



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:44 am GMT

PDB ID : 5L5L
Title : Plexin A4 full extracellular region, domains 1 to 8 modeled, data to 8 angstrom, spacegroup P2(1)
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
Deposited on : 2016-05-28
Resolution : 8.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

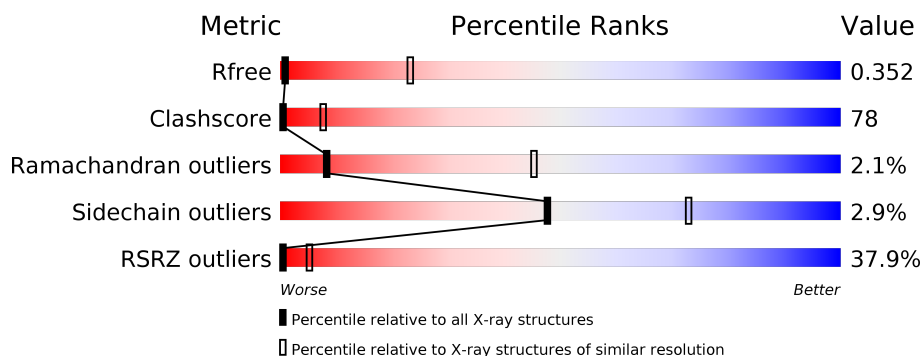
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 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}	100719	1100 (10.00-3.70)
Clashscore	112137	1036 (11.50-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)
RSRZ outliers	101464	1004 (11.50-3.72)

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

Mol	Chain	Length	Quality of chain
1	A	1207	<div> <div>33%</div> <div>27%</div> <div>52%</div> <div>17%</div> </div>
1	B	1207	<div> <div>27%</div> <div>25%</div> <div>47%</div> <div>24%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15030 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1000	Total	C	N	O	S	0	0	0
			7841	4938	1356	1482	65			
1	B	915	Total	C	N	O	S	0	0	0
			7189	4533	1239	1357	60			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2
B	33	GLU	-	expression tag	UNP Q80UG2
B	34	THR	-	expression tag	UNP Q80UG2
B	35	GLY	-	expression tag	UNP Q80UG2
B	1230	GLY	-	expression tag	UNP Q80UG2
B	1231	ARG	-	expression tag	UNP Q80UG2
B	1232	THR	-	expression tag	UNP Q80UG2
B	1233	LYS	-	expression tag	UNP Q80UG2
B	1234	HIS	-	expression tag	UNP Q80UG2
B	1235	HIS	-	expression tag	UNP Q80UG2
B	1236	HIS	-	expression tag	UNP Q80UG2
B	1237	HIS	-	expression tag	UNP Q80UG2
B	1238	HIS	-	expression tag	UNP Q80UG2

Continued on next page...

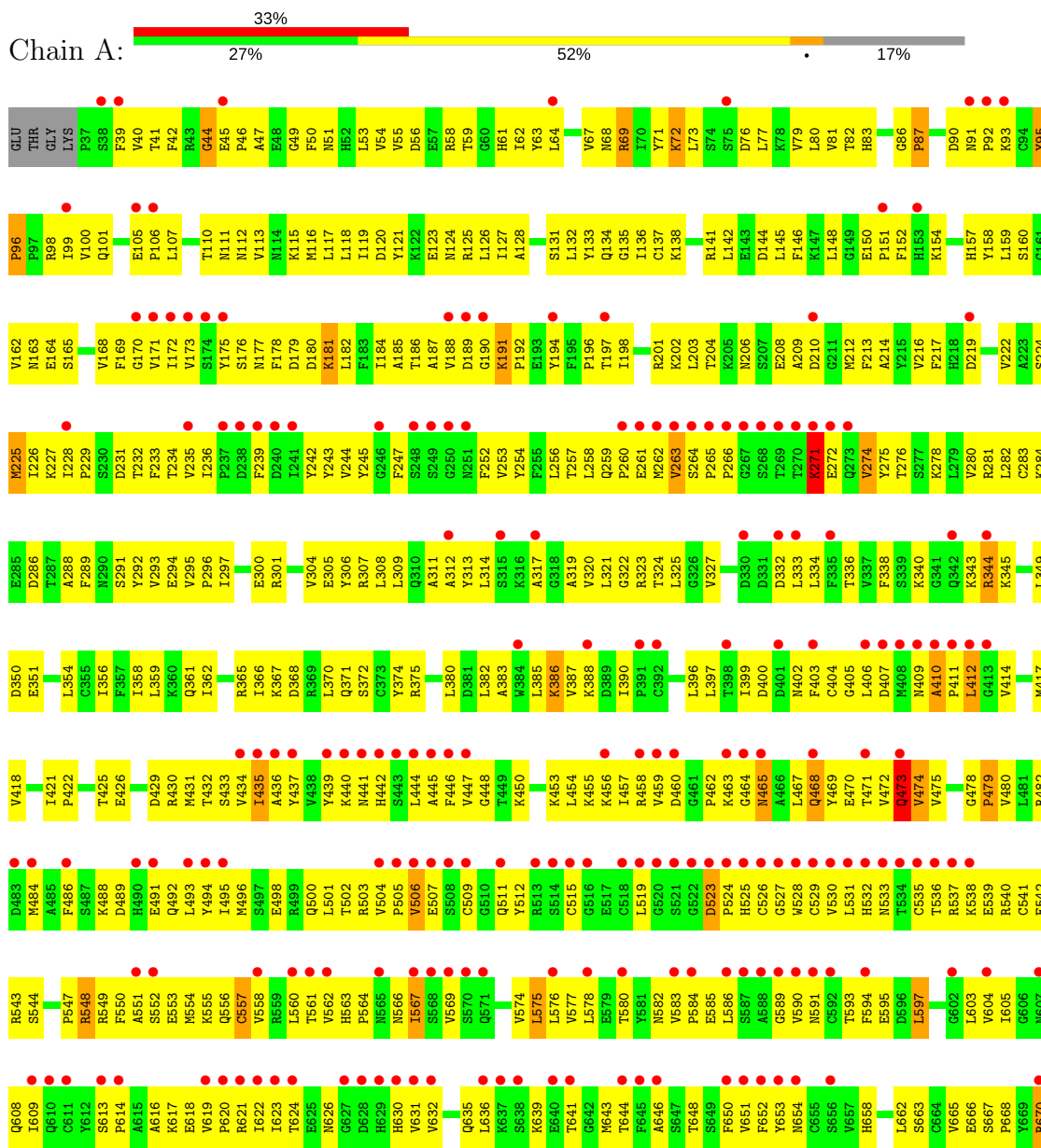
Continued from previous page...

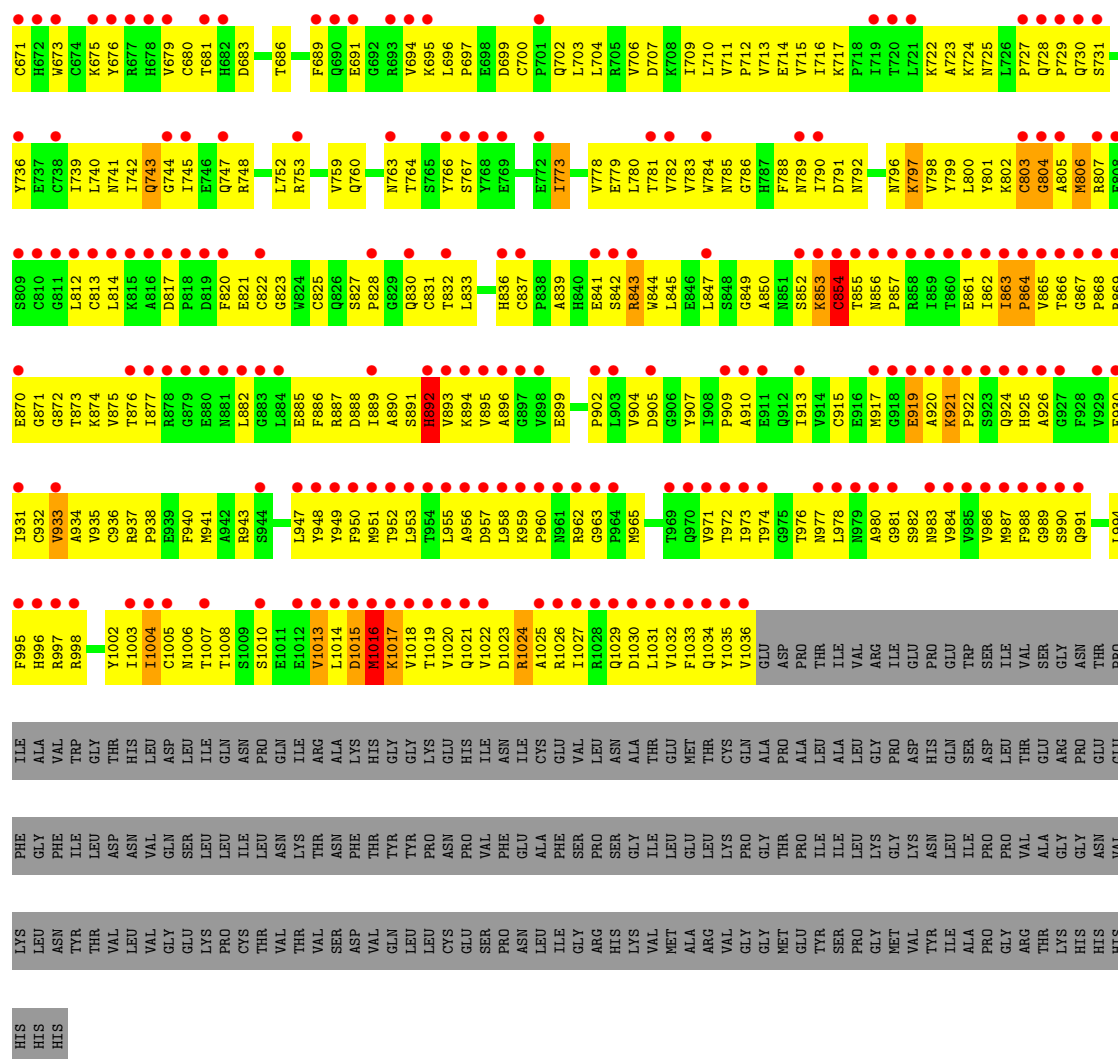
Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP Q80UG2

3 Residue-property plots

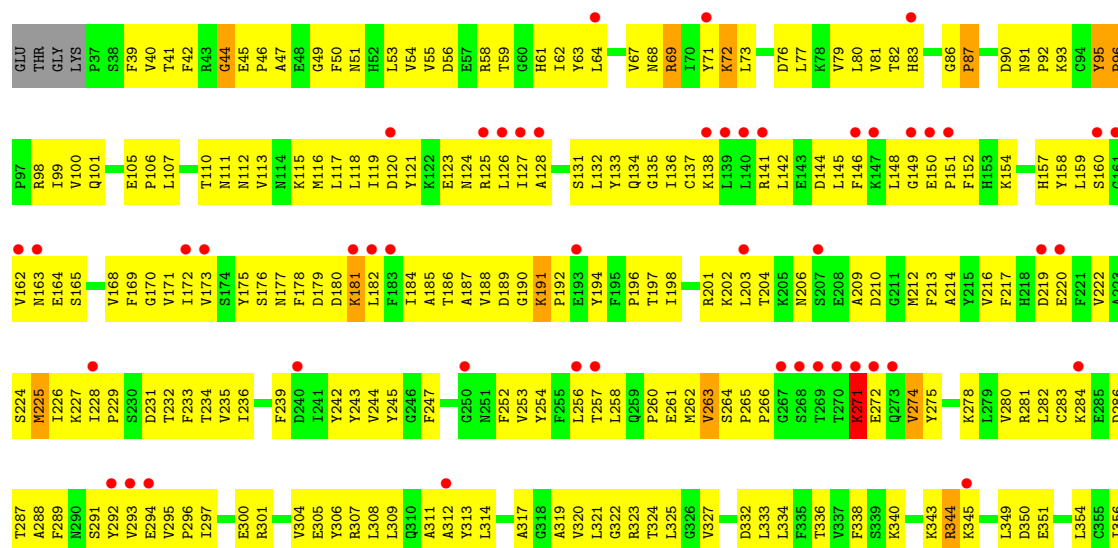
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Plexin-A4





• Molecule 1: Plexin-A4



HIS	HIS	HIS	HIS	C836	T873	L812	I745	T681	K617	Q556	L493	K431	F357
ARG	ARG	C813	E746	H662	E618	C813	E746	H662	E618	C557	Y494	T432	I358
ALA	ALA	L814	R747	D683	V619	L814	R747	D683	V619	R558	I495	S433	I358
SER	PRO	R815	R748	P684	P620	R815	R748	P684	P620	R559	M496	V434	K360
PRO	GLY	D817	V749	H685	R621	D817	V749	H685	R621	L560	S497	I435	Q361
SER	SER	A818	P750	T686	T622	A818	P750	T686	T622	T561	E498	A436	I362
TYR	TYR	P818	A751	H686	T623	P818	A751	H686	T623	V562	R499	Y437	R365
ILE	ILE	D819	R752	F689	T624	D819	R752	F689	T624	H563	Q500	Y439	R366
ILE	ILE	F820	L753	Q690	E625	F820	L753	Q690	E625	P564	L501	K440	I366
CYS	CYS	E821		E691	N626	E821		E691	N626	N566	T502	N441	K367
ASN	ASN	C822	V759	G692		C822	V759	G692		N566	R503	D368	D368
THR	THR	G823	Q760	H694	H629	G823	Q760	H694	H629	S568	V504	H442	R369
THR	THR	N824	C761	K695	H630	N824	C761	K695	H630	V569	P505	S443	L370
SER	SER	C825	Q762	K696	V631	C825	Q762	K696	V631	S570	E508	L444	Q371
GLY	GLY	C826	N763	L696	V632	C826	N763	L696	V632	Q571	S507	A445	C372
GLY	GLY	S827	T764	P697	L634	S827	T764	P697	L634	Y572	C509	F446	C373
GLY	GLY	P828	S765	E698	L634	P828	S765	E698	L634	Y573	G510	V447	S374
VAL	VAL	G829	Y766	D699	Q635	G829	Y766	D699	Q635	V574	Q511	Q448	R375
THR	THR	H832	S767	C700	L636	H832	S767	C700	L636	V574	Q511	T449	R375
THR	THR	V833	Y768	P701	K637	V833	Y768	P701	K637	L575	Y512	K450	L380
ALA	ALA	K834		Q702	S638	K834		Q702	S638	L576	C515	D381	D381
ASP	ASP	H835	M771	L703	K639	H835	M771	L703	K639	V577		L382	L382
ASP	ASP	A836	E772	L704	E640	A836	E772	L704	E640	L578		L454	A383
LEU	LEU	L833				L833						K455	W384
LYS	LYS	H836	I773	R705	T641	H836	I773	R705	T641	E579	L519	K456	L385
VAL	VAL	C837	N774	V706	H642	C837	N774	V706	H642	Y581	G520	L457	L386
ASN	ASN	P838	N775	D707	H643	P838	N775	D707	H643	N582	S521	K386	K386
ARG	ARG	A839	L776	I708	T644	A839	L776	I708	T644	N582	G522	R458	V387
GLY	GLY	H840	P777	R709	P645	H840	P777	R709	P645	D523	D523	V459	K388
GLY	GLY	E841	P778	L710	A646	E841	P778	L710	A646	P584	H525	D460	D389
ALA	ALA	S842	E779	V711	S647	S842	E779	V711	S647	E585	C526	G461	I390
ALA	ALA	R843	L780	P712	T648	R843	L780	P712	T648	S587	G527	P462	L396
SER	SER	D844	T781	V713	S649	D844	T781	V713	S649	A588	W528	G464	L397
GLY	GLY	L845	V782	E714	P650	L845	V782	E714	P650	G589	C530	N485	T399
GLY	GLY	E846	V783	V715	V651	E846	V783	V715	V651	V590	V530	L466	L399
THR	THR	S848	N785	I716	P652	S848	N785	I716	P652	N591	L531	L467	D401
THR	THR	Q849	G786	K717	Y653	Q849	G786	K717	Y653	C592	H532	D468	D401
ILE	ILE	A850	H787	F718	N654	A850	H787	F718	N654	T593	N533	N402	N402
THR	THR	H851	F788	I719		H851	F788	I719		F594	T594	E470	F403
GLY	GLY	C852	N789	T720	H658	C852	N789	T720	H658	E595	C535	T471	C404
THR	THR	K853	N790	L721	N659	K853	N790	L721	N659	D596	T536	V472	G405
ASN	ASN	C854	I791	K722	S660	C854	I791	K722	S660	L597	R537	Q473	L406
ASN	ASN	T855	D791	A723	C661	T855	D791	A723	C661	S598	K538	V474	L406
LEU	LEU	N856	N792	K724	S663	N856	N792	K724	S663	E599	E539	V475	N409
ASN	ASN	P857		N725	S663	P857		N725	S663	M600	R540	A410	A410
ALA	ALA	H858	N796	L726	C664	H858	N796	L726	C664	D601	C541	P411	P411
ALA	ALA	R858	K797	P727	V665	R858	K797	P727	V665	G602	E542	P479	L412
GLY	GLY	L859	V798	Q728	E666	L859	V798	Q728	E666	L603	R543	V480	G413
SER	SER	T860	Y799	P729	S667	T860	Y799	P729	S667	V604	S544	L481	V414
ASN	ASN	E861	L800	Q730	P668	E861	L800	Q730	P668	I605	E545	R482	V414
VAL	VAL	T862	Y801	Q730	V669	T862	Y801	Q730	V669	Q608	E546	D483	M417
VAL	VAL	L863	K802	S731	R670	L863	K802	S731	R670	I609	P547	M484	V418
VAL	VAL	P864	C803		C671	P864	C803		C671	Q610	R548	A485	V418
MET	MET	H864	C804	Y736	H672	H864	C804	Y736	H672	Q611	R549	F486	I421
GLU	GLU	V865	G804	E737	H673	V865	G804	E737	H673	C611	F550	S487	T425
TRP	TRP	T866	A805	C738	H673	T866	A805	C738	H673	Y612	S552	D489	E426
ASP	ASP	G867	M806	L739	C674	G867	M806	L739	C674	S613	E553	H490	D429
THR	THR	P868	R807	L740	K675	P868	R807	L740	K675	P614	M554	E491	D429
GLN	GLN	H869	B807	L741	H676	H869	B807	L741	H676	A616	K555	Q492	
VAL	VAL	R869	E868	N741		R869	E868	N741					
SER	SER	C870	S809	I742		C870	S809	I742					
GLY	GLY	E870	C810	Q743		E870	C810	Q743					
ASN	ASN	H871	C810	Q743		H871	C810	Q743					
THR	THR	G872	G811	G744		G872	G811	G744					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.18Å 241.00Å 144.07Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	47.74 – 8.00 47.74 – 8.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.74-8.00) 99.5 (47.74-8.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 8.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.349 , 0.349 0.344 , 0.352	Depositor DCC
R_{free} test set	488 reflections (4.86%)	DCC
Wilson B-factor (Å ²)	450.9	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 550.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.70	EDS
Total number of atoms	15030	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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

5.1 Standard geometry

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	1.01	5/8007 (0.1%)	1.36	27/10846 (0.2%)
1	B	1.00	5/7344 (0.1%)	1.32	24/9943 (0.2%)
All	All	1.01	10/15351 (0.1%)	1.34	51/20789 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	VAL	C-N	23.13	1.87	1.34
1	B	506	VAL	C-N	21.10	1.82	1.34
1	A	557	CYS	C-N	-20.82	0.86	1.34
1	B	557	CYS	C-N	-17.13	0.94	1.34
1	A	700	CYS	C-N	-15.63	1.04	1.34
1	B	700	CYS	C-N	15.54	1.63	1.34
1	B	49	GLY	CA-C	6.43	1.62	1.51
1	A	49	GLY	CA-C	6.42	1.62	1.51
1	A	49	GLY	C-N	5.06	1.45	1.34
1	B	49	GLY	C-N	5.05	1.45	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	747	GLN	CG-CD-OE1	-38.83	43.94	121.60
1	A	747	GLN	CG-CD-OE1	-38.81	43.98	121.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	TYR	O-C-N	-33.42	69.23	122.70
1	B	557	CYS	O-C-N	-31.89	71.68	122.70
1	A	653	TYR	CA-C-N	23.37	168.61	117.20
1	A	854	CYS	O-C-N	-23.21	85.56	122.70
1	A	557	CYS	O-C-N	18.53	152.35	122.70
1	B	557	CYS	CA-C-N	17.95	156.70	117.20
1	B	700	CYS	C-N-CD	-17.94	81.14	120.60
1	A	557	CYS	CA-C-N	-17.52	78.65	117.20
1	B	506	VAL	O-C-N	17.20	150.23	122.70
1	A	854	CYS	C-N-CA	16.73	163.51	121.70
1	A	653	TYR	C-N-CA	16.67	163.37	121.70
1	B	506	VAL	CA-C-N	-16.51	80.87	117.20
1	B	506	VAL	C-N-CA	-14.85	84.57	121.70
1	A	506	VAL	O-C-N	-14.82	98.98	122.70
1	A	854	CYS	CA-C-N	13.98	147.96	117.20
1	A	557	CYS	C-N-CA	-13.97	86.77	121.70
1	B	557	CYS	C-N-CA	11.36	150.09	121.70
1	B	747	GLN	CG-CD-NE2	-9.58	93.70	116.70
1	A	747	GLN	CG-CD-NE2	-9.56	93.76	116.70
1	A	700	CYS	O-C-N	-8.60	104.76	121.10
1	A	479	PRO	N-CA-C	8.18	133.37	112.10
1	B	479	PRO	N-CA-C	8.16	133.31	112.10
1	A	843	ARG	C-N-CA	7.76	141.10	121.70
1	B	843	ARG	C-N-CA	7.75	141.07	121.70
1	A	747	GLN	OE1-CD-NE2	6.89	137.74	121.90
1	A	478	GLY	CA-C-O	-6.87	108.23	120.60
1	B	478	GLY	CA-C-O	-6.85	108.27	120.60
1	B	747	GLN	OE1-CD-NE2	6.84	137.63	121.90
1	B	473	GLN	C-N-CA	-6.70	104.95	121.70
1	A	473	GLN	C-N-CA	-6.69	104.97	121.70
1	B	892	HIS	CA-CB-CG	6.59	124.81	113.60
1	A	892	HIS	CA-CB-CG	6.57	124.77	113.60
1	B	700	CYS	CA-C-N	-6.33	99.38	117.10
1	A	225	MET	CG-SD-CE	-5.72	91.05	100.20
1	B	225	MET	CG-SD-CE	-5.71	91.06	100.20
1	A	409	ASN	C-N-CA	5.67	135.87	121.70
1	B	409	ASN	C-N-CA	5.66	135.85	121.70
1	A	49	GLY	C-N-CA	5.62	135.74	121.70
1	B	49	GLY	C-N-CA	5.57	135.63	121.70
1	B	700	CYS	O-C-N	-5.55	110.55	121.10
1	A	700	CYS	CA-C-N	5.48	132.43	117.10
1	B	274	VAL	CG1-CB-CG2	5.47	119.65	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	VAL	CG1-CB-CG2	5.45	119.61	110.90
1	B	919	GLU	C-N-CA	5.27	134.88	121.70
1	A	919	GLU	C-N-CA	5.24	134.81	121.70
1	B	676	TYR	CA-CB-CG	-5.12	103.67	113.40
1	A	676	TYR	CA-CB-CG	-5.11	103.70	113.40
1	A	803	CYS	C-N-CA	5.09	132.98	122.30
1	B	803	CYS	C-N-CA	5.08	132.96	122.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	854	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	Peptide
1	B	557	CYS	Mainchain
1	B	700	CYS	Mainchain
1	B	863	ILE	Peptide
1	B	95	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7710	1244	29
1	B	7189	0	7050	1075	59
All	All	15030	0	14760	2319	61

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 78.

