



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 11:54 pm GMT

PDB ID : 6TGB
EMDB ID : EMD-10497
Title : CryoEM structure of the binary DOCK2-ELMO1 complex
Authors : Chang, L.; Yang, J.; Chang, J.H.; Zhang, Z.; Boland, A.; McLaughlin, S.H.;
Abu-Thuraia, A.; Killoran, R.C.; Smith, M.J.; Cote, J.F.; Barford, D.
Deposited on : 2019-11-15
Resolution : 5.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

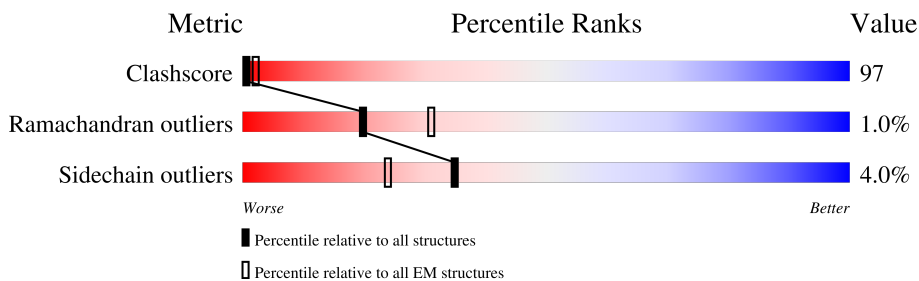
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.50 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1830	
1	D	1830	
2	B	727	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18649 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Deducator of cytokinesis protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1450	10203	6463	1792	1894	54	0	0
1	D	411	3379	2175	550	632	22	0	0

There are 1048 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207A	UNK	ASP	conflict	UNP Q92608
A	207B	UNK	TYR	conflict	UNP Q92608
A	207C	UNK	ALA	conflict	UNP Q92608
A	207D	UNK	MET	conflict	UNP Q92608
A	207E	UNK	TYR	conflict	UNP Q92608
A	207F	UNK	SER	conflict	UNP Q92608
A	207G	UNK	ARG	conflict	UNP Q92608
A	207H	UNK	ILE	conflict	UNP Q92608
A	207I	UNK	SER	conflict	UNP Q92608
A	207J	UNK	SER	conflict	UNP Q92608
A	207K	UNK	SER	conflict	UNP Q92608
A	207L	UNK	PRO	conflict	UNP Q92608
A	207M	UNK	THR	conflict	UNP Q92608
A	207N	UNK	HIS	conflict	UNP Q92608
A	207O	UNK	SER	conflict	UNP Q92608
A	207P	UNK	LEU	conflict	UNP Q92608
A	207Q	UNK	TYR	conflict	UNP Q92608
A	207R	UNK	VAL	conflict	UNP Q92608
A	207S	UNK	PHE	conflict	UNP Q92608
A	207T	UNK	VAL	conflict	UNP Q92608
A	207U	UNK	ARG	conflict	UNP Q92608
A	207V	UNK	ASN	conflict	UNP Q92608
A	207W	UNK	PHE	conflict	UNP Q92608
A	207X	UNK	VAL	conflict	UNP Q92608
A	207Y	UNK	CYS	conflict	UNP Q92608
A	207Z	UNK	ARG	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	208A	UNK	ILE	conflict	UNP Q92608
A	208B	UNK	GLY	conflict	UNP Q92608
A	208C	UNK	GLU	conflict	UNP Q92608
A	208D	UNK	ASP	conflict	UNP Q92608
A	208E	UNK	ALA	conflict	UNP Q92608
A	208F	UNK	GLU	conflict	UNP Q92608
A	208G	UNK	LEU	conflict	UNP Q92608
A	208H	UNK	PHE	conflict	UNP Q92608
A	208I	UNK	MET	conflict	UNP Q92608
A	208J	UNK	SER	conflict	UNP Q92608
A	208K	UNK	LEU	conflict	UNP Q92608
A	208L	UNK	TYR	conflict	UNP Q92608
A	208M	UNK	ASP	conflict	UNP Q92608
A	208N	UNK	PRO	conflict	UNP Q92608
A	208O	UNK	ASN	conflict	UNP Q92608
A	208P	UNK	LYS	conflict	UNP Q92608
A	208Q	UNK	GLN	conflict	UNP Q92608
A	208R	UNK	THR	conflict	UNP Q92608
A	208S	UNK	VAL	conflict	UNP Q92608
A	208T	UNK	ILE	conflict	UNP Q92608
A	208U	UNK	SER	conflict	UNP Q92608
A	208V	UNK	GLU	conflict	UNP Q92608
A	208W	UNK	ASN	conflict	UNP Q92608
A	208X	UNK	TYR	conflict	UNP Q92608
A	208Y	UNK	LEU	conflict	UNP Q92608
A	208Z	UNK	VAL	conflict	UNP Q92608
A	209A	UNK	ARG	conflict	UNP Q92608
A	209B	UNK	TRP	conflict	UNP Q92608
A	209C	UNK	GLY	conflict	UNP Q92608
A	209D	UNK	SER	conflict	UNP Q92608
A	209E	UNK	ARG	conflict	UNP Q92608
A	209F	UNK	GLY	conflict	UNP Q92608
A	209G	UNK	PHE	conflict	UNP Q92608
A	209H	UNK	PRO	conflict	UNP Q92608
A	209I	UNK	LYS	conflict	UNP Q92608
A	209J	UNK	GLU	conflict	UNP Q92608
A	209K	UNK	ILE	conflict	UNP Q92608
A	209L	UNK	GLU	conflict	UNP Q92608
A	209M	UNK	MET	conflict	UNP Q92608
A	209N	UNK	LEU	conflict	UNP Q92608
A	209O	UNK	ASN	conflict	UNP Q92608
A	209P	UNK	ASN	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	209Q	UNK	LEU	conflict	UNP Q92608
A	209R	UNK	LYS	conflict	UNP Q92608
A	209S	UNK	VAL	conflict	UNP Q92608
A	219	UNK	VAL	conflict	UNP Q92608
A	220	UNK	PHE	conflict	UNP Q92608
A	221	UNK	THR	conflict	UNP Q92608
A	222	UNK	ASP	conflict	UNP Q92608
A	223	UNK	LEU	conflict	UNP Q92608
A	224	UNK	GLY	conflict	UNP Q92608
A	225	UNK	ASN	conflict	UNP Q92608
A	226	UNK	LYS	conflict	UNP Q92608
A	227	UNK	ASP	conflict	UNP Q92608
A	228	UNK	LEU	conflict	UNP Q92608
A	229	UNK	ASN	conflict	UNP Q92608
A	230	UNK	ARG	conflict	UNP Q92608
A	231	UNK	ASP	conflict	UNP Q92608
A	232	UNK	LYS	conflict	UNP Q92608
A	233	UNK	ILE	conflict	UNP Q92608
A	234	UNK	TYR	conflict	UNP Q92608
A	235	UNK	LEU	conflict	UNP Q92608
A	236	UNK	ILE	conflict	UNP Q92608
A	237	UNK	CYS	conflict	UNP Q92608
A	238	UNK	GLN	conflict	UNP Q92608
A	239	UNK	ILE	conflict	UNP Q92608
A	240	UNK	VAL	conflict	UNP Q92608
A	241	UNK	ARG	conflict	UNP Q92608
A	242	UNK	VAL	conflict	UNP Q92608
A	243	UNK	GLY	conflict	UNP Q92608
A	244	UNK	LYS	conflict	UNP Q92608
A	245	UNK	MET	conflict	UNP Q92608
A	246	UNK	ASP	conflict	UNP Q92608
A	247	UNK	LEU	conflict	UNP Q92608
A	248	UNK	LYS	conflict	UNP Q92608
A	249	UNK	ASP	conflict	UNP Q92608
A	250	UNK	THR	conflict	UNP Q92608
A	251	UNK	GLY	conflict	UNP Q92608
A	252	UNK	ALA	conflict	UNP Q92608
A	253	UNK	LYS	conflict	UNP Q92608
A	254	UNK	LYS	conflict	UNP Q92608
A	255	UNK	CYS	conflict	UNP Q92608
A	256	UNK	THR	conflict	UNP Q92608
A	257	UNK	GLN	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	UNK	GLY	conflict	UNP Q92608
A	259	UNK	LEU	conflict	UNP Q92608
A	260	UNK	ARG	conflict	UNP Q92608
A	261	UNK	ARG	conflict	UNP Q92608
A	262	UNK	PRO	conflict	UNP Q92608
A	263	UNK	PHE	conflict	UNP Q92608
A	264	UNK	GLY	conflict	UNP Q92608
A	265	UNK	VAL	conflict	UNP Q92608
A	266	UNK	ALA	conflict	UNP Q92608
A	267	UNK	VAL	conflict	UNP Q92608
A	268	UNK	MET	conflict	UNP Q92608
A	269	UNK	ASP	conflict	UNP Q92608
A	270	UNK	ILE	conflict	UNP Q92608
A	271	UNK	THR	conflict	UNP Q92608
A	272	UNK	ASP	conflict	UNP Q92608
A	273	UNK	ILE	conflict	UNP Q92608
A	274	UNK	ILE	conflict	UNP Q92608
A	275	UNK	LYS	conflict	UNP Q92608
A	276	UNK	GLY	conflict	UNP Q92608
A	277	UNK	LYS	conflict	UNP Q92608
A	278	UNK	ALA	conflict	UNP Q92608
A	279	UNK	GLU	conflict	UNP Q92608
A	280	UNK	SER	conflict	UNP Q92608
A	281	UNK	ASP	conflict	UNP Q92608
A	282	UNK	GLU	conflict	UNP Q92608
A	283	UNK	GLU	conflict	UNP Q92608
A	284	UNK	LYS	conflict	UNP Q92608
A	285	UNK	GLN	conflict	UNP Q92608
A	286	UNK	HIS	conflict	UNP Q92608
A	287	UNK	PHE	conflict	UNP Q92608
A	288	UNK	ILE	conflict	UNP Q92608
A	289	UNK	PRO	conflict	UNP Q92608
A	290	UNK	PHE	conflict	UNP Q92608
A	291	UNK	HIS	conflict	UNP Q92608
A	292	UNK	PRO	conflict	UNP Q92608
A	293	UNK	VAL	conflict	UNP Q92608
A	294	UNK	THR	conflict	UNP Q92608
A	295	UNK	ALA	conflict	UNP Q92608
A	296	UNK	GLU	conflict	UNP Q92608
A	297	UNK	ASN	conflict	UNP Q92608
A	298	UNK	ASP	conflict	UNP Q92608
A	299	UNK	PHE	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	300	UNK	LEU	conflict	UNP Q92608
A	301	UNK	HIS	conflict	UNP Q92608
A	302	UNK	SER	conflict	UNP Q92608
A	303	UNK	LEU	conflict	UNP Q92608
A	304	UNK	LEU	conflict	UNP Q92608
A	318	UNK	GLY	conflict	UNP Q92608
A	319	UNK	LYS	conflict	UNP Q92608
A	320	UNK	VAL	conflict	UNP Q92608
A	321	UNK	ILE	conflict	UNP Q92608
A	322	UNK	ALA	conflict	UNP Q92608
A	323	UNK	SER	conflict	UNP Q92608
A	324	UNK	LYS	conflict	UNP Q92608
A	325	UNK	GLY	conflict	UNP Q92608
A	326	UNK	ASP	conflict	UNP Q92608
A	327	UNK	SER	conflict	UNP Q92608
A	328	UNK	GLY	conflict	UNP Q92608
A	329	UNK	GLY	conflict	UNP Q92608
A	330	UNK	GLN	conflict	UNP Q92608
A	331	UNK	GLY	conflict	UNP Q92608
A	332	UNK	LEU	conflict	UNP Q92608
A	333	UNK	TRP	conflict	UNP Q92608
A	334	UNK	VAL	conflict	UNP Q92608
A	335	UNK	THR	conflict	UNP Q92608
A	336	UNK	MET	conflict	UNP Q92608
A	337	UNK	LYS	conflict	UNP Q92608
A	338	UNK	MET	conflict	UNP Q92608
A	339	UNK	LEU	conflict	UNP Q92608
A	340	UNK	VAL	conflict	UNP Q92608
A	341	UNK	GLY	conflict	UNP Q92608
A	342	UNK	ASP	conflict	UNP Q92608
A	343	UNK	ILE	conflict	UNP Q92608
A	344	UNK	ILE	conflict	UNP Q92608
A	345	UNK	GLN	conflict	UNP Q92608
A	346	UNK	ILE	conflict	UNP Q92608
A	347	UNK	ARG	conflict	UNP Q92608
A	348	UNK	LYS	conflict	UNP Q92608
A	349	UNK	ASP	conflict	UNP Q92608
A	350	UNK	TYR	conflict	UNP Q92608
A	351	UNK	PRO	conflict	UNP Q92608
A	377	UNK	HIS	conflict	UNP Q92608
A	378	UNK	LEU	conflict	UNP Q92608
A	379	UNK	VAL	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	UNK	ASP	conflict	UNP Q92608
A	381	UNK	ARG	conflict	UNP Q92608
A	382	UNK	THR	conflict	UNP Q92608
A	383	UNK	THR	conflict	UNP Q92608
A	384	UNK	VAL	conflict	UNP Q92608
A	385	UNK	VAL	conflict	UNP Q92608
A	386	UNK	ALA	conflict	UNP Q92608
A	387	UNK	ARG	conflict	UNP Q92608
A	388	UNK	LYS	conflict	UNP Q92608
A	389	UNK	LEU	conflict	UNP Q92608
A	609A	UNK	LYS	conflict	UNP Q92608
A	609B	UNK	LEU	conflict	UNP Q92608
A	609C	UNK	THR	conflict	UNP Q92608
A	609D	UNK	GLN	conflict	UNP Q92608
A	609E	UNK	ASN	conflict	UNP Q92608
A	609F	UNK	VAL	conflict	UNP Q92608
A	609G	UNK	GLY	conflict	UNP Q92608
A	609H	UNK	LEU	conflict	UNP Q92608
A	609I	UNK	LEU	conflict	UNP Q92608
A	609J	UNK	GLY	conflict	UNP Q92608
A	609K	UNK	LEU	conflict	UNP Q92608
A	609L	UNK	LEU	conflict	UNP Q92608
A	609M	UNK	LYS	conflict	UNP Q92608
A	609N	UNK	TRP	conflict	UNP Q92608
A	609O	UNK	ARG	conflict	UNP Q92608
A	609P	UNK	MET	conflict	UNP Q92608
A	609Q	UNK	LYS	conflict	UNP Q92608
A	609R	UNK	PRO	conflict	UNP Q92608
A	609S	UNK	GLN	conflict	UNP Q92608
A	609T	UNK	LEU	conflict	UNP Q92608
A	609U	UNK	LEU	conflict	UNP Q92608
A	609V	UNK	GLN	conflict	UNP Q92608
A	609W	UNK	GLU	conflict	UNP Q92608
A	609X	UNK	ASN	conflict	UNP Q92608
A	609Y	UNK	LEU	conflict	UNP Q92608
A	609Z	UNK	GLU	conflict	UNP Q92608
A	610A	UNK	LYS	conflict	UNP Q92608
A	610B	UNK	LEU	conflict	UNP Q92608
A	610C	UNK	LYS	conflict	UNP Q92608
A	610D	UNK	ILE	conflict	UNP Q92608
A	610E	UNK	VAL	conflict	UNP Q92608
A	610F	UNK	ASP	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	626	UNK	GLY	conflict	UNP Q92608
A	627	UNK	GLU	conflict	UNP Q92608
A	628	UNK	GLU	conflict	UNP Q92608
A	629	UNK	VAL	conflict	UNP Q92608
A	630	UNK	VAL	conflict	UNP Q92608
A	631	UNK	LYS	conflict	UNP Q92608
A	632	UNK	PHE	conflict	UNP Q92608
A	633	UNK	LEU	conflict	UNP Q92608
A	634	UNK	GLN	conflict	UNP Q92608
A	635	UNK	ASP	conflict	UNP Q92608
A	636	UNK	THR	conflict	UNP Q92608
A	637	UNK	LEU	conflict	UNP Q92608
A	638	UNK	ASP	conflict	UNP Q92608
A	639	UNK	ALA	conflict	UNP Q92608
A	640	UNK	LEU	conflict	UNP Q92608
A	641	UNK	PHE	conflict	UNP Q92608
A	642	UNK	ASN	conflict	UNP Q92608
A	679A	UNK	HIS	conflict	UNP Q92608
A	679B	UNK	PHE	conflict	UNP Q92608
A	679C	UNK	ASN	conflict	UNP Q92608
A	679D	UNK	THR	conflict	UNP Q92608
A	679E	UNK	VAL	conflict	UNP Q92608
A	679F	UNK	LEU	conflict	UNP Q92608
A	679G	UNK	GLU	conflict	UNP Q92608
A	679H	UNK	ALA	conflict	UNP Q92608
A	679I	UNK	TYR	conflict	UNP Q92608
A	679J	UNK	ILE	conflict	UNP Q92608
A	679K	UNK	GLN	conflict	UNP Q92608
A	679L	UNK	GLN	conflict	UNP Q92608
A	679M	UNK	HIS	conflict	UNP Q92608
A	679N	UNK	PHE	conflict	UNP Q92608
A	679O	UNK	SER	conflict	UNP Q92608
A	679P	UNK	ALA	conflict	UNP Q92608
A	679Q	UNK	THR	conflict	UNP Q92608
A	688	UNK	LEU	conflict	UNP Q92608
A	689	UNK	ALA	conflict	UNP Q92608
A	690	UNK	TYR	conflict	UNP Q92608
A	691	UNK	LYS	conflict	UNP Q92608
A	692	UNK	LYS	conflict	UNP Q92608
A	693	UNK	LEU	conflict	UNP Q92608
A	694	UNK	MET	conflict	UNP Q92608
A	695	UNK	THR	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	696	UNK	VAL	conflict	UNP Q92608
A	697	UNK	LEU	conflict	UNP Q92608
A	698	UNK	LYS	conflict	UNP Q92608
A	699	UNK	THR	conflict	UNP Q92608
A	700	UNK	TYR	conflict	UNP Q92608
A	701	UNK	LEU	conflict	UNP Q92608
A	702	UNK	ASP	conflict	UNP Q92608
A	703	UNK	THR	conflict	UNP Q92608
A	704	UNK	SER	conflict	UNP Q92608
A	705	UNK	SER	conflict	UNP Q92608
A	706	UNK	ARG	conflict	UNP Q92608
A	707	UNK	GLY	conflict	UNP Q92608
A	708	UNK	GLU	conflict	UNP Q92608
A	709	UNK	GLN	conflict	UNP Q92608
A	710	UNK	CYS	conflict	UNP Q92608
A	711	UNK	GLU	conflict	UNP Q92608
A	712	UNK	PRO	conflict	UNP Q92608
A	713	UNK	ILE	conflict	UNP Q92608
A	714	UNK	LEU	conflict	UNP Q92608
A	715	UNK	ARG	conflict	UNP Q92608
A	716	UNK	THR	conflict	UNP Q92608
A	717	UNK	LEU	conflict	UNP Q92608
A	718	UNK	LYS	conflict	UNP Q92608
A	719	UNK	ALA	conflict	UNP Q92608
A	720	UNK	LEU	conflict	UNP Q92608
A	721	UNK	GLU	conflict	UNP Q92608
A	722	UNK	TYR	conflict	UNP Q92608
A	723	UNK	VAL	conflict	UNP Q92608
A	724	UNK	PHE	conflict	UNP Q92608
A	725	UNK	LYS	conflict	UNP Q92608
A	726	UNK	PHE	conflict	UNP Q92608
A	727	UNK	ILE	conflict	UNP Q92608
A	728	UNK	VAL	conflict	UNP Q92608
A	729	UNK	ARG	conflict	UNP Q92608
A	730	UNK	SER	conflict	UNP Q92608
A	731	UNK	ARG	conflict	UNP Q92608
A	732	UNK	THR	conflict	UNP Q92608
A	733	UNK	LEU	conflict	UNP Q92608
A	734	UNK	PHE	conflict	UNP Q92608
A	735	UNK	SER	conflict	UNP Q92608
A	736	UNK	GLN	conflict	UNP Q92608
A	742	UNK	LEU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	743	UNK	TYR	conflict	UNP Q92608
A	744	UNK	GLU	conflict	UNP Q92608
A	745	UNK	GLY	conflict	UNP Q92608
A	746	UNK	LYS	conflict	UNP Q92608
A	747	UNK	GLU	conflict	UNP Q92608
A	748	UNK	GLN	conflict	UNP Q92608
A	749	UNK	MET	conflict	UNP Q92608
A	750	UNK	GLU	conflict	UNP Q92608
A	751	UNK	PHE	conflict	UNP Q92608
A	752	UNK	GLU	conflict	UNP Q92608
A	753	UNK	GLU	conflict	UNP Q92608
A	754	UNK	SER	conflict	UNP Q92608
A	755	UNK	MET	conflict	UNP Q92608
A	756	UNK	ARG	conflict	UNP Q92608
A	757	UNK	ARG	conflict	UNP Q92608
A	758	UNK	LEU	conflict	UNP Q92608
A	759	UNK	PHE	conflict	UNP Q92608
A	760	UNK	GLU	conflict	UNP Q92608
A	761	UNK	SER	conflict	UNP Q92608
A	762	UNK	ILE	conflict	UNP Q92608
A	763	UNK	ASN	conflict	UNP Q92608
A	764	UNK	ASN	conflict	UNP Q92608
A	765	UNK	LEU	conflict	UNP Q92608
A	766	UNK	MET	conflict	UNP Q92608
A	767	UNK	LYS	conflict	UNP Q92608
A	768	UNK	SER	conflict	UNP Q92608
A	769	UNK	GLN	conflict	UNP Q92608
A	770	UNK	TYR	conflict	UNP Q92608
A	771	UNK	LYS	conflict	UNP Q92608
A	772	UNK	THR	conflict	UNP Q92608
A	773	UNK	THR	conflict	UNP Q92608
A	774	UNK	ILE	conflict	UNP Q92608
A	775	UNK	LEU	conflict	UNP Q92608
A	776	UNK	LEU	conflict	UNP Q92608
A	777	UNK	GLN	conflict	UNP Q92608
A	778	UNK	VAL	conflict	UNP Q92608
A	779	UNK	ALA	conflict	UNP Q92608
A	780	UNK	ALA	conflict	UNP Q92608
A	781	UNK	LEU	conflict	UNP Q92608
A	782	UNK	LYS	conflict	UNP Q92608
A	783	UNK	TYR	conflict	UNP Q92608
A	784	UNK	ILE	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	UNK	PRO	conflict	UNP Q92608
A	786	UNK	SER	conflict	UNP Q92608
A	787	UNK	VAL	conflict	UNP Q92608
A	788	UNK	LEU	conflict	UNP Q92608
A	789	UNK	HIS	conflict	UNP Q92608
A	790	UNK	ASP	conflict	UNP Q92608
A	791	UNK	VAL	conflict	UNP Q92608
A	792	UNK	GLU	conflict	UNP Q92608
A	793	UNK	MET	conflict	UNP Q92608
A	794	UNK	VAL	conflict	UNP Q92608
A	795	UNK	PHE	conflict	UNP Q92608
A	796	UNK	ASP	conflict	UNP Q92608
A	797	UNK	ALA	conflict	UNP Q92608
A	798	UNK	LYS	conflict	UNP Q92608
A	799	UNK	LEU	conflict	UNP Q92608
A	801	UNK	LEU	conflict	UNP Q92608
A	802	UNK	SER	conflict	UNP Q92608
A	803	UNK	GLN	conflict	UNP Q92608
A	804	UNK	LEU	conflict	UNP Q92608
A	805	UNK	LEU	conflict	UNP Q92608
A	806	UNK	TYR	conflict	UNP Q92608
A	807	UNK	GLU	conflict	UNP Q92608
A	808	UNK	PHE	conflict	UNP Q92608
A	809	UNK	TYR	conflict	UNP Q92608
A	810	UNK	THR	conflict	UNP Q92608
A	811	UNK	CYS	conflict	UNP Q92608
A	812	UNK	ILE	conflict	UNP Q92608
A	813	UNK	PRO	conflict	UNP Q92608
A	814	UNK	PRO	conflict	UNP Q92608
A	815	UNK	VAL	conflict	UNP Q92608
A	816	UNK	LYS	conflict	UNP Q92608
A	817	UNK	LEU	conflict	UNP Q92608
A	818	UNK	GLN	conflict	UNP Q92608
A	819	UNK	LYS	conflict	UNP Q92608
A	820	UNK	GLN	conflict	UNP Q92608
A	821	UNK	LYS	conflict	UNP Q92608
A	822	UNK	VAL	conflict	UNP Q92608
A	823	UNK	GLN	conflict	UNP Q92608
A	824	UNK	SER	conflict	UNP Q92608
A	825	UNK	MET	conflict	UNP Q92608
A	826	UNK	ASN	conflict	UNP Q92608
A	827	UNK	GLU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	828	UNK	ILE	conflict	UNP Q92608
A	829	UNK	VAL	conflict	UNP Q92608
A	830	UNK	GLN	conflict	UNP Q92608
A	831	UNK	SER	conflict	UNP Q92608
A	832	UNK	ASN	conflict	UNP Q92608
A	833	UNK	LEU	conflict	UNP Q92608
A	834	UNK	PHE	conflict	UNP Q92608
A	835	UNK	LYS	conflict	UNP Q92608
A	836	UNK	LYS	conflict	UNP Q92608
A	837	UNK	GLN	conflict	UNP Q92608
A	838	UNK	GLU	conflict	UNP Q92608
A	839	UNK	CYS	conflict	UNP Q92608
A	840	UNK	ARG	conflict	UNP Q92608
A	841	UNK	ASP	conflict	UNP Q92608
A	842	UNK	ILE	conflict	UNP Q92608
A	843	UNK	LEU	conflict	UNP Q92608
A	844	UNK	LEU	conflict	UNP Q92608
A	845	UNK	PRO	conflict	UNP Q92608
A	846	UNK	VAL	conflict	UNP Q92608
A	847	UNK	ILE	conflict	UNP Q92608
A	848	UNK	THR	conflict	UNP Q92608
A	849	UNK	LYS	conflict	UNP Q92608
A	850	UNK	GLU	conflict	UNP Q92608
A	851	UNK	LEU	conflict	UNP Q92608
A	852	UNK	LYS	conflict	UNP Q92608
A	853	UNK	GLU	conflict	UNP Q92608
A	854	UNK	LEU	conflict	UNP Q92608
A	855	UNK	LEU	conflict	UNP Q92608
A	856	UNK	GLU	conflict	UNP Q92608
A	857	UNK	GLN	conflict	UNP Q92608
A	858	UNK	LYS	conflict	UNP Q92608
A	859	UNK	ASP	conflict	UNP Q92608
A	860	UNK	ASP	conflict	UNP Q92608
A	861	UNK	MET	conflict	UNP Q92608
A	862	UNK	GLN	conflict	UNP Q92608
A	863	UNK	HIS	conflict	UNP Q92608
A	864	UNK	GLN	conflict	UNP Q92608
A	865	UNK	VAL	conflict	UNP Q92608
A	866	UNK	LEU	conflict	UNP Q92608
A	867	UNK	GLU	conflict	UNP Q92608
A	868	UNK	ARG	conflict	UNP Q92608
A	869	UNK	LYS	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	870	UNK	TYR	conflict	UNP Q92608
A	871	UNK	CYS	conflict	UNP Q92608
A	872	UNK	VAL	conflict	UNP Q92608
A	873	UNK	GLU	conflict	UNP Q92608
A	874	UNK	LEU	conflict	UNP Q92608
A	875	UNK	LEU	conflict	UNP Q92608
A	876	UNK	ASN	conflict	UNP Q92608
A	877	UNK	SER	conflict	UNP Q92608
A	878	UNK	ILE	conflict	UNP Q92608
A	879	UNK	LEU	conflict	UNP Q92608
A	880	UNK	GLU	conflict	UNP Q92608
A	881	UNK	VAL	conflict	UNP Q92608
A	882	UNK	LEU	conflict	UNP Q92608
A	883	UNK	SER	conflict	UNP Q92608
A	884	UNK	TYR	conflict	UNP Q92608
A	885	UNK	GLN	conflict	UNP Q92608
A	886	UNK	ASP	conflict	UNP Q92608
A	887	UNK	ALA	conflict	UNP Q92608
A	888	UNK	ALA	conflict	UNP Q92608
A	889	UNK	PHE	conflict	UNP Q92608
A	890	UNK	THR	conflict	UNP Q92608
A	891	UNK	TYR	conflict	UNP Q92608
A	892	UNK	HIS	conflict	UNP Q92608
A	896	UNK	HIS	conflict	UNP Q92608
A	897	UNK	ILE	conflict	UNP Q92608
A	898	UNK	GLN	conflict	UNP Q92608
A	899	UNK	GLU	conflict	UNP Q92608
A	900	UNK	ILE	conflict	UNP Q92608
A	901	UNK	MET	conflict	UNP Q92608
A	902	UNK	VAL	conflict	UNP Q92608
A	903	UNK	GLN	conflict	UNP Q92608
A	904	UNK	LEU	conflict	UNP Q92608
A	905	UNK	LEU	conflict	UNP Q92608
A	906	UNK	ARG	conflict	UNP Q92608
A	907	UNK	THR	conflict	UNP Q92608
A	908	UNK	VAL	conflict	UNP Q92608
A	909	UNK	ASN	conflict	UNP Q92608
A	910	UNK	ARG	conflict	UNP Q92608
A	911	UNK	THR	conflict	UNP Q92608
A	912	UNK	VAL	conflict	UNP Q92608
A	913	UNK	ILE	conflict	UNP Q92608
A	914	UNK	THR	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	915	UNK	MET	conflict	UNP Q92608
A	916	UNK	GLY	conflict	UNP Q92608
A	917	UNK	ARG	conflict	UNP Q92608
A	918	UNK	ASP	conflict	UNP Q92608
A	919	UNK	HIS	conflict	UNP Q92608
A	920	UNK	ILE	conflict	UNP Q92608
A	921	UNK	LEU	conflict	UNP Q92608
A	922	UNK	ILE	conflict	UNP Q92608
A	923	UNK	SER	conflict	UNP Q92608
A	934	UNK	HIS	conflict	UNP Q92608
A	935	UNK	PHE	conflict	UNP Q92608
A	936	UNK	VAL	conflict	UNP Q92608
A	937	UNK	ALA	conflict	UNP Q92608
A	938	UNK	CYS	conflict	UNP Q92608
A	939	UNK	MET	conflict	UNP Q92608
A	940	UNK	THR	conflict	UNP Q92608
A	941	UNK	ALA	conflict	UNP Q92608
A	942	UNK	ILE	conflict	UNP Q92608
A	943	UNK	LEU	conflict	UNP Q92608
A	944	UNK	ASN	conflict	UNP Q92608
A	945	UNK	GLN	conflict	UNP Q92608
A	946	UNK	MET	conflict	UNP Q92608
A	947	UNK	GLY	conflict	UNP Q92608
A	948	UNK	ASP	conflict	UNP Q92608
A	949	UNK	GLN	conflict	UNP Q92608
A	950	UNK	HIS	conflict	UNP Q92608
A	951	UNK	TYR	conflict	UNP Q92608
A	952	UNK	SER	conflict	UNP Q92608
A	953	UNK	PHE	conflict	UNP Q92608
A	954	UNK	TYR	conflict	UNP Q92608
A	955	UNK	ILE	conflict	UNP Q92608
A	956	UNK	GLU	conflict	UNP Q92608
A	957	UNK	THR	conflict	UNP Q92608
A	958	UNK	PHE	conflict	UNP Q92608
A	959	UNK	GLN	conflict	UNP Q92608
A	960	UNK	THR	conflict	UNP Q92608
D	208	UNK	ASP	conflict	UNP Q92608
D	209	UNK	TYR	conflict	UNP Q92608
D	210	UNK	ALA	conflict	UNP Q92608
D	211	UNK	MET	conflict	UNP Q92608
D	212	UNK	TYR	conflict	UNP Q92608
D	213	UNK	SER	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	214	UNK	ARG	conflict	UNP Q92608
D	215	UNK	ILE	conflict	UNP Q92608
D	216	UNK	SER	conflict	UNP Q92608
D	217	UNK	SER	conflict	UNP Q92608
D	218	UNK	SER	conflict	UNP Q92608
D	219	UNK	PRO	conflict	UNP Q92608
D	220	UNK	THR	conflict	UNP Q92608
D	221	UNK	HIS	conflict	UNP Q92608
D	222	UNK	SER	conflict	UNP Q92608
D	223	UNK	LEU	conflict	UNP Q92608
D	224	UNK	TYR	conflict	UNP Q92608
D	225	UNK	VAL	conflict	UNP Q92608
D	226	UNK	PHE	conflict	UNP Q92608
D	227	UNK	VAL	conflict	UNP Q92608
D	228	UNK	ARG	conflict	UNP Q92608
D	229	UNK	ASN	conflict	UNP Q92608
D	230	UNK	PHE	conflict	UNP Q92608
D	231	UNK	VAL	conflict	UNP Q92608
D	232	UNK	CYS	conflict	UNP Q92608
D	233	UNK	ARG	conflict	UNP Q92608
D	234	UNK	ILE	conflict	UNP Q92608
D	235	UNK	GLY	conflict	UNP Q92608
D	236	UNK	GLU	conflict	UNP Q92608
D	237	UNK	ASP	conflict	UNP Q92608
D	238	UNK	ALA	conflict	UNP Q92608
D	239	UNK	GLU	conflict	UNP Q92608
D	240	UNK	LEU	conflict	UNP Q92608
D	241	UNK	PHE	conflict	UNP Q92608
D	242	UNK	MET	conflict	UNP Q92608
D	243	UNK	SER	conflict	UNP Q92608
D	244	UNK	LEU	conflict	UNP Q92608
D	245	UNK	TYR	conflict	UNP Q92608
D	246	UNK	ASP	conflict	UNP Q92608
D	247	UNK	PRO	conflict	UNP Q92608
D	248	UNK	ASN	conflict	UNP Q92608
D	249	UNK	LYS	conflict	UNP Q92608
D	250	UNK	GLN	conflict	UNP Q92608
D	251	UNK	THR	conflict	UNP Q92608
D	252	UNK	VAL	conflict	UNP Q92608
D	253	UNK	ILE	conflict	UNP Q92608
D	254	UNK	SER	conflict	UNP Q92608
D	255	UNK	GLU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	256	UNK	ASN	conflict	UNP Q92608
D	257	UNK	TYR	conflict	UNP Q92608
D	258	UNK	LEU	conflict	UNP Q92608
D	259	UNK	VAL	conflict	UNP Q92608
D	260	UNK	ARG	conflict	UNP Q92608
D	261	UNK	TRP	conflict	UNP Q92608
D	262	UNK	GLY	conflict	UNP Q92608
D	263	UNK	SER	conflict	UNP Q92608
D	264	UNK	ARG	conflict	UNP Q92608
D	265	UNK	GLY	conflict	UNP Q92608
D	266	UNK	PHE	conflict	UNP Q92608
D	267	UNK	PRO	conflict	UNP Q92608
D	268	UNK	LYS	conflict	UNP Q92608
D	269	UNK	GLU	conflict	UNP Q92608
D	270	UNK	ILE	conflict	UNP Q92608
D	271	UNK	GLU	conflict	UNP Q92608
D	272	UNK	MET	conflict	UNP Q92608
D	273	UNK	LEU	conflict	UNP Q92608
D	274	UNK	ASN	conflict	UNP Q92608
D	275	UNK	ASN	conflict	UNP Q92608
D	276	UNK	LEU	conflict	UNP Q92608
D	277	UNK	LYS	conflict	UNP Q92608
D	278	UNK	VAL	conflict	UNP Q92608
D	279	UNK	VAL	conflict	UNP Q92608
D	280	UNK	PHE	conflict	UNP Q92608
D	281	UNK	THR	conflict	UNP Q92608
D	282	UNK	ASP	conflict	UNP Q92608
D	283	UNK	LEU	conflict	UNP Q92608
D	284	UNK	GLY	conflict	UNP Q92608
D	285	UNK	ASN	conflict	UNP Q92608
D	286	UNK	LYS	conflict	UNP Q92608
D	287	UNK	ASP	conflict	UNP Q92608
D	288	UNK	LEU	conflict	UNP Q92608
D	289	UNK	ASN	conflict	UNP Q92608
D	290	UNK	ARG	conflict	UNP Q92608
D	291	UNK	ASP	conflict	UNP Q92608
D	292	UNK	LYS	conflict	UNP Q92608
D	293	UNK	ILE	conflict	UNP Q92608
D	294	UNK	TYR	conflict	UNP Q92608
D	295	UNK	LEU	conflict	UNP Q92608
D	296	UNK	ILE	conflict	UNP Q92608
D	297	UNK	CYS	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	298	UNK	GLN	conflict	UNP Q92608
D	299	UNK	ILE	conflict	UNP Q92608
D	300	UNK	VAL	conflict	UNP Q92608
D	301	UNK	ARG	conflict	UNP Q92608
D	302	UNK	VAL	conflict	UNP Q92608
D	303	UNK	GLY	conflict	UNP Q92608
D	304	UNK	LYS	conflict	UNP Q92608
D	305	UNK	MET	conflict	UNP Q92608
D	306	UNK	ASP	conflict	UNP Q92608
D	307	UNK	LEU	conflict	UNP Q92608
D	308	UNK	LYS	conflict	UNP Q92608
D	309	UNK	ASP	conflict	UNP Q92608
D	310	UNK	THR	conflict	UNP Q92608
D	311	UNK	GLY	conflict	UNP Q92608
D	312	UNK	ALA	conflict	UNP Q92608
D	313	UNK	LYS	conflict	UNP Q92608
D	314	UNK	LYS	conflict	UNP Q92608
D	315	UNK	CYS	conflict	UNP Q92608
D	316	UNK	THR	conflict	UNP Q92608
D	317	UNK	GLN	conflict	UNP Q92608
D	318	UNK	GLY	conflict	UNP Q92608
D	319	UNK	LEU	conflict	UNP Q92608
D	320	UNK	ARG	conflict	UNP Q92608
D	321	UNK	ARG	conflict	UNP Q92608
D	322	UNK	PRO	conflict	UNP Q92608
D	323	UNK	PHE	conflict	UNP Q92608
D	324	UNK	GLY	conflict	UNP Q92608
D	325	UNK	VAL	conflict	UNP Q92608
D	326	UNK	ALA	conflict	UNP Q92608
D	327	UNK	VAL	conflict	UNP Q92608
D	328	UNK	MET	conflict	UNP Q92608
D	329	UNK	ASP	conflict	UNP Q92608
D	330	UNK	ILE	conflict	UNP Q92608
D	331	UNK	THR	conflict	UNP Q92608
D	332	UNK	ASP	conflict	UNP Q92608
D	333	UNK	ILE	conflict	UNP Q92608
D	334	UNK	ILE	conflict	UNP Q92608
D	335	UNK	LYS	conflict	UNP Q92608
D	336	UNK	GLY	conflict	UNP Q92608
D	337	UNK	LYS	conflict	UNP Q92608
D	338	UNK	ALA	conflict	UNP Q92608
D	339	UNK	GLU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	340	UNK	SER	conflict	UNP Q92608
D	341	UNK	ASP	conflict	UNP Q92608
D	342	UNK	GLU	conflict	UNP Q92608
D	343	UNK	GLU	conflict	UNP Q92608
D	344	UNK	LYS	conflict	UNP Q92608
D	345	UNK	GLN	conflict	UNP Q92608
D	346	UNK	HIS	conflict	UNP Q92608
D	347	UNK	PHE	conflict	UNP Q92608
D	348	UNK	ILE	conflict	UNP Q92608
D	349	UNK	PRO	conflict	UNP Q92608
D	350	UNK	PHE	conflict	UNP Q92608
D	351	UNK	HIS	conflict	UNP Q92608
D	352	UNK	PRO	conflict	UNP Q92608
D	353	UNK	VAL	conflict	UNP Q92608
D	354	UNK	THR	conflict	UNP Q92608
D	355	UNK	ALA	conflict	UNP Q92608
D	356	UNK	GLU	conflict	UNP Q92608
D	357	UNK	ASN	conflict	UNP Q92608
D	358	UNK	ASP	conflict	UNP Q92608
D	359	UNK	PHE	conflict	UNP Q92608
D	360	UNK	LEU	conflict	UNP Q92608
D	361	UNK	HIS	conflict	UNP Q92608
D	362	UNK	SER	conflict	UNP Q92608
D	363	UNK	LEU	conflict	UNP Q92608
D	364	UNK	LEU	conflict	UNP Q92608
D	365	UNK	GLY	conflict	UNP Q92608
D	366	UNK	LYS	conflict	UNP Q92608
D	367	UNK	VAL	conflict	UNP Q92608
D	368	UNK	ILE	conflict	UNP Q92608
D	369	UNK	ALA	conflict	UNP Q92608
D	370	UNK	SER	conflict	UNP Q92608
D	371	UNK	LYS	conflict	UNP Q92608
D	372	UNK	GLY	conflict	UNP Q92608
D	373	UNK	ASP	conflict	UNP Q92608
D	374	UNK	SER	conflict	UNP Q92608
D	375	UNK	GLY	conflict	UNP Q92608
D	376	UNK	GLY	conflict	UNP Q92608
D	377	UNK	GLN	conflict	UNP Q92608
D	378	UNK	GLY	conflict	UNP Q92608
D	379	UNK	LEU	conflict	UNP Q92608
D	380	UNK	TRP	conflict	UNP Q92608
D	381	UNK	VAL	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	382	UNK	THR	conflict	UNP Q92608
D	383	UNK	MET	conflict	UNP Q92608
D	384	UNK	LYS	conflict	UNP Q92608
D	385	UNK	MET	conflict	UNP Q92608
D	386	UNK	LEU	conflict	UNP Q92608
D	387	UNK	VAL	conflict	UNP Q92608
D	388	UNK	GLY	conflict	UNP Q92608
D	389	UNK	ASP	conflict	UNP Q92608
D	390	UNK	ILE	conflict	UNP Q92608
D	391	UNK	ILE	conflict	UNP Q92608
D	392	UNK	GLN	conflict	UNP Q92608
D	393	UNK	ILE	conflict	UNP Q92608
D	394	UNK	ARG	conflict	UNP Q92608
D	395	UNK	LYS	conflict	UNP Q92608
D	396	UNK	ASP	conflict	UNP Q92608
D	397	UNK	TYR	conflict	UNP Q92608
D	398	UNK	PRO	conflict	UNP Q92608
D	399	UNK	HIS	conflict	UNP Q92608
D	400	UNK	LEU	conflict	UNP Q92608
D	401	UNK	VAL	conflict	UNP Q92608
D	402	UNK	ASP	conflict	UNP Q92608
D	403	UNK	ARG	conflict	UNP Q92608
D	404	UNK	THR	conflict	UNP Q92608
D	405	UNK	THR	conflict	UNP Q92608
D	406	UNK	VAL	conflict	UNP Q92608
D	407	UNK	VAL	conflict	UNP Q92608
D	408	UNK	ALA	conflict	UNP Q92608
D	409	UNK	ARG	conflict	UNP Q92608
D	410	UNK	LYS	conflict	UNP Q92608
D	411	UNK	LEU	conflict	UNP Q92608
D	610	UNK	LYS	conflict	UNP Q92608
D	611	UNK	LEU	conflict	UNP Q92608
D	612	UNK	THR	conflict	UNP Q92608
D	613	UNK	GLN	conflict	UNP Q92608
D	614	UNK	ASN	conflict	UNP Q92608
D	615	UNK	VAL	conflict	UNP Q92608
D	616	UNK	GLY	conflict	UNP Q92608
D	617	UNK	LEU	conflict	UNP Q92608
D	618	UNK	LEU	conflict	UNP Q92608
D	619	UNK	GLY	conflict	UNP Q92608
D	620	UNK	LEU	conflict	UNP Q92608
D	621	UNK	LEU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	622	UNK	LYS	conflict	UNP Q92608
D	623	UNK	TRP	conflict	UNP Q92608
D	624	UNK	ARG	conflict	UNP Q92608
D	625	UNK	MET	conflict	UNP Q92608
D	626	UNK	LYS	conflict	UNP Q92608
D	627	UNK	PRO	conflict	UNP Q92608
D	628	UNK	GLN	conflict	UNP Q92608
D	629	UNK	LEU	conflict	UNP Q92608
D	630	UNK	LEU	conflict	UNP Q92608
D	631	UNK	GLN	conflict	UNP Q92608
D	632	UNK	GLU	conflict	UNP Q92608
D	633	UNK	ASN	conflict	UNP Q92608
D	634	UNK	LEU	conflict	UNP Q92608
D	635	UNK	GLU	conflict	UNP Q92608
D	636	UNK	LYS	conflict	UNP Q92608
D	637	UNK	LEU	conflict	UNP Q92608
D	638	UNK	LYS	conflict	UNP Q92608
D	639	UNK	ILE	conflict	UNP Q92608
D	640	UNK	VAL	conflict	UNP Q92608
D	641	UNK	ASP	conflict	UNP Q92608
D	642	UNK	GLY	conflict	UNP Q92608
D	643	UNK	GLU	conflict	UNP Q92608
D	644	UNK	GLU	conflict	UNP Q92608
D	645	UNK	VAL	conflict	UNP Q92608
D	646	UNK	VAL	conflict	UNP Q92608
D	647	UNK	LYS	conflict	UNP Q92608
D	648	UNK	PHE	conflict	UNP Q92608
D	649	UNK	LEU	conflict	UNP Q92608
D	650	UNK	GLN	conflict	UNP Q92608
D	651	UNK	ASP	conflict	UNP Q92608
D	652	UNK	THR	conflict	UNP Q92608
D	653	UNK	LEU	conflict	UNP Q92608
D	654	UNK	ASP	conflict	UNP Q92608
D	655	UNK	ALA	conflict	UNP Q92608
D	656	UNK	LEU	conflict	UNP Q92608
D	657	UNK	PHE	conflict	UNP Q92608
D	658	UNK	ASN	conflict	UNP Q92608
D	691	UNK	HIS	conflict	UNP Q92608
D	692	UNK	PHE	conflict	UNP Q92608
D	693	UNK	ASN	conflict	UNP Q92608
D	694	UNK	THR	conflict	UNP Q92608
D	695	UNK	VAL	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	696	UNK	LEU	conflict	UNP Q92608
D	697	UNK	GLU	conflict	UNP Q92608
D	698	UNK	ALA	conflict	UNP Q92608
D	699	UNK	TYR	conflict	UNP Q92608
D	700	UNK	ILE	conflict	UNP Q92608
D	701	UNK	GLN	conflict	UNP Q92608
D	702	UNK	GLN	conflict	UNP Q92608
D	703	UNK	HIS	conflict	UNP Q92608
D	704	UNK	PHE	conflict	UNP Q92608
D	705	UNK	SER	conflict	UNP Q92608
D	706	UNK	ALA	conflict	UNP Q92608
D	707	UNK	THR	conflict	UNP Q92608
D	708	UNK	LEU	conflict	UNP Q92608
D	709	UNK	ALA	conflict	UNP Q92608
D	710	UNK	TYR	conflict	UNP Q92608
D	711	UNK	LYS	conflict	UNP Q92608
D	712	UNK	LYS	conflict	UNP Q92608
D	713	UNK	LEU	conflict	UNP Q92608
D	714	UNK	MET	conflict	UNP Q92608
D	715	UNK	THR	conflict	UNP Q92608
D	716	UNK	VAL	conflict	UNP Q92608
D	717	UNK	LEU	conflict	UNP Q92608
D	718	UNK	LYS	conflict	UNP Q92608
D	719	UNK	THR	conflict	UNP Q92608
D	720	UNK	TYR	conflict	UNP Q92608
D	721	UNK	LEU	conflict	UNP Q92608
D	722	UNK	ASP	conflict	UNP Q92608
D	723	UNK	THR	conflict	UNP Q92608
D	724	UNK	SER	conflict	UNP Q92608
D	725	UNK	SER	conflict	UNP Q92608
D	726	UNK	ARG	conflict	UNP Q92608
D	727	UNK	GLY	conflict	UNP Q92608
D	728	UNK	GLU	conflict	UNP Q92608
D	729	UNK	GLN	conflict	UNP Q92608
D	730	UNK	CYS	conflict	UNP Q92608
D	731	UNK	GLU	conflict	UNP Q92608
D	732	UNK	PRO	conflict	UNP Q92608
D	733	UNK	ILE	conflict	UNP Q92608
D	734	UNK	LEU	conflict	UNP Q92608
D	735	UNK	ARG	conflict	UNP Q92608
D	736	UNK	THR	conflict	UNP Q92608
D	737	UNK	LEU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	738	UNK	LYS	conflict	UNP Q92608
D	739	UNK	ALA	conflict	UNP Q92608
D	740	UNK	LEU	conflict	UNP Q92608
D	741	UNK	GLU	conflict	UNP Q92608
D	742	UNK	TYR	conflict	UNP Q92608
D	743	UNK	VAL	conflict	UNP Q92608
D	744	UNK	PHE	conflict	UNP Q92608
D	745	UNK	LYS	conflict	UNP Q92608
D	746	UNK	PHE	conflict	UNP Q92608
D	747	UNK	ILE	conflict	UNP Q92608
D	748	UNK	VAL	conflict	UNP Q92608
D	749	UNK	ARG	conflict	UNP Q92608
D	750	UNK	SER	conflict	UNP Q92608
D	751	UNK	ARG	conflict	UNP Q92608
D	752	UNK	THR	conflict	UNP Q92608
D	753	UNK	LEU	conflict	UNP Q92608
D	754	UNK	PHE	conflict	UNP Q92608
D	755	UNK	SER	conflict	UNP Q92608
D	756	UNK	GLN	conflict	UNP Q92608
D	757	UNK	LEU	conflict	UNP Q92608
D	758	UNK	TYR	conflict	UNP Q92608
D	759	UNK	GLU	conflict	UNP Q92608
D	760	UNK	GLY	conflict	UNP Q92608
D	761	UNK	LYS	conflict	UNP Q92608
D	762	UNK	GLU	conflict	UNP Q92608
D	763	UNK	GLN	conflict	UNP Q92608
D	764	UNK	MET	conflict	UNP Q92608
D	765	UNK	GLU	conflict	UNP Q92608
D	766	UNK	PHE	conflict	UNP Q92608
D	767	UNK	GLU	conflict	UNP Q92608
D	768	UNK	GLU	conflict	UNP Q92608
D	769	UNK	SER	conflict	UNP Q92608
D	770	UNK	MET	conflict	UNP Q92608
D	771	UNK	ARG	conflict	UNP Q92608
D	772	UNK	ARG	conflict	UNP Q92608
D	773	UNK	LEU	conflict	UNP Q92608
D	774	UNK	PHE	conflict	UNP Q92608
D	775	UNK	GLU	conflict	UNP Q92608
D	776	UNK	SER	conflict	UNP Q92608
D	777	UNK	ILE	conflict	UNP Q92608
D	778	UNK	ASN	conflict	UNP Q92608
D	779	UNK	ASN	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	780	UNK	LEU	conflict	UNP Q92608
D	781	UNK	MET	conflict	UNP Q92608
D	782	UNK	LYS	conflict	UNP Q92608
D	783	UNK	SER	conflict	UNP Q92608
D	784	UNK	GLN	conflict	UNP Q92608
D	785	UNK	TYR	conflict	UNP Q92608
D	786	UNK	LYS	conflict	UNP Q92608
D	787	UNK	THR	conflict	UNP Q92608
D	788	UNK	THR	conflict	UNP Q92608
D	789	UNK	ILE	conflict	UNP Q92608
D	790	UNK	LEU	conflict	UNP Q92608
D	791	UNK	LEU	conflict	UNP Q92608
D	792	UNK	GLN	conflict	UNP Q92608
D	793	UNK	VAL	conflict	UNP Q92608
D	794	UNK	ALA	conflict	UNP Q92608
D	795	UNK	ALA	conflict	UNP Q92608
D	796	UNK	LEU	conflict	UNP Q92608
D	797	UNK	LYS	conflict	UNP Q92608
D	798	UNK	TYR	conflict	UNP Q92608
D	799	UNK	ILE	conflict	UNP Q92608
D	800	UNK	PRO	conflict	UNP Q92608
D	801	UNK	SER	conflict	UNP Q92608
D	802	UNK	VAL	conflict	UNP Q92608
D	803	UNK	LEU	conflict	UNP Q92608
D	804	UNK	HIS	conflict	UNP Q92608
D	805	UNK	ASP	conflict	UNP Q92608
D	806	UNK	VAL	conflict	UNP Q92608
D	807	UNK	GLU	conflict	UNP Q92608
D	808	UNK	MET	conflict	UNP Q92608
D	809	UNK	VAL	conflict	UNP Q92608
D	810	UNK	PHE	conflict	UNP Q92608
D	811	UNK	ASP	conflict	UNP Q92608
D	812	UNK	ALA	conflict	UNP Q92608
D	813	UNK	LYS	conflict	UNP Q92608
D	814	UNK	LEU	conflict	UNP Q92608
D	815	UNK	LEU	conflict	UNP Q92608
D	816	UNK	SER	conflict	UNP Q92608
D	817	UNK	GLN	conflict	UNP Q92608
D	818	UNK	LEU	conflict	UNP Q92608
D	819	UNK	LEU	conflict	UNP Q92608
D	820	UNK	TYR	conflict	UNP Q92608
D	821	UNK	GLU	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	822	UNK	PHE	conflict	UNP Q92608
D	823	UNK	TYR	conflict	UNP Q92608
D	824	UNK	THR	conflict	UNP Q92608
D	825	UNK	CYS	conflict	UNP Q92608
D	826	UNK	ILE	conflict	UNP Q92608
D	827	UNK	PRO	conflict	UNP Q92608
D	828	UNK	PRO	conflict	UNP Q92608
D	829	UNK	VAL	conflict	UNP Q92608
D	830	UNK	LYS	conflict	UNP Q92608
D	831	UNK	LEU	conflict	UNP Q92608
D	832	UNK	GLN	conflict	UNP Q92608
D	833	UNK	LYS	conflict	UNP Q92608
D	834	UNK	GLN	conflict	UNP Q92608
D	835	UNK	LYS	conflict	UNP Q92608
D	836	UNK	VAL	conflict	UNP Q92608
D	837	UNK	GLN	conflict	UNP Q92608
D	838	UNK	SER	conflict	UNP Q92608
D	839	UNK	MET	conflict	UNP Q92608
D	840	UNK	ASN	conflict	UNP Q92608
D	841	UNK	GLU	conflict	UNP Q92608
D	842	UNK	ILE	conflict	UNP Q92608
D	843	UNK	VAL	conflict	UNP Q92608
D	844	UNK	GLN	conflict	UNP Q92608
D	845	UNK	SER	conflict	UNP Q92608
D	846	UNK	ASN	conflict	UNP Q92608
D	847	UNK	LEU	conflict	UNP Q92608
D	848	UNK	PHE	conflict	UNP Q92608
D	849	UNK	LYS	conflict	UNP Q92608
D	850	UNK	LYS	conflict	UNP Q92608
D	851	UNK	GLN	conflict	UNP Q92608
D	852	UNK	GLU	conflict	UNP Q92608
D	853	UNK	CYS	conflict	UNP Q92608
D	854	UNK	ARG	conflict	UNP Q92608
D	855	UNK	ASP	conflict	UNP Q92608
D	856	UNK	ILE	conflict	UNP Q92608
D	857	UNK	LEU	conflict	UNP Q92608
D	858	UNK	LEU	conflict	UNP Q92608
D	859	UNK	PRO	conflict	UNP Q92608
D	860	UNK	VAL	conflict	UNP Q92608
D	861	UNK	ILE	conflict	UNP Q92608
D	862	UNK	THR	conflict	UNP Q92608
D	863	UNK	LYS	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	864	UNK	GLU	conflict	UNP Q92608
D	865	UNK	LEU	conflict	UNP Q92608
D	866	UNK	LYS	conflict	UNP Q92608
D	867	UNK	GLU	conflict	UNP Q92608
D	868	UNK	LEU	conflict	UNP Q92608
D	869	UNK	LEU	conflict	UNP Q92608
D	870	UNK	GLU	conflict	UNP Q92608
D	871	UNK	GLN	conflict	UNP Q92608
D	872	UNK	LYS	conflict	UNP Q92608
D	873	UNK	ASP	conflict	UNP Q92608
D	874	UNK	ASP	conflict	UNP Q92608
D	875	UNK	MET	conflict	UNP Q92608
D	876	UNK	GLN	conflict	UNP Q92608
D	877	UNK	HIS	conflict	UNP Q92608
D	878	UNK	GLN	conflict	UNP Q92608
D	879	UNK	VAL	conflict	UNP Q92608
D	880	UNK	LEU	conflict	UNP Q92608
D	881	UNK	GLU	conflict	UNP Q92608
D	882	UNK	ARG	conflict	UNP Q92608
D	883	UNK	LYS	conflict	UNP Q92608
D	884	UNK	TYR	conflict	UNP Q92608
D	885	UNK	CYS	conflict	UNP Q92608
D	886	UNK	VAL	conflict	UNP Q92608
D	887	UNK	GLU	conflict	UNP Q92608
D	888	UNK	LEU	conflict	UNP Q92608
D	889	UNK	LEU	conflict	UNP Q92608
D	890	UNK	ASN	conflict	UNP Q92608
D	891	UNK	SER	conflict	UNP Q92608
D	892	UNK	ILE	conflict	UNP Q92608
D	893	UNK	LEU	conflict	UNP Q92608
D	894	UNK	GLU	conflict	UNP Q92608
D	895	UNK	VAL	conflict	UNP Q92608
D	896	UNK	LEU	conflict	UNP Q92608
D	897	UNK	SER	conflict	UNP Q92608
D	898	UNK	TYR	conflict	UNP Q92608
D	899	UNK	GLN	conflict	UNP Q92608
D	900	UNK	ASP	conflict	UNP Q92608
D	901	UNK	ALA	conflict	UNP Q92608
D	902	UNK	ALA	conflict	UNP Q92608
D	903	UNK	PHE	conflict	UNP Q92608
D	904	UNK	THR	conflict	UNP Q92608
D	905	UNK	TYR	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	906	UNK	HIS	conflict	UNP Q92608
D	907	UNK	HIS	conflict	UNP Q92608
D	908	UNK	ILE	conflict	UNP Q92608
D	909	UNK	GLN	conflict	UNP Q92608
D	910	UNK	GLU	conflict	UNP Q92608
D	911	UNK	ILE	conflict	UNP Q92608
D	912	UNK	MET	conflict	UNP Q92608
D	913	UNK	VAL	conflict	UNP Q92608
D	914	UNK	GLN	conflict	UNP Q92608
D	915	UNK	LEU	conflict	UNP Q92608
D	916	UNK	LEU	conflict	UNP Q92608
D	917	UNK	ARG	conflict	UNP Q92608
D	918	UNK	THR	conflict	UNP Q92608
D	919	UNK	VAL	conflict	UNP Q92608
D	920	UNK	ASN	conflict	UNP Q92608
D	921	UNK	ARG	conflict	UNP Q92608
D	922	UNK	THR	conflict	UNP Q92608
D	923	UNK	VAL	conflict	UNP Q92608
D	924	UNK	ILE	conflict	UNP Q92608
D	925	UNK	THR	conflict	UNP Q92608
D	926	UNK	MET	conflict	UNP Q92608
D	927	UNK	GLY	conflict	UNP Q92608
D	928	UNK	ARG	conflict	UNP Q92608
D	929	UNK	ASP	conflict	UNP Q92608
D	930	UNK	HIS	conflict	UNP Q92608
D	931	UNK	ILE	conflict	UNP Q92608
D	932	UNK	LEU	conflict	UNP Q92608
D	933	UNK	ILE	conflict	UNP Q92608
D	934	UNK	SER	conflict	UNP Q92608
D	935	UNK	HIS	conflict	UNP Q92608
D	936	UNK	PHE	conflict	UNP Q92608
D	937	UNK	VAL	conflict	UNP Q92608
D	938	UNK	ALA	conflict	UNP Q92608
D	939	UNK	CYS	conflict	UNP Q92608
D	940	UNK	MET	conflict	UNP Q92608
D	941	UNK	THR	conflict	UNP Q92608
D	942	UNK	ALA	conflict	UNP Q92608
D	943	UNK	ILE	conflict	UNP Q92608
D	944	UNK	LEU	conflict	UNP Q92608
D	945	UNK	ASN	conflict	UNP Q92608
D	946	UNK	GLN	conflict	UNP Q92608
D	947	UNK	MET	conflict	UNP Q92608

