.47	0.44
1:E:69:MET:HE3	1:E:107:VAL:HG22	2.00	0.44
1:E:707:ALA:C	1:E:709:ASN:H	2.19	0.44
1:E:748:THR:HG21	1:E:790:VAL:HG22	2.00	0.44
1:E:792:ASN:HB2	1:E:796:GLU:O	2.16	0.44
1:F:612:VAL:CG1	1:F:615:PHE:HB3	2.47	0.44
1:F:61:VAL:HG22	1:F:118:LEU:HD22	1.99	0.44
1:F:569:GLN:HA	1:F:634:TRP:HH2	1.82	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:B:61:VAL:CG2	1:B:122:VAL:HG21	2.47	0.44
1:B:133:VAL:HG12	1:B:135:ASN:OD1	2.18	0.44
1:B:528:GLU:CD	1:B:967:ARG:HG3	2.38	0.44
1:B:55:GLU:C	1:B:57:VAL:H	2.20	0.44
1:B:709:ASN:OD1	1:B:710:PRO:HD2	2.16	0.44
1:C:306:ILE:O	1:C:306:ILE:HG13	2.17	0.44
1:C:370:ILE:O	1:C:373:PRO:HD2	2.18	0.44
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.17	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:E:188:LEU:HD23	1:E:266:ALA:HB2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:HIS:C	1:E:340:VAL:H	2.20	0.44
1:E:72:ILE:CD1	1:E:75:LEU:HD13	2.46	0.44
1:F:111:LEU:C	1:F:113:LEU:N	2.71	0.44
1:A:10:ILE:HG13	1:A:10:ILE:O	2.17	0.44
1:A:146:ASP:C	1:A:148:SER:N	2.71	0.44
1:A:738:LEU:HD22	1:A:798:VAL:HG11	1.99	0.44
1:A:887:LEU:HD23	1:A:887:LEU:HA	1.78	0.44
1:B:568:ASP:O	1:B:634:TRP:CH2	2.70	0.44
1:C:404:LEU:HD13	1:C:449:LEU:HD13	1.98	0.44
1:C:278:ASN:HB2	1:C:613:THR:CG2	2.48	0.44
1:C:652:GLN:HG3	1:C:714:ARG:NH1	2.31	0.44
1:D:363:ARG:NH2	2:D:2026:LMT:O3B	2.49	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:D:861:LEU:O	1:D:865:GLU:HB2	2.18	0.44
1:D:891:TYR:OH	1:D:942:ILE:HA	2.18	0.44
1:E:559:ILE:CD1	1:E:560:PRO:HD2	2.48	0.44
1:F:503:GLY:C	1:F:505:HIS:H	2.21	0.44
1:F:652:GLN:HG3	1:F:714:ARG:NH1	2.32	0.44
1:F:982:LEU:O	1:F:985:VAL:HG22	2.18	0.44
1:A:330:THR:N	1:A:331:PRO:CD	2.80	0.44
1:A:333:VAL:O	1:A:337:ILE:HG12	2.17	0.44
1:B:189:ASP:HB3	1:B:192:LYS:HB3	1.99	0.44
2:B:2033:LMT:H111	2:B:2033:LMT:H71	1.98	0.44
1:B:223:PRO:HG3	1:C:275:TYR:CD2	2.53	0.44
1:B:314:GLU:N	1:B:315:PRO:CD	2.80	0.44
1:B:418:ARG:O	1:B:422:GLU:HG3	2.17	0.44
1:C:186:ILE:CG2	1:C:268:VAL:HG22	2.46	0.44
1:D:157:TYR:O	1:D:158:ILE:C	2.55	0.44
1:D:631:LEU:HD22	1:D:644:VAL:HG23	2.00	0.44
1:D:668:PRO:HA	1:D:669:PRO:HD3	1.75	0.44
1:F:186:ILE:CG2	1:F:268:VAL:HG22	2.48	0.44
1:F:65:ILE:HD11	1:F:90:ILE:HG12	2.00	0.44
1:F:720:MET:SD	1:F:720:MET:N	2.81	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:B:438:ILE:O	1:B:439:GLN:C	2.56	0.44
1:C:39:ALA:HA	1:C:40:PRO:HD3	1.78	0.44
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.58	0.44
1:C:572:LEU:HB3	1:C:629:ILE: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:45:VAL:HB	1:C:90:ILE:HG13	2.00	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:D:357:LEU:HD22	1:D:357:LEU:O	2.18	0.44
1:D:38:ILE:HD13	1:D:38:ILE:H	1.83	0.44
1:D:747:SER:O	1:D:751:ILE:HG13	2.17	0.44
1:D:974:VAL:O	1:D:978:LEU:HB2	2.17	0.44
1:E:544:ILE:O	1:E:548:ILE:HG12	2.17	0.44
1:E:692:HIS:CD2	1:E:692:HIS:C	2.90	0.44
1:F:282:ASN:HD22	1:F:599:LEU:HD11	1.83	0.44
1:A:108:GLN:HA	1:A:111:LEU:HB3	2.00	0.44
1:A:228:GLN:NE2	1:A:230:LEU:H	2.06	0.44
1:B:412:VAL:HG11	1:B:489:THR:OG1	2.18	0.44
1:B:492:LEU:O	1:B:496:MET:HG3	2.18	0.44
1:B:577:GLN:HG3	1:B:616:ASN:ND2	2.32	0.44
1:B:652:GLN:O	1:B:656:PHE:HB2	2.17	0.44
1:B:578:THR:HA	1:B:661:ALA:HA	1.99	0.44
1:B:748:THR:HG21	1:B:790:VAL:HG22	2.00	0.44
1:B:958:ILE:HG12	1:B:959:VAL:H	1.81	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:D:655:PHE:HD2	1:D:658:PHE:CE2	2.36	0.44
1:D:738:LEU:HD22	1:D:798:VAL:HG11	1.98	0.44
1:E:189:ASP:HB3	1:E:192:LYS:HB3	1.98	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:E:577:GLN:HG3	1:E:616:ASN:ND2	2.33	0.44
1:F:138:MET:O	1:F:291:ILE:HG12	2.18	0.44
1:F:408:ASP:OD1	1:F:445:ILE:HD11	2.18	0.44
1:F:709:ASN:HA	1:F:710:PRO:HD3	1.72	0.44
1:F:755:SER:HB3	1:F:773:GLN:HE21	1.83	0.44
1:F:783:ASP:C	1:F:785:LEU:H	2.19	0.44
1:A:1009:MET:O	1:A:1013:THR:HG23	2.17	0.44
1:A:534:ILE:HD11	1:A:1022:LEU:HG	2.00	0.44
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.99	0.44
1:A:984:VAL:HG13	1:A:987:LEU:HD12	2.00	0.44
1:C:102:ILE:HD12	1:C:103:ALA:N	2.33	0.44
1:C:155:SER:O	1:C:159:VAL:HG23	2.18	0.44
1:C:683:PHE:CE1	1:C:818:TYR:CE2	3.05	0.44
1:C:783:ASP:C	1:C:785:LEU:H	2.20	0.44
1:E:740:VAL:HG23	1:E:792:ASN:ND2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:943:LEU:O	1:E:947:PHE:HD1	2.01	0.44
1:F:281:PHE:CZ	1:F:324:VAL:HG11	2.53	0.44
1:A:237:LYS:HD3	1:B:746:ASN:HD21	1.82	0.43
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:A:631:LEU:HD22	1:A:644:VAL:HG23	1.99	0.43
1:B:240:LEU:HD22	1:B:245:GLN:HE21	1.83	0.43
1:B:942:ILE:O	1:B:946:GLU:HB2	2.17	0.43
1:C:425:LEU:HD23	1:C:426:SER:H	1.82	0.43
1:C:197:GLN:HA	1:C:797:MET:SD	2.58	0.43
1:C:726:TYR:CZ	1:C:808:TRP:CZ3	3.05	0.43
1:C:418:ARG:CZ	1:C:968:MET:HB3	2.48	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:D:872:ALA:N	1:D:873:PRO:CD	2.81	0.43
1:D:887:LEU:HD21	1:D:942:ILE:CD1	2.47	0.43
1:E:528:GLU:CD	1:E:967:ARG:HG3	2.39	0.43
1:F:156:ASN:OD1	1:F:180:SER:O	2.36	0.43
1:F:682:LEU:O	1:F:683:PHE:HD2	2.01	0.43
1:A:190:PRO:C	1:A:192:LYS:H	2.21	0.43
1:A:175:PHE:HD1	1:A:289:ILE:HD11	1.84	0.43
1:A:745:ILE:O	1:A:749:VAL:HG23	2.17	0.43
1:A:861:LEU:O	1:A:865:GLU:HB2	2.18	0.43
1:A:872:ALA:N	1:A:873:PRO:CD	2.82	0.43
1:B:293:LEU:HD13	1:B:294:ALA:O	2.18	0.43
1:B:34:GLN:CB	1:B:333:VAL:HG22	2.48	0.43
1:B:338:HIS:C	1:B:340:VAL:H	2.21	0.43
1:B:391:ASN:ND2	1:B:394:THR:H	2.16	0.43
1:B:442:LEU:O	1:B:445:ILE:HG12	2.18	0.43
1:C:15:ILE:HD13	1:C:487:ILE:HD12	2.00	0.43
1:C:300:LEU:O	1:C:304:LYS:HG3	2.18	0.43
1:C:973:ILE:HG13	1:C:973:ILE:O	2.18	0.43
1:D:712:LEU:HD21	1:D:842:ALA:HB1	1.99	0.43
1:D:859:THR:CG2	1:D:860:GLY:N	2.80	0.43
1:D:909:ILE:C	1:D:911:ALA:N	2.72	0.43
2:E:2032:LMT:H1B	2:E:2032:LMT:O3'	2.19	0.43
1:E:215:SER:HB2	1:F:750:SER:CB	2.47	0.43
1:F:424:GLY:HA3	1:F:502:LYS:HG3	2.00	0.43
1:F:578:THR:CG2	1:F:623:SER:HB2	2.46	0.43
1:F:734:LYS:HD3	1:F:802:ALA:O	2.18	0.43
1:A:181:GLN:HG3	1:A:768:LYS:NZ	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ASN:N	1:A:254:ASN:ND2	2.64	0.43
1:A:25:LEU:HA	1:A:25:LEU:HD12	1.86	0.43
1:A:541:TYR:HA	1:A:544:ILE:HG23	1.99	0.43
1:B:414:GLU:HG3	1:B:415:ASN:N	2.33	0.43
1:B:575:GLN:NE2	1:B:617:PHE:HB2	2.34	0.43
1:B:712:LEU:HD21	1:B:843:VAL:CG2	2.48	0.43
1:B:182:TYR:HB2	1:B:768:LYS:HZ3	1.82	0.43
1:C:313:LEU:O	1:C:317:MET:HG3	2.18	0.43
1:C:762:ILE:H	1:C:762:ILE:HG12	1.51	0.43
1:D:207:ILE:H	1:D:207:ILE:HG12	1.47	0.43
1:D:379:THR:HA	1:D:382:VAL:HG23	2.00	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:E:104:GLN:O	1:E:107:VAL:HG12	2.18	0.43
1:E:690:VAL:O	1:E:691:GLY:O	2.36	0.43
1:F:1:MET:O	1:F:2:SER:C	2.57	0.43
1:F:958:ILE:HD13	1:F:959:VAL:H	1.84	0.43
1:A:234:ILE:HA	1:B:726:TYR:O	2.18	0.43
1:A:358:PHE:CG	1:A:975:MET:HB2	2.53	0.43
1:A:784:ASP:O	1:A:787:LYS:HB3	2.18	0.43
1:B:105:VAL:CG1	1:B:106:GLN:N	2.81	0.43
1:B:254:ASN:HB2	1:B:258:SER:OG	2.18	0.43
1:B:520:PHE:O	1:B:523:THR:HG22	2.18	0.43
1:B:544:ILE:O	1:B:548:ILE:HG12	2.18	0.43
1:A:219:LEU:HD11	1:B:726:TYR:CD2	2.54	0.43
1:B:552:MET:HE3	1:B:908:VAL:HB	2.00	0.43
1:C:438:ILE:O	1:C:440:GLY:N	2.51	0.43
1:C:687:GLN:CD	1:C:855:GLY:HA3	2.39	0.43
1:C:838:ASP:O	1:C:841:ALA:HB3	2.18	0.43
1:D:780:MET:HB3	1:F:228:GLN:HE21	1.82	0.43
1:E:240:LEU:HD22	1:E:245:GLN:HE21	1.84	0.43
1:E:375:VAL:O	1:E:379:THR:HB	2.19	0.43
1:E:410:ILE:HD11	1:E:976:THR:CG2	2.32	0.43
1:E:418:ARG:O	1:E:422:GLU:HG3	2.18	0.43
1:E:951:LEU:C	1:E:953:GLU:N	2.71	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:F:99:ASP:O	1:F:102:ILE:HG13	2.18	0.43
1:A:184:MET:HG2	1:A:246:PHE:CE1	2.53	0.43
1:A:32:VAL:HG22	1:A:390:ILE:HB	2.00	0.43
1:A:31:PRO:HG2	1:A:389:SER:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:LEU:HD12	1:A:881:LEU:O	2.19	0.43
1:B:145:THR:HB	1:B:320:GLY:HA2	1.99	0.43
1:B:579:PRO:HD3	1:B:660:ASP:O	2.19	0.43
1:A:131:LYS:NZ	1:B:73:ASP:OD2	2.52	0.43
1:B:753:TRP:CZ2	1:B:785:LEU:HA	2.42	0.43
1:C:83:ASN:OD1	1:C:814:LYS:HG2	2.18	0.43
1:C:65:ILE:HD11	1:C:90:ILE:HG12	2.00	0.43
1:D:190:PRO:HG2	1:D:787:LYS:HG2	2.01	0.43
1:D:316:PHE:CD2	1:E:687:GLN:HG3	2.54	0.43
1:D:533:SER:O	1:D:537:HIS:N	2.31	0.43
1:D:592:ASP:O	1:D:595:ARG:HB2	2.18	0.43
1:D:572:LEU:HD12	1:D:666:PHE:O	2.18	0.43
1:D:810:TYR:O	1:D:810:TYR:CD2	2.71	0.43
1:E:145:THR:HB	1:E:320:GLY:HA2	2.01	0.43
1:F:219:LEU:HG	1:F:234:ILE:CG2	2.48	0.43
1:A:219:LEU:HG	1:A:234:ILE:HG23	2.00	0.43
1:A:594:MET:HG3	1:A:655:PHE:CZ	2.54	0.43
1:B:702:PHE:CE2	1:B:826:ILE:CD1	3.02	0.43
1:B:757:TYR:CZ	1:B:769:ARG:HG3	2.53	0.43
1:B:818:TYR:O	1:B:819:ASN:HB2	2.19	0.43
1:B:987:LEU:HD13	1:B:1001:ILE:HD11	2.00	0.43
1:C:1013:THR:O	1:C:1017:ILE:HG12	2.19	0.43
1:C:219:LEU:HG	1:C:234:ILE:CG2	2.49	0.43
1:C:451:ALA:HB1	1:C:882:VAL:HG12	2.00	0.43
1:B:219:LEU:HD12	1:C:726:TYR:CE1	2.54	0.43
1:C:447:MET:HE1	1:C:886:CYS:HB3	1.98	0.43
1:C:891:TYR:O	1:C:892:GLU:C	2.57	0.43
1:D:242:THR:CG2	1:D:245:GLN:HG3	2.49	0.43
1:D:310:ILE:HD13	1:D:323:VAL:HG11	2.01	0.43
1:D:49:TYR:CD1	1:D:52:ALA:HB2	2.53	0.43
1:D:594:MET:HG3	1:D:655:PHE:CZ	2.53	0.43
1:D:650:ARG:HB2	1:D:650:ARG:HH11	1.84	0.43
1:D:189:ASP:HB2	1:D:775:ARG:HD3	2.01	0.43
1:E:125:GLN:NE2	1:E:769:ARG:NH1	2.51	0.43
1:E:619:GLY:HA3	1:E:720:MET:SD	2.59	0.43
1:F:368:PRO:HG3	1:F:413:VAL:HG21	2.01	0.43
1:A:70:ASN:HB2	1:C:167:SER:HB2	2.00	0.43
1:B:151:LYS:HD2	1:B:151:LYS:H	1.83	0.43
1:B:178:PHE:HE2	1:B:277:ILE:HD12	1.83	0.43
1:B:470:PHE:O	1:B:473:THR:HG22	2.19	0.43
1:C:281:PHE:CZ	1:C:324:VAL:HG11	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:330:THR:N	1:D:331:PRO:CD	2.82	0.43
1:D:370:ILE:HD11	1:D:488:LEU:CD1	2.47	0.43
1:D:31:PRO:HG2	1:D:389:SER:HB3	2.01	0.43
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.99	0.43
1:D:454:LEU:HD23	1:D:454:LEU:HA	1.74	0.43
1:D:616:ASN:HD22	1:D:616:ASN:HA	1.63	0.43
1:E:1016:ALA:O	1:E:1020:VAL:HG23	2.18	0.43
1:E:105:VAL:HG13	1:E:106:GLN:N	2.34	0.43
1:E:204:SER:O	1:E:207:ILE:HG12	2.19	0.43
1:E:254:ASN:HB2	1:E:258:SER:OG	2.19	0.43
1:E:412:VAL:HG13	1:E:435:MET:CE	2.49	0.43
1:E:712:LEU:HD21	1:E:843:VAL:CG2	2.47	0.43
1:E:552:MET:HE3	1:E:908:VAL:HB	2.00	0.43
1:F:10:ILE:O	1:F:14:VAL:HG23	2.19	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:B:391:ASN:ND2	1:B:393:LEU:H	2.13	0.43
1:D:146:ASP:C	1:D:148:SER:N	2.71	0.43
1:D:318:PRO:O	1:D:320:GLY:N	2.51	0.43
1:E:108:GLN:HG2	1:F:112:GLN:OE1	2.18	0.43
1:E:515:TRP:CH2	1:E:519:MET:HG3	2.54	0.43
1:E:757:TYR:CZ	1:E:769:ARG:HG3	2.53	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:F:555:MET:O	1:F:559:ILE:HG23	2.19	0.43
1:A:188:LEU:HG	1:A:772:LEU:HD21	2.00	0.43
1:B:120:GLN:O	1:B:124:ARG:HG3	2.19	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:B:228:GLN:HE21	1:B:231:ASN:HD21	1.67	0.43
1:B:682:LEU:HD11	1:B:856:TYR:CD2	2.53	0.43
1:C:184:MET:HE1	1:C:268:VAL:HG13	2.01	0.43
1:C:563:PHE:CD2	1:C:564:LEU:HG	2.54	0.43
1:C:958:ILE:HD13	1:C:959:VAL:H	1.84	0.43
1:D:108:GLN:HA	1:D:111:LEU:HB3	1.99	0.43
1:D:184:MET:HG2	1:D:246:PHE:CE1	2.54	0.43
1:D:306:ILE:O	1:D:310:ILE:HG23	2.18	0.43
1:D:731:ASP:CB	1:D:734:LYS:HB2	2.38	0.43
1:D:755:SER:HA	1:D:773:GLN:HG3	2.01	0.43
1:E:143:VAL:HG22	1:E:322:LYS:O	2.19	0.43
1:E:317:MET:HE1	1:E:323:VAL:HG23	2.00	0.43
1:E:330:THR:N	1:E:331:PRO:CD	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:415:ASN:ND2	1:E:434:SER:HB2	2.26	0.43
1:E:184:MET:HB2	1:E:770:VAL:HG22	2.01	0.43
1:E:958:ILE:HD13	1:E:958:ILE:H	1.80	0.43
1:F:99:ASP:HA	1:F:100:PRO:HD3	1.92	0.43
1:F:321:MET:HB3	1:F:321:MET:HE2	1.90	0.43
1:F:90:ILE:O	1:F:90:ILE:HD12	2.18	0.43
1:F:958:ILE:N	1:F:958:ILE:HD13	2.34	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:A:128:ARG:NH2	1:A:175:PHE:CE2	2.87	0.43
1:A:655:PHE:HD2	1:A:658:PHE:CE2	2.36	0.43
1:B:158:ILE:O	1:B:163:GLN:HB2	2.19	0.43
1:B:164:ASP:HB3	1:B:165:PRO:HD3	2.01	0.43
1:B:142:VAL:HG12	1:B:288:GLY:HA2	2.00	0.43
1:B:303:ALA:O	1:B:307:ARG:HB2	2.19	0.43
1:B:410:ILE:HD11	1:B:976:THR:CG2	2.31	0.43
1:B:79:SER:HB2	1:B:818:TYR:HD1	1.83	0.43
1:C:150:THR:HG22	1:C:153:ASP:CG	2.39	0.43
1:C:671:VAL:O	1:C:674:LEU:HB2	2.19	0.43
1:C:695:LEU:O	1:C:698:ALA:HB3	2.19	0.43
1:C:929:GLY:HA2	1:C:932:THR:CG2	2.49	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:D:683:PHE:CZ	1:D:825:GLU:HB2	2.54	0.43
1:E:105:VAL:CG1	1:E:106:GLN:N	2.81	0.43
1:E:470:PHE:O	1:E:473:THR:HG22	2.18	0.43
1:E:8:ARG:N	1:E:9:PRO:HD3	2.34	0.43
1:E:987:LEU:HD13	1:E:1001:ILE:HD11	2.01	0.43
1:F:111:LEU:O	1:F:113:LEU:N	2.51	0.43
1:F:300:LEU:O	1:F:304:LYS:HG3	2.19	0.43
1:F:695:LEU:O	1:F:698:ALA:HB3	2.19	0.43
1:A:523:THR:O	1:A:524:THR:C	2.57	0.42
1:A:682:LEU:HD21	1:A:856:TYR:HD1	1.84	0.42
1:A:711:ALA:HA	1:A:834:LEU:CD2	2.49	0.42
2:B:2033:LMT:H62	2:B:2033:LMT:C12	2.46	0.42
1:B:352:PHE:CD1	1:B:365:THR:CG2	3.02	0.42
1:B:515:TRP:CH2	1:B:519:MET:HG3	2.54	0.42
1:C:456:MET:HB2	1:C:467:TYR:HB3	2.00	0.42
1:C:903:VAL:O	1:C:906:LEU:HB2	2.18	0.42
1:D:936:LEU:HD12	1:D:1009:MET:CE	2.48	0.42
1:D:776:PRO:O	1:D:780:MET:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:818:TYR:OH	1:D:859:THR:OG1	2.28	0.42
1:D:682:LEU:CD2	1:D:856:TYR:HB2	2.44	0.42
1:E:228:GLN:HE21	1:E:231:ASN:HD21	1.68	0.42
1:E:46:GLN:HA	1:E:88:MET:HE3	2.01	0.42
1:E:521:LEU:O	1:E:525:HIS:ND1	2.50	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
1:A:1001:ILE:CG2	1:A:1002:GLY:N	2.82	0.42
1:A:634:TRP:O	1:A:638:PRO:HG3	2.19	0.42
1:A:695:LEU:HD13	1:A:699:ARG:NH2	2.34	0.42
1:A:76:ARG:HD3	1:A:95:GLU:OE1	2.19	0.42
1:A:794:LYS:CD	1:A:795:GLY:H	2.29	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:B:204:SER:O	1:B:207:ILE:HG12	2.19	0.42
1:B:314:GLU:HA	1:B:317:MET:HE2	2.01	0.42
1:B:541:TYR:O	1:B:1019:TRP:CZ3	2.72	0.42
1:B:840:MET:O	1:B:844:GLU:HG3	2.19	0.42
1:C:324:VAL:HG12	1:C:325:TYR:N	2.34	0.42
1:C:667:ALA:HA	1:C:668:PRO:HD3	1.84	0.42
1:C:712:LEU:HD12	1:C:715:VAL:HG21	2.00	0.42
1:D:453:PHE:CG	1:D:474:ILE:HD11	2.54	0.42
1:D:530:GLY:O	1:D:531:VAL:C	2.57	0.42
1:D:969:ARG:O	1:D:972:PRO:HD2	2.19	0.42
1:E:445:ILE:HD12	1:E:939:LYS:HG3	2.00	0.42
1:E:375:VAL:HG22	1:E:484:VAL:HG21	2.01	0.42
1:E:569:GLN:O	1:E:571:VAL:N	2.45	0.42
1:E:280:GLN:HB2	1:E:611:THR:HG23	2.00	0.42
1:F:185:ARG:HD3	1:F:771:TYR:HB2	2.01	0.42
1:F:438:ILE:O	1:F:440:GLY:N	2.53	0.42
1:F:687:GLN:CD	1:F:855:GLY:HA3	2.39	0.42
1:F:757:TYR:OH	1:F:760:ASP:OD1	2.33	0.42
1:F:803:PHE:O	1:F:804:ALA:HB2	2.19	0.42
1:A:532:ALA:O	1:A:533:SER:C	2.58	0.42
1:A:655:PHE:CG	1:A:663:VAL:HG11	2.55	0.42
1:A:683:PHE:CZ	1:A:825:GLU:HB2	2.54	0.42
1:A:694:VAL:O	1:A:697:GLN:HB3	2.20	0.42
1:B:228:GLN:NE2	1:B:231:ASN:HD21	2.17	0.42
1:B:412:VAL:HG13	1:B:435:MET:CE	2.49	0.42
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.89	0.42
1:B:631:LEU:CD1	1:B:644:VAL:HG22	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:TYR:CE1	1:C:1023:PHE:HZ	2.37	0.42
1:C:734:LYS:HD3	1:C:802:ALA:O	2.18	0.42
1:C:755:SER:HB3	1:C:773:GLN:HE21	1.83	0.42
1:D:110:LYS:HA	1:D:110:LYS:HD2	1.85	0.42
1:E:172:VAL:HG22	1:E:306:ILE:CG2	2.49	0.42
2:E:2033:LMT:H111	2:E:2033:LMT:C7	2.48	0.42
1:E:352:PHE:CD1	1:E:365:THR:CG2	3.03	0.42
1:E:738:LEU:C	1:E:792:ASN:HD21	2.23	0.42
1:E:681:ASP:CB	1:E:827:LEU:HD13	2.44	0.42
1:F:291:ILE:CD1	1:F:306:ILE:HD12	2.45	0.42
1:F:184:MET:H	1:F:761:PHE:HE1	1.67	0.42
1:F:903:VAL:O	1:F:906:LEU:HB2	2.19	0.42
1:A:944:ILE:HD11	1:A:1020:VAL:CG1	2.50	0.42
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.78	0.42
1:A:532:ALA:O	1:A:535:LEU:N	2.36	0.42
1:A:906:LEU:N	1:A:906:LEU:HD23	2.33	0.42
1:A:909:ILE:C	1:A:911:ALA:N	2.72	0.42
1:B:298:ASN:O	1:B:302:THR:HG22	2.17	0.42
1:B:172:VAL:HG22	1:B:306:ILE:CG2	2.50	0.42
1:B:30:LEU:HD23	1:B:31:PRO:HD2	2.02	0.42
1:B:409:ALA:O	1:B:413:VAL:HG23	2.19	0.42
1:B:568:ASP:HB3	1:B:634:TRP:CZ3	2.37	0.42
1:B:62:VAL:HG23	1:B:88:MET:HG3	1.99	0.42
1:B:942:ILE:H	1:B:942:ILE:HG12	1.50	0.42
1:C:424:GLY:HA3	1:C:502:LYS:HG3	2.01	0.42
1:C:690:VAL:HB	1:C:691:GLY:H	1.64	0.42
1:C:803:PHE:O	1:C:804:ALA:HB2	2.19	0.42
1:D:154:LEU:CD1	1:D:286:ALA:HA	2.48	0.42
1:D:168:ARG:HD3	1:E:75:LEU:HD21	2.02	0.42
1:D:568:ASP:O	1:D:569:GLN:HB2	2.20	0.42
1:D:610:PHE:HB3	1:D:628:PHE:HB2	2.00	0.42
1:D:815:LEU:HA	1:D:815:LEU:HD12	1.89	0.42
1:E:151:LYS:HD2	1:E:151:LYS:H	1.84	0.42
1:E:461:GLY:O	1:E:465:VAL:HG23	2.19	0.42
1:E:446:ALA:HB2	1:E:482:VAL:HG21	2.01	0.42
1:E:515:TRP:O	1:E:519:MET:HG2	2.19	0.42
1:E:592:ASP:CG	1:E:595:ARG:HH12	2.23	0.42
1:E:753:TRP:CZ2	1:E:785:LEU:HA	2.42	0.42
1:E:55:GLU:HG2	1:E:815:LEU:HD11	2.01	0.42
1:E:840:MET:O	1:E:844:GLU:HG3	2.19	0.42
1:E:909:ILE:HG13	1:E:910:GLY:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:OD1	1:F:814:LYS:HG2	2.20	0.42
1:A:167:SER:O	1:B:70:ASN:HB2	2.19	0.42
1:A:453:PHE:CG	1:A:474:ILE:HD11	2.54	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
1:A:859:THR:CG2	1:A:860:GLY:N	2.81	0.42
2:B:2032:LMT:H101	2:B:2032:LMT:H72	1.74	0.42
1:B:330:THR:N	1:B:331:PRO:CD	2.82	0.42
1:B:370:ILE:O	1:B:373:PRO:HD2	2.20	0.42
1:B:376:LEU:HD22	1:B:398:MET:HE2	2.02	0.42
1:B:726:TYR:HE2	1:B:785:LEU:CD1	2.32	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: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:D:682:LEU:HD21	1:D:856:TYR:HD1	1.84	0.42
1:E:89:THR:HG21	2:E:2033:LMT:H82	2.02	0.42
1:E:314:GLU:N	1:E:315:PRO:CD	2.82	0.42
1:D:223:PRO:O	1:E:779:ARG:NH2	2.52	0.42
1:E:812:SER:HA	1:E:813:PRO:HD3	1.73	0.42
1:F:1013:THR:O	1:F:1017:ILE:HG12	2.20	0.42
1:F:563:PHE:CD2	1:F:564:LEU:HG	2.55	0.42
1:F:578:THR:HG22	1:F:623:SER:CB	2.46	0.42
1:A:306:ILE:O	1:A:310:ILE:HG23	2.20	0.42
1:A:49:TYR:CD1	1:A:52:ALA:HB2	2.55	0.42
1:A:578:THR:OG1	1:A:587:THR:HG22	2.19	0.42
1:A:755:SER:HA	1:A:773:GLN:HG3	2.00	0.42
1:B:1001:ILE:O	1:B:1005:VAL:HG23	2.19	0.42
1:B:564:LEU:HD21	1:B:670:SER:HB3	2.01	0.42
1:C:1005:VAL:HG12	1:C:1006:ILE:N	2.35	0.42
1:C:17:LEU:HD23	1:C:20:MET:CE	2.49	0.42
1:D:164:ASP:HB2	1:D:165:PRO:HD3	2.01	0.42
1:D:958:ILE:N	1:D:958:ILE:HD13	2.35	0.42
1:E:303:ALA:O	1:E:307:ARG:HB2	2.19	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:F:306:ILE:HG13	1:F:306:ILE:O	2.19	0.42
1:F:695:LEU:HD12	1:F:696:LEU:N	2.34	0.42
1:F:891:TYR:O	1:F:892:GLU:C	2.58	0.42
1:A:405:LEU:C	1:A:405:LEU:HD22	2.39	0.42
1:A:747:SER:O	1:A:751:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:LEU:HA	1:A:885:LEU:HD12	1.77	0.42
1:B:367:ILE:HG12	1:B:367:ILE:H	1.63	0.42
1:B:454:LEU:HD23	1:B:454:LEU:HA	1.82	0.42
1:B:56:THR:O	1:B:56:THR:HG22	2.20	0.42
1:C:981:ILE:HG22	1:C:1006:ILE:HB	2.00	0.42