All (2319) 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:868:PRO:HD2	1:A:981:GLY:CA	1.32	1.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:CD	1:A:981:GLY:CA	1.87	1.50
1:A:873:THR:CA	1:A:982:SER:HB2	1.46	1.43
1:A:873:THR:HA	1:A:982:SER:CB	1.48	1.40
1:B:506:VAL:HG22	1:B:525:HIS:NE2	1.33	1.38
1:B:629:HIS:CE1	1:B:669:TYR:OH	1.76	1.37
1:B:629:HIS:ND1	1:B:669:TYR:OH	1.56	1.34
1:A:870:GLU:CD	1:A:1025:ALA:HB2	1.46	1.33
1:A:868:PRO:HD3	1:A:981:GLY:N	1.06	1.33
1:B:506:VAL:N	1:B:507:GLU:N	1.77	1.29
1:B:506:VAL:C	1:B:507:GLU:N	1.82	1.28
1:A:868:PRO:CD	1:A:981:GLY:N	1.88	1.27
1:A:506:VAL:C	1:A:507:GLU:N	1.87	1.26
1:B:700:CYS:O	1:B:725:ASN:HB2	1.38	1.23
1:A:870:GLU:HB3	1:A:1024:ARG:CG	1.70	1.22
1:B:809:SER:CB	1:B:881:ASN:OD1	1.89	1.19
1:B:809:SER:HB2	1:B:881:ASN:CG	1.62	1.18
1:A:569:VAL:CG2	1:A:654:ASN:HB2	1.71	1.18
1:A:867:GLY:HA2	1:A:981:GLY:N	1.59	1.17
1:A:359:LEU:HD12	1:A:362:ILE:HD11	1.24	1.17
1:B:118:LEU:HD12	1:B:172:ILE:HD12	1.17	1.17
1:B:456:LYS:HD2	1:B:523:ASP:OD2	1.44	1.17
1:A:868:PRO:HD3	1:A:980:ALA:C	1.63	1.17
1:B:676:TYR:CE1	1:B:730:GLN:HG2	1.80	1.15
1:B:295:VAL:HG12	1:B:414:VAL:HG11	1.27	1.14
1:B:802:LYS:C	1:B:803:CYS:N	2.01	1.14
1:A:453:LYS:HG2	1:A:472:VAL:HG22	1.25	1.14
1:B:359:LEU:HD12	1:B:362:ILE:HD11	1.24	1.14
1:B:506:VAL:CG2	1:B:525:HIS:NE2	2.11	1.14
1:A:324:THR:HB	1:A:462:PRO:HB3	1.27	1.13
1:A:458:ARG:HD2	1:A:524:PRO:HB3	1.31	1.12
1:A:118:LEU:HD12	1:A:172:ILE:HD12	1.17	1.12
1:A:435:ILE:HG22	1:A:446:PHE:HB2	1.22	1.12
1:A:295:VAL:HG12	1:A:414:VAL:HG11	1.27	1.12
1:B:453:LYS:HG2	1:B:472:VAL:HG22	1.25	1.12
1:B:809:SER:HB2	1:B:881:ASN:OD1	0.95	1.11
1:B:435:ILE:HG22	1:B:446:PHE:HB2	1.22	1.11
1:A:533:ASN:ND2	1:A:644:THR:O	1.83	1.11
1:A:595:GLU:HB2	1:A:597:LEU:HD23	1.32	1.11
1:B:676:TYR:CD1	1:B:730:GLN:CG	2.33	1.11
1:B:469:TYR:HB2	1:B:523:ASP:OD1	1.50	1.10
1:B:595:GLU:HB2	1:B:597:LEU:HD23	1.32	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:806:MET:H	1:A:806:MET:HE3	1.14	1.10
1:B:324:THR:HB	1:B:462:PRO:HB3	1.27	1.09
1:B:806:MET:HE3	1:B:806:MET:H	1.14	1.09
1:A:868:PRO:CD	1:A:981:GLY:HA3	1.61	1.09
1:A:871:GLY:O	1:A:1023:ASP:CB	2.00	1.09
1:B:444:LEU:HD23	1:B:524:PRO:CG	1.83	1.08
1:A:1017:LYS:HE2	1:A:1017:LYS:H	1.18	1.08
1:B:676:TYR:CE1	1:B:730:GLN:CG	2.37	1.08
1:A:868:PRO:HD2	1:A:981:GLY:HA2	1.17	1.08
1:A:474:VAL:HG12	1:A:475:VAL:HG23	1.33	1.08
1:B:468:GLN:HG3	1:B:523:ASP:HA	1.16	1.07
1:B:469:TYR:CB	1:B:523:ASP:OD1	2.02	1.07
1:B:506:VAL:C	1:B:507:GLU:CA	2.21	1.07
1:A:870:GLU:CB	1:A:1024:ARG:HG2	1.84	1.07
1:B:474:VAL:HG12	1:B:475:VAL:HG23	1.33	1.07
1:A:549:ARG:HD3	1:A:584:PRO:CB	1.84	1.06
1:A:440:LYS:HB2	1:A:538:LYS:NZ	1.68	1.06
1:A:439:TYR:CE2	1:A:538:LYS:NZ	2.23	1.05
1:B:506:VAL:CA	1:B:507:GLU:N	2.17	1.05
1:B:676:TYR:CD1	1:B:730:GLN:HG3	1.91	1.05
1:A:569:VAL:HG21	1:A:654:ASN:HB2	1.32	1.04
1:B:506:VAL:HG22	1:B:525:HIS:CE1	1.92	1.04
1:B:444:LEU:HD23	1:B:524:PRO:HG3	1.37	1.03
1:B:494:TYR:HB3	1:B:501:LEU:HD21	1.40	1.03
1:B:301:ARG:HD2	1:B:425:THR:HG21	1.37	1.03
1:B:620:PRO:HA	1:B:623:ILE:HG13	1.41	1.03
1:A:46:PRO:HG2	1:A:69:ARG:HG3	1.41	1.02
1:A:301:ARG:HD2	1:A:425:THR:HG21	1.37	1.02
1:A:560:LEU:HD23	1:A:648:THR:HG23	1.37	1.02
1:A:440:LYS:HD2	1:A:538:LYS:HD3	1.37	1.02
1:A:871:GLY:O	1:A:1023:ASP:CG	1.98	1.01
1:A:620:PRO:HA	1:A:623:ILE:HG13	1.41	1.01
1:A:867:GLY:CA	1:A:981:GLY:H	1.72	1.01
1:A:494:TYR:HB3	1:A:501:LEU:HD21	1.40	1.01
1:B:676:TYR:CD1	1:B:730:GLN:HG2	1.94	1.00
1:B:560:LEU:HD23	1:B:648:THR:HG23	1.37	1.00
1:B:46:PRO:HG2	1:B:69:ARG:HG3	1.41	1.00
1:A:873:THR:OG1	1:A:981:GLY:HA2	1.60	0.99
1:B:117:LEU:HD11	1:B:126:LEU:HD21	1.45	0.99
1:A:117:LEU:HD11	1:A:126:LEU:HD21	1.45	0.99
1:A:870:GLU:CB	1:A:1024:ARG:CG	2.40	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ILE:HA	1:B:626:ASN:HD21	1.28	0.99
1:A:870:GLU:HB3	1:A:1024:ARG:HG2	1.01	0.99
1:A:868:PRO:HD3	1:A:981:GLY:CA	1.73	0.99
1:A:458:ARG:HD2	1:A:524:PRO:CB	1.92	0.98
1:B:548:ARG:HG3	1:B:583:VAL:C	1.84	0.98
1:B:444:LEU:HD12	1:B:446:PHE:CE1	1.98	0.98
1:B:862:ILE:HG22	1:B:877:ILE:HA	1.46	0.98
1:A:870:GLU:CD	1:A:1025:ALA:CB	2.33	0.97
1:A:444:LEU:HD12	1:A:446:PHE:CE1	1.98	0.97
1:A:870:GLU:OE1	1:A:1025:ALA:HB2	1.62	0.97
1:A:563:HIS:HB3	1:A:564:PRO:HD3	1.44	0.97
1:B:563:HIS:HB3	1:B:564:PRO:HD3	1.44	0.97
1:A:623:ILE:HA	1:A:626:ASN:HD21	1.28	0.96
1:A:862:ILE:HG22	1:A:877:ILE:HA	1.46	0.96
1:B:662:LEU:HD23	1:B:791:ASP:OD2	1.65	0.96
1:B:566:ASN:HA	1:B:651:VAL:HG23	1.49	0.95
1:B:458:ARG:HD2	1:B:524:PRO:HB3	1.45	0.95
1:B:629:HIS:CG	1:B:669:TYR:OH	2.15	0.95
1:A:566:ASN:HA	1:A:651:VAL:HG23	1.49	0.95
1:B:506:VAL:C	1:B:507:GLU:HA	1.84	0.95
1:A:440:LYS:HB2	1:A:538:LYS:HZ2	1.27	0.94
1:B:505:PRO:C	1:B:507:GLU:N	2.19	0.94
1:A:42:PHE:HE1	1:A:79:VAL:HG22	1.31	0.94
1:A:870:GLU:OE2	1:A:1025:ALA:HB2	1.65	0.94
1:A:868:PRO:HD2	1:A:981:GLY:HA3	1.16	0.94
1:A:994:LEU:HD11	1:A:1006:ASN:HD22	1.31	0.94
1:A:72:LYS:HE3	1:A:80:LEU:HD13	1.49	0.94
1:A:871:GLY:O	1:A:1023:ASP:HB3	1.68	0.93
1:B:62:ILE:CG1	1:B:73:LEU:HB2	1.98	0.93
1:B:42:PHE:HE1	1:B:79:VAL:HG22	1.31	0.93
1:A:297:ILE:HG22	1:A:418:VAL:CG1	1.97	0.93
1:A:870:GLU:CG	1:A:1024:ARG:HG3	1.97	0.93
1:B:456:LYS:CD	1:B:523:ASP:OD2	2.15	0.93
1:B:297:ILE:HG22	1:B:418:VAL:HG12	1.49	0.93
1:B:804:GLY:HA2	1:B:806:MET:SD	2.09	0.93
1:A:62:ILE:CG1	1:A:73:LEU:HB2	1.98	0.93
1:A:440:LYS:HD2	1:A:538:LYS:CD	1.98	0.93
1:A:804:GLY:HA2	1:A:806:MET:SD	2.09	0.93
1:B:297:ILE:HG22	1:B:418:VAL:CG1	1.97	0.93
1:B:865:VAL:HG13	1:B:866:THR:HG23	1.50	0.93
1:A:297:ILE:HG22	1:A:418:VAL:HG12	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:ILE:HG22	1:B:876:THR:HB	1.48	0.92
1:A:863:ILE:HG22	1:A:876:THR:HB	1.48	0.92
1:A:39:PHE:CE2	1:A:473:GLN:HG3	2.05	0.92
1:B:72:LYS:HE3	1:B:80:LEU:HD13	1.49	0.92
1:B:271:LYS:HG3	1:B:272:GLU:H	1.34	0.92
1:A:435:ILE:HD13	1:A:436:ALA:H	1.34	0.92
1:B:527:GLY:HA3	1:B:550:PHE:CZ	2.04	0.92
1:A:239:PHE:HA	1:A:260:PRO:HG2	1.51	0.92
1:A:865:VAL:HG13	1:A:866:THR:HG23	1.50	0.92
1:B:39:PHE:CE2	1:B:473:GLN:HG3	2.05	0.92
1:A:933:VAL:HG23	1:A:934:ALA:H	1.35	0.91
1:B:239:PHE:HA	1:B:260:PRO:HG2	1.51	0.91
1:A:870:GLU:HG2	1:A:1024:ARG:C	1.91	0.91
1:B:806:MET:SD	1:B:807:ARG:HG3	2.11	0.91
1:B:435:ILE:HD13	1:B:436:ALA:H	1.34	0.91
1:A:806:MET:SD	1:A:807:ARG:HG3	2.11	0.91
1:A:527:GLY:HA3	1:A:550:PHE:CZ	2.05	0.90
1:A:447:VAL:HG22	1:A:455:LYS:HB2	1.53	0.90
1:A:549:ARG:HD3	1:A:584:PRO:HB2	1.53	0.90
1:B:933:VAL:HG23	1:B:934:ALA:H	1.36	0.90
1:A:271:LYS:HG3	1:A:272:GLU:H	1.34	0.90
1:A:359:LEU:CD1	1:A:362:ILE:HD11	2.02	0.89
1:A:447:VAL:CG2	1:A:455:LYS:HB2	2.03	0.89
1:A:972:THR:HG23	1:A:1002:TYR:CE1	2.07	0.89
1:A:873:THR:C	1:A:982:SER:HB2	1.91	0.89
1:B:653:TYR:HE2	1:B:682:HIS:ND1	1.69	0.89
1:A:453:LYS:CG	1:A:472:VAL:HG22	2.03	0.88
1:B:447:VAL:CG2	1:B:455:LYS:HB2	2.03	0.88
1:B:453:LYS:CG	1:B:472:VAL:HG22	2.03	0.88
1:B:95:TYR:CD2	1:B:96:PRO:HD3	2.08	0.88
1:B:447:VAL:HG22	1:B:455:LYS:HB2	1.53	0.88
1:B:802:LYS:O	1:B:803:CYS:N	2.06	0.88
1:B:181:LYS:CD	1:B:202:LYS:HA	2.04	0.88
1:A:870:GLU:OE2	1:A:1025:ALA:CB	2.22	0.88
1:B:359:LEU:CD1	1:B:362:ILE:HD11	2.02	0.88
1:A:863:ILE:HG23	1:A:864:PRO:HD2	1.55	0.88
1:B:892:HIS:HB2	1:B:932:CYS:O	1.74	0.88
1:A:446:PHE:HD2	1:A:454:LEU:HD21	1.38	0.87
1:B:847:LEU:HG	1:B:850:ALA:H	1.39	0.87
1:B:486:PHE:CD1	1:B:493:LEU:HD13	2.09	0.87
1:A:532:HIS:HA	1:A:641:THR:OG1	1.73	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:HIS:HB2	1:A:932:CYS:O	1.73	0.87
1:A:95:TYR:CD2	1:A:96:PRO:HD3	2.08	0.87
1:A:867:GLY:HA2	1:A:981:GLY:H	0.77	0.87
1:A:486:PHE:CD1	1:A:493:LEU:HD13	2.09	0.87
1:B:468:GLN:HG3	1:B:523:ASP:CA	2.03	0.87
1:B:863:ILE:HG23	1:B:864:PRO:HD2	1.56	0.86
1:B:110:THR:CG2	1:B:132:LEU:HD21	2.05	0.86
1:B:439:TYR:CE2	1:B:538:LYS:NZ	2.42	0.86
1:A:39:PHE:CE1	1:A:505:PRO:HD2	2.10	0.86
1:A:959:LYS:HB2	1:A:972:THR:HB	1.57	0.86
1:A:110:THR:CG2	1:A:132:LEU:HD21	2.05	0.86
1:A:181:LYS:CD	1:A:202:LYS:HA	2.04	0.86
1:A:833:LEU:HB2	1:A:836:HIS:HD2	1.39	0.86
1:B:446:PHE:HD2	1:B:454:LEU:HD21	1.38	0.86
1:B:603:LEU:HD23	1:B:604:VAL:N	1.90	0.86
1:B:699:ASP:HA	1:B:725:ASN:OD1	1.74	0.86
1:A:370:LEU:CD1	1:A:399:ILE:HD12	2.06	0.86
1:B:256:LEU:HB3	1:B:309:LEU:HD22	1.56	0.86
1:B:435:ILE:CG2	1:B:446:PHE:HB2	2.06	0.86
1:B:833:LEU:HB2	1:B:836:HIS:HD2	1.39	0.86
1:B:295:VAL:HA	1:B:414:VAL:CG2	2.05	0.86
1:A:118:LEU:HD13	1:A:119:ILE:N	1.91	0.86
1:A:295:VAL:HA	1:A:414:VAL:CG2	2.05	0.86
1:B:100:VAL:HG12	1:B:101:GLN:HG3	1.58	0.86
1:B:473:GLN:CG	1:B:504:VAL:HG22	2.06	0.86
1:B:700:CYS:HB3	1:B:701:PRO:CD	1.92	0.86
1:B:847:LEU:HD12	1:B:852:SER:HB3	1.58	0.86
1:A:603:LEU:HD23	1:A:604:VAL:N	1.90	0.85
1:B:370:LEU:CD1	1:B:399:ILE:HD12	2.05	0.85
1:B:531:LEU:O	1:B:641:THR:OG1	1.94	0.85
1:B:847:LEU:HD11	1:B:850:ALA:HA	1.58	0.85
1:A:100:VAL:HG12	1:A:101:GLN:HG3	1.58	0.85
1:B:676:TYR:HE1	1:B:730:GLN:HG2	1.41	0.85
1:B:133:TYR:CG	1:B:136:ILE:HG12	2.12	0.85
1:A:882:LEU:HB2	1:A:910:ALA:HA	1.58	0.85
1:A:847:LEU:HD12	1:A:852:SER:HB3	1.58	0.85
1:A:133:TYR:CG	1:A:136:ILE:HG12	2.12	0.85
1:A:706:VAL:HG22	1:A:707:ASP:H	1.42	0.85
1:A:473:GLN:CG	1:A:504:VAL:HG22	2.06	0.85
1:A:42:PHE:CZ	1:A:45:GLU:HB2	2.12	0.84
1:A:847:LEU:HG	1:A:850:ALA:H	1.39	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD13	1:B:119:ILE:N	1.91	0.84
1:B:39:PHE:CE1	1:B:505:PRO:HD2	2.11	0.84
1:A:256:LEU:HB3	1:A:309:LEU:HD22	1.56	0.84
1:B:548:ARG:HG3	1:B:583:VAL:O	1.77	0.84
1:A:989:GLY:HA2	1:A:1017:LYS:HE3	1.57	0.84
1:B:42:PHE:CZ	1:B:45:GLU:HB2	2.12	0.84
1:B:356:ILE:CG2	1:B:421:ILE:HB	2.07	0.84
1:B:295:VAL:CG1	1:B:414:VAL:HG11	2.07	0.84
1:B:50:PHE:HB2	1:B:498:GLU:O	1.78	0.84
1:B:40:VAL:CG1	1:B:503:ARG:HB3	2.08	0.84
1:B:653:TYR:C	1:B:654:ASN:N	2.31	0.83
1:A:40:VAL:CG1	1:A:503:ARG:HB3	2.08	0.83
1:B:295:VAL:HA	1:B:414:VAL:HG22	1.60	0.83
1:A:229:PRO:O	1:A:232:THR:HG22	1.79	0.83
1:A:356:ILE:CG2	1:A:421:ILE:HB	2.07	0.83
1:A:336:THR:O	1:A:354:LEU:HD12	1.78	0.83
1:A:863:ILE:CG2	1:A:876:THR:HB	2.07	0.83
1:A:971:VAL:HG22	1:A:1005:CYS:O	1.78	0.83
1:B:706:VAL:HG22	1:B:707:ASP:H	1.42	0.83
1:A:118:LEU:HD12	1:A:172:ILE:CD1	2.05	0.83
1:B:830:GLN:HG2	1:B:831:CYS:H	1.43	0.83
1:B:474:VAL:HG22	1:B:495:ILE:HG21	1.61	0.83
1:B:118:LEU:HD12	1:B:172:ILE:CD1	2.05	0.83
1:B:336:THR:O	1:B:354:LEU:HD12	1.78	0.83
1:B:358:ILE:HG23	1:B:361:GLN:H	1.44	0.83
1:A:397:LEU:HD23	1:A:399:ILE:HD13	1.61	0.83
1:A:42:PHE:CE1	1:A:79:VAL:HG22	2.14	0.83
1:A:847:LEU:HD11	1:A:850:ALA:HA	1.58	0.83
1:A:996:HIS:HB3	1:A:1004:ILE:HG23	1.59	0.83
1:B:229:PRO:O	1:B:232:THR:HG22	1.79	0.83
1:A:295:VAL:CG1	1:A:414:VAL:HG11	2.07	0.83
1:B:133:TYR:CB	1:B:136:ILE:HG12	2.09	0.83
1:A:440:LYS:CD	1:A:538:LYS:HD3	2.08	0.82
1:A:474:VAL:HG22	1:A:495:ILE:HG21	1.61	0.82
1:B:397:LEU:HD23	1:B:399:ILE:HD13	1.61	0.82
1:B:53:LEU:HD23	1:B:54:VAL:N	1.94	0.82
1:A:358:ILE:HG23	1:A:361:GLN:H	1.44	0.82
1:A:951:MET:C	1:A:952:THR:N	2.32	0.82
1:B:295:VAL:HG12	1:B:414:VAL:CG1	2.09	0.82
1:A:435:ILE:CG2	1:A:446:PHE:HB2	2.06	0.82
1:A:548:ARG:HG3	1:A:583:VAL:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:785:ASN:HB3	1:B:788:PHE:CD2	2.14	0.82
1:B:863:ILE:CG2	1:B:876:THR:HB	2.07	0.82
1:A:987:MET:HB2	1:A:1019:THR:CG2	2.09	0.82
1:A:44:GLY:HA2	1:A:50:PHE:CE2	2.15	0.82
1:A:53:LEU:HD23	1:A:54:VAL:N	1.94	0.82
1:A:44:GLY:HA2	1:A:50:PHE:HE2	1.44	0.82
1:B:44:GLY:HA2	1:B:50:PHE:CE2	2.15	0.82
1:A:133:TYR:CB	1:A:136:ILE:HG12	2.09	0.82
1:A:785:ASN:HB3	1:A:788:PHE:CD2	2.14	0.82
1:A:295:VAL:HA	1:A:414:VAL:HG22	1.60	0.82
1:A:50:PHE:HB2	1:A:498:GLU:O	1.78	0.82
1:A:991:GLN:CG	1:A:1008:THR:HG21	2.10	0.82
1:A:439:TYR:CE2	1:A:538:LYS:CE	2.63	0.82
1:B:185:ALA:HB1	1:B:243:TYR:CE1	2.15	0.82
1:A:397:LEU:HD23	1:A:399:ILE:CD1	2.10	0.81
1:B:882:LEU:HB2	1:B:910:ALA:HA	1.58	0.81
1:A:225:MET:HE1	1:A:227:LYS:HG3	1.63	0.81
1:A:994:LEU:HD11	1:A:1006:ASN:HB2	1.63	0.81
1:B:356:ILE:HG22	1:B:421:ILE:HB	1.61	0.81
1:B:62:ILE:HG13	1:B:73:LEU:HB2	1.62	0.81
1:A:889:ILE:HG23	1:A:892:HIS:CE1	2.16	0.81
1:B:154:LYS:HD3	1:B:210:ASP:OD1	1.81	0.81
1:B:397:LEU:HD23	1:B:399:ILE:CD1	2.11	0.81
1:B:863:ILE:HG13	1:B:864:PRO:HD3	1.62	0.81
1:A:458:ARG:HD2	1:A:524:PRO:CG	2.10	0.81
1:B:42:PHE:CE1	1:B:79:VAL:HG22	2.14	0.81
1:A:440:LYS:CB	1:A:538:LYS:NZ	2.44	0.81
1:A:154:LYS:HD3	1:A:210:ASP:OD1	1.81	0.80
1:B:154:LYS:HB2	1:B:157:HIS:CD2	2.16	0.80
1:B:324:THR:HB	1:B:462:PRO:CB	2.10	0.80
1:A:185:ALA:HB1	1:A:243:TYR:CE1	2.15	0.80
1:A:623:ILE:HD12	1:A:624:THR:N	1.96	0.80
1:B:486:PHE:CE1	1:B:493:LEU:HD13	2.16	0.80
1:B:889:ILE:HG23	1:B:892:HIS:CE1	2.16	0.80
1:A:830:GLN:HG2	1:A:831:CYS:H	1.43	0.80
1:A:356:ILE:HG22	1:A:421:ILE:HB	1.61	0.80
1:A:486:PHE:CE1	1:A:493:LEU:HD13	2.16	0.80
1:B:444:LEU:HD13	1:B:445:ALA:N	1.97	0.80
1:B:623:ILE:HD12	1:B:624:THR:N	1.96	0.80
1:A:620:PRO:HA	1:A:623:ILE:CG1	2.12	0.80
1:B:314:LEU:HD11	1:B:332:ASP:HB3	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:PRO:HB3	1:B:233:PHE:CE1	2.17	0.80
1:B:653:TYR:HE2	1:B:682:HIS:HD1	1.27	0.80
1:A:994:LEU:CD1	1:A:1006:ASN:HB2	2.12	0.79
1:B:620:PRO:HA	1:B:623:ILE:CG1	2.12	0.79
1:A:192:PRO:HB3	1:A:233:PHE:CE1	2.17	0.79
1:B:239:PHE:CE1	1:B:260:PRO:HD2	2.17	0.79
1:B:317:ALA:HB1	1:B:321:LEU:HB3	1.64	0.79
1:B:380:LEU:HD12	1:B:386:LYS:HE3	1.64	0.79
1:A:321:LEU:HD12	1:A:462:PRO:HG2	1.64	0.79
1:A:591:ASN:OD1	1:A:639:LYS:HE2	1.83	0.79
1:A:926:ALA:HB1	1:A:947:LEU:HD12	1.63	0.79
1:B:699:ASP:CA	1:B:725:ASN:OD1	2.29	0.79
1:A:154:LYS:HB2	1:A:157:HIS:CD2	2.16	0.79
1:A:370:LEU:HD12	1:A:399:ILE:HD12	1.64	0.79
1:A:951:MET:HG2	1:A:977:ASN:CG	2.03	0.79
1:B:370:LEU:HD12	1:B:399:ILE:HD12	1.63	0.79
1:A:239:PHE:CE1	1:A:260:PRO:HD2	2.17	0.79
1:A:244:VAL:HG13	1:A:482:ARG:NH1	1.98	0.79
1:B:244:VAL:HG13	1:B:482:ARG:NH1	1.98	0.79
1:A:324:THR:HB	1:A:462:PRO:CB	2.10	0.79
1:A:444:LEU:HD13	1:A:445:ALA:N	1.97	0.79
1:A:863:ILE:HG13	1:A:864:PRO:HD3	1.62	0.79
1:B:591:ASN:OD1	1:B:639:LYS:HE2	1.83	0.79
1:A:62:ILE:HG13	1:A:73:LEU:HB2	1.62	0.79
1:B:319:ALA:H	1:B:441:ASN:HD22	1.31	0.79
1:B:44:GLY:HA2	1:B:50:PHE:HE2	1.44	0.79
1:B:926:ALA:HB1	1:B:947:LEU:HD12	1.63	0.79
1:A:715:VAL:HG21	1:A:717:LYS:HD2	1.65	0.78
1:B:453:LYS:HE3	1:B:472:VAL:CG2	2.13	0.78
1:B:715:VAL:HG21	1:B:717:LYS:HD2	1.65	0.78
1:A:319:ALA:H	1:A:441:ASN:HD22	1.31	0.78
1:A:440:LYS:CB	1:A:538:LYS:HZ3	1.96	0.78
1:A:231:ASP:O	1:A:234:THR:HG22	1.84	0.78
1:A:295:VAL:HG12	1:A:414:VAL:CG1	2.09	0.78
1:A:847:LEU:CG	1:A:850:ALA:HA	2.13	0.78
1:B:320:VAL:HG21	1:B:442:HIS:CD2	2.19	0.78
1:A:453:LYS:HE3	1:A:472:VAL:CG2	2.13	0.78
1:A:320:VAL:HG21	1:A:442:HIS:CD2	2.19	0.78
1:A:742:ILE:HB	1:A:745:ILE:O	1.84	0.78
1:A:873:THR:HA	1:A:982:SER:HB2	0.82	0.78
1:B:469:TYR:HB3	1:B:523:ASP:OD1	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ILE:HB	1:B:745:ILE:O	1.84	0.78
1:A:380:LEU:HD12	1:A:386:LYS:HE3	1.64	0.78
1:A:868:PRO:CG	1:A:981:GLY:HA3	2.12	0.78
1:B:56:ASP:OD2	1:B:142:LEU:HD11	1.83	0.78
1:B:321:LEU:HD12	1:B:462:PRO:HG2	1.64	0.78
1:A:972:THR:HA	1:A:1002:TYR:HE1	1.47	0.78
1:A:181:LYS:NZ	1:A:216:VAL:HG23	1.98	0.78
1:A:327:VAL:HG12	1:A:358:ILE:HD11	1.66	0.78
1:B:439:TYR:OH	1:B:538:LYS:HE3	1.83	0.78
1:A:439:TYR:CZ	1:A:538:LYS:CE	2.67	0.78
1:A:870:GLU:HG2	1:A:1025:ALA:N	1.98	0.78
1:A:51:ASN:HD21	1:A:67:VAL:HG23	1.49	0.78
1:A:994:LEU:O	1:A:994:LEU:HD12	1.84	0.78
1:B:847:LEU:CG	1:B:850:ALA:HA	2.13	0.78
1:A:314:LEU:HD11	1:A:332:ASP:HB3	1.64	0.77
1:A:710:LEU:HD12	1:A:710:LEU:O	1.84	0.77
1:A:284:LYS:HD3	1:A:284:LYS:O	1.84	0.77
1:B:168:VAL:HG23	1:B:185:ALA:O	1.84	0.77
1:B:51:ASN:HD21	1:B:67:VAL:HG23	1.50	0.77
1:A:1014:LEU:H	1:A:1014:LEU:HD22	1.48	0.77
1:A:1016:MET:HG2	1:A:1035:TYR:CE2	2.19	0.77
1:A:327:VAL:CG1	1:A:358:ILE:HD11	2.14	0.77
1:B:327:VAL:CG1	1:B:358:ILE:HD11	2.14	0.77
1:A:56:ASP:OD2	1:A:142:LEU:HD11	1.83	0.77
1:B:710:LEU:O	1:B:710:LEU:HD12	1.84	0.77
1:B:595:GLU:CB	1:B:597:LEU:HD23	2.14	0.77
1:B:231:ASP:O	1:B:234:THR:HG22	1.84	0.77
1:B:327:VAL:HG12	1:B:358:ILE:HD11	1.65	0.77
1:B:567:ILE:HD13	1:B:567:ILE:H	1.50	0.77
1:A:168:VAL:HG23	1:A:185:ALA:O	1.84	0.77
1:B:662:LEU:HD11	1:B:702:GLN:NE2	1.99	0.77
1:A:317:ALA:HB1	1:A:321:LEU:HB3	1.64	0.77
1:A:547:PRO:O	1:A:548:ARG:HG2	1.84	0.77
1:A:870:GLU:HG3	1:A:1024:ARG:HG3	1.64	0.77
1:B:204:THR:HG21	1:B:209:ALA:HB3	1.66	0.77
1:B:181:LYS:NZ	1:B:216:VAL:HG23	1.98	0.77
1:B:359:LEU:HD12	1:B:362:ILE:CD1	2.10	0.77
1:A:1021:GLN:HG2	1:A:1026:ARG:HG3	1.67	0.77
1:B:403:PHE:CE1	1:B:406:LEU:HD23	2.20	0.77
1:A:567:ILE:H	1:A:567:ILE:HD13	1.50	0.76
1:A:549:ARG:HD3	1:A:584:PRO:HB3	1.66	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:LYS:O	1:B:284:LYS:HD3	1.84	0.76
1:A:120:ASP:OD2	1:A:123:GLU:HG3	1.86	0.76
1:A:403:PHE:CE1	1:A:406:LEU:HD23	2.20	0.76
1:A:439:TYR:OH	1:A:538:LYS:HE3	1.84	0.76
1:A:460:ASP:HB3	1:A:464:GLY:N	2.00	0.76
1:B:780:LEU:O	1:B:780:LEU:HD12	1.86	0.76
1:B:847:LEU:CD1	1:B:850:ALA:HA	2.16	0.76
1:A:873:THR:HA	1:A:982:SER:CA	2.15	0.76
1:B:172:ILE:HG12	1:B:182:LEU:HD13	1.68	0.76
1:B:616:ALA:O	1:B:620:PRO:HD2	1.85	0.76
1:A:359:LEU:HD12	1:A:362:ILE:CD1	2.09	0.76
1:A:616:ALA:O	1:A:620:PRO:HD2	1.85	0.76
1:A:780:LEU:HD12	1:A:780:LEU:O	1.86	0.76
1:B:120:ASP:OD2	1:B:123:GLU:HG3	1.86	0.76
1:B:460:ASP:HB3	1:B:464:GLY:N	2.00	0.76
1:B:64:LEU:HD12	1:B:496:MET:CE	2.16	0.76
1:A:873:THR:OG1	1:A:981:GLY:CA	2.34	0.76
1:A:1010:SER:HB2	1:A:1035:TYR:CE2	2.20	0.75
1:A:256:LEU:CB	1:A:309:LEU:HD22	2.16	0.75
1:A:42:PHE:HZ	1:A:45:GLU:HB2	1.50	0.75
1:A:869:ARG:O	1:A:920:ALA:HB3	1.86	0.75
1:A:868:PRO:HG2	1:A:1022:VAL:HG22	1.65	0.75
1:A:172:ILE:HG12	1:A:182:LEU:HD13	1.68	0.75
1:A:458:ARG:CD	1:A:524:PRO:HB3	2.12	0.75
1:A:919:GLU:HB3	1:A:1024:ARG:HH11	1.51	0.75
1:B:278:LYS:HE3	1:B:296:PRO:HG3	1.67	0.75
1:B:547:PRO:O	1:B:548:ARG:HG2	1.84	0.75
1:B:806:MET:HE3	1:B:806:MET:N	1.99	0.75
1:B:847:LEU:HD12	1:B:852:SER:CB	2.16	0.75
1:A:874:LYS:N	1:A:982:SER:HB2	2.02	0.75
1:B:506:VAL:HG22	1:B:525:HIS:CD2	2.21	0.75
1:B:785:ASN:HB3	1:B:788:PHE:HD2	1.48	0.75
1:B:873:THR:HB	1:B:917:MET:CE	2.17	0.75
1:A:204:THR:HG21	1:A:209:ALA:HB3	1.66	0.75
1:A:847:LEU:CD1	1:A:850:ALA:HA	2.16	0.75
1:A:278:LYS:HE3	1:A:296:PRO:HG3	1.67	0.75
1:A:473:GLN:CB	1:A:504:VAL:HG22	2.17	0.75
1:B:323:ARG:HG3	1:B:324:THR:N	2.02	0.75
1:B:473:GLN:CB	1:B:504:VAL:HG22	2.17	0.75
1:B:784:TRP:HD1	1:B:790:ILE:HD11	1.51	0.75
1:B:806:MET:H	1:B:806:MET:CE	1.97	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:PHE:HB3	1:B:454:LEU:HD11	1.69	0.75
1:B:448:GLY:HA3	1:B:480:VAL:HG21	1.68	0.75
1:A:188:VAL:HG22	1:A:191:LYS:H	1.52	0.75
1:A:278:LYS:HG2	1:A:296:PRO:HA	1.69	0.75
1:A:64:LEU:HD12	1:A:496:MET:CE	2.16	0.75
1:A:739:ILE:CD1	1:A:748:ARG:HG2	2.17	0.75
1:A:847:LEU:HD12	1:A:852:SER:CB	2.16	0.75
1:B:699:ASP:C	1:B:725:ASN:OD1	2.26	0.75
1:B:700:CYS:CB	1:B:701:PRO:CD	2.50	0.75
1:A:323:ARG:HG3	1:A:324:THR:N	2.02	0.74
1:A:623:ILE:HA	1:A:626:ASN:ND2	2.01	0.74
1:A:683:ASP:O	1:A:686:THR:HG22	1.87	0.74
1:A:873:THR:HB	1:A:917:MET:CE	2.17	0.74
1:B:196:PRO:HB3	1:B:225:MET:HE1	1.68	0.74
1:A:321:LEU:CD1	1:A:462:PRO:HG2	2.17	0.74
1:B:202:LYS:HD3	1:B:214:ALA:HB3	1.69	0.74
1:B:256:LEU:CB	1:B:309:LEU:HD22	2.16	0.74
1:B:42:PHE:HZ	1:B:45:GLU:HB2	1.50	0.74
1:B:321:LEU:CD1	1:B:462:PRO:HG2	2.17	0.74
1:B:869:ARG:O	1:B:920:ALA:HB3	1.86	0.74
1:A:99:ILE:HD11	1:A:152:PHE:HB2	1.69	0.74
1:A:785:ASN:HB3	1:A:788:PHE:HD2	1.48	0.74
1:A:151:PRO:HB2	1:A:157:HIS:ND1	2.02	0.74
1:B:623:ILE:HA	1:B:626:ASN:ND2	2.01	0.74
1:A:868:PRO:HG2	1:A:1022:VAL:CG2	2.17	0.74
1:A:448:GLY:HA3	1:A:480:VAL:HG21	1.68	0.74
1:B:151:PRO:HB2	1:B:157:HIS:ND1	2.03	0.74
1:B:188:VAL:HG22	1:B:191:LYS:H	1.52	0.74
1:A:1010:SER:HB2	1:A:1035:TYR:CZ	2.23	0.74
1:B:814:LEU:HB3	1:B:847:LEU:HB2	1.70	0.74
1:A:567:ILE:HD12	1:A:650:PHE:CZ	2.22	0.74
1:B:185:ALA:HB1	1:B:243:TYR:CZ	2.23	0.74
1:B:548:ARG:CG	1:B:584:PRO:HA	2.16	0.74
1:A:324:THR:HG21	1:A:462:PRO:HA	1.70	0.73
1:B:278:LYS:HG2	1:B:296:PRO:HA	1.68	0.73
1:B:739:ILE:CD1	1:B:748:ARG:HG2	2.17	0.73
1:A:185:ALA:HB1	1:A:243:TYR:CZ	2.23	0.73
1:A:569:VAL:CB	1:A:654:ASN:HB2	2.17	0.73
1:B:548:ARG:HG3	1:B:584:PRO:N	2.03	0.73
1:B:562:VAL:HG22	1:B:578:LEU:CD2	2.18	0.73
1:A:562:VAL:HG22	1:A:578:LEU:CD2	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:HB3	1:A:847:LEU:HB2	1.70	0.73
1:B:324:THR:HG21	1:B:462:PRO:HA	1.70	0.73
1:A:435:ILE:HD13	1:A:436:ALA:N	2.03	0.73
1:A:446:PHE:HB3	1:A:454:LEU:HD11	1.69	0.73
1:A:704:LEU:HD11	1:A:724:LYS:HE3	1.69	0.73
1:B:439:TYR:OH	1:B:538:LYS:CE	2.37	0.73
1:A:154:LYS:H	1:A:157:HIS:HD2	1.36	0.73
1:A:958:LEU:HD22	1:A:960:PRO:O	1.87	0.73
1:B:683:ASP:O	1:B:686:THR:HG22	1.88	0.73
1:A:225:MET:CE	1:A:227:LYS:HG3	2.19	0.73
1:B:468:GLN:CG	1:B:523:ASP:HA	2.08	0.73
1:B:225:MET:CE	1:B:227:LYS:HG3	2.19	0.73
1:A:446:PHE:CD2	1:A:454:LEU:HD21	2.24	0.73
1:B:225:MET:HE1	1:B:227:LYS:HG3	1.70	0.73
1:B:435:ILE:HD13	1:B:436:ALA:N	2.03	0.73
1:B:46:PRO:HG2	1:B:69:ARG:CG	2.17	0.73
1:A:548:ARG:O	1:A:584:PRO:HD3	1.88	0.73
1:B:39:PHE:CD2	1:B:473:GLN:HG3	2.23	0.73
1:B:567:ILE:HD12	1:B:650:PHE:CZ	2.22	0.73
1:B:704:LEU:HD11	1:B:724:LYS:HE3	1.69	0.73
1:A:670:ARG:HA	1:A:670:ARG:HE	1.54	0.72
1:A:46:PRO:HG2	1:A:69:ARG:CG	2.17	0.72
1:B:184:ILE:O	1:B:184:ILE:HD12	1.89	0.72
1:A:1030:ASP:O	1:A:1032:VAL:HG23	1.89	0.72
1:A:181:LYS:HZ3	1:A:216:VAL:HG23	1.54	0.72
1:A:184:ILE:HD12	1:A:184:ILE:O	1.89	0.72
1:A:784:TRP:HD1	1:A:790:ILE:HD11	1.51	0.72
1:A:73:LEU:HD22	1:A:79:VAL:HA	1.72	0.72
1:B:99:ILE:HD11	1:B:152:PHE:HB2	1.69	0.72
1:B:670:ARG:HA	1:B:670:ARG:HE	1.55	0.72
1:A:822:CYS:HA	1:A:833:LEU:HD23	1.70	0.72
1:A:994:LEU:HD11	1:A:1006:ASN:ND2	2.05	0.72
1:B:181:LYS:HD2	1:B:202:LYS:HA	1.71	0.72
1:B:822:CYS:HA	1:B:833:LEU:HD23	1.70	0.72
1:A:558:VAL:HG11	1:A:646:ALA:HB2	1.71	0.72
1:B:261:GLU:HA	1:B:264:SER:O	1.89	0.72
1:A:202:LYS:HD3	1:A:214:ALA:HB3	1.69	0.72
1:B:115:LYS:HB3	1:B:168:VAL:HG11	1.71	0.72
1:A:39:PHE:CD2	1:A:473:GLN:HG3	2.23	0.72
1:A:619:VAL:HB	1:A:620:PRO:HD3	1.72	0.72
1:A:832:THR:CG2	1:A:836:HIS:HB2	2.20	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ARG:HG3	1:B:468:GLN:OE1	1.90	0.72
1:B:704:LEU:HB2	1:B:722:LYS:HG3	1.72	0.72
1:A:261:GLU:HA	1:A:264:SER:O	1.89	0.71
1:A:595:GLU:CB	1:A:597:LEU:HD23	2.14	0.71
1:A:937:ARG:CG	1:A:938:PRO:HD2	2.20	0.71
1:B:93:LYS:HD2	1:B:105:GLU:OE1	1.90	0.71
1:B:446:PHE:HZ	1:B:506:VAL:HG23	1.55	0.71
1:B:595:GLU:HG2	1:B:632:VAL:HG13	1.72	0.71
1:A:519:LEU:HD12	1:A:552:SER:O	1.90	0.71
1:A:806:MET:H	1:A:806:MET:CE	1.97	0.71
1:B:380:LEU:HB2	1:B:386:LYS:CE	2.20	0.71
1:B:471:THR:HG23	1:B:473:GLN:HE22	1.55	0.71
1:A:1017:LYS:H	1:A:1017:LYS:CE	2.01	0.71
1:A:321:LEU:HG	1:A:325:LEU:CD1	2.20	0.71
1:B:832:THR:CG2	1:B:836:HIS:HB2	2.20	0.71
1:A:595:GLU:HG2	1:A:632:VAL:HG13	1.72	0.71
1:A:847:LEU:CD1	1:A:852:SER:HB3	2.20	0.71
1:B:937:ARG:CG	1:B:938:PRO:HD2	2.20	0.71
1:A:989:GLY:HA2	1:A:1017:LYS:CE	2.20	0.71
1:A:370:LEU:HD21	1:A:374:TYR:HE1	1.55	0.71
1:B:563:HIS:HB2	1:B:577:VAL:CG1	2.21	0.71
1:B:619:VAL:HB	1:B:620:PRO:HD3	1.72	0.71
1:B:847:LEU:CD1	1:B:852:SER:HB3	2.20	0.71
1:A:321:LEU:HG	1:A:325:LEU:HD11	1.71	0.71
1:B:188:VAL:HG13	1:B:190:GLY:H	1.56	0.71
1:B:321:LEU:HG	1:B:325:LEU:CD1	2.20	0.71
1:A:1016:MET:O	1:A:1032:VAL:HG13	1.91	0.71
1:A:304:VAL:HG11	1:A:351:GLU:OE2	1.91	0.71
1:A:40:VAL:HG12	1:A:503:ARG:HB3	1.73	0.71
1:B:450:LYS:HA	1:B:479:PRO:HB3	1.73	0.71
1:A:1004:ILE:HD13	1:A:1005:CYS:N	2.06	0.71
1:A:380:LEU:HB2	1:A:386:LYS:CE	2.20	0.71
1:A:474:VAL:HG21	1:A:495:ILE:HD13	1.72	0.71
1:A:515:CYS:O	1:A:519:LEU:HD23	1.91	0.71
1:A:704:LEU:HB2	1:A:722:LYS:HG3	1.71	0.71
1:A:806:MET:HE3	1:A:806:MET:N	1.99	0.71
1:B:474:VAL:HG21	1:B:495:ILE:HD13	1.72	0.71
1:B:575:LEU:HD22	1:B:575:LEU:H	1.56	0.71
1:A:962:ARG:HB3	1:A:1034:GLN:HG3	1.73	0.70
1:B:154:LYS:H	1:B:157:HIS:HD2	1.36	0.70
1:B:72:LYS:HE3	1:B:80:LEU:CD1	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ARG:HG3	1:A:468:GLN:OE1	1.90	0.70
1:B:321:LEU:HG	1:B:325:LEU:HD11	1.71	0.70
1:A:115:LYS:HB3	1:A:168:VAL:HG11	1.71	0.70
1:A:446:PHE:HZ	1:A:506:VAL:HG23	1.55	0.70
1:A:480:VAL:HB	1:A:484:MET:CE	2.21	0.70
1:A:507:GLU:HG3	1:A:537:ARG:HG3	1.74	0.70
1:A:556:GLN:O	1:A:582:ASN:HB3	1.91	0.70
1:B:281:ARG:HB3	1:B:293:VAL:CG1	2.22	0.70
1:B:304:VAL:HG11	1:B:351:GLU:OE2	1.91	0.70
1:A:281:ARG:HB3	1:A:293:VAL:CG1	2.22	0.70
1:A:563:HIS:HB2	1:A:577:VAL:CG1	2.21	0.70
1:B:519:LEU:HD12	1:B:552:SER:O	1.90	0.70
1:A:471:THR:HG23	1:A:473:GLN:HE22	1.55	0.70
1:B:370:LEU:HD21	1:B:374:TYR:HE1	1.55	0.70
1:A:63:TYR:C	1:A:64:LEU:HD22	2.12	0.70
1:A:39:PHE:HE1	1:A:505:PRO:HD2	1.56	0.70
1:A:93:LYS:HD2	1:A:105:GLU:OE1	1.91	0.70
1:A:1016:MET:HE3	1:A:1017:LYS:C	2.12	0.70
1:A:181:LYS:HD2	1:A:202:LYS:HA	1.71	0.70
1:B:847:LEU:HD21	1:B:850:ALA:HA	1.73	0.70
1:A:42:PHE:HE1	1:A:79:VAL:CG2	2.05	0.70
1:B:216:VAL:HG12	1:B:224:SER:OG	1.92	0.70
1:B:480:VAL:HB	1:B:484:MET:CE	2.21	0.70
1:A:873:THR:HG23	1:A:981:GLY:C	2.11	0.70
1:B:551:ALA:HA	1:B:556:GLN:OE1	1.92	0.70
1:A:367:LYS:HE2	1:A:399:ILE:O	1.91	0.69
1:A:474:VAL:CG1	1:A:475:VAL:HG23	2.18	0.69
1:A:450:LYS:HA	1:A:479:PRO:HB3	1.73	0.69
1:A:551:ALA:HA	1:A:556:GLN:OE1	1.92	0.69
1:B:558:VAL:HG11	1:B:646:ALA:HB2	1.71	0.69
1:B:73:LEU:HD22	1:B:79:VAL:HA	1.72	0.69
1:A:72:LYS:HE3	1:A:80:LEU:CD1	2.22	0.69
1:A:739:ILE:HB	1:A:781:THR:CG2	2.22	0.69
1:B:110:THR:HG22	1:B:132:LEU:HD21	1.73	0.69
1:B:63:TYR:C	1:B:64:LEU:HD22	2.12	0.69
1:B:367:LYS:HE2	1:B:399:ILE:O	1.91	0.69
1:B:515:CYS:O	1:B:519:LEU:HD23	1.91	0.69
1:A:847:LEU:HD21	1:A:850:ALA:HA	1.73	0.69
1:B:40:VAL:HG12	1:B:503:ARG:HB3	1.73	0.69
1:A:1016:MET:HG2	1:A:1035:TYR:HE2	1.57	0.69
1:A:216:VAL:HG12	1:A:224:SER:OG	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HB2	1:A:386:LYS:HE3	1.74	0.69
1:A:439:TYR:CZ	1:A:538:LYS:HE3	2.28	0.69
1:A:560:LEU:CD2	1:A:648:THR:HG23	2.19	0.69
1:A:188:VAL:HG13	1:A:190:GLY:H	1.56	0.69
1:A:473:GLN:OE1	1:A:504:VAL:HG13	1.93	0.69
1:A:435:ILE:HD12	1:A:486:PHE:CD1	2.27	0.69
1:A:802:LYS:C	1:A:803:CYS:N	2.46	0.69
1:A:873:THR:HG23	1:A:982:SER:N	2.07	0.69
1:B:473:GLN:OE1	1:B:504:VAL:HG13	1.93	0.69
1:A:595:GLU:CG	1:A:632:VAL:HG13	2.22	0.69
1:A:959:LYS:CB	1:A:972:THR:HB	2.21	0.69
1:A:988:PHE:HB3	1:A:1016:MET:SD	2.33	0.69
1:B:453:LYS:HE3	1:B:472:VAL:HG21	1.73	0.69
1:A:958:LEU:HD23	1:A:959:LYS:N	2.08	0.69
1:B:380:LEU:HB2	1:B:386:LYS:HE3	1.74	0.69
1:A:133:TYR:CD2	1:A:136:ILE:HG12	2.28	0.69
1:A:133:TYR:HB2	1:A:136:ILE:HG12	1.75	0.69
1:B:133:TYR:CD2	1:B:136:ILE:HG12	2.28	0.69
1:A:196:PRO:HB3	1:A:225:MET:HE1	1.73	0.68
1:B:446:PHE:CD2	1:B:454:LEU:HD21	2.24	0.68
1:B:507:GLU:HG3	1:B:537:ARG:HG3	1.74	0.68
1:A:453:LYS:HE3	1:A:472:VAL:HG21	1.73	0.68
1:B:46:PRO:HG3	1:B:69:ARG:HD2	1.75	0.68
1:A:972:THR:HG23	1:A:1002:TYR:CD1	2.28	0.68
1:B:739:ILE:HB	1:B:781:THR:CG2	2.23	0.68
1:B:412:LEU:H	1:B:412:LEU:HD13	1.59	0.68
1:A:773:ILE:HD13	1:A:773:ILE:H	1.59	0.68
1:B:474:VAL:CG1	1:B:475:VAL:HG23	2.18	0.68
1:B:773:ILE:HD13	1:B:773:ILE:H	1.59	0.68
1:A:110:THR:HG22	1:A:132:LEU:HD21	1.74	0.68
1:A:323:ARG:HG3	1:A:324:THR:H	1.58	0.68
1:A:689:PHE:CD1	1:A:691:GLU:HG2	2.28	0.68
1:A:703:LEU:HD13	1:A:723:ALA:HB2	1.76	0.68
1:B:435:ILE:HD12	1:B:486:PHE:CD1	2.27	0.68
1:A:594:PHE:O	1:A:595:GLU:HG2	1.94	0.68
1:A:867:GLY:HA3	1:A:948:TYR:OH	1.94	0.68
1:B:190:GLY:HA2	1:B:233:PHE:CE2	2.29	0.68
1:B:548:ARG:NE	1:B:583:VAL:O	2.26	0.68
1:B:595:GLU:CG	1:B:632:VAL:HG13	2.22	0.68
1:A:53:LEU:HB2	1:A:496:MET:HE1	1.76	0.68
1:B:594:PHE:O	1:B:595:GLU:HG2	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:700:CYS:O	1:B:725:ASN:CB	2.30	0.68
1:A:190:GLY:HA2	1:A:233:PHE:CE2	2.29	0.68
1:A:40:VAL:HG11	1:A:503:ARG:NE	2.09	0.68
1:A:555:LYS:HG3	1:A:556:GLN:N	2.09	0.68
1:A:830:GLN:HG2	1:A:831:CYS:N	2.09	0.68
1:B:98:ARG:HE	1:B:107:LEU:CD1	2.07	0.68
1:B:689:PHE:CD1	1:B:691:GLU:HG2	2.28	0.68
1:B:830:GLN:HG2	1:B:831:CYS:N	2.09	0.68
1:A:575:LEU:HD22	1:A:575:LEU:H	1.56	0.68
1:A:73:LEU:CD2	1:A:79:VAL:HA	2.23	0.68
1:B:323:ARG:HG3	1:B:324:THR:H	1.58	0.68
1:B:62:ILE:HD11	1:B:73:LEU:HD12	1.76	0.68
1:B:62:ILE:O	1:B:62:ILE:HG13	1.94	0.68
1:A:867:GLY:C	1:A:980:ALA:HB1	2.14	0.67
1:A:962:ARG:HB3	1:A:1034:GLN:CG	2.23	0.67
1:B:548:ARG:HG3	1:B:584:PRO:CA	2.25	0.67
1:A:1013:VAL:HG22	1:A:1014:LEU:H	1.60	0.67
1:A:532:HIS:O	1:A:641:THR:HG21	1.94	0.67
1:B:42:PHE:HE1	1:B:79:VAL:CG2	2.05	0.67
1:B:560:LEU:CD2	1:B:648:THR:HG23	2.19	0.67
1:B:863:ILE:HG23	1:B:864:PRO:CD	2.23	0.67
1:A:46:PRO:HG3	1:A:69:ARG:HD2	1.75	0.67
1:B:460:ASP:HB3	1:B:463:LYS:HB3	1.77	0.67
1:B:867:GLY:HA3	1:B:948:TYR:OH	1.94	0.67
1:A:531:LEU:HG	1:A:584:PRO:HG2	1.77	0.67
1:A:951:MET:HG3	1:A:952:THR:N	2.09	0.67
1:A:98:ARG:HE	1:A:107:LEU:HD11	1.60	0.67
1:B:98:ARG:HE	1:B:107:LEU:HD11	1.60	0.67
1:A:137:CYS:HB2	1:A:213:PHE:CZ	2.30	0.67
1:A:321:LEU:O	1:A:325:LEU:HG	1.95	0.67
1:A:460:ASP:HB3	1:A:463:LYS:HB3	1.77	0.67
1:B:555:LYS:HG3	1:B:556:GLN:N	2.09	0.67
1:A:994:LEU:CD1	1:A:1006:ASN:HD22	2.07	0.67
1:A:863:ILE:HG23	1:A:864:PRO:CD	2.23	0.67
1:B:321:LEU:O	1:B:325:LEU:HG	1.95	0.67
1:B:595:GLU:HG2	1:B:632:VAL:CG1	2.25	0.67
1:B:62:ILE:HD12	1:B:64:LEU:HD21	1.75	0.67
1:B:73:LEU:CD2	1:B:79:VAL:HA	2.24	0.67
1:A:62:ILE:HD11	1:A:73:LEU:HD12	1.76	0.67
1:B:53:LEU:HB2	1:B:496:MET:HE1	1.77	0.67
1:A:62:ILE:HD12	1:A:64:LEU:HD21	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:LEU:CD1	1:B:333:LEU:HD11	2.25	0.66
1:A:98:ARG:HE	1:A:107:LEU:CD1	2.07	0.66
1:A:595:GLU:HG2	1:A:632:VAL:CG1	2.25	0.66
1:A:847:LEU:HG	1:A:850:ALA:N	2.10	0.66
1:B:703:LEU:HD13	1:B:723:ALA:HB2	1.76	0.66
1:B:847:LEU:HG	1:B:850:ALA:N	2.10	0.66
1:A:532:HIS:HA	1:A:641:THR:CG2	2.25	0.66
1:A:873:THR:HG1	1:A:981:GLY:HA2	1.61	0.66
1:B:133:TYR:HB2	1:B:136:ILE:HG12	1.75	0.66
1:B:863:ILE:HG13	1:B:864:PRO:CD	2.25	0.66
1:B:40:VAL:HG11	1:B:503:ARG:NE	2.09	0.66
1:B:98:ARG:HH21	1:B:107:LEU:HD12	1.60	0.66
1:A:98:ARG:HH21	1:A:107:LEU:HD12	1.59	0.66
1:A:239:PHE:CD1	1:A:260:PRO:HD2	2.30	0.66
1:A:566:ASN:HA	1:A:651:VAL:CG2	2.25	0.66
1:A:955:LEU:HG	1:A:973:ILE:CG2	2.24	0.66
1:B:133:TYR:HB2	1:B:136:ILE:H	1.61	0.66
1:A:446:PHE:CZ	1:A:486:PHE:HZ	2.13	0.66
1:B:739:ILE:HD12	1:B:748:ARG:HG2	1.76	0.66
1:B:854:CYS:C	1:B:855:THR:N	2.49	0.66
1:B:809:SER:CB	1:B:881:ASN:CG	2.47	0.66
1:A:325:LEU:CD1	1:A:333:LEU:HD11	2.25	0.66
1:A:739:ILE:HD12	1:A:748:ARG:HG2	1.76	0.66
1:A:863:ILE:HG13	1:A:864:PRO:CD	2.25	0.66
1:A:567:ILE:HD13	1:A:651:VAL:O	1.96	0.66
1:B:181:LYS:HD3	1:B:202:LYS:HA	1.78	0.66
1:B:137:CYS:HB2	1:B:213:PHE:CZ	2.30	0.66
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.78	0.66
1:B:548:ARG:HG3	1:B:584:PRO:HA	1.78	0.66
1:A:1016:MET:CE	1:A:1033:PHE:HB3	2.25	0.66
1:A:892:HIS:NE2	1:A:931:ILE:HB	2.11	0.66
1:B:110:THR:HB	1:B:132:LEU:CD2	2.26	0.66
1:B:629:HIS:CE1	1:B:669:TYR:CZ	2.69	0.66
1:A:261:GLU:HG2	1:A:264:SER:C	2.17	0.65
1:A:296:PRO:HD2	1:A:414:VAL:CG2	2.27	0.65
1:B:261:GLU:HG2	1:B:264:SER:C	2.17	0.65
1:A:216:VAL:HG12	1:A:224:SER:CB	2.26	0.65
1:A:412:LEU:HD13	1:A:412:LEU:H	1.59	0.65
1:A:474:VAL:HG12	1:A:475:VAL:CG2	2.21	0.65
1:A:782:VAL:HG23	1:A:790:ILE:HB	1.78	0.65
1:A:797:LYS:HD2	1:A:797:LYS:N	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:GLU:CB	1:A:1024:ARG:HG3	2.17	0.65
1:B:239:PHE:CD1	1:B:260:PRO:HD2	2.30	0.65
1:B:782:VAL:HG23	1:B:790:ILE:HB	1.78	0.65
1:A:133:TYR:HB2	1:A:136:ILE:H	1.61	0.65
1:A:62:ILE:HG13	1:A:62:ILE:O	1.94	0.65
1:A:432:THR:OG1	1:A:480:VAL:HG23	1.96	0.65
1:A:473:GLN:HG2	1:A:504:VAL:HG22	1.79	0.65
1:B:676:TYR:HD1	1:B:730:GLN:CG	2.08	0.65
1:B:847:LEU:CD2	1:B:850:ALA:HA	2.27	0.65
1:A:181:LYS:HD3	1:A:202:LYS:HA	1.78	0.65
1:A:154:LYS:H	1:A:157:HIS:CD2	2.15	0.65
1:B:265:PRO:HD3	1:B:274:VAL:CG2	2.27	0.65
1:B:446:PHE:CZ	1:B:486:PHE:HZ	2.14	0.65
1:B:675:LYS:HE3	1:B:694:VAL:HG22	1.79	0.65
1:A:110:THR:HB	1:A:132:LEU:CD2	2.26	0.65
1:A:453:LYS:HG2	1:A:472:VAL:CG2	2.16	0.65
1:A:706:VAL:HG13	1:A:707:ASP:O	1.96	0.65
1:B:216:VAL:HG12	1:B:224:SER:CB	2.26	0.65
1:A:872:GLY:HA3	1:A:1023:ASP:OD1	1.97	0.65
1:A:807:ARG:HD3	1:A:812:LEU:C	2.18	0.65
1:B:653:TYR:OH	1:B:682:HIS:CE1	2.50	0.65
1:B:807:ARG:HD3	1:B:812:LEU:C	2.17	0.65
1:A:368:ASP:O	1:A:371:GLN:HG2	1.97	0.64
1:A:675:LYS:HE3	1:A:694:VAL:HG22	1.79	0.64
1:B:432:THR:OG1	1:B:480:VAL:HG23	1.96	0.64
1:A:405:GLY:O	1:A:406:LEU:HD22	1.98	0.64
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.78	0.64
1:B:39:PHE:HE1	1:B:505:PRO:HD2	1.57	0.64
1:B:405:GLY:O	1:B:406:LEU:HD22	1.98	0.64
1:A:105:GLU:HB3	1:A:106:PRO:HD2	1.80	0.64
1:A:265:PRO:HD3	1:A:274:VAL:CG2	2.27	0.64
1:A:309:LEU:HD11	1:A:311:ALA:O	1.98	0.64
1:A:926:ALA:HB1	1:A:947:LEU:CD1	2.27	0.64
1:B:186:THR:HG22	1:B:187:ALA:N	2.12	0.64
1:B:320:VAL:O	1:B:323:ARG:HG2	1.98	0.64
1:B:474:VAL:HG12	1:B:475:VAL:CG2	2.21	0.64
1:B:53:LEU:HB2	1:B:496:MET:CE	2.28	0.64
1:B:567:ILE:HD13	1:B:651:VAL:O	1.96	0.64
1:A:186:THR:HG22	1:A:187:ALA:N	2.12	0.64
1:A:53:LEU:HB2	1:A:496:MET:CE	2.28	0.64
1:A:620:PRO:CA	1:A:623:ILE:HG13	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HG	1:A:64:LEU:CD1	2.28	0.64
1:B:797:LYS:N	1:B:797:LYS:HD2	2.11	0.64
1:B:926:ALA:HB1	1:B:947:LEU:CD1	2.27	0.64
1:A:175:TYR:HD2	1:A:179:ASP:HB3	1.63	0.64
1:A:460:ASP:CB	1:A:463:LYS:HB3	2.28	0.64
1:B:473:GLN:HG2	1:B:504:VAL:HG22	1.79	0.64
1:B:469:TYR:HB3	1:B:523:ASP:CG	2.18	0.64
1:B:175:TYR:HD2	1:B:179:ASP:HB3	1.63	0.64
1:B:296:PRO:HD2	1:B:414:VAL:CG2	2.27	0.64
1:B:460:ASP:CB	1:B:463:LYS:HB3	2.28	0.64
1:B:505:PRO:CB	1:B:507:GLU:O	2.46	0.64
1:A:566:ASN:HB3	1:A:651:VAL:HG21	1.80	0.64
1:A:847:LEU:CD2	1:A:850:ALA:HA	2.27	0.64
1:B:56:ASP:OD1	1:B:119:ILE:HD12	1.98	0.64
1:A:741:ASN:O	1:A:778:VAL:HG13	1.98	0.64
1:B:105:GLU:HB3	1:B:106:PRO:HD2	1.80	0.64
1:B:473:GLN:HB2	1:B:504:VAL:HG22	1.80	0.64
1:B:566:ASN:HA	1:B:651:VAL:CG2	2.25	0.64
1:A:56:ASP:OD1	1:A:119:ILE:HD12	1.98	0.64
1:B:118:LEU:HG	1:B:172:ILE:HG13	1.80	0.64
1:B:154:LYS:H	1:B:157:HIS:CD2	2.15	0.64
1:B:309:LEU:HD11	1:B:311:ALA:O	1.98	0.64
1:B:53:LEU:HG	1:B:64:LEU:CD1	2.28	0.64
1:B:706:VAL:HG13	1:B:707:ASP:O	1.96	0.64
1:B:713:VAL:HG12	1:B:714:GLU:HG3	1.79	0.64
1:B:806:MET:HG2	1:B:807:ARG:HG3	1.80	0.64
1:A:405:GLY:C	1:A:406:LEU:HD22	2.19	0.63
1:B:185:ALA:HB1	1:B:243:TYR:CD1	2.33	0.63
1:B:653:TYR:CE2	1:B:682:HIS:ND1	2.60	0.63
1:B:892:HIS:NE2	1:B:931:ILE:HB	2.11	0.63