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	948	UNK	GLY	conflict	UNP Q92608
D	949	UNK	ASP	conflict	UNP Q92608
D	950	UNK	GLN	conflict	UNP Q92608
D	951	UNK	HIS	conflict	UNP Q92608
D	952	UNK	TYR	conflict	UNP Q92608
D	953	UNK	SER	conflict	UNP Q92608
D	954	UNK	PHE	conflict	UNP Q92608
D	955	UNK	TYR	conflict	UNP Q92608
D	956	UNK	ILE	conflict	UNP Q92608
D	957	UNK	GLU	conflict	UNP Q92608
D	958	UNK	THR	conflict	UNP Q92608
D	959	UNK	PHE	conflict	UNP Q92608
D	960	UNK	GLN	conflict	UNP Q92608
D	961	UNK	THR	conflict	UNP Q92608

- Molecule 2 is a protein called Engulfment and cell motility protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	680	5067	3276	844	918	29	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	139	LEU	ARG	conflict	UNP Q92556

I548	K349	Q550	Q551	R552	L553	N554	R555	L556	V557	E558	G559	T560	C561	F562	R563	K564	L565	N566	A567	R568	R569	R570	Q571	D572	K573	F574	W575	Y576	C577	R578	L579	N582	H583	K584	V585	L586	H587	Y588	G589	D590	L591	E592	E593	S594	P595	Q596	G597	E598	V599	P600	H601	D602	S603	L604	Q605	D606	K607	L608		
P609	V610	A611	D612	I613	K614	A615	V616	V617	T618	G619	K620	D621	C622	P623	H624	MET	LYS	GLU	LYS	LYS	GLY	ALA	LEU	LYS	GLN	N634	K635	E636	V637	L638	E639	L640	A641	F642	S643	I644	L645	Y646	D647	S648	N649	C650	Q651	L652	N653	F654	I655	A656	P657	D658	K659	H660	E661	Y662	C663	I664	W665	T666	D667	G668
L669	M670	A671	L672	L673	G674	K675	D676	M677	M678	S679	D680	L681	T682	R683	N684	D685	L686	D687	T688	L689	L690	S691	M692	E693	I694	K695	L696	R697	L698	L699	D700	L701	E702	N703	I704	Q705	I706	P707	D708	A709	P710	P711	P712	I713	P714	K715	E716	P717	S718	N719	Y720	D721	F722	V723	Y724	D725	C726	ASN		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	154428	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.101	Depositor
Minimum map value	-0.031	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	403.25998, 403.25998, 403.25998	wwPDB
Map dimensions	282, 282, 282	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	Depositor

5 Model quality i

5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.97	11/8363 (0.1%)	0.76	15/11315 (0.1%)
1	D	0.58	1/3467 (0.0%)	0.62	1/4695 (0.0%)
2	B	2.03	9/5160 (0.2%)	0.77	14/6971 (0.2%)
All	All	1.33	21/16990 (0.1%)	0.74	30/22981 (0.1%)

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	16
1	D	0	2
2	B	0	11
All	All	0	29

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	722	PHE	CB-CG	81.33	2.89	1.51
2	B	724	TYR	CD1-CE1	63.56	2.34	1.39
2	B	724	TYR	CD2-CE2	59.40	2.28	1.39
1	A	4	TRP	CE3-CZ3	41.80	2.09	1.38
2	B	724	TYR	CE1-CZ	39.52	1.90	1.38
2	B	724	TYR	CE2-CZ	39.15	1.89	1.38
2	B	724	TYR	CG-CD1	31.34	1.79	1.39
2	B	724	TYR	CG-CD2	31.30	1.79	1.39
1	A	4	TRP	CE2-CZ2	27.00	1.85	1.39
1	A	4	TRP	CZ3-CH2	26.56	1.82	1.40
1	A	4	TRP	CD2-CE2	18.47	1.63	1.41
1	A	4	TRP	CZ2-CH2	14.41	1.64	1.37
1	A	5	ARG	C-N	13.05	1.64	1.34
1	A	4	TRP	CD2-CE3	12.79	1.59	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	LYS	N-CA	10.54	1.67	1.46
2	B	722	PHE	CG-CD1	10.29	1.54	1.38
2	B	722	PHE	CG-CD2	8.80	1.51	1.38
1	A	1481	TRP	CB-CG	-6.99	1.37	1.50
1	A	1249	TRP	CB-CG	-6.98	1.37	1.50
1	A	102	TRP	CB-CG	-6.98	1.37	1.50
1	D	1481	TRP	CB-CG	-5.57	1.40	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	ARG	C-N-CA	14.35	157.57	121.70
2	B	722	PHE	CB-CG-CD1	11.35	128.75	120.80
2	B	722	PHE	CD1-CG-CD2	-10.65	104.45	118.30
2	B	492	LEU	CA-CB-CG	-8.67	95.36	115.30
2	B	722	PHE	CB-CG-CD2	8.30	126.61	120.80
2	B	294	LEU	CA-CB-CG	-7.89	97.16	115.30
1	A	1280	LEU	CA-CB-CG	-7.73	97.51	115.30
1	A	1042	LEU	CA-CB-CG	6.82	130.98	115.30
2	B	232	LEU	CA-CB-CG	-6.58	100.17	115.30
1	A	175	PRO	N-CA-CB	6.41	110.99	103.30
1	A	207	PRO	N-CA-CB	5.98	110.48	103.30
1	A	414	PRO	N-CA-CB	5.83	110.30	103.30
2	B	722	PHE	CA-CB-CG	5.76	127.72	113.90
1	A	1153	LEU	CA-CB-CG	-5.67	102.26	115.30
2	B	30	LEU	CA-CB-CG	5.52	128.00	115.30
2	B	305	LEU	CA-CB-CG	-5.45	102.77	115.30
1	A	6	LYS	CB-CA-C	-5.42	99.55	110.40
2	B	724	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	A	131	LEU	CA-CB-CG	-5.42	102.84	115.30
2	B	722	PHE	CG-CD1-CE1	5.41	126.75	120.80
1	A	1157	LEU	CA-CB-CG	-5.40	102.88	115.30
2	B	724	TYR	CD1-CG-CD2	5.37	123.80	117.90
1	D	1227	LEU	CA-CB-CG	-5.37	102.95	115.30
2	B	400	LEU	CA-CB-CG	-5.32	103.06	115.30
1	A	6	LYS	N-CA-C	5.21	125.08	111.00
2	B	297	LEU	CA-CB-CG	-5.21	103.31	115.30
1	A	1415	LEU	CA-CB-CG	-5.17	103.42	115.30
1	A	1132	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	A	4	TRP	CE3-CZ3-CH2	-5.09	115.60	121.20
1	A	419	PRO	N-CA-CB	5.07	109.38	103.30

There are no chirality outliers.

All (29) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1042	LEU	Peptide
1	A	1047	PHE	Peptide
1	A	1223	TYR	Peptide
1	A	1309	GLU	Peptide
1	A	1428	ASP	Peptide
1	A	40	THR	Peptide
1	A	418	MET	Peptide
1	A	439	ASN	Peptide
1	A	45	TYR	Peptide
1	A	478	SER	Peptide
1	A	482	TYR	Peptide
1	A	5	ARG	Peptide
1	A	524	GLU	Peptide
1	A	547	HIS	Peptide
1	A	548	ASP	Peptide
1	A	597	ARG	Peptide
2	B	120	PHE	Peptide
2	B	171	VAL	Peptide
2	B	354	ARG	Peptide
2	B	56	SER	Peptide
2	B	57	SER	Peptide
2	B	621	ASP	Peptide
2	B	622	CYS	Peptide
2	B	647	ASP	Peptide
2	B	680	ASP	Peptide
2	B	720	TYR	Peptide
2	B	723	VAL	Peptide
1	D	1248	THR	Peptide
1	D	1427	PRO	Peptide

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10203	0	8228	1869	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3379	0	3224	591	0
2	B	5067	0	4741	1047	0
All	All	18649	0	16193	3370	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 97.