1:C:667:ALA:O	1:C:678:THR:HG22	2.19	0.42
1:C:695:LEU:HD12	1:C:696:LEU:N	2.35	0.42
1:C:789:TYR:HE2	1:C:799:PRO:HG3	1.85	0.42
1:C:958:ILE:HD13	1:C:958:ILE:N	2.35	0.42
1:C:94:PHE:HB3	1:C:98:THR:HG21	2.02	0.42
1:E:237:LYS:NZ	1:F:742:LEU:HD22	2.35	0.42
1:E:391:ASN:ND2	1:E:393:LEU:H	2.16	0.42
1:E:455:PRO:HG2	1:E:879:SER:HB3	2.02	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:A:186:ILE:O	1:A:186:ILE:HG22	2.18	0.42
1:A:415:ASN:HA	1:A:418:ARG:HD2	2.01	0.42
1:A:65:ILE:HD13	1:A:66:GLU:N	2.34	0.42
1:A:681:ASP:OD1	1:A:859:THR:HG22	2.20	0.42
1:A:887:LEU:CD2	1:A:942:ILE:HD12	2.50	0.42
1:A:974:VAL:O	1:A:978:LEU:HB2	2.20	0.42
1:B:1011:THR:O	1:B:1015:LEU:HB2	2.20	0.42
1:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.42
1:B:278:ASN:O	1:B:612:VAL:HA	2.19	0.42
1:C:138:MET:O	1:C:291:ILE:HG12	2.20	0.42
1:C:368:PRO:HG3	1:C:413:VAL:HG21	2.00	0.42
1:C:555:MET:O	1:C:559:ILE:HG23	2.19	0.42
1:C:698:ALA:O	1:C:702:PHE:HB2	2.19	0.42
1:C:861:LEU:HD23	1:C:861:LEU:O	2.20	0.42
1:D:137:LEU:HD11	1:D:330:THR:HG23	2.02	0.42
1:D:336:SER:O	1:D:340:VAL:HG23	2.19	0.42
1:D:456:MET:CE	1:D:931:LEU:HD12	2.49	0.42
1:D:523:THR:O	1:D:524:THR:C	2.56	0.42
1:D:745:ILE:HA	1:D:748:THR:HG22	2.02	0.42
1:D:984:VAL:HG13	1:D:987:LEU:HD12	2.00	0.42
1:E:910:GLY:HA3	1:E:1011:THR:CG2	2.50	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD12	1.88	0.42
1:E:702:PHE:CE2	1:E:826:ILE:CD1	3.03	0.42
1:A:910:GLY:HA3	1:A:1011:THR:HG21	2.02	0.42
1:A:356:TYR:C	1:A:356:TYR:CD1	2.93	0.42
1:A:456:MET:CE	1:A:931:LEU:HD12	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLY:O	1:A:534:ILE:HG22	2.19	0.42
1:A:616:ASN:N	1:A:619:GLY:O	2.50	0.42
1:A:197:GLN:CB	1:A:797:MET:HE3	2.50	0.42
1:B:944:ILE:HD11	1:B:1020:VAL:HB	2.02	0.42
1:B:48:SER:O	1:B:50:PRO:HD3	2.20	0.42
1:B:559:ILE:CD1	1:B:560:PRO:HD2	2.49	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:D:542:LEU:HD12	1:D:1022:LEU:HD13	2.02	0.42
1:D:181:GLN:HE21	1:D:181:GLN:H	1.67	0.42
1:D:541:TYR:HA	1:D:544:ILE:HG23	2.00	0.42
1:D:70:ASN:HB2	1:F:167:SER:HB2	2.01	0.42
1:D:753:TRP:HZ3	1:D:779:ARG:CB	2.29	0.42
1:D:188:LEU:HG	1:D:772:LEU:CD2	2.50	0.42
1:E:204:SER:O	1:E:208:GLN:HG3	2.20	0.42
1:F:150:THR:HG22	1:F:153:ASP:CG	2.40	0.42
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.42
1:F:418:ARG:CZ	1:F:968:MET:HB3	2.49	0.42
1:A:936:LEU:HD12	1:A:1009:MET:HE1	2.01	0.42
1:A:13:TRP:CE2	2:A:2026:LMT:C1	3.03	0.42
1:A:242:THR:CG2	1:A:245:GLN:HG3	2.48	0.42
1:A:261:ARG:CZ	1:A:263:LYS:HZ3	2.33	0.42
1:A:275:TYR:CG	1:C:223:PRO:HG3	2.55	0.42
1:A:341:VAL:O	1:A:344:LEU:HB2	2.20	0.42
1:A:88:MET:C	1:A:88:MET:SD	2.98	0.42
1:A:90:ILE:C	1:A:90:ILE:HD12	2.39	0.42
1:B:222:LEU:HD12	1:C:276:SER:HA	2.02	0.42
1:B:375:VAL:O	1:B:379:THR:HB	2.20	0.42
1:B:587:THR:HG23	1:B:588:GLN:N	2.35	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:C:749:VAL:HG22	1:C:800:PHE:HZ	1.85	0.42
1:C:984:VAL:C	1:C:986:PRO:HD2	2.40	0.42
1:D:944:ILE:HD11	1:D:1020:VAL:CG1	2.50	0.42
1:D:396:PHE:HA	1:D:399:VAL:HG12	2.02	0.42
1:D:976:THR:CG2	1:D:977:SER:N	2.83	0.42
1:E:228:GLN:NE2	1:E:231:ASN:HD21	2.17	0.42
1:E:303:ALA:HB2	1:E:330:THR:HG21	2.01	0.42
1:E:352:PHE:CD2	1:E:352:PHE:C	2.93	0.42
1:E:367:ILE:HB	1:E:368:PRO:CD	2.40	0.42
1:F:34:GLN:HG2	1:F:35:TYR:CD1	2.55	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:F:671:VAL:O	1:F:674:LEU:HB2	2.20	0.42
1:F:698:ALA:O	1:F:702:PHE:HB2	2.20	0.42
1:A:253:VAL:HG12	1:A:259:GLN:CB	2.37	0.41
1:A:354:VAL:HG11	1:A:979:ALA:CA	2.50	0.41
1:A:356:TYR:O	1:A:356:TYR:CD1	2.72	0.41
1:A:866:ARG:HA	1:A:866:ARG:HD2	1.78	0.41
1:A:930:LEU:HD23	1:A:930:LEU:HA	1.83	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:B:280:GLN:HB2	1:B:611:THR:HG23	2.02	0.41
1:B:943:LEU:O	1:B:947:PHE:HD1	2.02	0.41
1:B:418:ARG:CZ	1:B:968:MET:CE	2.97	0.41
1:D:175:PHE:HD1	1:D:289:ILE:HD11	1.84	0.41
1:D:47:VAL:HG12	1:D:88:MET:HG3	2.00	0.41
1:D:881:LEU:O	1:D:881:LEU:HD12	2.20	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:E:746:ASN:O	1:E:749:VAL:HG12	2.19	0.41
1:F:1013:THR:O	1:F:1017:ILE:HG23	2.20	0.41
1:F:39:ALA:HA	1:F:40:PRO:HD3	1.78	0.41
1:F:488:LEU:HD22	1:F:492:LEU:HG	2.02	0.41
1:F:520:PHE:O	1:F:524:THR:HG23	2.20	0.41
1:F:712:LEU:HD12	1:F:715:VAL:HG21	2.02	0.41
1:A:378:GLY:O	1:A:382:VAL:HG23	2.20	0.41
1:A:789:TYR:HE2	1:A:799:PRO:HG3	1.81	0.41
1:A:864:GLU:C	1:A:866:ARG:H	2.24	0.41
1:A:453:PHE:CE2	1:A:932:THR:HG22	2.54	0.41
1:B:534:ILE:CG2	1:B:1022:LEU:HD23	2.44	0.41
1:B:237:LYS:NZ	1:C:742:LEU:HD22	2.35	0.41
1:B:278:ASN:HB2	1:B:588:GLN:HE21	1.85	0.41
1:B:685:GLN:HE22	1:B:818:TYR:HD2	1.66	0.41
1:B:958:ILE:CG1	1:B:959:VAL:N	2.82	0.41
1:C:652:GLN:HE22	1:C:664:PHE:HB3	1.85	0.41
1:C:75:LEU:C	1:C:75:LEU:HD23	2.40	0.41
1:D:634:TRP:O	1:D:638:PRO:HG3	2.20	0.41
1:D:866:ARG:HD2	1:D:866:ARG:HA	1.78	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:E:587:THR:HG23	1:E:588:GLN:N	2.35	0.41
1:E:860:GLY:C	1:E:862:SER:N	2.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:324:VAL:HG12	1:F:325:TYR:N	2.35	0.41
1:F:559:ILE:HA	1:F:560:PRO:HD3	1.87	0.41
1:F:652:GLN:HE22	1:F:664:PHE:HB3	1.86	0.41
1:F:667:ALA:HA	1:F:668:PRO:HD3	1.83	0.41
1:F:197:GLN:HA	1:F:797:MET:SD	2.60	0.41
1:F:749:VAL:HG22	1:F:800:PHE:HZ	1.84	0.41
1:F:838:ASP:O	1:F:841:ALA:HB3	2.20	0.41
1:A:155:SER:OG	1:A:180:SER:N	2.54	0.41
1:A:355:MET:HE2	1:A:355:MET:HB3	1.90	0.41
1:A:472:ILE:C	1:A:472:ILE:HD12	2.41	0.41
1:A:578:THR:CG2	1:A:579:PRO:CD	2.94	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:B:108:GLN:HG2	1:C:112:GLN:OE1	2.20	0.41
1:B:204:SER:O	1:B:208:GLN:HG3	2.19	0.41
1:B:563:PHE:O	1:B:923:ASP:HA	2.20	0.41
1:B:673:GLU:O	1:B:674:LEU:C	2.59	0.41
1:B:784:ASP:HA	1:B:787:LYS:HE3	2.02	0.41
1:B:951:LEU:C	1:B:953:GLU:N	2.73	0.41
1:C:357:LEU:O	1:C:357:LEU:HD22	2.20	0.41
1:C:90:ILE:C	1:C:90:ILE:HD12	2.41	0.41
1:C:930:LEU:HA	1:C:930:LEU:HD23	1.86	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:D:90:ILE:HD12	1:D:90:ILE:C	2.39	0.41
1:E:44:ALA:CB	1:E:132:ALA:HB2	2.50	0.41
1:E:186:ILE:CG2	1:E:268:VAL:HG22	2.48	0.41
1:E:521:LEU:HD22	1:E:525:HIS:CE1	2.56	0.41
1:E:278:ASN:HB2	1:E:588:GLN:HE21	1.86	0.41
1:E:702:PHE:CD2	1:E:826:ILE:HD12	2.55	0.41
1:F:181:GLN:HB3	1:F:181:GLN:HE21	1.67	0.41
1:F:214:ILE:HG13	1:F:237:LYS:HB2	2.03	0.41
1:F:451:ALA:HB1	1:F:882:VAL:HG12	2.02	0.41
1:F:56:THR:O	1:F:60:THR:HG22	2.21	0.41
1:F:896:ILE:N	1:F:897:PRO:CD	2.83	0.41
1:B:154:LEU:CD1	1:B:286:ALA:HA	2.51	0.41
1:B:184:MET:HB2	1:B:770:VAL:HG22	2.01	0.41
1:B:843:VAL:HA	1:B:846:ILE:HG12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:MET:HE2	1:B:88:MET:HB3	1.90	0.41
1:C:367:ILE:HG22	1:C:492:LEU:HB3	2.02	0.41
1:C:971:ARG:CB	1:C:972:PRO:HD3	2.50	0.41
1:D:283:GLY:HA2	1:D:595:ARG:NE	2.35	0.41
1:D:333:VAL:O	1:D:337:ILE:HG12	2.20	0.41
1:D:445:ILE:HG13	1:D:446:ALA:N	2.36	0.41
1:D:479:ALA:O	1:D:483:ILE:HG22	2.20	0.41
1:D:694:VAL:O	1:D:697:GLN:HB3	2.21	0.41
1:D:76:ARG:HD3	1:D:95:GLU:OE1	2.21	0.41
1:D:887:LEU:CD2	1:D:942:ILE:HD12	2.50	0.41
1:E:438:ILE:O	1:E:439:GLN:C	2.58	0.41
1:E:616:ASN:HB2	1:E:619:GLY:O	2.20	0.41
1:E:239:ARG:HD2	1:E:762:ILE:HG23	2.03	0.41
1:F:357:LEU:O	1:F:357:LEU:HD22	2.20	0.41
1:F:367:ILE:HG22	1:F:492:LEU:HB3	2.01	0.41
1:F:445:ILE:N	1:F:942:ILE:HD11	2.35	0.41
1:F:812:SER:HA	1:F:813:PRO:HD3	1.92	0.41
1:F:683:PHE:CG	1:F:818:TYR:CE1	3.09	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:B:910:GLY:HA3	1:B:1011:THR:CG2	2.50	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:B:909:ILE:HG13	1:B:910:GLY:N	2.36	0.41
1:D:406:VAL:O	1:D:410:ILE:HG12	2.19	0.41
1:D:681:ASP:OD1	1:D:859:THR:HG22	2.20	0.41
1:D:896:ILE:HD12	1:D:945:VAL:CG2	2.50	0.41
1:E:534:ILE:CG2	1:E:1022:LEU:HD23	2.42	0.41
1:F:330:THR:N	1:F:331:PRO:CD	2.84	0.41
1:F:454:LEU:HA	1:F:454:LEU:HD23	1.60	0.41
1:F:742:LEU:HD23	1:F:745:ILE:HD11	2.02	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:A:30:LEU:HA	1:A:31:PRO:HD2	1.86	0.41
1:A:357:LEU:O	1:A:357:LEU:HD22	2.21	0.41
1:A:896:ILE:HD12	1:A:945:VAL:CG2	2.50	0.41
1:A:985:VAL:O	1:A:989:ILE:HG12	2.20	0.41
1:B:907:GLY:HA2	1:B:1011:THR:HG23	2.02	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
1:C:766:ARG:O	1:C:768:LYS:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:TYR:CG	1:F:223:PRO:HG3	2.55	0.41
1:D:38:ILE:HB	1:D:462:SER:OG	2.20	0.41
1:D:88:MET:SD	1:D:90:ILE:HG22	2.61	0.41
1:E:454:LEU:HA	1:E:454:LEU:HD23	1.83	0.41
1:E:784:ASP:HA	1:E:787:LYS:HE3	2.01	0.41
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:F:363:ARG:O	1:F:367:ILE:HD13	2.21	0.41
1:F:652:GLN:OE1	1:F:652:GLN:HA	2.19	0.41
1:F:789:TYR:CE2	1:F:799:PRO:HG3	2.56	0.41
1:A:100:PRO:HB3	1:A:295:THR:CG2	2.51	0.41
1:A:479:ALA:O	1:A:483:ILE:HG22	2.21	0.41
1:A:610:PHE:HB3	1:A:628:PHE:HB2	2.03	0.41
1:B:143:VAL:HG22	1:B:322:LYS:O	2.21	0.41
1:B:463:THR:O	1:B:466:ILE:HG12	2.20	0.41
1:B:527:TYR:CZ	1:B:966:CYS:HB3	2.56	0.41
1:C:150:THR:OG1	1:C:151:LYS:N	2.54	0.41
1:C:7:ASP:C	1:C:8:ARG:HG3	2.41	0.41
1:C:896:ILE:N	1:C:897:PRO:CD	2.84	0.41
1:D:222:LEU:HA	1:D:223:PRO:C	2.41	0.41
1:D:655:PHE:CG	1:D:663:VAL:HG11	2.55	0.41
1:D:973:ILE:H	1:D:973:ILE:HG12	1.67	0.41
1:E:278:ASN:O	1:E:612:VAL:HA	2.21	0.41
1:F:17:LEU:HD23	1:F:20:MET:CE	2.50	0.41
1:F:522:SER:O	1:F:525:HIS:HB2	2.21	0.41
1:F:929:GLY:HA2	1:F:932:THR:CG2	2.50	0.41
1:A:445:ILE:HG13	1:A:446:ALA:N	2.34	0.41
1:A:457:ALA:O	1:A:468:ARG:HD3	2.20	0.41
1:A:332:VAL:HG23	1:A:634:TRP:CZ2	2.56	0.41
1:A:650:ARG:HH11	1:A:650:ARG:HB2	1.86	0.41
1:A:699:ARG:NH2	1:A:824:MET:CG	2.77	0.41
1:A:6:ILE:HD12	1:A:6:ILE:N	2.36	0.41
1:A:745:ILE:HA	1:A:748:THR:HG22	2.03	0.41
1:B:515:TRP:O	1:B:519:MET:HG2	2.20	0.41
1:A:224:ALA:CB	1:B:780:MET:HE1	2.49	0.41
1:B:527:TYR:HE2	1:B:966:CYS:HB3	1.83	0.41
1:C:184:MET:H	1:C:761:PHE:HE1	1.67	0.41
1:A:780:MET:HB3	1:C:228:GLN:HE21	1.85	0.41
1:C:520:PHE:O	1:C:524:THR:HG23	2.21	0.41
1:C:553:ILE:HG12	1:C:553:ILE:H	1.73	0.41
1:C:652:GLN:HA	1:C:652:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:TYR:CE2	1:C:799:PRO:HG3	2.56	0.41
1:C:881:LEU:O	1:C:885:LEU:HG	2.21	0.41
1:C:930:LEU:O	1:C:933:THR:HB	2.20	0.41
1:D:631:LEU:CD2	1:D:644:VAL:HG23	2.51	0.41
1:D:864:GLU:C	1:D:866:ARG:H	2.24	0.41
1:E:164:ASP:HB3	1:E:165:PRO:HD3	2.03	0.41
1:E:641:GLU:O	1:E:650:ARG:NH2	2.54	0.41
1:F:187:TRP:O	1:F:266:ALA:HB1	2.21	0.41
1:F:489:THR:HA	1:F:492:LEU:HD12	2.03	0.41
1:F:545:TYR:CE1	1:F:1023:PHE:HZ	2.39	0.41
1:F:5:PHE:CD1	1:F:487:ILE:HG23	2.56	0.41
1:F:184:MET:CB	1:F:770:VAL:HG12	2.46	0.41
1:F:843:VAL:O	1:F:847:VAL:HG23	2.21	0.41
1:F:881:LEU:O	1:F:885:LEU:HG	2.20	0.41
1:A:766:ARG:HE	1:B:67:GLN:NE2	2.19	0.41
1:A:712:LEU:CD2	1:A:838:ASP:HB3	2.51	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:B:99:ASP:OD2	1:B:101:ASP:HB2	2.21	0.41
1:B:757:TYR:CE1	1:B:769:ARG:CG	3.03	0.41
1:B:685:GLN:HB3	1:B:823:ALA:HB2	2.03	0.41
1:C:652:GLN:HE22	1:C:664:PHE:CB	2.34	0.41
1:C:726:TYR:HB3	1:C:727:LYS:H	1.70	0.41
1:C:915:THR:HG23	1:C:920:LEU:HB2	2.01	0.41
1:D:306:ILE:HG13	1:D:307:ARG:N	2.36	0.41
1:D:355:MET:HE1	1:D:406:VAL:HG11	2.02	0.41
1:D:356:TYR:CD1	1:D:356:TYR:C	2.94	0.41
1:D:457:ALA:O	1:D:468:ARG:HD3	2.21	0.41
1:E:374:VAL:CG1	1:E:375:VAL:N	2.84	0.41
1:E:563:PHE:O	1:E:923:ASP:HA	2.21	0.41
1:F:150:THR:OG1	1:F:151:LYS:N	2.54	0.41
1:F:370:ILE:O	1:F:373:PRO:HD2	2.20	0.41
1:F:690:VAL:HG12	1:F:694:VAL:HG21	2.03	0.41
1:F:789:TYR:HE2	1:F:799:PRO:HG3	1.84	0.41
1:A:137:LEU:HD11	1:A:330:THR:HG23	2.02	0.41
2:A:2026:LMT:C8	2:A:2026:LMT:C12	2.98	0.41
1:A:295:THR:HG23	1:A:295:THR:O	2.20	0.41
1:A:437:GLN:HE21	1:A:437:GLN:HB3	1.65	0.41
1:A:616:ASN:HA	1:A:616:ASN:HD22	1.65	0.41
1:A:879:SER:O	1:A:883:VAL:HG23	2.20	0.41
1:B:222:LEU:HA	1:B:223:PRO:C	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PRO:HG2	1:B:879:SER:HB3	2.02	0.41
1:A:233:THR:CG2	1:B:725:GLN:HG2	2.47	0.41
1:B:683:PHE:O	1:B:856:TYR:HA	2.21	0.41
1:C:489:THR:HA	1:C:492:LEU:HD12	2.03	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:C:918:ARG:O	1:C:918:ARG:HG2	2.21	0.41
1:D:220:GLY:O	1:D:221:GLY:C	2.59	0.41
1:D:587:THR:HG21	1:D:622:GLN:O	2.21	0.41
1:D:591:VAL:HG11	1:D:611:THR:CG2	2.51	0.41
1:D:902:LEU:HD23	1:D:1023:PHE:CD1	2.56	0.41
1:D:930:LEU:HD23	1:D:930:LEU:HA	1.84	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:143:VAL:HG12	1:E:286:ALA:HB2	2.03	0.41
1:E:293:LEU:HD13	1:E:294:ALA:O	2.20	0.41
1:E:527:TYR:CZ	1:E:966:CYS:HB3	2.55	0.41
1:F:362:PHE:HA	1:F:365:THR:HG22	2.03	0.41
1:A:1003:THR:CG2	1:A:1004:GLY:N	2.84	0.41
1:A:38:ILE:HB	1:A:462:SER:OG	2.21	0.41
1:A:578:THR:HG22	1:A:579:PRO:CD	2.50	0.41
1:A:631:LEU:CD2	1:A:644:VAL:HG23	2.51	0.41
1:A:69:MET:HE1	1:A:107:VAL:HG13	2.04	0.41
1:A:728:LEU:HA	1:A:728:LEU:HD23	1.83	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:B:483:ILE:O	1:B:487:ILE:HD13	2.21	0.41
1:C:111:LEU:O	1:C:113:LEU:N	2.53	0.41
1:C:548:ILE:HD11	1:C:906:LEU:CD2	2.47	0.41
1:C:52:ALA:HB1	1:C:56:THR:CG2	2.51	0.41
1:C:579:PRO:HG3	1:C:660:ASP:OD2	2.21	0.41
1:C:445:ILE:N	1:C:942:ILE:HD11	2.36	0.41
1:D:1001:ILE:CG2	1:D:1002:GLY:N	2.82	0.41
1:D:192:LYS:O	1:D:193:LEU:C	2.59	0.41
1:D:376:LEU:HA	1:D:379:THR:HG22	2.03	0.41
1:D:527:TYR:O	1:D:531:VAL:N	2.45	0.41
1:D:579:PRO:HD3	1:D:661:ALA:HA	2.03	0.41
1:D:812:SER:HA	1:D:813:PRO:HD3	1.80	0.41
1:E:1001:ILE:HG13	1:E:1002:GLY:H	1.85	0.41
1:E:47:VAL:HG22	1:E:127:ILE:HG23	2.03	0.41
1:F:52:ALA:HB1	1:F: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:A:43:ILE:HG12	1:A:104:GLN:HA	2.03	0.40
1:A:127:ILE:O	1:B:113:LEU:HG	2.21	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:B:616:ASN:HB2	1:B:619:GLY:O	2.21	0.40
1:B:936:LEU:HA	1:B:936:LEU:HD23	1.93	0.40
1:C:488:LEU:HD22	1:C:492:LEU:HG	2.03	0.40
1:C:690:VAL:HG12	1:C:694:VAL:HG21	2.02	0.40
1:C:742:LEU:HD23	1:C:745:ILE:HD11	2.02	0.40
1:C:836:SER:O	1:C:840:MET:HG3	2.21	0.40
1:D:295:THR:HG23	1:D:295:THR:O	2.21	0.40
1:D:438:ILE:O	1:D:438:ILE:HD12	2.21	0.40
1:D:455:PRO:HG2	1:D:879:SER:HA	2.03	0.40
1:E:116:PRO:HA	1:E:123:GLN:NE2	2.35	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:E:958:ILE:CG1	1:E:959:VAL:N	2.83	0.40
1:F:1001:ILE:HG13	1:F:1002:GLY:N	2.36	0.40
1:F:667:ALA:O	1:F:678:THR:HG22	2.20	0.40
1:A:310:ILE:HD13	1:A:323:VAL:HG11	2.03	0.40
1:A:375:VAL:O	1:A:379:THR:HG22	2.22	0.40
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.83	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
2:B:2033:LMT:O5B	2:B:2033:LMT:H5'	2.21	0.40
1:D:293:LEU:HD21	1:D:297:ALA:HB3	2.04	0.40
1:D:351:VAL:O	1:D:355:MET:HG2	2.22	0.40
1:D:609:VAL:HG13	1:D:629:ILE:HD13	2.02	0.40
1:D:787:LYS:HE2	1:D:787:LYS:HB2	1.84	0.40
1:D:354:VAL:HG11	1:D:979:ALA:CA	2.51	0.40
1:E:492:LEU:O	1:E:496:MET:HG3	2.21	0.40
1:E:575:GLN:NE2	1:E:617:PHE:HB2	2.36	0.40
1:D:131:LYS:NZ	1:E:73:ASP:OD2	2.51	0.40
1:E:929:GLY:C	1:E:932:THR:HG22	2.42	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:F:94:PHE:HB3	1:F:98:THR:HG21	2.02	0.40
1:A:188:LEU:HG	1:A:772:LEU:CD2	2.51	0.40
1:A:438:ILE:C	1:A:438:ILE:HD12	2.41	0.40
1:A:609:VAL:HG13	1:A:629:ILE:HD13	2.03	0.40
1:A:62:VAL:HG12	1:A:63:GLN:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:THR:HG22	1:B:201:GLY:N	2.37	0.40
1:B:256:ASP:OD1	1:B:256:ASP:N	2.54	0.40
1:B:641:GLU:O	1:B:650:ARG:NH2	2.54	0.40
1:C:182:TYR:HD2	1:C:271:GLY:O	2.04	0.40
1:C:363:ARG:O	1:C:367:ILE:HD13	2.22	0.40
1:C:431:ALA:O	1:C:432:ARG:C	2.59	0.40
1:C:2:SER:O	1:C:6:ILE:HG13	2.21	0.40
1:D:273:GLN:NE2	1:D:769:ARG:NH1	2.67	0.40
1:D:563:PHE:O	1:D:563:PHE:CD2	2.74	0.40
1:D:600:GLU:HA	1:D:600:GLU:OE1	2.21	0.40
1:E:43:ILE:CG2	1:E:107:VAL:HG11	2.23	0.40
1:E:154:LEU:CD1	1:E:286:ALA:HA	2.51	0.40
1:E:428:ARG:N	1:E:428:ARG:HD2	2.27	0.40
1:E:463:THR:O	1:E:466:ILE:HG12	2.21	0.40
1:E:690:VAL:HG13	1:E:690:VAL:O	2.20	0.40
1:E:85:ASP:OD1	1:E:85:ASP:N	2.50	0.40
1:F:90:ILE:C	1:F:90:ILE:HD12	2.42	0.40
1:A:137:LEU:HD22	1:A:293:LEU:HD12	2.04	0.40
1:A:415:ASN:O	1:A:416:VAL:C	2.59	0.40
1:A:68:GLN:O	1:A:110:LYS:HG3	2.21	0.40
1:A:924:VAL:HG23	1:A:925:PHE:N	2.36	0.40
1:B:352:PHE:HD1	1:B:365:THR:CG2	2.34	0.40
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.02	0.40
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.37	0.40
1:C:185:ARG:HD3	1:C:771:TYR:HB2	2.03	0.40
1:C:479:ALA:O	1:C:483:ILE:HG23	2.22	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:D:581:GLY:N	1:D:723:GLU:OE1	2.54	0.40
1:D:63:GLN:O	1:D:67:GLN:HG3	2.21	0.40
1:D:701:LYS:HB3	1:D:701:LYS:HE2	1.91	0.40
1:D:763:ASP:CB	1:D:768:LYS:HD2	2.52	0.40
1:D:49:TYR:O	1:D:86:GLY:HA3	2.22	0.40
1:D:78:ILE:HG13	1:D:90:ILE:HD11	2.02	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:E:88:MET:HB3	1:E:88:MET:HE2	1.89	0.40
1:F:792:ASN:C	1:F:794:LYS:H	2.24	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.22	0.40
1:A:353:LEU:HA	1:A:353:LEU:HD13	1.86	0.40
1:A:396:PHE:HA	1:A:399:VAL:HG12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:GLU:O	1:A:597:TYR:C	2.60	0.40
1:A:780:MET:HE3	1:C:224:ALA:CA	2.51	0.40
1:A:455:PRO:HG2	1:A:879:SER:HA	2.02	0.40
1:B:44:ALA:CB	1:B:132:ALA:HB2	2.52	0.40
1:B:162:ILE:O	1:B:166:LEU:HB2	2.22	0.40
1:A:223:PRO:HD3	1:B:275:TYR:CG	2.56	0.40
1:B:352:PHE:C	1:B:352:PHE:CD2	2.95	0.40
1:B:702:PHE:CD2	1:B:826:ILE:HD12	2.56	0.40
1:B:864:GLU:O	1:B:865:GLU:C	2.60	0.40
1:B:890:LEU:CD1	1:B:891:TYR:CE2	3.05	0.40
1:C:362:PHE:HA	1:C:365:THR:HG22	2.04	0.40
1:C:438:ILE:C	1:C:440:GLY:N	2.75	0.40
1:C:840:MET:O	1:C:844:GLU:HG3	2.22	0.40
1:C:939:LYS:HB3	1:C:939:LYS:HE3	1.90	0.40
1:D:415:ASN:HA	1:D:418:ARG:HD2	2.02	0.40
1:D:579:PRO:HA	1:D:580:PRO:HD3	1.94	0.40
1:D:713:GLN:O	1:D:714:ARG:HB2	2.22	0.40
1:D:754:GLY:O	1:D:755:SER:O	2.39	0.40
1:D:528:GLU:OE2	1:D:967:ARG:NH2	2.55	0.40
1:D:985:VAL:N	1:D:986:PRO:CD	2.85	0.40
1:E:99:ASP:OD2	1:E:101:ASP:HB2	2.21	0.40
1:E:158:ILE:O	1:E:163:GLN:HB2	2.22	0.40
1:F:175:PHE:CD2	1:F:175:PHE:C	2.94	0.40
1:F:668:PRO:HA	1:F:669:PRO:HD3	1.75	0.40
1:F:757:TYR:HE1	1:F:769:ARG:CG	2.35	0.40
1:F:75:LEU:HD23	1:F:75:LEU:C	2.41	0.40
1:F:753:TRP:HZ2	1:F:785:LEU:HA	1.86	0.40
1:F:939:LYS:NZ	1:F:976:THR:HG21	2.33	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%)	2	14
1	B	1028/1052 (98%)	863 (84%)	147 (14%)	18 (2%)	8	37
1	C	1028/1052 (98%)	859 (84%)	143 (14%)	26 (2%)	5	28
1	D	990/1052 (94%)	820 (83%)	132 (13%)	38 (4%)	3	18
1	E	1006/1052 (96%)	847 (84%)	141 (14%)	18 (2%)	8	37
1	F	1028/1052 (98%)	866 (84%)	136 (13%)	26 (2%)	5	28
All	All	6079/6312 (96%)	5085 (84%)	822 (14%)	172 (3%)	5	25