1:B:368:ASP:O	1:B:371:GLN:HG2	1.97	0.63
1:B:405:GLY:C	1:B:406:LEU:HD22	2.19	0.63
1:B:446:PHE:CE1	1:B:486:PHE:HZ	2.16	0.63
1:B:480:VAL:HG11	1:B:495:ILE:HD11	1.81	0.63
1:B:653:TYR:CE2	1:B:682:HIS:CE1	2.87	0.63
1:B:894:LYS:HD3	1:B:899:GLU:HA	1.81	0.63
1:A:320:VAL:O	1:A:323:ARG:HG2	1.98	0.63
1:B:181:LYS:HE2	1:B:202:LYS:HG2	1.80	0.63
1:A:1002:TYR:CZ	1:A:1004:ILE:HB	2.32	0.63
1:A:118:LEU:HG	1:A:172:ILE:HG13	1.80	0.63
1:A:713:VAL:HG12	1:A:714:GLU:HG3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:LEU:O	1:A:998:ARG:HD2	1.98	0.63
1:B:620:PRO:CA	1:B:623:ILE:HG13	2.23	0.63
1:A:806:MET:HG2	1:A:807:ARG:HG3	1.80	0.63
1:B:386:LYS:HG3	1:B:386:LYS:O	1.99	0.63
1:B:41:THR:HG22	1:B:502:THR:HA	1.81	0.63
1:B:446:PHE:CZ	1:B:506:VAL:HG23	2.33	0.63
1:B:566:ASN:HB3	1:B:651:VAL:HG21	1.79	0.63
1:A:933:VAL:HG23	1:A:934:ALA:N	2.10	0.63
1:A:1014:LEU:HD22	1:A:1014:LEU:N	2.14	0.63
1:A:295:VAL:HA	1:A:414:VAL:HG21	1.81	0.63
1:A:446:PHE:CE1	1:A:486:PHE:HZ	2.16	0.63
1:A:894:LYS:HD3	1:A:899:GLU:HA	1.80	0.63
1:A:40:VAL:HG11	1:A:503:ARG:CZ	2.29	0.63
1:B:448:GLY:CA	1:B:480:VAL:HG21	2.29	0.63
1:B:575:LEU:N	1:B:575:LEU:HD22	2.14	0.63
1:A:1015:ASP:O	1:A:1016:MET:HB3	1.98	0.62
1:A:197:THR:HG21	1:A:228:ILE:HD11	1.81	0.62
1:B:741:ASN:O	1:B:778:VAL:HG13	1.98	0.62
1:B:949:TYR:HE2	1:B:951:MET:CE	2.12	0.62
1:A:180:ASP:O	1:A:181:LYS:HG2	1.99	0.62
1:A:185:ALA:HB1	1:A:243:TYR:CD1	2.33	0.62
1:A:372:SER:O	1:A:375:ARG:HB2	1.99	0.62
1:B:180:ASP:O	1:B:181:LYS:HG2	1.99	0.62
1:B:295:VAL:HA	1:B:414:VAL:HG21	1.81	0.62
1:B:474:VAL:CG2	1:B:495:ILE:HD13	2.29	0.62
1:A:949:TYR:HE2	1:A:951:MET:CE	2.12	0.62
1:B:458:ARG:HG3	1:B:468:GLN:CD	2.20	0.62
1:A:382:LEU:HD23	1:A:385:LEU:HB3	1.81	0.62
1:A:439:TYR:OH	1:A:538:LYS:CE	2.47	0.62
1:A:492:GLN:HG2	1:A:503:ARG:CG	2.29	0.62
1:B:469:TYR:HE2	1:B:471:THR:HB	1.65	0.62
1:B:432:THR:HG1	1:B:480:VAL:HG23	1.65	0.62
1:A:458:ARG:HG3	1:A:468:GLN:CD	2.20	0.62
1:A:448:GLY:CA	1:A:480:VAL:HG21	2.28	0.62
1:A:446:PHE:CZ	1:A:506:VAL:HG23	2.33	0.62
1:B:320:VAL:HG21	1:B:442:HIS:HD2	1.64	0.62
1:A:575:LEU:HD22	1:A:575:LEU:N	2.14	0.62
1:B:933:VAL:HG23	1:B:934:ALA:N	2.10	0.62
1:B:296:PRO:HB2	1:B:417:MET:SD	2.39	0.62
1:B:40:VAL:HG11	1:B:503:ARG:CZ	2.29	0.62
1:A:386:LYS:O	1:A:386:LYS:HG3	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:N	1:B:696:LEU:HD12	2.15	0.62
1:B:806:MET:CG	1:B:807:ARG:HG3	2.30	0.62
1:B:474:VAL:HG22	1:B:495:ILE:CG2	2.29	0.62
1:B:492:GLN:HG2	1:B:503:ARG:CG	2.29	0.62
1:B:855:THR:HG23	1:B:856:ASN:OD1	2.00	0.62
1:A:182:LEU:HG	1:A:184:ILE:HG23	1.82	0.61
1:A:473:GLN:HB2	1:A:504:VAL:HG22	1.80	0.61
1:A:72:LYS:CD	1:A:80:LEU:HD12	2.30	0.61
1:B:382:LEU:HD23	1:B:385:LEU:HB3	1.81	0.61
1:B:715:VAL:CG2	1:B:717:LYS:HD2	2.30	0.61
1:A:855:THR:HG23	1:A:856:ASN:OD1	1.99	0.61
1:B:372:SER:O	1:B:375:ARG:HB2	1.99	0.61
1:A:110:THR:HG22	1:A:111:ASN:N	2.14	0.61
1:B:204:THR:HG22	1:B:212:MET:SD	2.40	0.61
1:A:181:LYS:HE2	1:A:202:LYS:HG2	1.80	0.61
1:A:296:PRO:HB2	1:A:417:MET:SD	2.39	0.61
1:A:1016:MET:HE2	1:A:1033:PHE:HB3	1.82	0.61
1:A:41:THR:HG22	1:A:502:THR:HA	1.81	0.61
1:A:873:THR:HG23	1:A:982:SER:CA	2.30	0.61
1:B:110:THR:HG22	1:B:111:ASN:N	2.14	0.61
1:B:706:VAL:HG22	1:B:707:ASP:N	2.12	0.61
1:A:175:TYR:CD2	1:A:179:ASP:HB3	2.36	0.61
1:A:204:THR:HG22	1:A:212:MET:SD	2.40	0.61
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.30	0.61
1:A:474:VAL:CG2	1:A:495:ILE:HD13	2.29	0.61
1:A:488:LYS:HG3	1:A:489:ASP:N	2.14	0.61
1:A:480:VAL:HG11	1:A:495:ILE:HD11	1.81	0.61
1:A:712:PRO:HG3	1:A:801:TYR:OH	2.01	0.61
1:A:806:MET:CG	1:A:807:ARG:HG3	2.30	0.61
1:B:833:LEU:HB2	1:B:836:HIS:CD2	2.29	0.61
1:A:119:ILE:HD13	1:A:121:TYR:CZ	2.36	0.61
1:A:532:HIS:HA	1:A:641:THR:HG21	1.82	0.61
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.30	0.61
1:B:41:THR:HG22	1:B:502:THR:HG23	1.83	0.61
1:A:257:THR:C	1:A:258:LEU:HD12	2.21	0.61
1:A:696:LEU:N	1:A:696:LEU:HD12	2.15	0.61
1:B:175:TYR:CD2	1:B:179:ASP:HB3	2.36	0.61
1:B:181:LYS:HZ3	1:B:216:VAL:HG23	1.66	0.61
1:B:333:LEU:CD2	1:B:358:ILE:HG13	2.31	0.61
1:B:46:PRO:HD2	1:B:71:TYR:CE1	2.35	0.61
1:B:847:LEU:HD11	1:B:850:ALA:CA	2.29	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:VAL:HG22	1:A:495:ILE:CG2	2.29	0.60
1:A:569:VAL:HB	1:A:654:ASN:HB2	1.83	0.60
1:A:665:VAL:HG12	1:A:697:PRO:HG3	1.83	0.60
1:A:706:VAL:HG22	1:A:707:ASP:N	2.12	0.60
1:B:488:LYS:HG3	1:B:489:ASP:N	2.14	0.60
1:A:313:TYR:CE1	1:A:435:ILE:HG12	2.37	0.60
1:A:469:TYR:HE2	1:A:471:THR:HB	1.65	0.60
1:A:870:GLU:CG	1:A:1025:ALA:N	2.64	0.60
1:B:444:LEU:CD2	1:B:524:PRO:HG3	2.23	0.60
1:B:548:ARG:HG2	1:B:584:PRO:HA	1.83	0.60
1:B:95:TYR:CG	1:B:96:PRO:HD3	2.36	0.60
1:A:715:VAL:CG2	1:A:717:LYS:HD2	2.30	0.60
1:B:99:ILE:HG13	1:B:100:VAL:N	2.16	0.60
1:B:257:THR:C	1:B:258:LEU:HD12	2.21	0.60
1:A:314:LEU:HD12	1:A:333:LEU:O	2.01	0.60
1:B:773:ILE:HD13	1:B:773:ILE:N	2.17	0.60
1:A:963:GLY:O	1:A:1036:VAL:HG22	2.01	0.60
1:A:919:GLU:HB3	1:A:1024:ARG:NH1	2.16	0.60
1:B:314:LEU:HD12	1:B:333:LEU:O	2.01	0.60
1:B:313:TYR:CE1	1:B:435:ILE:HG12	2.37	0.60
1:B:712:PRO:HG3	1:B:801:TYR:OH	2.01	0.60
1:A:333:LEU:CD2	1:A:358:ILE:HG13	2.31	0.60
1:A:46:PRO:HD2	1:A:71:TYR:CE1	2.35	0.60
1:A:773:ILE:HD13	1:A:773:ILE:N	2.17	0.60
1:B:46:PRO:HD2	1:B:71:TYR:CZ	2.36	0.60
1:A:403:PHE:CZ	1:A:406:LEU:HD23	2.37	0.60
1:A:320:VAL:HG21	1:A:442:HIS:HD2	1.64	0.60
1:A:62:ILE:HD13	1:A:77:LEU:CD2	2.32	0.60
1:A:630:HIS:HD2	1:A:632:VAL:CG2	2.15	0.60
1:B:181:LYS:HZ2	1:B:216:VAL:HG23	1.64	0.60
1:B:495:ILE:CG2	1:B:502:THR:HB	2.32	0.60
1:B:182:LEU:HG	1:B:184:ILE:HG23	1.82	0.60
1:B:323:ARG:HH21	1:B:463:LYS:HD2	1.67	0.60
1:B:119:ILE:HD13	1:B:121:TYR:CZ	2.36	0.60
1:B:171:VAL:O	1:B:182:LEU:HD12	2.02	0.60
1:B:403:PHE:CZ	1:B:406:LEU:HD23	2.37	0.60
1:B:469:TYR:CE2	1:B:471:THR:HB	2.36	0.60
1:B:665:VAL:HG12	1:B:697:PRO:HG3	1.83	0.60
1:B:662:LEU:HD11	1:B:702:GLN:HE22	1.65	0.60
1:B:72:LYS:CD	1:B:80:LEU:HD12	2.30	0.60
1:A:1029:GLN:HG2	1:A:1030:ASP:H	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HG13	1:B:388:LYS:HG3	1.83	0.60
1:A:1002:TYR:CE2	1:A:1004:ILE:HB	2.37	0.59
1:A:991:GLN:HG3	1:A:1008:THR:HG21	1.84	0.59
1:B:154:LYS:N	1:B:157:HIS:HD2	2.00	0.59
1:A:387:VAL:HG13	1:A:388:LYS:HG3	1.83	0.59
1:A:469:TYR:CE2	1:A:471:THR:HB	2.36	0.59
1:A:566:ASN:CA	1:A:651:VAL:HG23	2.28	0.59
1:A:95:TYR:CG	1:A:96:PRO:HD3	2.36	0.59
1:A:99:ILE:HG13	1:A:100:VAL:N	2.16	0.59
1:B:243:TYR:CD2	1:B:257:THR:HG22	2.37	0.59
1:B:873:THR:HB	1:B:917:MET:HE2	1.84	0.59
1:A:271:LYS:HG3	1:A:272:GLU:N	2.13	0.59
1:A:432:THR:HG1	1:A:480:VAL:HG23	1.65	0.59
1:A:457:ILE:HG12	1:A:467:LEU:HD13	1.84	0.59
1:A:560:LEU:HD23	1:A:648:THR:CG2	2.25	0.59
1:A:847:LEU:HD11	1:A:850:ALA:CA	2.29	0.59
1:B:197:THR:HG21	1:B:228:ILE:HD11	1.82	0.59
1:B:239:PHE:CA	1:B:260:PRO:HG2	2.30	0.59
1:B:387:VAL:HG13	1:B:388:LYS:N	2.18	0.59
1:B:665:VAL:HG11	1:B:697:PRO:HD3	1.84	0.59
1:A:243:TYR:CD2	1:A:257:THR:HG22	2.37	0.59
1:A:46:PRO:HD2	1:A:71:TYR:CZ	2.37	0.59
1:A:904:VAL:HG13	1:A:905:ASP:N	2.18	0.59
1:A:931:ILE:O	1:A:931:ILE:HG13	2.02	0.59
1:A:40:VAL:HG13	1:A:503:ARG:HB3	1.85	0.59
1:A:41:THR:HG22	1:A:502:THR:HG23	1.82	0.59
1:A:62:ILE:HD12	1:A:501:LEU:CD1	2.33	0.59
1:A:833:LEU:HB2	1:A:836:HIS:CD2	2.28	0.59
1:A:987:MET:HB2	1:A:1019:THR:HG23	1.83	0.59
1:A:994:LEU:CG	1:A:1006:ASN:HB2	2.31	0.59
1:B:453:LYS:HG2	1:B:472:VAL:CG2	2.16	0.59
1:B:548:ARG:CG	1:B:583:VAL:O	2.50	0.59
1:B:904:VAL:HG13	1:B:905:ASP:N	2.18	0.59
1:A:196:PRO:HB3	1:A:225:MET:CE	2.33	0.59
1:A:889:ILE:HD12	1:A:907:TYR:CZ	2.38	0.59
1:B:473:GLN:H	1:B:473:GLN:NE2	2.01	0.59
1:B:630:HIS:HD2	1:B:632:VAL:CG2	2.15	0.59
1:B:931:ILE:HG13	1:B:931:ILE:O	2.02	0.59
1:A:972:THR:HA	1:A:1002:TYR:CE1	2.32	0.59
1:B:62:ILE:HD13	1:B:77:LEU:CD2	2.32	0.59
1:A:439:TYR:CZ	1:A:538:LYS:NZ	2.70	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ARG:HH21	1:A:463:LYS:HD2	1.67	0.59
1:A:563:HIS:HB3	1:A:564:PRO:CD	2.28	0.59
1:B:349:LEU:HD22	1:B:349:LEU:N	2.18	0.59
1:B:578:LEU:HD13	1:B:636:LEU:HD21	1.85	0.59
1:A:814:LEU:HD22	1:A:847:LEU:N	2.18	0.59
1:A:959:LYS:CG	1:A:972:THR:HB	2.33	0.59
1:B:40:VAL:HG13	1:B:503:ARG:HB3	1.85	0.59
1:B:937:ARG:HG2	1:B:938:PRO:HD2	1.85	0.59
1:A:171:VAL:O	1:A:182:LEU:HD12	2.02	0.58
1:A:495:ILE:CG2	1:A:502:THR:HB	2.32	0.58
1:A:530:VAL:HG11	1:A:584:PRO:HD2	1.84	0.58
1:A:759:VAL:HG12	1:A:760:GLN:N	2.18	0.58
1:A:955:LEU:CD1	1:A:973:ILE:HG23	2.33	0.58
1:B:457:ILE:HG12	1:B:467:LEU:HD13	1.84	0.58
1:B:814:LEU:HD22	1:B:847:LEU:N	2.18	0.58
1:A:387:VAL:HG13	1:A:388:LYS:N	2.18	0.58
1:A:62:ILE:HG12	1:A:73:LEU:HB2	1.84	0.58
1:A:870:GLU:CG	1:A:1024:ARG:CG	2.69	0.58
1:B:271:LYS:HG3	1:B:272:GLU:N	2.13	0.58
1:A:349:LEU:N	1:A:349:LEU:HD22	2.18	0.58
1:A:665:VAL:HG11	1:A:697:PRO:HD3	1.84	0.58
1:B:560:LEU:HD23	1:B:648:THR:CG2	2.25	0.58
1:A:110:THR:HB	1:A:132:LEU:HD23	1.85	0.58
1:A:506:VAL:HG22	1:A:525:HIS:NE2	2.18	0.58
1:B:263:VAL:O	1:B:263:VAL:HG12	2.04	0.58
1:B:426:GLU:HA	1:B:426:GLU:OE1	2.04	0.58
1:B:198:ILE:HB	1:B:226:ILE:CG2	2.34	0.58
1:A:350:ASP:HA	1:A:430:ARG:HB2	1.86	0.58
1:A:473:GLN:H	1:A:473:GLN:NE2	2.01	0.58
1:A:949:TYR:CE2	1:A:951:MET:HE1	2.38	0.58
1:B:188:VAL:HG22	1:B:191:LYS:N	2.18	0.58
1:B:653:TYR:HE2	1:B:682:HIS:CE1	2.21	0.58
1:B:832:THR:HG23	1:B:836:HIS:HB2	1.85	0.58
1:B:889:ILE:HD12	1:B:907:TYR:CZ	2.38	0.58
1:A:426:GLU:OE1	1:A:426:GLU:HA	2.04	0.58
1:A:430:ARG:HH21	1:A:432:THR:HG22	1.68	0.58
1:A:578:LEU:HD13	1:A:636:LEU:HD21	1.85	0.58
1:A:814:LEU:HD22	1:A:847:LEU:H	1.68	0.58
1:A:873:THR:HA	1:A:982:SER:N	2.17	0.58
1:B:110:THR:HB	1:B:132:LEU:HD23	1.85	0.58
1:B:196:PRO:HB3	1:B:225:MET:CE	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASN:HD21	1:B:67:VAL:CG2	2.15	0.58
1:B:759:VAL:HG12	1:B:760:GLN:N	2.18	0.58
1:A:1021:GLN:CG	1:A:1026:ARG:HG3	2.34	0.58
1:A:456:LYS:O	1:A:468:GLN:HG2	2.04	0.58
1:A:585:GLU:OE1	1:A:585:GLU:HA	2.04	0.58
1:A:873:THR:HG23	1:A:982:SER:HA	1.86	0.58
1:B:254:TYR:CZ	1:B:281:ARG:HD2	2.39	0.58
1:B:430:ARG:HH21	1:B:432:THR:HG22	1.68	0.58
1:B:62:ILE:HD12	1:B:501:LEU:CD1	2.33	0.58
1:A:972:THR:CA	1:A:1002:TYR:HE1	2.15	0.58
1:B:456:LYS:O	1:B:468:GLN:HG2	2.04	0.58
1:B:566:ASN:CA	1:B:651:VAL:HG23	2.28	0.58
1:A:254:TYR:CZ	1:A:281:ARG:HD2	2.39	0.57
1:A:703:LEU:HD21	1:A:782:VAL:HG21	1.86	0.57
1:B:505:PRO:HB2	1:B:507:GLU:O	2.03	0.57
1:A:937:ARG:HG2	1:A:938:PRO:HD2	1.85	0.57
1:A:458:ARG:HD2	1:A:524:PRO:HG3	1.86	0.57
1:A:994:LEU:HG	1:A:1006:ASN:HB2	1.87	0.57
1:A:1018:VAL:HG13	1:A:1018:VAL:O	2.04	0.57
1:A:892:HIS:CE1	1:A:931:ILE:HB	2.40	0.57
1:A:874:LYS:N	1:A:982:SER:CB	2.66	0.57
1:B:350:ASP:HA	1:B:430:ARG:HB2	1.86	0.57
1:A:154:LYS:N	1:A:157:HIS:HD2	2.00	0.57
1:A:265:PRO:HD3	1:A:274:VAL:HG21	1.87	0.57
1:B:370:LEU:HD21	1:B:374:TYR:CE1	2.39	0.57
1:A:198:ILE:HB	1:A:226:ILE:CG2	2.34	0.57
1:A:262:MET:HG3	1:A:262:MET:O	2.05	0.57
1:A:532:HIS:HA	1:A:641:THR:CB	2.35	0.57
1:A:188:VAL:HG22	1:A:191:LYS:N	2.18	0.57
1:A:263:VAL:O	1:A:263:VAL:HG12	2.04	0.57
1:A:370:LEU:HD21	1:A:374:TYR:CE1	2.39	0.57
1:A:324:THR:CG2	1:A:462:PRO:HA	2.34	0.57
1:A:458:ARG:CG	1:A:524:PRO:HG3	2.34	0.57
1:A:51:ASN:HD21	1:A:67:VAL:CG2	2.15	0.57
1:A:832:THR:HG23	1:A:836:HIS:HB2	1.85	0.57
1:B:265:PRO:HD3	1:B:274:VAL:HG21	1.87	0.57
1:B:433:SER:HB3	1:B:484:MET:SD	2.45	0.57
1:B:42:PHE:CE2	1:B:50:PHE:HZ	2.23	0.57
1:A:239:PHE:CA	1:A:260:PRO:HG2	2.30	0.57
1:A:459:VAL:O	1:A:459:VAL:HG23	2.05	0.57
1:A:45:GLU:HB3	1:A:46:PRO:CD	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:VAL:HG22	1:B:435:ILE:N	2.20	0.57
1:B:459:VAL:HG23	1:B:459:VAL:O	2.05	0.57
1:A:446:PHE:CE1	1:A:486:PHE:CZ	2.93	0.57
1:B:262:MET:O	1:B:262:MET:HG3	2.05	0.57
1:A:1013:VAL:HG22	1:A:1014:LEU:N	2.19	0.56
1:A:926:ALA:CB	1:A:947:LEU:HD12	2.35	0.56
1:B:665:VAL:CG1	1:B:697:PRO:HD3	2.35	0.56
1:A:435:ILE:CG2	1:A:486:PHE:HE1	2.19	0.56
1:A:501:LEU:HD23	1:A:502:THR:H	1.70	0.56
1:A:820:PHE:O	1:A:821:GLU:HB3	2.05	0.56
1:B:444:LEU:HD23	1:B:524:PRO:CD	2.35	0.56
1:A:305:GLU:O	1:A:340:LYS:HG3	2.06	0.56
1:A:434:VAL:HG22	1:A:435:ILE:N	2.20	0.56
1:B:53:LEU:HG	1:B:64:LEU:HD13	1.87	0.56
1:B:882:LEU:N	1:B:882:LEU:HD12	2.21	0.56
1:A:882:LEU:HD12	1:A:882:LEU:N	2.21	0.56
1:B:116:MET:HG3	1:B:117:LEU:N	2.20	0.56
1:B:41:THR:CG2	1:B:502:THR:HG23	2.36	0.56
1:A:42:PHE:CE2	1:A:50:PHE:HZ	2.23	0.56
1:A:955:LEU:HG	1:A:973:ILE:HG23	1.86	0.56
1:B:305:GLU:O	1:B:340:LYS:HG3	2.06	0.56
1:B:45:GLU:HB3	1:B:46:PRO:CD	2.35	0.56
1:B:785:ASN:HD22	1:B:788:PHE:HE2	1.54	0.56
1:B:885:GLU:HG3	1:B:887:ARG:H	1.70	0.56
1:A:665:VAL:CG1	1:A:697:PRO:HD3	2.35	0.56
1:B:585:GLU:OE1	1:B:585:GLU:HA	2.04	0.56
1:B:700:CYS:HB3	1:B:701:PRO:HD2	1.81	0.56
1:B:710:LEU:HB2	1:B:801:TYR:HE1	1.70	0.56
1:B:814:LEU:HD22	1:B:847:LEU:H	1.69	0.56
1:A:865:VAL:HG13	1:A:866:THR:N	2.21	0.56
1:B:892:HIS:CE1	1:B:931:ILE:HB	2.40	0.56
1:A:474:VAL:CG2	1:A:495:ILE:HG21	2.35	0.56
1:A:785:ASN:ND2	1:A:788:PHE:HE2	2.03	0.56
1:B:446:PHE:CE1	1:B:486:PHE:CZ	2.93	0.56
1:B:324:THR:CG2	1:B:462:PRO:HA	2.34	0.56
1:B:526:CYS:HB3	1:B:535:CYS:SG	2.46	0.56
1:B:804:GLY:HA2	1:B:806:MET:CE	2.36	0.56
1:A:226:ILE:O	1:A:226:ILE:HG23	2.06	0.56
1:A:321:LEU:HD12	1:A:462:PRO:CG	2.34	0.56
1:A:41:THR:CG2	1:A:502:THR:HG23	2.35	0.56
1:A:549:ARG:HA	1:A:584:PRO:HB3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:VAL:HB	1:A:654:ASN:CB	2.36	0.56
1:A:885:GLU:HG3	1:A:887:ARG:H	1.70	0.56
1:B:118:LEU:HB3	1:B:127:ILE:CG2	2.36	0.56
1:B:435:ILE:CG2	1:B:486:PHE:HE1	2.19	0.56
1:B:567:ILE:N	1:B:567:ILE:HD13	2.20	0.56
1:B:569:VAL:HG21	1:B:654:ASN:HB2	1.87	0.56
1:A:118:LEU:HB3	1:A:127:ILE:CG2	2.36	0.56
1:A:42:PHE:HE2	1:A:50:PHE:HZ	1.54	0.56
1:A:526:CYS:HB3	1:A:535:CYS:SG	2.46	0.56
1:A:567:ILE:HD13	1:A:567:ILE:N	2.20	0.56
1:A:983:ASN:O	1:A:1022:VAL:HG23	2.06	0.56
1:A:447:VAL:HG23	1:A:447:VAL:O	2.06	0.56
1:A:53:LEU:HG	1:A:64:LEU:HD13	1.87	0.56
1:A:46:PRO:CG	1:A:69:ARG:HD2	2.36	0.56
1:B:505:PRO:HB3	1:B:507:GLU:O	2.04	0.56
1:B:785:ASN:ND2	1:B:788:PHE:HE2	2.03	0.56
1:B:865:VAL:HG13	1:B:866:THR:N	2.21	0.56
1:A:1022:VAL:HG13	1:A:1022:VAL:O	2.06	0.55
1:A:433:SER:HB3	1:A:484:MET:SD	2.45	0.55
1:A:710:LEU:HB2	1:A:801:TYR:HE1	1.70	0.55
1:A:704:LEU:HD11	1:A:724:LYS:CE	2.35	0.55
1:A:460:ASP:OD2	1:A:463:LYS:HB3	2.06	0.55
1:A:873:THR:HB	1:A:917:MET:HE2	1.86	0.55
1:A:949:TYR:HE2	1:A:951:MET:HE1	1.71	0.55
1:B:46:PRO:CG	1:B:69:ARG:HD2	2.36	0.55
1:A:474:VAL:HG12	1:A:475:VAL:N	2.21	0.55
1:A:435:ILE:HD12	1:A:486:PHE:HD1	1.70	0.55
1:A:548:ARG:HG3	1:A:583:VAL:C	2.26	0.55
1:A:619:VAL:CB	1:A:620:PRO:HD3	2.36	0.55
1:A:845:LEU:HD13	1:A:845:LEU:C	2.26	0.55
1:B:412:LEU:N	1:B:412:LEU:HD13	2.21	0.55
1:B:501:LEU:HD23	1:B:502:THR:H	1.70	0.55
1:B:62:ILE:HG12	1:B:73:LEU:HB2	1.84	0.55
1:B:807:ARG:HD3	1:B:812:LEU:O	2.07	0.55
1:A:382:LEU:HD23	1:A:385:LEU:CB	2.36	0.55
1:B:110:THR:HG22	1:B:111:ASN:H	1.72	0.55
1:B:190:GLY:O	1:B:192:PRO:HD3	2.07	0.55
1:B:359:LEU:HA	1:B:362:ILE:HG12	1.89	0.55
1:B:447:VAL:O	1:B:447:VAL:HG23	2.06	0.55
1:B:474:VAL:CG2	1:B:495:ILE:HG21	2.34	0.55
1:B:713:VAL:HG13	1:B:766:TYR:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LEU:HD21	1:B:782:VAL:HG21	1.86	0.55
1:A:448:GLY:HA3	1:A:480:VAL:CG2	2.37	0.55
1:B:51:ASN:ND2	1:B:67:VAL:HG23	2.20	0.55
1:B:710:LEU:HB2	1:B:801:TYR:CE1	2.42	0.55
1:B:820:PHE:O	1:B:821:GLU:HB3	2.06	0.55
1:B:845:LEU:C	1:B:845:LEU:HD13	2.26	0.55
1:B:91:ASN:CG	1:B:92:PRO:HD2	2.27	0.55
1:B:949:TYR:HE2	1:B:951:MET:HE2	1.71	0.55
1:A:1014:LEU:H	1:A:1014:LEU:CD2	2.17	0.55
1:A:713:VAL:HG13	1:A:766:TYR:O	2.06	0.55
1:A:825:CYS:HB3	1:A:828:PRO:HG2	1.89	0.55
1:A:861:GLU:HG3	1:A:862:ILE:N	2.21	0.55
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.27	0.55
1:B:280:VAL:HG12	1:B:281:ARG:N	2.22	0.55
1:B:72:LYS:HD2	1:B:80:LEU:HB2	1.87	0.55
1:A:168:VAL:HG22	1:A:169:PHE:N	2.22	0.55
1:A:190:GLY:O	1:A:192:PRO:HD3	2.07	0.55
1:A:280:VAL:HG12	1:A:281:ARG:N	2.22	0.55
1:A:509:CYS:HB3	1:A:535:CYS:SG	2.47	0.55
1:B:226:ILE:O	1:B:226:ILE:HG23	2.06	0.55
1:B:380:LEU:HB2	1:B:386:LYS:HE2	1.87	0.55
1:B:42:PHE:HE2	1:B:50:PHE:HZ	1.54	0.55
1:A:116:MET:HG3	1:A:117:LEU:N	2.21	0.55
1:B:242:TYR:CD1	1:B:345:LYS:HE2	2.41	0.55
1:B:619:VAL:CB	1:B:620:PRO:HD3	2.36	0.55
1:B:937:ARG:HG3	1:B:938:PRO:HD2	1.89	0.55
1:A:988:PHE:HD2	1:A:1016:MET:SD	2.30	0.55
1:A:242:TYR:CD1	1:A:345:LYS:HE2	2.41	0.55
1:A:380:LEU:HB2	1:A:386:LYS:HE2	1.87	0.55
1:B:380:LEU:CD1	1:B:386:LYS:HE3	2.37	0.55
1:B:501:LEU:HD23	1:B:502:THR:N	2.22	0.55
1:A:239:PHE:HA	1:A:260:PRO:CG	2.32	0.55
1:A:370:LEU:HD13	1:A:370:LEU:O	2.07	0.55
1:A:501:LEU:HD23	1:A:502:THR:N	2.22	0.55
1:A:72:LYS:HD2	1:A:80:LEU:HB2	1.87	0.55
1:A:804:GLY:HA2	1:A:806:MET:CE	2.36	0.55
1:A:1016:MET:HE3	1:A:1017:LYS:CA	2.38	0.54
1:A:597:LEU:HD22	1:A:597:LEU:N	2.21	0.54
1:B:168:VAL:HG22	1:B:169:PHE:N	2.22	0.54
1:B:370:LEU:HD13	1:B:370:LEU:O	2.07	0.54
1:B:597:LEU:N	1:B:597:LEU:HD22	2.21	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:HD11	1:B:724:LYS:CE	2.35	0.54
1:A:785:ASN:HD22	1:A:788:PHE:HE2	1.54	0.54
1:A:797:LYS:HD2	1:A:797:LYS:H	1.72	0.54
1:B:382:LEU:HD23	1:B:385:LEU:CB	2.37	0.54
1:B:435:ILE:HD12	1:B:486:PHE:HD1	1.71	0.54
1:B:930:GLU:OE2	1:B:941:MET:HG3	2.07	0.54
1:A:471:THR:CG2	1:A:473:GLN:HE22	2.20	0.54
1:A:46:PRO:CG	1:A:69:ARG:HG3	2.27	0.54
1:A:709:ILE:O	1:A:799:TYR:HD1	1.91	0.54
1:A:72:LYS:HD2	1:A:80:LEU:HD12	1.90	0.54
1:A:710:LEU:HB2	1:A:801:TYR:CE1	2.41	0.54
1:A:874:LYS:H	1:A:982:SER:CB	2.20	0.54
1:B:236:ILE:O	1:B:236:ILE:HG23	2.07	0.54
1:B:370:LEU:C	1:B:370:LEU:HD13	2.27	0.54
1:B:440:LYS:HB2	1:B:538:LYS:NZ	2.22	0.54
1:B:72:LYS:HD2	1:B:80:LEU:HD12	1.90	0.54
1:A:301:ARG:CD	1:A:425:THR:HG21	2.26	0.54
1:A:556:GLN:O	1:A:582:ASN:CB	2.56	0.54
1:A:947:LEU:CD2	1:A:947:LEU:H	2.21	0.54
1:B:460:ASP:OD2	1:B:463:LYS:HB3	2.06	0.54
1:A:151:PRO:O	1:A:157:HIS:HB3	2.07	0.54
1:A:359:LEU:HA	1:A:362:ILE:HG12	1.89	0.54
1:A:63:TYR:CE2	1:A:72:LYS:HG2	2.43	0.54
1:B:474:VAL:HG12	1:B:475:VAL:N	2.21	0.54
1:B:509:CYS:HB3	1:B:535:CYS:SG	2.47	0.54
1:A:412:LEU:C	1:A:412:LEU:HD22	2.28	0.54
1:A:994:LEU:HD11	1:A:1006:ASN:CB	2.37	0.54
1:B:412:LEU:HD22	1:B:412:LEU:C	2.28	0.54
1:B:426:GLU:HG2	1:B:429:ASP:O	2.08	0.54
1:A:495:ILE:O	1:A:495:ILE:HG23	2.08	0.54
1:A:699:ASP:HA	1:A:725:ASN:OD1	2.07	0.54
1:A:739:ILE:HB	1:A:781:THR:HG22	1.90	0.54
1:B:154:LYS:HB2	1:B:157:HIS:HD2	1.70	0.54
1:B:151:PRO:O	1:B:157:HIS:HB3	2.08	0.54
1:B:471:THR:CG2	1:B:473:GLN:HE22	2.20	0.54
1:A:236:ILE:O	1:A:236:ILE:HG23	2.07	0.54
1:A:370:LEU:HD13	1:A:370:LEU:C	2.27	0.54
1:A:429:ASP:OD1	1:A:450:LYS:HB3	2.08	0.54
1:A:930:GLU:OE2	1:A:941:MET:HG3	2.07	0.54
1:B:370:LEU:HD11	1:B:399:ILE:HD12	1.88	0.54
1:B:797:LYS:HD2	1:B:797:LYS:H	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:GLY:O	1:A:159:LEU:HD13	2.08	0.54
1:A:175:TYR:HB3	1:A:179:ASP:HB3	1.89	0.54
1:A:412:LEU:HD13	1:A:412:LEU:N	2.21	0.54
1:A:531:LEU:O	1:A:641:THR:OG1	2.25	0.54
1:A:662:LEU:HD23	1:A:791:ASP:OD2	2.08	0.54
1:A:780:LEU:HD12	1:A:780:LEU:C	2.27	0.54
1:B:861:GLU:HG3	1:B:862:ILE:N	2.21	0.54
1:A:370:LEU:HD11	1:A:399:ILE:HD12	1.88	0.54
1:A:51:ASN:ND2	1:A:67:VAL:HG23	2.20	0.54
1:B:175:TYR:HB3	1:B:179:ASP:HB3	1.89	0.54
1:B:716:ILE:HG12	1:B:763:ASN:HB3	1.90	0.54
1:B:780:LEU:C	1:B:780:LEU:HD12	2.27	0.54
1:B:825:CYS:HB3	1:B:828:PRO:HG2	1.89	0.54
1:B:301:ARG:CD	1:B:425:THR:HG21	2.26	0.53
1:B:921:LYS:N	1:B:922:PRO:HD2	2.23	0.53
1:B:947:LEU:CD2	1:B:947:LEU:H	2.21	0.53
1:A:110:THR:HG22	1:A:111:ASN:H	1.72	0.53
1:A:225:MET:HE1	1:A:227:LYS:CG	2.37	0.53
1:A:957:ASP:O	1:A:974:THR:HG22	2.08	0.53
1:A:955:LEU:CG	1:A:973:ILE:HG23	2.38	0.53
1:B:63:TYR:CE2	1:B:72:LYS:HG2	2.43	0.53
1:B:926:ALA:CB	1:B:947:LEU:HD12	2.35	0.53
1:B:925:HIS:O	1:B:950:PHE:HD2	1.91	0.53
1:A:739:ILE:HB	1:A:781:THR:HG23	1.90	0.53
1:A:921:LYS:N	1:A:922:PRO:HD2	2.23	0.53
1:A:924:GLN:O	1:A:925:HIS:HB2	2.09	0.53
1:A:426:GLU:HG2	1:A:429:ASP:O	2.08	0.53
1:A:589:GLY:HA3	1:A:639:LYS:HG3	1.90	0.53
1:A:807:ARG:HD3	1:A:812:LEU:O	2.07	0.53
1:A:867:GLY:CA	1:A:981:GLY:N	2.49	0.53
1:B:429:ASP:OD1	1:B:450:LYS:HB3	2.08	0.53
1:B:623:ILE:C	1:B:623:ILE:HD12	2.28	0.53
1:B:924:GLN:O	1:B:925:HIS:HB2	2.09	0.53
1:A:321:LEU:CD2	1:A:325:LEU:HD11	2.39	0.53
1:A:533:ASN:HD22	1:A:643:MET:HB3	1.73	0.53
1:A:827:SER:HB2	1:A:828:PRO:HD3	1.91	0.53
1:B:181:LYS:CE	1:B:202:LYS:HG2	2.39	0.53
1:B:371:GLN:O	1:B:375:ARG:HG3	2.09	0.53
1:B:385:LEU:HD13	1:B:385:LEU:C	2.29	0.53
1:B:578:LEU:HB2	1:B:609:ILE:HB	1.91	0.53
1:B:709:ILE:O	1:B:799:TYR:HD1	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB3	1:A:243:TYR:CG	2.44	0.53
1:A:509:CYS:HB2	1:A:536:THR:HA	1.91	0.53
1:A:623:ILE:HD12	1:A:623:ILE:C	2.29	0.53
1:A:679:VAL:HG12	1:A:680:CYS:N	2.23	0.53
1:A:716:ILE:HG12	1:A:763:ASN:HB3	1.90	0.53
1:B:278:LYS:HG2	1:B:296:PRO:CA	2.38	0.53
1:B:321:LEU:CD2	1:B:325:LEU:HD11	2.39	0.53
1:B:563:HIS:HB3	1:B:564:PRO:CD	2.28	0.53
1:A:190:GLY:HA2	1:A:233:PHE:HE2	1.73	0.53
1:A:549:ARG:CD	1:A:584:PRO:HB2	2.33	0.53
1:A:805:ALA:H	1:A:806:MET:CE	2.22	0.53
1:B:356:ILE:HG22	1:B:421:ILE:O	2.09	0.53
1:B:448:GLY:HA3	1:B:480:VAL:CG2	2.37	0.53
1:B:39:PHE:CD1	1:B:505:PRO:HD2	2.44	0.53
1:B:739:ILE:HB	1:B:781:THR:HG22	1.90	0.53
1:B:947:LEU:HD23	1:B:947:LEU:O	2.09	0.53
1:A:997:ARG:H	1:A:1004:ILE:CG2	2.22	0.53
1:A:119:ILE:O	1:A:119:ILE:HG23	2.09	0.53
1:A:356:ILE:HG22	1:A:421:ILE:O	2.09	0.53
1:A:385:LEU:HD13	1:A:385:LEU:C	2.29	0.53
1:A:925:HIS:O	1:A:950:PHE:HD2	1.91	0.53
1:A:958:LEU:HD23	1:A:959:LYS:H	1.73	0.53
1:A:963:GLY:C	1:A:1036:VAL:HG22	2.29	0.53
1:B:198:ILE:HB	1:B:226:ILE:HG22	1.91	0.53
1:B:308:LEU:O	1:B:338:PHE:HA	2.09	0.53
1:B:716:ILE:HG23	1:B:716:ILE:O	2.09	0.53
1:A:575:LEU:H	1:A:575:LEU:CD2	2.22	0.53
1:A:937:ARG:HG3	1:A:938:PRO:HD2	1.89	0.53
1:A:1032:VAL:HG12	1:A:1033:PHE:N	2.23	0.53
1:A:308:LEU:O	1:A:338:PHE:HA	2.09	0.53
1:A:40:VAL:HG11	1:A:503:ARG:NH2	2.24	0.53
1:A:578:LEU:HB2	1:A:609:ILE:HB	1.91	0.53
1:A:805:ALA:N	1:A:806:MET:HE3	2.24	0.53
1:A:807:ARG:HD2	1:A:813:CYS:HA	1.90	0.53
1:B:882:LEU:HD13	1:B:910:ALA:O	2.09	0.53
1:A:181:LYS:CE	1:A:202:LYS:HG2	2.39	0.52
1:A:580:THR:HG21	1:A:583:VAL:HG11	1.91	0.52
1:A:806:MET:HG2	1:A:807:ARG:CG	2.39	0.52
1:A:875:VAL:HG22	1:A:915:CYS:O	2.09	0.52
1:A:933:VAL:HG22	1:A:940:PHE:HB3	1.91	0.52
1:B:40:VAL:HG11	1:B:503:ARG:NH2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:THR:HG23	1:A:1019:THR:O	2.10	0.52
1:A:716:ILE:HG23	1:A:716:ILE:O	2.09	0.52
1:A:947:LEU:O	1:A:947:LEU:HD23	2.09	0.52
1:A:952:THR:HG23	1:A:952:THR:O	2.08	0.52
1:A:959:LYS:HG2	1:A:972:THR:CG2	2.39	0.52
1:B:439:TYR:CZ	1:B:538:LYS:CE	2.92	0.52
1:B:495:ILE:HG23	1:B:495:ILE:O	2.08	0.52
1:B:64:LEU:N	1:B:64:LEU:HD22	2.24	0.52
1:B:783:VAL:HG12	1:B:784:TRP:N	2.25	0.52
1:B:807:ARG:HD2	1:B:813:CYS:HA	1.90	0.52
1:A:1004:ILE:HG23	1:A:1004:ILE:O	2.08	0.52
1:A:281:ARG:O	1:A:282:LEU:HD23	2.09	0.52
1:A:827:SER:HB2	1:A:828:PRO:CD	2.39	0.52
1:B:135:GLY:O	1:B:159:LEU:HD13	2.08	0.52
1:B:321:LEU:HD12	1:B:462:PRO:CG	2.34	0.52
1:B:679:VAL:HG12	1:B:680:CYS:N	2.23	0.52
1:B:185:ALA:HB3	1:B:243:TYR:CG	2.44	0.52
1:B:589:GLY:HA3	1:B:639:LYS:HG3	1.90	0.52
1:B:739:ILE:HB	1:B:781:THR:HG23	1.90	0.52
1:B:827:SER:HB2	1:B:828:PRO:CD	2.40	0.52
1:A:42:PHE:HZ	1:A:45:GLU:CB	2.22	0.52
1:B:127:ILE:O	1:B:127:ILE:HG23	2.09	0.52
1:B:281:ARG:O	1:B:282:LEU:HD23	2.09	0.52
1:A:296:PRO:HD2	1:A:414:VAL:HG22	1.92	0.52
1:A:371:GLN:O	1:A:375:ARG:HG3	2.09	0.52
1:A:868:PRO:CG	1:A:1022:VAL:HG21	2.40	0.52
1:A:882:LEU:HD13	1:A:910:ALA:O	2.09	0.52
1:B:630:HIS:HD2	1:B:632:VAL:HG23	1.73	0.52
1:B:875:VAL:HG22	1:B:915:CYS:O	2.09	0.52
1:A:560:LEU:HG	1:A:648:THR:HG21	1.92	0.52
1:B:396:LEU:C	1:B:396:LEU:HD13	2.30	0.52
1:B:439:TYR:CZ	1:B:538:LYS:NZ	2.75	0.52
1:A:593:THR:HG23	1:A:593:THR:O	2.10	0.52
1:A:64:LEU:N	1:A:64:LEU:HD22	2.24	0.52
1:A:566:ASN:HB3	1:A:651:VAL:CG2	2.40	0.52
1:B:228:ILE:HG22	1:B:233:PHE:CE1	2.45	0.52
1:B:472:VAL:HG12	1:B:472:VAL:O	2.09	0.52
1:B:575:LEU:CD2	1:B:575:LEU:H	2.22	0.52
1:B:59:THR:HB	1:B:61:HIS:CE1	2.45	0.52
1:A:198:ILE:HB	1:A:226:ILE:HG22	1.91	0.52
1:A:472:VAL:O	1:A:472: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:A:39:PHE:CD1	1:A:505:PRO:HD2	2.44	0.52
1:A:553:GLU:HG3	1:A:554:MET:N	2.24	0.52
1:B:322:GLY:CA	1:B:327:VAL:HG22	2.40	0.52
1:B:560:LEU:HG	1:B:648:THR:HG21	1.92	0.52
1:B:806:MET:HG2	1:B:807:ARG:CG	2.39	0.52
1:A:322:GLY:CA	1:A:327:VAL:HG22	2.40	0.52
1:A:712:PRO:O	1:A:715:VAL:HG22	2.09	0.52
1:A:873:THR:CG2	1:A:981:GLY:C	2.78	0.52
1:A:956:ALA:O	1:A:1031:LEU:HD11	2.10	0.52
1:B:171:VAL:HG12	1:B:172:ILE:N	2.25	0.52
1:B:64:LEU:HD11	1:B:501:LEU:HD12	1.92	0.52
1:B:509:CYS:HB2	1:B:536:THR:HA	1.91	0.52
1:B:580:THR:HG21	1:B:583:VAL:HG11	1.92	0.52
1:B:827:SER:HB2	1:B:828:PRO:HD3	1.91	0.52
1:A:870:GLU:CD	1:A:1025:ALA:CA	2.78	0.51
1:A:171:VAL:HG12	1:A:172:ILE:N	2.26	0.51
1:A:473:GLN:CD	1:A:504:VAL:HG13	2.31	0.51
1:A:54:VAL:HG22	1:A:55:VAL:N	2.25	0.51
1:A:64:LEU:HD11	1:A:501:LEU:HD12	1.92	0.51
1:A:716:ILE:CG1	1:A:763:ASN:HB3	2.41	0.51
1:A:986:VAL:HG12	1:A:988:PHE:CE1	2.45	0.51
1:B:444:LEU:HD12	1:B:446:PHE:CZ	2.44	0.51
1:A:127:ILE:O	1:A:127:ILE:HG23	2.09	0.51
1:A:154:LYS:HB2	1:A:157:HIS:HD2	1.71	0.51
1:A:185:ALA:CB	1:A:243:TYR:CG	2.94	0.51
1:A:228:ILE:HG22	1:A:233:PHE:CE1	2.45	0.51
1:B:712:PRO:O	1:B:715:VAL:HG22	2.09	0.51
1:B:805:ALA:H	1:B:806:MET:CE	2.22	0.51
1:A:93:LYS:HD3	1:A:105:GLU:OE2	2.10	0.51
1:A:712:PRO:HG3	1:A:801:TYR:CZ	2.45	0.51
1:B:119:ILE:HG23	1:B:119:ILE:O	2.09	0.51
1:B:553:GLU:HG3	1:B:554:MET:N	2.24	0.51
1:B:567:ILE:CD1	1:B:650:PHE:CE2	2.94	0.51
1:A:468:GLN:HG3	1:A:523:ASP:HA	1.92	0.51
1:B:418:VAL:O	1:B:418:VAL:HG13	2.11	0.51
1:B:468:GLN:HB2	1:B:522:GLY:C	2.30	0.51
1:B:519:LEU:N	1:B:519:LEU:HD22	2.26	0.51
1:B:695:LYS:CB	1:B:696:LEU:HD12	2.41	0.51
1:B:727:PRO:O	1:B:729:PRO:HD3	2.10	0.51
1:A:216:VAL:HG13	1:A:217:PHE:N	2.26	0.51
1:A:53:LEU:HG	1:A:64:LEU:HD11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LYS:CB	1:A:696:LEU:HD12	2.41	0.51
1:A:984:VAL:HG11	1:A:998:ARG:HD3	1.91	0.51
1:B:265:PRO:HD3	1:B:274:VAL:HG22	1.92	0.51
1:B:541:CYS:SG	1:B:550:PHE:HD2	2.33	0.51
1:B:712:PRO:HG3	1:B:801:TYR:CZ	2.45	0.51
1:B:716:ILE:CG1	1:B:763:ASN:HB3	2.40	0.51
1:B:933:VAL:HG22	1:B:940:PHE:HB3	1.91	0.51
1:A:805:ALA:H	1:A:806:MET:HE3	1.75	0.51
1:B:184:ILE:C	1:B:184:ILE:HD12	2.31	0.51
1:B:53:LEU:HD23	1:B:53:LEU:C	2.31	0.51
1:B:54:VAL:HG22	1:B:55:VAL:N	2.25	0.51
1:A:997:ARG:H	1:A:1004:ILE:HG23	1.75	0.51
1:A:278:LYS:HG2	1:A:296:PRO:CA	2.39	0.51
1:A:370:LEU:HD11	1:A:374:TYR:CE1	2.46	0.51
1:A:790:ILE:HD12	1:A:790:ILE:N	2.25	0.51
1:A:889:ILE:CD1	1:A:907:TYR:CE1	2.94	0.51
1:B:426:GLU:HG3	1:B:429:ASP:H	1.75	0.51
1:B:548:ARG:O	1:B:584:PRO:HD3	2.11	0.51
1:B:823:GLY:HA3	1:B:844:TRP:CZ2	2.46	0.51
1:B:930:GLU:HG3	1:B:941:MET:SD	2.51	0.51
1:A:133:TYR:O	1:A:134:GLN:HB2	2.11	0.51
1:A:396:LEU:C	1:A:396:LEU:HD13	2.30	0.51
1:A:473:GLN:HB2	1:A:504:VAL:CG2	2.40	0.51
1:B:239:PHE:HA	1:B:260:PRO:CG	2.33	0.51
1:B:284:LYS:HD3	1:B:284:LYS:C	2.31	0.51
1:B:370:LEU:HD11	1:B:374:TYR:CE1	2.46	0.51
1:A:418:VAL:O	1:A:418:VAL:HG13	2.10	0.51
1:A:519:LEU:N	1:A:519:LEU:HD22	2.26	0.51
1:A:59:THR:HB	1:A:61:HIS:CE1	2.45	0.51
1:A:630:HIS:HD2	1:A:632:VAL:HG23	1.73	0.51
1:A:567:ILE:CD1	1:A:650:PHE:CE2	2.94	0.51
1:A:727:PRO:O	1:A:729:PRO:HD3	2.10	0.51
1:A:76:ASP:O	1:A:77:LEU:HB2	2.11	0.51
1:A:847:LEU:HG	1:A:850:ALA:HA	1.91	0.51
1:B:296:PRO:HD2	1:B:414:VAL:HG22	1.92	0.51
1:B:527:GLY:HA3	1:B:550:PHE:CE1	2.45	0.51
1:B:53:LEU:HG	1:B:64:LEU:HD11	1.92	0.51
1:B:703:LEU:N	1:B:703:LEU:HD22	2.26	0.51
1:B:847:LEU:HG	1:B:850:ALA:HA	1.91	0.51
1:A:507:GLU:HG3	1:A:537:ARG:CG	2.41	0.51
1:A:807:ARG:HD3	1:A:812:LEU:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ALA:CB	1:B:243:TYR:CG	2.94	0.51
1:B:93:LYS:HD3	1:B:105:GLU:OE2	2.10	0.51
1:A:358:ILE:CG2	1:A:361:GLN:HB2	2.41	0.50
1:A:541:CYS:SG	1:A:550:PHE:HD2	2.33	0.50
1:A:823:GLY:HA3	1:A:844:TRP:CZ2	2.46	0.50
1:A:870:GLU:OE2	1:A:1025:ALA:CA	2.58	0.50
1:A:987:MET:HB2	1:A:1019:THR:HG22	1.91	0.50
1:B:204:THR:HG23	1:B:206:ASN:O	2.11	0.50
1:B:228:ILE:CG2	1:B:233:PHE:CE1	2.94	0.50
1:B:566:ASN:HB3	1:B:651:VAL:CG2	2.40	0.50
1:B:689:PHE:CE1	1:B:691:GLU:CG	2.94	0.50
1:B:790:ILE:HD12	1:B:790:ILE:N	2.25	0.50
1:B:807:ARG:HD3	1:B:812:LEU:HB3	1.93	0.50
1:B:895:VAL:O	1:B:896:ALA:HB3	2.11	0.50
1:A:204:THR:HG23	1:A:206:ASN:O	2.11	0.50
1:A:469:TYR:HB2	1:A:523:ASP:OD2	2.11	0.50
1:A:783:VAL:HG12	1:A:784:TRP:N	2.25	0.50
1:A:798:VAL:O	1:A:798:VAL:HG13	2.10	0.50
1:A:930:GLU:HG3	1:A:941:MET:SD	2.51	0.50
1:B:119:ILE:CG2	1:B:121:TYR:CE1	2.95	0.50
1:B:300:GLU:HG2	1:B:305:GLU:HA	1.93	0.50
1:B:400:ASP:HB2	1:B:402:ASN:OD1	2.11	0.50
1:A:1004:ILE:HD13	1:A:1004:ILE:C	2.32	0.50
1:A:1029:GLN:HG2	1:A:1030:ASP:N	2.26	0.50
1:A:228:ILE:CG2	1:A:233:PHE:CE1	2.94	0.50
1:A:265:PRO:HD3	1:A:274:VAL:HG22	1.92	0.50
1:A:284:LYS:HD3	1:A:284:LYS:C	2.31	0.50
1:A:703:LEU:HD22	1:A:703:LEU:N	2.26	0.50
1:A:785:ASN:HB3	1:A:788:PHE:CE2	2.46	0.50
1:B:370:LEU:CD1	1:B:374:TYR:CD1	2.95	0.50
1:B:370:LEU:HD13	1:B:374:TYR:CD1	2.46	0.50
1:B:473:GLN:HB2	1:B:504:VAL:CG2	2.40	0.50
1:A:185:ALA:CB	1:A:243:TYR:CD2	2.94	0.50
1:A:261:GLU:HG2	1:A:265:PRO:N	2.25	0.50
1:A:53:LEU:HD23	1:A:53:LEU:C	2.31	0.50
1:A:689:PHE:CE1	1:A:691:GLU:CG	2.94	0.50
1:A:782:VAL:CG2	1:A:790:ILE:HB	2.41	0.50
1:A:894:LYS:CD	1:A:899:GLU:HA	2.41	0.50
1:B:295:VAL:O	1:B:295:VAL:HG23	2.12	0.50
1:B:785:ASN:HB3	1:B:788:PHE:CE2	2.46	0.50
1:B:853:LYS:H	1:B:853:LYS:HD2	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ILE:HD12	1:A:184:ILE:C	2.31	0.50
1:A:370:LEU:CD1	1:A:374:TYR:CD1	2.95	0.50
1:A:439:TYR:CE2	1:A:538:LYS:HE2	2.43	0.50
1:B:412:LEU:HD22	1:B:412:LEU:O	2.11	0.50
1:B:541:CYS:CB	1:B:544:SER:HB3	2.42	0.50
1:B:76:ASP:O	1:B:77:LEU:HB2	2.11	0.50
1:A:1029:GLN:CG	1:A:1030:ASP:H	2.24	0.50
1:A:662:LEU:CD2	1:A:791:ASP:OD2	2.60	0.50
1:A:895:VAL:O	1:A:896:ALA:HB3	2.11	0.50
1:A:868:PRO:CD	1:A:980:ALA:C	2.54	0.50
1:B:133:TYR:O	1:B:134:GLN:HB2	2.11	0.50
1:B:185:ALA:CB	1:B:243:TYR:CD2	2.94	0.50
1:B:261:GLU:HG2	1:B:265:PRO:N	2.25	0.50
1:B:403:PHE:CE1	1:B:406:LEU:CD2	2.94	0.50
1:B:473:GLN:CD	1:B:504:VAL:HG13	2.31	0.50
1:B:491:GLU:O	1:B:506:VAL:HG12	2.11	0.50
1:B:64:LEU:HB2	1:B:71:TYR:HD2	1.77	0.50
1:A:110:THR:CB	1:A:132:LEU:HD21	2.42	0.50
1:A:185:ALA:HB1	1:A:243:TYR:CE2	2.47	0.50
1:A:39:PHE:CD2	1:A:473:GLN:CG	2.95	0.50
1:A:491:GLU:O	1:A:506:VAL:HG12	2.11	0.50
1:A:527:GLY:HA3	1:A:550:PHE:CE1	2.45	0.50
1:A:673:TRP:HB3	1:A:694:VAL:HB	1.94	0.50
1:A:81:VAL:HG12	1:A:82:THR:N	2.26	0.50
1:B:358:ILE:CG2	1:B:361:GLN:HB2	2.41	0.50
1:B:457:ILE:HG12	1:B:467:LEU:CD1	2.42	0.50
1:B:798:VAL:HG13	1:B:798:VAL:O	2.10	0.50
1:A:320:VAL:HG23	1:A:441:ASN:HB3	1.94	0.50
1:A:40:VAL:HG21	1:A:76:ASP:O	2.12	0.50
1:A:736:TYR:CD2	1:A:784:TRP:HB3	2.47	0.50
1:B:889:ILE:CD1	1:B:907:TYR:CE1	2.94	0.50
1:A:119:ILE:CG2	1:A:121:TYR:CE1	2.95	0.50
1:A:300:GLU:HG2	1:A:305:GLU:HA	1.93	0.50
1:A:370:LEU:HD13	1:A:374:TYR:CD1	2.46	0.50
1:A:433:SER:HB3	1:A:484:MET:HE3	1.93	0.50
1:A:892:HIS:HD2	1:A:893:VAL:N	2.10	0.50
1:A:986:VAL:CG1	1:A:988:PHE:CE1	2.94	0.50
1:B:593:THR:O	1:B:593:THR:HG23	2.10	0.50
1:B:736:TYR:CD2	1:B:784:TRP:HB3	2.47	0.50
1:B:81:VAL:HG12	1:B:82:THR:N	2.26	0.50
1:B:841:GLU:HG3	1:B:842:SER:H	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:CD1	1:A:386:LYS:HE3	2.37	0.49
1:A:457:ILE:HG12	1:A:467:LEU:CD1	2.42	0.49
1:A:597:LEU:HD22	1:A:597:LEU:H	1.78	0.49
1:B:278:LYS:CE	1:B:296:PRO:HG3	2.41	0.49
1:B:882:LEU:HD23	1:B:913:ILE:HD11	1.94	0.49
1:A:265:PRO:CD	1:A:274:VAL:HG22	2.42	0.49
1:A:426:GLU:HG3	1:A:429:ASP:H	1.75	0.49
1:A:444:LEU:HD12	1:A:446:PHE:CZ	2.44	0.49
1:A:623:ILE:HD12	1:A:624:THR:CA	2.42	0.49
1:A:976:THR:HG22	1:A:977:ASN:N	2.27	0.49
1:B:623:ILE:HD12	1:B:624:THR:CA	2.42	0.49
1:B:790:ILE:H	1:B:790:ILE:HD12	1.77	0.49
1:B:856:ASN:N	1:B:857:PRO:HD3	2.27	0.49
1:B:892:HIS:HD2	1:B:893:VAL:N	2.10	0.49
1:A:105:GLU:CB	1:A:106:PRO:HD2	2.42	0.49
1:A:234:THR:HG23	1:A:235:VAL:N	2.26	0.49
1:A:400:ASP:HB2	1:A:402:ASN:OD1	2.11	0.49
1:B:234:THR:HG23	1:B:235:VAL:N	2.27	0.49
1:B:333:LEU:HD21	1:B:358:ILE:HG13	1.94	0.49
1:B:597:LEU:H	1:B:597:LEU:CD2	2.26	0.49
1:B:59:THR:HB	1:B:61:HIS:ND1	2.27	0.49
1:B:792:ASN:HD21	1:B:796:ASN:N	2.10	0.49
1:B:894:LYS:CD	1:B:899:GLU:HA	2.41	0.49
1:A:333:LEU:HD21	1:A:358:ILE:HG13	1.94	0.49
1:A:792:ASN:HD21	1:A:796:ASN:N	2.10	0.49
1:B:185:ALA:HB1	1:B:243:TYR:CE2	2.47	0.49
1:B:265:PRO:HB2	1:B:266:PRO:HD2	1.94	0.49
1:B:713:VAL:HG13	1:B:767:SER:HA	1.94	0.49
1:A:412:LEU:O	1:A:412:LEU:HD22	2.11	0.49
1:A:790:ILE:H	1:A:790:ILE:HD12	1.77	0.49
1:A:955:LEU:HD11	1:A:973:ILE:HG23	1.94	0.49
1:B:312:ALA:HB1	1:B:334:LEU:HD11	1.94	0.49
1:B:475:VAL:HG22	1:B:500:GLN:OE1	2.13	0.49
1:B:40:VAL:HG21	1:B:76:ASP:O	2.12	0.49
1:A:132:LEU:HD11	1:A:163:ASN:HD22	1.77	0.49
1:A:185:ALA:HA	1:A:197:THR:O	2.13	0.49
1:A:475:VAL:HG22	1:A:500:GLN:OE1	2.13	0.49
1:A:597:LEU:CD2	1:A:597:LEU:H	2.26	0.49
1:A:532:HIS:CA	1:A:641:THR:HG21	2.43	0.49
1:A:782:VAL:HG23	1:A:782:VAL:O	2.12	0.49
1:B:110:THR:CB	1:B:132:LEU:HD21	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TYR:HB3	1:B:136:ILE:HG23	1.94	0.49
1:B:265:PRO:CD	1:B:274:VAL:HG22	2.42	0.49
1:B:374:TYR:CE2	1:B:397:LEU:HD22	2.48	0.49
1:B:782:VAL:HG23	1:B:782:VAL:O	2.12	0.49
1:A:1002:TYR:OH	1:A:1004:ILE:HB	2.12	0.49
1:A:1021:GLN:HG2	1:A:1026:ARG:CG	2.41	0.49
1:A:254:TYR:CE2	1:A:281:ARG:HD2	2.48	0.49
1:A:295:VAL:O	1:A:295:VAL:HG23	2.12	0.49
1:A:374:TYR:CE2	1:A:397:LEU:HD22	2.48	0.49
1:A:995:PHE:HZ	1:A:998:ARG:HB2	1.77	0.49
1:B:444:LEU:CD2	1:B:524:PRO:CD	2.91	0.49
1:B:548:ARG:CD	1:B:583:VAL:O	2.60	0.49
1:A:541:CYS:CB	1:A:544:SER:HB3	2.42	0.49
1:A:841:GLU:HG3	1:A:842:SER:H	1.78	0.49
1:A:889:ILE:O	1:A:892:HIS:HB3	2.13	0.49
1:B:132:LEU:HD11	1:B:163:ASN:HD22	1.77	0.49
1:B:190:GLY:C	1:B:192:PRO:HD3	2.33	0.49
1:B:216:VAL:HG13	1:B:217:PHE:N	2.26	0.49
1:B:433:SER:HB3	1:B:484:MET:HE3	1.95	0.49
1:B:889:ILE:O	1:B:892:HIS:HB3	2.13	0.49
1:A:265:PRO:HB2	1:A:266:PRO:HD2	1.94	0.49
1:A:991:GLN:CB	1:A:1008:THR:HG21	2.42	0.49
1:B:473:GLN:HB3	1:B:502:THR:HG21	1.94	0.49
1:B:590:VAL:HG12	1:B:591:ASN:N	2.27	0.49
1:B:847:LEU:HG	1:B:850:ALA:CA	2.42	0.49
1:A:133:TYR:HB3	1:A:136:ILE:HG23	1.94	0.49
1:A:853:LYS:HD2	1:A:853:LYS:H	1.76	0.49