All (3370) 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)
2:B:724:TYR:CD1	2:B:724:TYR:CG	1.79	1.66
2:B:724:TYR:CG	2:B:724:TYR:CD2	1.79	1.64
2:B:724:TYR:CE2	2:B:724:TYR:CZ	1.89	1.61
1:A:4:TRP:CH2	1:A:4:TRP:CZ3	1.82	1.60
1:A:4:TRP:CE2	1:A:4:TRP:CZ2	1.85	1.58
2:B:724:TYR:CZ	2:B:724:TYR:CE1	1.89	1.56
1:A:4:TRP:CZ3	1:A:4:TRP:CE3	2.09	1.41
1:A:4:TRP:CE2	2:B:722:PHE:CG	2.10	1.39
1:A:6:LYS:N	2:B:724:TYR:CE2	1.90	1.34
1:A:6:LYS:N	2:B:724:TYR:CZ	1.95	1.32
1:A:6:LYS:N	2:B:724:TYR:CD2	1.96	1.31
1:A:6:LYS:N	2:B:724:TYR:CE1	2.03	1.26
1:A:4:TRP:CD2	2:B:722:PHE:CG	2.24	1.25
1:A:4:TRP:CZ2	2:B:722:PHE:CG	2.25	1.25
2:B:195:ILE:O	2:B:199:GLN:HB2	1.35	1.25
2:B:724:TYR:CD2	2:B:724:TYR:CE2	2.28	1.22
1:A:4:TRP:CE3	2:B:722:PHE:CG	2.28	1.21
1:A:4:TRP:CZ3	2:B:722:PHE:CB	2.22	1.21
1:A:4:TRP:CZ3	2:B:722:PHE:CG	2.27	1.21
1:D:1306:GLU:O	1:D:1310:MET:HB2	1.36	1.20
1:A:4:TRP:CH2	2:B:722:PHE:CG	2.30	1.19
1:A:6:LYS:N	2:B:724:TYR:CD1	2.11	1.17
1:A:6:LYS:N	2:B:724:TYR:CG	2.12	1.17
1:A:4:TRP:CE3	2:B:722:PHE:CB	2.29	1.16
2:B:724:TYR:CD1	2:B:724:TYR:CE1	2.34	1.15
2:B:12:ILE:O	2:B:19:PRO:HA	1.46	1.14
1:A:4:TRP:HA	2:B:723:VAL:HA	1.25	1.12
1:A:4:TRP:CH2	2:B:722:PHE:CB	2.32	1.11
1:A:4:TRP:CZ2	2:B:722:PHE:CB	2.36	1.09
1:A:4:TRP:CZ2	2:B:722:PHE:CD1	2.40	1.09
1:A:445:ASN:HB2	1:A:514:ARG:O	1.51	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:O	1:A:102:TRP:HB2	1.53	1.08
1:A:6:LYS:HA	2:B:724:TYR:CG	1.88	1.08
1:A:1175:VAL:O	1:A:1179:LYS:HB2	1.53	1.08
1:A:4:TRP:CE3	2:B:722:PHE:CD2	2.44	1.05
1:A:1566:LEU:O	1:A:1569:LEU:HB3	1.58	1.04
1:A:4:TRP:CH2	2:B:722:PHE:HB3	1.93	1.03
1:A:4:TRP:CE2	2:B:722:PHE:CB	2.40	1.02
1:D:1547:GLU:HA	1:D:1551:PHE:HB2	1.40	1.02
1:A:5:ARG:C	2:B:724:TYR:CD1	2.34	1.01
2:B:561:CYS:HA	2:B:576:TYR:HA	1.40	1.01
1:A:4:TRP:CD2	2:B:722:PHE:CB	2.43	1.01
1:A:1125:PHE:O	1:A:1128:PHE:HB3	1.61	1.01
2:B:38:CYS:HB3	2:B:43:LEU:HB2	1.43	1.00
2:B:409:HIS:HA	2:B:467:TRP:HZ2	1.24	0.99
1:A:1210:PHE:HA	1:A:1213:ASP:HB3	1.43	0.99
2:B:699:LEU:HA	2:B:702:GLU:HG2	1.43	0.99
2:B:97:MET:O	2:B:101:LEU:HB3	1.64	0.98
2:B:12:ILE:HB	2:B:20:LYS:O	1.61	0.98
1:A:1211:TYR:O	1:A:1215:ASN:N	1.97	0.98
1:A:4:TRP:CE3	2:B:722:PHE:HB2	1.93	0.97
1:A:289:UNK:HA	1:A:331:UNK:HA	1.43	0.97
1:A:1581:GLY:O	1:A:1585:LYS:N	1.98	0.96
1:A:5:ARG:C	2:B:724:TYR:CE1	2.39	0.96
1:A:182:SER:HA	1:A:185:HIS:HD2	1.29	0.95
1:A:1471:THR:HA	1:A:1485:VAL:H	1.30	0.95
1:A:6:LYS:CA	2:B:724:TYR:CD1	2.49	0.95
2:B:62:THR:O	2:B:66:ARG:N	1.99	0.95
1:A:547:HIS:HA	1:A:573:HIS:CE1	2.02	0.94
1:A:41:CYS:HB2	1:A:44:TRP:HB2	1.47	0.93
1:A:1467:THR:HA	1:A:1488:SER:O	1.67	0.93
2:B:298:GLN:HE22	2:B:442:HIS:H	1.04	0.93
2:B:195:ILE:O	2:B:199:GLN:CB	2.17	0.93
2:B:299:VAL:HG12	2:B:303:ASN:HD21	1.34	0.93
2:B:550:GLN:HA	2:B:553:LEU:HD12	1.50	0.93
2:B:329:ARG:O	2:B:333:ASP:N	2.02	0.92
1:D:1306:GLU:O	1:D:1310:MET:CB	2.17	0.92
1:D:1579:PHE:O	1:D:1583:GLY:N	2.03	0.92
1:A:227:UNK:HA	1:A:381:UNK:HA	1.49	0.92
2:B:254:ALA:O	2:B:259:ARG:NH2	2.03	0.92
1:A:82:PRO:O	1:A:85:ILE:N	2.02	0.92
1:A:1584:ILE:O	1:A:1588:GLU:N	2.02	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:GLN:NE2	2:B:322:ASP:OD1	2.03	0.92
2:B:313:MET:H	2:B:372:THR:HA	1.33	0.91
2:B:49:PHE:HA	2:B:78:THR:O	1.70	0.91
1:D:1211:TYR:HB2	1:D:1220:TYR:HD1	1.36	0.91
2:B:331:ALA:HA	2:B:396:ILE:HG12	1.51	0.91
1:A:1334:LYS:HE3	1:D:1316:GLU:HA	1.53	0.91
1:A:274:UNK:N	1:A:348:UNK:O	2.05	0.90
1:A:1202:SER:O	1:A:1206:ASN:ND2	2.04	0.90
2:B:118:GLN:HA	2:B:121:ILE:HD12	1.53	0.90
1:D:1567:THR:O	1:D:1571:ASP:N	2.05	0.90
1:A:41:CYS:HA	2:B:723:VAL:HG22	1.54	0.90
2:B:7:ILE:HD13	2:B:25:ASP:HA	1.55	0.89
1:A:5:ARG:O	2:B:724:TYR:CD1	2.25	0.89
1:A:1216:ARG:O	1:A:1220:TYR:N	2.05	0.89
2:B:548:ILE:O	2:B:552:ARG:NH1	2.06	0.89
2:B:645:LEU:HA	2:B:651:GLN:HB2	1.53	0.89
1:A:22:SER:H	1:A:26:GLN:HB2	1.37	0.88
1:A:1128:PHE:O	1:A:1132:ILE:N	2.05	0.88
1:A:1563:GLN:O	1:A:1566:LEU:HB2	1.74	0.88
1:D:1298:ILE:O	1:D:1325:GLN:NE2	2.07	0.87
1:A:5:ARG:C	2:B:724:TYR:CG	2.45	0.87
1:D:1244:LEU:HD22	1:D:1280:LEU:HD11	1.54	0.87
1:A:40:THR:HA	1:A:45:TYR:HA	1.54	0.87
1:A:1127:LYS:O	1:A:1131:GLU:N	2.07	0.87
1:D:1444:TYR:O	1:D:1467:THR:N	2.07	0.87
1:A:1417:GLU:HA	1:A:1422:LYS:HE3	1.57	0.87
2:B:110:LEU:O	2:B:113:ASP:N	2.07	0.87
1:D:1352:PHE:HB2	1:D:1357:ARG:HB3	1.53	0.87
1:A:1081:LYS:HE2	1:A:1115:MET:HA	1.56	0.86
2:B:557:VAL:HA	2:B:579:LEU:HB3	1.57	0.86
1:A:6:LYS:CA	2:B:724:TYR:CG	2.59	0.86
1:A:1207:LEU:HD22	1:A:1208:LEU:HD22	1.58	0.86
1:A:1231:HIS:NE2	1:A:1478:ILE:O	2.09	0.86
1:A:1525:ASN:O	1:A:1529:MET:HB3	1.76	0.86
1:A:950:UNK:O	1:A:954:UNK:N	2.09	0.86
1:A:1009:GLU:O	1:A:1013:GLN:NE2	2.07	0.86
2:B:292:HIS:ND1	2:B:438:CYS:O	2.08	0.85
2:B:641:ALA:O	2:B:662:TYR:OH	1.94	0.85
1:A:100:SER:O	1:A:104:GLN:NE2	2.09	0.85
2:B:487:GLN:O	2:B:491:ALA:N	2.09	0.85
1:A:449:ILE:N	1:A:510:MET:O	2.09	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:ALA:O	1:A:1548:LYS:N	2.10	0.85
1:D:1339:LYS:HE3	1:D:1368:TYR:HA	1.58	0.85
1:A:106:TYR:HH	2:B:552:ARG:HH12	1.24	0.85
1:A:549:LEU:HA	1:A:572:ARG:HB2	1.57	0.85
1:A:1196:SER:O	1:A:1200:ARG:N	2.10	0.85
2:B:488:VAL:O	2:B:492:LEU:N	2.09	0.85
1:A:1524:ILE:O	1:A:1528:SER:N	2.09	0.85
1:D:1319:SER:HA	1:D:1322:LEU:HD12	1.58	0.85
2:B:640:LEU:HD22	2:B:656:ALA:HB3	1.57	0.84
2:B:484:VAL:O	2:B:487:GLN:HB2	1.77	0.84
2:B:642:PHE:O	2:B:654:PHE:HB2	1.76	0.84
1:A:1350:GLN:HA	1:A:1357:ARG:HD3	1.59	0.84
1:A:425:ASP:HA	1:A:494:LYS:HE3	1.60	0.84
1:A:774:UNK:O	1:A:778:UNK:N	2.11	0.83
2:B:412:PRO:HB2	2:B:415:ARG:HB3	1.57	0.83
1:A:1277:LYS:HA	1:A:1280:LEU:HD12	1.57	0.83
2:B:568:ARG:O	2:B:571:GLN:NE2	2.10	0.83
1:A:432:GLN:HB2	1:A:600:PHE:HD1	1.44	0.83
1:A:1066:ILE:O	1:A:1069:SER:OG	1.95	0.83
1:A:1447:PRO:HB2	1:A:1449:ARG:HH12	1.41	0.83
1:A:1586:ILE:HA	1:A:1589:LYS:HD2	1.60	0.83
1:A:1573:ILE:O	1:A:1576:GLN:HB3	1.77	0.83
1:D:1211:TYR:HB3	1:D:1216:ARG:HB3	1.61	0.83
1:A:1322:LEU:HD22	1:D:1326:ALA:HB2	1.59	0.83
1:A:36:ARG:NH2	1:A:37:ILE:O	2.12	0.83
1:A:1024:GLN:HA	1:A:1027:ASN:HD22	1.43	0.83
1:A:1129:GLU:O	1:A:1132:ILE:HG22	1.79	0.83
1:A:4:TRP:CE2	2:B:722:PHE:N	2.46	0.83
1:D:1461:SER:HG	1:D:1463:TRP:HE1	1.23	0.83
1:A:447:GLU:HG3	1:A:477:ARG:HB3	1.60	0.82
1:D:1196:SER:N	1:D:1199:ASN:OD1	2.12	0.82
1:A:242:UNK:HA	1:A:297:UNK:HA	1.60	0.82
1:A:1210:PHE:O	1:A:1214:ASN:ND2	2.13	0.82
1:D:1396:ASP:HA	1:D:1399:LYS:HG3	1.60	0.82
1:A:4:TRP:CZ2	2:B:722:PHE:HD1	1.95	0.82
1:A:508:ARG:HH22	1:A:562:ALA:HA	1.43	0.82
2:B:331:ALA:HB1	2:B:399:VAL:HG11	1.62	0.82
1:A:977:LYS:HG2	1:A:1032:LEU:HD13	1.61	0.82
1:A:1072:ASP:HA	1:A:1075:TYR:CE1	2.15	0.82
1:A:166:ARG:NH1	1:A:167:ASP:O	2.12	0.81
1:D:1228:ARG:NH1	1:D:1229:ASP:OD1	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1316:GLU:OE1	1:D:1316:GLU:N	2.13	0.81
1:A:533:LYS:NZ	1:A:537:GLU:OE1	2.12	0.81
1:A:1042:LEU:HD22	1:A:1046:GLN:HG2	1.61	0.81
1:A:1253:TRP:HE3	1:A:1274:ARG:HB2	1.43	0.81
2:B:216:TYR:OH	2:B:250:LEU:O	1.99	0.81
2:B:534:LEU:HA	2:B:537:LYS:HD3	1.63	0.81
1:A:572:ARG:NH1	1:A:597:ARG:O	2.13	0.81
1:A:1043:GLN:O	1:A:1046:GLN:NE2	2.14	0.81
2:B:606:ASP:OD2	2:B:607:LYS:NZ	2.12	0.81
1:A:5:ARG:C	2:B:724:TYR:CD2	2.53	0.81
1:A:1354:SER:O	1:A:1359:LYS:NZ	2.12	0.81
1:A:1595:LEU:O	1:A:1599:HIS:N	2.14	0.81
2:B:320:GLN:HA	2:B:323:ILE:HD12	1.62	0.81
1:A:429:THR:O	1:A:603:SER:N	2.13	0.81
1:A:1225:TYR:O	1:A:1228:ARG:HG2	1.81	0.81
1:A:1350:GLN:O	1:A:1357:ARG:NH1	2.14	0.81
2:B:369:MET:O	2:B:373:GLN:NE2	2.13	0.81
2:B:692:MET:HA	2:B:695:LYS:HD3	1.61	0.81
1:A:1217:GLU:N	1:A:1217:GLU:OE1	2.14	0.81
1:A:1315:TYR:HA	1:A:1318:LEU:HD23	1.62	0.81
1:A:1278:GLU:HA	1:A:1281:TYR:HD2	1.45	0.81
2:B:306:GLU:O	2:B:310:MET:N	2.14	0.81
1:D:1394:PRO:HB2	1:D:1398:VAL:HG21	1.63	0.81
1:A:1007:PHE:O	1:A:1010:THR:OG1	1.99	0.81
2:B:106:ASP:O	2:B:109:SER:OG	1.99	0.81
2:B:599:VAL:HG22	2:B:601:HIS:HD2	1.46	0.81
2:B:193:ILE:H	2:B:198:LEU:HD22	1.46	0.80
2:B:356:TYR:O	2:B:364:HIS:ND1	2.14	0.80
1:A:1296:GLU:N	1:A:1296:GLU:OE1	2.11	0.80
1:D:1465:GLU:HA	1:D:1490:THR:O	1.81	0.80
1:A:1316:GLU:O	1:A:1319:SER:OG	1.99	0.80
2:B:56:SER:O	2:B:58:ASN:N	2.14	0.80
2:B:199:GLN:OE1	2:B:200:ARG:NH2	2.14	0.80
2:B:356:TYR:HA	2:B:359:LEU:HD13	1.62	0.80
1:A:4:TRP:CE2	2:B:722:PHE:CD1	2.69	0.80
1:A:430:LEU:HD21	1:A:600:PHE:HB3	1.63	0.80
1:A:1418:HIS:H	1:A:1422:LYS:HG3	1.45	0.80
1:A:19:PHE:O	1:A:29:LEU:N	2.14	0.80
1:D:1613:VAL:O	1:D:1617:TYR:N	2.15	0.80
1:A:1090:GLY:O	1:A:1093:LEU:N	2.14	0.80
1:A:1098:ILE:N	1:A:1102:GLU:OE2	2.14	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1539:VAL:HG23	1:A:1540:MET:HG3	1.63	0.80
1:D:1440:GLN:NE2	1:D:1471:THR:O	2.15	0.79
1:D:1248:THR:HB	1:D:1277:LYS:HE3	1.63	0.79
2:B:536:LEU:HD12	2:B:539:LYS:HB2	1.62	0.79
1:A:5:ARG:C	2:B:724:TYR:CZ	2.54	0.79
1:A:504:ARG:HD3	1:A:504:ARG:H	1.46	0.79
1:A:1372:GLU:OE1	1:A:1372:GLU:N	2.15	0.79
2:B:318:GLN:O	2:B:321:ARG:N	2.16	0.79
1:A:1205:VAL:HG22	1:A:1209:ASN:HD21	1.46	0.79
1:A:1301:CYS:HA	1:A:1304:LEU:HG	1.65	0.79
1:A:1238:THR:OG1	1:A:1239:GLU:OE1	1.99	0.79
1:A:1342:TYR:CE1	1:A:1413:PRO:HG3	2.17	0.79
2:B:617:VAL:HG21	2:B:621:ASP:HB2	1.65	0.79
1:A:1281:TYR:HA	1:A:1284:ILE:HD12	1.64	0.79
1:A:1289:ASP:OD1	1:A:1294:TRP:NE1	2.15	0.79
1:A:1480:ARG:HB2	1:A:1481:TRP:CE3	2.17	0.79
1:A:1239:GLU:HA	1:A:1242:TYR:HD2	1.48	0.79
1:A:1350:GLN:N	1:A:1401:ALA:O	2.16	0.78
2:B:298:GLN:NE2	2:B:442:HIS:H	1.80	0.78
1:D:1415:LEU:HD22	1:D:1435:LYS:HA	1.64	0.78
1:A:439:ASN:ND2	1:A:441:THR:OG1	2.17	0.78
1:D:1350:GLN:HA	1:D:1357:ARG:HH21	1.47	0.78
1:D:1453:VAL:HG22	1:D:1461:SER:HB3	1.65	0.78
1:A:1216:ARG:NE	1:A:1216:ARG:HA	1.96	0.78
1:A:6:LYS:CA	2:B:724:TYR:CE1	2.67	0.78
1:A:1157:LEU:O	1:A:1161:ALA:HB2	1.84	0.78
1:A:1337:ARG:HD2	1:A:1433:PHE:HB2	1.66	0.78
1:A:1412:GLN:N	1:A:1443:HIS:O	2.12	0.78
1:A:913:UNK:HA	1:A:968:PHE:CZ	2.18	0.78
1:A:1254:SER:O	1:A:1273:HIS:ND1	2.13	0.78
2:B:548:ILE:HD11	2:B:685:ASP:HB2	1.66	0.78
1:D:1342:TYR:OH	1:D:1436:SER:O	2.01	0.78
1:A:1209:ASN:HA	1:A:1212:LYS:HE2	1.64	0.78
1:A:232:UNK:N	1:A:272:UNK:O	2.17	0.77
1:A:473:MET:N	1:A:476:TYR:OH	2.16	0.77
2:B:287:ASN:O	2:B:291:ALA:N	2.16	0.77
2:B:376:PRO:HB2	2:B:379:LEU:HB3	1.67	0.77
1:A:501:ASP:HA	1:A:504:ARG:CZ	2.14	0.77
1:A:998:ARG:O	1:A:1001:LEU:HB3	1.83	0.77
2:B:306:GLU:HA	2:B:309:MET:HB3	1.65	0.77
2:B:460:ILE:HD12	2:B:463:LEU:HD13	1.65	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1443:HIS:HB3	1:D:1466:ARG:HD2	1.65	0.77
1:A:156:ASN:O	1:A:160:GLU:N	2.17	0.77
1:A:536:LYS:N	1:A:540:THR:O	2.16	0.77
1:A:1382:PHE:HB2	1:A:1385:ALA:HB2	1.67	0.77
2:B:551:GLN:OE1	2:B:552:ARG:NH1	2.18	0.77
1:A:106:TYR:OH	2:B:548:ILE:HA	1.84	0.77
1:A:1443:HIS:HB3	1:A:1466:ARG:HH21	1.49	0.77
2:B:530:SER:HB3	2:B:533:ILE:HD12	1.66	0.77
1:D:1304:LEU:HB3	1:D:1308:TYR:CZ	2.20	0.77
1:D:1453:VAL:HG13	1:D:1460:ALA:HB3	1.66	0.77
1:A:966:VAL:HG13	1:A:1025:LEU:HD22	1.67	0.77
1:A:1179:LYS:HA	1:A:1182:LEU:HD12	1.67	0.77
1:A:1214:ASN:OD1	1:A:1216:ARG:HG2	1.85	0.77
2:B:194:ASP:HB3	2:B:197:ILE:HG12	1.65	0.77
2:B:245:ALA:HA	2:B:248:ASN:HD22	1.50	0.77
1:A:1132:ILE:O	1:A:1136:LEU:N	2.13	0.77
1:A:1601:ARG:NH1	1:A:1601:ARG:O	2.18	0.77
2:B:551:GLN:HB3	2:B:552:ARG:NH1	1.99	0.77
1:D:1511:MET:SD	1:D:1514:ASN:ND2	2.57	0.77
1:A:6:LYS:HA	2:B:724:TYR:CD1	2.20	0.77
1:A:1313:PHE:HD2	1:D:1427:PRO:HD2	1.49	0.77
1:A:1394:PRO:O	1:A:1399:LYS:NZ	2.18	0.77
1:D:1428:ASP:O	1:D:1431:ILE:N	2.18	0.77
1:A:635:UNK:O	1:A:639:UNK:N	2.18	0.76
1:A:1328:PHE:O	1:A:1331:SER:N	2.18	0.76
2:B:186:SER:O	2:B:190:LYS:N	2.17	0.76
2:B:402:ASN:HB3	2:B:410:GLU:HA	1.67	0.76
2:B:292:HIS:NE2	2:B:436:GLU:HA	2.00	0.76
1:A:4:TRP:CZ3	2:B:722:PHE:HB3	2.17	0.76
1:A:106:TYR:OH	2:B:552:ARG:NH1	2.18	0.76
2:B:174:ASP:OD1	2:B:174:ASP:N	2.16	0.76
1:A:1152:LEU:O	1:A:1155:SER:OG	2.03	0.76
1:D:1301:CYS:HB2	1:D:1325:GLN:NE2	2.01	0.76
1:A:4:TRP:CE3	2:B:722:PHE:HD2	2.03	0.76
1:A:1235:ASP:OD1	1:A:1237:TYR:OH	2.03	0.76
1:A:1591:VAL:HG23	1:A:1595:LEU:HG	1.68	0.76
1:D:1254:SER:H	1:D:1273:HIS:HB2	1.48	0.76
1:D:1370:ARG:HG3	1:D:1372:GLU:H	1.49	0.76
1:D:1611:MET:O	1:D:1615:LYS:N	2.17	0.76
1:A:1200:ARG:NH2	1:A:1233:ASP:OD2	2.19	0.76
2:B:402:ASN:ND2	2:B:411:CYS:SG	2.59	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1227:LEU:HA	1:D:1230:LEU:HB2	1.67	0.76
1:A:546:PHE:O	1:A:573:HIS:NE2	2.18	0.76
1:A:46:ARG:HE	2:B:726:CYS:HB3	1.50	0.76
1:A:1576:GLN:HG2	1:A:1580:LEU:HG	1.65	0.76
2:B:181:ILE:HA	2:B:184:ILE:HG12	1.67	0.76
1:A:2:ALA:H	2:B:721:ASP:HB3	1.52	0.75
1:A:110:LYS:HE2	1:A:112:GLU:HG2	1.68	0.75
1:D:1583:GLY:O	1:D:1587:HIS:N	2.18	0.75
1:A:1506:ASN:HA	1:A:1509:ILE:HD12	1.68	0.75
1:A:1568:HIS:O	1:A:1571:ASP:HB3	1.86	0.75
1:A:1582:ALA:O	1:A:1585:LYS:HB2	1.86	0.75
1:D:1222:ARG:HG2	1:D:1226:LYS:HE3	1.66	0.75
1:A:6:LYS:CA	2:B:724:TYR:CD2	2.70	0.75
1:A:969:LEU:O	1:A:972:THR:OG1	2.03	0.75
1:A:1248:THR:HA	1:A:1251:LEU:HD22	1.68	0.75
1:A:1595:LEU:HD12	1:A:1598:PHE:HB3	1.67	0.75
1:A:1525:ASN:O	1:A:1529:MET:CB	2.34	0.75
2:B:360:GLY:O	2:B:413:PHE:N	2.19	0.75
1:D:1464:ILE:O	1:D:1491:THR:HA	1.87	0.75
2:B:356:TYR:HB3	2:B:361:PHE:HE2	1.51	0.75
1:D:1275:GLN:HA	1:D:1278:GLU:HB3	1.69	0.75
2:B:225:ILE:O	2:B:228:LEU:N	2.20	0.75
2:B:437:THR:O	2:B:563:ARG:NH1	2.19	0.75
2:B:452:PHE:O	2:B:455:PHE:N	2.19	0.75
2:B:564:LYS:HB2	2:B:573:LYS:HA	1.68	0.75
1:D:1248:THR:HG22	1:D:1251:LEU:HB3	1.68	0.75
1:A:471:LYS:O	1:A:476:TYR:OH	2.03	0.75
2:B:477:PHE:O	2:B:480:VAL:HB	1.87	0.75
1:D:1563:GLN:HA	1:D:1566:LEU:HB2	1.69	0.75
1:A:45:TYR:HE2	1:A:61:LYS:HA	1.52	0.75
1:A:330:UNK:O	1:A:334:UNK:N	2.20	0.75
2:B:296:VAL:HG12	2:B:300:LEU:HD21	1.68	0.75
1:D:1244:LEU:HB3	1:D:1280:LEU:HD21	1.69	0.75
1:A:1445:SER:OG	1:A:1466:ARG:NH1	2.20	0.75
1:A:1457:ASN:HB3	1:A:1549:ALA:HB2	1.68	0.75
2:B:156:SER:O	2:B:160:THR:OG1	2.03	0.74
1:A:95:LEU:HA	1:A:98:TRP:HB2	1.69	0.74
1:A:1297:ALA:HA	1:A:1300:LEU:HD22	1.68	0.74
1:A:1375:GLN:NE2	1:A:1379:MET:SD	2.60	0.74
2:B:88:LEU:HD22	2:B:103:ALA:HB1	1.69	0.74
2:B:451:SER:HA	2:B:454:GLU:HG2	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TRP:O	1:A:102:TRP:CB	2.35	0.74
2:B:38:CYS:O	2:B:43:LEU:N	2.20	0.74
1:D:1462:MET:HB2	1:D:1494:PRO:HB3	1.70	0.74
1:A:974:ILE:HA	1:A:977:LYS:HD2	1.67	0.74
1:A:4:TRP:CE2	2:B:722:PHE:CA	2.71	0.74
1:A:102:TRP:CZ2	1:A:118:GLN:HB2	2.22	0.74
1:A:1221:ILE:HA	1:A:1224:LEU:HD12	1.69	0.74
1:A:1542:GLY:O	1:A:1546:TYR:N	2.16	0.74
2:B:310:MET:C	2:B:374:THR:HG21	2.08	0.74
1:D:1288:PHE:O	1:D:1292:LYS:N	2.19	0.74
1:A:12:HIS:HB2	1:A:69:VAL:HG21	1.69	0.74
1:A:536:LYS:HE2	1:A:543:HIS:HD2	1.53	0.74
1:A:548:ASP:H	1:A:573:HIS:HE1	1.34	0.74
1:A:970:MET:HG3	1:A:1028:ASN:HD22	1.52	0.74
1:A:1127:LYS:HA	1:A:1130:ASN:ND2	2.01	0.74
1:A:1392:SER:OG	1:A:1393:ALA:N	2.20	0.74
1:A:237:UNK:HA	1:A:263:UNK:N	2.03	0.74
1:A:1433:PHE:HE1	1:A:1437:ASN:HB2	1.52	0.74
1:D:1211:TYR:O	1:D:1215:ASN:N	2.21	0.74
1:D:1471:THR:HG22	1:D:1484:VAL:HG13	1.69	0.74
1:A:129:SER:O	1:A:133:SER:N	2.19	0.74
2:B:7:ILE:HA	2:B:24:ILE:O	1.87	0.74
1:A:444:ARG:HG3	1:A:513:HIS:HA	1.67	0.74
1:A:1231:HIS:O	1:A:1236:ASN:ND2	2.20	0.74
1:A:105:LEU:O	1:A:109:SER:N	2.20	0.73
1:A:1212:LYS:NZ	1:A:1220:TYR:OH	2.16	0.73
1:A:1347:TYR:HB3	1:A:1352:PHE:HD2	1.53	0.73
1:A:1195:GLU:O	1:A:1200:ARG:NH1	2.21	0.73
2:B:54:ALA:H	2:B:75:LEU:HA	1.52	0.73
2:B:546:GLU:HA	2:B:549:LYS:HD2	1.69	0.73
1:A:1308:TYR:CG	1:A:1318:LEU:HB2	2.22	0.73
1:A:1601:ARG:NH1	1:A:1605:CYS:SG	2.62	0.73
1:D:1582:ALA:O	1:D:1585:LYS:HB3	1.87	0.73
1:D:1595:LEU:O	1:D:1599:HIS:N	2.21	0.73
1:A:547:HIS:HA	1:A:573:HIS:HE1	1.51	0.73
1:A:935:UNK:O	1:A:939:UNK:N	2.21	0.73
1:A:714:UNK:O	1:A:718:UNK:N	2.21	0.73
1:A:1350:GLN:OE1	1:A:1400:ASN:HA	1.88	0.73
2:B:298:GLN:O	2:B:301:THR:OG1	2.06	0.73
1:D:1231:HIS:CE1	1:D:1236:ASN:HD22	2.05	0.73
1:D:1238:THR:OG1	1:D:1239:GLU:OE1	2.07	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:O	2:B:207:SER:OG	2.05	0.73
2:B:503:LYS:HA	2:B:506:LEU:HG	1.68	0.73
2:B:622:CYS:HB3	2:B:624:HIS:CE1	2.23	0.73
1:D:1546:TYR:O	1:D:1551:PHE:N	2.20	0.73
2:B:372:THR:OG1	2:B:373:GLN:NE2	2.22	0.73
1:A:246:UNK:O	1:A:250:UNK:N	2.21	0.73
1:A:1378:LEU:HD23	1:A:1406:ILE:HG23	1.71	0.73
2:B:10:VAL:HG12	2:B:22:MET:O	1.89	0.73
1:A:130:GLN:O	1:A:133:SER:OG	2.06	0.73
2:B:129:LEU:HD22	2:B:158:THR:HG23	1.69	0.73
2:B:618:THR:HA	2:B:642:PHE:HA	1.70	0.73
1:A:965:LEU:O	1:A:969:LEU:HG	1.89	0.72
1:A:1293:MET:SD	1:A:1337:ARG:NH1	2.61	0.72
1:D:1353:PRO:HD2	1:D:1356:LEU:HB2	1.71	0.72
1:D:1573:ILE:O	1:D:1576:GLN:HB3	1.88	0.72
1:A:688:UNK:O	1:A:692:UNK:N	2.21	0.72
1:A:689:UNK:O	1:A:693:UNK:N	2.23	0.72
2:B:256:ASP:O	2:B:260:GLN:N	2.21	0.72
2:B:551:GLN:HB3	2:B:552:ARG:HH12	1.52	0.72
1:A:896:UNK:O	1:A:900:UNK:N	2.21	0.72
1:A:907:UNK:O	1:A:910:UNK:N	2.22	0.72
1:A:1065:LEU:HA	1:A:1068:PHE:CD2	2.25	0.72
1:A:1470:VAL:O	1:A:1485:VAL:N	2.22	0.72
1:A:4:TRP:CZ3	2:B:722:PHE:HB2	2.22	0.72
1:A:5:ARG:C	2:B:724:TYR:CE2	2.62	0.72
1:A:1083:CYS:O	1:A:1087:GLY:N	2.22	0.72
1:A:1342:TYR:OH	1:A:1436:SER:O	2.07	0.72
1:A:1349:GLY:N	1:A:1398:VAL:O	2.23	0.72
2:B:199:GLN:HB3	2:B:200:ARG:CZ	2.20	0.72
2:B:298:GLN:HE22	2:B:442:HIS:N	1.84	0.72
2:B:488:VAL:HA	2:B:491:ALA:HB3	1.71	0.72
1:D:1584:ILE:O	1:D:1587:HIS:HB3	1.89	0.72
1:A:5:ARG:O	2:B:724:TYR:CE1	2.41	0.72
2:B:31:SER:HA	2:B:34:ILE:HB	1.69	0.72
2:B:206:GLU:O	2:B:209:VAL:HB	1.88	0.72
1:D:1316:GLU:O	1:D:1319:SER:OG	2.07	0.72
1:A:1220:TYR:HD2	1:A:1224:LEU:HD11	1.54	0.72
1:A:343:UNK:HA	1:A:382:UNK:HA	1.71	0.72
1:A:466:VAL:HB	1:A:471:LYS:HB2	1.70	0.72
1:A:1239:GLU:HA	1:A:1242:TYR:CD2	2.24	0.72
1:A:1440:GLN:HB2	1:A:1474:LYS:HA	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:UNK:H	1:A:349:UNK:HA	1.53	0.72
1:A:424:ASN:HD22	1:A:426:ILE:HD11	1.55	0.72
1:A:715:UNK:O	1:A:719:UNK:N	2.23	0.72
2:B:639:GLU:OE1	2:B:639:GLU:N	2.21	0.72
1:A:14:VAL:HG21	1:A:67:LYS:HE3	1.72	0.71
1:A:964:GLU:HG2	1:A:966:VAL:H	1.55	0.71
1:A:155:GLY:O	1:A:159:LEU:N	2.22	0.71
1:A:187:HIS:CE1	1:A:992:MET:HB2	2.25	0.71
1:A:1296:GLU:O	1:A:1299:SER:OG	2.07	0.71
2:B:292:HIS:HA	2:B:439:ASN:HA	1.71	0.71
1:D:1317:LEU:HD12	1:D:1320:GLN:HB2	1.73	0.71
1:A:1245:LEU:O	1:A:1249:TRP:CB	2.38	0.71
1:A:1532:ASN:HA	1:A:1535:VAL:HG12	1.71	0.71
1:A:432:GLN:HB2	1:A:600:PHE:CD1	2.25	0.71
1:A:1072:ASP:O	1:A:1076:LYS:CB	2.38	0.71
1:A:1375:GLN:HB2	1:A:1408:CYS:HG	1.56	0.71
1:D:1487:MET:N	1:D:1487:MET:SD	2.63	0.71
2:B:376:PRO:HD3	2:B:418:ILE:HG23	1.72	0.71
1:D:1231:HIS:NE2	1:D:1239:GLU:HG2	2.05	0.71
1:A:1353:PRO:O	1:A:1357:ARG:N	2.23	0.71
2:B:424:LEU:O	2:B:428:LEU:HG	1.90	0.71
1:D:1344:ALA:HB2	1:D:1411:VAL:HG13	1.72	0.71
1:A:1126:LYS:O	1:A:1130:ASN:N	2.20	0.71
2:B:551:GLN:HA	2:B:554:ASN:ND2	2.06	0.71
1:A:572:ARG:HD3	1:A:599:VAL:HG22	1.73	0.70
1:A:716:UNK:O	1:A:720:UNK:N	2.23	0.70
1:A:1537:PRO:HA	1:A:1540:MET:O	1.91	0.70
1:A:1610:LYS:NZ	1:A:1611:MET:SD	2.63	0.70
2:B:97:MET:O	2:B:101:LEU:CB	2.39	0.70
2:B:425:CYS:O	2:B:429:LYS:N	2.24	0.70
1:A:531:TYR:OH	1:A:564:ALA:O	2.02	0.70
1:A:1551:PHE:HE1	1:A:1566:LEU:HB3	1.56	0.70
2:B:582:ASN:CG	2:B:584:LYS:H	1.95	0.70
2:B:705:GLN:NE2	2:B:706:ILE:O	2.24	0.70
1:A:1570:LYS:HA	1:A:1573:ILE:HD12	1.74	0.70
1:A:13:GLY:N	1:A:35:VAL:O	2.24	0.70
1:A:43:ASP:O	1:A:60:PRO:HA	1.91	0.70
1:A:49:LEU:HB3	1:A:52:HIS:HD2	1.57	0.70
1:A:1109:PRO:HB3	1:A:1160:CYS:SG	2.32	0.70
1:A:1239:GLU:OE1	1:A:1239:GLU:N	2.18	0.70
2:B:498:SER:O	2:B:502:PHE:N	2.23	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:GLU:O	1:A:129:SER:OG	2.05	0.70
2:B:291:ALA:HA	2:B:294:LEU:HD12	1.74	0.70
1:D:1245:LEU:O	1:D:1249:TRP:N	2.12	0.70
1:A:106:TYR:HH	2:B:552:ARG:NH1	1.88	0.70
1:A:1475:LEU:HD12	1:A:1476:PRO:HA	1.74	0.70
2:B:6:ASP:O	2:B:26:GLN:N	2.24	0.70
2:B:564:LYS:N	2:B:573:LYS:O	2.23	0.70
1:A:696:UNK:O	1:A:700:UNK:N	2.24	0.70
1:A:1171:VAL:O	1:A:1174:PHE:HB2	1.92	0.70
1:A:1173:ASN:HA	1:A:1176:ASN:ND2	2.05	0.70
1:A:1197:LYS:O	1:A:1201:MET:HG2	1.92	0.70
2:B:196:SER:O	2:B:200:ARG:HG2	1.92	0.70
2:B:198:LEU:O	2:B:201:SER:OG	2.09	0.70
1:A:973:PHE:HA	1:A:976:PHE:CD2	2.26	0.70
2:B:251:PHE:CZ	2:B:262:MET:HG2	2.27	0.70
2:B:458:ILE:HG23	2:B:506:LEU:HD11	1.72	0.70
1:D:1242:TYR:HA	1:D:1245:LEU:HD12	1.74	0.70
1:A:480:VAL:HG13	1:A:514:ARG:HH12	1.56	0.69
1:A:508:ARG:NH1	1:A:559:MET:O	2.25	0.69
1:A:1427:PRO:HG2	1:D:1313:PHE:HB2	1.72	0.69
1:D:1208:LEU:HD21	1:D:1224:LEU:HD23	1.74	0.69
1:D:1357:ARG:NH1	1:D:1358:ASN:OD1	2.24	0.69
1:D:1462:MET:H	1:D:1494:PRO:HG3	1.57	0.69
1:A:126:GLU:HG3	1:A:127:TRP:CD1	2.26	0.69
1:A:1204:THR:O	1:A:1207:LEU:HB3	1.92	0.69
1:A:1316:GLU:O	1:A:1320:GLN:NE2	2.26	0.69
1:A:1536:ASP:HB3	1:A:1539:VAL:HG22	1.73	0.69
2:B:574:PHE:HB3	2:B:591:LEU:HB2	1.74	0.69
1:A:1433:PHE:CE1	1:A:1437:ASN:HB2	2.27	0.69
2:B:184:ILE:HA	2:B:187:PHE:CD2	2.27	0.69
1:A:84:GLU:OE1	1:A:84:GLU:N	2.19	0.69
1:A:780:UNK:O	1:A:784:UNK:N	2.25	0.69
1:A:1397:ASP:O	1:A:1401:ALA:N	2.25	0.69
1:D:1556:VAL:O	1:D:1563:GLN:NE2	2.25	0.69
1:A:41:CYS:O	1:A:44:TRP:N	2.24	0.69
1:A:1314:ASP:OD1	1:A:1315:TYR:N	2.25	0.69
1:D:1396:ASP:O	1:D:1400:ASN:N	2.26	0.69
1:A:62:SER:HB3	2:B:713:ILE:HA	1.75	0.69
1:A:452:VAL:O	1:A:460:LEU:N	2.26	0.69
1:A:1240:ALA:O	1:A:1243:THR:OG1	2.05	0.69
1:A:1244:LEU:HB3	1:A:1284:ILE:HG12	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1484:VAL:HG12	1:D:1486:HIS:H	1.58	0.69
1:A:4:TRP:CZ3	2:B:722:PHE:CD2	2.81	0.69
1:A:5:ARG:HD3	2:B:723:VAL:HB	1.75	0.69
1:A:1433:PHE:O	1:A:1436:SER:N	2.26	0.69
1:A:1446:ARG:H	1:A:1464:ILE:HG23	1.58	0.69
2:B:24:ILE:HG23	2:B:33:ILE:HD12	1.75	0.69
2:B:113:ASP:CG	2:B:116:PHE:HB3	2.13	0.69
1:D:1421:PHE:HE2	1:D:1434:TYR:HE2	1.41	0.69
1:A:27:LEU:N	1:A:58:ILE:O	2.24	0.69
1:A:49:LEU:HB2	1:A:52:HIS:HB2	1.74	0.69
1:A:1205:VAL:HG13	1:A:1206:ASN:H	1.57	0.69
2:B:477:PHE:O	2:B:481:MET:HG2	1.92	0.69
1:D:1244:LEU:HD12	1:D:1287:TYR:HE2	1.57	0.69
1:D:1252:LYS:O	1:D:1273:HIS:HB3	1.93	0.68
1:D:1372:GLU:OE1	1:D:1372:GLU:N	2.26	0.68
1:D:1412:GLN:O	1:D:1443:HIS:N	2.22	0.68
1:D:1454:ASP:OD2	1:D:1457:ASN:ND2	2.27	0.68
1:D:1462:MET:N	1:D:1494:PRO:HG3	2.08	0.68
1:D:1572:LEU:O	1:D:1576:GLN:N	2.25	0.68
1:A:1024:GLN:O	1:A:1024:GLN:NE2	2.27	0.68
2:B:224:THR:HG1	2:B:227:GLN:H	1.41	0.68
1:A:1350:GLN:HB2	1:A:1402:PRO:HA	1.76	0.68
1:A:1395:GLY:O	1:A:1399:LYS:N	2.27	0.68
2:B:582:ASN:OD1	2:B:583:HIS:N	2.27	0.68
1:D:1348:TYR:HB3	1:D:1399:LYS:HA	1.75	0.68
1:D:1352:PHE:CB	1:D:1357:ARG:HB3	2.22	0.68
1:A:4:TRP:CZ2	2:B:722:PHE:N	2.60	0.68
1:A:45:TYR:CE2	1:A:61:LYS:HA	2.28	0.68
1:A:181:ILE:O	1:A:184:PHE:N	2.26	0.68
1:A:384:UNK:O	1:A:386:UNK:N	2.27	0.68
1:A:1384:ASN:HD22	1:A:1404:GLN:HG3	1.57	0.68
1:A:1441:ARG:HA	1:A:1469:PHE:O	1.93	0.68
1:A:1445:SER:HB3	1:A:1464:ILE:HG21	1.75	0.68
2:B:409:HIS:ND1	2:B:472:ALA:O	2.26	0.68
1:A:112:GLU:HG2	1:A:113:ARG:H	1.58	0.68
1:A:1443:HIS:HB3	1:A:1466:ARG:HE	1.59	0.68
2:B:177:SER:O	2:B:181:ILE:N	2.23	0.68
1:D:1562:ASP:O	1:D:1566:LEU:N	2.25	0.68
1:D:1578:PRO:O	1:D:1582:ALA:N	2.26	0.68
1:A:473:MET:HB2	1:A:476:TYR:CE1	2.29	0.68
1:A:542:LEU:HD21	1:A:571:TYR:HE1	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:MET:HA	1:A:997:ASN:ND2	2.08	0.68
1:A:994:MET:HA	1:A:997:ASN:HD21	1.59	0.68
2:B:489:MET:O	2:B:493:THR:N	2.25	0.68
2:B:530:SER:O	2:B:534:LEU:N	2.25	0.68
1:D:1428:ASP:OD1	1:D:1429:GLN:N	2.27	0.68
1:A:985:TYR:HB3	1:A:989:TRP:CE3	2.28	0.68
1:A:1352:PHE:O	1:A:1357:ARG:NH1	2.27	0.68
1:A:1510:LEU:O	1:A:1514:ASN:ND2	2.27	0.68
2:B:357:LYS:HA	2:B:364:HIS:CG	2.29	0.68
1:A:1246:LEU:O	1:A:1249:TRP:HB3	1.94	0.68
1:A:1358:ASN:ND2	1:A:1399:LYS:O	2.24	0.68
1:A:4:TRP:HA	2:B:723:VAL:CA	2.14	0.68
1:A:105:LEU:HD22	1:A:110:LYS:HB3	1.76	0.68
1:A:545:GLY:N	1:A:604:THR:OG1	2.26	0.68
2:B:90:GLU:O	2:B:94:SER:N	2.27	0.68
1:D:1251:LEU:HG	1:D:1277:LYS:HD2	1.77	0.68
1:A:30:GLN:N	1:A:33:ASP:OD2	2.28	0.67
1:A:125:MET:SD	2:B:695:LYS:HG2	2.34	0.67
1:A:548:ASP:OD2	1:A:573:HIS:NE2	2.27	0.67
1:A:1362:ILE:O	1:A:1481:TRP:HB2	1.94	0.67
1:D:1354:SER:OG	1:D:1355:PHE:N	2.27	0.67
1:D:1364:ARG:HD2	1:D:1475:LEU:HG	1.75	0.67
1:A:44:TRP:CZ2	2:B:716:GLU:HB2	2.29	0.67
1:A:1068:PHE:O	1:A:1071:ARG:HG2	1.94	0.67
2:B:576:TYR:HB3	2:B:591:LEU:HG	1.76	0.67
1:D:1447:PRO:HA	1:D:1464:ILE:HA	1.75	0.67
1:A:453:CYS:HA	1:A:459:THR:HA	1.76	0.67
1:A:626:UNK:O	1:A:630:UNK:N	2.27	0.67
1:A:1440:GLN:NE2	1:A:1471:THR:O	2.28	0.67
1:A:112:GLU:H	1:A:112:GLU:CD	1.98	0.67
1:A:450:MET:O	1:A:475:GLU:HA	1.94	0.67
1:A:874:UNK:O	1:A:878:UNK:N	2.28	0.67
1:A:1034:VAL:O	1:A:1038:THR:OG1	2.12	0.67
1:A:1150:MET:HA	1:A:1153:LEU:HD12	1.77	0.67
1:A:1546:TYR:O	1:A:1550:PHE:N	2.25	0.67
1:D:1205:VAL:O	1:D:1209:ASN:ND2	2.27	0.67
1:A:1026:TRP:O	1:A:1029:TYR:HB3	1.92	0.67
2:B:7:ILE:N	2:B:26:GLN:HG2	2.09	0.67
2:B:207:SER:O	2:B:210:LEU:N	2.27	0.67
1:D:1371:ARG:NH2	1:D:1375:GLN:OE1	2.26	0.67
1:D:1531:LEU:O	1:D:1535:VAL:HB	1.94	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:UNK:N	1:A:384:UNK:O	2.28	0.67
1:A:1333:MET:HB3	1:D:1315:TYR:HB2	1.77	0.67
2:B:66:ARG:HA	2:B:69:ILE:HG13	1.77	0.67
1:A:985:TYR:HB3	1:A:989:TRP:HE3	1.60	0.67
1:A:1149:TYR:O	1:A:1153:LEU:HG	1.94	0.67
1:A:1338:PRO:HB3	1:A:1368:TYR:CE2	2.30	0.67
1:A:1494:PRO:O	1:A:1497:ASN:HB3	1.95	0.67
2:B:111:SER:OG	2:B:164:GLU:HB2	1.95	0.67
2:B:416:SER:HA	2:B:477:PHE:HZ	1.59	0.67
2:B:473:THR:OG1	2:B:475:GLU:OE1	2.08	0.67
2:B:566:ASN:O	2:B:569:ARG:NH2	2.27	0.67
1:D:1357:ARG:H	1:D:1359:LYS:HZ3	1.43	0.67
1:A:1195:GLU:O	1:A:1197:LYS:N	2.27	0.67
1:A:1308:TYR:HD1	1:A:1314:ASP:HB3	1.58	0.67
1:A:1469:PHE:HD1	1:A:1487:MET:HG2	1.59	0.67
2:B:202:LEU:HA	2:B:205:LEU:HD12	1.76	0.67
1:D:1444:TYR:N	1:D:1467:THR:O	2.28	0.67
1:A:1017:GLU:O	1:A:1018:HIS:ND1	2.27	0.67
1:A:1136:LEU:HD22	1:A:1182:LEU:HD21	1.76	0.67
2:B:688:THR:O	2:B:691:SER:OG	2.09	0.67
1:D:1398:VAL:HG13	1:D:1405:TYR:HB2	1.77	0.67
1:A:1146:ASP:O	1:A:1149:TYR:N	2.20	0.67
1:A:1418:HIS:CD2	1:A:1434:TYR:HB3	2.30	0.67
2:B:575:TRP:HA	2:B:590:ASP:HA	1.77	0.67
1:D:1239:GLU:HG3	1:D:1478:ILE:HA	1.77	0.67
1:D:1500:GLU:O	1:D:1504:THR:HG23	1.95	0.67
1:A:25:PRO:O	1:A:58:ILE:N	2.27	0.66
2:B:139:LEU:HD22	2:B:155:LEU:HD13	1.76	0.66
2:B:510:SER:HB3	2:B:514:ILE:HD11	1.76	0.66
1:D:1445:SER:HA	1:D:1466:ARG:HA	1.77	0.66
1:A:350:UNK:HA	1:A:481:TYR:HD1	1.61	0.66
1:A:1068:PHE:HA	1:A:1071:ARG:NE	2.09	0.66
2:B:183:LYS:O	2:B:186:SER:OG	2.12	0.66
1:D:1577:ILE:O	1:D:1581:GLY:N	2.20	0.66
1:A:116:GLN:O	1:A:120:MET:HG3	1.95	0.66
1:A:1077:LEU:HD13	1:A:1080:ASN:HB3	1.77	0.66
1:A:1146:ASP:OD1	1:A:1149:TYR:N	2.29	0.66
1:A:1317:LEU:HA	1:A:1320:GLN:OE1	1.95	0.66
2:B:306:GLU:HG2	2:B:310:MET:HG2	1.77	0.66
2:B:416:SER:HA	2:B:477:PHE:CZ	2.30	0.66
1:A:5:ARG:CA	2:B:724:TYR:CE2	2.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:HIS:CD2	1:A:524:GLU:HB2	2.30	0.66
1:A:1184:LYS:HA	1:A:1187:ASP:OD2	1.96	0.66
1:A:1245:LEU:O	1:A:1249:TRP:HB2	1.95	0.66
1:A:1348:TYR:O	1:A:1405:TYR:HB2	1.94	0.66
1:A:1361:PHE:HB2	1:A:1363:TYR:HE1	1.59	0.66
1:A:1486:HIS:HE1	1:A:1488:SER:HB3	1.60	0.66
2:B:166:MET:HA	2:B:171:VAL:HG21	1.77	0.66
2:B:206:GLU:O	2:B:210:LEU:HG	1.94	0.66
2:B:673:LEU:HD23	2:B:675:LYS:HE2	1.76	0.66
1:A:23:GLY:N	1:A:26:GLN:O	2.27	0.66
1:A:147:LYS:O	1:A:150:SER:OG	2.14	0.66
1:A:1334:LYS:HZ1	1:D:1315:TYR:C	1.99	0.66
1:D:1256:GLU:H	1:D:1273:HIS:H	1.42	0.66
1:D:1307:GLN:O	1:D:1312:ILE:N	2.21	0.66
1:A:11:ARG:O	1:A:36:ARG:HD2	1.96	0.66
1:A:265:UNK:N	1:A:267:UNK:O	2.29	0.66
1:A:1186:LEU:HA	1:A:1189:ARG:HB3	1.76	0.66
1:A:1201:MET:SD	1:A:1230:LEU:HB3	2.35	0.66
1:A:1216:ARG:HB3	1:A:1219:MET:HB2	1.77	0.66
1:A:1382:PHE:HB3	1:A:1404:GLN:OE1	1.95	0.66
1:D:1348:TYR:HB2	1:D:1398:VAL:HG12	1.77	0.66
1:A:14:VAL:HG12	1:A:34:VAL:HG22	1.78	0.66
1:A:1242:TYR:OH	1:A:1476:PRO:O	2.13	0.66
2:B:409:HIS:HA	2:B:467:TRP:CZ2	2.17	0.66
1:A:990:MET:O	1:A:994:MET:HB3	1.96	0.66
1:A:1211:TYR:HB3	1:A:1220:TYR:CD1	2.30	0.66
1:A:1297:ALA:O	1:A:1300:LEU:HB2	1.96	0.66
1:A:1391:THR:HA	1:A:1407:GLN:HB2	1.78	0.66
1:A:1428:ASP:O	1:A:1431:ILE:N	2.19	0.66
1:A:116:GLN:O	1:A:119:SER:OG	2.14	0.66
1:A:778:UNK:O	1:A:782:UNK:N	2.29	0.66
1:A:1170:SER:HA	1:A:1173:ASN:ND2	2.10	0.66
1:A:1281:TYR:O	1:A:1284:ILE:HB	1.96	0.66
1:A:1414:VAL:HG22	1:A:1443:HIS:CD2	2.30	0.66
1:A:1424:LYS:NZ	1:A:1425:PRO:O	2.25	0.66
1:A:1496:GLU:O	1:A:1500:GLU:HG3	1.96	0.66
2:B:188:VAL:HA	2:B:198:LEU:HD21	1.77	0.66
2:B:576:TYR:OH	2:B:578:ARG:NE	2.28	0.66
1:A:527:PHE:HA	1:A:553:LYS:HD3	1.77	0.65
1:A:1254:SER:H	1:A:1273:HIS:CE1	2.14	0.65
1:A:1293:MET:O	1:A:1295:GLU:N	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:LEU:HD12	1:A:1321:ASN:ND2	2.12	0.65
2:B:87:GLN:HB3	2:B:91:ARG:CZ	2.25	0.65
2:B:695:LYS:O	2:B:699:LEU:HG	1.94	0.65
1:A:113:ARG:O	1:A:117:VAL:HG23	1.96	0.65
1:A:1497:ASN:O	1:A:1501:THR:HG23	1.97	0.65
2:B:162:PHE:HA	2:B:165:LEU:HD12	1.78	0.65
2:B:225:ILE:HA	2:B:228:LEU:HG	1.78	0.65
2:B:603:SER:O	2:B:606:ASP:HB2	1.96	0.65
1:D:1308:TYR:HA	1:D:1312:ILE:HG12	1.77	0.65
1:A:1042:LEU:HD13	1:A:1046:GLN:HB2	1.79	0.65
2:B:208:MET:HA	2:B:211:ASN:ND2	2.11	0.65
1:A:5:ARG:HA	2:B:724:TYR:CD2	2.31	0.65
1:A:12:HIS:NE2	1:A:36:ARG:HB2	2.12	0.65
1:A:1424:LYS:HE2	1:A:1425:PRO:HG2	1.78	0.65
2:B:225:ILE:O	2:B:229:ILE:HG13	1.96	0.65
1:D:1248:THR:HG22	1:D:1251:LEU:HD23	1.79	0.65
1:D:1272:THR:O	1:D:1276:LEU:HD13	1.95	0.65
1:A:565:TYR:HA	1:A:568:LEU:HD12	1.76	0.65
1:A:1557:ARG:NH1	1:A:1558:ASP:OD1	2.30	0.65
2:B:37:VAL:O	2:B:40:GLY:N	2.30	0.65
2:B:695:LYS:HA	2:B:698:LEU:HG	1.79	0.65
1:A:4:TRP:CD2	2:B:722:PHE:CD2	2.82	0.65
1:A:430:LEU:HG	1:A:601:SER:O	1.97	0.65
1:A:1171:VAL:HA	1:A:1174:PHE:CD1	2.31	0.65
1:A:1196:SER:O	1:A:1199:ASN:N	2.29	0.65
1:A:1246:LEU:HD11	1:A:1478:ILE:HD12	1.79	0.65
1:A:1496:GLU:HA	1:A:1499:ILE:HD12	1.78	0.65
2:B:292:HIS:O	2:B:296:VAL:HG23	1.96	0.65
1:D:1248:THR:HG21	1:D:1280:LEU:HD22	1.77	0.65
1:A:350:UNK:HA	1:A:481:TYR:CD1	2.32	0.65
1:A:1341:ASP:HB3	1:A:1343:PHE:CE1	2.32	0.65
2:B:466:THR:O	2:B:470:MET:N	2.29	0.65
2:B:548:ILE:HG23	2:B:552:ARG:CZ	2.26	0.65
2:B:658:ASP:OD1	2:B:661:GLU:N	2.17	0.65
1:D:1580:LEU:O	1:D:1584:ILE:N	2.30	0.65
1:A:548:ASP:N	1:A:573:HIS:HE1	1.95	0.65
1:A:1133:ILE:O	1:A:1136:LEU:HB2	1.97	0.65
1:A:1180:GLY:O	1:A:1184:LYS:HG2	1.97	0.65
2:B:360:GLY:N	2:B:364:HIS:HE1	1.95	0.65
1:D:1605:CYS:HA	1:D:1608:ASN:ND2	2.12	0.65
1:A:460:LEU:O	1:A:474:ASN:ND2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:ILE:HG22	1:A:465:CYS:H	1.62	0.65
1:A:1198:ASP:OD1	1:A:1198:ASP:N	2.30	0.65
1:A:1313:PHE:CD2	1:D:1427:PRO:HD2	2.31	0.65
2:B:276:LEU:O	2:B:281:ARG:N	2.20	0.65
1:A:1140:VAL:HG11	1:A:1185:LEU:HB3	1.79	0.64
1:A:1543:PHE:O	1:A:1546:TYR:HB2	1.97	0.64
2:B:401:GLU:HB3	2:B:405:ARG:HH21	1.60	0.64
1:D:1244:LEU:HB3	1:D:1284:ILE:HD11	1.78	0.64
1:D:1357:ARG:O	1:D:1359:LYS:NZ	2.24	0.64
1:A:118:GLN:HG3	1:A:122:TYR:CE2	2.32	0.64
1:A:546:PHE:HD1	1:A:601:SER:HB2	1.62	0.64
2:B:292:HIS:HB2	2:B:439:ASN:OD1	1.97	0.64
1:A:223:UNK:HA	1:A:386:UNK:N	2.12	0.64
1:A:1200:ARG:O	1:A:1204:THR:OG1	2.14	0.64
2:B:272:ARG:NE	2:B:449:ASP:OD1	2.31	0.64
2:B:295:TYR:O	2:B:299:VAL:HG23	1.98	0.64
2:B:532:PRO:HA	2:B:535:GLU:HG3	1.80	0.64
2:B:681:LEU:HD12	2:B:684:ASN:HD22	1.62	0.64
1:D:1601:ARG:NH1	1:D:1605:CYS:SG	2.71	0.64
1:A:1607:LYS:O	1:A:1611:MET:HG2	1.98	0.64
1:A:5:ARG:HA	2:B:724:TYR:CE2	2.33	0.64
1:A:1275:GLN:NE2	1:A:1279:THR:OG1	2.30	0.64
1:A:1607:LYS:HA	1:A:1610:LYS:HD3	1.80	0.64
2:B:670:ASN:HD22	2:B:677:MET:HA	1.63	0.64
1:D:1201:MET:HG2	1:D:1230:LEU:HD13	1.79	0.64
1:A:15:ALA:HB3	1:A:33:ASP:H	1.61	0.64
1:A:103:LYS:O	1:A:106:TYR:HB3	1.97	0.64
1:A:563:SER:OG	1:A:590:GLY:O	2.11	0.64
2:B:204:ILE:O	2:B:208:MET:HG3	1.98	0.64
2:B:452:PHE:CE1	2:B:456:PHE:HB2	2.33	0.64
1:D:1284:ILE:HA	1:D:1287:TYR:CD2	2.33	0.64
1:A:97:GLU:O	1:A:100:SER:OG	2.13	0.64
1:A:1227:LEU:HA	1:A:1230:LEU:HG	1.80	0.64
2:B:188:VAL:HA	2:B:198:LEU:HD11	1.79	0.64
2:B:439:ASN:OD1	2:B:563:ARG:NH2	2.31	0.64
1:D:1208:LEU:HA	1:D:1211:TYR:CD2	2.32	0.64
1:D:1580:LEU:HD22	1:D:1584:ILE:HG13	1.80	0.64
1:A:19:PHE:H	1:A:29:LEU:HB2	1.63	0.64
1:A:65:HIS:HE1	1:A:67:LYS:HB3	1.62	0.64
1:A:65:HIS:CE1	1:A:67:LYS:HB3	2.32	0.64
1:A:1023:PHE:O	1:A:1026:TRP:HB2	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1441:ARG:HG2	1:A:1470:VAL:HG12	1.79	0.64
2:B:166:MET:HA	2:B:171:VAL:HG11	1.80	0.64
2:B:660:HIS:O	2:B:664:ILE:HG12	1.98	0.64
1:D:1592:SER:HB3	1:D:1595:LEU:HG	1.79	0.64
1:A:144:LEU:O	1:A:148:VAL:HG23	1.97	0.64
1:A:1010:THR:OG1	1:A:1011:MET:N	2.29	0.64
1:A:1036:PHE:O	1:A:1039:GLN:N	2.27	0.64
1:A:1238:THR:HG1	1:A:1239:GLU:H	1.46	0.64
1:D:1607:LYS:O	1:D:1611:MET:HG2	1.97	0.64
1:A:1178:VAL:O	1:A:1182:LEU:HG	1.98	0.64
2:B:224:THR:OG1	2:B:227:GLN:N	2.19	0.64
2:B:226:GLY:HA2	2:B:229:ILE:HD12	1.79	0.64
2:B:414:GLY:O	2:B:417:SER:OG	2.15	0.64
1:D:1203:CYS:HA	1:D:1206:ASN:HD22	1.62	0.64
1:A:4:TRP:CH2	2:B:722:PHE:CD1	2.81	0.63
1:A:37:ILE:HA	1:A:47:GLY:HA3	1.79	0.63
1:A:1049:HIS:HA	1:A:1052:TYR:CD2	2.33	0.63
2:B:501:GLN:O	2:B:504:SER:OG	2.07	0.63
1:D:1285:ILE:HG13	1:D:1286:GLY:H	1.63	0.63
1:D:1553:GLU:N	1:D:1553:GLU:OE1	2.31	0.63
1:A:1200:ARG:HB3	1:A:1201:MET:HE2	1.80	0.63
1:A:1322:LEU:HD21	1:D:1322:LEU:C	2.18	0.63
1:A:1480:ARG:HB2	1:A:1481:TRP:HE3	1.61	0.63
1:A:1609:LEU:HA	1:A:1612:LYS:HD2	1.80	0.63
2:B:541:GLN:HE21	2:B:690:LEU:HD22	1.64	0.63
1:D:1525:ASN:O	1:D:1529:MET:HB2	1.99	0.63
1:A:1239:GLU:O	1:A:1243:THR:HG23	1.98	0.63
1:A:1253:TRP:CE3	1:A:1274:ARG:HB2	2.31	0.63
2:B:542:PRO:HA	2:B:545:LEU:HD12	1.78	0.63
1:D:1446:ARG:O	1:D:1464:ILE:HG13	1.99	0.63
1:A:155:GLY:O	1:A:158:ILE:N	2.31	0.63
1:A:767:UNK:O	1:A:770:UNK:CB	2.47	0.63
1:A:1201:MET:O	1:A:1204:THR:N	2.31	0.63
2:B:314:ASP:O	2:B:320:GLN:NE2	2.31	0.63
1:D:1303:GLU:O	1:D:1306:GLU:HB3	1.98	0.63
1:A:990:MET:O	1:A:994:MET:CB	2.46	0.63
1:A:1071:ARG:HG3	1:A:1075:TYR:CE2	2.34	0.63
2:B:303:ASN:HB3	2:B:431:GLY:HA2	1.80	0.63
1:D:1281:TYR:CD1	1:D:1284:ILE:HD12	2.34	0.63
1:D:1553:GLU:O	1:D:1557:ARG:HG2	1.99	0.63
1:A:111:LYS:HA	1:A:114:PHE:HB3	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLY:H	1:A:486:GLN:CD	2.01	0.63
1:A:1136:LEU:HD11	1:A:1178:VAL:HG13	1.81	0.63
1:A:1479:LEU:HD12	1:A:1480:ARG:H	1.64	0.63
2:B:272:ARG:HD2	2:B:446:PHE:HA	1.80	0.63
1:D:1211:TYR:HB2	1:D:1220:TYR:CD1	2.27	0.63
1:D:1220:TYR:O	1:D:1224:LEU:HG	1.97	0.63
1:D:1223:TYR:HA	1:D:1226:LYS:HG2	1.80	0.63
1:D:1479:LEU:HD12	1:D:1480:ARG:H	1.64	0.63
1:A:970:MET:HG3	1:A:1028:ASN:ND2	2.13	0.63
1:A:1207:LEU:HD21	1:A:1223:TYR:CD1	2.33	0.63
1:A:1275:GLN:NE2	1:A:1278:GLU:OE1	2.31	0.63
2:B:232:LEU:HD23	2:B:240:GLN:HA	1.81	0.63
2:B:237:GLN:O	2:B:241:THR:OG1	2.16	0.63
1:D:1555:TYR:CD2	1:D:1566:LEU:HD21	2.33	0.63
1:A:182:SER:HA	1:A:185:HIS:CD2	2.22	0.63
1:A:502:MET:HG2	1:A:534:LEU:HD23	1.80	0.63
1:A:433:GLY:N	1:A:486:GLN:OE1	2.30	0.63
1:A:1009:GLU:O	1:A:1012:ASN:HB3	1.99	0.63
1:A:1208:LEU:HD13	1:A:1211:TYR:HD2	1.64	0.63
1:A:1248:THR:O	1:A:1251:LEU:N	2.28	0.63
2:B:166:MET:HB3	2:B:173:TRP:CH2	2.34	0.63
2:B:199:GLN:HG2	2:B:242:TYR:CE2	2.34	0.63
2:B:361:PHE:HA	2:B:414:GLY:H	1.63	0.63
2:B:462:LEU:HA	2:B:465:LYS:HD3	1.81	0.63
1:D:1333:MET:SD	1:D:1429:GLN:HB3	2.39	0.63
2:B:64:LYS:O	2:B:68:GLU:N	2.32	0.62
2:B:299:VAL:O	2:B:303:ASN:ND2	2.31	0.62
1:A:505:ILE:O	1:A:534:LEU:HD13	1.99	0.62
1:A:1414:VAL:HG22	1:A:1443:HIS:NE2	2.14	0.62
1:A:1587:HIS:HE1	1:A:1595:LEU:HD21	1.63	0.62
2:B:199:GLN:HG3	2:B:239:ILE:HD13	1.81	0.62
2:B:202:LEU:HD13	2:B:242:TYR:HB3	1.81	0.62
2:B:402:ASN:OD1	2:B:405:ARG:NE	2.33	0.62
2:B:560:THR:H	2:B:577:CYS:HB3	1.64	0.62
1:D:1319:SER:O	1:D:1323:ILE:HG12	1.98	0.62
1:D:1371:ARG:HH12	1:D:1375:GLN:HB2	1.63	0.62
1:A:1296:GLU:O	1:A:1299:SER:N	2.32	0.62
1:A:1348:TYR:CZ	1:A:1394:PRO:HG3	2.34	0.62
1:A:1375:GLN:HB2	1:A:1408:CYS:SG	2.38	0.62
1:A:1582:ALA:HA	1:A:1585:LYS:HE2	1.81	0.62
1:D:1253:TRP:O	1:D:1274:ARG:NH1	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1577:ILE:HG21	1:D:1610:LYS:HG3	1.79	0.62
1:A:5:ARG:CA	2:B:724:TYR:CD2	2.82	0.62
1:A:45:TYR:CE2	1:A:64:ILE:HG13	2.35	0.62
1:A:152:ILE:O	1:A:156:ASN:ND2	2.32	0.62
1:A:1009:GLU:C	1:A:1013:GLN:HE22	2.03	0.62
1:A:1373:ASP:O	1:A:1377:GLN:HB2	2.00	0.62
2:B:381:LEU:O	2:B:384:MET:HG2	1.98	0.62
2:B:388:ALA:O	2:B:392:GLN:N	2.32	0.62
1:A:153:ASP:HA	1:A:156:ASN:HD22	1.63	0.62
1:A:1339:LYS:HG2	1:A:1340:PRO:HD2	1.80	0.62
1:D:1201:MET:SD	1:D:1230:LEU:HB3	2.40	0.62
1:D:1280:LEU:O	1:D:1283:THR:OG1	2.12	0.62
1:A:37:ILE:HD12	1:A:66:ILE:HD11	1.80	0.62
1:A:274:UNK:N	1:A:349:UNK:HA	2.15	0.62
1:A:1108:ILE:HA	1:A:1111:PHE:CD2	2.35	0.62
1:A:1239:GLU:O	1:A:1242:TYR:HB2	1.98	0.62
2:B:440:ASP:OD1	2:B:440:ASP:N	2.33	0.62
1:A:775:UNK:O	1:A:779:UNK:N	2.33	0.62
1:A:1237:TYR:HB3	1:A:1287:TYR:HD1	1.63	0.62
1:A:1354:SER:HA	1:A:1357:ARG:HB2	1.81	0.62
1:A:1379:MET:HA	1:A:1385:ALA:CB	2.29	0.62
1:A:1543:PHE:O	1:A:1547:GLU:N	2.28	0.62
1:A:1006:LYS:O	1:A:1010:THR:HG23	2.00	0.62
1:A:1255:ASP:N	1:A:1255:ASP:OD1	2.32	0.62
1:A:1341:ASP:HB3	1:A:1343:PHE:HE1	1.64	0.62
1:A:1429:GLN:HA	1:A:1432:ASN:ND2	2.15	0.62
2:B:575:TRP:HA	2:B:591:LEU:N	2.14	0.62
1:A:7:ALA:O	1:A:36:ARG:NH2	2.30	0.62
1:A:446:VAL:C	1:A:478:SER:HB2	2.20	0.62
1:A:1188:TYR:O	1:A:1192:MET:N	2.32	0.62
1:A:1248:THR:HA	1:A:1251:LEU:HD13	1.82	0.62
1:A:105:LEU:HA	1:A:108:ALA:HB3	1.82	0.62
1:A:1352:PHE:O	1:A:1357:ARG:HG3	2.00	0.62
1:A:1577:ILE:HA	1:A:1580:LEU:HD12	1.82	0.62
2:B:670:ASN:O	2:B:675:LYS:N	2.28	0.62
1:A:462:ASN:HA	1:A:473:MET:C	2.20	0.61
1:A:548:ASP:H	1:A:573:HIS:CE1	2.17	0.61