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%)	2	13
1	B	841/860 (98%)	736 (88%)	105 (12%)	4	20
1	C	841/860 (98%)	755 (90%)	86 (10%)	7	28
1	D	816/860 (95%)	695 (85%)	121 (15%)	3	14
1	E	829/860 (96%)	727 (88%)	102 (12%)	4	21
1	F	841/860 (98%)	751 (89%)	90 (11%)	6	26
All	All	4991/5160 (97%)	4361 (87%)	630 (13%)	4	20

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	E	2032	-	36,36,36	0.62	1 (2%)	47,47,47	1.40	5 (10%)
2	LMT	D	2026	-	36,36,36	0.71	1 (2%)	47,47,47	1.76	8 (17%)
2	LMT	E	2033	-	36,36,36	1.11	4 (11%)	47,47,47	3.55	18 (38%)
2	LMT	B	2033	-	36,36,36	1.19	3 (8%)	47,47,47	3.63	19 (40%)
2	LMT	A	2026	-	36,36,36	0.57	0	47,47,47	1.44	6 (12%)
2	LMT	B	2032	-	36,36,36	0.76	1 (2%)	47,47,47	2.01	9 (19%)
2	LMT	B	2031	-	36,36,36	0.97	1 (2%)	47,47,47	1.42	9 (19%)
2	LMT	E	2031	-	36,36,36	0.89	1 (2%)	47,47,47	1.81	9 (19%)