1:A:868:PRO:HG2	1:A:981:GLY:HA3	1.91	0.49
1:B:182:LEU:HD21	1:B:184:ILE:HG21	1.94	0.49
1:B:190:GLY:HA2	1:B:233:PHE:HE2	1.73	0.49
1:B:662:LEU:HD23	1:B:791:ASP:CG	2.32	0.49
1:B:809:SER:CB	1:B:881:ASN:ND2	2.75	0.49
1:A:603:LEU:C	1:A:603:LEU:HD23	2.33	0.48
1:A:856:ASN:N	1:A:857:PRO:HD3	2.27	0.48
1:A:863:ILE:HG13	1:A:864:PRO:N	2.28	0.48
1:A:99:ILE:HD11	1:A:152:PHE:CB	2.41	0.48
1:B:39:PHE:CD2	1:B:473:GLN:CG	2.95	0.48
1:B:506:VAL:O	1:B:525:HIS:CE1	2.66	0.48
1:B:541:CYS:SG	1:B:550:PHE:CD2	3.06	0.48
1:B:863:ILE:HG13	1:B:864:PRO:N	2.28	0.48
1:B:907:TYR:CZ	1:B:909:PRO:HA	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:CG	1:A:1022:VAL:CG2	2.88	0.48
1:A:473:GLN:CD	1:A:504:VAL:HG22	2.33	0.48
1:A:59:THR:HB	1:A:61:HIS:ND1	2.27	0.48
1:A:790:ILE:HG22	1:A:791:ASP:N	2.29	0.48
1:A:847:LEU:HG	1:A:850:ALA:CA	2.42	0.48
1:B:160:SER:OG	1:B:162:VAL:HG23	2.13	0.48
1:B:949:TYR:CE2	1:B:951:MET:CE	2.95	0.48
1:A:1020:VAL:HG13	1:A:1020:VAL:O	2.13	0.48
1:A:590:VAL:HG12	1:A:591:ASN:N	2.27	0.48
1:A:713:VAL:HG13	1:A:767:SER:HA	1.94	0.48
1:A:882:LEU:HD23	1:A:913:ILE:HD11	1.94	0.48
1:B:185:ALA:HA	1:B:197:THR:O	2.13	0.48
1:B:435:ILE:HG21	1:B:486:PHE:CE1	2.48	0.48
1:B:603:LEU:HD23	1:B:603:LEU:C	2.33	0.48
1:B:673:TRP:HB3	1:B:694:VAL:HB	1.94	0.48
1:A:239:PHE:CD1	1:A:260:PRO:HG2	2.48	0.48
1:A:321:LEU:CG	1:A:325:LEU:HD11	2.40	0.48
1:A:991:GLN:HB3	1:A:1008:THR:HG21	1.96	0.48
1:B:254:TYR:CE2	1:B:281:ARG:HD2	2.48	0.48
1:B:239:PHE:CD1	1:B:260:PRO:HG2	2.48	0.48
1:B:320:VAL:HG23	1:B:441:ASN:HB3	1.94	0.48
1:B:781:THR:HG23	1:B:781:THR:O	2.12	0.48
1:B:807:ARG:HB3	1:B:812:LEU:HB2	1.95	0.48
1:A:435:ILE:HG21	1:A:486:PHE:CE1	2.48	0.48
1:A:473:GLN:HB3	1:A:502:THR:HG21	1.94	0.48
1:A:681:THR:HG21	1:A:686:THR:HG21	1.94	0.48
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.48
1:A:716:ILE:HD11	1:A:763:ASN:HB3	1.95	0.48
1:A:781:THR:O	1:A:781:THR:HG23	2.12	0.48
1:B:258:LEU:HD12	1:B:258:LEU:N	2.29	0.48
1:B:453:LYS:HE3	1:B:472:VAL:HG22	1.94	0.48
1:B:715:VAL:HG23	1:B:715:VAL:O	2.13	0.48
1:A:182:LEU:HD21	1:A:184:ILE:HG21	1.94	0.48
1:A:567:ILE:HD12	1:A:650:PHE:CE2	2.49	0.48
1:B:716:ILE:HD11	1:B:763:ASN:HB3	1.95	0.48
1:B:935:VAL:HG12	1:B:936:CYS:N	2.28	0.48
1:A:190:GLY:C	1:A:192:PRO:HD3	2.33	0.48
1:A:312:ALA:HB1	1:A:334:LEU:HD11	1.94	0.48
1:A:144:ASP:O	1:A:145:LEU:HB2	2.13	0.48
1:A:543:ARG:HH11	1:A:549:ARG:HH22	1.62	0.48
1:A:626:ASN:ND2	1:A:630:HIS:HB2	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HB2	1:A:71:TYR:HD2	1.77	0.48
1:A:807:ARG:HB3	1:A:812:LEU:HB2	1.95	0.48
1:A:935:VAL:HG12	1:A:936:CYS:N	2.28	0.48
1:B:144:ASP:O	1:B:145:LEU:HB2	2.13	0.48
1:B:42:PHE:HZ	1:B:45:GLU:CB	2.22	0.48
1:B:626:ASN:ND2	1:B:630:HIS:HB2	2.29	0.48
1:B:782:VAL:CG2	1:B:790:ILE:HB	2.41	0.48
1:B:783:VAL:HG13	1:B:788:PHE:O	2.13	0.48
1:B:471:THR:HG23	1:B:473:GLN:NE2	2.27	0.48
1:A:710:LEU:HD13	1:A:801:TYR:OH	2.13	0.48
1:A:1010:SER:HB2	1:A:1035:TYR:CD2	2.49	0.47
1:A:361:GLN:HE21	1:A:365:ARG:HH21	1.61	0.47
1:A:469:TYR:CB	1:A:523:ASP:OD2	2.62	0.47
1:A:704:LEU:H	1:A:723:ALA:HA	1.79	0.47
1:A:987:MET:HE3	1:A:990:SER:HA	1.95	0.47
1:B:440:LYS:O	1:B:440:LYS:HG2	2.14	0.47
1:B:561:THR:HG22	1:B:562:VAL:N	2.29	0.47
1:B:681:THR:HG21	1:B:686:THR:HG21	1.95	0.47
1:B:710:LEU:HD13	1:B:801:TYR:OH	2.13	0.47
1:A:124:ASN:OD1	1:A:142:LEU:HB3	2.14	0.47
1:A:258:LEU:HD12	1:A:258:LEU:N	2.28	0.47
1:A:440:LYS:HG2	1:A:440:LYS:O	2.14	0.47
1:A:541:CYS:SG	1:A:550:PHE:CD2	3.07	0.47
1:A:862:ILE:CG2	1:A:877:ILE:HG23	2.44	0.47
1:A:907:TYR:CZ	1:A:909:PRO:HA	2.48	0.47
1:A:991:GLN:HA	1:A:991:GLN:OE1	2.13	0.47
1:B:124:ASN:OD1	1:B:142:LEU:HB3	2.15	0.47
1:B:430:ARG:HG2	1:B:431:MET:O	2.14	0.47
1:B:814:LEU:HD11	1:B:845:LEU:CD1	2.44	0.47
1:A:468:GLN:HB3	1:A:468:GLN:HE21	1.47	0.47
1:A:695:LYS:HB2	1:A:696:LEU:HD12	1.97	0.47
1:A:728:GLN:HA	1:A:753:ARG:NH2	2.30	0.47
1:A:953:LEU:HB3	1:A:977:ASN:O	2.14	0.47
1:B:113:VAL:HG11	1:B:165:SER:HB3	1.97	0.47
1:B:361:GLN:HE21	1:B:365:ARG:HH21	1.61	0.47
1:B:473:GLN:CD	1:B:504:VAL:HG22	2.34	0.47
1:B:507:GLU:HG3	1:B:537:ARG:CG	2.40	0.47
1:B:698:GLU:O	1:B:725:ASN:OD1	2.32	0.47
1:B:728:GLN:HA	1:B:753:ARG:NH2	2.29	0.47
1:A:991:GLN:HG2	1:A:1008:THR:HG21	1.96	0.47
1:A:783:VAL:HG13	1:A:788:PHE:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:VAL:HG23	1:A:984:VAL:O	2.14	0.47
1:A:997:ARG:HG2	1:A:998:ARG:N	2.30	0.47
1:B:98:ARG:NH2	1:B:107:LEU:HD12	2.29	0.47
1:B:175:TYR:CG	1:B:176:SER:N	2.82	0.47
1:B:543:ARG:HH11	1:B:549:ARG:HH22	1.62	0.47
1:A:264:SER:HA	1:A:265:PRO:HA	1.53	0.47
1:A:40:VAL:HG11	1:A:503:ARG:HE	1.79	0.47
1:A:458:ARG:CD	1:A:524:PRO:HG3	2.44	0.47
1:A:702:GLN:O	1:A:723:ALA:HB1	2.14	0.47
1:A:715:VAL:HG23	1:A:715:VAL:O	2.13	0.47
1:A:863:ILE:CG1	1:A:864:PRO:HD3	2.39	0.47
1:A:175:TYR:CG	1:A:176:SER:N	2.82	0.47
1:A:430:ARG:HG2	1:A:431:MET:O	2.14	0.47
1:A:77:LEU:HD22	1:A:501:LEU:HD13	1.96	0.47
1:A:68:ASN:ND2	1:A:87:PRO:HD3	2.29	0.47
1:B:118:LEU:HD13	1:B:118:LEU:C	2.34	0.47
1:B:380:LEU:HD12	1:B:390:ILE:CG2	2.45	0.47
1:B:469:TYR:HB3	1:B:523:ASP:OD2	2.15	0.47
1:B:480:VAL:HB	1:B:484:MET:HE1	1.94	0.47
1:B:597:LEU:H	1:B:597:LEU:HD22	1.78	0.47
1:B:699:ASP:O	1:B:725:ASN:CB	2.63	0.47
1:B:745:ILE:O	1:B:745:ILE:HG23	2.14	0.47
1:A:333:LEU:CD2	1:A:358:ILE:HA	2.45	0.47
1:A:569:VAL:HG23	1:A:654:ASN:HB2	1.80	0.47
1:A:72:LYS:O	1:A:80:LEU:HB2	2.15	0.47
1:A:745:ILE:O	1:A:745:ILE:HG23	2.15	0.47
1:A:814:LEU:HD11	1:A:845:LEU:CD1	2.44	0.47
1:A:987:MET:CE	1:A:990:SER:HA	2.45	0.47
1:B:372:SER:HA	1:B:375:ARG:NE	2.29	0.47
1:B:704:LEU:H	1:B:723:ALA:HA	1.79	0.47
1:B:702:GLN:O	1:B:723:ALA:HB1	2.14	0.47
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.75	0.47
1:B:262:MET:O	1:B:263:VAL:HB	2.14	0.47
1:B:569:VAL:CG1	1:B:620:PRO:HG3	2.45	0.47
1:B:947:LEU:HD23	1:B:947:LEU:H	1.80	0.47
1:A:253:VAL:O	1:A:253:VAL:HG23	2.15	0.47
1:A:453:LYS:HE3	1:A:472:VAL:HG22	1.94	0.47
1:A:843:ARG:NH1	1:A:843:ARG:HB2	2.30	0.47
1:A:892:HIS:CD2	1:A:893:VAL:CG2	2.98	0.47
1:A:958:LEU:HD13	1:A:1033:PHE:HD1	1.79	0.47
1:B:253:VAL:O	1:B:253:VAL:HG23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PHE:HE1	1:B:406:LEU:HD23	1.75	0.47
1:B:45:GLU:HB3	1:B:46:PRO:HD3	1.97	0.47
1:B:740:LEU:HD12	1:B:740:LEU:N	2.29	0.47
1:B:790:ILE:HG22	1:B:791:ASP:N	2.28	0.47
1:A:245:TYR:CE2	1:A:247:PHE:HD2	2.33	0.47
1:A:569:VAL:CG1	1:A:620:PRO:HG3	2.45	0.47
1:A:873:THR:CG2	1:A:982:SER:N	2.78	0.47
1:B:68:ASN:ND2	1:B:87:PRO:HD3	2.30	0.47
1:A:1020:VAL:HG13	1:A:1027:ILE:HG12	1.96	0.47
1:A:160:SER:OG	1:A:162:VAL:HG23	2.14	0.47
1:A:495:ILE:HG22	1:A:502:THR:HB	1.96	0.47
1:A:561:THR:HG22	1:A:562:VAL:N	2.28	0.47
1:A:947:LEU:N	1:A:947:LEU:HD23	2.30	0.47
1:B:105:GLU:CB	1:B:106:PRO:HD2	2.42	0.47
1:B:333:LEU:CD2	1:B:358:ILE:HA	2.45	0.47
1:B:343:LYS:HG2	1:B:344:ARG:HG2	1.97	0.47
1:B:82:THR:O	1:B:82:THR:HG23	2.14	0.47
1:A:118:LEU:C	1:A:118:LEU:HD13	2.34	0.46
1:A:372:SER:HA	1:A:375:ARG:NE	2.30	0.46
1:B:244:VAL:HB	1:B:309:LEU:HD23	1.97	0.46
1:B:783:VAL:HG11	1:B:786:GLY:O	2.15	0.46
1:B:843:ARG:HB2	1:B:843:ARG:NH1	2.30	0.46
1:B:862:ILE:CG2	1:B:877:ILE:HG23	2.44	0.46
1:B:863:ILE:CG1	1:B:864:PRO:HD3	2.39	0.46
1:A:181:LYS:HZ2	1:A:216:VAL:HG23	1.77	0.46
1:A:403:PHE:HE1	1:A:406:LEU:HD23	1.75	0.46
1:A:68:ASN:HB3	1:A:86:GLY:HA3	1.97	0.46
1:A:949:TYR:CE2	1:A:951:MET:CE	2.95	0.46
1:A:873:THR:HG23	1:A:981:GLY:O	2.14	0.46
1:B:567:ILE:HD12	1:B:650:PHE:CE2	2.49	0.46
1:B:72:LYS:O	1:B:80:LEU:HB2	2.15	0.46
1:A:244:VAL:HB	1:A:309:LEU:HD23	1.97	0.46
1:B:286:ASP:OD1	1:B:288:ALA:HB3	2.15	0.46
1:B:380:LEU:CB	1:B:386:LYS:HE3	2.44	0.46
1:B:505:PRO:HB2	1:B:507:GLU:C	2.35	0.46
1:A:1007:THR:HG22	1:A:1008:THR:O	2.15	0.46
1:A:532:HIS:CA	1:A:641:THR:OG1	2.57	0.46
1:A:82:THR:O	1:A:82:THR:HG23	2.14	0.46
1:B:321:LEU:CG	1:B:325:LEU:HD11	2.40	0.46
1:A:252:PHE:CD1	1:A:283:CYS:HA	2.50	0.46
1:A:503:ARG:O	1:A:505:PRO:HD3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:CD	1:A:584:PRO:CB	2.76	0.46
1:A:549:ARG:HA	1:A:584:PRO:HG3	1.97	0.46
1:A:862:ILE:HG22	1:A:877:ILE:CA	2.32	0.46
1:A:873:THR:HG22	1:A:874:LYS:N	2.31	0.46
1:B:159:LEU:HG	1:B:201:ARG:HH12	1.81	0.46
1:B:245:TYR:CD2	1:B:312:ALA:HB3	2.51	0.46
1:B:296:PRO:CD	1:B:414:VAL:HG22	2.45	0.46
1:B:468:GLN:O	1:B:521:SER:O	2.34	0.46
1:B:68:ASN:HB3	1:B:86:GLY:HA3	1.97	0.46
1:B:660:SER:HB2	1:B:791:ASP:OD1	2.16	0.46
1:B:892:HIS:CD2	1:B:893:VAL:CG2	2.98	0.46
1:A:1015:ASP:H	1:A:1035:TYR:H	1.63	0.46
1:A:265:PRO:CB	1:A:266:PRO:HD2	2.45	0.46
1:A:296:PRO:CD	1:A:414:VAL:HG22	2.46	0.46
1:A:492:GLN:HG2	1:A:503:ARG:HG2	1.98	0.46
1:B:46:PRO:CG	1:B:69:ARG:HG3	2.27	0.46
1:B:77:LEU:HD22	1:B:501:LEU:HD13	1.96	0.46
1:B:902:PRO:HA	1:B:915:CYS:HA	1.97	0.46
1:B:99:ILE:HD11	1:B:152:PHE:CB	2.41	0.46
1:A:113:VAL:HG11	1:A:165:SER:HB3	1.96	0.46
1:A:226:ILE:HD11	1:A:385:LEU:CD2	2.46	0.46
1:A:444:LEU:HD13	1:A:445:ALA:H	1.79	0.46
1:A:62:ILE:CD1	1:A:77:LEU:CD2	2.94	0.46
1:A:62:ILE:HD11	1:A:73:LEU:CD1	2.45	0.46
1:A:873:THR:OG1	1:A:982:SER:N	2.48	0.46
1:B:295:VAL:CA	1:B:414:VAL:HG21	2.45	0.46
1:A:262:MET:O	1:A:263:VAL:HB	2.14	0.46
1:A:274:VAL:HG23	1:A:275:TYR:N	2.30	0.46
1:A:295:VAL:CA	1:A:414:VAL:HG21	2.45	0.46
1:A:343:LYS:HG2	1:A:344:ARG:HG2	1.97	0.46
1:A:947:LEU:H	1:A:947:LEU:HD23	1.80	0.46
1:B:495:ILE:HG22	1:B:502:THR:HB	1.96	0.46
1:B:594:PHE:CZ	1:B:614:PRO:HD3	2.51	0.46
1:A:403:PHE:CE1	1:A:406:LEU:CD2	2.94	0.46
1:A:437:TYR:CE2	1:A:439:TYR:HB2	2.51	0.46
1:B:245:TYR:CE2	1:B:247:PHE:HD2	2.34	0.46
1:B:278:LYS:HD3	1:B:294:GLU:HG2	1.98	0.46
1:B:46:PRO:HD2	1:B:71:TYR:OH	2.16	0.46
1:B:91:ASN:OD1	1:B:92:PRO:HD2	2.16	0.46
1:A:870:GLU:CA	1:A:1024:ARG:HG2	2.43	0.46
1:A:286:ASP:OD1	1:A:288:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD12	1:A:390:ILE:CG2	2.45	0.46
1:A:902:PRO:HA	1:A:915:CYS:HA	1.98	0.46
1:B:118:LEU:CD1	1:B:172:ILE:HD12	2.12	0.46
1:B:225:MET:HE1	1:B:227:LYS:CG	2.45	0.46
1:B:361:GLN:O	1:B:365:ARG:HG2	2.16	0.46
1:A:327:VAL:HG11	1:A:358:ILE:HD11	1.97	0.45
1:A:624:THR:O	1:A:624:THR:HG23	2.15	0.45
1:A:828:PRO:HG3	1:A:837:CYS:SG	2.56	0.45
1:A:892:HIS:CD2	1:A:893:VAL:HG22	2.51	0.45
1:B:252:PHE:CD1	1:B:283:CYS:HA	2.50	0.45
1:B:435:ILE:HG23	1:B:486:PHE:HE1	1.81	0.45
1:B:439:TYR:CE2	1:B:538:LYS:CE	2.99	0.45
1:B:689:PHE:CE1	1:B:691:GLU:HG2	2.50	0.45
1:B:62:ILE:CD1	1:B:73:LEU:HB2	2.47	0.45
1:B:743:GLN:HG2	1:B:744:GLY:N	2.31	0.45
1:A:110:THR:CB	1:A:132:LEU:CD2	2.95	0.45
1:A:435:ILE:HG23	1:A:486:PHE:HE1	1.81	0.45
1:A:480:VAL:HB	1:A:484:MET:HE1	1.97	0.45
1:A:563:HIS:CB	1:A:577:VAL:HG12	2.46	0.45
1:A:532:HIS:C	1:A:641:THR:HG21	2.36	0.45
1:A:870:GLU:OE2	1:A:1025:ALA:HA	2.16	0.45
1:A:890:ALA:O	1:A:891:SER:HB2	2.17	0.45
1:B:265:PRO:CB	1:B:266:PRO:HD2	2.45	0.45
1:A:1020:VAL:CG1	1:A:1027:ILE:CG1	2.95	0.45
1:A:380:LEU:CB	1:A:386:LYS:HE3	2.43	0.45
1:A:45:GLU:HB3	1:A:46:PRO:HD3	1.97	0.45
1:B:118:LEU:HB3	1:B:127:ILE:HG22	1.98	0.45
1:B:663:SER:O	1:B:667:SER:HB2	2.17	0.45
1:B:695:LYS:HB2	1:B:696:LEU:HD12	1.96	0.45
1:A:361:GLN:O	1:A:365:ARG:HG2	2.16	0.45
1:A:458:ARG:HG3	1:A:468:GLN:NE2	2.32	0.45
1:A:469:TYR:CG	1:A:470:GLU:N	2.84	0.45
1:A:689:PHE:CE1	1:A:691:GLU:HG2	2.50	0.45
1:A:783:VAL:HG11	1:A:786:GLY:O	2.16	0.45
1:B:256:LEU:HD22	1:B:256:LEU:N	2.31	0.45
1:B:435:ILE:HG21	1:B:486:PHE:HE1	1.81	0.45
1:B:58:ARG:HG2	1:B:58:ARG:NH1	2.31	0.45
1:B:62:ILE:HD11	1:B:73:LEU:CD1	2.45	0.45
1:B:828:PRO:HG3	1:B:837:CYS:SG	2.56	0.45
1:B:892:HIS:CD2	1:B:893:VAL:N	2.85	0.45
1:A:159:LEU:HG	1:A:201:ARG:HH12	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HD22	1:A:256:LEU:N	2.31	0.45
1:A:288:ALA:O	1:A:289:PHE:HB2	2.17	0.45
1:A:322:GLY:HA2	1:A:327:VAL:HG22	1.99	0.45
1:A:511:GLN:HG3	1:A:512:TYR:CD2	2.51	0.45
1:A:743:GLN:HG2	1:A:744:GLY:N	2.31	0.45
1:B:563:HIS:CB	1:B:577:VAL:HG12	2.46	0.45
1:B:624:THR:O	1:B:624:THR:HG23	2.15	0.45
1:B:62:ILE:CD1	1:B:77:LEU:CD2	2.94	0.45
1:B:805:ALA:N	1:B:806:MET:HE3	2.31	0.45
1:A:1014:LEU:HD12	1:A:1035:TYR:O	2.16	0.45
1:A:118:LEU:HB3	1:A:127:ILE:HG22	1.98	0.45
1:A:278:LYS:CE	1:A:296:PRO:HG3	2.41	0.45
1:A:245:TYR:CD2	1:A:312:ALA:HB3	2.51	0.45
1:A:506:VAL:O	1:A:507:GLU:N	2.39	0.45
1:A:695:LYS:C	1:A:696:LEU:HD12	2.37	0.45
1:B:442:HIS:CD2	1:B:458:ARG:HH21	2.35	0.45
1:B:503:ARG:O	1:B:505:PRO:HD3	2.15	0.45
1:B:671:CYS:HB3	1:B:680:CYS:SG	2.57	0.45
1:B:873:THR:HG22	1:B:874:LYS:N	2.31	0.45
1:B:892:HIS:CD2	1:B:893:VAL:HG22	2.51	0.45
1:B:947:LEU:HD23	1:B:947:LEU:N	2.30	0.45
1:A:358:ILE:CG2	1:A:361:GLN:CB	2.95	0.45
1:A:53:LEU:HD12	1:A:501:LEU:HG	1.99	0.45
1:A:539:GLU:HG3	1:A:540:ARG:N	2.31	0.45
1:A:594:PHE:CZ	1:A:614:PRO:HD3	2.51	0.45
1:A:46:PRO:HD2	1:A:71:TYR:OH	2.16	0.45
1:B:118:LEU:O	1:B:127:ILE:HG22	2.17	0.45
1:B:226:ILE:HD11	1:B:385:LEU:CD2	2.46	0.45
1:B:40:VAL:HG11	1:B:503:ARG:HE	1.80	0.45
1:B:62:ILE:CD1	1:B:501:LEU:CD1	2.95	0.45
1:B:635:GLN:HB3	1:B:644:THR:HB	1.99	0.45
1:B:890:ALA:O	1:B:891:SER:HB2	2.17	0.45
1:A:182:LEU:HB2	1:A:203:LEU:HD11	1.99	0.45
1:A:62:ILE:CD1	1:A:501:LEU:CD1	2.95	0.45
1:A:663:SER:O	1:A:667:SER:HB2	2.16	0.45
1:A:715:VAL:HG21	1:A:717:LYS:CD	2.44	0.45
1:A:841:GLU:HG3	1:A:842:SER:N	2.32	0.45
1:A:955:LEU:CD1	1:A:973:ILE:CG2	2.94	0.45
1:B:133:TYR:CG	1:B:136:ILE:CG1	2.94	0.45
1:B:464:GLY:O	1:B:465:ASN:HB3	2.17	0.45
1:A:492:GLN:HG2	1:A:503:ARG:HD2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:THR:CB	1:A:982:SER:N	2.80	0.45
1:B:192:PRO:HB3	1:B:233:PHE:CZ	2.51	0.45
1:B:288:ALA:O	1:B:289:PHE:HB2	2.17	0.45
1:B:492:GLN:HG2	1:B:503:ARG:HG2	1.98	0.45
1:B:511:GLN:HG3	1:B:512:TYR:CD2	2.51	0.45
1:B:539:GLU:HG3	1:B:540:ARG:N	2.31	0.45
1:B:814:LEU:HB2	1:B:884:LEU:HD11	1.98	0.45
1:A:118:LEU:CD1	1:A:172:ILE:HD12	2.12	0.45
1:A:531:LEU:HG	1:A:584:PRO:CG	2.46	0.45
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.16	0.45
1:B:327:VAL:HG11	1:B:358:ILE:HD11	1.97	0.45
1:B:468:GLN:HB3	1:B:468:GLN:HE21	1.47	0.45
1:B:862:ILE:HG22	1:B:877:ILE:CA	2.32	0.45
1:A:464:GLY:O	1:A:465:ASN:HB3	2.17	0.44
1:A:703:LEU:CD2	1:A:790:ILE:CG2	2.95	0.44
1:A:778:VAL:O	1:A:797:LYS:HB2	2.17	0.44
1:B:295:VAL:CB	1:B:414:VAL:HG21	2.48	0.44
1:B:469:TYR:CG	1:B:470:GLU:N	2.84	0.44
1:B:586:LEU:HD13	1:B:590:VAL:HG21	1.99	0.44
1:B:703:LEU:CD2	1:B:790:ILE:CG2	2.95	0.44
1:B:832:THR:HG21	1:B:836:HIS:CB	2.48	0.44
1:A:151:PRO:HB2	1:A:157:HIS:CE1	2.52	0.44
1:A:247:PHE:CD1	1:A:314:LEU:HD22	2.52	0.44
1:A:278:LYS:HD3	1:A:294:GLU:HG2	1.98	0.44
1:A:252:PHE:HD1	1:A:283:CYS:HA	1.82	0.44
1:A:471:THR:HG23	1:A:473:GLN:NE2	2.27	0.44
1:A:564:PRO:HB2	1:A:576:LEU:CD2	2.48	0.44
1:A:567:ILE:HD11	1:A:652:PHE:CD1	2.53	0.44
1:A:892:HIS:CD2	1:A:893:VAL:N	2.85	0.44
1:B:162:VAL:HG21	1:B:187:ALA:HB3	1.99	0.44
1:B:252:PHE:HD1	1:B:283:CYS:HA	1.82	0.44
1:B:305:GLU:HG2	1:B:307:ARG:HG2	1.99	0.44
1:B:291:SER:HB3	1:B:404:CYS:O	2.18	0.44
1:B:458:ARG:HG3	1:B:468:GLN:NE2	2.32	0.44
1:B:53:LEU:HD12	1:B:501:LEU:HG	1.99	0.44
1:B:492:GLN:HG2	1:B:503:ARG:HD2	1.98	0.44
1:B:566:ASN:CB	1:B:651:VAL:CG2	2.95	0.44
1:A:189:ASP:HB3	1:A:191:LYS:HD3	1.99	0.44
1:B:597:LEU:HG	1:B:622:ILE:HG12	1.99	0.44
1:A:291:SER:HB3	1:A:404:CYS:O	2.18	0.44
1:A:566:ASN:CB	1:A:651:VAL:CG2	2.94	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:PRO:HG2	1:A:1022:VAL:HG21	1.94	0.44
1:A:995:PHE:CZ	1:A:998:ARG:HB2	2.52	0.44
1:B:182:LEU:HB2	1:B:203:LEU:HD11	1.99	0.44
1:B:247:PHE:CD1	1:B:314:LEU:HD22	2.52	0.44
1:B:264:SER:HA	1:B:265:PRO:HA	1.53	0.44
1:B:370:LEU:CD2	1:B:374:TYR:HE1	2.27	0.44
1:B:437:TYR:CE2	1:B:439:TYR:HB2	2.51	0.44
1:B:567:ILE:HD11	1:B:652:PHE:CD1	2.53	0.44
1:B:695:LYS:C	1:B:696:LEU:HD12	2.37	0.44
1:B:805:ALA:H	1:B:806:MET:HE3	1.82	0.44
1:A:116:MET:SD	1:A:169:PHE:HA	2.57	0.44
1:A:262:MET:SD	1:A:383:ALA:HB3	2.57	0.44
1:A:541:CYS:HB3	1:A:544:SER:HB3	1.99	0.44
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.31	0.44
1:A:53:LEU:CG	1:A:64:LEU:CD1	2.96	0.44
1:A:889:ILE:CD1	1:A:907:TYR:CZ	3.01	0.44
1:A:958:LEU:HD13	1:A:1033:PHE:CD1	2.53	0.44
1:B:116:MET:SD	1:B:169:PHE:HA	2.57	0.44
1:A:281:ARG:NH1	1:A:366:ILE:HG21	2.33	0.44
1:A:306:TYR:HE1	1:A:351:GLU:HG2	1.83	0.44
1:A:635:GLN:HB3	1:A:644:THR:HB	1.99	0.44
1:A:671:CYS:HB3	1:A:680:CYS:SG	2.57	0.44
1:A:951:MET:HG2	1:A:977:ASN:OD1	2.17	0.44
1:B:179:ASP:O	1:B:180:ASP:HB3	2.17	0.44
1:B:185:ALA:CB	1:B:243:TYR:CD1	3.00	0.44
1:B:262:MET:SD	1:B:383:ALA:HB3	2.58	0.44
1:A:98:ARG:NH2	1:A:107:LEU:HD12	2.29	0.44
1:A:179:ASP:O	1:A:180:ASP:HB3	2.17	0.44
1:A:40:VAL:HG13	1:A:40:VAL:O	2.17	0.44
1:A:421:ILE:HA	1:A:422:PRO:HD2	1.84	0.44
1:A:586:LEU:HD13	1:A:590:VAL:HG21	1.99	0.44
1:A:597:LEU:HG	1:A:622:ILE:HG12	1.99	0.44
1:A:72:LYS:CE	1:A:80:LEU:CD1	2.95	0.44
1:B:117:LEU:HD11	1:B:126:LEU:CD2	2.31	0.44
1:B:119:ILE:HG23	1:B:121:TYR:CE1	2.53	0.44
1:B:173:VAL:O	1:B:173:VAL:HG23	2.18	0.44
1:B:256:LEU:CB	1:B:309:LEU:CD2	2.94	0.44
1:B:281:ARG:NH1	1:B:366:ILE:HG21	2.33	0.44
1:B:676:TYR:CE1	1:B:730:GLN:CD	2.90	0.44
1:B:699:ASP:O	1:B:725:ASN:HB3	2.18	0.44
1:B:62:ILE:CD1	1:B:73:LEU:HD12	2.45	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:O	1:A:127:ILE:HG22	2.17	0.44
1:A:133:TYR:CG	1:A:136:ILE:CG1	2.94	0.44
1:A:162:VAL:HG21	1:A:187:ALA:HB3	1.99	0.44
1:A:217:PHE:CE2	1:A:219:ASP:HB2	2.53	0.44
1:A:889:ILE:HA	1:A:892:HIS:ND1	2.33	0.44
1:B:110:THR:CB	1:B:132:LEU:CD2	2.95	0.44
1:B:274:VAL:HG23	1:B:275:TYR:N	2.30	0.44
1:B:322:GLY:HA2	1:B:327:VAL:HG22	1.99	0.44
1:B:332:ASP:O	1:B:333:LEU:HD23	2.18	0.44
1:B:42:PHE:CZ	1:B:45:GLU:CB	2.95	0.44
1:B:564:PRO:HB2	1:B:576:LEU:CD2	2.48	0.44
1:B:55:VAL:HG22	1:B:62:ILE:HG22	2.00	0.44
1:A:442:HIS:CD2	1:A:458:ARG:HH21	2.35	0.44
1:A:528:TRP:HZ2	1:A:533:ASN:OD1	2.01	0.44
1:A:569:VAL:CG2	1:A:654:ASN:CB	2.65	0.44
1:A:574:VAL:HG22	1:A:613:SER:OG	2.17	0.44
1:A:713:VAL:O	1:A:714:GLU:HB2	2.18	0.44
1:B:358:ILE:CG2	1:B:361:GLN:CB	2.95	0.44
1:B:743:GLN:H	1:B:743:GLN:CD	2.21	0.44
1:B:778:VAL:O	1:B:797:LYS:HB2	2.17	0.44
1:B:863:ILE:HG22	1:B:876:THR:CB	2.35	0.44
1:B:889:ILE:CD1	1:B:907:TYR:CZ	3.01	0.44
1:A:332:ASP:O	1:A:333:LEU:HD23	2.18	0.43
1:A:53:LEU:HD11	1:A:501:LEU:HD11	2.00	0.43
1:A:567:ILE:HD11	1:A:650:PHE:CE2	2.53	0.43
1:A:574:VAL:CG2	1:A:613:SER:HB3	2.48	0.43
1:A:62:ILE:CD1	1:A:73:LEU:HD12	2.45	0.43
1:A:764:THR:CG2	1:A:766:TYR:CZ	3.01	0.43
1:A:874:LYS:H	1:A:982:SER:HB2	1.80	0.43
1:B:189:ASP:HB3	1:B:191:LYS:HD3	1.99	0.43
1:B:306:TYR:HE1	1:B:351:GLU:HG2	1.83	0.43
1:B:53:LEU:HD11	1:B:501:LEU:HD11	2.00	0.43
1:B:711:VAL:HG21	1:B:798:VAL:CG2	2.48	0.43
1:B:841:GLU:HG3	1:B:842:SER:N	2.32	0.43
1:A:711:VAL:HG21	1:A:798:VAL:CG2	2.48	0.43
1:A:832:THR:HG21	1:A:836:HIS:CB	2.48	0.43
1:B:541:CYS:HB3	1:B:544:SER:HB3	1.99	0.43
1:A:119:ILE:HG23	1:A:121:TYR:CE1	2.53	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HG13	2.00	0.43
1:A:589:GLY:C	1:A:639:LYS:HG2	2.39	0.43
1:B:151:PRO:HB2	1:B:157:HIS:CE1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:THR:HG22	1:B:324:THR:O	2.18	0.43
1:B:555:LYS:NZ	1:B:556:GLN:HG2	2.33	0.43
1:B:574:VAL:HG22	1:B:613:SER:OG	2.17	0.43
1:B:764:THR:CG2	1:B:766:TYR:CZ	3.01	0.43
1:B:889:ILE:HA	1:B:892:HIS:ND1	2.33	0.43
1:A:1016:MET:HE2	1:A:1033:PHE:H	1.84	0.43
1:A:1031:LEU:HD22	1:A:1031:LEU:N	2.34	0.43
1:A:1014:LEU:HA	1:A:1035:TYR:HB2	2.00	0.43
1:A:435:ILE:CD1	1:A:486:PHE:HD1	2.31	0.43
1:A:590:VAL:CG1	1:A:591:ASN:N	2.82	0.43
1:A:62:ILE:CD1	1:A:501:LEU:HD13	2.49	0.43
1:A:531:LEU:C	1:A:641:THR:HG1	2.19	0.43
1:A:743:GLN:CD	1:A:743:GLN:H	2.22	0.43
1:A:839:ALA:HB1	1:A:841:GLU:O	2.18	0.43
1:B:296:PRO:HB2	1:B:417:MET:CE	2.48	0.43
1:B:370:LEU:HD12	1:B:399:ILE:HG23	2.00	0.43
1:B:456:LYS:HD3	1:B:523:ASP:OD2	2.10	0.43
1:B:527:GLY:HA3	1:B:550:PHE:HZ	1.72	0.43
1:B:528:TRP:HZ2	1:B:533:ASN:OD1	2.01	0.43
1:B:563:HIS:CB	1:B:577:VAL:CG1	2.95	0.43
1:B:589:GLY:C	1:B:639:LYS:HG2	2.39	0.43
1:A:173:VAL:HG23	1:A:173:VAL:O	2.18	0.43
1:A:224:SER:HA	1:A:289:PHE:CD1	2.54	0.43
1:A:501:LEU:CD2	1:A:502:THR:N	2.81	0.43
1:A:832:THR:CG2	1:A:836:HIS:CB	2.95	0.43
1:B:333:LEU:HD23	1:B:358:ILE:HG13	2.00	0.43
1:B:458:ARG:HB2	1:B:468:GLN:HE22	1.83	0.43
1:B:574:VAL:CG2	1:B:613:SER:HB3	2.48	0.43
1:B:839:ALA:HB1	1:B:841:GLU:O	2.18	0.43
1:A:978:LEU:HD13	1:A:1003:ILE:HG13	2.01	0.43
1:A:100:VAL:HG21	1:A:158:TYR:OH	2.19	0.43
1:A:962:ARG:HD3	1:A:1034:GLN:HE21	1.83	0.43
1:A:128:ALA:O	1:A:138:LYS:HG2	2.19	0.43
1:A:162:VAL:HG12	1:A:164:GLU:H	1.84	0.43
1:A:295:VAL:CB	1:A:414:VAL:HG21	2.48	0.43
1:A:296:PRO:HB2	1:A:417:MET:CE	2.48	0.43
1:A:470:GLU:HG2	1:A:471:THR:N	2.34	0.43
1:A:716:ILE:CD1	1:A:763:ASN:HB3	2.49	0.43
1:B:117:LEU:HG	1:B:126:LEU:HD11	2.01	0.43
1:B:217:PHE:CE2	1:B:219:ASP:HB2	2.53	0.43
1:B:281:ARG:HB3	1:B:293:VAL:HG11	1.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:O	1:B:40:VAL:HG13	2.17	0.43
1:B:435:ILE:CD1	1:B:486:PHE:HD1	2.31	0.43
1:B:440:LYS:HB2	1:B:538:LYS:HZ2	1.84	0.43
1:B:764:THR:HG23	1:B:766:TYR:CZ	2.54	0.43
1:B:95:TYR:HA	1:B:95:TYR:HD1	1.70	0.43
1:A:965:MET:HG3	1:A:1010:SER:O	2.18	0.43
1:A:962:ARG:CB	1:A:1034:GLN:HG3	2.45	0.43
1:A:185:ALA:CB	1:A:243:TYR:CE2	3.02	0.43
1:A:305:GLU:HG2	1:A:307:ARG:HG2	1.99	0.43
1:A:764:THR:HG23	1:A:766:TYR:CZ	2.54	0.43
1:B:119:ILE:HG21	1:B:121:TYR:CE1	2.54	0.43
1:B:460:ASP:CG	1:B:463:LYS:HB3	2.39	0.43
1:B:542:GLU:HG2	1:B:543:ARG:HG3	2.01	0.43
1:B:549:ARG:HD3	1:B:584:PRO:CB	2.48	0.43
1:A:1010:SER:HB2	1:A:1035:TYR:CE1	2.52	0.43
1:A:1016:MET:CE	1:A:1033:PHE:CB	2.94	0.43
1:A:555:LYS:NZ	1:A:556:GLN:HG2	2.33	0.43
1:A:562:VAL:HG22	1:A:578:LEU:HD22	1.98	0.43
1:A:620:PRO:O	1:A:623:ILE:HG13	2.18	0.43
1:A:72:LYS:CD	1:A:80:LEU:CD1	2.97	0.43
1:B:506:VAL:CG2	1:B:525:HIS:CE1	2.81	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HA	2.01	0.43
1:A:62:ILE:CD1	1:A:64:LEU:HD21	2.46	0.43
1:A:789:ASN:HD22	1:A:790:ILE:N	2.17	0.43
1:B:100:VAL:HG21	1:B:158:TYR:OH	2.19	0.43
1:B:234:THR:CG2	1:B:235:VAL:N	2.82	0.43
1:B:358:ILE:HG23	1:B:358:ILE:O	2.18	0.43
1:B:506:VAL:HG21	1:B:525:HIS:NE2	2.22	0.43
1:B:620:PRO:O	1:B:623:ILE:HG13	2.18	0.43
1:B:949:TYR:CE2	1:B:951:MET:HE2	2.53	0.43
1:A:112:ASN:ND2	1:A:133:TYR:HE2	2.17	0.43
1:A:117:LEU:HG	1:A:126:LEU:HD11	2.01	0.43
1:A:186:THR:CG2	1:A:187:ALA:N	2.81	0.43
1:A:281:ARG:HB3	1:A:293:VAL:HG11	1.97	0.43
1:A:617:LYS:HG3	1:A:618:GLU:N	2.34	0.43
1:A:55:VAL:HG22	1:A:62:ILE:HG22	2.00	0.43
1:A:805:ALA:N	1:A:806:MET:CE	2.82	0.43
1:A:885:GLU:HG3	1:A:886:PHE:N	2.34	0.43
1:B:123:GLU:HB2	1:B:125:ARG:HG2	2.01	0.43
1:B:470:GLU:HG2	1:B:471:THR:N	2.34	0.43
1:B:501:LEU:CD2	1:B:502:THR:N	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:LYS:HG3	1:B:618:GLU:N	2.34	0.43
1:B:789:ASN:HD22	1:B:790:ILE:N	2.17	0.43
1:A:665:VAL:HG11	1:A:697:PRO:CD	2.48	0.42
1:A:98:ARG:HE	1:A:107:LEU:HD12	1.83	0.42
1:B:90:ASP:C	1:B:107:LEU:HD22	2.39	0.42
1:B:128:ALA:O	1:B:138:LYS:HG2	2.19	0.42
1:B:62:ILE:CD1	1:B:501:LEU:HD13	2.49	0.42
1:B:713:VAL:O	1:B:714:GLU:HB2	2.18	0.42
1:A:192:PRO:HB3	1:A:233:PHE:CZ	2.51	0.42
1:A:90:ASP:C	1:A:107:LEU:HD22	2.39	0.42
1:A:972:THR:HG23	1:A:1002:TYR:HE1	1.72	0.42
1:B:133:TYR:CB	1:B:136:ILE:HG23	2.49	0.42
1:B:178:PHE:O	1:B:178:PHE:HD1	2.02	0.42
1:B:543:ARG:HB2	1:B:549:ARG:NH1	2.34	0.42
1:B:567:ILE:HD11	1:B:650:PHE:CE2	2.53	0.42
1:B:665:VAL:HG11	1:B:697:PRO:CD	2.48	0.42
1:A:1032:VAL:CG1	1:A:1033:PHE:N	2.82	0.42
1:A:110:THR:HG21	1:A:132:LEU:HD21	1.97	0.42
1:A:458:ARG:HB2	1:A:468:GLN:HE22	1.83	0.42
1:A:541:CYS:HB2	1:A:544:SER:HB3	2.01	0.42
1:A:630:HIS:CD2	1:A:632:VAL:CG2	3.00	0.42
1:A:889:ILE:HG23	1:A:892:HIS:NE2	2.33	0.42
1:B:185:ALA:CB	1:B:243:TYR:CE2	3.02	0.42
1:B:358:ILE:HG23	1:B:361:GLN:N	2.24	0.42
1:B:605:ILE:O	1:B:608:GLN:HG2	2.20	0.42
1:B:689:PHE:HD1	1:B:691:GLU:HG2	1.80	0.42
1:A:1029:GLN:CG	1:A:1030:ASP:N	2.83	0.42
1:A:119:ILE:HG21	1:A:121:TYR:CE1	2.54	0.42
1:A:225:MET:CE	1:A:227:LYS:CG	2.94	0.42
1:A:370:LEU:HD12	1:A:399:ILE:HG23	2.00	0.42
1:A:471:THR:HG21	1:A:473:GLN:OE1	2.19	0.42
1:A:567:ILE:CD1	1:A:567:ILE:N	2.82	0.42
1:A:710:LEU:HD12	1:A:710:LEU:C	2.40	0.42
1:A:865:VAL:CG1	1:A:866:THR:N	2.82	0.42
1:A:953:LEU:HD12	1:A:978:LEU:HD23	2.01	0.42
1:A:868:PRO:CD	1:A:981:GLY:HA2	1.99	0.42
1:B:224:SER:HA	1:B:289:PHE:CD1	2.54	0.42
1:B:662:LEU:HD23	1:B:791:ASP:CB	2.48	0.42
1:A:962:ARG:HD3	1:A:1034:GLN:NE2	2.34	0.42
1:A:169:PHE:CD2	1:A:170:GLY:N	2.84	0.42
1:A:178:PHE:O	1:A:178:PHE:HD1	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HG23	1:A:361:GLN:N	2.24	0.42
1:A:358:ILE:HG23	1:A:358:ILE:O	2.18	0.42
1:A:955:LEU:CG	1:A:973:ILE:CG2	2.95	0.42
1:B:216:VAL:CG1	1:B:217:PHE:N	2.82	0.42
1:B:333:LEU:HD23	1:B:358:ILE:HA	2.01	0.42
1:B:567:ILE:N	1:B:567:ILE:CD1	2.82	0.42
1:B:590:VAL:CG1	1:B:591:ASN:N	2.82	0.42
1:B:759:VAL:CG1	1:B:760:GLN:N	2.81	0.42
1:B:885:GLU:HG3	1:B:886:PHE:N	2.34	0.42
1:B:889:ILE:HG23	1:B:892:HIS:NE2	2.33	0.42
1:A:1007:THR:HG22	1:A:1008:THR:N	2.33	0.42
1:A:123:GLU:HB2	1:A:125:ARG:HG2	2.01	0.42
1:A:460:ASP:CG	1:A:463:LYS:HB3	2.39	0.42
1:A:435:ILE:HG21	1:A:486:PHE:HE1	1.81	0.42
1:A:543:ARG:HB2	1:A:549:ARG:NH1	2.34	0.42
1:A:959:LYS:HG2	1:A:972:THR:HG21	2.01	0.42
1:B:112:ASN:ND2	1:B:133:TYR:HE2	2.17	0.42
1:B:186:THR:CG2	1:B:187:ALA:N	2.81	0.42
1:B:471:THR:HG21	1:B:473:GLN:OE1	2.19	0.42
1:B:68:ASN:CB	1:B:86:GLY:HA3	2.50	0.42
1:A:256:LEU:CB	1:A:309:LEU:CD2	2.94	0.42
1:A:549:ARG:CD	1:A:584:PRO:HB3	2.42	0.42
1:A:830:GLN:CG	1:A:831:CYS:H	2.24	0.42
1:B:321:LEU:HD23	1:B:333:LEU:CD1	2.50	0.42
1:A:542:GLU:HG2	1:A:543:ARG:HG3	2.00	0.42
1:A:845:LEU:HD11	1:A:852:SER:OG	2.20	0.42
1:B:458:ARG:HD2	1:B:524:PRO:CB	2.31	0.42
1:B:437:TYR:HH	1:B:525:HIS:CD2	2.37	0.42
1:B:653:TYR:CZ	1:B:682:HIS:CE1	3.07	0.42
1:B:700:CYS:HA	1:B:701:PRO:HD3	1.45	0.42
1:A:234:THR:CG2	1:A:235:VAL:N	2.82	0.42
1:A:324:THR:HG22	1:A:324:THR:O	2.18	0.42
1:A:370:LEU:CD2	1:A:374:TYR:HE1	2.28	0.42
1:A:562:VAL:HG22	1:A:578:LEU:HD23	1.99	0.42
1:A:566:ASN:CA	1:A:651:VAL:CG2	2.95	0.42
1:A:783:VAL:CG1	1:A:784:TRP:N	2.83	0.42
1:B:446:PHE:CB	1:B:454:LEU:HD11	2.43	0.42
1:B:562:VAL:HG22	1:B:578:LEU:HD23	1.99	0.42
1:B:563:HIS:HB2	1:B:577:VAL:HG13	2.01	0.42
1:A:380:LEU:HD22	1:A:412:LEU:HB3	2.02	0.42
1:A:662:LEU:O	1:A:666:GLU:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:CD1	1:A:73:LEU:HB2	2.47	0.42
1:A:888:ASP:OD1	1:A:889:ILE:HG13	2.20	0.42
1:A:920:ALA:C	1:A:922:PRO:HD2	2.41	0.42
1:B:39:PHE:CZ	1:B:473:GLN:HG3	2.53	0.42
1:B:528:TRP:CZ2	1:B:533:ASN:OD1	2.73	0.42
1:B:783:VAL:CG1	1:B:784:TRP:N	2.83	0.42
1:B:926:ALA:HB2	1:B:949:TYR:CD1	2.55	0.42
1:A:412:LEU:CD1	1:A:412:LEU:N	2.83	0.41
1:A:440:LYS:HD2	1:A:538:LYS:HD2	1.93	0.41
1:A:605:ILE:O	1:A:608:GLN:HG2	2.19	0.41
1:A:67:VAL:CG1	1:A:111:ASN:HB3	2.50	0.41
1:B:162:VAL:HG12	1:B:164:GLU:H	1.84	0.41
1:B:177:ASN:O	1:B:178:PHE:CG	2.73	0.41
1:B:256:LEU:HD12	1:B:297:ILE:HD11	2.02	0.41
1:B:575:LEU:N	1:B:575:LEU:CD2	2.83	0.41
1:B:623:ILE:HD12	1:B:624:THR:HA	2.02	0.41
1:B:64:LEU:HD12	1:B:496:MET:HE3	1.98	0.41
1:B:817:ASP:OD1	1:B:820:PHE:CD2	2.73	0.41
1:A:216:VAL:CG1	1:A:217:PHE:N	2.82	0.41
1:A:44:GLY:O	1:A:47:ALA:HA	2.20	0.41
1:A:440:LYS:HB3	1:A:538:LYS:HZ3	1.79	0.41
1:A:817:ASP:OD1	1:A:820:PHE:CD2	2.73	0.41
1:A:68:ASN:CB	1:A:86:GLY:HA3	2.50	0.41
1:A:959:LYS:CG	1:A:972:THR:CB	2.97	0.41
1:B:159:LEU:HG	1:B:201:ARG:NH1	2.35	0.41
1:B:403:PHE:CE2	1:B:405:GLY:HA2	2.55	0.41
1:B:492:GLN:HB3	1:B:503:ARG:HG3	2.02	0.41
1:B:728:GLN:HG3	1:B:753:ARG:NH2	2.35	0.41
1:B:716:ILE:CD1	1:B:763:ASN:HB3	2.49	0.41
1:B:72:LYS:CE	1:B:80:LEU:CD1	2.95	0.41
1:A:1016:MET:HE2	1:A:1033:PHE:CB	2.49	0.41
1:A:177:ASN:O	1:A:178:PHE:CG	2.73	0.41
1:A:387:VAL:CG1	1:A:388:LYS:N	2.82	0.41
1:A:446:PHE:CD1	1:A:446:PHE:N	2.88	0.41
1:A:569:VAL:HB	1:A:654:ASN:CG	2.41	0.41
1:A:728:GLN:HG3	1:A:753:ARG:NH2	2.35	0.41
1:B:412:LEU:N	1:B:412:LEU:CD1	2.83	0.41
1:B:444:LEU:HD23	1:B:524:PRO:HG2	1.91	0.41
1:B:619:VAL:HB	1:B:620:PRO:CD	2.47	0.41
1:B:865:VAL:CG1	1:B:866:THR:N	2.82	0.41
1:A:111:ASN:O	1:A:132:LEU:HD13	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:VAL:HG22	1:A:188:VAL:O	2.21	0.41
1:A:307:ARG:HA	1:A:307:ARG:HD3	1.88	0.41
1:A:349:LEU:CD2	1:A:349:LEU:N	2.84	0.41
1:A:403:PHE:CE2	1:A:405:GLY:HA2	2.55	0.41
1:A:563:HIS:HB2	1:A:577:VAL:HG13	2.01	0.41
1:A:631:VAL:HG13	1:A:631:VAL:O	2.19	0.41
1:A:711:VAL:HB	1:A:800:LEU:HD23	2.02	0.41
1:A:926:ALA:HB2	1:A:949:TYR:CD1	2.55	0.41
1:A:978:LEU:HA	1:A:978:LEU:HD23	1.93	0.41
1:B:110:THR:HG21	1:B:132:LEU:HD21	1.97	0.41
1:B:225:MET:CE	1:B:227:LYS:CG	2.94	0.41
1:B:446:PHE:CD1	1:B:446:PHE:N	2.89	0.41
1:B:562:VAL:HG22	1:B:578:LEU:HD22	1.98	0.41
1:B:679:VAL:CG1	1:B:680:CYS:N	2.82	0.41
1:B:862:ILE:HG21	1:B:877:ILE:HG12	2.03	0.41
1:B:920:ALA:C	1:B:922:PRO:HD2	2.40	0.41
1:A:988:PHE:CB	1:A:1016:MET:SD	3.06	0.41
1:A:1031:LEU:H	1:A:1031:LEU:HD22	1.84	0.41
1:A:133:TYR:CB	1:A:136:ILE:HG23	2.49	0.41
1:A:159:LEU:HG	1:A:201:ARG:NH1	2.36	0.41
1:A:226:ILE:HD11	1:A:385:LEU:HD23	2.03	0.41
1:A:531:LEU:HA	1:A:531:LEU:HD23	1.91	0.41
1:B:137:CYS:SG	1:B:159:LEU:CD1	3.09	0.41
1:B:280:VAL:CG1	1:B:281:ARG:N	2.83	0.41
1:B:380:LEU:HD22	1:B:412:LEU:HB3	2.02	0.41
1:B:631:VAL:HG13	1:B:631:VAL:O	2.19	0.41
1:B:803:CYS:SG	1:B:832:THR:HA	2.61	0.41
1:B:949:TYR:CE2	1:B:951:MET:HE1	2.55	0.41
1:A:446:PHE:CB	1:A:454:LEU:HD11	2.43	0.41
1:A:703:LEU:HD13	1:A:723:ALA:CB	2.47	0.41
1:A:862:ILE:HG21	1:A:877:ILE:HG12	2.03	0.41
1:A:958:LEU:HD22	1:A:960:PRO:N	2.35	0.41
1:A:959:LYS:CG	1:A:972:THR:HG21	2.51	0.41
1:B:185:ALA:HB3	1:B:243:TYR:CD2	2.56	0.41
1:B:444:LEU:HD12	1:B:446:PHE:CD1	2.51	0.41
1:B:444:LEU:HD13	1:B:445:ALA:H	1.79	0.41
1:B:453:LYS:CE	1:B:472:VAL:HG22	2.51	0.41
1:B:506:VAL:CG1	1:B:507:GLU:N	2.84	0.41
1:B:541:CYS:HB2	1:B:544:SER:HB3	2.01	0.41
1:B:551:ALA:HB1	1:B:556:GLN:HB2	2.03	0.41
1:B:778:VAL:HG12	1:B:779:GLU:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:ALA:N	1:B:806:MET:CE	2.82	0.41
1:B:888:ASP:OD1	1:B:889:ILE:HG13	2.20	0.41
1:A:380:LEU:CB	1:A:386:LYS:CE	2.95	0.41
1:A:492:GLN:HB3	1:A:503:ARG:HG3	2.02	0.41
1:A:679:VAL:CG1	1:A:680:CYS:N	2.82	0.41
1:A:759:VAL:CG1	1:A:760:GLN:N	2.81	0.41
1:A:95:TYR:CG	1:A:96:PRO:CD	3.03	0.41
1:B:137:CYS:O	1:B:150:GLU:HG3	2.20	0.41
1:B:387:VAL:CG1	1:B:388:LYS:N	2.82	0.41
1:B:44:GLY:O	1:B:47:ALA:HA	2.20	0.41
1:B:658:HIS:ND1	1:B:663:SER:HB3	2.36	0.41
1:B:67:VAL:CG1	1:B:111:ASN:HB3	2.50	0.41
1:A:972:THR:CG2	1:A:1002:TYR:CE1	2.93	0.41
1:A:988:PHE:CD2	1:A:1016:MET:SD	3.12	0.41
1:A:137:CYS:O	1:A:150:GLU:HG3	2.20	0.41
1:A:185:ALA:HB3	1:A:243:TYR:CD2	2.56	0.41
1:A:188:VAL:CG2	1:A:191:LYS:HB2	2.51	0.41
1:A:280:VAL:CG1	1:A:281:ARG:N	2.83	0.41
1:B:492:GLN:CG	1:B:503:ARG:HD2	2.51	0.41
1:B:95:TYR:CG	1:B:96:PRO:CD	3.03	0.41
1:A:137:CYS:SG	1:A:159:LEU:CD1	3.09	0.41
1:A:236:ILE:CG2	1:A:239:PHE:HB2	2.51	0.41
1:A:480:VAL:HB	1:A:484:MET:HE2	2.01	0.41
1:A:492:GLN:CG	1:A:503:ARG:HD2	2.51	0.41
1:A:528:TRP:CZ2	1:A:533:ASN:OD1	2.73	0.41
1:B:188:VAL:CG2	1:B:191:LYS:HB2	2.51	0.41
1:B:226:ILE:HD11	1:B:385:LEU:HD23	2.03	0.41
1:B:239:PHE:CD1	1:B:260:PRO:CD	3.03	0.41
1:B:696:LEU:HA	1:B:697:PRO:HD3	1.87	0.41
1:B:710:LEU:C	1:B:710:LEU:HD12	2.40	0.41
1:B:832:THR:HG21	1:B:836:HIS:HB2	1.99	0.41
1:B:843:ARG:CZ	1:B:843:ARG:CB	2.99	0.41
1:A:117:LEU:HD11	1:A:126:LEU:CD2	2.31	0.41
1:A:619:VAL:HB	1:A:620:PRO:CD	2.47	0.41
1:A:623:ILE:HD12	1:A:624:THR:HA	2.01	0.41
1:A:953:LEU:HA	1:A:977:ASN:HB2	2.02	0.41
1:A:959:LYS:HG2	1:A:972:THR:HB	2.02	0.41
1:B:111:ASN:O	1:B:132:LEU:HD13	2.20	0.41
1:B:236:ILE:CG2	1:B:239:PHE:HB2	2.51	0.41
1:B:349:LEU:CD2	1:B:349:LEU:N	2.84	0.41
1:B:560:LEU:CG	1:B:648:THR:CG2	2.98	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ASP:HA	1:B:684:PRO:HD3	1.83	0.41
1:B:703:LEU:HD13	1:B:723:ALA:CB	2.47	0.41
1:B:901:SER:HA	1:B:902:PRO:HD2	1.89	0.41
1:A:111:ASN:O	1:A:132:LEU:HD22	2.21	0.41
1:A:95:TYR:CE2	1:A:194:TYR:CD1	3.09	0.41
1:A:252:PHE:HE1	1:A:283:CYS:SG	2.44	0.41
1:A:256:LEU:HD12	1:A:297:ILE:HD11	2.01	0.41
1:A:321:LEU:HD23	1:A:333:LEU:CD1	2.50	0.41
1:A:551:ALA:HB1	1:A:556:GLN:HB2	2.03	0.41
1:A:560:LEU:CG	1:A:648:THR:CG2	2.98	0.41
1:A:658:HIS:ND1	1:A:663:SER:HB3	2.36	0.41
1:A:778:VAL:HG12	1:A:779:GLU:O	2.20	0.41
1:A:832:THR:HG21	1:A:836:HIS:HB2	1.99	0.41
1:B:469:TYR:CZ	1:B:470:GLU:O	2.74	0.41
1:B:560:LEU:HB3	1:B:648:THR:CG2	2.51	0.41
1:B:711:VAL:HB	1:B:800:LEU:HD23	2.02	0.41
1:A:313:TYR:CZ	1:A:435:ILE:CD1	3.05	0.40
1:B:141:ARG:HB3	1:B:144:ASP:OD1	2.21	0.40
1:B:188:VAL:HG22	1:B:188:VAL:O	2.21	0.40
1:B:667:SER:HB3	1:B:668:PRO:CD	2.51	0.40
1:B:832:THR:CG2	1:B:836:HIS:CB	2.95	0.40
1:A:185:ALA:CB	1:A:243:TYR:CD1	3.00	0.40
1:A:45:GLU:CB	1:A:46:PRO:CD	3.00	0.40
1:A:469:TYR:CZ	1:A:470:GLU:O	2.74	0.40
1:A:667:SER:HB3	1:A:668:PRO:CD	2.51	0.40
1:A:873:THR:OG1	1:A:981:GLY:C	2.59	0.40
1:A:955:LEU:HD23	1:A:957:ASP:N	2.37	0.40
1:B:169:PHE:CD2	1:B:170:GLY:N	2.84	0.40
1:B:219:ASP:HB3	1:B:222:VAL:H	1.86	0.40
1:B:242:TYR:CE1	1:B:345:LYS:HE2	2.56	0.40
1:B:44:GLY:CA	1:B:50:PHE:HE2	2.23	0.40
1:A:131:SER:O	1:A:133:TYR:CD2	2.74	0.40
1:A:453:LYS:CE	1:A:472:VAL:HG22	2.51	0.40
1:A:527:GLY:HA3	1:A:550:PHE:HZ	1.72	0.40
1:B:172:ILE:CG1	1:B:182:LEU:HD13	2.46	0.40
1:B:95:TYR:CE2	1:B:194:TYR:CD1	3.09	0.40
1:B:282:LEU:HD23	1:B:292:TYR:HA	2.03	0.40
1:B:450:LYS:CA	1:B:479:PRO:HB3	2.49	0.40
1:B:62:ILE:CD1	1:B:64:LEU:HD21	2.46	0.40
1:B:662:LEU:O	1:B:666:GLU:HB3	2.20	0.40
1:A:188:VAL:HG13	1:A:189:ASP:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASP:HB3	1:A:222:VAL:H	1.86	0.40
1:A:259:GLN:HA	1:A:260:PRO:HD3	1.82	0.40
1:A:276:THR:HB	1:A:278:LYS:HZ2	1.86	0.40
1:A:455:LYS:HB3	1:A:467:LEU:CD1	2.52	0.40
1:A:773:ILE:N	1:A:773:ILE:CD1	2.82	0.40
1:A:803:CYS:SG	1:A:832:THR:HA	2.61	0.40
1:A:904:VAL:CG1	1:A:905:ASP:N	2.82	0.40
1:A:896:ALA:HB1	1:A:924:GLN:OE1	2.22	0.40
1:B:313:TYR:CZ	1:B:435:ILE:CD1	3.04	0.40
1:B:410:ALA:CB	1:B:411:PRO:CD	2.98	0.40
1:B:660:SER:HB2	1:B:791:ASP:OD2	2.22	0.40
1:B:904:VAL:CG1	1:B:905:ASP:N	2.82	0.40
1:A:282:LEU:HD23	1:A:292:TYR:HA	2.03	0.40
1:A:242:TYR:CE1	1:A:345:LYS:HE2	2.56	0.40
1:A:847:LEU:CD1	1:A:850:ALA:CA	2.94	0.40
1:A:943:ARG:HB2	1:A:943:ARG:CZ	2.51	0.40
1:B:131:SER:O	1:B:133:TYR:CD2	2.74	0.40
1:B:53:LEU:CG	1:B:64:LEU:CD1	2.96	0.40
1:B:681:THR:OG1	1:B:686:THR:HG21	2.21	0.40
1:B:81:VAL:CG1	1:B:82:THR:N	2.85	0.40
1:B:889:ILE:HD12	1:B:907:TYR:CE1	2.56	0.40
1:B:943:ARG:CZ	1:B:943:ARG:HB2	2.51	0.40