1:A:1020:ASN:C	1:A:1022:GLU:H	2.02	0.61
2:B:486:GLU:O	2:B:490:ARG:N	2.25	0.61
1:A:445:ASN:ND2	1:A:481:TYR:O	2.32	0.61
1:A:779:UNK:O	1:A:783:UNK:N	2.32	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:LYS:HG3	2:B:374:THR:HG23	1.81	0.61
1:D:1307:GLN:HB3	1:D:1312:ILE:HG23	1.81	0.61
1:A:102:TRP:NE1	1:A:114:PHE:O	2.28	0.61
1:A:444:ARG:HH21	1:A:447:GLU:C	2.03	0.61
1:A:445:ASN:CB	1:A:514:ARG:O	2.40	0.61
1:D:1390:THR:OG1	1:D:1407:GLN:NE2	2.33	0.61
2:B:168:HIS:O	2:B:170:ILE:N	2.33	0.61
1:D:1211:TYR:CD2	1:D:1220:TYR:HA	2.35	0.61
1:D:1354:SER:O	1:D:1359:LYS:NZ	2.32	0.61
1:D:1370:ARG:HB3	1:D:1373:ASP:CG	2.21	0.61
1:A:93:THR:HA	1:A:96:TRP:HD1	1.65	0.61
1:A:112:GLU:OE1	1:A:112:GLU:N	2.18	0.61
1:A:964:GLU:OE1	1:A:964:GLU:N	2.33	0.61
1:A:997:ASN:OD1	1:A:998:ARG:N	2.33	0.61
1:A:1000:PHE:O	1:A:1004:ILE:HG12	1.99	0.61
2:B:212:SER:OG	2:B:213:HIS:N	2.32	0.61
2:B:245:ALA:HB2	2:B:293:GLN:HG2	1.82	0.61
2:B:577:CYS:HA	2:B:588:TYR:HA	1.80	0.61
1:A:288:UNK:O	1:A:331:UNK:N	2.33	0.61
1:A:1181:LEU:O	1:A:1185:LEU:HG	2.00	0.61
1:A:1242:TYR:O	1:A:1246:LEU:HG	2.00	0.61
2:B:614:LYS:O	2:B:673:LEU:HD21	2.00	0.61
1:D:1349:GLY:HA2	1:D:1401:ALA:H	1.64	0.61
1:A:83:ALA:HA	1:A:86:PRO:HG2	1.81	0.61
1:A:991:ALA:O	1:A:994:MET:N	2.34	0.61
1:D:1238:THR:OG1	1:D:1239:GLU:N	2.32	0.61
1:D:1332:ILE:HG13	1:D:1333:MET:H	1.65	0.61
1:D:1348:TYR:HD1	1:D:1358:ASN:HD22	1.46	0.61
1:D:1582:ALA:O	1:D:1586:ILE:HG13	2.00	0.61
1:A:6:LYS:C	2:B:724:TYR:CE1	2.74	0.61
1:A:12:HIS:HA	1:A:36:ARG:HA	1.82	0.61
1:A:454:ALA:HA	1:A:505:ILE:HG22	1.81	0.61
1:A:1222:ARG:O	1:A:1226:LYS:HG3	2.00	0.61
2:B:587:HIS:HA	2:B:606:ASP:O	2.00	0.61
1:A:452:VAL:HG21	1:A:463:ALA:HB3	1.83	0.61
1:A:1208:LEU:C	1:A:1212:LYS:HZ3	2.04	0.61
2:B:259:ARG:HA	2:B:262:MET:HE3	1.81	0.61
2:B:420:LEU:O	2:B:424:LEU:HG	2.01	0.61
2:B:443:PRO:HA	2:B:446:PHE:HD1	1.66	0.61
1:A:36:ARG:CZ	1:A:38:GLN:HA	2.31	0.61
1:A:90:GLU:O	1:A:94:THR:OG1	2.12	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1049:HIS:HA	1:A:1052:TYR:HD2	1.65	0.61
1:A:1156:ILE:HA	1:A:1159:GLU:OE2	2.01	0.61
1:A:1282:GLU:HA	1:A:1285:ILE:HG12	1.81	0.61
1:A:1424:LYS:HG2	1:A:1425:PRO:HD2	1.83	0.61
2:B:234:GLY:O	2:B:240:GLN:NE2	2.34	0.61
1:D:1611:MET:HA	1:D:1614:GLU:HB2	1.82	0.61
2:B:12:ILE:CB	2:B:20:LYS:O	2.45	0.60
2:B:33:ILE:HA	2:B:36:GLU:HB3	1.81	0.60
2:B:328:ARG:HG3	2:B:359:LEU:HD21	1.81	0.60
1:A:46:ARG:CG	1:A:56:GLN:HG2	2.30	0.60
1:A:272:UNK:N	1:A:480:VAL:O	2.35	0.60
1:A:773:UNK:O	1:A:777:UNK:N	2.33	0.60
1:A:973:PHE:HB2	1:A:1028:ASN:ND2	2.16	0.60
1:A:1175:VAL:O	1:A:1179:LYS:CB	2.41	0.60
1:D:1418:HIS:HB2	1:D:1421:PHE:H	1.66	0.60
1:D:1577:ILE:HG13	1:D:1613:VAL:HG11	1.84	0.60
1:A:11:ARG:O	1:A:37:ILE:N	2.35	0.60
1:A:96:TRP:CH2	2:B:696:LEU:HB3	2.36	0.60
1:A:424:ASN:HB3	1:A:496:ALA:HB1	1.83	0.60
1:A:1348:TYR:CD1	1:A:1399:LYS:HG2	2.36	0.60
1:A:1516:TYR:CZ	1:A:1522:LEU:HB2	2.37	0.60
2:B:53:HIS:HA	2:B:75:LEU:CD1	2.30	0.60
1:D:1430:ILE:HG13	1:D:1431:ILE:N	2.14	0.60
1:A:6:LYS:HA	2:B:724:TYR:CD2	2.35	0.60
1:A:37:ILE:HA	1:A:47:GLY:CA	2.32	0.60
1:A:457:GLY:CA	1:A:508:ARG:HE	2.15	0.60
1:A:964:GLU:HG2	1:A:966:VAL:N	2.17	0.60
1:A:990:MET:HA	1:A:993:SER:OG	2.02	0.60
1:A:1090:GLY:HA2	1:A:1093:LEU:HD12	1.83	0.60
1:A:1361:PHE:CD1	1:A:1481:TRP:CD1	2.90	0.60
1:A:1366:LYS:N	1:A:1369:GLU:OE2	2.34	0.60
2:B:115:THR:OG1	2:B:116:PHE:N	2.32	0.60
1:D:1335:ILE:O	1:D:1429:GLN:NE2	2.34	0.60
1:D:1513:ILE:HG13	1:D:1514:ASN:N	2.17	0.60
1:A:82:PRO:O	1:A:86:PRO:HD2	2.02	0.60
1:A:455:GLU:OE2	1:A:533:LYS:HG3	2.02	0.60
1:A:531:TYR:CZ	1:A:565:TYR:HB3	2.37	0.60
1:A:1155:SER:OG	1:A:1156:ILE:N	2.34	0.60
1:A:1294:TRP:CE3	1:A:1332:ILE:HD11	2.36	0.60
1:A:1363:TYR:HA	1:A:1481:TRP:CB	2.31	0.60
2:B:118:GLN:O	2:B:122:ASN:ND2	2.35	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLN:HG2	2:B:242:TYR:CD2	2.37	0.60
2:B:354:ARG:C	2:B:356:TYR:H	2.03	0.60
2:B:652:LEU:HB3	2:B:654:PHE:CE2	2.36	0.60
1:D:1308:TYR:HA	1:D:1312:ILE:CG1	2.31	0.60
1:A:555:ASP:O	1:A:559:MET:HG2	2.01	0.60
1:A:713:UNK:O	1:A:717:UNK:N	2.34	0.60
1:A:977:LYS:HZ1	1:A:1031:HIS:HB2	1.67	0.60
1:A:1326:ALA:O	1:A:1330:GLU:N	2.23	0.60
2:B:8:VAL:HG22	2:B:26:GLN:OE1	2.00	0.60
1:D:1244:LEU:HD13	1:D:1280:LEU:HG	1.83	0.60
1:D:1440:GLN:HG3	1:D:1471:THR:OG1	2.02	0.60
1:A:67:LYS:NZ	2:B:701:LEU:HA	2.16	0.60
1:A:1180:GLY:HA2	1:A:1183:GLU:OE2	2.01	0.60
2:B:256:ASP:HA	2:B:259:ARG:HB3	1.84	0.60
2:B:579:LEU:HB2	2:B:586:LEU:HD12	1.83	0.60
1:A:82:PRO:HD2	1:A:85:ILE:HD12	1.84	0.60
1:A:431:LEU:HD21	1:A:603:SER:HB3	1.83	0.60
2:B:329:ARG:NH2	2:B:330:ILE:HA	2.17	0.60
1:D:1467:THR:HA	1:D:1488:SER:O	2.02	0.60
1:A:1208:LEU:O	1:A:1212:LYS:HG2	2.02	0.60
2:B:51:LEU:O	2:B:61:ILE:HG12	2.02	0.60
2:B:399:VAL:O	2:B:403:SER:OG	2.11	0.60
2:B:560:THR:N	2:B:577:CYS:HB3	2.17	0.60
1:A:39:GLU:O	1:A:46:ARG:N	2.25	0.59
1:A:453:CYS:HB2	1:A:457:GLY:C	2.23	0.59
1:A:555:ASP:HB2	1:A:558:LYS:HB3	1.84	0.59
1:A:1449:ARG:HG3	1:A:1462:MET:HG3	1.84	0.59
1:A:1547:GLU:O	1:A:1552:THR:HG23	2.02	0.59
2:B:322:ASP:OD1	2:B:322:ASP:N	2.34	0.59
1:A:88:ALA:C	1:A:128:ARG:HH21	2.06	0.59
1:A:511:PHE:H	1:A:512:ARG:NH1	1.99	0.59
1:A:526:ASN:O	1:A:553:LYS:HD3	2.02	0.59
1:A:544:ASP:N	1:A:544:ASP:OD1	2.21	0.59
1:A:964:GLU:C	1:A:966:VAL:H	2.05	0.59
1:A:1056:LEU:HA	1:A:1059:TYR:O	2.02	0.59
1:A:1127:LYS:O	1:A:1130:ASN:HB2	2.02	0.59
1:A:1174:PHE:HB3	1:A:1179:LYS:NZ	2.17	0.59
1:A:1327:LYS:C	1:A:1330:GLU:HB3	2.23	0.59
1:A:1371:ARG:NH1	1:A:1371:ARG:O	2.35	0.59
1:A:1542:GLY:N	1:A:1545:LYS:HG2	2.17	0.59
2:B:211:ASN:HB2	2:B:215:LEU:HD12	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:HIS:O	2:B:282:ALA:HB2	2.02	0.59
2:B:555:ARG:HA	2:B:558:GLU:CD	2.22	0.59
1:A:426:ILE:H	1:A:494:LYS:HE3	1.66	0.59
1:A:455:GLU:HA	1:A:506:HIS:CE1	2.38	0.59
1:A:529:MET:SD	1:A:530:SER:N	2.75	0.59
1:A:1175:VAL:HA	1:A:1179:LYS:CE	2.33	0.59
2:B:467:TRP:CE3	2:B:472:ALA:HB3	2.37	0.59
2:B:562:PHE:HB2	2:B:575:TRP:CE2	2.37	0.59
2:B:562:PHE:N	2:B:575:TRP:O	2.35	0.59
1:D:1319:SER:O	1:D:1322:LEU:HB2	2.02	0.59
1:A:1051:LYS:O	1:A:1055:ILE:HG12	2.03	0.59
2:B:564:LYS:NZ	2:B:572:ASP:O	2.28	0.59
2:B:685:ASP:O	2:B:689:LEU:HG	2.03	0.59
1:D:1440:GLN:O	1:D:1471:THR:OG1	2.12	0.59
1:A:102:TRP:HZ2	1:A:118:GLN:HB2	1.65	0.59
1:A:121:MET:O	1:A:125:MET:HG3	2.02	0.59
1:A:1011:MET:HA	1:A:1014:LYS:HZ3	1.67	0.59
2:B:48:TYR:O	2:B:80:SER:N	2.35	0.59
2:B:220:ALA:HA	2:B:223:ILE:HG12	1.85	0.59
2:B:467:TRP:O	2:B:471:ARG:N	2.36	0.59
1:A:40:THR:HA	1:A:45:TYR:CD1	2.37	0.59
1:A:508:ARG:NH2	1:A:562:ALA:HA	2.14	0.59
1:A:1188:TYR:HA	1:A:1191:VAL:HG22	1.84	0.59
1:A:1529:MET:HE1	2:B:40:GLY:HA2	1.83	0.59
2:B:85:ALA:HB1	2:B:123:LEU:HD22	1.85	0.59
1:D:1296:GLU:O	1:D:1300:LEU:HG	2.03	0.59
1:D:1581:GLY:HA3	1:D:1610:LYS:HZ3	1.66	0.59
1:A:91:VAL:O	1:A:95:LEU:HG	2.01	0.59
1:A:571:TYR:HB2	1:A:574:HIS:CG	2.37	0.59
1:A:1247:HIS:CE1	1:A:1280:LEU:HD13	2.37	0.59
1:A:1252:LYS:O	1:A:1273:HIS:NE2	2.35	0.59
1:A:1479:LEU:HD21	1:A:1481:TRP:CE2	2.38	0.59
2:B:39:ASP:N	2:B:39:ASP:OD1	2.32	0.59
2:B:652:LEU:HG	2:B:653:ASN:O	2.02	0.59
1:A:115:LEU:O	1:A:118:GLN:HB3	2.03	0.59
1:A:973:PHE:HB2	1:A:1028:ASN:HD21	1.67	0.59
2:B:247:ILE:HA	2:B:250:LEU:HG	1.85	0.59
1:A:138:LYS:N	1:A:138:LYS:HD2	2.16	0.59
1:A:429:THR:N	1:A:603:SER:O	2.33	0.59
1:A:535:MET:HA	1:A:541:THR:HA	1.84	0.59
1:A:1571:ASP:OD1	1:A:1620:ARG:NH1	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:GLN:HB3	2:B:91:ARG:NH2	2.17	0.59
2:B:479:LYS:HA	2:B:482:GLN:HB2	1.85	0.59
2:B:697:ARG:N	2:B:697:ARG:HD2	2.17	0.59
1:A:39:GLU:HB3	1:A:46:ARG:HB3	1.85	0.59
1:A:1315:TYR:HB3	1:D:1329:TYR:HB3	1.83	0.59
1:D:1207:LEU:HD13	1:D:1210:PHE:HD2	1.68	0.59
1:A:22:SER:N	1:A:26:GLN:HB2	2.12	0.58
1:A:1275:GLN:O	1:A:1278:GLU:HB3	2.03	0.58
1:A:1418:HIS:ND1	1:A:1434:TYR:HD2	2.00	0.58
2:B:139:LEU:HD13	2:B:155:LEU:HD22	1.84	0.58
2:B:575:TRP:HZ3	2:B:588:TYR:HB2	1.68	0.58
2:B:679:SER:O	2:B:682:THR:N	2.31	0.58
1:D:1279:THR:O	1:D:1283:THR:HG23	2.03	0.58
1:A:6:LYS:CA	2:B:724:TYR:CZ	2.85	0.58
1:A:82:PRO:HG2	1:A:85:ILE:HG13	1.84	0.58
1:A:118:GLN:HG3	1:A:122:TYR:HE2	1.68	0.58
1:A:1182:LEU:O	1:A:1186:LEU:HG	2.03	0.58
1:A:1412:GLN:HB2	1:A:1443:HIS:HB2	1.85	0.58
2:B:478:ASN:OD1	2:B:478:ASN:N	2.36	0.58
2:B:568:ARG:HB2	2:B:569:ARG:HD3	1.85	0.58
1:D:1281:TYR:CE1	1:D:1284:ILE:HD12	2.39	0.58
1:A:1361:PHE:CG	1:A:1481:TRP:CD1	2.91	0.58
1:D:1298:ILE:HG21	1:D:1329:TYR:HE2	1.68	0.58
1:D:1348:TYR:CD1	1:D:1358:ASN:HA	2.38	0.58
1:D:1530:LEU:O	1:D:1534:ILE:HG22	2.03	0.58
1:D:1569:LEU:HG	1:D:1573:ILE:HD11	1.85	0.58
1:A:542:LEU:HD21	1:A:571:TYR:CE1	2.38	0.58
1:A:1085:ILE:HD12	1:A:1085:ILE:H	1.67	0.58
1:A:1172:GLU:OE2	1:A:1176:ASN:ND2	2.35	0.58
1:A:1178:VAL:HG12	1:A:1182:LEU:HD11	1.84	0.58
1:D:1459:PHE:HB3	1:D:1550:PHE:CE1	2.38	0.58
1:D:1486:HIS:HE2	1:D:1488:SER:HB3	1.67	0.58
1:A:530:SER:HA	1:A:552:LEU:HD12	1.85	0.58
1:A:1348:TYR:HB3	1:A:1398:VAL:O	2.04	0.58
1:A:1605:CYS:HA	1:A:1608:ASN:ND2	2.18	0.58
2:B:196:SER:HA	2:B:200:ARG:NH2	2.19	0.58
2:B:483:VAL:O	2:B:486:GLU:HB2	2.04	0.58
2:B:588:TYR:OH	2:B:608:LEU:HB2	2.04	0.58
2:B:658:ASP:CG	2:B:660:HIS:HB3	2.23	0.58
2:B:722:PHE:HD2	2:B:725:ASP:HA	1.68	0.58
1:D:1446:ARG:HG3	1:D:1465:GLU:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1211:TYR:O	1:A:1214:ASN:N	2.33	0.58
1:A:1234:CYS:HB3	1:A:1236:ASN:HD21	1.68	0.58
1:A:1247:HIS:HE1	1:A:1280:LEU:HD22	1.67	0.58
1:A:1417:GLU:OE2	1:A:1419:PRO:HA	2.04	0.58
2:B:315:PRO:HD3	2:B:372:THR:CG2	2.33	0.58
2:B:329:ARG:HH21	2:B:330:ILE:HG12	1.67	0.58
2:B:544:ILE:HG22	2:B:689:LEU:HD12	1.84	0.58
1:A:563:SER:HA	1:A:566:LEU:HB2	1.86	0.58
1:A:1178:VAL:HB	1:A:1179:LYS:HZ3	1.69	0.58
2:B:259:ARG:HG3	2:B:262:MET:SD	2.44	0.58
2:B:464:ASN:O	2:B:468:LYS:HD2	2.03	0.58
2:B:681:LEU:O	2:B:684:ASN:HB3	2.04	0.58
1:A:106:TYR:HA	1:A:111:LYS:HZ2	1.68	0.58
1:A:142:LYS:HG3	1:A:143:GLU:N	2.19	0.58
1:A:533:LYS:HZ3	1:A:537:GLU:HA	1.68	0.58
1:A:595:SER:O	1:A:597:ARG:NH1	2.34	0.58
1:A:1579:PHE:HA	1:A:1582:ALA:HB3	1.83	0.58
2:B:435:SER:H	2:B:634:ASN:ND2	2.02	0.58
2:B:690:LEU:O	2:B:694:ILE:HG12	2.03	0.58
1:D:1196:SER:OG	1:D:1197:LYS:N	2.37	0.58
1:A:136:LEU:HB3	1:A:140:GLU:CG	2.34	0.58
1:A:854:UNK:O	1:A:858:UNK:CB	2.52	0.58
1:A:966:VAL:HA	1:A:969:LEU:HD12	1.86	0.58
1:A:1081:LYS:NZ	1:A:1117:CYS:HB3	2.18	0.58
1:A:1339:LYS:HD3	1:A:1340:PRO:O	2.02	0.58
1:A:1413:PRO:HA	1:A:1442:PHE:CD2	2.39	0.58
1:A:1546:TYR:HA	1:A:1550:PHE:HD2	1.69	0.58
2:B:411:CYS:HB2	2:B:413:PHE:CE1	2.38	0.58
2:B:572:ASP:CG	2:B:601:HIS:HE1	2.06	0.58
1:D:1376:MET:SD	1:D:1377:GLN:N	2.77	0.58
1:A:14:VAL:HB	2:B:701:LEU:HD11	1.86	0.58
1:A:226:UNK:N	1:A:382:UNK:O	2.36	0.58
1:A:1588:GLU:N	1:A:1599:HIS:HE1	2.02	0.58
2:B:356:TYR:HB3	2:B:361:PHE:CE2	2.37	0.58
2:B:388:ALA:HA	2:B:395:TYR:CG	2.39	0.58
1:D:1469:PHE:HA	1:D:1486:HIS:O	2.03	0.58
1:A:19:PHE:N	1:A:29:LEU:O	2.36	0.57
1:A:443:GLN:HG2	1:A:485:LYS:NZ	2.19	0.57
1:A:453:CYS:SG	1:A:457:GLY:HA2	2.44	0.57
1:A:543:HIS:HA	1:A:606:VAL:HG11	1.85	0.57
1:A:889:UNK:C	1:A:891:UNK:N	2.66	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:TYR:CE2	1:A:1224:LEU:HD21	2.39	0.57
1:A:1234:CYS:O	1:A:1366:LYS:NZ	2.36	0.57
1:A:1343:PHE:CD1	1:A:1410:THR:HA	2.39	0.57
1:A:1364:ARG:HB2	1:A:1475:LEU:HD21	1.85	0.57
2:B:10:VAL:HG22	2:B:11:ALA:O	2.04	0.57
2:B:129:LEU:HD13	2:B:162:PHE:HB2	1.86	0.57
1:D:1574:ALA:O	1:D:1578:PRO:HD3	2.04	0.57
1:A:1237:TYR:HA	1:A:1240:ALA:HB3	1.86	0.57
1:A:1424:LYS:HD2	1:D:1313:PHE:CE1	2.40	0.57
1:A:1426:VAL:HG22	1:D:1313:PHE:CZ	2.40	0.57
1:A:1580:LEU:O	1:A:1584:ILE:N	2.20	0.57
2:B:669:LEU:HD23	2:B:672:LEU:HD12	1.85	0.57
1:D:1495:LEU:O	1:D:1499:ILE:HG12	2.04	0.57
1:A:8:ASP:HA	1:A:36:ARG:HH12	1.69	0.57
1:A:274:UNK:C	1:A:349:UNK:HA	2.35	0.57
1:A:1134:LEU:O	1:A:1137:ASP:HB3	2.05	0.57
1:A:1220:TYR:O	1:A:1224:LEU:HG	2.04	0.57
1:A:1278:GLU:O	1:A:1281:TYR:HB2	2.04	0.57
2:B:543:GLU:O	2:B:547:LEU:HG	2.04	0.57
2:B:575:TRP:HE3	2:B:589:GLY:O	1.87	0.57
2:B:642:PHE:CZ	2:B:654:PHE:HB3	2.38	0.57
1:D:1345:VAL:HB	1:D:1347:TYR:OH	2.03	0.57
1:A:136:LEU:HB3	1:A:140:GLU:HG2	1.86	0.57
1:A:443:GLN:N	1:A:483:GLN:HE22	2.03	0.57
1:A:1148:GLN:O	1:A:1151:GLN:HB3	2.04	0.57
1:A:1310:MET:O	1:A:1313:PHE:HE1	1.87	0.57
1:A:1384:ASN:ND2	1:A:1404:GLN:HG3	2.20	0.57
2:B:476:ASP:O	2:B:480:VAL:HG23	2.02	0.57
2:B:513:GLU:HG3	2:B:514:ILE:HD13	1.86	0.57
1:D:1319:SER:CA	1:D:1322:LEU:HD12	2.33	0.57
1:D:1418:HIS:ND1	1:D:1421:PHE:HB2	2.18	0.57
1:A:6:LYS:CA	2:B:724:TYR:CE2	2.88	0.57
1:A:1088:MET:SD	1:A:1091:PRO:HB2	2.44	0.57
1:A:1207:LEU:HD11	1:A:1223:TYR:HD1	1.68	0.57
1:A:1486:HIS:CE1	1:A:1488:SER:HB3	2.39	0.57
2:B:444:MET:O	2:B:447:THR:OG1	2.21	0.57
2:B:668:GLY:O	2:B:672:LEU:HG	2.04	0.57
1:D:1241:ALA:HB1	1:D:1284:ILE:HG23	1.85	0.57
1:D:1475:LEU:HD12	1:D:1476:PRO:HA	1.86	0.57
1:A:536:LYS:HG3	1:A:542:LEU:HA	1.86	0.57
1:A:1087:GLY:O	1:A:1091:PRO:HG2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1403:GLY:HA3	1:A:1405:TYR:CZ	2.39	0.57
1:A:1443:HIS:HB3	1:A:1466:ARG:NH2	2.17	0.57
1:A:1479:LEU:C	1:A:1481:TRP:H	2.08	0.57
1:A:1584:ILE:HG23	1:A:1599:HIS:NE2	2.19	0.57
2:B:114:VAL:HG23	2:B:168:HIS:HB3	1.86	0.57
2:B:304:LEU:HB2	2:B:305:LEU:HG	1.86	0.57
1:D:1244:LEU:HD12	1:D:1287:TYR:CE2	2.38	0.57
1:D:1364:ARG:NH2	1:D:1437:ASN:OD1	2.27	0.57
1:A:446:VAL:O	1:A:478:SER:HB2	2.04	0.57
1:A:598:ASP:HB3	1:A:600:PHE:CE2	2.40	0.57
1:A:1342:TYR:OH	1:A:1437:ASN:OD1	2.12	0.57
1:A:1342:TYR:C	1:A:1343:PHE:HD1	2.07	0.57
1:A:1557:ARG:HG3	1:A:1558:ASP:N	2.18	0.57
2:B:107:LEU:HA	2:B:110:LEU:HG	1.87	0.57
2:B:309:MET:HE1	2:B:430:VAL:HB	1.87	0.57
2:B:562:PHE:HD2	2:B:575:TRP:O	1.88	0.57
1:D:1198:ASP:HA	1:D:1201:MET:HG3	1.85	0.57
1:D:1224:LEU:O	1:D:1228:ARG:HB2	2.04	0.57
1:D:1418:HIS:HB2	1:D:1421:PHE:N	2.20	0.57
1:A:92:THR:HG22	1:A:96:TRP:NE1	2.20	0.57
1:A:1301:CYS:CA	1:A:1304:LEU:HG	2.35	0.57
2:B:673:LEU:HB3	2:B:675:LYS:HG3	1.86	0.57
1:D:1197:LYS:O	1:D:1201:MET:HE3	2.04	0.57
1:D:1222:ARG:O	1:D:1226:LYS:HG2	2.05	0.57
1:D:1237:TYR:CZ	1:D:1290:LYS:HD2	2.40	0.57
1:D:1551:PHE:CD1	1:D:1566:LEU:HD12	2.39	0.57
1:A:27:LEU:HD22	1:A:56:GLN:HA	1.85	0.57
1:A:101:ILE:HA	1:A:104:GLN:HG2	1.86	0.57
1:A:444:ARG:NH1	1:A:511:PHE:HB3	2.20	0.57
1:A:1575:TRP:HE3	1:A:1620:ARG:HB3	1.69	0.57
2:B:255:PRO:O	2:B:259:ARG:N	2.20	0.57
2:B:568:ARG:C	2:B:569:ARG:HD3	2.24	0.57
1:A:11:ARG:HA	1:A:36:ARG:NH2	2.20	0.57
1:A:154:TYR:O	1:A:157:LYS:HB3	2.04	0.57
1:A:1593:ASP:OD1	1:A:1593:ASP:N	2.38	0.57
1:D:1225:TYR:O	1:D:1228:ARG:HB3	2.04	0.57
1:A:1209:ASN:HA	1:A:1212:LYS:CE	2.34	0.56
2:B:100:LYS:O	2:B:104:LEU:CB	2.53	0.56
2:B:415:ARG:NH2	2:B:477:PHE:HB3	2.21	0.56
2:B:590:ASP:HB3	2:B:601:HIS:CE1	2.40	0.56
1:D:1466:ARG:NE	1:D:1468:SER:OG	2.37	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1562:ASP:O	1:D:1565:LYS:HB2	2.04	0.56
1:A:448:VAL:O	1:A:477:ARG:HA	2.05	0.56
1:A:1312:ILE:HG23	1:A:1314:ASP:H	1.69	0.56
1:A:1447:PRO:HA	1:A:1464:ILE:HG12	1.87	0.56
2:B:90:GLU:CD	2:B:91:ARG:HG3	2.25	0.56
2:B:277:THR:O	2:B:281:ARG:HB2	2.04	0.56
2:B:486:GLU:O	2:B:490:ARG:HG3	2.05	0.56
1:D:1421:PHE:CE2	1:D:1434:TYR:HE2	2.21	0.56
1:D:1547:GLU:O	1:D:1552:THR:N	2.32	0.56
1:A:89:GLN:O	1:A:92:THR:HB	2.05	0.56
1:A:112:GLU:O	1:A:115:LEU:HG	2.04	0.56
1:A:118:GLN:HA	1:A:121:MET:HE3	1.87	0.56
1:A:432:GLN:HE22	1:A:599:VAL:HG12	1.71	0.56
1:A:1048:SER:OG	1:A:1049:HIS:N	2.37	0.56
1:A:1255:ASP:HA	1:A:1274:ARG:H	1.70	0.56
1:A:1427:PRO:HD2	1:D:1313:PHE:CD1	2.40	0.56
2:B:8:VAL:HB	2:B:71:ASN:OD1	2.05	0.56
2:B:119:GLU:HA	2:B:122:ASN:HD22	1.70	0.56
2:B:131:GLN:O	2:B:133:VAL:N	2.38	0.56
2:B:219:VAL:O	2:B:223:ILE:HG23	2.05	0.56
2:B:386:TYR:CD2	2:B:453:GLU:HG2	2.40	0.56
2:B:541:GLN:HG2	2:B:686:LEU:HD11	1.87	0.56
2:B:548:ILE:HG12	2:B:552:ARG:NH2	2.20	0.56
2:B:564:LYS:HG3	2:B:575:TRP:HD1	1.70	0.56
2:B:575:TRP:HA	2:B:591:LEU:H	1.70	0.56
2:B:576:TYR:O	2:B:589:GLY:N	2.36	0.56
2:B:617:VAL:CG2	2:B:621:ASP:HB2	2.34	0.56
1:D:1211:TYR:HD2	1:D:1220:TYR:HA	1.70	0.56
1:D:1557:ARG:NH1	1:D:1558:ASP:OD1	2.39	0.56
1:A:41:CYS:HA	2:B:723:VAL:CG2	2.33	0.56
1:A:456:ASP:OD1	1:A:562:ALA:N	2.39	0.56
1:A:536:LYS:HE2	1:A:543:HIS:CD2	2.38	0.56
1:A:977:LYS:HE3	1:A:1032:LEU:HB2	1.88	0.56
1:A:1043:GLN:HG2	1:A:1098:ILE:HB	1.86	0.56
1:A:1175:VAL:HA	1:A:1179:LYS:CD	2.35	0.56
1:A:1208:LEU:HD12	1:A:1220:TYR:CD2	2.41	0.56
1:A:1222:ARG:O	1:A:1225:TYR:HB2	2.05	0.56
2:B:448:HIS:HB3	2:B:451:SER:HA	1.87	0.56
1:D:1386:GLU:HB3	1:D:1405:TYR:CD1	2.41	0.56
1:D:1492:ILE:HD12	1:D:1496:GLU:HB2	1.86	0.56
1:D:1576:GLN:HG2	1:D:1577:ILE:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:TYR:O	1:A:428:ILE:HD13	2.06	0.56
1:A:1479:LEU:HD11	1:A:1481:TRP:CH2	2.41	0.56
1:A:1579:PHE:HA	1:A:1582:ALA:CB	2.36	0.56
2:B:31:SER:HA	2:B:34:ILE:HD12	1.88	0.56
1:D:1254:SER:N	1:D:1273:HIS:HB2	2.19	0.56
1:D:1614:GLU:HA	1:D:1618:GLY:HA2	1.88	0.56
1:A:1196:SER:OG	1:A:1199:ASN:HB2	2.04	0.56
1:A:1205:VAL:HG22	1:A:1209:ASN:ND2	2.20	0.56
2:B:14:TRP:CD2	2:B:15:PRO:HD2	2.41	0.56
2:B:537:LYS:HB3	2:B:541:GLN:NE2	2.21	0.56
1:A:19:PHE:HB3	1:A:29:LEU:HB2	1.88	0.56
1:A:110:LYS:HG3	1:A:113:ARG:HB3	1.87	0.56
1:A:232:UNK:O	1:A:272:UNK:HA	2.05	0.56
1:A:285:UNK:O	1:A:289:UNK:N	2.39	0.56
1:A:1174:PHE:O	1:A:1178:VAL:HB	2.06	0.56
1:A:1188:TYR:OH	1:A:1192:MET:SD	2.53	0.56
1:A:1342:TYR:HE1	1:A:1413:PRO:HG3	1.69	0.56
2:B:265:ILE:O	2:B:269:LYS:HG2	2.05	0.56
2:B:556:LEU:HD22	2:B:665:TRP:CE3	2.41	0.56
1:D:1231:HIS:HE1	1:D:1236:ASN:HD22	1.50	0.56
1:D:1281:TYR:O	1:D:1285:ILE:HG23	2.05	0.56
1:A:430:LEU:HA	1:A:602:ILE:HA	1.88	0.56
1:A:547:HIS:HB2	1:A:602:ILE:HD12	1.88	0.56
1:A:1153:LEU:O	1:A:1157:LEU:HG	2.06	0.56
1:A:1421:PHE:HB2	1:A:1431:ILE:HD13	1.88	0.56
2:B:50:ALA:HB2	2:B:81:PRO:HD3	1.88	0.56
2:B:585:VAL:HG22	2:B:609:PRO:HA	1.88	0.56
1:D:1300:LEU:O	1:D:1304:LEU:HG	2.06	0.56
1:D:1361:PHE:O	1:D:1362:ILE:HD13	2.06	0.56
1:A:455:GLU:O	1:A:508:ARG:NH2	2.39	0.56
1:A:1371:ARG:NH1	1:A:1372:GLU:HA	2.21	0.56
2:B:567:ALA:O	2:B:573:LYS:HB2	2.06	0.56
2:B:575:TRP:HB2	2:B:590:ASP:HA	1.86	0.56
1:D:1220:TYR:CE2	1:D:1224:LEU:HD21	2.41	0.56
1:D:1370:ARG:HG3	1:D:1372:GLU:N	2.21	0.56
1:A:1174:PHE:HB3	1:A:1179:LYS:HZ1	1.70	0.56
1:A:1346:GLY:HA2	1:A:1360:VAL:HG22	1.87	0.56
1:A:1592:SER:H	1:A:1595:LEU:HD23	1.71	0.56
1:A:1610:LYS:NZ	1:A:1614:GLU:OE1	2.37	0.56
2:B:286:ILE:O	2:B:595:PRO:HA	2.06	0.56
1:D:1416:ASP:OD1	1:D:1417:GLU:N	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ARG:NH1	2:B:723:VAL:HG21	2.21	0.55
1:A:43:ASP:HA	1:A:61:LYS:H	1.71	0.55
1:A:117:VAL:O	1:A:121:MET:HG3	2.06	0.55
1:A:474:ASN:OD1	1:A:475:GLU:N	2.40	0.55
1:A:1132:ILE:O	1:A:1135:LYS:CB	2.54	0.55
1:A:1294:TRP:CD1	1:A:1328:PHE:CG	2.94	0.55
1:A:1519:ASP:OD1	1:A:1521:THR:N	2.39	0.55
1:A:1541:GLY:O	1:A:1544:ALA:N	2.36	0.55
2:B:696:LEU:HA	2:B:699:LEU:HD12	1.87	0.55
1:D:1345:VAL:HG21	1:D:1363:TYR:CD1	2.40	0.55
1:A:18:ASN:OD1	1:A:31:ILE:N	2.38	0.55
1:A:143:GLU:HA	1:A:146:GLN:OE1	2.05	0.55
1:A:187:HIS:O	1:A:190:ALA:HB3	2.07	0.55
1:A:1106:ALA:HA	1:A:1156:ILE:HD11	1.88	0.55
1:A:1136:LEU:O	1:A:1139:GLU:CB	2.54	0.55
1:A:1288:PHE:CE1	1:A:1293:MET:HB3	2.40	0.55
1:A:1371:ARG:HH12	1:A:1376:MET:HE2	1.71	0.55
2:B:402:ASN:HA	2:B:405:ARG:HE	1.70	0.55
1:D:1301:CYS:HB3	1:D:1321:ASN:OD1	2.06	0.55
1:A:93:THR:O	1:A:96:TRP:HB2	2.06	0.55
1:A:444:ARG:HG2	1:A:446:VAL:HA	1.88	0.55
1:A:1035:ALA:O	1:A:1038:THR:OG1	2.23	0.55
1:A:1614:GLU:HG2	1:A:1619:VAL:HG12	1.88	0.55
2:B:290:MET:O	2:B:294:LEU:HG	2.06	0.55
1:D:1294:TRP:CZ3	1:D:1331:SER:HB2	2.42	0.55
1:A:1126:LYS:HD2	1:A:1126:LYS:C	2.27	0.55
1:A:1504:THR:HA	1:A:1507:GLU:HG2	1.88	0.55
2:B:195:ILE:HA	2:B:239:ILE:HD11	1.88	0.55
2:B:201:SER:OG	2:B:202:LEU:N	2.38	0.55
2:B:478:ASN:HB2	2:B:482:GLN:NE2	2.22	0.55
2:B:551:GLN:NE2	2:B:555:ARG:HH11	2.04	0.55
2:B:722:PHE:CG	2:B:722:PHE:CB	2.89	0.55
1:A:14:VAL:HG22	1:A:67:LYS:HG2	1.89	0.55
1:A:142:LYS:HG3	1:A:143:GLU:H	1.71	0.55
1:A:142:LYS:HA	1:A:145:LYS:HE2	1.86	0.55
1:A:435:PHE:CD2	1:A:444:ARG:HB3	2.41	0.55
1:A:986:PRO:HD2	1:A:989:TRP:CE3	2.41	0.55
1:A:1088:MET:HG3	1:A:1092:ILE:HG13	1.88	0.55
1:A:1208:LEU:HD13	1:A:1211:TYR:CD2	2.41	0.55
1:A:1537:PRO:HA	1:A:1540:MET:C	2.27	0.55
2:B:548:ILE:O	2:B:552:ARG:HG2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1330:GLU:O	1:D:1334:LYS:HE3	2.06	0.55
1:D:1345:VAL:HA	1:D:1408:CYS:SG	2.47	0.55
1:A:38:GLN:NE2	2:B:726:CYS:SG	2.79	0.55
1:A:445:ASN:HB2	1:A:514:ARG:C	2.27	0.55
1:A:569:PRO:HG2	1:A:575:VAL:HA	1.86	0.55
1:A:656:ASP:O	1:A:660:ILE:N	2.39	0.55
1:A:957:UNK:O	1:A:959:UNK:N	2.39	0.55
1:A:1148:GLN:O	1:A:1152:LEU:HG	2.07	0.55
1:A:1308:TYR:CD1	1:A:1314:ASP:HB3	2.42	0.55
1:A:1348:TYR:CE1	1:A:1358:ASN:HA	2.42	0.55
1:A:1353:PRO:HA	1:A:1357:ARG:NH2	2.21	0.55
1:A:1361:PHE:HA	1:A:1483:GLU:HA	1.89	0.55
2:B:55:ASP:OD1	2:B:55:ASP:N	2.39	0.55
2:B:279:VAL:O	2:B:286:ILE:HD11	2.07	0.55
1:D:1220:TYR:CD2	1:D:1224:LEU:HD21	2.42	0.55
1:A:87:LEU:O	1:A:91:VAL:HG23	2.06	0.55
1:A:294:UNK:O	1:A:296:UNK:N	2.40	0.55
1:A:450:MET:HG2	1:A:509:PHE:CE2	2.42	0.55
1:A:1129:GLU:O	1:A:1133:ILE:HG12	2.07	0.55
1:A:1429:GLN:NE2	1:A:1429:GLN:O	2.40	0.55
2:B:181:ILE:HG22	2:B:222:GLU:HG3	1.88	0.55
2:B:616:VAL:HG22	2:B:644:ILE:HG23	1.88	0.55
1:D:1227:LEU:HA	1:D:1230:LEU:HD12	1.89	0.55
1:A:511:PHE:H	1:A:512:ARG:HH12	1.54	0.55
1:A:771:UNK:O	1:A:774:UNK:CB	2.55	0.55
1:A:1175:VAL:HA	1:A:1179:LYS:HE2	1.89	0.55
2:B:216:TYR:CZ	2:B:253:LYS:HB2	2.42	0.55
2:B:356:TYR:HD1	2:B:359:LEU:HD22	1.71	0.55
2:B:541:GLN:HE21	2:B:690:LEU:CD2	2.19	0.55
1:D:1216:ARG:HG2	1:D:1219:MET:HB3	1.88	0.55
1:D:1413:PRO:HG2	1:D:1436:SER:OG	2.07	0.55
1:D:1568:HIS:O	1:D:1572:LEU:N	2.37	0.55
1:A:139:ASP:HA	1:A:142:LYS:HE3	1.89	0.55
1:A:513:HIS:HB2	1:A:524:GLU:H	1.71	0.55
2:B:45:ASN:O	2:B:48:TYR:N	2.29	0.55
2:B:185:ALA:O	2:B:189:ASN:CB	2.55	0.55
1:D:1216:ARG:O	1:D:1220:TYR:HB2	2.07	0.55
1:D:1229:ASP:O	1:D:1232:LEU:HB3	2.07	0.55
1:D:1254:SER:O	1:D:1274:ARG:N	2.39	0.55
1:A:64:ILE:HG22	1:A:66:ILE:HG12	1.89	0.55
1:A:90:GLU:O	1:A:93:THR:OG1	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:THR:OG1	1:A:128:ARG:NH2	2.40	0.55
1:A:328:UNK:O	1:A:330:UNK:N	2.40	0.55
1:A:435:PHE:C	1:A:437:LYS:H	2.11	0.55
1:A:1200:ARG:HE	1:A:1230:LEU:HD22	1.72	0.55
1:A:1278:GLU:HA	1:A:1281:TYR:CD2	2.34	0.55
1:A:1357:ARG:O	1:A:1359:LYS:NZ	2.28	0.55
2:B:481:MET:HA	2:B:484:VAL:HB	1.89	0.55
2:B:562:PHE:O	2:B:575:TRP:N	2.40	0.55
1:D:1247:HIS:O	1:D:1250:LEU:N	2.29	0.55
1:A:1001:LEU:HD23	1:A:1002:ARG:N	2.22	0.54
1:A:1091:PRO:O	1:A:1095:MET:HG2	2.07	0.54
1:A:1442:PHE:O	1:A:1468:SER:OG	2.18	0.54
2:B:318:GLN:NE2	2:B:321:ARG:HB2	2.23	0.54
1:D:1388:MET:HB2	1:D:1407:GLN:HG2	1.89	0.54
1:D:1463:TRP:CZ3	1:D:1494:PRO:HD3	2.42	0.54
1:D:1563:GLN:HA	1:D:1566:LEU:HD23	1.89	0.54
2:B:205:LEU:O	2:B:209:VAL:HG23	2.07	0.54
1:D:1305:ALA:HA	1:D:1308:TYR:HB2	1.89	0.54
1:D:1306:GLU:HA	1:D:1310:MET:HE1	1.89	0.54
1:A:426:ILE:HB	1:A:495:VAL:O	2.07	0.54
1:A:1109:PRO:HG2	1:A:1110:ILE:HD12	1.89	0.54
1:A:1229:ASP:HA	1:A:1232:LEU:HD12	1.90	0.54
1:A:1361:PHE:CD1	1:A:1481:TRP:HD1	2.26	0.54
1:A:1394:PRO:HG2	1:A:1399:LYS:NZ	2.23	0.54
1:A:1551:PHE:CE2	1:A:1617:TYR:HE2	2.26	0.54
2:B:63:GLU:O	2:B:67:ASN:N	2.39	0.54
2:B:537:LYS:HE3	2:B:690:LEU:HD21	1.88	0.54
2:B:564:LYS:HZ2	2:B:575:TRP:HB3	1.71	0.54
1:D:1546:TYR:HA	1:D:1550:PHE:HD1	1.71	0.54
1:A:47:GLY:H	1:A:59:PHE:HE2	1.51	0.54
1:A:94:THR:HG22	1:A:98:TRP:CE2	2.42	0.54
1:A:971:GLU:O	1:A:975:MET:HG2	2.07	0.54
1:A:1163:GLU:H	1:A:1165:PRO:HD3	1.70	0.54
1:A:1294:TRP:O	1:A:1297:ALA:N	2.41	0.54
1:A:1471:THR:OG1	1:A:1483:GLU:O	2.23	0.54
1:A:1552:THR:O	1:A:1556:VAL:HG23	2.07	0.54
2:B:261:GLU:HA	2:B:264:ASN:ND2	2.22	0.54
2:B:371:PHE:C	2:B:373:GLN:H	2.09	0.54
2:B:402:ASN:HD21	2:B:464:ASN:ND2	2.05	0.54
1:D:1284:ILE:HA	1:D:1287:TYR:HB2	1.88	0.54
1:D:1306:GLU:HA	1:D:1310:MET:CE	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:LEU:HD11	1:A:59:PHE:CD1	2.42	0.54
1:A:41:CYS:CA	2:B:723:VAL:HG22	2.34	0.54
1:A:46:ARG:HG3	1:A:56:GLN:HG2	1.88	0.54
1:A:976:PHE:O	1:A:980:ILE:HG13	2.07	0.54
1:A:998:ARG:C	1:A:998:ARG:HD3	2.27	0.54
1:A:1570:LYS:O	1:A:1574:ALA:N	2.31	0.54
2:B:287:ASN:H	2:B:290:MET:HE3	1.72	0.54
2:B:376:PRO:HG3	2:B:380:ALA:HB2	1.90	0.54
2:B:551:GLN:O	2:B:555:ARG:HG2	2.07	0.54
2:B:619:GLY:N	2:B:641:ALA:O	2.26	0.54
2:B:622:CYS:HA	2:B:653:ASN:OD1	2.07	0.54
1:D:1370:ARG:HB3	1:D:1373:ASP:OD2	2.08	0.54
1:A:542:LEU:O	1:A:606:VAL:HG21	2.07	0.54
1:A:1214:ASN:HB2	1:A:1216:ARG:NH1	2.23	0.54
1:A:1223:TYR:HA	1:A:1226:LYS:HD3	1.88	0.54
1:A:1288:PHE:HZ	1:A:1296:GLU:OE1	1.90	0.54
1:A:1414:VAL:HG11	1:A:1441:ARG:NH1	2.22	0.54
2:B:224:THR:O	2:B:227:GLN:HB2	2.08	0.54
2:B:270:GLN:O	2:B:273:SER:N	2.35	0.54
2:B:529:GLN:HA	2:B:534:LEU:HD13	1.88	0.54
2:B:613:ILE:HA	2:B:646:TYR:CB	2.37	0.54
2:B:636:GLU:H	2:B:636:GLU:CD	2.08	0.54
1:D:1361:PHE:HB3	1:D:1481:TRP:CD1	2.42	0.54
1:A:153:ASP:HA	1:A:156:ASN:ND2	2.23	0.54
1:A:452:VAL:HG23	1:A:474:ASN:HB2	1.89	0.54
1:A:498:PRO:O	1:A:501:ASP:N	2.41	0.54
1:A:547:HIS:HB2	1:A:602:ILE:HB	1.90	0.54
1:A:558:LYS:HD3	1:A:592:LEU:HB2	1.89	0.54
1:A:1247:HIS:CE1	1:A:1280:LEU:HD22	2.42	0.54
1:A:1301:CYS:CB	1:A:1321:ASN:HD21	2.21	0.54
1:A:1553:GLU:O	1:A:1557:ARG:HG2	2.08	0.54
1:D:1208:LEU:HD13	1:D:1223:TYR:CB	2.38	0.54
1:D:1350:GLN:OE1	1:D:1400:ASN:HA	2.08	0.54
1:D:1448:VAL:HG23	1:D:1463:TRP:HB2	1.90	0.54
1:A:160:GLU:O	1:A:161:LEU:HD23	2.07	0.54
1:A:965:LEU:C	1:A:969:LEU:HG	2.28	0.54
1:A:1243:THR:HA	1:A:1246:LEU:HD12	1.88	0.54
1:A:1577:ILE:O	1:A:1579:PHE:N	2.41	0.54
2:B:108:ALA:HB2	2:B:157:PHE:HB3	1.90	0.54
2:B:218:LYS:O	2:B:222:GLU:N	2.41	0.54
2:B:323:ILE:HG21	2:B:381:LEU:HD21	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:SER:H	2:B:634:ASN:HD21	1.55	0.54
1:D:1321:ASN:O	1:D:1324:GLN:HB3	2.07	0.54
1:D:1364:ARG:HH11	1:D:1475:LEU:HG	1.73	0.54
1:D:1498:ALA:O	1:D:1501:THR:OG1	2.25	0.54
1:A:428:ILE:O	1:A:429:THR:OG1	2.17	0.54
1:A:447:GLU:HA	1:A:478:SER:H	1.73	0.54
1:A:448:VAL:HG12	1:A:478:SER:OG	2.08	0.54
1:A:1415:LEU:HD11	1:A:1418:HIS:NE2	2.23	0.54
1:A:1524:ILE:HG13	1:A:1527:LEU:HB3	1.89	0.54
2:B:375:PRO:HB2	2:B:422:LYS:HB2	1.89	0.54
2:B:448:HIS:CD2	2:B:449:ASP:H	2.26	0.54
2:B:459:CYS:O	2:B:463:LEU:HB2	2.08	0.54
1:D:1301:CYS:HA	1:D:1304:LEU:HG	1.90	0.54
1:D:1317:LEU:HA	1:D:1320:GLN:HG2	1.90	0.54
1:D:1426:VAL:HG11	1:D:1431:ILE:HD13	1.90	0.54
1:D:1450:ARG:HB2	1:D:1463:TRP:CD1	2.43	0.54
1:A:35:VAL:HG12	1:A:49:LEU:HA	1.90	0.54
1:A:113:ARG:O	1:A:116:GLN:HB3	2.08	0.54
1:A:187:HIS:ND1	1:A:989:TRP:CG	2.76	0.54
1:A:425:ASP:CA	1:A:494:LYS:HE3	2.36	0.54
1:A:1200:ARG:HG2	1:A:1230:LEU:HD13	1.90	0.54
2:B:53:HIS:HA	2:B:75:LEU:HD12	1.88	0.54
2:B:360:GLY:CA	2:B:364:HIS:HE1	2.21	0.54
1:A:19:PHE:HD2	1:A:29:LEU:HG	1.73	0.53
1:A:40:THR:O	2:B:723:VAL:HG22	2.08	0.53
1:A:100:SER:HA	1:A:103:LYS:HE2	1.89	0.53
1:A:820:UNK:O	1:A:823:UNK:N	2.42	0.53
1:A:1322:LEU:HA	1:A:1325:GLN:CD	2.28	0.53
2:B:361:PHE:H	2:B:364:HIS:CE1	2.26	0.53
2:B:417:SER:O	2:B:421:THR:OG1	2.23	0.53
2:B:483:VAL:HA	2:B:486:GLU:CD	2.29	0.53
1:D:1247:HIS:NE2	1:D:1251:LEU:HB2	2.23	0.53
1:A:102:TRP:HE1	1:A:114:PHE:C	2.12	0.53
1:A:464:ILE:HG22	1:A:465:CYS:N	2.22	0.53
1:A:548:ASP:HB3	1:A:599:VAL:HG13	1.90	0.53
1:A:1004:ILE:HA	1:A:1007:PHE:CD2	2.42	0.53
1:A:1315:TYR:OH	1:D:1430:ILE:HG21	2.08	0.53
1:A:1327:LYS:O	1:A:1330:GLU:HB3	2.09	0.53
1:A:1585:LYS:O	1:A:1588:GLU:HB2	2.08	0.53
2:B:272:ARG:HA	2:B:275:ILE:HD12	1.89	0.53
2:B:575:TRP:CA	2:B:590:ASP:HA	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1208:LEU:HD13	1:D:1223:TYR:HB2	1.90	0.53
1:D:1231:HIS:CE1	1:D:1239:GLU:HG2	2.43	0.53
1:D:1412:GLN:HG2	1:D:1443:HIS:HB2	1.89	0.53
1:A:433:GLY:HA3	1:A:489:TRP:HE1	1.73	0.53
1:A:985:TYR:CZ	1:A:992:MET:HG3	2.43	0.53
1:A:1343:PHE:CE1	1:A:1410:THR:HG23	2.43	0.53
1:A:1362:ILE:HD11	1:A:1469:PHE:CD2	2.43	0.53
1:A:1445:SER:HB3	1:A:1464:ILE:HD13	1.90	0.53
1:A:1504:THR:O	1:A:1508:LYS:HG3	2.08	0.53
1:A:1587:HIS:O	1:A:1591:VAL:N	2.41	0.53
2:B:306:GLU:O	2:B:310:MET:HG2	2.08	0.53
2:B:561:CYS:HA	2:B:576:TYR:CA	2.26	0.53
2:B:561:CYS:CA	2:B:576:TYR:HA	2.26	0.53
2:B:582:ASN:O	2:B:584:LYS:HG3	2.08	0.53
2:B:699:LEU:HD23	2:B:702:GLU:OE2	2.08	0.53
1:D:1248:THR:HA	1:D:1251:LEU:HB3	1.91	0.53
1:A:609:THR:HA	1:A:668:TYR:OH	2.07	0.53
1:A:946:UNK:O	1:A:949:UNK:N	2.42	0.53
1:A:1255:ASP:N	1:A:1274:ARG:HG2	2.23	0.53
1:A:1303:GLU:O	1:A:1306:GLU:HB2	2.08	0.53
2:B:130:THR:HB	2:B:134:GLU:OE1	2.09	0.53
2:B:267:ALA:O	2:B:270:GLN:N	2.42	0.53
2:B:576:TYR:CG	2:B:577:CYS:N	2.76	0.53
1:D:1208:LEU:HD22	1:D:1227:LEU:HD12	1.90	0.53
1:D:1509:ILE:O	1:D:1513:ILE:HG23	2.09	0.53
1:A:84:GLU:O	1:A:87:LEU:HB3	2.08	0.53
1:A:137:PRO:HG2	1:A:140:GLU:HB2	1.90	0.53
1:A:146:GLN:O	1:A:149:THR:OG1	2.20	0.53
1:A:385:UNK:O	1:A:387:UNK:N	2.41	0.53
1:A:992:MET:O	1:A:995:VAL:HG13	2.09	0.53
1:A:1061:ASP:O	1:A:1064:ARG:HB2	2.07	0.53
1:A:1216:ARG:HA	1:A:1216:ARG:HE	1.72	0.53
2:B:276:LEU:HD12	2:B:280:ILE:HB	1.90	0.53
1:A:118:GLN:O	1:A:122:TYR:HD2	1.92	0.53
1:A:798:UNK:O	1:A:802:UNK:N	2.41	0.53
1:A:1165:PRO:O	1:A:1168:ALA:HB3	2.08	0.53
1:A:1207:LEU:HD11	1:A:1223:TYR:CD1	2.43	0.53
1:A:1412:GLN:O	1:A:1443:HIS:N	2.30	0.53
2:B:288:ASN:C	2:B:593:GLU:HG2	2.29	0.53
2:B:502:PHE:HA	2:B:505:LYS:HB2	1.91	0.53
1:D:1345:VAL:HG21	1:D:1363:TYR:CG	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1365:GLY:HA2	1:D:1374:PHE:CE1	2.43	0.53
1:A:40:THR:CA	1:A:45:TYR:HA	2.32	0.53
1:A:126:GLU:OE2	1:A:130:GLN:NE2	2.42	0.53
1:A:424:ASN:O	1:A:494:LYS:NZ	2.28	0.53
1:A:965:LEU:HB3	1:A:969:LEU:HD21	1.89	0.53
1:A:1066:ILE:O	1:A:1070:ILE:HG12	2.08	0.53
1:A:1244:LEU:HB3	1:A:1284:ILE:CG1	2.37	0.53
2:B:178:VAL:O	2:B:182:LYS:HG3	2.07	0.53
2:B:571:GLN:O	2:B:573:LYS:N	2.36	0.53
1:D:1204:THR:HG23	1:D:1227:LEU:HD11	1.91	0.53
1:D:1363:TYR:HA	1:D:1481:TRP:HB3	1.90	0.53
1:D:1484:VAL:HG12	1:D:1486:HIS:N	2.23	0.53
1:A:86:PRO:O	1:A:90:GLU:HG2	2.09	0.53
1:A:648:ILE:O	1:A:652:HIS:N	2.42	0.53
1:A:1020:ASN:C	1:A:1022:GLU:N	2.62	0.53
1:A:1206:ASN:HA	1:A:1209:ASN:ND2	2.24	0.53
1:A:1456:GLU:OE1	1:A:1456:GLU:N	2.42	0.53
1:A:1541:GLY:HA3	1:A:1545:LYS:NZ	2.24	0.53
2:B:229:ILE:HG22	2:B:233:GLN:OE1	2.08	0.53
2:B:247:ILE:O	2:B:250:LEU:HB2	2.09	0.53
2:B:289:GLU:N	2:B:593:GLU:HG2	2.24	0.53
2:B:453:GLU:HA	2:B:456:PHE:HB3	1.90	0.53
2:B:658:ASP:OD2	2:B:660:HIS:HB3	2.09	0.53
1:A:43:ASP:C	1:A:60:PRO:HA	2.29	0.53
1:A:162:ASP:N	1:A:162:ASP:OD1	2.42	0.53
1:A:569:PRO:HD2	1:A:575:VAL:HG12	1.90	0.53
1:A:1210:PHE:CA	1:A:1213:ASP:HB3	2.27	0.53
1:A:1371:ARG:HH12	1:A:1376:MET:CE	2.22	0.53
1:A:1401:ALA:HB3	1:A:1405:TYR:HE2	1.74	0.53
1:A:1414:VAL:HG22	1:A:1443:HIS:CE1	2.44	0.53
1:A:1601:ARG:HH11	1:A:1601:ARG:C	2.12	0.53
2:B:332:PHE:CE1	2:B:400:LEU:HD21	2.44	0.53
2:B:435:SER:C	2:B:437:THR:H	2.12	0.53
2:B:468:LYS:C	2:B:471:ARG:H	2.11	0.53
2:B:567:ALA:H	2:B:573:LYS:HE3	1.73	0.53
2:B:575:TRP:CB	2:B:590:ASP:HA	2.38	0.53
1:D:1243:THR:HA	1:D:1246:LEU:HD12	1.90	0.53
1:D:1531:LEU:HD12	1:D:1587:HIS:CD2	2.44	0.53
1:A:29:LEU:HD21	1:A:59:PHE:CG	2.44	0.53
1:A:69:VAL:C	1:A:81:ILE:HD12	2.29	0.53
1:A:443:GLN:HG2	1:A:485:LYS:HZ2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLY:H	1:A:559:MET:CE	2.22	0.53
1:A:1023:PHE:HZ	1:A:1079:GLN:O	1.92	0.53
1:A:1301:CYS:HA	1:A:1304:LEU:CG	2.38	0.53
1:A:1361:PHE:HB2	1:A:1363:TYR:CE1	2.41	0.53
1:A:1372:GLU:N	1:A:1372:GLU:CD	2.62	0.53
2:B:274:ILE:H	2:B:274:ILE:HD12	1.73	0.53
1:D:1256:GLU:N	1:D:1272:THR:HA	2.24	0.53
1:D:1301:CYS:O	1:D:1304:LEU:HB2	2.09	0.53
1:D:1565:LYS:O	1:D:1568:HIS:HB3	2.09	0.53
1:A:47:GLY:O	1:A:56:GLN:HG3	2.09	0.52
1:A:105:LEU:HD22	1:A:110:LYS:CB	2.39	0.52
1:A:1029:TYR:OH	1:A:1073:MET:HG3	2.09	0.52
2:B:14:TRP:CE3	2:B:15:PRO:HD2	2.44	0.52
2:B:120:PHE:CD1	2:B:123:LEU:HB2	2.44	0.52
2:B:388:ALA:HB2	2:B:395:TYR:CZ	2.44	0.52
2:B:613:ILE:HA	2:B:646:TYR:HB3	1.92	0.52
2:B:670:ASN:HD21	2:B:678:MET:HG2	1.74	0.52
2:B:718:SER:HA	2:B:720:TYR:CZ	2.44	0.52
1:D:1363:TYR:CD1	1:D:1481:TRP:CD2	2.98	0.52
1:A:303:UNK:C	1:A:318:UNK:HA	2.39	0.52
1:A:431:LEU:HD21	1:A:603:SER:H	1.72	0.52
1:A:976:PHE:HB2	1:A:1032:LEU:HD21	1.91	0.52
1:A:1002:ARG:HA	1:A:1005:ASN:ND2	2.24	0.52
1:A:1010:THR:HG1	1:A:1011:MET:H	1.57	0.52
1:A:1272:THR:O	1:A:1276:LEU:HG	2.09	0.52
2:B:113:ASP:OD1	2:B:115:THR:N	2.43	0.52
2:B:116:PHE:HA	2:B:119:GLU:HB3	1.91	0.52
2:B:118:GLN:O	2:B:121:ILE:HB	2.09	0.52
2:B:247:ILE:HA	2:B:250:LEU:CG	2.38	0.52
2:B:363:ASN:HD21	2:B:365:VAL:HG22	1.75	0.52
1:D:1299:SER:HA	1:D:1302:LYS:HE2	1.90	0.52
1:D:1355:PHE:HA	1:D:1359:LYS:HE2	1.91	0.52
1:A:43:ASP:HA	1:A:61:LYS:HB2	1.90	0.52
1:A:46:ARG:HG2	1:A:56:GLN:HG2	1.91	0.52
1:A:519:SER:C	1:A:521:ASP:H	2.13	0.52
1:A:1148:GLN:HA	1:A:1151:GLN:HB3	1.90	0.52
1:A:1231:HIS:CD2	1:A:1239:GLU:HB2	2.44	0.52
1:A:1245:LEU:O	1:A:1249:TRP:HB3	2.09	0.52
1:A:1254:SER:C	1:A:1273:HIS:HD1	2.08	0.52
1:A:1309:GLU:O	1:A:1313:PHE:HD1	1.92	0.52
1:A:1432:ASN:OD1	1:A:1432:ASN:N	2.39	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1198:ASP:HA	1:D:1201:MET:CG	2.39	0.52
1:D:1348:TYR:HA	1:D:1358:ASN:HD22	1.73	0.52
1:D:1446:ARG:C	1:D:1464:ILE:HG13	2.30	0.52
1:A:42:GLY:O	1:A:61:LYS:HB2	2.08	0.52
1:A:91:VAL:O	1:A:94:THR:HB	2.10	0.52
1:A:977:LYS:CG	1:A:1032:LEU:HD13	2.38	0.52
1:A:1007:PHE:C	1:A:1010:THR:HG1	2.09	0.52
1:A:1334:LYS:HG2	1:D:1316:GLU:HG3	1.92	0.52
1:A:1379:MET:HA	1:A:1385:ALA:HB1	1.90	0.52
1:A:1546:TYR:HA	1:A:1550:PHE:CD2	2.44	0.52
1:A:1551:PHE:CE1	1:A:1566:LEU:HB3	2.41	0.52
2:B:481:MET:O	2:B:484:VAL:HB	2.10	0.52
2:B:528:PHE:HA	2:B:533:ILE:HG21	1.91	0.52
1:D:1300:LEU:HA	1:D:1303:GLU:OE1	2.09	0.52
1:D:1308:TYR:CD2	1:D:1318:LEU:HA	2.45	0.52
1:D:1364:ARG:N	1:D:1480:ARG:O	2.43	0.52
1:D:1471:THR:HA	1:D:1485:VAL:H	1.73	0.52
1:A:7:ALA:HB1	1:A:37:ILE:HG22	1.92	0.52
1:A:8:ASP:O	1:A:11:ARG:HG2	2.09	0.52
1:A:426:ILE:HG22	1:A:428:ILE:HD11	1.92	0.52
1:A:636:UNK:O	1:A:640:UNK:HA	2.10	0.52
1:A:1133:ILE:O	1:A:1137:ASP:N	2.28	0.52
1:A:1332:ILE:HB	1:D:1315:TYR:CE2	2.44	0.52
1:A:1394:PRO:HG2	1:A:1399:LYS:HZ2	1.75	0.52
1:A:1516:TYR:OH	1:A:1522:LEU:HB2	2.10	0.52
2:B:154:MET:HG2	2:B:157:PHE:CD2	2.45	0.52
2:B:289:GLU:O	2:B:292:HIS:HB3	2.10	0.52
1:D:1360:VAL:HG22	1:D:1483:GLU:OE2	2.09	0.52
1:D:1573:ILE:O	1:D:1577:ILE:HG12	2.09	0.52
1:D:1608:ASN:HB3	1:D:1612:LYS:NZ	2.25	0.52
1:A:17:TYR:HD1	1:A:31:ILE:HD12	1.73	0.52
1:A:450:MET:HE1	1:A:464:ILE:HG21	1.92	0.52
1:A:884:UNK:O	1:A:887:UNK:N	2.42	0.52
2:B:53:HIS:CD2	2:B:58:ASN:HA	2.45	0.52
2:B:116:PHE:O	2:B:120:PHE:HB2	2.10	0.52
2:B:214:ASP:HA	2:B:217:GLN:CD	2.30	0.52
2:B:496:PRO:HG3	2:B:502:PHE:CE1	2.44	0.52
2:B:588:TYR:O	2:B:606:ASP:HA	2.09	0.52
2:B:724:TYR:CD2	2:B:724:TYR:CB	2.79	0.52
1:D:1361:PHE:HD1	1:D:1482:PHE:O	1.92	0.52
1:D:1424:LYS:O	1:D:1426:VAL:HG23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1461:SER:OG	1:D:1463:TRP:NE1	2.22	0.52
1:A:429:THR:HG22	1:A:431:LEU:HD23	1.92	0.52
1:A:1567:THR:OG1	1:A:1568:HIS:N	2.43	0.52
2:B:614:LYS:NZ	2:B:648:SER:HA	2.25	0.52
2:B:694:ILE:HA	2:B:697:ARG:HD3	1.91	0.52
1:D:1307:GLN:NE2	1:D:1311:GLU:HG3	2.25	0.52
1:D:1339:LYS:NZ	1:D:1341:ASP:OD1	2.41	0.52
1:A:432:GLN:NE2	1:A:601:SER:H	2.06	0.52
1:A:1071:ARG:HA	1:A:1074:TRP:HB3	1.92	0.52
1:A:1094:GLU:O	1:A:1102:GLU:HG2	2.10	0.52
1:A:1183:GLU:HA	1:A:1186:LEU:HD12	1.92	0.52
1:A:1255:ASP:HB2	1:A:1272:THR:HA	1.90	0.52
1:A:1418:HIS:N	1:A:1422:LYS:HG3	2.20	0.52
1:D:1255:ASP:HA	1:D:1272:THR:HB	1.91	0.52
1:D:1371:ARG:NH1	1:D:1375:GLN:HB2	2.24	0.52
1:D:1516:TYR:CE2	1:D:1522:LEU:HD13	2.44	0.52
1:A:93:THR:O	1:A:97:GLU:HG3	2.10	0.52
1:A:130:GLN:HB3	1:A:136:LEU:HD11	1.91	0.52
1:A:976:PHE:HD2	1:A:1032:LEU:HD21	1.73	0.52
1:A:1363:TYR:HA	1:A:1481:TRP:HB3	1.92	0.52
1:A:1432:ASN:O	1:A:1435:LYS:HB3	2.10	0.52
2:B:184:ILE:HD13	2:B:187:PHE:CE2	2.45	0.52
2:B:360:GLY:N	2:B:364:HIS:CE1	2.77	0.52
2:B:450:ARG:O	2:B:453:GLU:N	2.43	0.52
2:B:543:GLU:O	2:B:546:GLU:HB3	2.10	0.52
1:D:1241:ALA:O	1:D:1245:LEU:HG	2.10	0.52
1:A:302:UNK:HA	1:A:319:UNK:C	2.40	0.52
1:A:444:ARG:HB2	1:A:513:HIS:CE1	2.45	0.52
1:A:464:ILE:HG23	1:A:495:VAL:HG22	1.90	0.52
1:A:970:MET:HA	1:A:973:PHE:CD2	2.45	0.52
1:A:1040:ASP:C	1:A:1042:LEU:N	2.63	0.52
1:A:1253:TRP:HA	1:A:1274:ARG:CB	2.40	0.52
1:A:1440:GLN:N	1:A:1474:LYS:HZ2	2.07	0.52
1:A:1445:SER:HA	1:A:1466:ARG:HA	1.92	0.52
1:A:1467:THR:CG2	1:A:1487:MET:HB3	2.40	0.52
2:B:479:LYS:O	2:B:483:VAL:N	2.29	0.52
2:B:564:LYS:H	2:B:573:LYS:C	2.12	0.52
1:D:1336:LEU:HA	1:D:1429:GLN:HE22	1.75	0.52
1:D:1412:GLN:CD	1:D:1444:TYR:HA	2.30	0.52
1:A:27:LEU:HB2	1:A:57:GLY:H	1.75	0.51
1:A:427:TYR:HB2	1:A:605:LEU:HB2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:989:TRP:N	1:A:989:TRP:CD1	2.76	0.51
1:A:1428:ASP:OD1	1:A:1429:GLN:N	2.43	0.51
1:A:1443:HIS:CB	1:A:1466:ARG:HE	2.23	0.51
2:B:91:ARG:O	2:B:94:SER:OG	2.12	0.51
1:D:1197:LYS:NZ	1:D:1198:ASP:OD1	2.40	0.51
1:D:1231:HIS:CD2	1:D:1239:GLU:HG2	2.44	0.51
1:D:1303:GLU:O	1:D:1307:GLN:HG2	2.11	0.51
1:D:1562:ASP:HA	1:D:1565:LYS:HE2	1.93	0.51
1:D:1606:PHE:CZ	1:D:1610:LYS:HD2	2.45	0.51
1:A:1450:ARG:HE	1:A:1463:TRP:HB2	1.75	0.51
1:A:1587:HIS:CD2	1:A:1599:HIS:CE1	2.98	0.51
2:B:73:THR:OG1	2:B:74:ILE:N	2.41	0.51
2:B:202:LEU:HD11	2:B:243:THR:HA	1.92	0.51
2:B:451:SER:HA	2:B:454:GLU:CG	2.37	0.51
2:B:457:CYS:O	2:B:460:ILE:HG22	2.10	0.51
2:B:479:LYS:HA	2:B:482:GLN:OE1	2.10	0.51
2:B:556:LEU:HD12	2:B:672:LEU:HD21	1.91	0.51
2:B:692:MET:HA	2:B:695:LYS:HB2	1.91	0.51