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	E	2032	-	-	5/21/61/61	0/2/2/2
2	LMT	D	2026	-	-	4/21/61/61	0/2/2/2
2	LMT	E	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	B	2033	-	-	7/21/61/61	0/2/2/2
2	LMT	A	2026	-	-	6/21/61/61	0/2/2/2
2	LMT	B	2032	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2031	-	-	1/21/61/61	0/2/2/2
2	LMT	E	2031	-	-	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	B	2033	LMT	O1'-C1'	4.28	1.47	1.40
2	E	2033	LMT	O1'-C1'	3.77	1.46	1.40
2	B	2032	LMT	O1'-C1'	3.68	1.46	1.40
2	B	2031	LMT	O1'-C1'	3.41	1.46	1.40
2	E	2031	LMT	O1'-C1'	3.16	1.45	1.40
2	B	2033	LMT	C4'-C5'	2.54	1.59	1.52
2	D	2026	LMT	O1'-C1'	2.43	1.44	1.40
2	E	2032	LMT	O1'-C1'	2.42	1.44	1.40
2	B	2033	LMT	O5'-C5'	2.13	1.49	1.44
2	E	2033	LMT	O5'-C5'	2.11	1.49	1.44
2	E	2033	LMT	O1B-C1B	2.07	1.47	1.41
2	E	2033	LMT	C4'-C5'	2.03	1.58	1.52