All (61) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:CE1	1:B:730:GLN:CD[1_655]	0.64	1.56
1:B:287:THR:OG1	1:B:840:HIS:CG[1_655]	0.67	1.53
1:A:146:PHE:CE1	1:B:730:GLN:OE1[1_655]	0.77	1.43
1:A:146:PHE:CD1	1:B:730:GLN:OE1[1_655]	0.78	1.42
1:B:287:THR:CA	1:B:840:HIS:NE2[1_655]	0.79	1.41
1:B:287:THR:CB	1:B:840:HIS:CG[1_655]	0.85	1.35
1:B:287:THR:CB	1:B:840:HIS:CD2[1_655]	0.93	1.27
1:B:287:THR:CA	1:B:840:HIS:CD2[1_655]	1.03	1.17
1:A:146:PHE:CZ	1:B:730:GLN:NE2[1_655]	1.20	1.00
1:B:287:THR:OG1	1:B:840:HIS:ND1[1_655]	1.52	0.68
1:A:407:ASP:OD2	1:A:926:ALA:O[1_554]	1.55	0.65
1:B:220:GLU:OE2	1:B:939:GLU:OE1[1_655]	1.56	0.64
1:A:148:LEU:O	1:B:728:GLN:OE1[1_655]	1.56	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:OG1	1:B:840:HIS:CB[1_655]	1.58	0.62
1:B:287:THR:OG1	1:B:840:HIS:CD2[1_655]	1.61	0.59
1:A:83:HIS:CE1	1:B:731:SER:OG[1_655]	1.62	0.58
1:B:219:ASP:OD1	1:B:826:GLN:OE1[1_655]	1.68	0.52
1:B:288:ALA:CB	1:B:841:GLU:OE1[1_655]	1.71	0.49
1:B:287:THR:CA	1:B:840:HIS:CE1[1_655]	1.74	0.46
1:A:146:PHE:CE1	1:B:730:GLN:CG[1_655]	1.75	0.45
1:A:146:PHE:CZ	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:A:146:PHE:CG	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:B:287:THR:CG2	1:B:840:HIS:CD2[1_655]	1.77	0.43
1:B:287:THR:CG2	1:B:840:HIS:C[1_655]	1.78	0.42
1:A:728:GLN:OE1	1:B:148:LEU:O[2_646]	1.83	0.37
1:A:730:GLN:OE1	1:B:146:PHE:CE1[2_646]	1.84	0.36
1:A:731:SER:OG	1:B:83:HIS:ND1[2_646]	1.85	0.35
1:B:219:ASP:OD1	1:B:826:GLN:CG[1_655]	1.86	0.34
1:A:146:PHE:CE1	1:B:730:GLN:NE2[1_655]	1.88	0.32
1:A:728:GLN:NE2	1:B:148:LEU:O[2_646]	1.89	0.31
1:B:217:PHE:CD1	1:B:827:SER:OG[1_655]	1.90	0.30
1:A:752:LEU:CD2	1:B:152:PHE:CE1[2_646]	1.91	0.29
1:B:287:THR:CB	1:B:840:HIS:CB[1_655]	1.91	0.29
1:B:287:THR:CB	1:B:840:HIS:ND1[1_655]	1.92	0.28
1:B:217:PHE:CE1	1:B:827:SER:OG[1_655]	1.93	0.27
1:A:208:GLU:OE2	1:B:728:GLN:NE2[1_655]	1.93	0.27
1:A:146:PHE:CD1	1:B:730:GLN:CD[1_655]	1.94	0.26
1:B:220:GLU:OE2	1:B:939:GLU:CD[1_655]	1.96	0.24
1:B:287:THR:N	1:B:840:HIS:NE2[1_655]	1.98	0.22
1:A:148:LEU:O	1:B:728:GLN:CD[1_655]	1.99	0.21
1:B:220:GLU:OE1	1:B:939:GLU:OE2[1_655]	2.00	0.20
1:B:287:THR:CA	1:B:840:HIS:CG[1_655]	2.01	0.19
1:A:730:GLN:NE2	1:B:146:PHE:CZ[2_646]	2.01	0.19
1:B:219:ASP:OD2	1:B:826:GLN:OE1[1_655]	2.01	0.19
1:B:287:THR:CB	1:B:840:HIS:NE2[1_655]	2.01	0.19
1:B:219:ASP:CG	1:B:826:GLN:OE1[1_655]	2.03	0.17
1:A:731:SER:OG	1:B:83:HIS:NE2[2_646]	2.03	0.17
1:B:219:ASP:CG	1:B:826:GLN:CD[1_655]	2.04	0.16
1:B:287:THR:O	1:B:840:HIS:NE2[1_655]	2.05	0.15
1:A:141:ARG:NH2	1:B:691:GLU:OE2[1_655]	2.06	0.14
1:A:208:GLU:OE2	1:B:728:GLN:CD[1_655]	2.08	0.12
1:A:728:GLN:CD	1:B:148:LEU:O[2_646]	2.09	0.11
1:B:287:THR:CG2	1:B:840:HIS:O[1_655]	2.09	0.11
1:A:407:ASP:OD1	1:A:924:GLN:OE1[1_554]	2.11	0.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:GLN:CD	1:B:146:PHE:CD1[2_646]	2.11	0.09
1:B:287:THR:CG2	1:B:840:HIS:CG[1_655]	2.12	0.08
1:B:287:THR:CG2	1:B:841:GLU:N[1_655]	2.13	0.07
1:A:208:GLU:OE1	1:B:753:ARG:NH2[1_655]	2.15	0.05
1:B:219:ASP:OD2	1:B:826:GLN:NE2[1_655]	2.16	0.04
1:A:728:GLN:OE1	1:B:148:LEU:C[2_646]	2.18	0.02
1:A:728:GLN:OE1	1:B:149:GLY:CA[2_646]	2.19	0.01