1:D:1201:MET:HG2	1:D:1230:LEU:HD22	1.92	0.51
1:A:445:ASN:ND2	1:A:481:TYR:H	2.09	0.51
1:A:991:ALA:O	1:A:995:VAL:HG12	2.11	0.51
1:A:1587:HIS:CE1	1:A:1595:LEU:HD21	2.45	0.51
2:B:156:SER:O	2:B:159:LEU:HG	2.10	0.51
2:B:162:PHE:O	2:B:166:MET:HG2	2.10	0.51
2:B:479:LYS:HA	2:B:482:GLN:CD	2.31	0.51
2:B:667:ASP:HA	2:B:670:ASN:ND2	2.25	0.51
2:B:722:PHE:CD2	2:B:725:ASP:HA	2.45	0.51
1:A:18:ASN:HB3	1:A:20:GLN:OE1	2.11	0.51
1:A:1066:ILE:HD11	1:A:1070:ILE:HD11	1.93	0.51
1:A:1227:LEU:HD12	1:A:1230:LEU:HB2	1.91	0.51
1:A:1363:TYR:HA	1:A:1481:TRP:HB2	1.92	0.51
1:A:1550:PHE:HB3	1:A:1566:LEU:HD11	1.92	0.51
2:B:311:THR:O	2:B:378:MET:HG2	2.10	0.51
2:B:386:TYR:CG	2:B:453:GLU:HG2	2.45	0.51
2:B:389:LYS:HD3	2:B:392:GLN:HE21	1.75	0.51
1:D:1201:MET:HA	1:D:1204:THR:HG22	1.91	0.51
1:D:1454:ASP:HB2	1:D:1457:ASN:O	2.11	0.51
1:D:1457:ASN:HA	1:D:1545:LYS:HD3	1.91	0.51
1:D:1583:GLY:HA2	1:D:1586:ILE:HD12	1.92	0.51
1:A:103:LYS:O	1:A:107:VAL:HG23	2.11	0.51
1:A:553:LYS:O	1:A:594:VAL:HB	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:LYS:HG2	1:A:1200:ARG:HH12	1.74	0.51
1:A:1371:ARG:NH1	1:A:1375:GLN:HB3	2.24	0.51
1:A:1547:GLU:HA	1:A:1551:PHE:HB2	1.92	0.51
2:B:287:ASN:O	2:B:290:MET:N	2.43	0.51
2:B:439:ASN:N	2:B:440:ASP:OD1	2.43	0.51
2:B:452:PHE:CZ	2:B:456:PHE:HB2	2.46	0.51
2:B:658:ASP:O	2:B:662:TYR:N	2.35	0.51
2:B:665:TRP:O	2:B:666:THR:C	2.47	0.51
1:D:1397:ASP:HA	1:D:1400:ASN:HB2	1.93	0.51
1:D:1494:PRO:O	1:D:1497:ASN:HB3	2.10	0.51
1:A:572:ARG:HH22	1:A:597:ARG:CA	2.24	0.51
1:A:957:UNK:C	1:A:959:UNK:N	2.71	0.51
1:A:968:PHE:O	1:A:972:THR:HG23	2.11	0.51
1:A:1321:ASN:O	1:A:1325:GLN:HG3	2.10	0.51
1:A:1535:VAL:HG11	1:A:1602:MET:HG3	1.91	0.51
1:A:1601:ARG:HA	1:A:1604:GLU:CD	2.31	0.51
2:B:356:TYR:O	2:B:359:LEU:HB2	2.11	0.51
2:B:370:ASP:C	2:B:373:GLN:HG2	2.31	0.51
2:B:382:ASP:HA	2:B:385:LEU:HD12	1.91	0.51
2:B:636:GLU:HA	2:B:639:GLU:OE2	2.10	0.51
1:D:1304:LEU:HB2	1:D:1321:ASN:ND2	2.25	0.51
1:A:1168:ALA:O	1:A:1172:GLU:HB2	2.10	0.51
1:A:1333:MET:SD	1:A:1429:GLN:HB3	2.50	0.51
2:B:292:HIS:O	2:B:295:TYR:HB3	2.10	0.51
1:A:6:LYS:CB	2:B:724:TYR:CE2	2.94	0.51
1:A:446:VAL:HB	1:A:478:SER:HB2	1.93	0.51
1:A:1196:SER:O	1:A:1196:SER:OG	2.24	0.51
1:A:1253:TRP:HA	1:A:1274:ARG:HB3	1.93	0.51
1:A:1255:ASP:H	1:A:1274:ARG:HG2	1.76	0.51
1:A:1315:TYR:HA	1:A:1318:LEU:HB3	1.93	0.51
1:A:1464:ILE:O	1:A:1492:ILE:HD12	2.11	0.51
1:A:1563:GLN:HA	1:A:1566:LEU:HD23	1.92	0.51
2:B:168:HIS:C	2:B:170:ILE:H	2.14	0.51
2:B:460:ILE:O	2:B:463:LEU:HB3	2.11	0.51
2:B:702:GLU:O	2:B:704:ILE:HG13	2.11	0.51
1:D:1499:ILE:HG13	1:D:1500:GLU:N	2.25	0.51
1:A:1:MET:SD	2:B:721:ASP:HB2	2.51	0.51
1:A:85:ILE:O	1:A:89:GLN:HG3	2.10	0.51
1:A:187:HIS:NE2	1:A:992:MET:HB2	2.25	0.51
1:A:251:UNK:O	1:A:253:UNK:N	2.44	0.51
1:A:532:VAL:HA	1:A:570:SER:OG	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:TRP:CZ2	1:A:1110:ILE:HD13	2.46	0.51
1:A:1191:VAL:O	1:A:1193:THR:N	2.43	0.51
1:A:1350:GLN:HA	1:A:1357:ARG:CD	2.38	0.51
1:A:1354:SER:O	1:A:1357:ARG:N	2.41	0.51
1:A:1391:THR:C	1:A:1407:GLN:HB2	2.32	0.51
1:A:1568:HIS:O	1:A:1572:LEU:HG	2.11	0.51
2:B:536:LEU:O	2:B:540:ILE:HG22	2.11	0.51
1:D:1285:ILE:HG13	1:D:1286:GLY:N	2.25	0.51
1:D:1324:GLN:HE22	1:D:1327:LYS:HZ1	1.58	0.51
1:A:43:ASP:OD1	1:A:61:LYS:N	2.44	0.51
1:A:121:MET:HA	1:A:124:LEU:HD12	1.93	0.51
1:A:433:GLY:O	1:A:486:GLN:HA	2.11	0.51
1:A:437:LYS:HG2	1:A:439:ASN:HA	1.93	0.51
1:A:513:HIS:N	1:A:523:GLY:HA2	2.26	0.51
1:A:572:ARG:HA	1:A:575:VAL:HG22	1.92	0.51
1:A:1282:GLU:O	1:A:1285:ILE:N	2.43	0.51
1:A:1340:PRO:HG3	1:A:1437:ASN:HD21	1.74	0.51
2:B:249:ALA:HA	2:B:252:LEU:HD12	1.92	0.51
2:B:288:ASN:HA	2:B:291:ALA:HB3	1.92	0.51
2:B:315:PRO:HB2	2:B:366:ASN:HD21	1.74	0.51
2:B:375:PRO:HG2	2:B:422:LYS:HD2	1.92	0.51
2:B:537:LYS:HG2	2:B:690:LEU:HD11	1.93	0.51
2:B:588:TYR:N	2:B:606:ASP:O	2.44	0.51
1:D:1277:LYS:HG2	1:D:1281:TYR:CE2	2.46	0.51
1:D:1323:ILE:O	1:D:1326:ALA:HB3	2.11	0.51
1:D:1496:GLU:HB3	1:D:1500:GLU:OE1	2.11	0.51
1:A:99:GLY:O	1:A:103:LYS:HE2	2.12	0.50
1:A:494:LYS:HE2	1:A:495:VAL:O	2.10	0.50
1:A:1080:ASN:O	1:A:1082:ILE:N	2.44	0.50
1:A:1227:LEU:O	1:A:1230:LEU:HB2	2.10	0.50
2:B:12:ILE:O	2:B:19:PRO:CA	2.37	0.50
2:B:24:ILE:HG12	2:B:33:ILE:HG21	1.93	0.50
2:B:207:SER:HG	2:B:208:MET:H	1.58	0.50
2:B:211:ASN:HB2	2:B:215:LEU:CD1	2.41	0.50
2:B:402:ASN:HA	2:B:405:ARG:NE	2.25	0.50
1:D:1301:CYS:HB2	1:D:1325:GLN:HE21	1.75	0.50
1:D:1446:ARG:CZ	1:D:1465:GLU:HB3	2.41	0.50
1:D:1591:VAL:HG21	1:D:1599:HIS:CE1	2.46	0.50
1:A:17:TYR:CD1	1:A:31:ILE:HD12	2.46	0.50
1:A:447:GLU:HB3	1:A:512:ARG:HB2	1.93	0.50
1:A:1061:ASP:CB	1:A:1064:ARG:HD3	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1515:GLN:OE1	1:A:1519:ASP:HB3	2.11	0.50
2:B:487:GLN:NE2	2:B:509:LEU:HD11	2.25	0.50
1:D:1569:LEU:O	1:D:1573:ILE:N	2.29	0.50
1:A:295:UNK:N	1:A:328:UNK:O	2.45	0.50
1:A:1043:GLN:OE1	1:A:1044:LEU:N	2.43	0.50
1:A:1443:HIS:HB3	1:A:1466:ARG:NE	2.25	0.50
1:A:1480:ARG:HB2	1:A:1481:TRP:CZ3	2.46	0.50
2:B:289:GLU:OE1	2:B:293:GLN:NE2	2.45	0.50
1:D:1301:CYS:HA	1:D:1304:LEU:CD1	2.42	0.50
1:D:1514:ASN:HA	1:D:1517:GLN:HB2	1.92	0.50
1:A:46:ARG:HG2	2:B:726:CYS:SG	2.51	0.50
1:A:148:VAL:O	1:A:152:ILE:HG23	2.11	0.50
1:A:1215:ASN:O	1:A:1217:GLU:N	2.45	0.50
1:A:1218:GLU:O	1:A:1221:ILE:HB	2.11	0.50
1:A:1244:LEU:HD22	1:A:1284:ILE:HA	1.93	0.50
1:A:1289:ASP:O	1:A:1292:LYS:N	2.38	0.50
1:A:1298:ILE:HD12	1:A:1298:ILE:H	1.76	0.50
1:A:1330:GLU:O	1:A:1335:ILE:N	2.45	0.50
1:A:98:TRP:O	1:A:101:ILE:HG12	2.11	0.50
1:A:179:SER:CB	1:A:183:LEU:H	2.24	0.50
1:A:548:ASP:HA	1:A:601:SER:HA	1.92	0.50
1:A:1040:ASP:C	1:A:1042:LEU:H	2.13	0.50
1:A:1168:ALA:O	1:A:1172:GLU:CB	2.59	0.50
1:A:1252:LYS:C	1:A:1277:LYS:HZ2	2.15	0.50
1:A:1391:THR:CA	1:A:1407:GLN:HB2	2.42	0.50
2:B:448:HIS:CE1	2:B:450:ARG:H	2.29	0.50
2:B:516:LYS:O	2:B:520:SER:CB	2.59	0.50
2:B:659:LYS:HA	2:B:662:TYR:HB2	1.92	0.50
2:B:724:TYR:CD1	2:B:724:TYR:CB	2.80	0.50
1:D:1282:GLU:C	1:D:1285:ILE:HG12	2.32	0.50
1:A:1125:PHE:O	1:A:1128:PHE:CB	2.49	0.50
1:A:1249:TRP:CD1	1:A:1250:LEU:HG	2.47	0.50
1:A:1323:ILE:HG22	1:A:1327:LYS:HE2	1.93	0.50
2:B:267:ALA:HA	2:B:271:LEU:HB3	1.94	0.50
2:B:303:ASN:OD1	2:B:431:GLY:N	2.43	0.50
2:B:623:PRO:HD2	2:B:653:ASN:HD21	1.77	0.50
1:A:8:ASP:OD1	1:A:8:ASP:N	2.44	0.50
1:A:67:LYS:HZ1	2:B:701:LEU:HA	1.76	0.50
1:A:187:HIS:HB3	1:A:989:TRP:CZ3	2.47	0.50
1:A:1027:ASN:HB3	1:A:1031:HIS:CE1	2.47	0.50
1:A:1524:ILE:HG23	1:A:1528:SER:OG	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:464:ASN:O	2:B:467:TRP:HB3	2.11	0.50
2:B:576:TYR:HB3	2:B:591:LEU:CG	2.41	0.50
2:B:662:TYR:O	2:B:666:THR:HG23	2.11	0.50
2:B:693:GLU:O	2:B:696:LEU:HB2	2.11	0.50
1:D:1357:ARG:H	1:D:1359:LYS:NZ	2.08	0.50
1:D:1364:ARG:CZ	1:D:1476:PRO:HG3	2.41	0.50
1:D:1479:LEU:HG	1:D:1481:TRP:H	1.77	0.50
1:D:1516:TYR:CZ	1:D:1522:LEU:HD13	2.47	0.50
1:A:12:HIS:CD2	1:A:36:ARG:HB2	2.47	0.50
1:A:40:THR:C	2:B:723:VAL:HG22	2.32	0.50
1:A:1177:LEU:HG	1:A:1178:VAL:N	2.27	0.50
1:A:1221:ILE:HG23	1:A:1225:TYR:CZ	2.46	0.50
1:A:1336:LEU:HD12	1:A:1429:GLN:OE1	2.12	0.50
2:B:11:ALA:HA	2:B:21:LEU:HD22	1.94	0.50
2:B:202:LEU:HD11	2:B:243:THR:CA	2.41	0.50
2:B:564:LYS:HG3	2:B:575:TRP:CD1	2.47	0.50
1:A:19:PHE:HA	1:A:63:PHE:HE2	1.77	0.50
1:A:92:THR:HG22	1:A:96:TRP:HE1	1.77	0.50
1:A:456:ASP:HA	1:A:508:ARG:HH21	1.76	0.50
1:A:705:UNK:O	1:A:707:UNK:N	2.45	0.50
1:A:1043:GLN:C	1:A:1046:GLN:HE22	2.15	0.50
1:A:1313:PHE:N	1:A:1313:PHE:CD1	2.79	0.50
1:A:1343:PHE:CD1	1:A:1410:THR:HG23	2.47	0.50
2:B:8:VAL:HG11	2:B:69:ILE:HG21	1.93	0.50
2:B:63:GLU:HA	2:B:66:ARG:HG2	1.94	0.50
2:B:556:LEU:HD11	2:B:668:GLY:HA3	1.94	0.50
2:B:693:GLU:OE2	2:B:697:ARG:NE	2.45	0.50
1:D:1237:TYR:CE2	1:D:1290:LYS:HB3	2.47	0.50
1:A:19:PHE:HB3	1:A:29:LEU:CG	2.42	0.49
1:A:262:UNK:N	1:A:265:UNK:HA	2.27	0.49
1:A:887:UNK:O	1:A:890:UNK:N	2.45	0.49
1:A:1280:LEU:O	1:A:1283:THR:OG1	2.25	0.49
1:A:1322:LEU:HA	1:A:1325:GLN:NE2	2.27	0.49
1:A:1345:VAL:HA	1:A:1407:GLN:O	2.11	0.49
1:A:1575:TRP:CE3	1:A:1620:ARG:HB3	2.47	0.49
1:A:1587:HIS:CD2	1:A:1599:HIS:CD2	3.00	0.49
2:B:287:ASN:H	2:B:290:MET:CE	2.25	0.49
2:B:309:MET:SD	2:B:425:CYS:HB3	2.52	0.49
2:B:466:THR:HA	2:B:469:GLU:CG	2.42	0.49
1:D:1244:LEU:CB	1:D:1284:ILE:HD11	2.41	0.49
1:D:1361:PHE:HB2	1:D:1363:TYR:CE1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1534:ILE:HD11	1:D:1576:GLN:NE2	2.27	0.49
1:A:230:UNK:HA	1:A:378:UNK:C	2.42	0.49
1:A:264:UNK:HA	1:A:268:UNK:HA	1.94	0.49
1:A:572:ARG:HH12	1:A:597:ARG:C	2.16	0.49
1:A:1338:PRO:HB3	1:A:1368:TYR:HE2	1.73	0.49
1:A:1343:PHE:CG	1:A:1410:THR:HA	2.47	0.49
1:A:1524:ILE:HD11	1:A:1527:LEU:HD22	1.93	0.49
1:A:1584:ILE:HG22	1:A:1588:GLU:OE1	2.13	0.49
2:B:241:THR:OG1	2:B:290:MET:SD	2.66	0.49
2:B:285:ALA:C	2:B:595:PRO:HB3	2.32	0.49
2:B:316:GLN:HA	2:B:321:ARG:HH22	1.78	0.49
2:B:331:ALA:O	2:B:396:ILE:HG23	2.12	0.49
2:B:360:GLY:HA3	2:B:413:PHE:CD2	2.47	0.49
2:B:579:LEU:HD21	2:B:583:HIS:HA	1.94	0.49
1:D:1243:THR:HG22	1:D:1246:LEU:HD12	1.92	0.49
1:A:768:UNK:C	1:A:770:UNK:N	2.73	0.49
1:A:1024:GLN:NE2	1:A:1027:ASN:HB2	2.28	0.49
1:A:1171:VAL:O	1:A:1175:VAL:HG23	2.12	0.49
1:A:1204:THR:HB	1:A:1227:LEU:HD13	1.94	0.49
1:A:1305:ALA:HA	1:A:1308:TYR:HB2	1.92	0.49
1:A:1375:GLN:HE22	1:A:1406:ILE:HG21	1.77	0.49
2:B:165:LEU:O	2:B:168:HIS:N	2.45	0.49
2:B:312:LYS:HB3	2:B:372:THR:HA	1.93	0.49
1:A:222:UNK:H	1:A:387:UNK:HA	1.76	0.49
1:A:1179:LYS:HD3	1:A:1179:LYS:N	2.28	0.49
1:A:1610:LYS:HZ3	1:A:1614:GLU:CD	2.13	0.49
2:B:84:ASN:O	2:B:88:LEU:HG	2.12	0.49
2:B:313:MET:N	2:B:372:THR:HA	2.16	0.49
1:D:1613:VAL:O	1:D:1618:GLY:N	2.44	0.49
1:A:4:TRP:HB3	2:B:724:TYR:HA	1.95	0.49
1:A:1046:GLN:O	1:A:1052:TYR:HB2	2.12	0.49
2:B:207:SER:OG	2:B:208:MET:N	2.46	0.49
2:B:311:THR:O	2:B:377:GLY:HA3	2.12	0.49
2:B:354:ARG:C	2:B:356:TYR:N	2.66	0.49
2:B:387:PHE:O	2:B:391:HIS:N	2.45	0.49
2:B:541:GLN:O	2:B:545:LEU:HG	2.13	0.49
2:B:577:CYS:SG	2:B:586:LEU:HD21	2.52	0.49
1:D:1212:LYS:C	1:D:1215:ASN:H	2.16	0.49
1:D:1557:ARG:NH2	1:D:1558:ASP:OD2	2.45	0.49
1:D:1577:ILE:HG22	1:D:1610:LYS:NZ	2.27	0.49
1:A:81:ILE:CG1	1:A:86:PRO:HD3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:PRO:HD2	1:A:489:TRP:HE1	1.77	0.49
1:A:1024:GLN:HA	1:A:1027:ASN:ND2	2.19	0.49
1:A:1166:THR:OG1	1:A:1167:ILE:HD12	2.12	0.49
1:A:1206:ASN:HB3	1:A:1210:PHE:CE2	2.47	0.49
1:A:1334:LYS:HE3	1:D:1316:GLU:CA	2.35	0.49
1:A:1339:LYS:NZ	1:A:1341:ASP:OD2	2.45	0.49
1:A:1401:ALA:HB3	1:A:1405:TYR:CE2	2.48	0.49
2:B:452:PHE:CE2	2:B:453:GLU:HG3	2.47	0.49
2:B:575:TRP:HB2	2:B:590:ASP:OD1	2.13	0.49
2:B:604:LEU:O	2:B:606:ASP:N	2.41	0.49
1:D:1301:CYS:O	1:D:1321:ASN:ND2	2.45	0.49
1:D:1331:SER:HA	1:D:1334:LYS:HZ2	1.77	0.49
1:D:1492:ILE:HG13	1:D:1493:SER:O	2.12	0.49
1:A:16:ILE:HD13	1:A:65:HIS:HB2	1.94	0.49
1:A:94:THR:O	1:A:98:TRP:CD1	2.65	0.49
1:A:96:TRP:CE3	2:B:696:LEU:HD22	2.47	0.49
1:A:133:SER:O	1:A:135:THR:HG23	2.12	0.49
1:A:139:ASP:O	1:A:142:LYS:NZ	2.33	0.49
1:A:572:ARG:HH22	1:A:597:ARG:HA	1.77	0.49
1:A:969:LEU:HB3	1:A:973:PHE:CZ	2.48	0.49
1:A:1047:PHE:O	1:A:1049:HIS:N	2.45	0.49
1:A:1124:ASP:O	1:A:1127:LYS:N	2.24	0.49
2:B:114:VAL:O	2:B:117:ALA:HB3	2.13	0.49
2:B:164:GLU:O	2:B:167:ASP:HB2	2.13	0.49
2:B:249:ALA:O	2:B:252:LEU:HB2	2.13	0.49
2:B:443:PRO:HA	2:B:446:PHE:CD1	2.46	0.49
2:B:448:HIS:CD2	2:B:449:ASP:N	2.81	0.49
2:B:466:THR:HA	2:B:469:GLU:HB2	1.94	0.49
2:B:545:LEU:HG	2:B:686:LEU:HD13	1.95	0.49
2:B:575:TRP:HB2	2:B:589:GLY:O	2.12	0.49
1:D:1301:CYS:HA	1:D:1304:LEU:HD12	1.94	0.49
1:A:102:TRP:CH2	1:A:118:GLN:HB2	2.48	0.49
1:A:120:MET:O	1:A:124:LEU:HG	2.13	0.49
1:A:127:TRP:HA	1:A:130:GLN:HB2	1.95	0.49
1:A:452:VAL:HA	1:A:507:LEU:HD23	1.95	0.49
1:A:513:HIS:CG	1:A:524:GLU:HB2	2.47	0.49
1:A:1180:GLY:C	1:A:1184:LYS:HE2	2.32	0.49
1:A:1274:ARG:HG3	1:A:1275:GLN:N	2.26	0.49
1:A:1388:MET:HE2	1:A:1405:TYR:HB3	1.95	0.49
1:A:1466:ARG:HG2	1:A:1467:THR:N	2.28	0.49
2:B:89:HIS:C	2:B:93:GLN:HB2	2.32	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:276:LEU:HA	2:B:280:ILE:HD12	1.94	0.49
2:B:612:ASP:OD2	2:B:613:ILE:N	2.45	0.49
2:B:614:LYS:HE3	2:B:647:ASP:HA	1.95	0.49
1:D:1239:GLU:HG3	1:D:1478:ILE:CA	2.40	0.49
1:D:1284:ILE:HG12	1:D:1287:TYR:HD2	1.78	0.49
1:D:1331:SER:HA	1:D:1334:LYS:NZ	2.27	0.49
1:A:86:PRO:HA	1:A:89:GLN:CD	2.33	0.49
1:A:127:TRP:CG	1:A:144:LEU:HD11	2.46	0.49
1:A:544:ASP:HA	1:A:547:HIS:HE1	1.77	0.49
1:A:811:UNK:O	1:A:815:UNK:N	2.46	0.49
1:A:1074:TRP:CE2	1:A:1107:THR:HA	2.48	0.49
1:A:1601:ARG:HA	1:A:1604:GLU:OE1	2.12	0.49
2:B:101:LEU:HA	2:B:154:MET:HG3	1.94	0.49
2:B:292:HIS:CE1	2:B:436:GLU:HA	2.46	0.49
2:B:315:PRO:HD3	2:B:372:THR:HG21	1.94	0.49
1:D:1324:GLN:HE22	1:D:1327:LYS:NZ	2.11	0.49
1:A:21:GLY:H	1:A:28:SER:HA	1.77	0.49
1:A:37:ILE:HD13	1:A:45:TYR:CD1	2.48	0.49
1:A:43:ASP:OD1	1:A:62:SER:N	2.46	0.49
1:A:127:TRP:HB3	1:A:144:LEU:HD21	1.95	0.49
1:A:446:VAL:HB	1:A:478:SER:CB	2.43	0.49
1:A:507:LEU:H	1:A:531:TYR:HB2	1.77	0.49
1:A:985:TYR:HE2	1:A:993:SER:HA	1.78	0.49
1:A:1231:HIS:CG	1:A:1239:GLU:HB2	2.48	0.49
1:A:1308:TYR:CD1	1:A:1318:LEU:HB2	2.48	0.49
1:A:1450:ARG:HG3	1:A:1463:TRP:CD2	2.48	0.49
2:B:84:ASN:HA	2:B:87:GLN:OE1	2.13	0.49
2:B:177:SER:O	2:B:181:ILE:HG12	2.13	0.49
2:B:180:PHE:CZ	2:B:184:ILE:HD11	2.48	0.49
2:B:386:TYR:OH	2:B:448:HIS:HE1	1.96	0.49
2:B:496:PRO:HG3	2:B:502:PHE:CD1	2.47	0.49
2:B:550:GLN:O	2:B:553:LEU:HB2	2.12	0.49
2:B:562:PHE:HE2	2:B:577:CYS:HB2	1.78	0.49
2:B:567:ALA:N	2:B:573:LYS:HZ1	2.11	0.49
1:D:1273:HIS:HA	1:D:1276:LEU:HB2	1.95	0.49
1:D:1333:MET:HA	1:D:1429:GLN:HG2	1.94	0.49
1:D:1557:ARG:O	1:D:1560:PRO:HD3	2.13	0.49
1:D:1559:HIS:ND1	1:D:1561:GLU:OE2	2.42	0.49
1:A:6:LYS:C	2:B:724:TYR:CD1	2.85	0.48
1:A:38:GLN:HG2	1:A:56:GLN:HE22	1.78	0.48
1:A:776:UNK:O	1:A:780:UNK:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1591:VAL:HG21	1:A:1596:ARG:HA	1.95	0.48
2:B:259:ARG:O	2:B:262:MET:HB3	2.12	0.48
2:B:634:ASN:HB3	2:B:636:GLU:OE1	2.12	0.48
1:D:1252:LYS:HE3	1:D:1254:SER:HB3	1.94	0.48
1:D:1272:THR:OG1	1:D:1275:GLN:OE1	2.25	0.48
1:D:1349:GLY:HA2	1:D:1401:ALA:N	2.27	0.48
1:D:1555:TYR:OH	1:D:1562:ASP:HB2	2.12	0.48
1:A:110:LYS:CG	1:A:113:ARG:HB3	2.42	0.48
1:A:571:TYR:HB3	1:A:573:HIS:ND1	2.27	0.48
1:A:1361:PHE:CB	1:A:1363:TYR:HE1	2.26	0.48
1:A:1397:ASP:CG	1:A:1401:ALA:HB2	2.33	0.48
2:B:124:ASP:HB3	2:B:127:SER:OG	2.14	0.48
2:B:251:PHE:HZ	2:B:263:ALA:HA	1.77	0.48
2:B:535:GLU:C	2:B:539:LYS:HE3	2.34	0.48
1:D:1304:LEU:HB3	1:D:1308:TYR:OH	2.13	0.48
1:D:1443:HIS:HA	1:D:1468:SER:HA	1.95	0.48
1:A:291:UNK:O	1:A:293:UNK:N	2.46	0.48
1:A:456:ASP:CA	1:A:508:ARG:HH21	2.27	0.48
1:A:1026:TRP:O	1:A:1030:PHE:CD2	2.66	0.48
1:A:1181:LEU:HG	1:A:1185:LEU:HD21	1.96	0.48
1:A:1211:TYR:CD2	1:A:1220:TYR:HA	2.48	0.48
1:A:1239:GLU:OE2	1:A:1480:ARG:HG2	2.13	0.48
1:A:1275:GLN:HG3	1:A:1276:LEU:HD23	1.95	0.48
1:A:1333:MET:SD	1:A:1430:ILE:HG23	2.53	0.48
1:A:1361:PHE:HD1	1:A:1482:PHE:C	2.16	0.48
1:A:1581:GLY:HA2	1:A:1584:ILE:HB	1.95	0.48
2:B:49:PHE:CA	2:B:78:THR:O	2.53	0.48
2:B:160:THR:O	2:B:163:VAL:HB	2.14	0.48
2:B:398:ILE:O	2:B:401:GLU:HB2	2.13	0.48
2:B:514:ILE:O	2:B:518:ARG:HG3	2.13	0.48
2:B:640:LEU:HD13	2:B:656:ALA:O	2.13	0.48
2:B:643:SER:OG	2:B:651:GLN:OE1	2.25	0.48
1:D:1208:LEU:HD12	1:D:1211:TYR:HD2	1.78	0.48
1:D:1236:ASN:O	1:D:1239:GLU:N	2.46	0.48
1:D:1332:ILE:HG13	1:D:1333:MET:N	2.28	0.48
1:D:1348:TYR:HB3	1:D:1399:LYS:CA	2.41	0.48
1:D:1446:ARG:O	1:D:1446:ARG:HD2	2.13	0.48
1:D:1532:ASN:O	1:D:1536:ASP:HB3	2.12	0.48
1:D:1540:MET:HG3	1:D:1541:GLY:N	2.28	0.48
1:A:551:VAL:HB	1:A:596:SER:HB2	1.94	0.48
1:A:1066:ILE:HD12	1:A:1069:SER:OG	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:TYR:HB3	1:A:1228:ARG:NH2	2.27	0.48
1:A:1272:THR:HB	1:A:1275:GLN:HB3	1.95	0.48
1:A:1288:PHE:CZ	1:A:1296:GLU:HB2	2.48	0.48
1:A:1429:GLN:HA	1:A:1432:ASN:HD21	1.75	0.48
2:B:471:ARG:CZ	2:B:471:ARG:HB3	2.43	0.48
2:B:478:ASN:OD1	2:B:479:LYS:HG3	2.13	0.48
1:D:1207:LEU:HA	1:D:1210:PHE:CD2	2.49	0.48
1:D:1216:ARG:CG	1:D:1219:MET:HB3	2.43	0.48
1:A:43:ASP:HA	1:A:61:LYS:CB	2.43	0.48
1:A:519:SER:O	1:A:520:LYS:HG2	2.14	0.48
1:A:555:ASP:HB2	1:A:558:LYS:CB	2.42	0.48
1:A:939:UNK:O	1:A:940:UNK:C	2.60	0.48
1:A:989:TRP:HB3	1:A:992:MET:HB3	1.94	0.48
1:A:1007:PHE:O	1:A:1011:MET:HG2	2.14	0.48
1:A:1527:LEU:O	1:A:1530:LEU:HB3	2.14	0.48
2:B:51:LEU:HD13	2:B:76:ARG:O	2.14	0.48
2:B:180:PHE:O	2:B:184:ILE:HG12	2.13	0.48
2:B:419:GLU:HG3	2:B:420:LEU:N	2.28	0.48
2:B:448:HIS:CE1	2:B:450:ARG:HB2	2.48	0.48
2:B:546:GLU:OE2	2:B:550:GLN:NE2	2.46	0.48
1:D:1251:LEU:HD12	1:D:1252:LYS:N	2.28	0.48
1:D:1307:GLN:HA	1:D:1311:GLU:H	1.78	0.48
1:A:9:LYS:O	1:A:11:ARG:N	2.47	0.48
1:A:24:ALA:HA	1:A:25:PRO:HA	1.61	0.48
1:A:512:ARG:NH1	1:A:526:ASN:H	2.12	0.48
1:A:965:LEU:O	1:A:968:PHE:N	2.46	0.48
1:A:1196:SER:HG	1:A:1200:ARG:H	1.61	0.48
2:B:669:LEU:HA	2:B:672:LEU:HG	1.96	0.48
1:A:19:PHE:CZ	1:A:21:GLY:HA3	2.48	0.48
1:A:1072:ASP:HA	1:A:1075:TYR:CZ	2.48	0.48
1:A:1247:HIS:CD2	1:A:1251:LEU:HD11	2.48	0.48
1:A:1313:PHE:CE2	1:D:1426:VAL:HA	2.48	0.48
2:B:198:LEU:C	2:B:201:SER:HG	2.11	0.48
2:B:371:PHE:O	2:B:377:GLY:HA2	2.13	0.48
2:B:475:GLU:CD	2:B:475:GLU:H	2.16	0.48
1:A:20:GLN:HA	1:A:28:SER:OG	2.13	0.48
1:A:49:LEU:HD12	1:A:55:LEU:HD23	1.96	0.48
1:A:1086:PRO:O	1:A:1088:MET:N	2.47	0.48
1:A:1088:MET:HE2	1:A:1092:ILE:HG13	1.95	0.48
1:A:1314:ASP:OD2	1:A:1317:LEU:HB2	2.13	0.48
1:A:1398:VAL:HA	1:A:1405:TYR:CE2	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1470:VAL:N	1:A:1484:VAL:HG13	2.29	0.48
1:A:1557:ARG:O	1:A:1560:PRO:HD3	2.14	0.48
2:B:53:HIS:HD2	2:B:58:ASN:HA	1.79	0.48
2:B:161:ALA:O	2:B:165:LEU:HG	2.14	0.48
2:B:167:ASP:N	2:B:167:ASP:OD1	2.46	0.48
2:B:172:SER:C	2:B:173:TRP:CD1	2.87	0.48
2:B:196:SER:HA	2:B:200:ARG:CZ	2.44	0.48
2:B:212:SER:H	2:B:215:LEU:HD12	1.79	0.48
2:B:556:LEU:HA	2:B:665:TRP:CH2	2.49	0.48
2:B:637:VAL:O	2:B:641:ALA:N	2.46	0.48
1:D:1391:THR:HA	1:D:1407:GLN:HB3	1.95	0.48
1:D:1395:GLY:O	1:D:1398:VAL:HB	2.12	0.48
1:D:1465:GLU:HA	1:D:1490:THR:C	2.33	0.48
1:A:11:ARG:HA	1:A:36:ARG:HH21	1.79	0.48
1:A:433:GLY:H	1:A:486:GLN:NE2	2.11	0.48
1:A:884:UNK:O	1:A:885:UNK:C	2.62	0.48
1:A:1068:PHE:HD1	1:A:1071:ARG:CZ	2.26	0.48
1:A:1471:THR:OG1	1:A:1472:ALA:N	2.44	0.48
1:A:1515:GLN:CD	1:A:1522:LEU:HD11	2.34	0.48
1:A:1543:PHE:HA	1:A:1546:TYR:HB2	1.95	0.48
2:B:313:MET:HB3	2:B:372:THR:HG22	1.95	0.48
1:D:1203:CYS:HA	1:D:1206:ASN:ND2	2.28	0.48
1:D:1203:CYS:O	1:D:1206:ASN:HB2	2.13	0.48
1:D:1556:VAL:HA	1:D:1563:GLN:HE21	1.77	0.48
1:A:781:UNK:O	1:A:784:UNK:CB	2.62	0.48
1:A:1085:ILE:HB	1:A:1086:PRO:HD3	1.95	0.48
1:A:1447:PRO:CA	1:A:1464:ILE:HG12	2.43	0.48
1:A:1449:ARG:HA	1:A:1462:MET:HG3	1.96	0.48
1:A:1450:ARG:HH21	1:A:1491:THR:HG21	1.78	0.48
1:A:1515:GLN:HG3	1:A:1516:TYR:CD1	2.49	0.48
2:B:227:GLN:O	2:B:230:PRO:HD2	2.14	0.48
2:B:266:LEU:O	2:B:271:LEU:HB2	2.13	0.48
2:B:292:HIS:CA	2:B:439:ASN:HA	2.43	0.48
2:B:361:PHE:HD2	2:B:364:HIS:ND1	2.11	0.48
2:B:492:LEU:HA	2:B:492:LEU:HD23	1.50	0.48
2:B:555:ARG:HA	2:B:558:GLU:OE1	2.13	0.48
2:B:579:LEU:HD13	2:B:586:LEU:HA	1.95	0.48
2:B:647:ASP:O	2:B:650:CYS:N	2.46	0.48
1:D:1208:LEU:HA	1:D:1211:TYR:CE2	2.49	0.48
1:D:1294:TRP:HZ3	1:D:1331:SER:HB2	1.78	0.48
1:D:1349:GLY:HA3	1:D:1401:ALA:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LEU:HB3	1:A:52:HIS:CD2	2.42	0.47
1:A:1196:SER:OG	1:A:1200:ARG:N	2.47	0.47
1:A:1218:GLU:HA	1:A:1221:ILE:HB	1.96	0.47
1:A:1549:ALA:HB3	1:A:1550:PHE:CE2	2.49	0.47
1:A:1582:ALA:HA	1:A:1585:LYS:HB2	1.96	0.47
1:A:1603:GLU:HA	1:A:1606:PHE:HB3	1.95	0.47
2:B:171:VAL:HG23	2:B:173:TRP:NE1	2.29	0.47
2:B:316:GLN:HA	2:B:321:ARG:NH2	2.28	0.47
2:B:374:THR:HG22	2:B:376:PRO:O	2.13	0.47
2:B:546:GLU:O	2:B:549:LYS:N	2.47	0.47
1:D:1386:GLU:O	1:D:1405:TYR:HA	2.14	0.47
1:A:6:LYS:HG2	2:B:724:TYR:CD2	2.49	0.47
1:A:101:ILE:CA	1:A:104:GLN:HG2	2.44	0.47
1:A:847:UNK:O	1:A:851:UNK:N	2.47	0.47
1:A:972:THR:HB	1:A:976:PHE:CZ	2.48	0.47
1:A:1124:ASP:N	1:A:1126:LYS:HG3	2.29	0.47
1:A:1469:PHE:CD1	1:A:1487:MET:HG2	2.46	0.47
1:A:1495:LEU:HG	1:A:1496:GLU:N	2.30	0.47
1:A:1559:HIS:HB3	1:A:1562:ASP:CG	2.35	0.47
2:B:38:CYS:HB2	2:B:46:HIS:CB	2.44	0.47
2:B:213:HIS:O	2:B:217:GLN:HG3	2.13	0.47
2:B:426:GLU:O	2:B:429:LYS:N	2.47	0.47
2:B:588:TYR:OH	2:B:607:LYS:O	2.32	0.47
1:D:1252:LYS:HE3	1:D:1252:LYS:HB2	1.53	0.47
1:D:1275:GLN:OE1	1:D:1275:GLN:N	2.42	0.47
1:D:1523:PRO:O	1:D:1526:PRO:HD2	2.14	0.47
1:A:183:LEU:O	1:A:186:ALA:HB3	2.14	0.47
1:A:444:ARG:HE	1:A:447:GLU:H	1.61	0.47
1:A:449:ILE:HB	1:A:510:MET:HB2	1.96	0.47
1:A:453:CYS:O	1:A:505:ILE:HB	2.14	0.47
1:A:973:PHE:O	1:A:977:LYS:HG3	2.13	0.47
1:A:1156:ILE:O	1:A:1159:GLU:HG2	2.13	0.47
1:A:1210:PHE:N	1:A:1210:PHE:CD1	2.80	0.47
1:A:1211:TYR:CD1	1:A:1216:ARG:HB2	2.49	0.47
2:B:326:GLU:O	2:B:330:ILE:HG13	2.13	0.47
2:B:671:ALA:HB2	2:B:677:MET:HE2	1.97	0.47
1:D:1244:LEU:O	1:D:1247:HIS:HB3	2.14	0.47
1:D:1272:THR:OG1	1:D:1275:GLN:NE2	2.46	0.47
1:D:1414:VAL:HB	1:D:1441:ARG:HB2	1.96	0.47
1:D:1470:VAL:O	1:D:1485:VAL:HB	2.14	0.47
1:D:1531:LEU:HD11	1:D:1584:ILE:HG12	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:SER:HB3	2:B:714:PRO:HD2	1.96	0.47
1:A:65:HIS:CE1	2:B:704:ILE:HD13	2.49	0.47
1:A:595:SER:O	1:A:595:SER:OG	2.30	0.47
1:A:657:GLU:O	1:A:660:ILE:N	2.48	0.47
1:A:829:UNK:O	1:A:832:UNK:N	2.48	0.47
1:A:1186:LEU:O	1:A:1189:ARG:HB3	2.13	0.47
1:A:1197:LYS:HA	1:A:1200:ARG:CZ	2.45	0.47
1:A:1330:GLU:HA	1:A:1334:LYS:HD2	1.96	0.47
1:A:1346:GLY:O	1:A:1407:GLN:HG2	2.14	0.47
1:A:1372:GLU:O	1:A:1376:MET:HG2	2.15	0.47
1:A:1501:THR:OG1	1:A:1502:MET:N	2.48	0.47
1:A:1574:ALA:HA	1:A:1577:ILE:HG12	1.96	0.47
2:B:199:GLN:O	2:B:202:LEU:HB3	2.14	0.47
2:B:226:GLY:HA2	2:B:229:ILE:CD1	2.44	0.47
2:B:540:ILE:HG12	2:B:544:ILE:HG12	1.97	0.47
2:B:557:VAL:HG13	2:B:579:LEU:O	2.14	0.47
2:B:609:PRO:HB2	2:B:612:ASP:OD1	2.15	0.47
1:D:1469:PHE:HB3	1:D:1484:VAL:HG11	1.96	0.47
1:A:96:TRP:CZ3	2:B:696:LEU:HD13	2.49	0.47
1:A:1226:LYS:HA	1:A:1229:ASP:OD2	2.15	0.47
1:A:1435:LYS:HD3	1:A:1436:SER:N	2.30	0.47
1:A:1459:PHE:HD2	1:A:1546:TYR:CE1	2.31	0.47
1:A:1585:LYS:HA	1:A:1588:GLU:HB2	1.96	0.47
2:B:62:THR:O	2:B:65:ASN:N	2.48	0.47
2:B:178:VAL:HA	2:B:181:ILE:HB	1.97	0.47
2:B:419:GLU:HG2	2:B:477:PHE:CZ	2.50	0.47
2:B:479:LYS:O	2:B:482:GLN:HB2	2.14	0.47
2:B:577:CYS:SG	2:B:586:LEU:HD11	2.54	0.47
2:B:585:VAL:HG13	2:B:608:LEU:H	1.80	0.47
2:B:687:ASP:OD1	2:B:690:LEU:HD23	2.15	0.47
1:D:1601:ARG:O	1:D:1604:GLU:HB3	2.15	0.47
1:A:152:ILE:HG13	1:A:153:ASP:OD1	2.14	0.47
1:A:433:GLY:HA3	1:A:487:PRO:HD2	1.97	0.47
1:A:517:LEU:HD12	1:A:518:GLU:HB3	1.95	0.47
1:A:554:GLY:H	1:A:559:MET:HE1	1.79	0.47
1:A:995:VAL:O	1:A:999:VAL:HG12	2.15	0.47
1:A:1479:LEU:H	1:A:1482:PHE:HE1	1.61	0.47
2:B:61:ILE:HA	2:B:65:ASN:CB	2.45	0.47
2:B:96:SER:O	2:B:100:LYS:N	2.44	0.47
2:B:292:HIS:CE1	2:B:436:GLU:C	2.88	0.47
2:B:326:GLU:OE1	2:B:329:ARG:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ALA:HB1	2:B:397:ARG:CZ	2.44	0.47
2:B:591:LEU:O	2:B:592:GLU:HG2	2.14	0.47
1:D:1343:PHE:CE2	1:D:1365:GLY:HA3	2.49	0.47
1:D:1569:LEU:O	1:D:1572:LEU:HB3	2.14	0.47
1:A:48:TYR:HB3	1:A:56:GLN:CD	2.34	0.47
1:A:62:SER:CB	2:B:713:ILE:HA	2.43	0.47
1:A:287:UNK:O	1:A:291:UNK:N	2.48	0.47
1:A:426:ILE:H	1:A:494:LYS:CE	2.28	0.47
1:A:802:UNK:O	1:A:803:UNK:C	2.62	0.47
1:A:937:UNK:O	1:A:940:UNK:N	2.48	0.47
1:A:939:UNK:O	1:A:942:UNK:N	2.48	0.47
1:A:975:MET:O	1:A:979:LEU:HD23	2.15	0.47
1:A:1201:MET:CE	1:A:1230:LEU:HB3	2.44	0.47
1:A:1244:LEU:O	1:A:1247:HIS:HB3	2.15	0.47
1:A:1251:LEU:HD21	1:A:1280:LEU:HD13	1.96	0.47
1:A:1253:TRP:CH2	1:A:1281:TYR:HE2	2.32	0.47
1:A:1334:LYS:NZ	1:D:1315:TYR:HB3	2.30	0.47
1:A:1426:VAL:HG13	1:D:1313:PHE:CG	2.49	0.47
1:A:1428:ASP:O	1:A:1430:ILE:N	2.48	0.47
1:A:1479:LEU:C	1:A:1481:TRP:N	2.68	0.47
1:A:1511:MET:HE3	1:A:1514:ASN:HB2	1.97	0.47
1:A:1532:ASN:O	1:A:1536:ASP:HB2	2.15	0.47
1:A:1599:HIS:O	1:A:1602:MET:HB3	2.14	0.47
2:B:120:PHE:O	2:B:124:ASP:N	2.47	0.47
2:B:172:SER:OG	2:B:173:TRP:N	2.47	0.47
2:B:224:THR:N	2:B:227:GLN:OE1	2.46	0.47
2:B:298:GLN:HB3	2:B:302:PHE:CE2	2.50	0.47
2:B:313:MET:SD	2:B:368:ALA:HB1	2.55	0.47
2:B:454:GLU:HB2	2:B:499:LEU:HD13	1.96	0.47
2:B:557:VAL:O	2:B:579:LEU:N	2.47	0.47
2:B:645:LEU:HA	2:B:651:GLN:CB	2.37	0.47
1:D:1206:ASN:HB3	1:D:1210:PHE:CE2	2.50	0.47
1:D:1253:TRP:HZ2	1:D:1281:TYR:CD2	2.33	0.47
1:D:1390:THR:O	1:D:1407:GLN:NE2	2.47	0.47
1:D:1411:VAL:HG12	1:D:1444:TYR:HB2	1.96	0.47
1:D:1412:GLN:OE1	1:D:1444:TYR:HA	2.15	0.47
1:D:1579:PHE:HA	1:D:1582:ALA:HB3	1.97	0.47
1:A:102:TRP:NE1	1:A:117:VAL:HB	2.29	0.47
1:A:424:ASN:HA	1:A:426:ILE:HD11	1.97	0.47
1:A:1034:VAL:HA	1:A:1037:ILE:HD11	1.96	0.47
1:A:1098:ILE:HG23	1:A:1101:ALA:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1108:ILE:N	1:A:1109:PRO:HD2	2.30	0.47
1:A:1183:GLU:OE2	1:A:1184:LYS:NZ	2.31	0.47
1:A:1315:TYR:OH	1:D:1430:ILE:HD13	2.15	0.47
2:B:74:ILE:C	2:B:75:LEU:HD22	2.35	0.47
2:B:202:LEU:CA	2:B:205:LEU:HD12	2.43	0.47
2:B:209:VAL:HG13	2:B:216:TYR:HD1	1.80	0.47
2:B:394:ALA:O	2:B:397:ARG:HB3	2.14	0.47
2:B:667:ASP:CG	2:B:678:MET:H	2.17	0.47
1:D:1294:TRP:HA	1:D:1297:ALA:HB3	1.96	0.47
1:D:1369:GLU:CD	1:D:1374:PHE:HD1	2.18	0.47
1:D:1417:GLU:CD	1:D:1417:GLU:H	2.18	0.47
1:A:19:PHE:CE2	1:A:60:PRO:HD3	2.50	0.47
1:A:48:TYR:CD2	1:A:53:LYS:HA	2.49	0.47
1:A:439:ASN:HB3	1:A:441:THR:O	2.15	0.47
1:A:531:TYR:CE2	1:A:565:TYR:HB3	2.50	0.47
1:A:886:UNK:O	1:A:887:UNK:C	2.62	0.47
1:A:1211:TYR:HB3	1:A:1220:TYR:HD1	1.78	0.47
1:A:1463:TRP:CD1	1:A:1494:PRO:HD3	2.49	0.47
1:A:1463:TRP:NE1	1:A:1494:PRO:HD3	2.29	0.47
1:A:1471:THR:HA	1:A:1485:VAL:N	2.13	0.47
1:A:1479:LEU:HD12	1:A:1480:ARG:N	2.29	0.47
1:A:1516:TYR:CD2	1:A:1520:GLU:HA	2.50	0.47
1:D:1363:TYR:HB2	1:D:1374:PHE:HE2	1.80	0.47
1:D:1540:MET:HG3	1:D:1541:GLY:H	1.80	0.47
1:A:10:GLU:O	1:A:37:ILE:HB	2.14	0.47
1:A:15:ALA:O	1:A:32:GLY:N	2.39	0.47
1:A:131:LEU:HG	1:A:144:LEU:HD23	1.96	0.47
1:A:547:HIS:H	1:A:602:ILE:H	1.63	0.47
1:A:823:UNK:C	1:A:825:UNK:H	2.28	0.47
1:A:1063:ARG:HA	1:A:1066:ILE:CG2	2.45	0.47
1:A:1342:TYR:C	1:A:1343:PHE:CD1	2.88	0.47
1:A:1347:TYR:HB3	1:A:1352:PHE:CD2	2.42	0.47
1:A:1375:GLN:HG2	1:A:1387:LYS:HE3	1.96	0.47
1:A:1547:GLU:HG3	1:A:1551:PHE:CD2	2.50	0.47
2:B:8:VAL:HA	2:B:71:ASN:HD21	1.78	0.47
2:B:114:VAL:HB	2:B:168:HIS:CE1	2.50	0.47
2:B:229:ILE:O	2:B:233:GLN:HG3	2.15	0.47
2:B:374:THR:HG22	2:B:376:PRO:C	2.34	0.47
2:B:569:ARG:CZ	2:B:571:GLN:HE22	2.27	0.47
2:B:584:LYS:O	2:B:610:VAL:N	2.42	0.47
2:B:661:GLU:HA	2:B:664:ILE:HB	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:666:THR:O	2:B:669:LEU:HB2	2.15	0.47
1:D:1509:ILE:HA	1:D:1512:MET:HB2	1.97	0.47
1:A:434:ASP:HB2	1:A:600:PHE:HZ	1.80	0.46
1:A:527:PHE:HD1	1:A:553:LYS:HE3	1.79	0.46
1:A:934:UNK:C	1:A:936:UNK:N	2.77	0.46
1:A:1068:PHE:HA	1:A:1071:ARG:HE	1.79	0.46
1:A:1090:GLY:O	1:A:1091:PRO:C	2.52	0.46
1:A:1093:LEU:H	1:A:1093:LEU:HG	1.47	0.46
1:A:1161:ALA:HB1	1:A:1168:ALA:HA	1.96	0.46
1:A:1524:ILE:O	1:A:1527:LEU:N	2.48	0.46
2:B:279:VAL:O	2:B:282:ALA:HB3	2.15	0.46
2:B:332:PHE:CZ	2:B:359:LEU:HD11	2.50	0.46
2:B:558:GLU:O	2:B:578:ARG:HA	2.15	0.46
2:B:564:LYS:NZ	2:B:575:TRP:HB3	2.29	0.46
1:D:1307:GLN:O	1:D:1311:GLU:N	2.44	0.46
1:D:1394:PRO:HD3	1:D:1407:GLN:OE1	2.15	0.46
1:A:39:GLU:HG2	1:A:46:ARG:N	2.30	0.46
1:A:110:LYS:NZ	1:A:113:ARG:HB2	2.30	0.46
1:A:944:UNK:O	1:A:945:UNK:C	2.63	0.46
1:A:1088:MET:HA	1:A:1091:PRO:HG2	1.96	0.46
1:A:1398:VAL:O	1:A:1405:TYR:HD2	1.98	0.46
1:A:1555:TYR:O	1:A:1559:HIS:HB2	2.16	0.46
1:A:1600:ASP:HA	1:A:1603:GLU:OE1	2.15	0.46
2:B:247:ILE:HG23	2:B:250:LEU:HD12	1.96	0.46
2:B:252:LEU:HA	2:B:252:LEU:HD23	1.64	0.46
2:B:295:TYR:HB2	2:B:440:ASP:O	2.15	0.46
2:B:375:PRO:HA	2:B:376:PRO:HA	1.66	0.46
2:B:409:HIS:HB3	2:B:467:TRP:HE1	1.80	0.46
1:D:1351:GLY:C	1:D:1404:GLN:HE21	2.18	0.46
1:D:1417:GLU:HB3	1:D:1422:LYS:HA	1.97	0.46
1:D:1534:ILE:HG23	1:D:1535:VAL:HG23	1.97	0.46
1:A:344:UNK:O	1:A:346:UNK:N	2.48	0.46
1:A:504:ARG:H	1:A:504:ARG:CD	2.24	0.46
1:A:1001:LEU:O	1:A:1002:ARG:C	2.52	0.46
1:A:1030:PHE:O	1:A:1034:VAL:HG12	2.15	0.46
1:A:1167:ILE:HD12	1:A:1167:ILE:H	1.80	0.46
1:A:1178:VAL:O	1:A:1181:LEU:HB3	2.16	0.46
1:A:1217:GLU:HG2	1:A:1218:GLU:HG2	1.97	0.46
1:A:1349:GLY:HA3	1:A:1405:TYR:CD2	2.50	0.46
1:A:1525:ASN:O	1:A:1529:MET:HB2	2.14	0.46
2:B:88:LEU:HD23	2:B:91:ARG:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1509:ILE:HA	1:D:1512:MET:CB	2.46	0.46
1:A:44:TRP:NE1	2:B:720:TYR:HE1	2.13	0.46
1:A:45:TYR:HE2	1:A:64:ILE:HG13	1.79	0.46
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.69	0.46
1:A:439:ASN:OD1	1:A:443:GLN:HA	2.16	0.46
1:A:487:PRO:HG2	1:A:489:TRP:CZ2	2.51	0.46
1:A:1225:TYR:HA	1:A:1228:ARG:NE	2.31	0.46
1:A:1358:ASN:OD1	1:A:1400:ASN:ND2	2.48	0.46
1:A:1503:SER:O	1:A:1506:ASN:N	2.49	0.46
2:B:111:SER:HB3	2:B:161:ALA:HA	1.96	0.46
2:B:198:LEU:HD12	2:B:198:LEU:HA	1.53	0.46
2:B:240:GLN:O	2:B:241:THR:C	2.54	0.46
2:B:274:ILE:HG23	2:B:278:HIS:CD2	2.51	0.46
2:B:314:ASP:O	2:B:317:ASP:HB3	2.14	0.46
2:B:363:ASN:CG	2:B:366:ASN:H	2.17	0.46
2:B:646:TYR:CE2	2:B:650:CYS:HB2	2.50	0.46
1:D:1301:CYS:HA	1:D:1304:LEU:CG	2.44	0.46
1:A:95:LEU:HA	1:A:98:TRP:CB	2.44	0.46
1:A:1138:HIS:HA	1:A:1141:GLU:CB	2.45	0.46
1:A:1164:HIS:ND1	1:A:1166:THR:HG23	2.30	0.46
1:A:1232:LEU:HD21	1:A:1287:TYR:OH	2.15	0.46
1:A:1354:SER:OG	1:A:1355:PHE:N	2.48	0.46
1:A:1414:VAL:HG23	1:A:1442:PHE:CA	2.46	0.46
1:A:1418:HIS:NE2	1:A:1434:TYR:HB3	2.29	0.46
2:B:125:GLY:O	2:B:129:LEU:HG	2.16	0.46
2:B:194:ASP:O	2:B:197:ILE:N	2.49	0.46
1:D:1577:ILE:HG22	1:D:1610:LYS:HZ1	1.79	0.46
1:A:158:ILE:O	1:A:159:LEU:HD23	2.15	0.46
1:A:450:MET:HB2	1:A:476:TYR:H	1.80	0.46
1:A:1071:ARG:HG3	1:A:1075:TYR:CZ	2.50	0.46
1:A:1082:ILE:H	1:A:1082:ILE:HD12	1.80	0.46
1:A:1125:PHE:N	1:A:1125:PHE:CD2	2.83	0.46
1:A:1181:LEU:HD21	1:A:1185:LEU:HD11	1.96	0.46
1:A:1292:LYS:HB2	1:A:1292:LYS:HE2	1.71	0.46
1:A:1331:SER:HA	1:A:1335:ILE:HD12	1.98	0.46
1:A:1340:PRO:HG3	1:A:1437:ASN:OD1	2.16	0.46
2:B:111:SER:CB	2:B:161:ALA:HA	2.45	0.46
2:B:216:TYR:CE2	2:B:253:LYS:HB2	2.51	0.46
2:B:313:MET:O	2:B:372:THR:HG22	2.16	0.46
2:B:478:ASN:O	2:B:482:GLN:N	2.27	0.46
2:B:561:CYS:SG	2:B:562:PHE:N	2.89	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1209:ASN:HA	1:D:1212:LYS:HE3	1.97	0.46
1:D:1355:PHE:O	1:D:1356:LEU:HD23	2.15	0.46
1:D:1465:GLU:CG	1:D:1489:GLN:HB3	2.46	0.46
1:A:46:ARG:HA	1:A:57:GLY:O	2.15	0.46
1:A:149:THR:HA	1:A:152:ILE:HD11	1.98	0.46
1:A:1062:MET:O	1:A:1066:ILE:HG22	2.15	0.46
1:A:1169:LYS:HE2	1:A:1173:ASN:OD1	2.16	0.46
1:A:1188:TYR:CZ	1:A:1192:MET:HB2	2.51	0.46
1:A:1223:TYR:CG	1:A:1226:LYS:HD3	2.51	0.46
1:A:1252:LYS:HB2	1:A:1273:HIS:CE1	2.50	0.46
1:A:1255:ASP:CB	1:A:1274:ARG:HG2	2.45	0.46
1:A:1301:CYS:HB3	1:A:1325:GLN:NE2	2.31	0.46
1:A:1315:TYR:CA	1:A:1318:LEU:HB3	2.45	0.46
1:A:1506:ASN:HD22	1:A:1576:GLN:HG3	1.81	0.46
2:B:218:LYS:O	2:B:222:GLU:HG2	2.15	0.46
2:B:401:GLU:O	2:B:404:SER:OG	2.34	0.46
2:B:562:PHE:HB2	2:B:575:TRP:CD1	2.50	0.46
1:D:1200:ARG:O	1:D:1204:THR:HG22	2.16	0.46
1:D:1248:THR:CG2	1:D:1280:LEU:HD22	2.45	0.46
1:A:19:PHE:HZ	1:A:26:GLN:HB3	1.80	0.46
1:A:65:HIS:ND1	1:A:65:HIS:O	2.48	0.46
1:A:1315:TYR:O	1:A:1319:SER:N	2.48	0.46
1:A:1332:ILE:HB	1:D:1315:TYR:CD2	2.51	0.46
1:A:1340:PRO:HG3	1:A:1437:ASN:ND2	2.31	0.46
1:A:1361:PHE:CB	1:A:1363:TYR:CE1	2.98	0.46
1:A:1470:VAL:H	1:A:1484:VAL:HG13	1.81	0.46
1:A:1537:PRO:HB3	1:A:1543:PHE:CZ	2.51	0.46
1:A:1601:ARG:HH12	1:A:1605:CYS:HB3	1.81	0.46
2:B:380:ALA:HA	2:B:383:ASN:ND2	2.31	0.46
2:B:510:SER:OG	2:B:513:GLU:N	2.47	0.46
2:B:579:LEU:HB2	2:B:586:LEU:CD1	2.44	0.46
1:D:1279:THR:HA	1:D:1282:GLU:OE1	2.16	0.46
1:D:1298:ILE:O	1:D:1302:LYS:HG3	2.16	0.46
1:D:1398:VAL:HA	1:D:1405:TYR:CD2	2.50	0.46
1:A:62:SER:CB	2:B:714:PRO:HD2	2.46	0.46
1:A:455:GLU:HA	1:A:506:HIS:ND1	2.30	0.46
1:A:1047:PHE:CB	1:A:1051:LYS:HB2	2.46	0.46
1:A:1199:ASN:HA	1:A:1202:SER:OG	2.16	0.46
1:A:1231:HIS:CE1	1:A:1479:LEU:HA	2.51	0.46
1:A:1235:ASP:HA	1:A:1237:TYR:CZ	2.51	0.46
1:A:1516:TYR:CZ	1:A:1522:LEU:HD12	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1601:ARG:HH12	1:A:1605:CYS:CB	2.29	0.46
2:B:51:LEU:HD13	2:B:76:ARG:C	2.37	0.46
2:B:275:ILE:O	2:B:279:VAL:HB	2.15	0.46
2:B:642:PHE:CD1	2:B:662:TYR:HE1	2.34	0.46
2:B:717:PRO:HB2	2:B:719:ASN:OD1	2.16	0.46
1:D:1273:HIS:HA	1:D:1276:LEU:HD22	1.98	0.46
1:D:1591:VAL:HG12	1:D:1592:SER:O	2.15	0.46
1:A:37:ILE:HG21	1:A:45:TYR:CE1	2.51	0.46
1:A:549:LEU:C	1:A:572:ARG:HD2	2.36	0.46
1:A:1074:TRP:CE3	1:A:1075:TYR:CD2	3.04	0.46
1:A:1179:LYS:CD	1:A:1179:LYS:N	2.78	0.46
1:A:1247:HIS:HE1	1:A:1280:LEU:HD13	1.78	0.46
1:A:1294:TRP:O	1:A:1295:GLU:C	2.53	0.46
1:A:1343:PHE:HA	1:A:1410:THR:HA	1.98	0.46
2:B:218:LYS:HA	2:B:221:GLN:CB	2.46	0.46
2:B:306:GLU:HB2	2:B:430:VAL:HG12	1.98	0.46
1:D:1251:LEU:HD12	1:D:1252:LYS:H	1.80	0.46
1:D:1254:SER:HG	1:D:1273:HIS:CG	2.35	0.46
1:D:1308:TYR:HB3	1:D:1318:LEU:HB2	1.98	0.46
1:D:1414:VAL:HG23	1:D:1441:ARG:C	2.37	0.46
1:D:1600:ASP:HA	1:D:1603:GLU:OE1	2.16	0.46
1:A:12:HIS:HA	1:A:35:VAL:O	2.15	0.45
1:A:17:TYR:CG	1:A:18:ASN:N	2.83	0.45
1:A:46:ARG:O	1:A:56:GLN:NE2	2.48	0.45
1:A:63:PHE:CZ	2:B:713:ILE:HB	2.51	0.45
1:A:546:PHE:HA	1:A:602:ILE:O	2.16	0.45
1:A:598:ASP:HB3	1:A:600:PHE:HE2	1.81	0.45
1:A:1169:LYS:HA	1:A:1172:GLU:HB3	1.98	0.45
1:A:1187:ASP:O	1:A:1191:VAL:HG22	2.16	0.45
1:A:1315:TYR:C	1:A:1318:LEU:HB3	2.36	0.45
1:A:1366:LYS:HG3	1:A:1480:ARG:CZ	2.45	0.45
1:A:1394:PRO:HG2	1:A:1399:LYS:HE3	1.98	0.45
1:A:1511:MET:HA	1:A:1514:ASN:HD22	1.80	0.45
1:A:1582:ALA:HA	1:A:1585:LYS:CE	2.44	0.45
2:B:62:THR:O	2:B:63:GLU:C	2.54	0.45
2:B:153:ASP:O	2:B:156:SER:OG	2.08	0.45
2:B:308:ARG:HA	2:B:311:THR:OG1	2.15	0.45
1:D:1522:LEU:HD23	1:D:1523:PRO:HD2	1.98	0.45
1:A:139:ASP:OD1	1:A:139:ASP:N	2.49	0.45
1:A:139:ASP:OD1	1:A:140:GLU:N	2.44	0.45
1:A:183:LEU:HG	1:A:992:MET:SD	2.56	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:THR:O	1:A:513:HIS:ND1	2.46	0.45
1:A:1302:LYS:O	1:A:1306:GLU:HG2	2.16	0.45
1:A:1414:VAL:HG23	1:A:1442:PHE:N	2.31	0.45
1:A:1430:ILE:HG21	1:D:1315:TYR:CZ	2.51	0.45
2:B:11:ALA:O	2:B:74:ILE:HG23	2.16	0.45
2:B:470:MET:SD	2:B:480:VAL:HG13	2.56	0.45
2:B:556:LEU:HD22	2:B:665:TRP:CZ3	2.51	0.45
1:D:1308:TYR:CD1	1:D:1312:ILE:HD11	2.52	0.45
1:A:769:UNK:O	1:A:772:UNK:CB	2.65	0.45
1:A:1412:GLN:HB2	1:A:1443:HIS:CB	2.45	0.45
1:A:1439:VAL:HG23	1:A:1442:PHE:CZ	2.51	0.45
1:A:1475:LEU:HA	1:A:1476:PRO:C	2.35	0.45
1:A:1479:LEU:O	1:A:1481:TRP:N	2.49	0.45
1:A:1531:LEU:HD13	1:A:1584:ILE:HG13	1.98	0.45
2:B:193:ILE:N	2:B:198:LEU:HD22	2.25	0.45
2:B:202:LEU:HD22	2:B:242:TYR:CD2	2.52	0.45
2:B:227:GLN:O	2:B:231:HIS:CD2	2.69	0.45
2:B:296:VAL:O	2:B:299:VAL:N	2.49	0.45
2:B:382:ASP:N	2:B:382:ASP:OD1	2.48	0.45
2:B:462:LEU:HA	2:B:465:LYS:HB3	1.97	0.45
2:B:544:ILE:CG2	2:B:686:LEU:HD12	2.46	0.45
1:D:1251:LEU:HD21	1:D:1277:LYS:N	2.31	0.45
1:D:1562:ASP:OD2	1:D:1565:LYS:HE3	2.15	0.45
1:D:1600:ASP:HA	1:D:1603:GLU:CD	2.36	0.45
1:A:131:LEU:HD23	1:A:131:LEU:HA	1.75	0.45
1:A:182:SER:CA	1:A:185:HIS:HD2	2.13	0.45
1:A:487:PRO:HD2	1:A:489:TRP:NE1	2.31	0.45
1:A:547:HIS:CD2	1:A:571:TYR:CZ	3.04	0.45
1:A:798:UNK:C	1:A:801:UNK:N	2.79	0.45
1:A:1374:PHE:CD2	1:A:1408:CYS:HB2	2.52	0.45
1:A:1529:MET:HB2	1:A:1529:MET:HE2	1.62	0.45
2:B:306:GLU:HG3	2:B:309:MET:HE2	1.99	0.45
1:D:1223:TYR:HA	1:D:1226:LYS:CG	2.46	0.45
1:D:1342:TYR:HE2	1:D:1436:SER:HB3	1.80	0.45
1:D:1512:MET:HE2	1:D:1527:LEU:HD13	1.99	0.45
1:A:47:GLY:CA	1:A:56:GLN:HE21	2.30	0.45
1:A:117:VAL:HA	1:A:120:MET:SD	2.56	0.45
1:A:157:LYS:C	1:A:159:LEU:H	2.20	0.45
1:A:536:LYS:HG2	1:A:542:LEU:HD12	1.98	0.45
1:A:829:UNK:C	1:A:831:UNK:N	2.78	0.45
1:A:1197:LYS:O	1:A:1201:MET:HE3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:CYS:O	1:A:1206:ASN:N	2.49	0.45
1:A:1229:ASP:HA	1:A:1232:LEU:HB2	1.99	0.45
1:A:1229:ASP:OD1	1:A:1229:ASP:N	2.50	0.45
2:B:185:ALA:HB2	2:B:222:GLU:HB3	1.98	0.45
2:B:297:LEU:HA	2:B:300:LEU:CD1	2.47	0.45
2:B:397:ARG:O	2:B:401:GLU:HG3	2.17	0.45
2:B:657:PRO:HG2	2:B:661:GLU:HG3	1.97	0.45
2:B:687:ASP:HA	2:B:690:LEU:HB3	1.98	0.45
1:D:1239:GLU:HG3	1:D:1478:ILE:C	2.36	0.45
1:D:1308:TYR:HE2	1:D:1321:ASN:CB	2.29	0.45
1:D:1357:ARG:O	1:D:1359:LYS:HG3	2.16	0.45
1:D:1371:ARG:HH21	1:D:1372:GLU:HG3	1.81	0.45
1:D:1492:ILE:HB	1:D:1496:GLU:HB2	1.97	0.45
1:D:1499:ILE:HG13	1:D:1500:GLU:HG3	1.99	0.45
1:D:1527:LEU:O	1:D:1530:LEU:HG	2.16	0.45
1:A:5:ARG:HD3	1:A:5:ARG:H	1.81	0.45
1:A:726:UNK:O	1:A:729:UNK:N	2.49	0.45
1:A:1096:THR:CB	1:A:1097:LEU:HD12	2.47	0.45
1:A:1253:TRP:CE3	1:A:1277:LYS:HD3	2.52	0.45
1:A:1313:PHE:CE2	1:D:1426:VAL:HG22	2.51	0.45
1:A:1424:LYS:O	1:A:1426:VAL:N	2.48	0.45
2:B:8:VAL:O	2:B:23:GLU:HA	2.16	0.45
2:B:402:ASN:C	2:B:404:SER:H	2.18	0.45
2:B:563:ARG:HG2	2:B:573:LYS:HG2	1.99	0.45
1:D:1226:LYS:O	1:D:1230:LEU:HG	2.17	0.45
1:D:1349:GLY:O	1:D:1357:ARG:NH2	2.49	0.45
1:A:43:ASP:HB3	2:B:717:PRO:HD3	1.98	0.45
1:A:93:THR:CA	1:A:96:TRP:HD1	2.28	0.45
1:A:426:ILE:HA	1:A:605:LEU:HD22	1.98	0.45
1:A:430:LEU:HD23	1:A:432:GLN:H	1.81	0.45
1:A:501:ASP:HA	1:A:504:ARG:NH1	2.31	0.45
1:A:802:UNK:O	1:A:804:UNK:N	2.49	0.45
1:A:1005:ASN:O	1:A:1008:ALA:HB3	2.17	0.45
1:A:1055:ILE:O	1:A:1059:TYR:N	2.45	0.45
1:A:1077:LEU:HD13	1:A:1080:ASN:CB	2.44	0.45
1:A:1083:CYS:C	1:A:1086:PRO:HD2	2.37	0.45
1:A:1156:ILE:HA	1:A:1159:GLU:CD	2.37	0.45
1:A:1196:SER:HG	1:A:1199:ASN:HB2	1.80	0.45
1:A:1435:LYS:NZ	1:A:1436:SER:HA	2.32	0.45
2:B:33:ILE:HG23	2:B:36:GLU:CD	2.37	0.45
2:B:53:HIS:HA	2:B:75:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:PHE:N	2:B:302:PHE:CD1	2.82	0.45