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2033	LMT	C1-O1'-C1'	14.36	137.65	113.84
2	E	2033	LMT	C1-O1'-C1'	13.64	136.47	113.84
2	B	2033	LMT	C1B-O1B-C4'	-10.03	93.14	117.96
2	E	2033	LMT	C1B-O1B-C4'	-9.66	94.06	117.96
2	B	2033	LMT	C3'-C4'-C5'	-7.90	92.81	110.93
2	E	2033	LMT	C3'-C4'-C5'	-7.84	92.95	110.93
2	B	2032	LMT	C1-O1'-C1'	-7.54	101.33	113.84
2	E	2031	LMT	C1-O1'-C1'	-6.67	102.78	113.84
2	E	2032	LMT	C1-O1'-C1'	-6.41	103.21	113.84
2	E	2033	LMT	O5'-C5'-C4'	6.10	122.62	109.75
2	B	2033	LMT	O5'-C5'-C4'	6.08	122.58	109.75
2	B	2032	LMT	C3'-C4'-C5'	-5.64	98.00	110.93
2	D	2026	LMT	O1'-C1'-C2'	5.63	117.10	108.30
2	E	2033	LMT	O1'-C1-C2	5.37	128.37	109.56
2	B	2033	LMT	O1B-C4'-C5'	4.88	122.81	109.45
2	E	2033	LMT	O1B-C4'-C5'	4.76	122.48	109.45
2	D	2026	LMT	O1'-C1-C2	-4.71	93.06	109.56
2	B	2033	LMT	O1B-C4'-C3'	-4.49	95.33	107.28
2	D	2026	LMT	O5'-C5'-C6'	-4.33	95.67	106.44
2	B	2033	LMT	O1'-C1-C2	4.28	124.58	109.56
2	B	2032	LMT	C6B-C5B-C4B	-4.24	103.08	113.00
2	E	2031	LMT	O5B-C5B-C6B	4.21	116.91	106.44
2	E	2033	LMT	O5'-C1'-O1'	4.14	119.78	109.97
2	E	2033	LMT	O1B-C1B-O5B	4.14	122.23	110.67
2	E	2031	LMT	O1'-C1-C2	4.04	123.72	109.56
2	B	2033	LMT	O5'-C1'-O1'	4.01	119.46	109.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2026	LMT	O1'-C1'-C2'	4.00	114.54	108.30
2	E	2033	LMT	C4B-C3B-C2B	-3.99	103.85	110.82
2	B	2033	LMT	O1B-C1B-O5B	3.95	121.71	110.67
2	B	2033	LMT	O1'-C1'-C2'	3.90	114.39	108.30
2	B	2033	LMT	C4B-C3B-C2B	-3.74	104.29	110.82
2	E	2033	LMT	O2B-C2B-C1B	3.66	118.93	110.05
2	E	2033	LMT	O1B-C4'-C3'	-3.59	97.73	107.28
2	E	2031	LMT	C6'-C5'-C4'	-3.57	102.94	113.33
2	E	2031	LMT	O1'-C1'-C2'	3.49	113.75	108.30
2	B	2033	LMT	C3B-C4B-C5B	-3.44	104.11	110.24
2	B	2033	LMT	O2B-C2B-C1B	3.43	118.39	110.05
2	E	2033	LMT	C3B-C4B-C5B	-3.39	104.19	110.24
2	D	2026	LMT	O1B-C4'-C5'	3.38	118.71	109.45
2	B	2031	LMT	C3'-C4'-C5'	-3.33	103.29	110.93
2	B	2032	LMT	O5'-C1'-O1'	3.33	117.85	109.97
2	D	2026	LMT	O5'-C1'-C2'	-3.28	103.40	110.35
2	B	2032	LMT	O1B-C1B-O5B	3.26	119.78	110.67
2	E	2033	LMT	O1'-C1'-C2'	3.25	113.38	108.30
2	D	2026	LMT	O5'-C1'-O1'	-3.21	102.36	109.97
2	E	2033	LMT	C1B-O5B-C5B	-3.18	107.44	113.69
2	B	2031	LMT	O5'-C1'-O1'	3.15	117.44	109.97
2	B	2033	LMT	O5B-C5B-C4B	3.09	115.31	109.69
2	A	2026	LMT	O1B-C4'-C3'	3.07	115.45	107.28
2	B	2033	LMT	C1B-O5B-C5B	-3.00	107.80	113.69
2	A	2026	LMT	O5'-C5'-C6'	-3.00	98.99	106.44
2	E	2032	LMT	O1B-C1B-O5B	-2.99	102.32	110.67
2	B	2033	LMT	C6B-C5B-C4B	-2.95	106.10	113.00
2	E	2033	LMT	C6B-C5B-C4B	-2.93	106.14	113.00
2	B	2033	LMT	O5'-C1'-C2'	-2.93	104.15	110.35
2	B	2033	LMT	C2'-C3'-C4'	2.92	116.36	109.68
2	B	2031	LMT	O1B-C4'-C5'	2.90	117.39	109.45
2	A	2026	LMT	O5'-C1'-O1'	-2.89	103.12	109.97
2	E	2033	LMT	O5B-C5B-C4B	2.84	114.85	109.69
2	E	2031	LMT	O1B-C1B-O5B	-2.79	102.87	110.67
2	E	2031	LMT	O1B-C4'-C3'	2.78	114.69	107.28
2	B	2031	LMT	C1-O1'-C1'	-2.73	109.31	113.84
2	A	2026	LMT	C6'-C5'-C4'	-2.73	105.38	113.33
2	E	2033	LMT	C2'-C3'-C4'	2.73	115.91	109.68
2	B	2031	LMT	O1B-C1B-O5B	2.63	118.01	110.67
2	E	2033	LMT	O5'-C1'-C2'	-2.56	104.92	110.35
2	E	2032	LMT	O1'-C1'-C2'	2.47	112.16	108.30
2	B	2031	LMT	C4B-C3B-C2B	-2.45	106.54	110.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2026	LMT	O1B-C1B-O5B	-2.45	103.83	110.67
2	E	2031	LMT	C1B-O1B-C4'	-2.44	111.92	117.96
2	E	2032	LMT	C1'-O5'-C5'	-2.44	108.90	113.69
2	E	2031	LMT	O1B-C1B-C2B	2.39	114.30	108.10
2	B	2032	LMT	C1B-C2B-C3B	2.35	114.89	110.00
2	B	2032	LMT	O1B-C1B-C2B	-2.35	102.02	108.10
2	D	2026	LMT	C6B-C5B-C4B	-2.30	107.61	113.00
2	B	2031	LMT	C1B-O1B-C4'	-2.27	112.35	117.96
2	B	2032	LMT	O1'-C1'-C2'	2.23	111.78	108.30
2	B	2032	LMT	C1B-O5B-C5B	2.23	118.06	113.69
2	B	2031	LMT	O5B-C1B-C2B	-2.18	105.74	110.35
2	B	2033	LMT	O2B-C2B-C3B	-2.17	105.34	110.35
2	E	2032	LMT	C9-C8-C7	-2.09	103.84	114.42
2	B	2031	LMT	C1B-C2B-C3B	2.05	114.27	110.00
2	D	2026	LMT	C4B-C3B-C2B	-2.03	107.28	110.82