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	994/1207 (82%)	923 (93%)	51 (5%)	20 (2%)	9	46
1	B	907/1207 (75%)	845 (93%)	43 (5%)	19 (2%)	8	45
All	All	1901/2414 (79%)	1768 (93%)	94 (5%)	39 (2%)	8	45

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN
1	A	804	GLY
1	A	864	PRO
1	B	96	PRO
1	B	181	LYS
1	B	191	LYS
1	B	410	ALA
1	B	465	ASN
1	B	557	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	700	CYS
1	B	701	PRO
1	B	804	GLY
1	B	864	PRO
1	A	87	PRO
1	B	87	PRO
1	A	271	LYS
1	A	474	VAL
1	A	557	CYS
1	A	849	GLY
1	A	1015	ASP
1	A	1016	MET
1	B	271	LYS
1	B	474	VAL
1	B	849	GLY
1	A	263	VAL
1	B	263	VAL
1	A	344	ARG
1	B	344	ARG
1	A	933	VAL
1	A	1013	VAL
1	B	933	VAL
1	A	44	GLY
1	A	921	LYS
1	B	921	LYS
1	B	44	GLY

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	888/1067 (83%)	861 (97%)	27 (3%)	46	72
1	B	812/1067 (76%)	789 (97%)	23 (3%)	49	74
All	All	1700/2134 (80%)	1650 (97%)	50 (3%)	48	73