1:D:1254:SER:H	1:D:1273:HIS:CB	2.23	0.45
1:D:1547:GLU:HA	1:D:1551:PHE:CB	2.29	0.45
1:A:81:ILE:HD11	1:A:89:GLN:HE22	1.82	0.45
1:A:97:GLU:O	1:A:101:ILE:HG23	2.16	0.45
1:A:541:THR:HG21	1:A:608:SER:HA	1.98	0.45
1:A:1034:VAL:HA	1:A:1037:ILE:HG12	1.98	0.45
1:A:1099:PRO:HA	1:A:1102:GLU:CD	2.37	0.45
1:A:1276:LEU:HG	1:A:1276:LEU:H	1.54	0.45
2:B:154:MET:HA	2:B:157:PHE:CD2	2.52	0.45
2:B:355:ASP:HB2	2:B:356:TYR:CE2	2.52	0.45
2:B:381:LEU:HA	2:B:384:MET:CE	2.47	0.45
2:B:561:CYS:SG	2:B:591:LEU:HD12	2.57	0.45
2:B:692:MET:O	2:B:695:LYS:HB2	2.16	0.45
2:B:695:LYS:HA	2:B:698:LEU:CD1	2.47	0.45
1:D:1292:LYS:O	1:D:1337:ARG:NH2	2.50	0.45
1:D:1456:GLU:O	1:D:1458:GLU:N	2.48	0.45
1:D:1560:PRO:HA	1:D:1563:GLN:NE2	2.31	0.45
1:D:1609:LEU:O	1:D:1613:VAL:HG12	2.17	0.45
1:A:86:PRO:O	1:A:89:GLN:N	2.50	0.45
1:A:451:CYS:SG	1:A:453:CYS:HB3	2.56	0.45
1:A:479:VAL:HG22	1:A:480:VAL:O	2.17	0.45
1:A:1099:PRO:HA	1:A:1102:GLU:HB2	1.99	0.45
1:A:1232:LEU:HD21	1:A:1287:TYR:CE1	2.52	0.45
1:A:1296:GLU:O	1:A:1300:LEU:HD13	2.17	0.45
1:A:1354:SER:HA	1:A:1357:ARG:HE	1.81	0.45
1:A:1397:ASP:O	1:A:1400:ASN:N	2.48	0.45
2:B:54:ALA:HB2	2:B:75:LEU:C	2.37	0.45
2:B:256:ASP:O	2:B:260:GLN:HG2	2.17	0.45
2:B:482:GLN:O	2:B:486:GLU:HG3	2.16	0.45
2:B:546:GLU:N	2:B:549:LYS:HZ2	2.14	0.45
2:B:564:LYS:HZ2	2:B:575:TRP:CB	2.30	0.45
2:B:572:ASP:OD2	2:B:601:HIS:HE1	2.00	0.45
1:D:1214:ASN:ND2	1:D:1216:ARG:HE	2.15	0.45
1:D:1354:SER:O	1:D:1357:ARG:HG2	2.17	0.45
1:D:1457:ASN:ND2	1:D:1548:LYS:O	2.50	0.45
1:D:1560:PRO:O	1:D:1562:ASP:N	2.50	0.45
1:D:1572:LEU:HD23	1:D:1573:ILE:N	2.32	0.45
1:A:88:ALA:O	1:A:92:THR:OG1	2.21	0.45
1:A:117:VAL:HG12	1:A:121:MET:SD	2.57	0.45
1:A:426:ILE:N	1:A:494:LYS:HE3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:VAL:HG23	1:A:572:ARG:NH2	2.32	0.45
1:A:886:UNK:O	1:A:889:UNK:N	2.50	0.45
1:A:977:LYS:NZ	1:A:1031:HIS:HB2	2.30	0.45
1:A:1074:TRP:CE3	1:A:1075:TYR:HD2	2.35	0.45
1:A:1127:LYS:HA	1:A:1130:ASN:HD22	1.81	0.45
1:A:1132:ILE:HG23	1:A:1136:LEU:HG	1.98	0.45
1:A:1163:GLU:N	1:A:1165:PRO:HD3	2.32	0.45
1:A:1363:TYR:CE2	1:A:1481:TRP:CD2	3.05	0.45
2:B:181:ILE:HA	2:B:184:ILE:CG1	2.43	0.45
2:B:199:GLN:HG2	2:B:242:TYR:CZ	2.51	0.45
2:B:640:LEU:HD23	2:B:640:LEU:HA	1.78	0.45
2:B:719:ASN:HB2	2:B:721:ASP:O	2.17	0.45
1:D:1256:GLU:HB2	1:D:1273:HIS:NE2	2.33	0.45
1:A:154:TYR:CZ	1:A:158:ILE:HD13	2.52	0.44
1:A:384:UNK:C	1:A:386:UNK:N	2.80	0.44
1:A:991:ALA:O	1:A:992:MET:C	2.56	0.44
1:A:1039:GLN:O	1:A:1041:SER:N	2.44	0.44
1:A:1194:ASP:C	1:A:1196:SER:H	2.20	0.44
1:A:1373:ASP:O	1:A:1377:GLN:CB	2.65	0.44
1:A:1380:THR:C	1:A:1382:PHE:H	2.19	0.44
1:A:1481:TRP:CD1	1:A:1481:TRP:C	2.88	0.44
2:B:42:SER:O	2:B:44:ALA:N	2.50	0.44
2:B:296:VAL:O	2:B:300:LEU:HG	2.16	0.44
2:B:363:ASN:OD1	2:B:365:VAL:HG22	2.17	0.44
2:B:532:PRO:HA	2:B:535:GLU:OE2	2.16	0.44
2:B:613:ILE:HA	2:B:646:TYR:HB2	1.99	0.44
1:D:1388:MET:CG	1:D:1405:TYR:HB3	2.47	0.44
1:D:1546:TYR:O	1:D:1550:PHE:HB2	2.18	0.44
1:A:19:PHE:HB3	1:A:29:LEU:CB	2.47	0.44
1:A:40:THR:HG23	2:B:723:VAL:CG2	2.47	0.44
1:A:449:ILE:O	1:A:509:PHE:HA	2.16	0.44
1:A:663:PHE:O	1:A:666:LEU:N	2.50	0.44
1:A:1126:LYS:HD2	1:A:1127:LYS:N	2.31	0.44
1:A:1153:LEU:O	1:A:1154:GLU:C	2.55	0.44
1:A:1156:ILE:HG23	1:A:1157:LEU:HG	1.99	0.44
1:A:1221:ILE:O	1:A:1224:LEU:HB2	2.16	0.44
1:A:1294:TRP:HE3	1:A:1332:ILE:HD11	1.82	0.44
1:A:1309:GLU:O	1:A:1313:PHE:CD1	2.70	0.44
1:A:1343:PHE:CD1	1:A:1343:PHE:N	2.83	0.44
1:A:1457:ASN:OD1	1:A:1459:PHE:HB2	2.17	0.44
1:A:1467:THR:HG21	1:A:1487:MET:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1614:GLU:HA	1:A:1618:GLY:O	2.17	0.44
2:B:424:LEU:HB3	2:B:428:LEU:HD11	1.98	0.44
2:B:484:VAL:HA	2:B:487:GLN:OE1	2.17	0.44
2:B:562:PHE:HB2	2:B:575:TRP:NE1	2.31	0.44
2:B:644:ILE:HB	2:B:654:PHE:CE2	2.52	0.44
2:B:646:TYR:HD2	2:B:647:ASP:CG	2.20	0.44
1:D:1198:ASP:HA	1:D:1201:MET:SD	2.57	0.44
1:D:1366:LYS:N	1:D:1369:GLU:OE1	2.32	0.44
1:A:149:THR:O	1:A:152:ILE:HG12	2.16	0.44
1:A:225:UNK:HA	1:A:384:UNK:N	2.32	0.44
1:A:456:ASP:HA	1:A:508:ARG:NH2	2.32	0.44
1:A:602:ILE:HG22	1:A:604:THR:HG23	1.98	0.44
1:A:1043:GLN:CG	1:A:1044:LEU:H	2.30	0.44
1:A:1161:ALA:O	1:A:1168:ALA:HB2	2.16	0.44
1:A:1201:MET:HE2	1:A:1230:LEU:HD13	1.98	0.44
1:A:1246:LEU:HD11	1:A:1478:ILE:CD1	2.46	0.44
1:A:1249:TRP:HD1	1:A:1250:LEU:HG	1.82	0.44
1:A:1510:LEU:HG	1:A:1514:ASN:HD21	1.82	0.44
2:B:199:GLN:HE22	2:B:238:GLU:CB	2.31	0.44
2:B:467:TRP:CD1	2:B:467:TRP:C	2.89	0.44
2:B:679:SER:O	2:B:682:THR:OG1	2.24	0.44
1:D:1486:HIS:NE2	1:D:1488:SER:HB3	2.32	0.44
1:D:1599:HIS:O	1:D:1603:GLU:HG3	2.17	0.44
1:A:37:ILE:HG12	1:A:59:PHE:HZ	1.81	0.44
1:A:110:LYS:HA	1:A:112:GLU:OE2	2.17	0.44
1:A:113:ARG:NH1	1:A:158:ILE:HD12	2.33	0.44
1:A:429:THR:HB	1:A:603:SER:OG	2.17	0.44
1:A:501:ASP:HA	1:A:504:ARG:NH2	2.32	0.44
1:A:511:PHE:O	1:A:512:ARG:NH1	2.48	0.44
1:A:964:GLU:C	1:A:966:VAL:N	2.69	0.44
1:A:1011:MET:SD	1:A:1014:LYS:HD2	2.57	0.44
1:A:1171:VAL:C	1:A:1174:PHE:HB2	2.37	0.44
1:A:1236:ASN:HB3	1:A:1239:GLU:OE1	2.17	0.44
1:A:1376:MET:N	1:A:1376:MET:SD	2.90	0.44
1:A:1378:LEU:HD11	1:A:1382:PHE:HE2	1.83	0.44
2:B:319:ALA:HA	2:B:322:ASP:CG	2.38	0.44
2:B:320:GLN:O	2:B:323:ILE:HB	2.17	0.44
2:B:452:PHE:CG	2:B:453:GLU:N	2.85	0.44
2:B:552:ARG:O	2:B:556:LEU:HG	2.18	0.44
1:D:1439:VAL:O	1:D:1474:LYS:HA	2.18	0.44
1:D:1475:LEU:CD1	1:D:1476:PRO:HA	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLY:HA2	1:A:56:GLN:HE21	1.82	0.44
1:A:512:ARG:NH2	1:A:526:ASN:HB2	2.33	0.44
1:A:1239:GLU:HA	1:A:1242:TYR:HB2	2.00	0.44
1:A:1275:GLN:NE2	1:A:1279:THR:HG1	2.15	0.44
2:B:372:THR:HG1	2:B:373:GLN:NE2	2.13	0.44
2:B:409:HIS:CE1	2:B:471:ARG:O	2.71	0.44
2:B:463:LEU:HD23	2:B:464:ASN:N	2.33	0.44
2:B:549:LYS:HA	2:B:552:ARG:HG2	1.98	0.44
2:B:585:VAL:HA	2:B:608:LEU:O	2.17	0.44
1:A:13:GLY:O	1:A:34:VAL:HA	2.17	0.44
1:A:15:ALA:CB	1:A:33:ASP:H	2.30	0.44
1:A:35:VAL:HA	1:A:48:TYR:O	2.17	0.44
1:A:41:CYS:H	1:A:44:TRP:C	2.20	0.44
1:A:107:VAL:HG13	2:B:554:ASN:HD21	1.83	0.44
1:A:541:THR:O	1:A:606:VAL:HG11	2.17	0.44
1:A:553:LYS:HB3	1:A:594:VAL:HB	2.00	0.44
1:A:1023:PHE:O	1:A:1027:ASN:N	2.49	0.44
1:A:1220:TYR:CD2	1:A:1224:LEU:HD11	2.42	0.44
1:A:1220:TYR:HE2	1:A:1224:LEU:HD21	1.81	0.44
1:A:1375:GLN:O	1:A:1379:MET:HG2	2.18	0.44
1:A:1459:PHE:HD2	1:A:1546:TYR:HE1	1.66	0.44
2:B:188:VAL:HG12	2:B:198:LEU:HD11	2.00	0.44
2:B:314:ASP:C	2:B:320:GLN:HE22	2.20	0.44
2:B:562:PHE:O	2:B:574:PHE:HA	2.18	0.44
1:D:1239:GLU:O	1:D:1243:THR:OG1	2.34	0.44
1:D:1245:LEU:O	1:D:1249:TRP:HB2	2.17	0.44
1:D:1343:PHE:CE1	1:D:1371:ARG:HA	2.53	0.44
1:D:1516:TYR:CE1	1:D:1527:LEU:HD13	2.53	0.44
1:A:499:ILE:O	1:A:502:MET:HB3	2.18	0.44
1:A:546:PHE:HB3	1:A:548:ASP:OD1	2.18	0.44
1:A:690:UNK:O	1:A:693:UNK:CB	2.66	0.44
1:A:1026:TRP:HB3	1:A:1030:PHE:CE2	2.52	0.44
1:A:1042:LEU:HD13	1:A:1046:GLN:HE21	1.82	0.44
1:A:1196:SER:HG	1:A:1200:ARG:N	2.15	0.44
1:A:1255:ASP:HB2	1:A:1272:THR:CA	2.47	0.44
1:A:1515:GLN:OE1	1:A:1522:LEU:HD11	2.18	0.44
1:A:1609:LEU:O	1:A:1613:VAL:HG12	2.18	0.44
2:B:38:CYS:HA	2:B:41:TRP:HB2	1.98	0.44
2:B:328:ARG:HD3	2:B:332:PHE:CD2	2.53	0.44
2:B:548:ILE:HG23	2:B:552:ARG:NH2	2.32	0.44
1:D:1522:LEU:HD21	1:D:1526:PRO:HG2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1557:ARG:HG3	1:D:1558:ASP:N	2.33	0.44
1:A:18:ASN:ND2	1:A:31:ILE:HB	2.33	0.44
1:A:89:GLN:O	1:A:93:THR:HG23	2.18	0.44
1:A:1181:LEU:HD23	1:A:1182:LEU:HG	1.99	0.44
1:A:1209:ASN:HB2	1:A:1210:PHE:CD1	2.53	0.44
1:A:1242:TYR:CZ	1:A:1476:PRO:O	2.70	0.44
1:A:1317:LEU:HD13	1:A:1320:GLN:OE1	2.18	0.44
1:A:1350:GLN:CD	1:A:1357:ARG:HD3	2.39	0.44
1:A:1527:LEU:O	1:A:1531:LEU:HG	2.18	0.44
2:B:63:GLU:CA	2:B:66:ARG:HG2	2.47	0.44
2:B:202:LEU:CD1	2:B:242:TYR:HB3	2.47	0.44
2:B:298:GLN:O	2:B:299:VAL:C	2.56	0.44
2:B:307:ASP:O	2:B:311:THR:N	2.51	0.44
2:B:436:GLU:H	2:B:436:GLU:HG2	1.54	0.44
1:D:1244:LEU:HD13	1:D:1280:LEU:CG	2.48	0.44
1:D:1352:PHE:N	1:D:1404:GLN:HE21	2.15	0.44
1:D:1508:LYS:HG3	1:D:1509:ILE:HD13	1.99	0.44
1:D:1510:LEU:O	1:D:1513:ILE:HG12	2.18	0.44
1:A:98:TRP:CD1	1:A:98:TRP:N	2.84	0.44
1:A:548:ASP:O	1:A:599:VAL:HG22	2.18	0.44
1:A:977:LYS:NZ	1:A:1028:ASN:HA	2.33	0.44
1:A:1081:LYS:HA	1:A:1084:PHE:HB3	2.00	0.44
1:A:1227:LEU:HD13	1:A:1230:LEU:HD12	1.99	0.44
1:A:1315:TYR:CG	1:D:1332:ILE:HD11	2.52	0.44
1:A:1331:SER:O	1:A:1332:ILE:HD13	2.18	0.44
1:A:1368:TYR:C	1:A:1370:ARG:HH12	2.20	0.44
2:B:41:TRP:O	2:B:42:SER:OG	2.31	0.44
2:B:54:ALA:N	2:B:75:LEU:HA	2.26	0.44
2:B:303:ASN:C	2:B:305:LEU:H	2.22	0.44
2:B:470:MET:SD	2:B:480:VAL:HG22	2.58	0.44
2:B:483:VAL:HA	2:B:486:GLU:CG	2.47	0.44
1:D:1298:ILE:HG21	1:D:1329:TYR:CE2	2.52	0.44
1:D:1327:LYS:HD2	1:D:1328:PHE:CD1	2.53	0.44
1:D:1493:SER:OG	1:D:1494:PRO:HD2	2.18	0.44
1:D:1588:GLU:HB2	1:D:1599:HIS:HE1	1.82	0.44
1:A:36:ARG:HB3	1:A:48:TYR:CZ	2.53	0.43
1:A:424:ASN:N	1:A:609:THR:O	2.50	0.43
1:A:461:PRO:HA	1:A:474:ASN:CG	2.38	0.43
1:A:497:VAL:CG1	1:A:501:ASP:HB2	2.48	0.43
1:A:506:HIS:HA	1:A:534:LEU:CD1	2.48	0.43
1:A:642:UNK:C	1:A:649:MET:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:UNK:O	1:A:938:UNK:N	2.51	0.43
1:A:1068:PHE:HD1	1:A:1071:ARG:NH2	2.15	0.43
1:A:1071:ARG:HA	1:A:1074:TRP:CB	2.47	0.43
1:A:1071:ARG:O	1:A:1074:TRP:HB3	2.17	0.43
1:A:1388:MET:HB2	1:A:1406:ILE:O	2.18	0.43
1:A:1577:ILE:C	1:A:1579:PHE:H	2.22	0.43
2:B:35:LYS:HA	2:B:46:HIS:CB	2.48	0.43
2:B:451:SER:CA	2:B:454:GLU:HG2	2.43	0.43
2:B:614:LYS:HZ2	2:B:648:SER:HA	1.81	0.43
1:D:1204:THR:OG1	1:D:1223:TYR:HD2	2.01	0.43
1:D:1465:GLU:HA	1:D:1491:THR:HA	1.99	0.43
1:A:12:HIS:CE1	1:A:36:ARG:HD3	2.53	0.43
1:A:14:VAL:CG2	1:A:67:LYS:HG2	2.48	0.43
1:A:147:LYS:HD2	1:A:147:LYS:HA	1.63	0.43
1:A:285:UNK:O	1:A:290:UNK:N	2.51	0.43
1:A:530:SER:OG	1:A:531:TYR:N	2.52	0.43
1:A:777:UNK:O	1:A:780:UNK:CB	2.66	0.43
1:A:818:UNK:O	1:A:819:UNK:C	2.63	0.43
1:A:973:PHE:HA	1:A:976:PHE:CE2	2.53	0.43
1:A:1001:LEU:HD23	1:A:1005:ASN:HD21	1.83	0.43
1:A:1342:TYR:CD1	1:A:1413:PRO:HG3	2.52	0.43
1:A:1355:PHE:CE2	1:A:1356:LEU:HD21	2.53	0.43
1:A:1367:GLU:OE1	1:A:1367:GLU:N	2.34	0.43
1:A:1424:LYS:HZ2	1:A:1426:VAL:HA	1.82	0.43
1:A:1450:ARG:HB2	1:A:1461:SER:O	2.17	0.43
1:A:1470:VAL:HG22	1:A:1486:HIS:O	2.17	0.43
2:B:156:SER:HA	2:B:159:LEU:HD21	2.00	0.43
2:B:297:LEU:O	2:B:301:THR:HG23	2.17	0.43
2:B:383:ASN:ND2	2:B:421:THR:HG23	2.33	0.43
2:B:396:ILE:HA	2:B:399:VAL:HB	2.00	0.43
2:B:425:CYS:HA	2:B:428:LEU:HD12	2.01	0.43
2:B:695:LYS:HA	2:B:698:LEU:CG	2.47	0.43
1:D:1241:ALA:HB2	1:D:1287:TYR:CD2	2.52	0.43
1:A:44:TRP:CE3	1:A:58:ILE:HG13	2.53	0.43
1:A:62:SER:OG	2:B:713:ILE:HG13	2.19	0.43
1:A:115:LEU:HA	1:A:118:GLN:HB3	1.99	0.43
1:A:435:PHE:CG	1:A:444:ARG:HB3	2.54	0.43
1:A:444:ARG:HH21	1:A:447:GLU:H	1.66	0.43
1:A:732:UNK:O	1:A:735:UNK:N	2.51	0.43
1:A:1084:PHE:HZ	1:A:1128:PHE:CD1	2.36	0.43
1:A:1205:VAL:HG13	1:A:1206:ASN:N	2.28	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:THR:OG1	1:A:1244:LEU:N	2.51	0.43
1:A:1559:HIS:HB3	1:A:1562:ASP:HB2	2.01	0.43
1:A:1583:GLY:O	1:A:1587:HIS:N	2.37	0.43
2:B:214:ASP:O	2:B:218:LYS:HD2	2.18	0.43
2:B:287:ASN:HA	2:B:595:PRO:N	2.33	0.43
2:B:318:GLN:HA	2:B:321:ARG:HD2	1.99	0.43
1:D:1284:ILE:O	1:D:1287:TYR:HB2	2.17	0.43
1:D:1494:PRO:HB2	1:D:1550:PHE:CZ	2.54	0.43
1:D:1593:ASP:O	1:D:1597:PRO:HD3	2.18	0.43
1:A:633:UNK:HA	1:A:636:UNK:CB	2.48	0.43
1:A:937:UNK:O	1:A:938:UNK:C	2.65	0.43
1:A:1248:THR:O	1:A:1251:LEU:HB2	2.19	0.43
1:A:1449:ARG:NH1	1:A:1462:MET:SD	2.91	0.43
1:A:1542:GLY:H	1:A:1545:LYS:HG2	1.79	0.43
2:B:194:ASP:HB3	2:B:197:ILE:CG1	2.42	0.43
2:B:227:GLN:O	2:B:231:HIS:NE2	2.51	0.43
2:B:466:THR:HA	2:B:469:GLU:HG3	2.00	0.43
1:D:1460:ALA:O	1:D:1494:PRO:HG2	2.18	0.43
1:A:19:PHE:CZ	1:A:60:PRO:HD3	2.52	0.43
1:A:111:LYS:O	1:A:114:PHE:HB3	2.19	0.43
1:A:998:ARG:NH1	1:A:1002:ARG:HB2	2.33	0.43
1:A:1134:LEU:HA	1:A:1137:ASP:HB3	2.01	0.43
1:A:1374:PHE:CE2	1:A:1408:CYS:HB2	2.53	0.43
1:A:1556:VAL:HG22	1:A:1563:GLN:CD	2.39	0.43
1:A:1591:VAL:HB	1:A:1599:HIS:HD1	1.83	0.43
2:B:131:GLN:C	2:B:133:VAL:H	2.21	0.43
2:B:309:MET:O	2:B:374:THR:HB	2.18	0.43
2:B:491:ALA:O	2:B:494:THR:CB	2.66	0.43
2:B:614:LYS:H	2:B:646:TYR:HA	1.84	0.43
1:D:1295:GLU:HB3	1:D:1296:GLU:OE2	2.18	0.43
1:D:1322:LEU:O	1:D:1323:ILE:C	2.57	0.43
1:D:1345:VAL:HG21	1:D:1363:TYR:CE1	2.53	0.43
1:A:44:TRP:HE3	1:A:59:PHE:CA	2.31	0.43
1:A:432:GLN:CD	1:A:600:PHE:HA	2.38	0.43
1:A:941:UNK:O	1:A:942:UNK:C	2.67	0.43
1:A:1163:GLU:O	1:A:1163:GLU:HG2	2.18	0.43
1:A:1172:GLU:O	1:A:1175:VAL:HB	2.19	0.43
1:A:1180:GLY:HA2	1:A:1183:GLU:CD	2.39	0.43
1:A:1212:LYS:N	1:A:1220:TYR:HE1	2.16	0.43
1:A:1256:GLU:H	1:A:1273:HIS:H	1.67	0.43
1:A:1355:PHE:O	1:A:1359:LYS:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:GLN:HE21	2:B:128:LEU:CD1	2.31	0.43
2:B:202:LEU:HD22	2:B:242:TYR:HD2	1.84	0.43
2:B:290:MET:HA	2:B:293:GLN:NE2	2.34	0.43
2:B:298:GLN:HB3	2:B:302:PHE:CZ	2.54	0.43
2:B:312:LYS:CE	2:B:374:THR:H	2.32	0.43
2:B:329:ARG:HH21	2:B:330:ILE:HA	1.83	0.43
2:B:331:ALA:HB1	2:B:399:VAL:HG21	1.99	0.43
2:B:587:HIS:ND1	2:B:607:LYS:HG2	2.33	0.43
2:B:652:LEU:HD23	2:B:654:PHE:CZ	2.54	0.43
2:B:673:LEU:HD23	2:B:675:LYS:CE	2.45	0.43
1:D:1211:TYR:O	1:D:1216:ARG:N	2.39	0.43
1:A:7:ALA:HB1	1:A:10:GLU:HB2	2.00	0.43
1:A:35:VAL:HG12	1:A:49:LEU:CA	2.49	0.43
1:A:106:TYR:HH	2:B:552:ARG:CZ	2.32	0.43
1:A:703:UNK:O	1:A:704:UNK:C	2.67	0.43
1:A:1125:PHE:CG	1:A:1126:LYS:N	2.86	0.43
2:B:34:ILE:O	2:B:37:VAL:HB	2.18	0.43
2:B:228:LEU:HA	2:B:231:HIS:HD2	1.83	0.43
2:B:271:LEU:HA	2:B:274:ILE:HD13	2.01	0.43
2:B:424:LEU:O	2:B:427:ILE:N	2.52	0.43
1:D:1349:GLY:CA	1:D:1401:ALA:HB3	2.48	0.43
1:A:125:MET:HE1	2:B:695:LYS:HE2	2.01	0.43
1:A:439:ASN:ND2	1:A:513:HIS:HE1	2.16	0.43
1:A:510:MET:C	1:A:511:PHE:CG	2.92	0.43
1:A:511:PHE:C	1:A:512:ARG:HH11	2.21	0.43
1:A:988:ASP:N	1:A:990:MET:HE3	2.34	0.43
1:A:1014:LYS:HG3	1:A:1015:PHE:N	2.34	0.43
1:A:1324:GLN:HA	1:A:1327:LYS:HE2	1.99	0.43
1:A:1334:LYS:HG2	1:D:1316:GLU:OE2	2.19	0.43
2:B:177:SER:OG	2:B:180:PHE:N	2.30	0.43
2:B:211:ASN:OD1	2:B:211:ASN:N	2.50	0.43
2:B:274:ILE:O	2:B:278:HIS:HD2	2.02	0.43
2:B:371:PHE:HE2	2:B:380:ALA:HB3	1.84	0.43
2:B:424:LEU:O	2:B:425:CYS:C	2.56	0.43
1:D:1209:ASN:O	1:D:1212:LYS:HG2	2.19	0.43
1:D:1439:VAL:HG23	1:D:1442:PHE:CE1	2.54	0.43
1:D:1463:TRP:CZ3	1:D:1493:SER:HA	2.54	0.43
1:D:1543:PHE:HB2	1:D:1546:TYR:CD2	2.54	0.43
1:A:462:ASN:N	1:A:474:ASN:HB3	2.34	0.43
1:A:571:TYR:HD2	1:A:573:HIS:HB2	1.84	0.43
1:A:1054:LYS:HD3	1:A:1055:ILE:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:GLU:O	1:A:1220:TYR:HB3	2.19	0.43
1:A:1256:GLU:H	1:A:1273:HIS:HB3	1.83	0.43
1:A:1350:GLN:HA	1:A:1357:ARG:HH11	1.82	0.43
2:B:8:VAL:HG11	2:B:69:ILE:CG2	2.49	0.43
2:B:173:TRP:HB3	2:B:208:MET:HE2	2.00	0.43
2:B:188:VAL:CA	2:B:198:LEU:HD11	2.47	0.43
2:B:545:LEU:O	2:B:548:ILE:HB	2.18	0.43
1:D:1299:SER:O	1:D:1302:LYS:HB2	2.19	0.43
1:D:1333:MET:SD	1:D:1430:ILE:HG23	2.59	0.43
1:A:48:TYR:HB3	1:A:56:GLN:CG	2.49	0.43
1:A:449:ILE:HD12	1:A:510:MET:HB2	2.00	0.43
1:A:533:LYS:NZ	1:A:537:GLU:HA	2.33	0.43
1:A:599:VAL:O	1:A:600:PHE:CG	2.72	0.43
1:A:889:UNK:O	1:A:891:UNK:N	2.52	0.43
1:A:1025:LEU:HD12	1:A:1025:LEU:HA	1.64	0.43
1:A:1084:PHE:CE1	1:A:1111:PHE:HB3	2.53	0.43
1:A:1128:PHE:CE2	1:A:1132:ILE:HD12	2.54	0.43
1:A:1166:THR:OG1	1:A:1167:ILE:N	2.52	0.43
1:A:1271:GLN:O	1:A:1273:HIS:N	2.51	0.43
1:A:1324:GLN:HA	1:A:1327:LYS:CE	2.48	0.43
1:A:1366:LYS:HG3	1:A:1480:ARG:NH2	2.34	0.43
1:A:1378:LEU:HD12	1:A:1378:LEU:HA	1.72	0.43
2:B:290:MET:O	2:B:293:GLN:N	2.52	0.43
2:B:361:PHE:N	2:B:364:HIS:CE1	2.86	0.43
2:B:443:PRO:O	2:B:447:THR:HG23	2.19	0.43
2:B:466:THR:HA	2:B:469:GLU:CB	2.49	0.43
2:B:532:PRO:HA	2:B:535:GLU:CG	2.49	0.43
2:B:565:LEU:HD23	2:B:565:LEU:H	1.84	0.43
2:B:567:ALA:HA	2:B:571:GLN:CD	2.39	0.43
2:B:586:LEU:HD12	2:B:586:LEU:HA	1.71	0.43
2:B:666:THR:OG1	2:B:667:ASP:N	2.52	0.43
2:B:685:ASP:O	2:B:686:LEU:C	2.57	0.43
1:D:1247:HIS:CD2	1:D:1247:HIS:C	2.91	0.43
1:D:1508:LYS:HG3	1:D:1509:ILE:N	2.34	0.43
1:A:222:UNK:O	1:A:387:UNK:HA	2.19	0.42
1:A:264:UNK:C	1:A:267:UNK:O	2.67	0.42
1:A:509:PHE:O	1:A:529:MET:HG2	2.18	0.42
1:A:1029:TYR:CE2	1:A:1073:MET:HG3	2.54	0.42
1:A:1084:PHE:HA	1:A:1087:GLY:HA3	1.99	0.42
1:A:1181:LEU:HD23	1:A:1182:LEU:N	2.34	0.42
1:A:1237:TYR:CD2	1:A:1290:LYS:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:ALA:HA	1:A:1244:LEU:HB2	2.01	0.42
1:A:1277:LYS:O	1:A:1280:LEU:HB2	2.19	0.42
1:A:1450:ARG:HG3	1:A:1463:TRP:CG	2.54	0.42
2:B:89:HIS:O	2:B:93:GLN:HB2	2.19	0.42
2:B:110:LEU:O	2:B:112:ARG:N	2.51	0.42
2:B:373:GLN:O	2:B:377:GLY:N	2.46	0.42
2:B:410:GLU:OE1	2:B:410:GLU:N	2.41	0.42
2:B:442:HIS:HB2	2:B:445:PHE:CD2	2.54	0.42
2:B:568:ARG:H	2:B:569:ARG:NH1	2.17	0.42
2:B:616:VAL:HG12	2:B:617:VAL:O	2.19	0.42
1:D:1344:ALA:HA	1:D:1362:ILE:HD13	2.01	0.42
1:D:1459:PHE:HB3	1:D:1550:PHE:CZ	2.54	0.42
1:D:1577:ILE:CG2	1:D:1610:LYS:HG3	2.47	0.42
1:D:1588:GLU:HA	1:D:1591:VAL:HG23	2.01	0.42
1:A:38:GLN:HG2	1:A:56:GLN:NE2	2.34	0.42
1:A:303:UNK:O	1:A:318:UNK:HA	2.18	0.42
1:A:544:ASP:OD2	1:A:606:VAL:N	2.37	0.42
1:A:552:LEU:HD11	1:A:565:TYR:CG	2.54	0.42
1:A:989:TRP:HB3	1:A:992:MET:CB	2.49	0.42
1:A:1081:LYS:HZ1	1:A:1117:CYS:HB3	1.83	0.42
1:A:1180:GLY:O	1:A:1184:LYS:HE2	2.19	0.42
1:A:1241:ALA:HA	1:A:1244:LEU:HD13	2.02	0.42
1:A:1322:LEU:HD23	1:A:1323:ILE:HD13	1.99	0.42
1:A:1397:ASP:OD1	1:A:1401:ALA:HB2	2.19	0.42
1:A:1450:ARG:H	1:A:1462:MET:HA	1.84	0.42
2:B:264:ASN:O	2:B:268:GLN:CB	2.66	0.42
2:B:332:PHE:CE2	2:B:359:LEU:HD11	2.54	0.42
2:B:470:MET:HG2	2:B:511:TYR:CE1	2.54	0.42
1:D:1312:ILE:HG13	1:D:1314:ASP:H	1.84	0.42
1:D:1342:TYR:HE1	1:D:1475:LEU:HD23	1.84	0.42
1:D:1492:ILE:HB	1:D:1496:GLU:CD	2.40	0.42
1:D:1502:MET:HE3	1:D:1572:LEU:HD21	1.99	0.42
1:A:96:TRP:CZ3	2:B:696:LEU:HB3	2.55	0.42
1:A:100:SER:C	1:A:102:TRP:H	2.22	0.42
1:A:480:VAL:HA	1:A:514:ARG:NH1	2.34	0.42
1:A:708:UNK:C	1:A:710:UNK:N	2.80	0.42
1:A:976:PHE:CD2	1:A:1032:LEU:HD21	2.54	0.42
1:A:1165:PRO:HA	1:A:1168:ALA:CB	2.49	0.42
1:A:1306:GLU:O	1:A:1310:MET:HG3	2.19	0.42
1:A:1348:TYR:CD1	1:A:1358:ASN:HA	2.53	0.42
1:A:1366:LYS:H	1:A:1480:ARG:NH2	2.17	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1457:ASN:HD22	1:A:1545:LYS:HB3	1.84	0.42
1:A:1467:THR:HG23	1:A:1488:SER:C	2.40	0.42
1:A:1509:ILE:O	1:A:1512:MET:HB2	2.19	0.42
1:A:1607:LYS:HA	1:A:1610:LYS:HB3	2.00	0.42
2:B:139:LEU:HD13	2:B:155:LEU:CD2	2.48	0.42
2:B:159:LEU:O	2:B:163:VAL:HG23	2.18	0.42
2:B:228:LEU:HD11	2:B:250:LEU:HD11	2.01	0.42
2:B:294:LEU:HD23	2:B:294:LEU:HA	1.68	0.42
2:B:398:ILE:HA	2:B:401:GLU:CD	2.40	0.42
2:B:574:PHE:HA	2:B:574:PHE:HD1	1.64	0.42
2:B:620:LYS:HG3	2:B:621:ASP:OD1	2.19	0.42
2:B:691:SER:HB2	2:B:695:LYS:NZ	2.33	0.42
1:D:1219:MET:O	1:D:1223:TYR:HD1	2.03	0.42
1:D:1248:THR:HA	1:D:1251:LEU:N	2.34	0.42
1:D:1308:TYR:O	1:D:1313:PHE:HA	2.19	0.42
1:D:1457:ASN:HA	1:D:1545:LYS:HZ2	1.84	0.42
1:D:1556:VAL:CA	1:D:1563:GLN:HE21	2.32	0.42
1:A:60:PRO:HG2	2:B:713:ILE:HD11	2.01	0.42
1:A:85:ILE:O	1:A:88:ALA:HB3	2.20	0.42
1:A:431:LEU:HG	1:A:601:SER:O	2.20	0.42
1:A:830:UNK:C	1:A:832:UNK:N	2.81	0.42
1:A:1011:MET:HA	1:A:1014:LYS:HG2	2.00	0.42
1:A:1095:MET:O	1:A:1149:TYR:CE1	2.72	0.42
1:A:1180:GLY:O	1:A:1181:LEU:C	2.57	0.42
1:A:1183:GLU:HG2	1:A:1184:LYS:N	2.33	0.42
1:A:1394:PRO:HG2	1:A:1399:LYS:CE	2.49	0.42
2:B:184:ILE:O	2:B:188:VAL:HG22	2.19	0.42
2:B:285:ALA:O	2:B:595:PRO:HB3	2.19	0.42
2:B:428:LEU:HG	2:B:428:LEU:H	1.52	0.42
2:B:618:THR:HB	2:B:662:TYR:OH	2.19	0.42
1:D:1342:TYR:CE1	1:D:1475:LEU:HD23	2.55	0.42
1:A:452:VAL:HA	1:A:507:LEU:CD2	2.49	0.42
1:A:502:MET:SD	1:A:534:LEU:HB3	2.58	0.42
1:A:965:LEU:HD13	1:A:965:LEU:HA	1.81	0.42
1:A:1132:ILE:O	1:A:1136:LEU:HG	2.19	0.42
1:A:1202:SER:HB2	1:A:1355:PHE:HE2	1.84	0.42
1:A:1252:LYS:O	1:A:1273:HIS:CE1	2.73	0.42
1:A:1348:TYR:CE2	1:A:1394:PRO:HG3	2.54	0.42
1:A:1522:LEU:H	1:A:1522:LEU:HG	1.47	0.42
1:A:1546:TYR:HD1	1:A:1550:PHE:CE2	2.37	0.42
1:A:1562:ASP:O	1:A:1564:ASP:N	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:THR:O	2:B:118:GLN:N	2.52	0.42
2:B:136:GLY:HA3	2:B:139:LEU:HD21	2.00	0.42
2:B:421:THR:O	2:B:424:LEU:HB2	2.19	0.42
2:B:447:THR:OG1	2:B:499:LEU:HG	2.18	0.42
2:B:551:GLN:NE2	2:B:555:ARG:HD3	2.35	0.42
2:B:691:SER:HB2	2:B:695:LYS:HZ2	1.85	0.42
2:B:716:GLU:HG3	2:B:716:GLU:O	2.18	0.42
1:D:1244:LEU:CD1	1:D:1287:TYR:HE2	2.28	0.42
1:D:1445:SER:HB2	1:D:1464:ILE:HD11	2.02	0.42
1:A:4:TRP:CZ2	2:B:722:PHE:CA	3.00	0.42
1:A:7:ALA:HB3	1:A:38:GLN:C	2.39	0.42
1:A:61:LYS:HE2	1:A:61:LYS:HB3	1.61	0.42
1:A:100:SER:O	1:A:104:GLN:HG2	2.19	0.42
1:A:187:HIS:CD2	1:A:992:MET:SD	3.13	0.42
1:A:433:GLY:CA	1:A:489:TRP:HE1	2.32	0.42
1:A:813:UNK:C	1:A:815:UNK:N	2.81	0.42
1:A:1200:ARG:HG2	1:A:1230:LEU:CD1	2.49	0.42
1:A:1214:ASN:O	1:A:1216:ARG:NH2	2.52	0.42
2:B:11:ALA:HA	2:B:21:LEU:CD2	2.49	0.42
2:B:259:ARG:HA	2:B:262:MET:HB3	2.02	0.42
2:B:374:THR:CG2	2:B:377:GLY:HA3	2.49	0.42
2:B:544:ILE:CG2	2:B:689:LEU:HD12	2.48	0.42
1:D:1241:ALA:HB2	1:D:1287:TYR:CB	2.49	0.42
1:D:1307:GLN:HA	1:D:1311:GLU:N	2.35	0.42
1:D:1314:ASP:OD1	1:D:1316:GLU:HB2	2.19	0.42
1:D:1498:ALA:HB2	1:D:1550:PHE:CE1	2.53	0.42
1:A:499:ILE:HG22	1:A:503:GLN:HE21	1.85	0.42
1:A:518:GLU:HA	1:A:522:LYS:NZ	2.33	0.42
1:A:531:TYR:C	1:A:531:TYR:CD1	2.93	0.42
1:A:549:LEU:O	1:A:599:VAL:HA	2.19	0.42
1:A:977:LYS:HE2	1:A:1031:HIS:HB2	2.02	0.42
1:A:1178:VAL:HB	1:A:1179:LYS:HD3	2.01	0.42
1:A:1292:LYS:N	1:A:1292:LYS:HD3	2.35	0.42
1:A:1308:TYR:OH	1:A:1317:LEU:HB3	2.20	0.42
1:A:1322:LEU:HD21	1:D:1322:LEU:O	2.19	0.42
1:A:1562:ASP:OD2	1:A:1562:ASP:N	2.51	0.42
1:A:1578:PRO:HB2	1:A:1579:PHE:CE1	2.55	0.42
2:B:245:ALA:O	2:B:248:ASN:HB2	2.19	0.42
2:B:300:LEU:O	2:B:301:THR:C	2.58	0.42
2:B:388:ALA:HB2	2:B:395:TYR:CE2	2.54	0.42
2:B:433:LEU:HA	2:B:433:LEU:HD23	1.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ILE:HA	2:B:463:LEU:HB3	2.02	0.42
2:B:620:LYS:O	2:B:623:PRO:HA	2.18	0.42
1:D:1294:TRP:CD2	1:D:1328:PHE:CD1	3.08	0.42
1:D:1342:TYR:CZ	1:D:1442:PHE:HZ	2.37	0.42
1:A:12:HIS:CE1	1:A:36:ARG:HB2	2.55	0.42
1:A:429:THR:HG1	1:A:493:VAL:H	1.68	0.42
1:A:443:GLN:H	1:A:483:GLN:HE22	1.64	0.42
1:A:1026:TRP:N	1:A:1026:TRP:CD1	2.87	0.42
1:A:1037:ILE:HG22	1:A:1066:ILE:HG21	2.00	0.42
1:A:1084:PHE:O	1:A:1087:GLY:N	2.52	0.42
1:A:1202:SER:CB	1:A:1355:PHE:HE2	2.33	0.42
1:A:1346:GLY:HA3	1:A:1407:GLN:HE21	1.85	0.42
1:A:1421:PHE:HB3	1:A:1426:VAL:HG21	2.01	0.42
2:B:173:TRP:HB3	2:B:208:MET:CE	2.50	0.42
2:B:278:HIS:CD2	2:B:278:HIS:H	2.37	0.42
2:B:295:TYR:O	2:B:298:GLN:HB2	2.19	0.42
2:B:450:ARG:HB3	2:B:453:GLU:CD	2.40	0.42
2:B:617:VAL:O	2:B:642:PHE:HB2	2.20	0.42
2:B:622:CYS:HB3	2:B:624:HIS:HE1	1.77	0.42
1:D:1303:GLU:HA	1:D:1306:GLU:HB3	2.01	0.42
1:D:1500:GLU:HA	1:D:1503:SER:OG	2.20	0.42
1:D:1564:ASP:O	1:D:1568:HIS:HB2	2.20	0.42
1:A:111:LYS:HA	1:A:114:PHE:CB	2.48	0.42
1:A:132:LEU:HA	1:A:132:LEU:HD23	1.72	0.42
1:A:439:ASN:HD21	1:A:513:HIS:HE1	1.66	0.42
1:A:1157:LEU:HG	1:A:1157:LEU:H	1.59	0.42
1:A:1158:MET:O	1:A:1161:ALA:HB3	2.20	0.42
1:A:1220:TYR:O	1:A:1223:TYR:N	2.50	0.42
1:A:1226:LYS:HG3	1:A:1226:LYS:H	1.56	0.42
1:A:1239:GLU:HG3	1:A:1477:GLY:O	2.20	0.42
1:A:1298:ILE:HG21	1:A:1329:TYR:OH	2.20	0.42
1:A:1334:LYS:HZ1	1:D:1315:TYR:HB3	1.85	0.42
1:A:1371:ARG:NH2	1:A:1372:GLU:OE2	2.53	0.42
1:A:1415:LEU:HD12	1:A:1415:LEU:HA	1.81	0.42
1:A:1553:GLU:OE1	1:A:1557:ARG:HD3	2.20	0.42
2:B:120:PHE:HA	2:B:123:LEU:HB2	2.01	0.42
2:B:462:LEU:HD11	2:B:509:LEU:HD13	2.02	0.42
2:B:466:THR:HG23	2:B:469:GLU:HB2	2.01	0.42
2:B:654:PHE:O	2:B:655:ILE:HD13	2.19	0.42
1:D:1397:ASP:OD1	1:D:1398:VAL:N	2.51	0.42
1:D:1544:ALA:O	1:D:1547:GLU:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TYR:HD1	1:A:56:GLN:NE2	2.18	0.42
1:A:117:VAL:O	1:A:118:GLN:C	2.57	0.42
1:A:124:LEU:HA	1:A:124:LEU:HD23	1.84	0.42
1:A:156:ASN:HA	1:A:159:LEU:HB2	2.01	0.42
1:A:1333:MET:HB2	1:A:1430:ILE:CG2	2.49	0.42
1:A:1575:TRP:HB2	1:A:1620:ARG:CZ	2.50	0.42
2:B:269:LYS:C	2:B:271:LEU:N	2.72	0.42
2:B:394:ALA:O	2:B:398:ILE:HG13	2.20	0.42
2:B:552:ARG:HG3	2:B:677:MET:CE	2.49	0.42
2:B:608:LEU:HD23	2:B:609:PRO:O	2.18	0.42
1:D:1604:GLU:OE2	1:D:1608:ASN:ND2	2.30	0.42
1:A:44:TRP:CZ3	1:A:60:PRO:HD3	2.55	0.41
1:A:137:PRO:HB2	1:A:139:ASP:OD1	2.20	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.69	0.41
1:A:181:ILE:O	1:A:184:PHE:HB3	2.19	0.41
1:A:772:UNK:O	1:A:775:UNK:CB	2.68	0.41
1:A:820:UNK:O	1:A:821:UNK:C	2.67	0.41
1:A:1034:VAL:HA	1:A:1037:ILE:CD1	2.49	0.41
1:A:1042:LEU:HB3	1:A:1046:GLN:NE2	2.35	0.41
1:A:1053:ASN:O	1:A:1056:LEU:HB3	2.20	0.41
1:A:1064:ARG:HB3	1:A:1068:PHE:CE2	2.55	0.41
1:A:1079:GLN:O	1:A:1082:ILE:HD13	2.19	0.41
1:A:1162:ALA:HA	1:A:1165:PRO:HG3	2.00	0.41
1:A:1281:TYR:O	1:A:1285:ILE:HG12	2.20	0.41
1:A:1294:TRP:CD1	1:A:1328:PHE:CD1	3.08	0.41
1:A:1385:ALA:HB1	1:A:1406:ILE:CD1	2.51	0.41
2:B:223:ILE:HA	2:B:227:GLN:OE1	2.20	0.41
2:B:299:VAL:O	2:B:302:PHE:HB2	2.20	0.41
2:B:315:PRO:O	2:B:321:ARG:NH2	2.53	0.41
2:B:354:ARG:CA	2:B:356:TYR:H	2.32	0.41
2:B:478:ASN:HB2	2:B:482:GLN:HE21	1.86	0.41
2:B:545:LEU:HB2	2:B:549:LYS:HZ2	1.84	0.41
2:B:696:LEU:HA	2:B:699:LEU:CD1	2.50	0.41
1:D:1247:HIS:CE1	1:D:1280:LEU:HD13	2.55	0.41
1:D:1421:PHE:CE2	1:D:1434:TYR:CE2	3.06	0.41
1:D:1432:ASN:HA	1:D:1435:LYS:HE2	2.01	0.41
1:D:1512:MET:HA	1:D:1515:GLN:HG3	2.02	0.41
1:A:27:LEU:HB2	1:A:57:GLY:N	2.35	0.41
1:A:100:SER:C	1:A:102:TRP:N	2.73	0.41
1:A:845:UNK:O	1:A:846:UNK:C	2.68	0.41
1:A:977:LYS:HG3	1:A:977:LYS:H	1.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:GLN:O	1:A:1027:ASN:N	2.53	0.41
1:A:1066:ILE:CD1	1:A:1070:ILE:HD11	2.50	0.41
1:A:1101:ALA:O	1:A:1103:LEU:N	2.53	0.41
1:A:1380:THR:C	1:A:1382:PHE:N	2.73	0.41
1:A:1384:ASN:HB3	1:A:1404:GLN:CD	2.41	0.41
1:A:1506:ASN:O	1:A:1509:ILE:HB	2.20	0.41
2:B:6:ASP:HA	2:B:26:GLN:HB2	2.01	0.41
2:B:380:ALA:HA	2:B:383:ASN:HD22	1.85	0.41
2:B:647:ASP:N	2:B:647:ASP:OD1	2.45	0.41
2:B:687:ASP:O	2:B:690:LEU:HB3	2.20	0.41
1:D:1208:LEU:HD12	1:D:1211:TYR:CD2	2.55	0.41
1:D:1308:TYR:HB2	1:D:1318:LEU:HD13	2.02	0.41
1:D:1516:TYR:OH	1:D:1522:LEU:HD22	2.20	0.41
1:A:86:PRO:O	1:A:87:LEU:C	2.59	0.41
1:A:115:LEU:HD12	1:A:116:GLN:N	2.35	0.41
1:A:435:PHE:CZ	1:A:446:VAL:HG22	2.55	0.41
1:A:437:LYS:O	1:A:439:ASN:N	2.53	0.41
1:A:1108:ILE:O	1:A:1111:PHE:HB2	2.20	0.41
1:A:1164:HIS:HA	1:A:1165:PRO:HD3	1.88	0.41
1:A:1296:GLU:O	1:A:1297:ALA:C	2.58	0.41
1:A:1361:PHE:HD1	1:A:1483:GLU:N	2.18	0.41
1:A:1376:MET:O	1:A:1379:MET:HB2	2.21	0.41
1:A:1475:LEU:CD1	1:A:1476:PRO:HA	2.45	0.41
1:A:1502:MET:O	1:A:1505:ALA:HB3	2.20	0.41
1:A:1579:PHE:HA	1:A:1582:ALA:H	1.85	0.41
2:B:36:GLU:HG2	2:B:37:VAL:N	2.34	0.41
2:B:120:PHE:CE2	2:B:125:GLY:HA3	2.55	0.41
2:B:124:ASP:O	2:B:128:LEU:HG	2.20	0.41
2:B:216:TYR:CE1	2:B:253:LYS:HB2	2.55	0.41
2:B:448:HIS:HB3	2:B:451:SER:CA	2.49	0.41
2:B:450:ARG:HB3	2:B:453:GLU:OE1	2.21	0.41
2:B:539:LYS:O	2:B:542:PRO:HD2	2.20	0.41
2:B:590:ASP:HB3	2:B:601:HIS:HE1	1.84	0.41
2:B:616:VAL:HG22	2:B:644:ILE:HA	2.02	0.41
1:D:1254:SER:OG	1:D:1273:HIS:CG	2.73	0.41
1:D:1345:VAL:HG21	1:D:1363:TYR:CD2	2.56	0.41
1:D:1409:PHE:CE1	1:D:1444:TYR:CG	3.08	0.41
1:D:1413:PRO:HG3	1:D:1442:PHE:CE2	2.55	0.41
1:D:1495:LEU:HD13	1:D:1555:TYR:OH	2.20	0.41
1:D:1504:THR:O	1:D:1508:LYS:HB3	2.21	0.41
1:A:4:TRP:CD2	2:B:722:PHE:CA	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD13	1:A:45:TYR:CE1	2.56	0.41
1:A:44:TRP:CE2	2:B:716:GLU:HB2	2.54	0.41
1:A:94:THR:HG22	1:A:98:TRP:NE1	2.36	0.41
1:A:106:TYR:HH	2:B:552:ARG:HH22	1.66	0.41
1:A:110:LYS:HG3	1:A:110:LYS:O	2.20	0.41
1:A:127:TRP:CD1	1:A:144:LEU:HD11	2.55	0.41
1:A:805:UNK:O	1:A:806:UNK:C	2.68	0.41
1:A:1058:LYS:HB3	1:A:1059:TYR:CE2	2.55	0.41
1:A:1188:TYR:CA	1:A:1191:VAL:HG22	2.48	0.41
1:A:1307:GLN:H	1:A:1307:GLN:HG2	1.58	0.41
1:A:1443:HIS:C	1:A:1469:PHE:HE2	2.23	0.41
2:B:33:ILE:HG23	2:B:36:GLU:OE1	2.20	0.41
2:B:116:PHE:HA	2:B:119:GLU:CB	2.50	0.41
2:B:116:PHE:CE1	2:B:120:PHE:HB2	2.55	0.41
2:B:311:THR:N	2:B:374:THR:HG21	2.35	0.41
2:B:318:GLN:CD	2:B:321:ARG:HB2	2.40	0.41
2:B:405:ARG:H	2:B:405:ARG:HG3	1.40	0.41
2:B:422:LYS:HA	2:B:425:CYS:SG	2.61	0.41
2:B:685:ASP:O	2:B:688:THR:N	2.52	0.41
1:D:1227:LEU:CA	1:D:1230:LEU:HB2	2.45	0.41
1:D:1462:MET:CB	1:D:1494:PRO:HB3	2.45	0.41
1:A:26:GLN:NE2	2:B:716:GLU:OE1	2.53	0.41
1:A:427:TYR:O	1:A:604:THR:HA	2.19	0.41
1:A:497:VAL:HG13	1:A:498:PRO:HD2	2.02	0.41
1:A:527:PHE:O	1:A:553:LYS:HB2	2.21	0.41
1:A:1126:LYS:NZ	1:A:1130:ASN:HD21	2.19	0.41
1:A:1418:HIS:H	1:A:1422:LYS:CG	2.25	0.41
1:A:1516:TYR:HD2	1:A:1520:GLU:HA	1.84	0.41
2:B:6:ASP:OD1	2:B:26:GLN:HB2	2.21	0.41
2:B:111:SER:OG	2:B:165:LEU:HG	2.20	0.41
2:B:545:LEU:HG	2:B:545:LEU:H	1.72	0.41
2:B:551:GLN:HE22	2:B:555:ARG:HH11	1.69	0.41
2:B:617:VAL:HG22	2:B:643:SER:O	2.20	0.41
2:B:668:GLY:O	2:B:671:ALA:HB3	2.21	0.41
1:D:1244:LEU:HA	1:D:1244:LEU:HD23	1.63	0.41
1:D:1316:GLU:N	1:D:1316:GLU:CD	2.67	0.41
1:D:1363:TYR:HD1	1:D:1481:TRP:CG	2.39	0.41
1:D:1426:VAL:H	1:D:1511:MET:CE	2.32	0.41
1:A:35:VAL:HG12	1:A:49:LEU:N	2.35	0.41
1:A:106:TYR:HH	2:B:552:ARG:NH2	2.18	0.41
1:A:436:ASP:OD1	1:A:527:PHE:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ASP:OD1	1:A:601:SER:HA	2.20	0.41
1:A:1165:PRO:HA	1:A:1168:ALA:HB2	2.02	0.41
1:A:1247:HIS:CG	1:A:1248:THR:N	2.87	0.41
1:A:1541:GLY:HA3	1:A:1545:LYS:HZ3	1.85	0.41
2:B:178:VAL:O	2:B:181:ILE:HB	2.20	0.41
2:B:184:ILE:HD13	2:B:187:PHE:HE2	1.86	0.41
2:B:317:ASP:HB3	2:B:320:GLN:NE2	2.36	0.41
2:B:361:PHE:CD2	2:B:363:ASN:O	2.74	0.41
2:B:371:PHE:C	2:B:373:GLN:N	2.71	0.41
2:B:545:LEU:HD21	2:B:686:LEU:HD22	2.02	0.41
2:B:576:TYR:HB3	2:B:591:LEU:CD2	2.50	0.41
2:B:590:ASP:O	2:B:591:LEU:HD23	2.21	0.41
2:B:658:ASP:O	2:B:661:GLU:N	2.53	0.41
2:B:663:CYS:SG	2:B:679:SER:HB3	2.60	0.41
2:B:682:THR:HA	2:B:685:ASP:OD2	2.21	0.41
1:D:1208:LEU:HD13	1:D:1223:TYR:HB3	2.02	0.41
1:D:1240:ALA:O	1:D:1243:THR:OG1	2.32	0.41
1:D:1308:TYR:HD2	1:D:1318:LEU:HA	1.85	0.41
1:D:1336:LEU:HA	1:D:1336:LEU:HD13	1.88	0.41
1:D:1336:LEU:HD13	1:D:1429:GLN:HE22	1.86	0.41
1:A:19:PHE:HB3	1:A:29:LEU:HG	2.03	0.41
1:A:86:PRO:C	1:A:90:GLU:HG2	2.40	0.41
1:A:164:ILE:HG22	1:A:165:VAL:O	2.21	0.41
1:A:518:GLU:HA	1:A:522:LYS:HZ2	1.84	0.41
1:A:1196:SER:O	1:A:1197:LYS:C	2.59	0.41
1:A:1298:ILE:HD12	1:A:1298:ILE:N	2.36	0.41
2:B:108:ALA:HB1	2:B:160:THR:HB	2.02	0.41
2:B:161:ALA:O	2:B:162:PHE:C	2.59	0.41
2:B:469:GLU:HB3	2:B:511:TYR:CD1	2.55	0.41
2:B:545:LEU:HD23	2:B:686:LEU:HB2	2.03	0.41
2:B:679:SER:OG	2:B:681:LEU:HB3	2.21	0.41
2:B:697:ARG:HA	2:B:700:ASP:OD2	2.21	0.41
1:D:1557:ARG:HG3	1:D:1558:ASP:H	1.85	0.41
1:A:4:TRP:CD1	2:B:722:PHE:O	2.74	0.41
1:A:45:TYR:CE2	1:A:64:ILE:HG21	2.56	0.41
1:A:187:HIS:HB3	1:A:989:TRP:CE3	2.56	0.41
1:A:541:THR:OG1	1:A:606:VAL:HG13	2.20	0.41
1:A:547:HIS:CE1	1:A:571:TYR:OH	2.74	0.41
1:A:813:UNK:O	1:A:814:UNK:C	2.66	0.41
1:A:1074:TRP:HZ2	1:A:1110:ILE:HD13	1.85	0.41
1:A:1089:VAL:HA	1:A:1092:ILE:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:VAL:HG22	1:A:1461:SER:OG	2.21	0.41
1:A:1577:ILE:O	1:A:1580:LEU:HB2	2.21	0.41
2:B:30:LEU:HG	2:B:66:ARG:CZ	2.50	0.41
2:B:554:ASN:OD1	2:B:554:ASN:N	2.51	0.41
2:B:567:ALA:HB1	2:B:571:GLN:HB2	2.02	0.41
2:B:606:ASP:CG	2:B:607:LYS:HG3	2.41	0.41
2:B:619:GLY:CA	2:B:638:LEU:HG	2.51	0.41
1:D:1353:PRO:HG2	1:D:1356:LEU:HD12	2.02	0.41
1:A:562:ALA:O	1:A:566:LEU:HG	2.20	0.41
1:A:1074:TRP:HZ2	1:A:1110:ILE:HB	1.86	0.41
1:A:1097:LEU:N	1:A:1102:GLU:OE2	2.53	0.41
1:A:1201:MET:HE1	1:A:1230:LEU:HB3	2.02	0.41
1:A:1216:ARG:NE	1:A:1216:ARG:CA	2.77	0.41
1:A:1224:LEU:HG	1:A:1224:LEU:H	1.62	0.41
1:A:1308:TYR:O	1:A:1314:ASP:N	2.53	0.41
1:A:1315:TYR:HE2	1:D:1333:MET:HG3	1.86	0.41
1:A:1322:LEU:HG	1:D:1322:LEU:HD23	2.03	0.41
1:A:1323:ILE:HG22	1:A:1327:LYS:CE	2.51	0.41
1:A:1353:PRO:HD2	1:A:1356:LEU:HD12	2.03	0.41
1:A:1428:ASP:O	1:A:1429:GLN:C	2.60	0.41
1:A:1435:LYS:HD3	1:A:1436:SER:HA	2.03	0.41
1:A:1465:GLU:HA	1:A:1491:THR:HA	2.02	0.41
1:A:1547:GLU:HA	1:A:1551:PHE:H	1.85	0.41
1:A:1614:GLU:O	1:A:1618:GLY:N	2.50	0.41
2:B:65:ASN:HA	2:B:68:GLU:CB	2.50	0.41
2:B:169:GLY:C	2:B:171:VAL:N	2.72	0.41
2:B:199:GLN:HE22	2:B:238:GLU:HB2	1.86	0.41
2:B:303:ASN:O	2:B:306:GLU:HB3	2.21	0.41
2:B:363:ASN:ND2	2:B:365:VAL:HG22	2.36	0.41
2:B:503:LYS:O	2:B:506:LEU:HB2	2.21	0.41
2:B:551:GLN:OE1	2:B:552:ARG:HD3	2.21	0.41
1:D:1283:THR:OG1	1:D:1284:ILE:N	2.53	0.41
1:D:1580:LEU:HD22	1:D:1584:ILE:CG1	2.48	0.41
1:A:19:PHE:CZ	1:A:26:GLN:HB3	2.55	0.41
1:A:27:LEU:HB3	1:A:59:PHE:HD2	1.86	0.41
1:A:44:TRP:CE3	1:A:59:PHE:HA	2.56	0.41
1:A:165:VAL:HB	1:A:167:ASP:OD1	2.20	0.41
1:A:454:ALA:HB3	1:A:458:LYS:HG2	2.03	0.41
1:A:455:GLU:O	1:A:562:ALA:HA	2.21	0.41
1:A:1253:TRP:CZ3	1:A:1277:LYS:HD3	2.56	0.41
1:A:1344:ALA:HB3	1:A:1409:PHE:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:HIS:C	2:B:294:LEU:N	2.74	0.41
2:B:376:PRO:HB2	2:B:379:LEU:CB	2.44	0.41
1:D:1247:HIS:HE2	1:D:1251:LEU:HB2	1.86	0.41
1:D:1307:GLN:C	1:D:1312:ILE:H	2.16	0.41
1:D:1349:GLY:H	1:D:1358:ASN:HD21	1.68	0.41
1:D:1387:LYS:H	1:D:1387:LYS:HG2	1.66	0.41
1:D:1425:PRO:HA	1:D:1514:ASN:HD22	1.85	0.41
1:A:424:ASN:H	1:A:609:THR:HB	1.86	0.40
1:A:457:GLY:N	1:A:508:ARG:HE	2.19	0.40
1:A:1208:LEU:HD12	1:A:1220:TYR:CE2	2.55	0.40
1:A:1246:LEU:C	1:A:1249:TRP:HB3	2.42	0.40
1:A:1250:LEU:HD23	1:A:1250:LEU:HA	1.65	0.40
1:A:1418:HIS:CE1	1:A:1434:TYR:O	2.74	0.40
2:B:56:SER:C	2:B:58:ASN:N	2.74	0.40
2:B:63:GLU:CD	2:B:63:GLU:H	2.25	0.40
2:B:116:PHE:CZ	2:B:120:PHE:CG	3.09	0.40
2:B:276:LEU:HA	2:B:280:ILE:HB	2.01	0.40
2:B:317:ASP:OD1	2:B:320:GLN:HG3	2.22	0.40
2:B:386:TYR:HE2	2:B:450:ARG:CZ	2.34	0.40
2:B:559:GLY:HA3	2:B:577:CYS:C	2.40	0.40
2:B:623:PRO:HD2	2:B:653:ASN:ND2	2.36	0.40
1:D:1236:ASN:OD1	1:D:1480:ARG:NH2	2.54	0.40
1:D:1307:GLN:C	1:D:1311:GLU:H	2.25	0.40
1:D:1389:ASN:CG	1:D:1390:THR:H	2.23	0.40
1:D:1464:ILE:N	1:D:1491:THR:HG23	2.36	0.40
1:A:165:VAL:HG11	1:A:175:PRO:N	2.36	0.40
1:A:802:UNK:C	1:A:804:UNK:N	2.83	0.40
1:A:1022:GLU:O	1:A:1026:TRP:CD2	2.74	0.40
1:A:1052:TYR:CG	1:A:1053:ASN:N	2.89	0.40
1:A:1174:PHE:C	1:A:1179:LYS:HZ3	2.23	0.40
1:A:1241:ALA:HB2	1:A:1288:PHE:N	2.36	0.40
1:A:1516:TYR:HA	1:A:1519:ASP:O	2.21	0.40
2:B:88:LEU:C	2:B:90:GLU:N	2.75	0.40
2:B:181:ILE:CA	2:B:184:ILE:HG12	2.46	0.40
2:B:361:PHE:CD2	2:B:364:HIS:ND1	2.87	0.40
2:B:470:MET:HG2	2:B:511:TYR:HE1	1.85	0.40
2:B:518:ARG:HB2	2:B:519:GLN:OE1	2.22	0.40
2:B:668:GLY:HA2	2:B:677:MET:HE1	2.02	0.40
1:D:1241:ALA:HB2	1:D:1287:TYR:HB3	2.03	0.40
1:D:1256:GLU:HB2	1:D:1273:HIS:CE1	2.56	0.40
1:D:1392:SER:O	1:D:1407:GLN:NE2	2.48	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1479:LEU:HD21	1:D:1481:TRP:CZ2	2.57	0.40
1:D:1502:MET:HE3	1:D:1572:LEU:CD2	2.51	0.40
1:D:1546:TYR:HA	1:D:1550:PHE:CD1	2.54	0.40
1:A:452:VAL:CG2	1:A:474:ASN:HB2	2.51	0.40
1:A:887:UNK:O	1:A:888:UNK:C	2.69	0.40
1:A:1169:LYS:CE	1:A:1173:ASN:HD21	2.34	0.40
1:A:1186:LEU:CA	1:A:1189:ARG:HB3	2.48	0.40
1:A:1204:THR:CB	1:A:1227:LEU:HD13	2.52	0.40
1:A:1209:ASN:HB2	1:A:1210:PHE:CE1	2.56	0.40
1:A:1536:ASP:CB	1:A:1539:VAL:HG22	2.48	0.40
2:B:60:TYR:CE2	2:B:81:PRO:HG3	2.56	0.40
2:B:214:ASP:HA	2:B:217:GLN:OE1	2.21	0.40
2:B:272:ARG:HD2	2:B:446:PHE:CA	2.48	0.40
2:B:329:ARG:HG2	2:B:333:ASP:HB2	2.03	0.40
2:B:588:TYR:CD2	2:B:605:GLN:C	2.94	0.40
1:D:1251:LEU:HG	1:D:1277:LYS:CD	2.50	0.40
1:D:1377:GLN:O	1:D:1380:THR:HB	2.21	0.40
1:D:1453:VAL:HG12	1:D:1454:ASP:N	2.36	0.40
1:D:1516:TYR:OH	1:D:1527:LEU:HB2	2.21	0.40
1:D:1582:ALA:O	1:D:1586:ILE:N	2.38	0.40
1:A:93:THR:HA	1:A:96:TRP:CD1	2.50	0.40
1:A:431:LEU:HD21	1:A:603:SER:N	2.37	0.40
1:A:462:ASN:OD1	1:A:473:MET:HA	2.21	0.40
1:A:511:PHE:HE2	1:A:529:MET:HA	1.85	0.40
1:A:941:UNK:O	1:A:944:UNK:N	2.55	0.40
1:A:1200:ARG:NE	1:A:1230:LEU:HD22	2.36	0.40
1:A:1238:THR:HG1	1:A:1239:GLU:N	2.17	0.40
1:A:1274:ARG:HG3	1:A:1274:ARG:HH11	1.87	0.40
1:A:1290:LYS:O	1:A:1292:LYS:NZ	2.28	0.40
1:A:1295:GLU:H	1:A:1295:GLU:HG2	1.47	0.40
1:A:1337:ARG:HD2	1:A:1433:PHE:CB	2.45	0.40
1:A:1403:GLY:HA3	1:A:1405:TYR:CE1	2.56	0.40
1:A:1563:GLN:NE2	1:A:1566:LEU:HG	2.37	0.40
2:B:249:ALA:HA	2:B:252:LEU:HB2	2.04	0.40
2:B:366:ASN:O	2:B:369:MET:HG2	2.21	0.40
2:B:604:LEU:C	2:B:606:ASP:N	2.74	0.40
2:B:618:THR:HA	2:B:642:PHE:CA	2.46	0.40
1:D:1415:LEU:HD13	1:D:1434:TYR:O	2.21	0.40
1:A:88:ALA:HB2	1:A:132:LEU:HD11	2.04	0.40
1:A:541:THR:HB	1:A:606:VAL:HG22	2.03	0.40
1:A:571:TYR:CD2	1:A:574:HIS:CE1	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:UNK:O	1:A:781:UNK:N	2.54	0.40
1:A:1371:ARG:O	1:A:1371:ARG:HD2	2.22	0.40
1:A:1444:TYR:C	1:A:1466:ARG:HG3	2.42	0.40
1:A:1516:TYR:CE1	1:A:1522:LEU:HD12	2.56	0.40
1:A:1551:PHE:CD1	1:A:1566:LEU:HD12	2.57	0.40
2:B:273:SER:O	2:B:276:LEU:HB3	2.21	0.40
2:B:327:LEU:HD22	2:B:385:LEU:CD2	2.52	0.40
2:B:402:ASN:CA	2:B:405:ARG:HE	2.34	0.40
2:B:663:CYS:HA	2:B:666:THR:OG1	2.22	0.40
2:B:694:ILE:HG12	2:B:694:ILE:H	1.70	0.40
1:D:1212:LYS:HA	1:D:1215:ASN:HA	2.03	0.40
1:D:1218:GLU:HA	1:D:1221:ILE:HB	2.03	0.40
1:D:1222:ARG:O	1:D:1225:TYR:HB2	2.21	0.40
1:D:1350:GLN:HA	1:D:1357:ARG:NH2	2.24	0.40
1:D:1418:HIS:H	1:D:1421:PHE:C	2.25	0.40
1:D:1454:ASP:HB2	1:D:1457:ASN:C	2.41	0.40
1:D:1512:MET:HA	1:D:1515:GLN:CD	2.42	0.40
1:D:1560:PRO:C	1:D:1562:ASP:H	2.25	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1027/1830 (56%)	719 (70%)	295 (29%)	13 (1%)	12	47
1	D	407/1830 (22%)	319 (78%)	87 (21%)	1 (0%)	47	81
2	B	672/727 (92%)	477 (71%)	187 (28%)	8 (1%)	13	49
All	All	2106/4387 (48%)	1515 (72%)	569 (27%)	22 (1%)	20	53