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2026	LMT	C2'-C1'-O1'-C1
2	D	2026	LMT	O5'-C1'-O1'-C1
2	E	2033	LMT	O5'-C1'-O1'-C1
2	E	2033	LMT	C2-C1-O1'-C1'
2	B	2033	LMT	O5'-C1'-O1'-C1
2	B	2033	LMT	C2-C1-O1'-C1'
2	A	2026	LMT	O5'-C1'-O1'-C1
2	B	2033	LMT	O5B-C1B-O1B-C4'
2	E	2033	LMT	O5B-C1B-O1B-C4'
2	B	2033	LMT	C3'-C4'-O1B-C1B
2	E	2033	LMT	C3'-C4'-O1B-C1B
2	D	2026	LMT	C3'-C4'-O1B-C1B
2	D	2026	LMT	C5'-C4'-O1B-C1B
2	A	2026	LMT	C2'-C1'-O1'-C1
2	E	2032	LMT	O5B-C5B-C6B-O6B
2	A	2026	LMT	O5B-C5B-C6B-O6B
2	E	2033	LMT	C2'-C1'-O1'-C1
2	B	2033	LMT	C2'-C1'-O1'-C1
2	E	2032	LMT	C2-C1-O1'-C1'
2	E	2032	LMT	C3'-C4'-O1B-C1B
2	E	2033	LMT	C2B-C1B-O1B-C4'
2	A	2026	LMT	C3'-C4'-O1B-C1B

Continued on next page...

Continued from previous page...

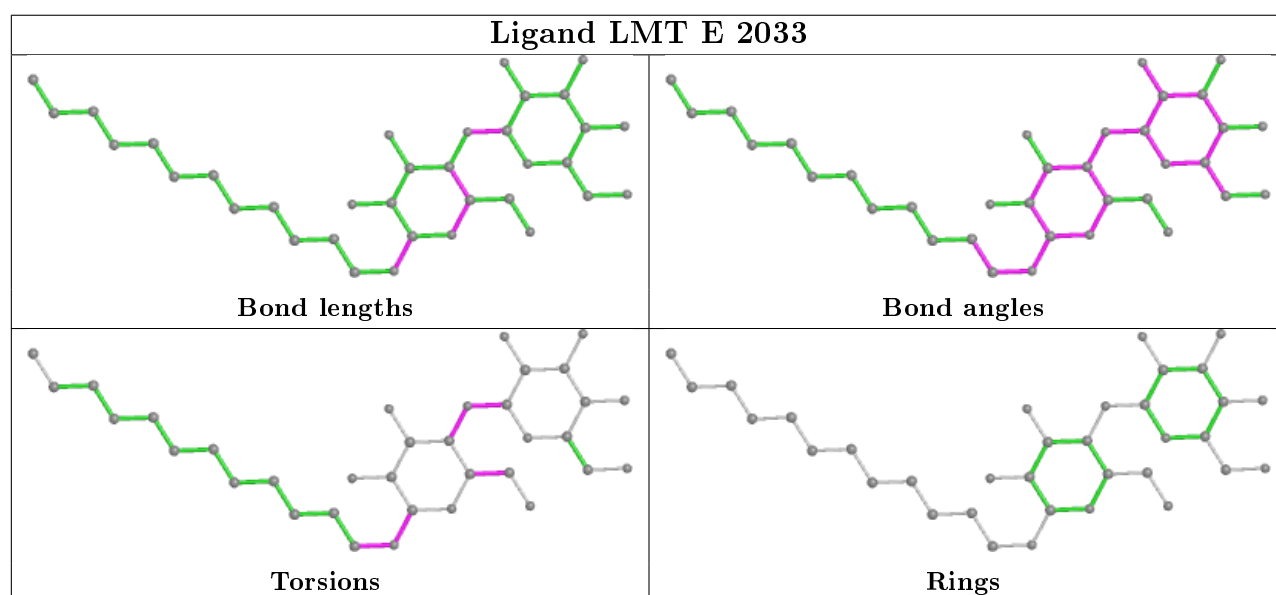
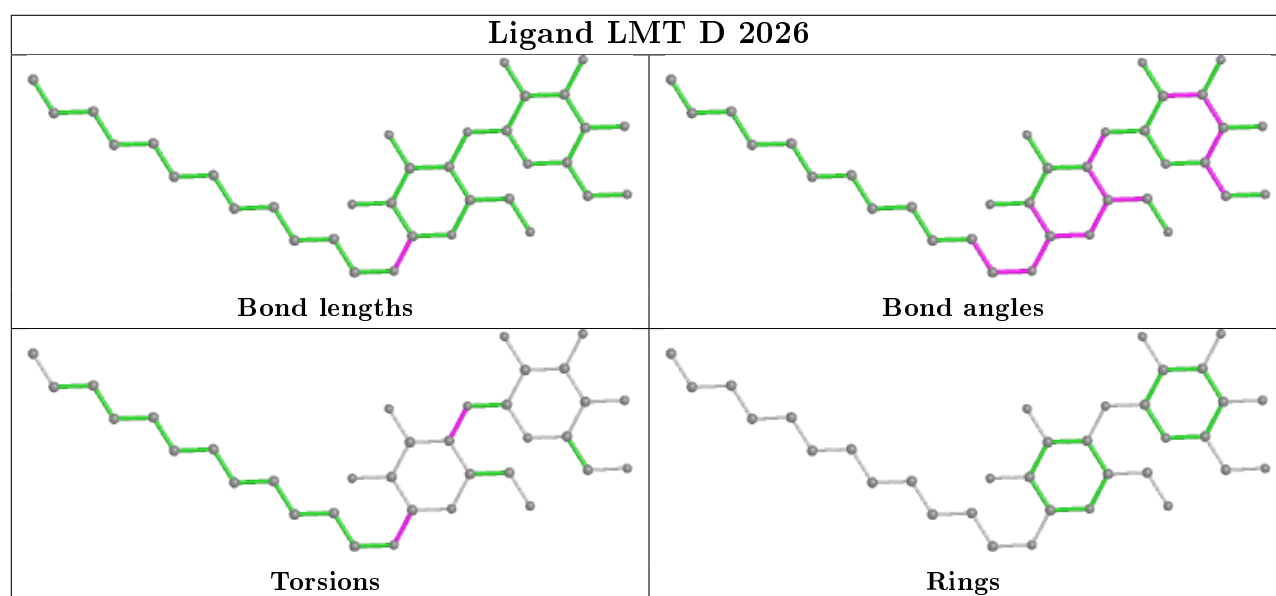
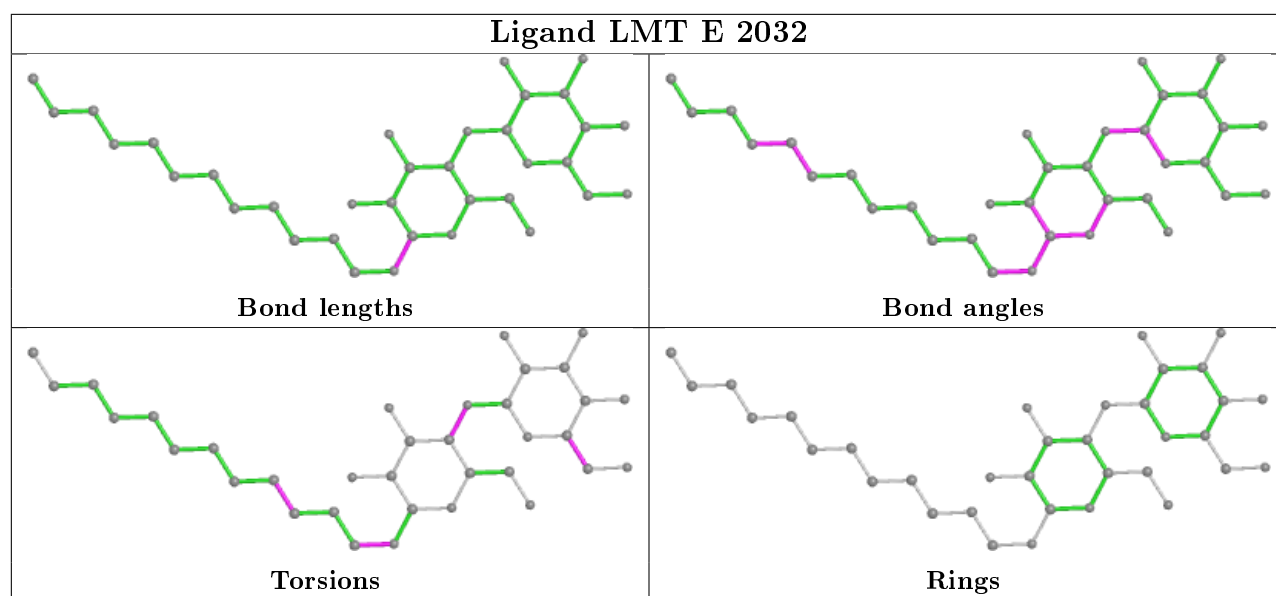
Mol	Chain	Res	Type	Atoms
2	E	2032	LMT	C2-C3-C4-C5
2	E	2032	LMT	C5'-C4'-O1B-C1B
2	E	2033	LMT	C4'-C5'-C6'-O6'
2	E	2031	LMT	C3'-C4'-O1B-C1B
2	B	2033	LMT	C4'-C5'-C6'-O6'
2	B	2033	LMT	C2B-C1B-O1B-C4'
2	B	2031	LMT	C3'-C4'-O1B-C1B
2	A	2026	LMT	C2B-C1B-O1B-C4'
2	A	2026	LMT	C5'-C4'-O1B-C1B