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	72	LYS
1	A	271	LYS
1	A	386	LYS
1	A	412	LEU
1	A	435	ILE
1	A	468	GLN
1	A	473	GLN
1	A	523	ASP
1	A	529	CYS
1	A	548	ARG
1	A	567	ILE
1	A	575	LEU
1	A	597	LEU
1	A	621	ARG
1	A	670	ARG
1	A	743	GLN
1	A	773	ILE
1	A	797	LYS
1	A	806	MET
1	A	853	LYS
1	A	854	CYS
1	A	892	HIS
1	A	1004	ILE
1	A	1016	MET
1	A	1017	LYS
1	A	1024	ARG
1	B	69	ARG
1	B	72	LYS
1	B	271	LYS
1	B	386	LYS
1	B	412	LEU
1	B	435	ILE
1	B	468	GLN
1	B	473	GLN
1	B	523	ASP
1	B	529	CYS
1	B	548	ARG
1	B	567	ILE
1	B	575	LEU
1	B	597	LEU
1	B	621	ARG
1	B	670	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	743	GLN
1	B	773	ILE
1	B	797	LYS
1	B	806	MET
1	B	853	LYS
1	B	854	CYS
1	B	892	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	101	GLN
1	A	157	HIS
1	A	163	ASN
1	A	273	GLN
1	A	361	GLN
1	A	441	ASN
1	A	442	HIS
1	A	473	GLN
1	A	500	GLN
1	A	533	ASN
1	A	626	ASN
1	A	630	HIS
1	A	672	HIS
1	A	685	ASN
1	A	690	GLN
1	A	702	GLN
1	A	728	GLN
1	A	747	GLN
1	A	789	ASN
1	A	792	ASN
1	A	826	GLN
1	A	836	HIS
1	A	892	HIS
1	A	970	GLN
1	A	983	ASN
1	A	1006	ASN
1	B	51	ASN
1	B	101	GLN
1	B	157	HIS
1	B	163	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	273	GLN
1	B	361	GLN
1	B	441	ASN
1	B	442	HIS
1	B	473	GLN
1	B	500	GLN
1	B	626	ASN
1	B	629	HIS
1	B	630	HIS
1	B	672	HIS
1	B	682	HIS
1	B	685	ASN
1	B	690	GLN
1	B	702	GLN
1	B	728	GLN
1	B	730	GLN
1	B	747	GLN
1	B	789	ASN
1	B	792	ASN
1	B	826	GLN
1	B	836	HIS
1	B	892	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	854:CYS	C	855:THR	N	2.49
1	A	802:LYS	C	803:CYS	N	2.46
1	A	951:MET	C	952:THR	N	2.32
1	B	653:TYR	C	654:ASN	N	2.31
1	B	802:LYS	C	803:CYS	N	2.01
1	A	506:VAL	C	507:GLU	N	1.87
1	B	506:VAL	C	507:GLU	N	1.82
1	B	700:CYS	C	701:PRO	N	1.63
1	A	700:CYS	C	701:PRO	N	1.04
1	B	557:CYS	C	558:VAL	N	0.94
1	A	557:CYS	C	558:VAL	N	0.86