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	VAL
1	A	414	PRO
1	A	1125	PHE
1	A	1196	SER
2	B	57	SER
2	B	722	PHE
2	B	724	TYR
1	A	206	GLN
1	A	1294	TRP
2	B	56	SER
1	A	413	PHE
1	A	1001	LEU
1	A	1087	GLY
1	A	1215	ASN
1	A	1497	ASN
2	B	289	GLU
2	B	647	ASP
1	A	1480	ARG
2	B	662	TYR
1	D	1332	ILE
1	A	1542	GLY
2	B	623	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	829/1180 (70%)	805 (97%)	24 (3%)	42	64
1	D	362/1180 (31%)	353 (98%)	9 (2%)	47	68
2	B	500/662 (76%)	465 (93%)	35 (7%)	15	41
All	All	1691/3022 (56%)	1623 (96%)	68 (4%)	35	56

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	162	ASP
1	A	166	ARG
1	A	451	CYS
1	A	478	SER
1	A	504	ARG
1	A	544	ASP
1	A	561	ASP
1	A	573	HIS
1	A	604	THR
1	A	1064	ARG
1	A	1126	LYS
1	A	1181	LEU
1	A	1204	THR
1	A	1213	ASP
1	A	1222	ARG
1	A	1228	ARG
1	A	1229	ASP
1	A	1273	HIS
1	A	1376	MET
1	A	1408	CYS
1	A	1432	ASN
1	A	1448	VAL
1	A	1601	ARG
2	B	6	ASP
2	B	13	GLU
2	B	39	ASP
2	B	55	ASP
2	B	63	GLU
2	B	90	GLU
2	B	174	ASP
2	B	200	ARG
2	B	300	LEU
2	B	306	GLU
2	B	317	ASP
2	B	322	ASP
2	B	328	ARG
2	B	329	ARG
2	B	333	ASP
2	B	355	ASP
2	B	370	ASP
2	B	405	ARG
2	B	440	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	452	PHE
2	B	456	PHE
2	B	471	ARG
2	B	476	ASP
2	B	513	GLU
2	B	518	ARG
2	B	554	ASN
2	B	569	ARG
2	B	574	PHE
2	B	576	TYR
2	B	588	TYR
2	B	624	HIS
2	B	647	ASP
2	B	662	TYR
2	B	685	ASP
2	B	722	PHE
1	D	1327	LYS
1	D	1331	SER
1	D	1339	LYS
1	D	1469	PHE
1	D	1486	HIS
1	D	1490	THR
1	D	1497	ASN
1	D	1565	LYS
1	D	1601	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	52	HIS
1	A	56	GLN
1	A	185	HIS
1	A	424	ASN
1	A	432	GLN
1	A	483	GLN
1	A	543	HIS
1	A	1005	ASN
1	A	1013	GLN
1	A	1024	GLN
1	A	1027	ASN
1	A	1046	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1130	ASN
1	A	1206	ASN
1	A	1209	ASN
1	A	1247	HIS
1	A	1275	GLN
1	A	1321	ASN
1	A	1358	ASN
1	A	1375	GLN
1	A	1384	ASN
1	A	1400	ASN
1	A	1412	GLN
1	A	1486	HIS
1	A	1514	ASN
1	A	1525	ASN
1	A	1559	HIS
1	A	1587	HIS
1	A	1599	HIS
2	B	53	HIS
2	B	93	GLN
2	B	122	ASN
2	B	231	HIS
2	B	248	ASN
2	B	278	HIS
2	B	298	GLN
2	B	373	GLN
2	B	383	ASN
2	B	392	GLN
2	B	402	ASN
2	B	448	HIS
2	B	482	GLN
2	B	541	GLN
2	B	571	GLN
2	B	601	HIS
2	B	660	HIS
2	B	670	ASN
2	B	684	ASN
1	D	1199	ASN
1	D	1206	ASN
1	D	1214	ASN
1	D	1231	HIS
1	D	1325	GLN
1	D	1358	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1400	ASN
1	D	1404	GLN
1	D	1407	GLN
1	D	1429	GLN
1	D	1432	ASN
1	D	1506	ASN
1	D	1514	ASN
1	D	1563	GLN
1	D	1587	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 monosaccharides 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	A	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	389:UNK	C	412:GLY	N	26.49
1	A	351:UNK	C	377:UNK	N	18.68
1	A	892:UNK	C	896:UNK	N	9.42
1	A	736:UNK	C	742:UNK	N	9.38
1	A	923:UNK	C	934:UNK	N	6.86
1	A	960:UNK	C	962:SER	N	4.36
1	A	304:UNK	C	318:UNK	N	3.56
1	A	1334:LYS	C	1335:ILE	N	3.31
1	A	5:ARG	C	6:LYS	N	1.64