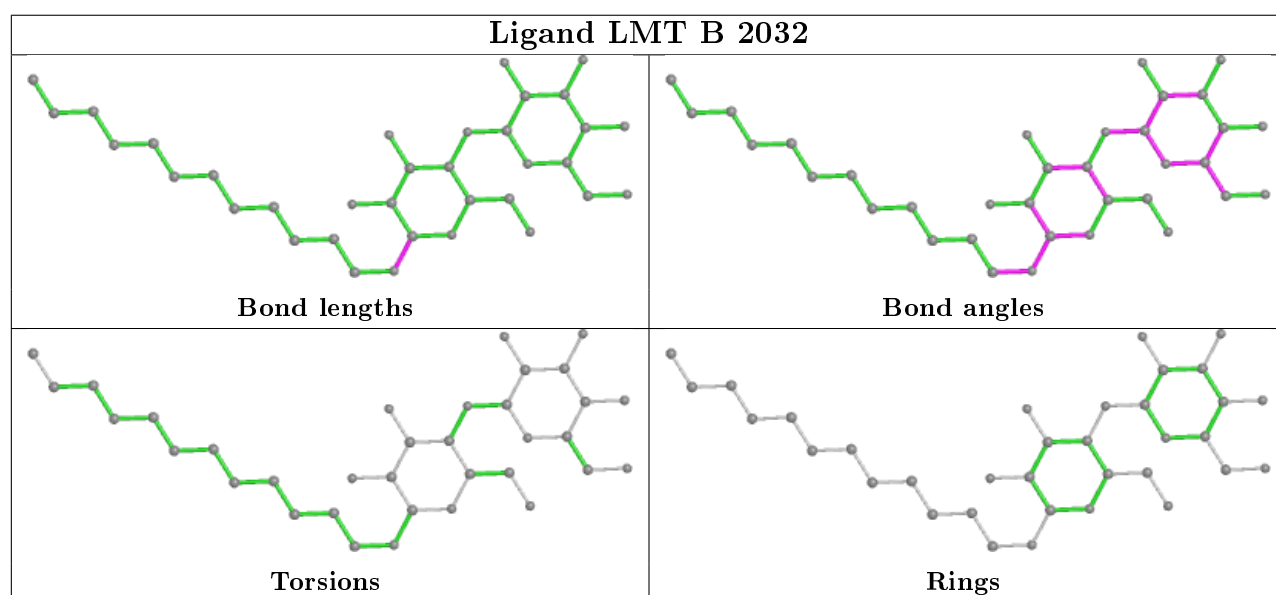
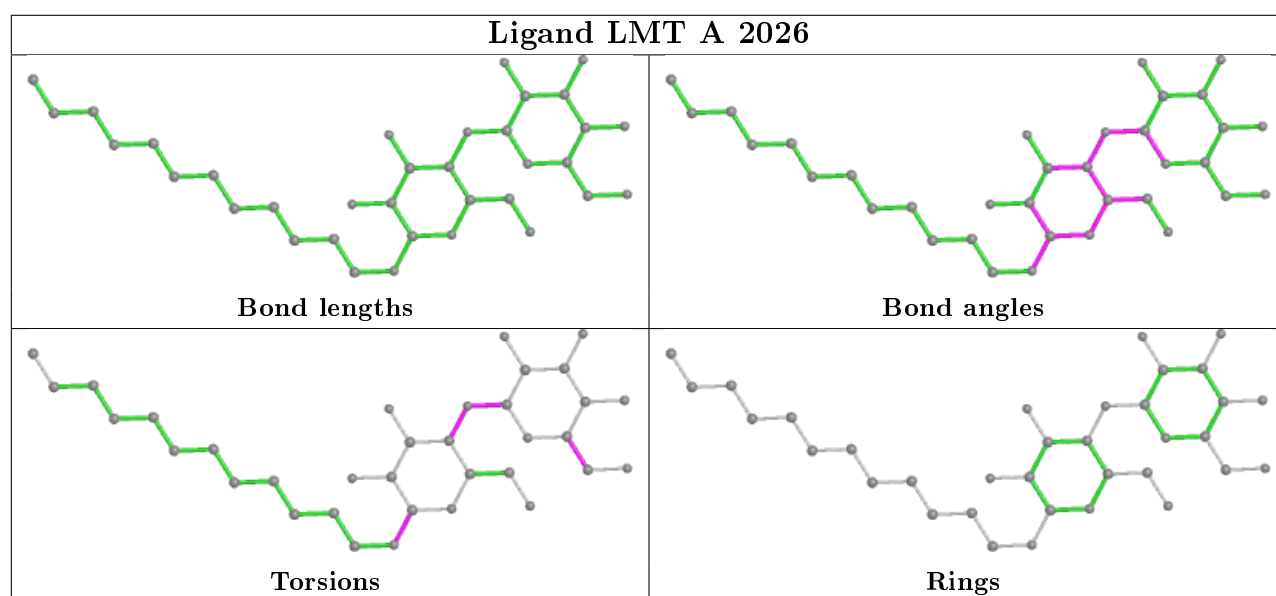
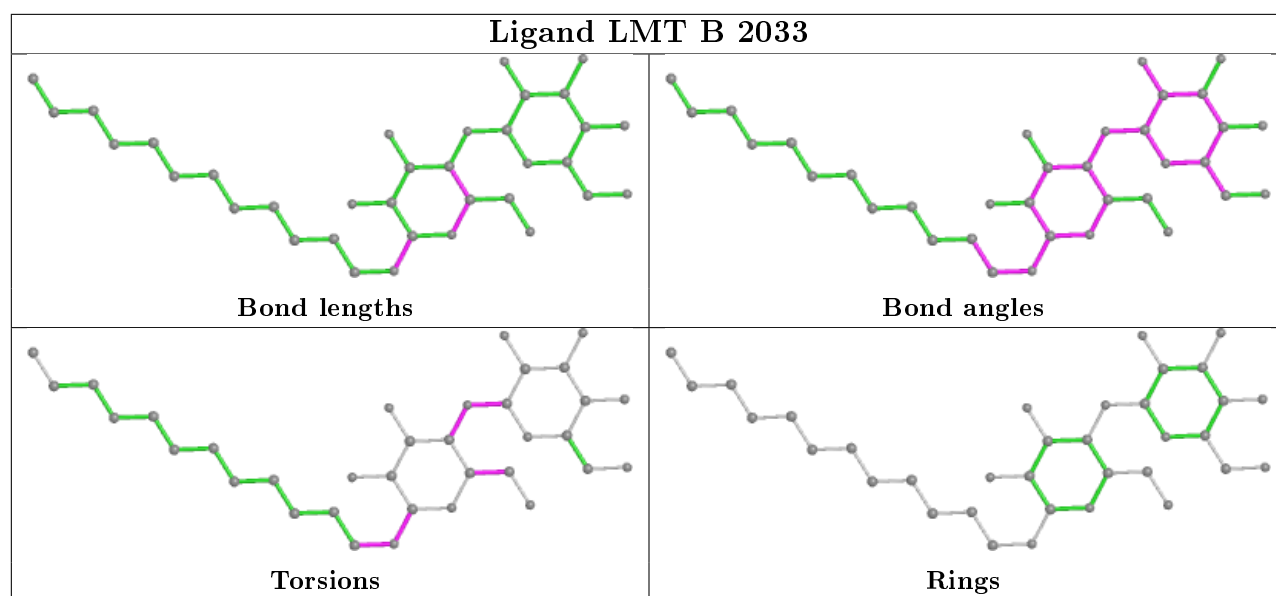
There are no ring outliers.

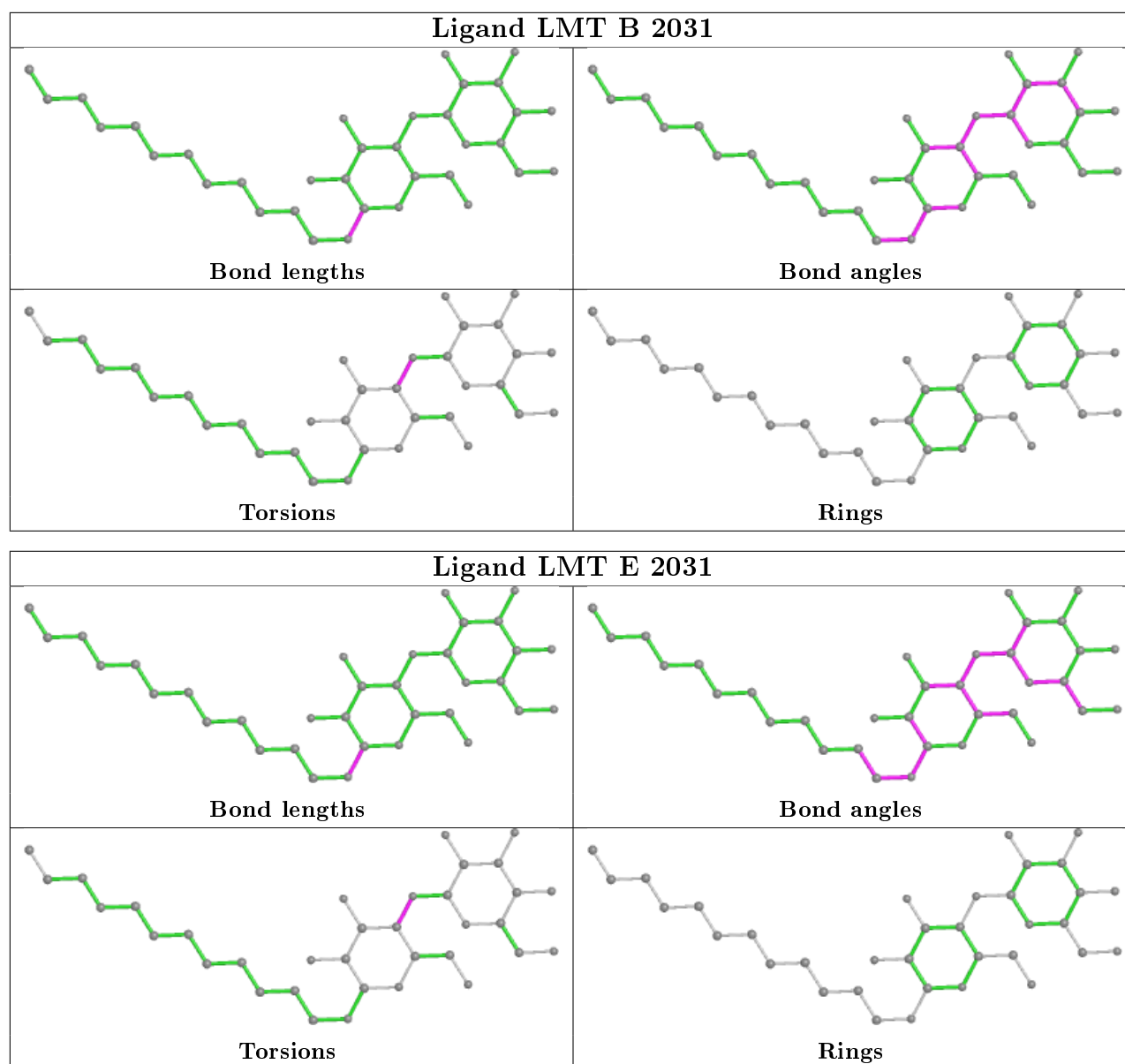
8 monomers are involved in 54 short contacts:

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

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.24	10 (0%)	82 59	54, 91, 132, 178	0
1	B	1030/1052 (97%)	-0.13	22 (2%)	63 34	53, 91, 143, 188	0
1	C	1028/1052 (97%)	-0.07	45 (4%)	34 13	58, 101, 178, 238	0
1	D	998/1052 (94%)	-0.28	19 (1%)	66 37	58, 91, 134, 179	0
1	E	1012/1052 (96%)	-0.15	38 (3%)	40 16	55, 93, 143, 189	0
1	F	1030/1052 (97%)	-0.09	46 (4%)	33 12	59, 100, 177, 238	0
All	All	6102/6312 (96%)	-0.16	180 (2%)	51 23	53, 94, 153, 238	0

All (180) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	803	PHE	7.4
1	E	260	VAL	6.6
1	E	251	LEU	6.0
1	C	778	ALA	6.0
1	F	753	TRP	5.3
1	F	660	ASP	5.2
1	C	503	GLY	5.0
1	A	841	ALA	4.8
1	F	640	GLY	4.8
1	C	783	ASP	4.7
1	D	585	GLU	4.6
1	C	505	HIS	4.6
1	D	252	LYS	4.6
1	F	745	ILE	4.3
1	F	659	LYS	4.3
1	F	744	ASP	4.3
1	E	506	GLY	4.2
1	E	834	LEU	4.2
1	B	140	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	203	VAL	4.1
1	E	833	GLY	4.0
1	F	251	LEU	4.0
1	E	252	LYS	4.0
1	E	732	ASP	3.9
1	C	790	VAL	3.9
1	C	638	PRO	3.9
1	B	162	ILE	3.9
1	B	678	THR	3.8
1	D	841	ALA	3.8
1	C	636	GLU	3.7
1	C	753	TRP	3.7
1	F	658	PHE	3.7
1	A	955	GLY	3.6
1	F	506	GLY	3.6
1	D	199	THR	3.6
1	E	250	LEU	3.6
1	D	635	GLU	3.5
1	D	785	LEU	3.5
1	E	229	GLN	3.5
1	C	721	SER	3.5
1	B	251	LEU	3.5
1	C	738	LEU	3.4
1	F	507	GLU	3.4
1	F	600	GLU	3.4
1	E	253	VAL	3.4
1	E	246	PHE	3.4
1	C	745	ILE	3.3
1	F	502	LYS	3.3
1	E	261	ARG	3.3
1	B	224	ALA	3.3
1	F	790	VAL	3.3
1	C	688	ALA	3.2
1	A	868	SER	3.2
1	E	507	GLU	3.2
1	C	507	GLU	3.2
1	C	805	THR	3.1
1	D	570	GLY	3.1
1	E	1030	LEU	3.1
1	B	141	GLY	3.1
1	E	600	GLU	3.1
1	B	237	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	199	THR	3.0
1	A	230	LEU	3.0
1	C	785	LEU	3.0
1	F	800	PHE	3.0
1	E	807	LYS	3.0
1	F	255	PRO	3.0
1	D	636	GLU	3.0
1	E	598	LEU	2.9
1	F	732	ASP	2.9
1	C	732	ASP	2.9
1	C	800	PHE	2.9
1	F	225	VAL	2.9
1	D	202	ASP	2.9
1	C	786	SER	2.9
1	F	250	LEU	2.8
1	C	200	PRO	2.8
1	C	198	LEU	2.8
1	E	262	LEU	2.8
1	C	147	GLY	2.8
1	A	147	GLY	2.8
1	F	261	ARG	2.7
1	C	265	VAL	2.7
1	D	840	MET	2.7
1	E	228	GLN	2.7
1	E	753	TRP	2.7
1	F	601	LYS	2.7
1	A	732	ASP	2.7
1	B	360	GLN	2.7
1	F	260	VAL	2.7
1	F	748	THR	2.7
1	F	591	VAL	2.7
1	C	794	LYS	2.6
1	D	264	ASP	2.6
1	E	655	PHE	2.6
1	C	259	GLN	2.6
1	D	251	LEU	2.6
1	B	498	LYS	2.6
1	B	289	ILE	2.6
1	E	561	THR	2.6
1	F	789	TYR	2.6
1	A	542	LEU	2.6
1	E	599	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	610	PHE	2.6
1	E	562	ALA	2.6
1	F	799	PRO	2.6
1	C	250	LEU	2.6
1	B	322	LYS	2.5
1	F	259	GLN	2.5
1	F	726	TYR	2.5
1	C	362	PHE	2.5
1	C	502	LYS	2.5
1	A	687	GLN	2.5
1	B	225	VAL	2.5
1	A	839	ALA	2.5
1	E	258	SER	2.5
1	E	708	GLN	2.4
1	E	704	MET	2.4
1	F	252	LYS	2.4
1	B	362	PHE	2.4
1	C	261	ARG	2.4
1	F	738	LEU	2.4
1	C	777	ASP	2.4
1	C	635	GLU	2.4
1	F	796	GLU	2.4
1	D	730	ILE	2.4
1	C	508	HIS	2.4
1	F	156	ASN	2.3
1	E	519	MET	2.3
1	E	805	THR	2.3
1	B	1030	LEU	2.3
1	C	854	VAL	2.3
1	F	788	TRP	2.3
1	C	730	ILE	2.3
1	E	788	TRP	2.3
1	F	224	ALA	2.3
1	F	265	VAL	2.3
1	C	600	GLU	2.3
1	D	248	ASN	2.3
1	F	258	SER	2.3
1	A	733	GLU	2.2
1	C	804	ALA	2.2
1	F	661	ALA	2.2
1	E	264	ASP	2.2
1	F	504	ASP	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	505	HIS	2.2
1	C	242	THR	2.2
1	F	200	PRO	2.2
1	C	251	LEU	2.2
1	F	246	PHE	2.2
1	C	726	TYR	2.2
1	E	832	PRO	2.2
1	D	690	VAL	2.2
1	C	728	LEU	2.2
1	B	581	GLY	2.2
1	E	509	LYS	2.2
1	B	587	THR	2.2
1	F	626	MET	2.2
1	B	250	LEU	2.2
1	D	583	SER	2.1
1	D	604	SER	2.1
1	B	260	VAL	2.1
1	C	801	ASN	2.1
1	B	263	LYS	2.1
1	D	263	LYS	2.1
1	F	253	VAL	2.1
1	B	849	GLN	2.1
1	E	849	GLN	2.1
1	E	778	ALA	2.1
1	F	226	LYS	2.1
1	C	852	LYS	2.1
1	F	262	LEU	2.1
1	C	640	GLY	2.1
1	F	188	LEU	2.1
1	E	254	ASN	2.1
1	E	266	ALA	2.1
1	E	697	GLN	2.0
1	B	800	PHE	2.0
1	C	743	ALA	2.0
1	D	160	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