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	1000/1207 (82%)	2.00	397 (39%) 0 5	195, 258, 410, 410	0
1	B	915/1207 (75%)	1.81	329 (35%) 0 5	209, 257, 329, 329	0
All	All	1915/2414 (79%)	1.91	726 (37%) 0 5	195, 257, 329, 410	0

All (726) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1029	GLN	16.5
1	A	269	THR	16.3
1	A	1018	VAL	14.5
1	A	270	THR	13.8
1	A	271	LYS	13.1
1	B	852	SER	12.9
1	A	268	SER	11.8
1	B	922	PRO	11.1
1	A	854	CYS	10.8
1	A	1031	LEU	10.4
1	A	1019	THR	10.3
1	A	1027	ILE	10.1
1	A	1020	VAL	10.0
1	B	854	CYS	9.7
1	A	1028	ARG	9.2
1	B	921	LYS	9.1
1	A	953	LEU	8.9
1	B	583	VAL	8.7
1	A	506	VAL	8.6
1	B	850	ALA	8.6
1	B	645	PHE	8.4
1	A	842	SER	8.4
1	B	923	SER	8.2
1	A	525	HIS	8.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	924	GLN	8.0
1	B	926	ALA	8.0
1	B	919	GLU	7.9
1	B	636	LEU	7.8
1	A	272	GLU	7.8
1	B	584	PRO	7.7
1	A	505	PRO	7.5
1	A	727	PRO	7.5
1	B	585	GLU	7.4
1	B	920	ALA	7.4
1	B	637	LYS	7.4
1	B	592	CYS	7.3
1	A	507	GLU	7.3
1	A	267	GLY	7.3
1	B	586	LEU	7.1
1	B	925	HIS	7.0
1	B	644	THR	7.0
1	B	851	ASN	6.9
1	A	952	THR	6.7
1	B	849	GLY	6.7
1	A	883	GLY	6.7
1	A	524	PRO	6.6
1	A	250	GLY	6.6
1	B	853	LYS	6.4
1	A	955	LEU	6.4
1	B	638	SER	6.4
1	B	720	THR	6.4
1	A	273	GLN	6.3
1	B	437	TYR	6.3
1	A	1017	LYS	6.2
1	A	881	ASN	6.1
1	A	645	PHE	6.1
1	B	412	LEU	6.1
1	B	604	VAL	6.0
1	B	622	ILE	6.0
1	B	640	GLU	6.0
1	B	591	ASN	6.0
1	A	590	VAL	5.9
1	B	862	ILE	5.9
1	A	882	LEU	5.9
1	B	589	GLY	5.9
1	B	568	SER	5.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	523	ASP	5.8
1	B	269	THR	5.8
1	A	988	PHE	5.8
1	A	1032	VAL	5.8
1	A	240	ASP	5.7
1	B	918	GLY	5.7
1	A	694	VAL	5.7
1	A	811	GLY	5.6
1	A	1030	ASP	5.6
1	B	884	LEU	5.6
1	B	646	ALA	5.6
1	B	650	PHE	5.6
1	A	853	LYS	5.6
1	B	870	GLU	5.6
1	B	847	LEU	5.6
1	B	548	ARG	5.6
1	B	590	VAL	5.6
1	B	814	LEU	5.5
1	A	238	ASP	5.5
1	A	986	VAL	5.5
1	B	803	CYS	5.5
1	A	927	GLY	5.5
1	A	1021	GLN	5.4
1	A	961	ASN	5.4
1	B	652	PHE	5.4
1	B	883	GLY	5.4
1	A	957	ASP	5.4
1	B	947	LEU	5.4
1	B	711	VAL	5.3
1	B	710	LEU	5.3
1	B	271	LYS	5.3
1	B	721	LEU	5.3
1	B	871	GLY	5.3
1	B	587	SER	5.3
1	A	249	SER	5.2
1	B	712	PRO	5.2
1	A	646	ALA	5.2
1	B	872	GLY	5.2
1	B	948	TYR	5.2
1	B	873	THR	5.2
1	A	852	SER	5.2
1	A	855	THR	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	268	SER	5.1
1	B	719	ILE	5.1
1	A	569	VAL	5.1
1	A	1033	PHE	5.1
1	B	917	MET	5.1
1	B	634	LEU	5.0
1	B	875	VAL	5.0
1	A	652	PHE	5.0
1	B	594	PHE	5.0
1	B	709	ILE	5.0
1	B	877	ILE	5.0
1	B	580	THR	4.9
1	B	869	ARG	4.9
1	A	960	PRO	4.9
1	B	571	GLN	4.9
1	B	801	TYR	4.9
1	B	767	SER	4.9
1	B	272	GLU	4.9
1	B	582	ASN	4.9
1	A	879	GLY	4.9
1	A	458	ARG	4.9
1	A	958	LEU	4.9
1	A	1026	ARG	4.9
1	B	613	SER	4.9
1	B	868	PRO	4.9
1	A	410	ALA	4.8
1	A	922	PRO	4.8
1	A	589	GLY	4.8
1	A	984	VAL	4.8
1	A	678	HIS	4.8
1	A	920	ALA	4.8
1	B	898	VAL	4.8
1	A	747	GLN	4.8
1	A	956	ALA	4.8
1	A	437	TYR	4.8
1	B	270	THR	4.8
1	B	413	GLY	4.8
1	B	950	PHE	4.8
1	A	810	CYS	4.8
1	A	963	GLY	4.7
1	A	508	SER	4.7
1	B	619	VAL	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1036	VAL	4.7
1	A	962	ARG	4.7
1	A	814	LEU	4.7
1	A	898	VAL	4.7
1	A	951	MET	4.7
1	A	868	PRO	4.7
1	B	558	VAL	4.7
1	A	973	ILE	4.7
1	B	802	LYS	4.7
1	A	526	CYS	4.7
1	A	989	GLY	4.7
1	A	1016	MET	4.7
1	B	864	PRO	4.7
1	B	766	TYR	4.6
1	A	530	VAL	4.6
1	B	882	LEU	4.6
1	A	980	ALA	4.6
1	B	774	ASN	4.6
1	A	977	ASN	4.6
1	A	1022	VAL	4.6
1	A	803	CYS	4.6
1	B	927	GLY	4.5
1	A	251	ASN	4.5
1	B	614	PRO	4.5
1	A	676	TYR	4.5
1	B	161	GLY	4.5
1	B	525	HIS	4.5
1	A	897	GLY	4.5
1	B	567	ILE	4.5
1	B	800	LEU	4.5
1	A	910	ALA	4.5
1	A	521	SER	4.5
1	A	836	HIS	4.5
1	A	950	PHE	4.5
1	B	775	ASN	4.5
1	B	524	PRO	4.5
1	B	707	ASP	4.5
1	B	752	LEU	4.4
1	A	640	GLU	4.4
1	B	899	GLU	4.4
1	B	588	ALA	4.4
1	B	782	VAL	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	695	LYS	4.4
1	B	897	GLY	4.4
1	A	619	VAL	4.3
1	A	591	ASN	4.3
1	B	620	PRO	4.3
1	A	987	MET	4.3
1	B	776	LEU	4.3
1	A	592	CYS	4.3
1	A	880	GLU	4.3
1	B	902	PRO	4.3
1	B	635	GLN	4.3
1	A	862	ILE	4.3
1	B	473	GLN	4.3
1	A	239	PHE	4.3
1	A	695	LYS	4.3
1	B	718	PRO	4.3
1	B	717	LYS	4.3
1	B	916	GLU	4.3
1	B	874	LYS	4.3
1	A	948	TYR	4.2
1	B	892	HIS	4.2
1	A	636	LEU	4.2
1	A	261	GLU	4.2
1	A	924	GLN	4.2
1	A	613	SER	4.2
1	A	409	ASN	4.2
1	B	798	VAL	4.2
1	B	593	THR	4.2
1	A	893	VAL	4.2
1	A	602	GLY	4.2
1	A	815	LYS	4.2
1	A	895	VAL	4.2
1	A	442	HIS	4.2
1	B	207	SER	4.2
1	A	767	SER	4.2
1	A	1034	GLN	4.2
1	B	694	VAL	4.2
1	B	761	CYS	4.2
1	B	599	GLU	4.1
1	A	263	VAL	4.1
1	A	411	PRO	4.1
1	B	747	GLN	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	672	HIS	4.1
1	A	877	ILE	4.1
1	B	609	ILE	4.1
1	B	895	VAL	4.1
1	A	808	GLU	4.1
1	A	971	VAL	4.1
1	A	527	GLY	4.0
1	A	190	GLY	4.0
1	B	846	GLU	4.0
1	B	642	GLY	4.0
1	B	727	PRO	4.0
1	B	267	GLY	4.0
1	A	954	THR	4.0
1	A	1025	ALA	4.0
1	A	522	GLY	4.0
1	B	842	SER	4.0
1	A	446	PHE	4.0
1	B	621	ARG	4.0
1	B	639	LYS	4.0
1	A	913	ILE	4.0
1	B	760	GLN	4.0
1	B	843	ARG	4.0
1	A	691	GLU	4.0
1	A	509	CYS	4.0
1	B	713	VAL	4.0
1	B	547	PRO	4.0
1	A	884	LEU	4.0
1	B	531	LEU	4.0
1	A	923	SER	4.0
1	B	820	PHE	4.0
1	B	546	GLU	3.9
1	A	456	LYS	3.9
1	A	931	ILE	3.9
1	A	266	PRO	3.9
1	B	708	LYS	3.9
1	B	736	TYR	3.9
1	B	762	GLN	3.9
1	B	790	ILE	3.9
1	A	675	LYS	3.9
1	B	411	PRO	3.9
1	A	859	ILE	3.9
1	B	750	PRO	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	926	ALA	3.9
1	A	537	ARG	3.9
1	A	892	HIS	3.9
1	A	248	SER	3.9
1	A	919	GLU	3.9
1	A	728	GLN	3.9
1	A	578	LEU	3.9
1	A	611	CYS	3.9
1	A	864	PRO	3.9
1	A	586	LEU	3.9
1	B	570	SER	3.9
1	B	618	GLU	3.8
1	B	777	PRO	3.8
1	B	889	ILE	3.8
1	A	650	PHE	3.8
1	A	412	LEU	3.8
1	A	495	ILE	3.8
1	A	1004	ILE	3.8
1	B	848	SER	3.8
1	A	970	GLN	3.8
1	B	549	ARG	3.8
1	A	391	PRO	3.8
1	B	643	MET	3.8
1	A	929	VAL	3.8
1	B	949	TYR	3.8
1	A	969	THR	3.7
1	B	566	ASN	3.7
1	A	623	ILE	3.7
1	A	330	ASP	3.7
1	B	915	CYS	3.7
1	A	262	MET	3.7
1	A	911	GLU	3.7
1	A	1003	ILE	3.7
1	A	444	LEU	3.7
1	A	473	GLN	3.7
1	A	983	ASN	3.7
1	B	796	ASN	3.7
1	A	869	ARG	3.7
1	A	622	ILE	3.7
1	B	598	SER	3.7
1	B	931	ILE	3.7
1	B	552	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	407	ASP	3.6
1	A	843	ARG	3.6
1	A	997	ARG	3.6
1	A	562	VAL	3.6
1	A	536	THR	3.6
1	A	439	TYR	3.6
1	A	174	SER	3.6
1	A	654	ASN	3.6
1	B	799	TYR	3.6
1	B	543	ARG	3.6
1	A	693	ARG	3.6
1	A	809	SER	3.6
1	A	443	SER	3.6
1	A	638	SER	3.5
1	A	628	ASP	3.5
1	A	153	HIS	3.5
1	A	949	TYR	3.5
1	A	189	ASP	3.5
1	A	730	GLN	3.5
1	A	804	GLY	3.5
1	A	985	VAL	3.5
1	B	578	LEU	3.5
1	B	738	CYS	3.4
1	B	900	CYS	3.4
1	A	847	LEU	3.4
1	A	558	VAL	3.4
1	B	293	VAL	3.4
1	B	602	GLY	3.4
1	B	572	TYR	3.4
1	B	273	GLN	3.4
1	A	1012	GLU	3.4
1	A	92	PRO	3.4
1	A	1035	TYR	3.4
1	B	859	ILE	3.4
1	A	587	SER	3.4
1	B	865	VAL	3.4
1	B	576	LEU	3.4
1	A	766	TYR	3.4
1	B	751	ALA	3.4
1	B	675	LYS	3.4
1	A	93	LYS	3.4
1	B	773	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1015	ASP	3.4
1	B	149	GLY	3.3
1	A	964	PRO	3.3
1	A	620	PRO	3.3
1	B	781	THR	3.3
1	B	890	ALA	3.3
1	A	520	GLY	3.3
1	A	972	THR	3.3
1	A	609	ILE	3.3
1	A	1014	LEU	3.3
1	A	677	ARG	3.3
1	B	867	GLY	3.3
1	B	768	TYR	3.3
1	B	845	LEU	3.3
1	B	706	VAL	3.3
1	A	930	GLU	3.3
1	A	830	GLN	3.3
1	B	740	LEU	3.3
1	B	676	TYR	3.2
1	A	624	THR	3.2
1	B	439	TYR	3.2
1	B	780	LEU	3.2
1	B	822	CYS	3.2
1	A	504	VAL	3.2
1	A	998	ARG	3.2
1	B	789	ASN	3.2
1	A	896	ALA	3.2
1	A	921	LYS	3.2
1	B	632	VAL	3.2
1	B	901	SER	3.2
1	A	816	ALA	3.2
1	B	929	VAL	3.2
1	B	183	PHE	3.2
1	A	614	PRO	3.2
1	B	162	VAL	3.2
1	B	126	LEU	3.1
1	B	836	HIS	3.1
1	B	601	ASP	3.1
1	A	995	PHE	3.1
1	A	630	HIS	3.1
1	A	866	THR	3.1
1	A	535	CYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	891	SER	3.1
1	A	408	MET	3.1
1	B	778	VAL	3.1
1	A	996	HIS	3.1
1	A	990	SER	3.1
1	A	484	MET	3.1
1	B	140	LEU	3.1
1	A	188	VAL	3.1
1	A	413	GLY	3.1
1	B	821	GLU	3.1
1	B	163	ASN	3.1
1	A	567	ILE	3.1
1	A	627	GLY	3.1
1	B	219	ASP	3.1
1	A	39	PHE	3.1
1	A	483	ASP	3.1
1	A	981	GLY	3.1
1	B	600	MET	3.1
1	B	569	VAL	3.1
1	B	817	ASP	3.1
1	A	631	VAL	3.1
1	A	679	VAL	3.1
1	A	576	LEU	3.1
1	B	64	LEU	3.1
1	A	552	SER	3.0
1	A	568	SER	3.0
1	A	75	SER	3.0
1	B	759	VAL	3.0
1	A	807	ARG	3.0
1	A	528	TRP	3.0
1	B	506	VAL	3.0
1	A	494	TYR	3.0
1	A	531	LEU	3.0
1	A	979	ASN	3.0
1	A	459	VAL	3.0
1	A	584	PRO	3.0
1	B	292	TYR	3.0
1	A	1007	THR	3.0
1	A	637	LYS	3.0
1	A	812	LEU	3.0
1	B	139	LEU	3.0
1	A	45	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	594	PHE	3.0
1	B	573	ASN	3.0
1	B	574	VAL	3.0
1	B	810	CYS	3.0
1	A	822	CYS	3.0
1	B	815	LYS	3.0
1	B	597	LEU	2.9
1	A	681	THR	2.9
1	A	959	LYS	2.9
1	B	816	ALA	2.9
1	B	797	LYS	2.9
1	B	446	PHE	2.9
1	A	246	GLY	2.9
1	B	610	GLN	2.9
1	A	463	LYS	2.9
1	A	867	GLY	2.9
1	A	644	THR	2.9
1	B	806	MET	2.9
1	A	671	CYS	2.9
1	B	905	ASP	2.9
1	B	611	CYS	2.9
1	A	832	THR	2.9
1	A	782	VAL	2.9
1	A	978	LEU	2.9
1	A	870	GLU	2.9
1	B	128	ALA	2.9
1	B	866	THR	2.9
1	B	595	GLU	2.9
1	A	925	HIS	2.9
1	B	913	ILE	2.9
1	A	210	ASP	2.8
1	A	91	ASN	2.8
1	A	515	CYS	2.8
1	B	763	ASN	2.8
1	A	909	PRO	2.8
1	B	722	LYS	2.8
1	B	138	LYS	2.8
1	A	769	GLU	2.8
1	A	570	SER	2.8
1	A	860	THR	2.8
1	B	764	THR	2.8
1	A	260	PRO	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	656	SER	2.8
1	B	903	LEU	2.8
1	A	534	THR	2.8
1	A	532	HIS	2.8
1	A	772	GLU	2.8
1	A	917	MET	2.8
1	B	125	ARG	2.8
1	A	689	PHE	2.8
1	B	807	ARG	2.8
1	A	241	ILE	2.7
1	B	951	MET	2.7
1	A	465	ASN	2.7
1	A	876	THR	2.7
1	B	703	LEU	2.7
1	A	105	GLU	2.7
1	A	511	GLN	2.7
1	A	106	PRO	2.7
1	B	564	PRO	2.7
1	B	542	GLU	2.7
1	A	789	ASN	2.7
1	A	551	ALA	2.7
1	B	181	LYS	2.7
1	A	1005	CYS	2.7
1	A	670	ARG	2.7
1	A	721	LEU	2.7
1	B	888	ASP	2.7
1	A	529	CYS	2.7
1	A	533	ASN	2.7
1	B	523	ASP	2.7
1	A	744	GLY	2.7
1	B	826	GLN	2.7
1	A	471	THR	2.7
1	A	493	LEU	2.7
1	B	715	VAL	2.6
1	A	690	GLN	2.6
1	B	603	LEU	2.6
1	A	38	SER	2.6
1	A	933	VAL	2.6
1	A	763	ASN	2.6
1	A	403	PHE	2.6
1	A	445	ALA	2.6
1	A	571	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	736	TYR	2.6
1	B	630	HIS	2.6
1	A	170	GLY	2.6
1	A	865	VAL	2.6
1	B	805	ALA	2.6
1	A	682	HIS	2.6
1	A	745	ILE	2.6
1	A	384	TRP	2.6
1	B	944	SER	2.6
1	A	264	SER	2.6
1	B	551	ALA	2.6
1	B	896	ALA	2.6
1	B	560	LEU	2.6
1	A	629	HIS	2.6
1	B	893	VAL	2.5
1	A	538	LYS	2.5
1	B	625	GLU	2.5
1	B	400	ASP	2.5
1	B	173	VAL	2.5
1	A	607	ASN	2.5
1	B	749	VAL	2.5
1	B	203	LEU	2.5
1	A	440	LYS	2.5
1	A	863	ILE	2.5
1	B	863	ILE	2.5
1	A	436	ALA	2.5
1	A	813	CYS	2.5
1	B	818	PRO	2.5
1	A	99	ILE	2.5
1	A	861	GLU	2.5
1	A	991	GLN	2.5
1	B	861	GLU	2.5
1	B	693	ARG	2.5
1	A	673	TRP	2.5
1	B	71	TYR	2.5
1	B	701	PRO	2.5
1	B	581	TYR	2.5
1	A	172	ILE	2.5
1	B	127	ILE	2.5
1	A	518	CYS	2.5
1	B	946	GLN	2.5
1	B	146	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	933	VAL	2.5
1	B	284	LYS	2.4
1	A	905	ASP	2.4
1	B	641	THR	2.4
1	A	265	PRO	2.4
1	A	781	THR	2.4
1	A	820	PHE	2.4
1	B	431	MET	2.4
1	B	904	VAL	2.4
1	A	588	ALA	2.4
1	A	1013	VAL	2.4
1	A	312	ALA	2.4
1	A	237	PRO	2.4
1	B	633	GLN	2.4
1	A	621	ARG	2.4
1	B	647	SER	2.4
1	A	228	ILE	2.4
1	B	876	THR	2.4
1	B	151	PRO	2.4
1	A	486	PHE	2.4
1	A	819	ASP	2.4
1	B	704	LEU	2.4
1	A	918	GLY	2.4
1	A	947	LEU	2.4
1	A	889	ILE	2.4
1	B	150	GLU	2.4
1	B	830	GLN	2.4
1	A	332	ASP	2.4
1	B	930	GLU	2.4
1	A	315	SER	2.4
1	B	120	ASP	2.3
1	B	612	TYR	2.3
1	A	857	PRO	2.3
1	A	856	ASN	2.3
1	A	333	LEU	2.3
1	A	604	VAL	2.3
1	A	902	PRO	2.3
1	A	583	VAL	2.3
1	A	858	ARG	2.3
1	A	175	TYR	2.3
1	A	194	TYR	2.3
1	A	894	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	182	LEU	2.3
1	B	345	LYS	2.3
1	B	881	ASN	2.3
1	B	83	HIS	2.3
1	B	742	ILE	2.3
1	A	701	PRO	2.3
1	B	160	SER	2.3
1	A	560	LEU	2.3
1	A	435	ILE	2.3
1	B	556	GLN	2.3
1	A	878	ARG	2.3
1	B	522	GLY	2.3
1	A	610	GLN	2.3
1	A	171	VAL	2.3
1	B	369	ARG	2.3
1	A	903	LEU	2.3
1	A	235	VAL	2.3
1	B	579	GLU	2.3
1	B	730	GLN	2.3
1	A	790	ILE	2.3
1	B	653	TYR	2.3
1	B	250	GLY	2.3
1	A	738	CYS	2.3
1	B	648	THR	2.2
1	A	64	LEU	2.2
1	B	172	ILE	2.2
1	B	811	GLY	2.2
1	A	460	ASP	2.2
1	B	617	LYS	2.2
1	A	317	ALA	2.2
1	B	444	LEU	2.2
1	A	729	PRO	2.2
1	A	447	VAL	2.2
1	A	720	THR	2.2
1	A	513	ARG	2.2
1	B	141	ARG	2.2
1	B	193	GLU	2.2
1	B	511	GLN	2.2
1	A	490	HIS	2.2
1	A	841	GLU	2.2
1	B	256	LEU	2.2
1	A	151	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	828	PRO	2.2
1	A	173	VAL	2.2
1	B	651	VAL	2.2
1	B	771	MET	2.2
1	B	257	THR	2.2
1	B	670	ARG	2.2
1	A	768	TYR	2.2
1	A	514	SER	2.2
1	B	312	ALA	2.2
1	B	832	THR	2.2
1	A	1010	SER	2.2
1	B	631	VAL	2.2
1	B	914	VAL	2.2
1	A	519	LEU	2.2
1	B	772	GLU	2.2
1	B	857	PRO	2.2
1	B	697	PRO	2.2
1	A	719	ILE	2.2
1	B	240	ASP	2.1
1	A	441	ASN	2.1
1	A	651	VAL	2.1
1	A	398	THR	2.1
1	B	624	THR	2.1
1	A	580	THR	2.1
1	B	894	LYS	2.1
1	B	147	LYS	2.1
1	A	817	ASP	2.1
1	B	596	ASP	2.1
1	A	805	ALA	2.1
1	B	791	ASP	2.1
1	A	219	ASP	2.1
1	B	831	CYS	2.1
1	A	335	PHE	2.1
1	B	294	GLU	2.1
1	A	837	CYS	2.1
1	B	403	PHE	2.1
1	A	388	LYS	2.1
1	B	804	GLY	2.1
1	A	434	VAL	2.1
1	A	468	GLN	2.1
1	B	692	GLY	2.1
1	B	702	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	753	ARG	2.1
1	A	974	THR	2.1
1	B	841	GLU	2.1
1	A	197	THR	2.1
1	A	344	ARG	2.1
1	A	464	GLY	2.1
1	B	228	ILE	2.1
1	A	632	VAL	2.0
1	B	649	SER	2.0
1	A	516	GLY	2.0
1	A	561	THR	2.0
1	A	818	PRO	2.0
1	B	672	HIS	2.0
1	A	944	SER	2.0
1	B	615	ALA	2.0
1	B	220	GLU	2.0
1	A	401	ASP	2.0
1	B	623	ILE	2.0
1	A	392	CYS	2.0
1	B	691	GLU	2.0
1	A	641	THR	2.0
1	A	784	TRP	2.0
1	A	406	LEU	2.0
1	A	565	ASN	2.0
1	A	342	GLN	2.0
1	A	731	SER	2.0
1	A	491	GLU	2.0
1	B	575	LEU	2.0
1	B	855	THR	2.0
1	A	653	TYR	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.