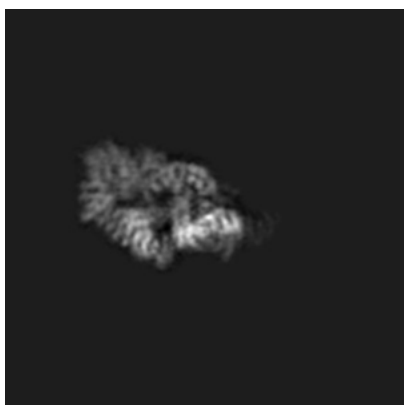
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10497. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

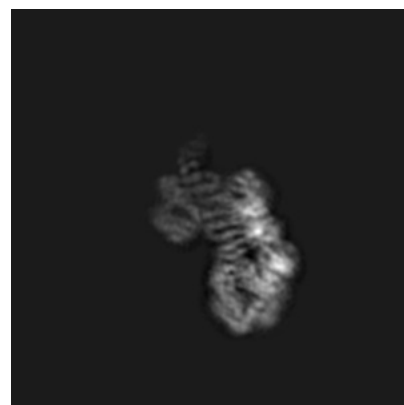
6.1.1 Primary map



X



Y

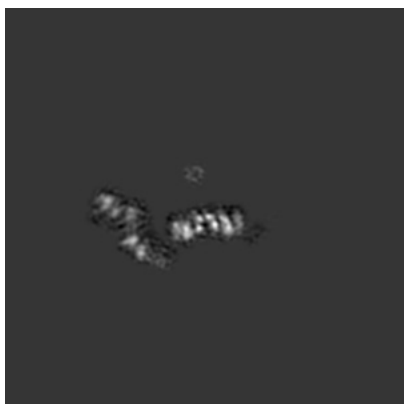


Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

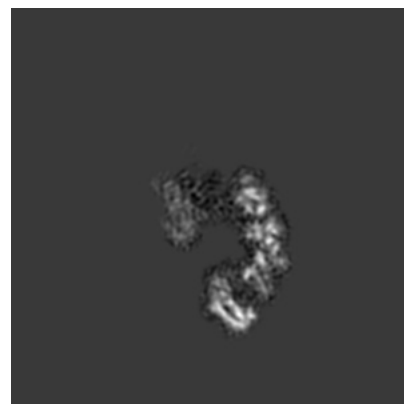
6.2.1 Primary map



X Index: 141



Y Index: 141

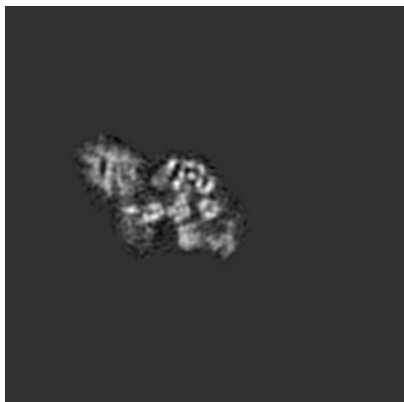


Z Index: 141

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 175



Y Index: 99

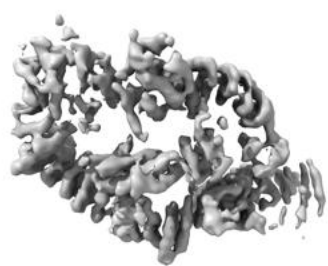


Z Index: 131

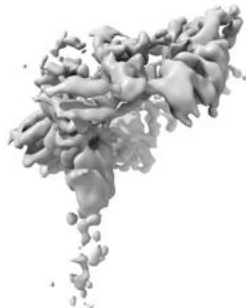
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

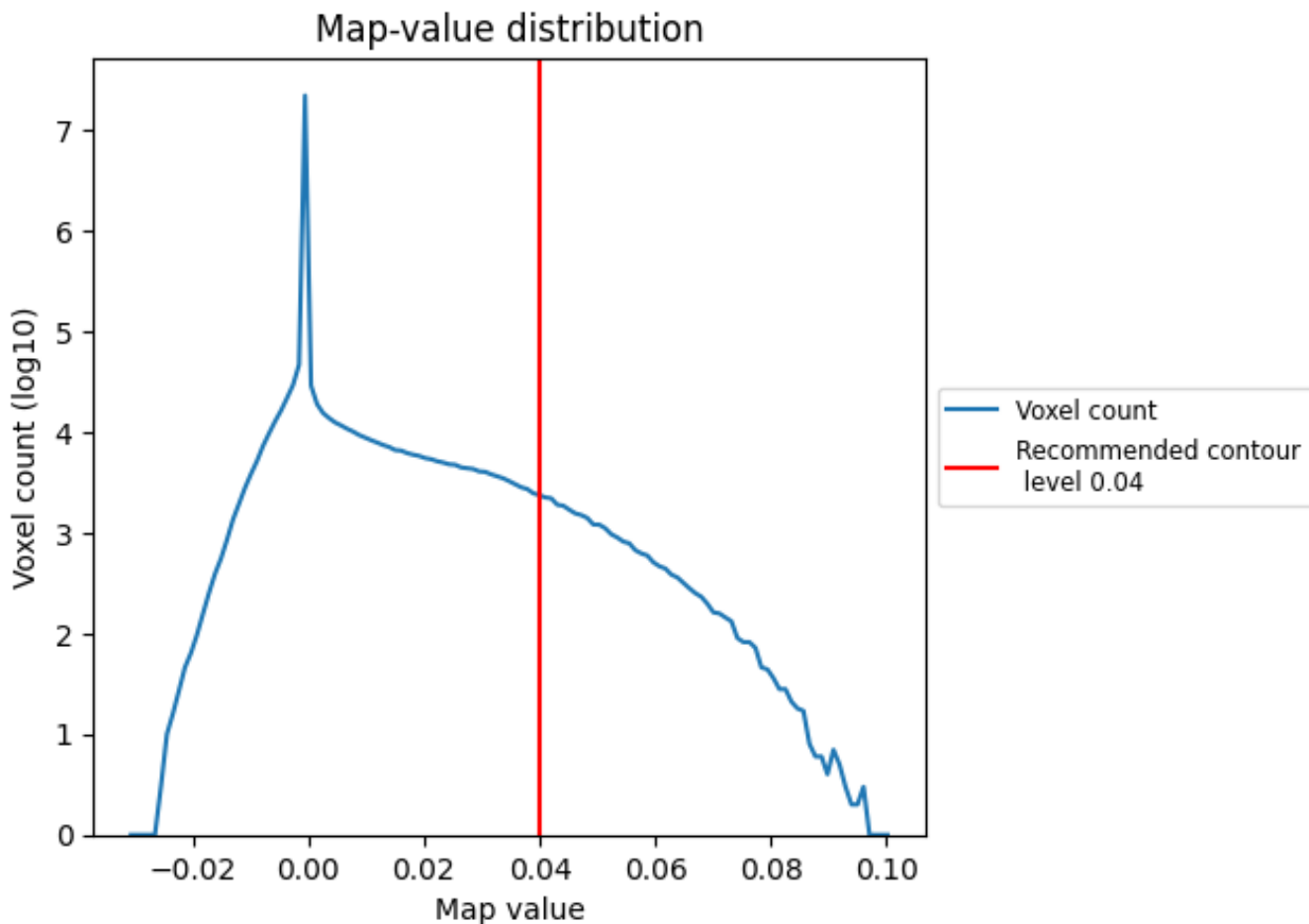
6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

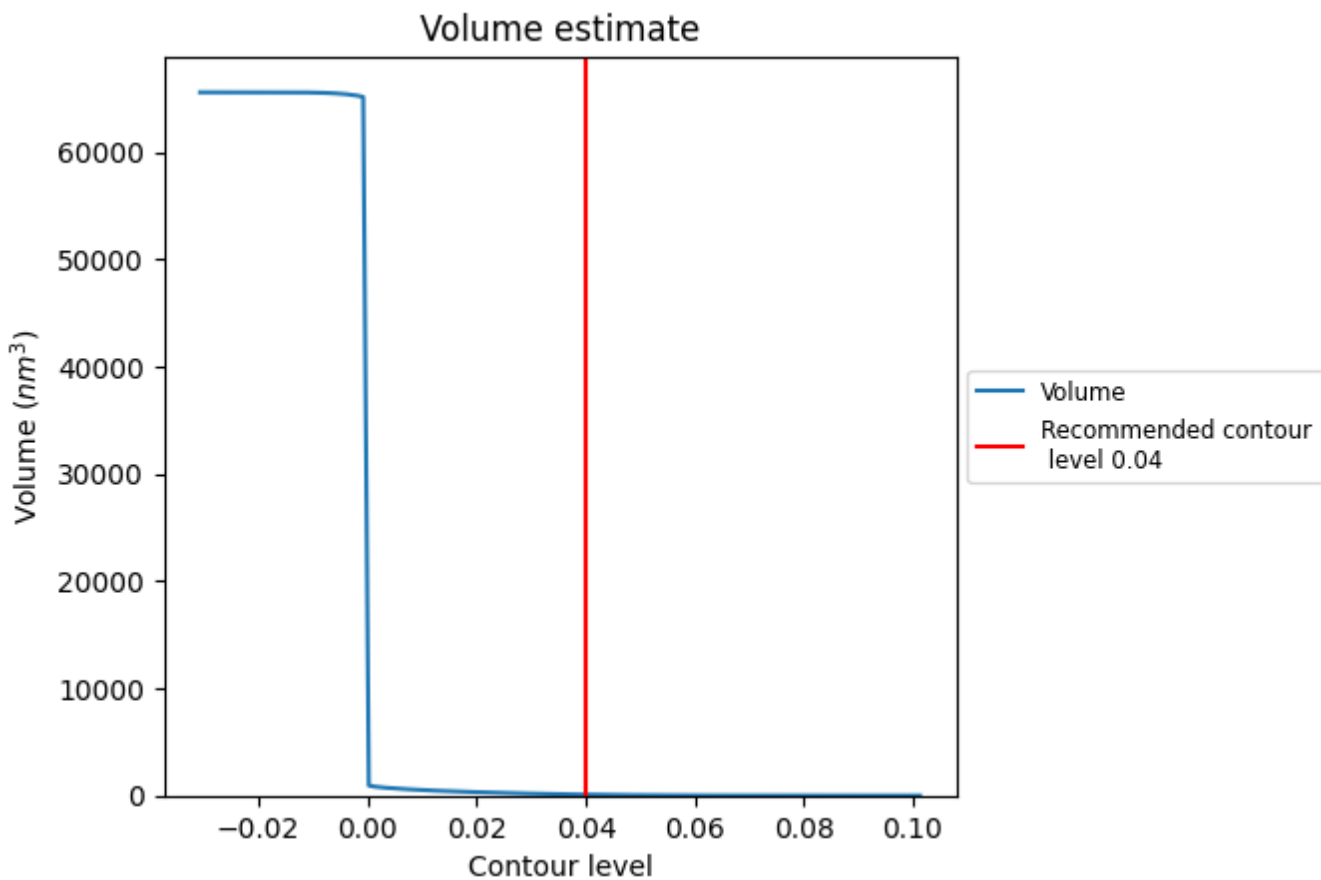
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

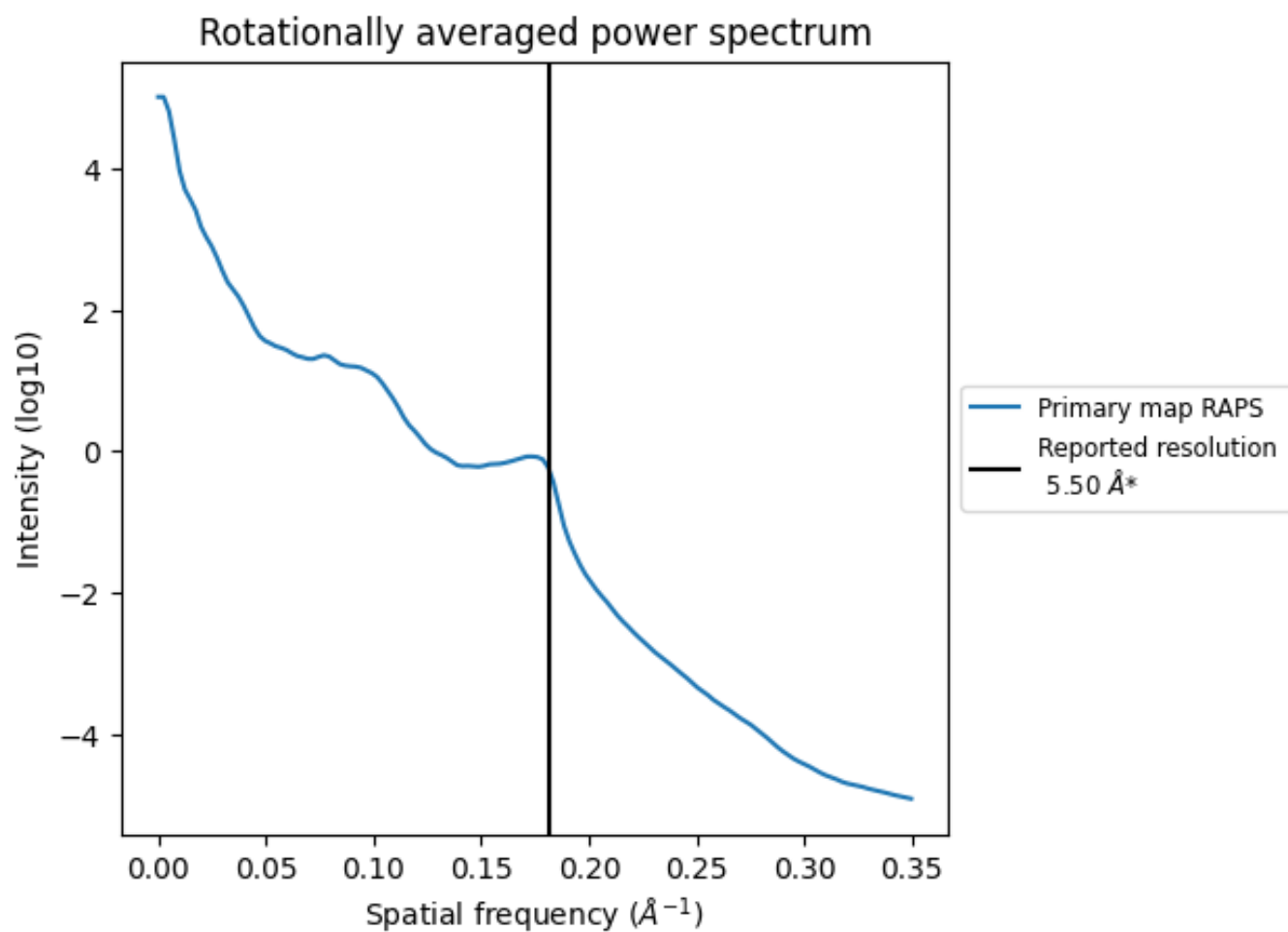
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 80 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.182\AA^{-1}

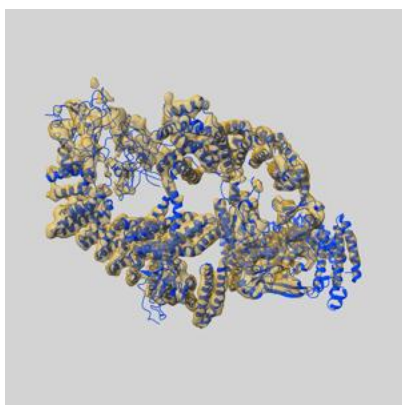
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

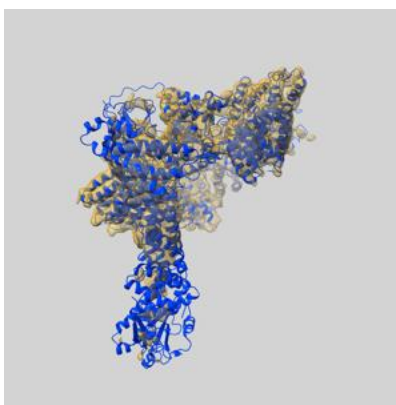
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10497 and PDB model 6TGB. Per-residue inclusion information can be found in section 3 on page 29.

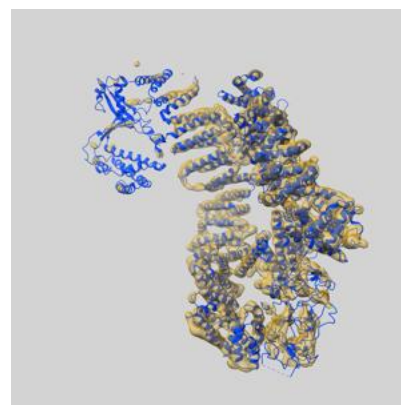
9.1 Map-model overlay [i](#)



X



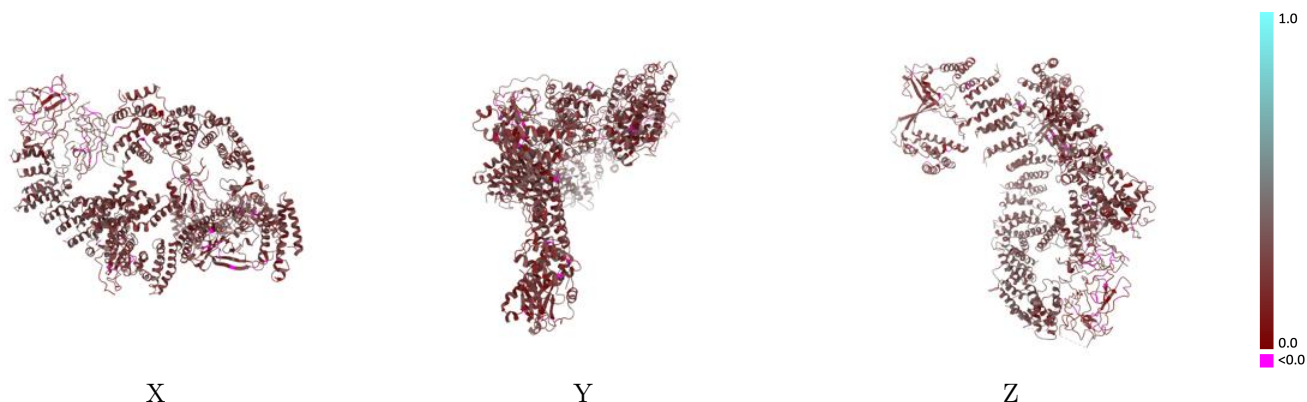
Y



Z

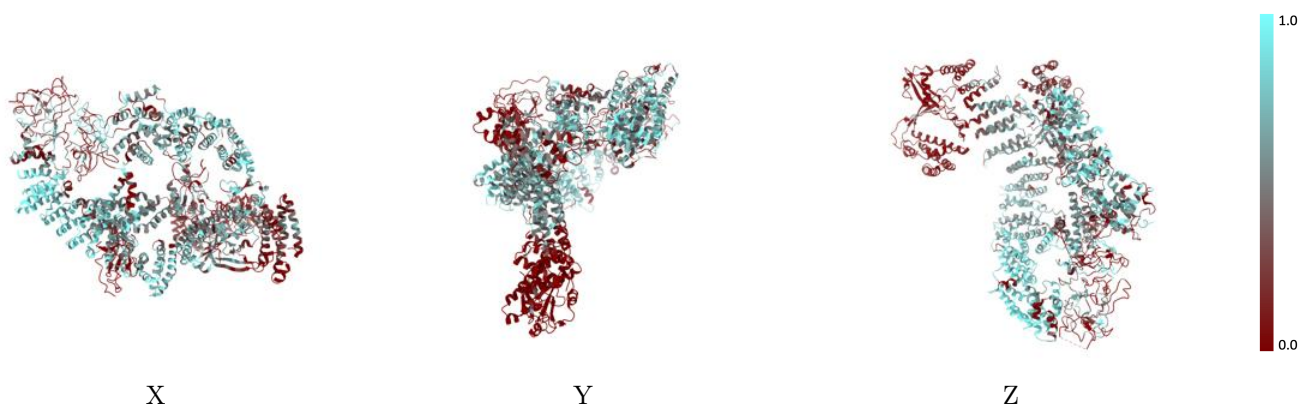
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [\(i\)](#)



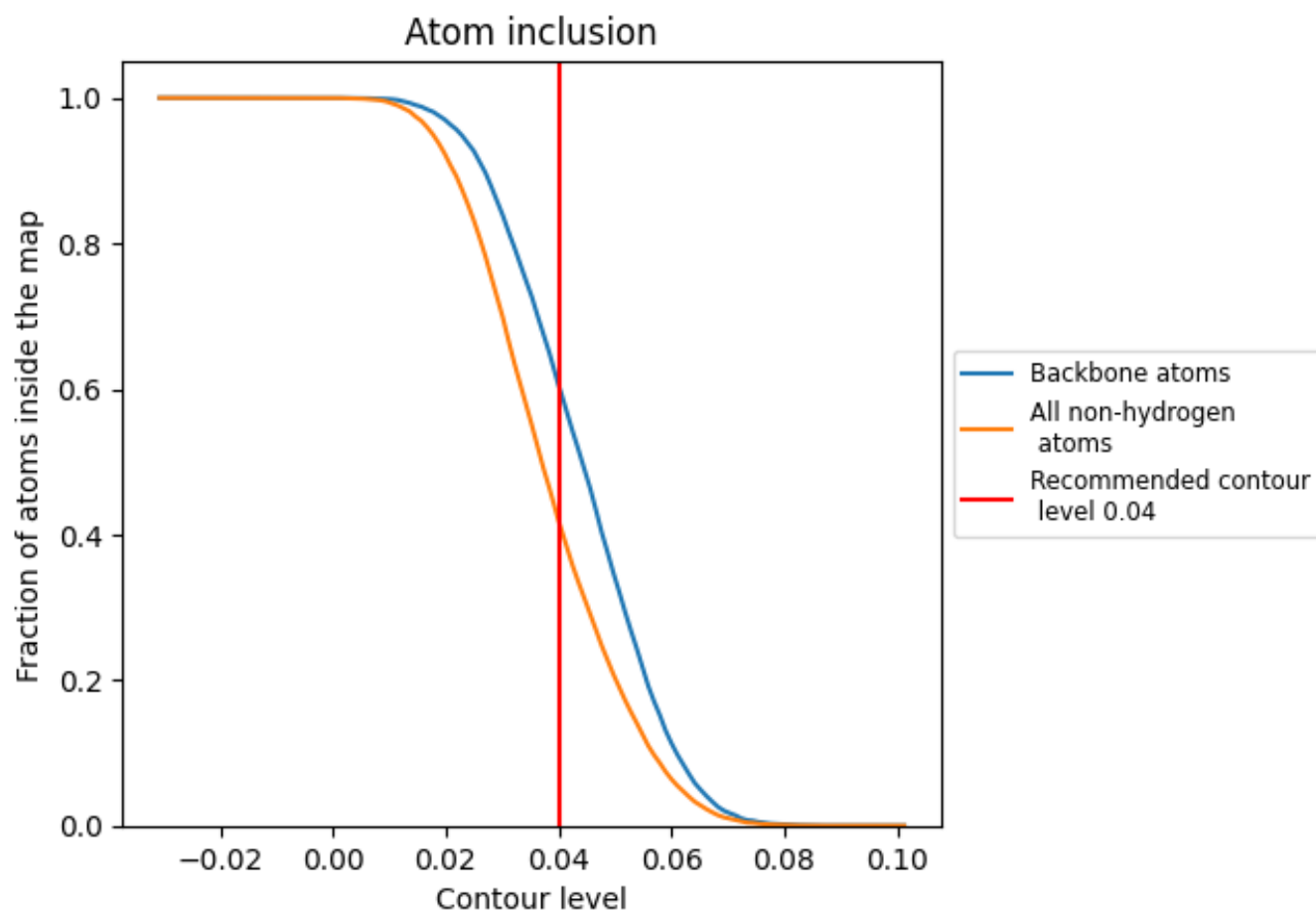
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).









9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 42% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4191	 0.2480
A	 0.4839	 0.2540
B	 0.5019	 0.2500
D	 0.0974	 0.2290