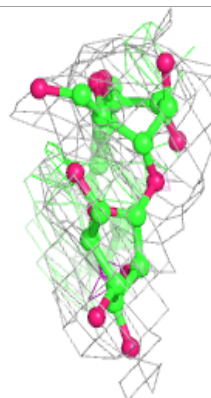
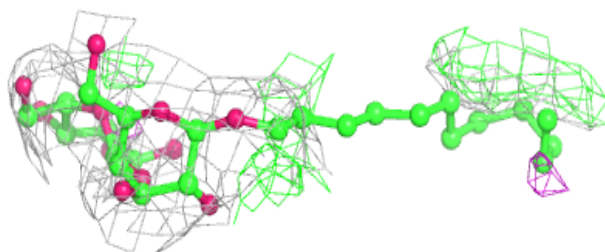
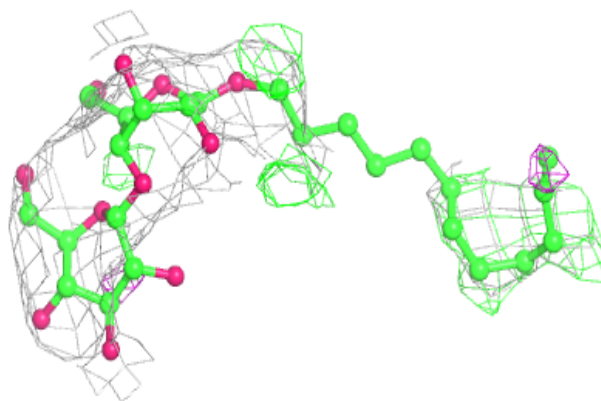
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	LMT	B	2033	35/35	0.72	0.42	100,155,176,183	0
2	LMT	E	2033	35/35	0.76	0.33	111,146,174,179	0
2	LMT	E	2031	35/35	0.85	0.23	72,95,121,130	0
2	LMT	B	2031	35/35	0.90	0.20	59,82,109,114	0
2	LMT	A	2026	35/35	0.90	0.21	80,110,145,173	0
2	LMT	D	2026	35/35	0.91	0.16	75,113,140,142	0
2	LMT	E	2032	35/35	0.93	0.23	66,90,115,128	0
2	LMT	B	2032	35/35	0.93	0.25	52,70,157,169	0

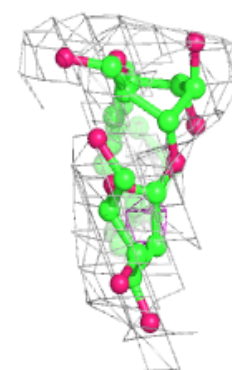
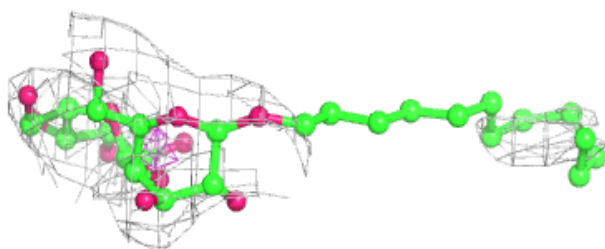
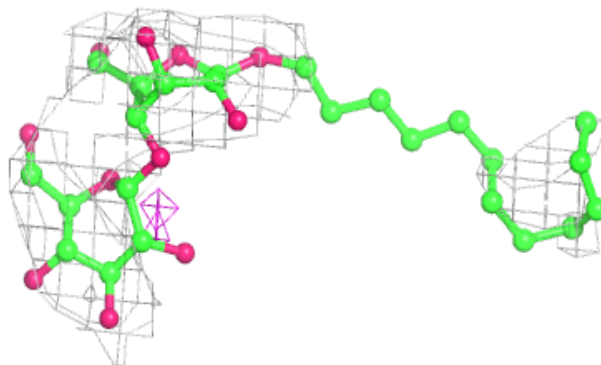
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT B 2033:

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

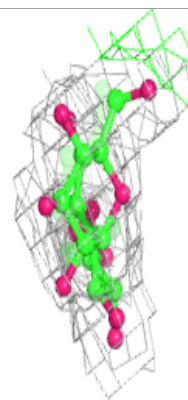
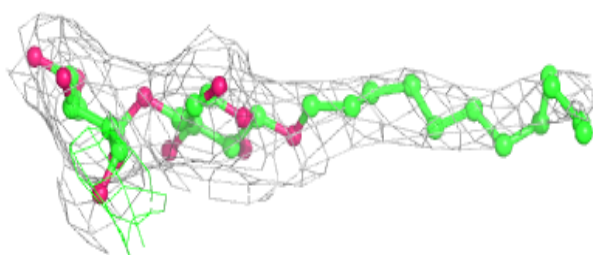
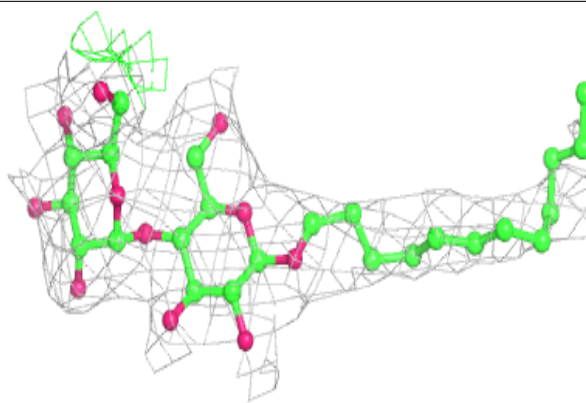
**Electron density around LMT E 2033:**

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

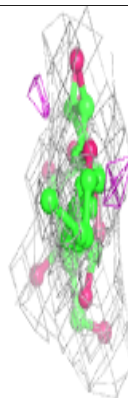
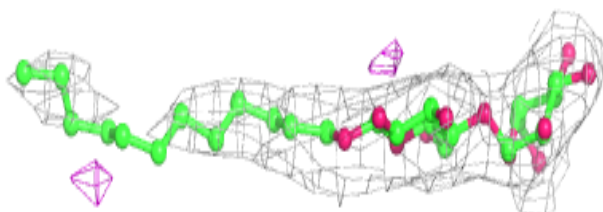
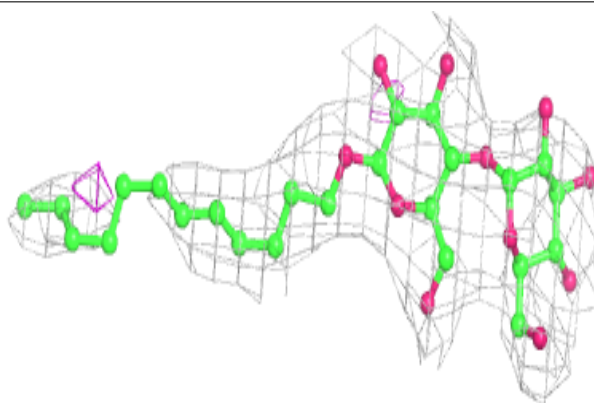


Electron density around LMT E 2031:

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

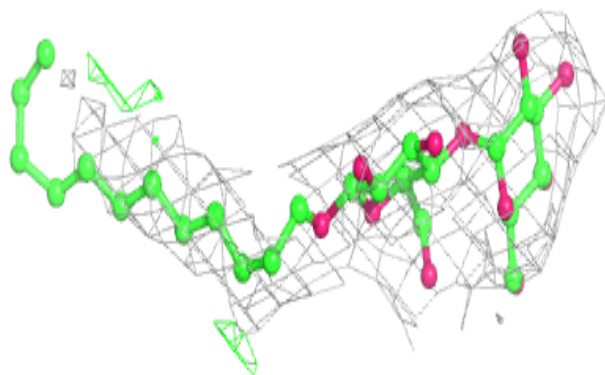
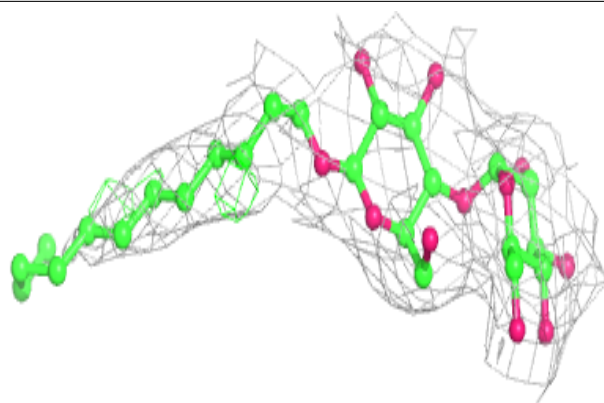
**Electron density around LMT B 2031:**

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

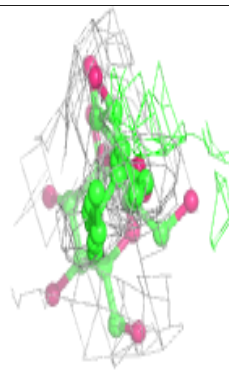
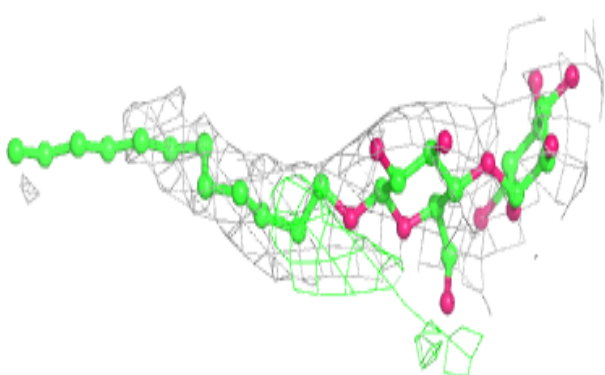
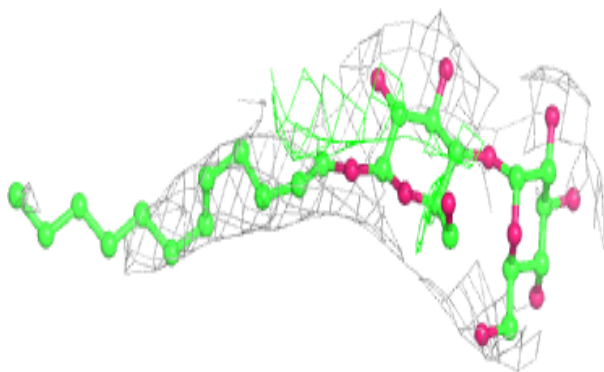


Electron density around LMT A 2026:

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

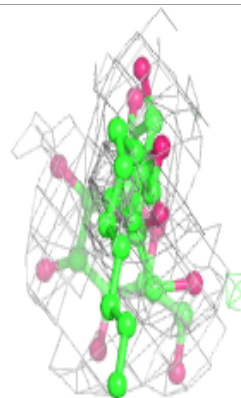
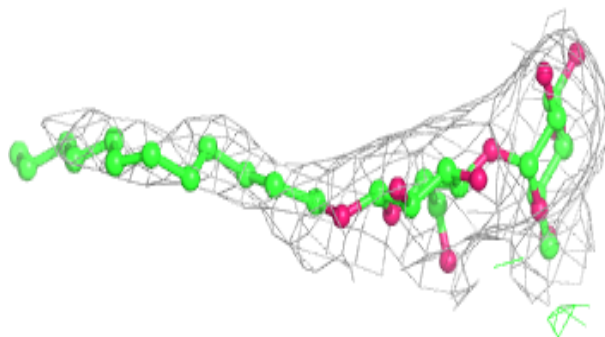
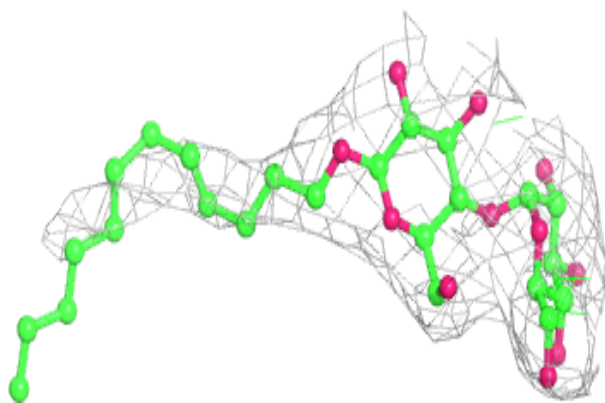
**Electron density around LMT D 2026:**

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

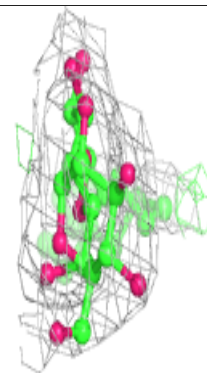
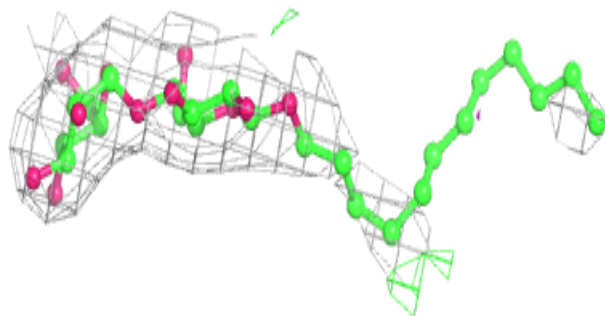
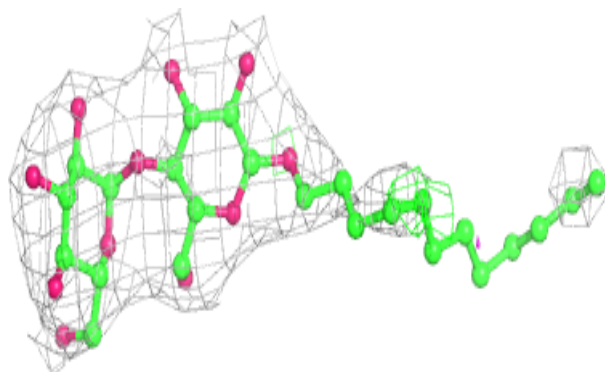


Electron density around LMT E 2032:

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

**Electron density around LMT B 2032:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.