



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 06:31 AM UTC

PDB ID : 5ND1 / pdb_00005nd1
EMDB ID : EMD-3619
Title : Viral evolution results in multiple, surface-allocated enzymatic activities in a fungal double-stranded RNA virus
Authors : Mata, C.P.; Luque, D.; Gomez Blanco, J.; Rodriguez, J.M.; Suzuki, N.; Ghabrial, S.A.; Carrascosa, J.L.; Trus, B.L.; Caston, J.R.
Deposited on : 2017-03-07
Resolution : 3.70 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.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

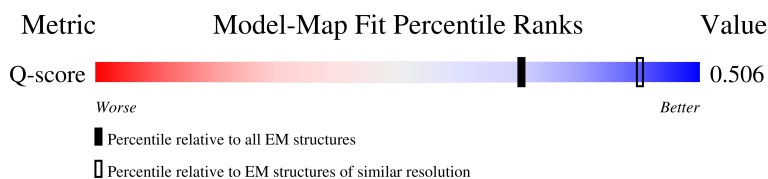
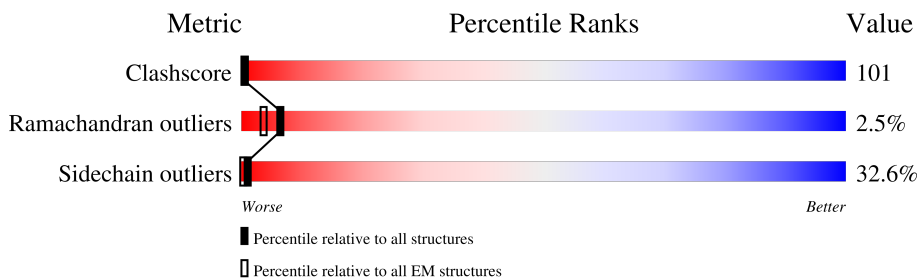
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	1357	
2	B	1059	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 14963 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 Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	972	Total	C	N	O	S	0	0
			7371	4561	1355	1400	55		

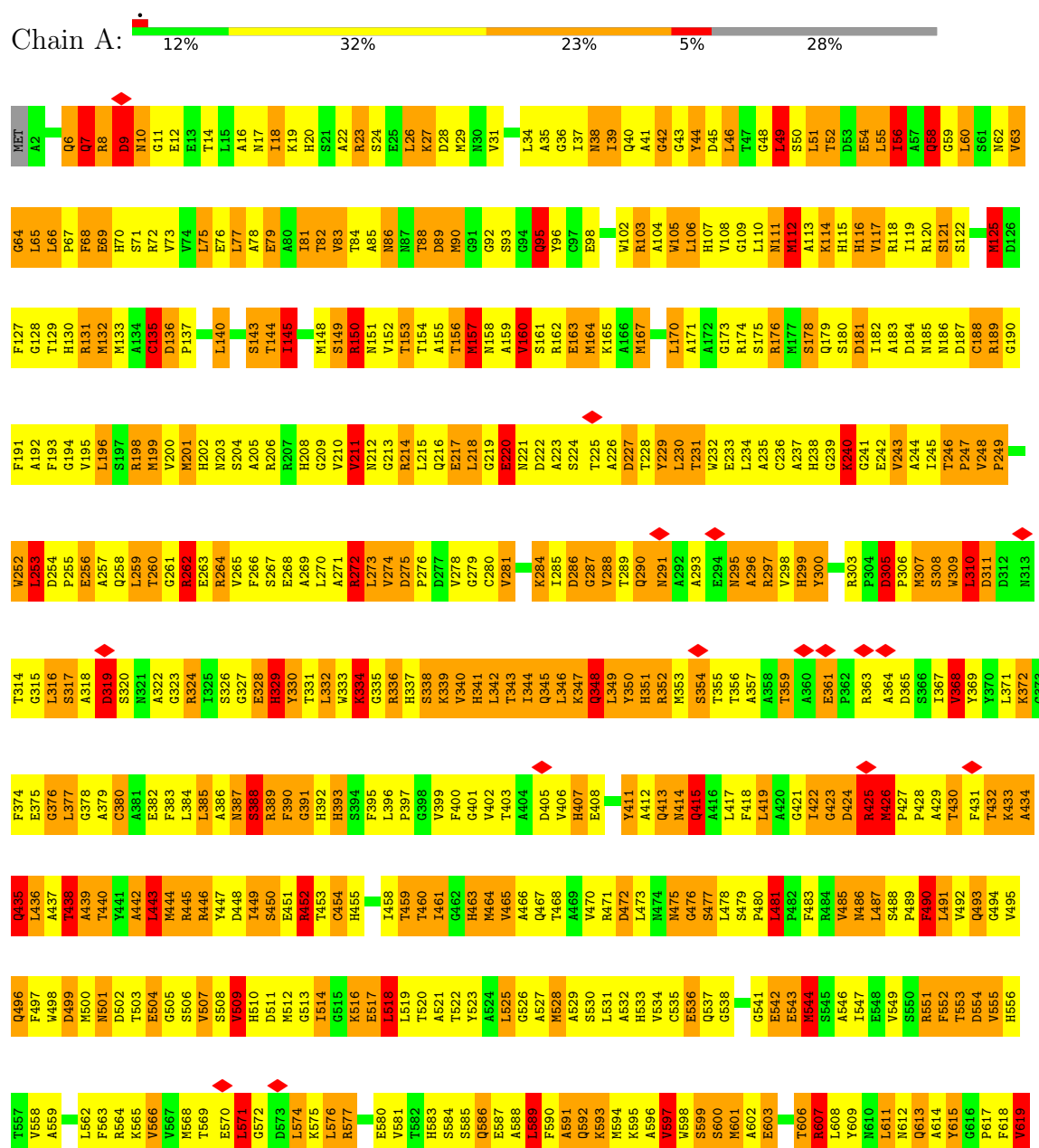
- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1005	Total	C	N	O	S	0	0
			7592	4717	1347	1480	48		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Capsid protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37531	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.7	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.371	Depositor
Minimum map value	-0.852	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.18	Depositor
Map size ($\text{\AA}$)	536.0, 536.0, 536.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.38	23/7511 (0.3%)	1.75	232/10188 (2.3%)
2	B	0.96	8/7739 (0.1%)	1.35	127/10515 (1.2%)
All	All	1.19	31/15250 (0.2%)	1.56	359/20703 (1.7%)

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	11
2	B	0	6
All	All	0	17

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	ALA	C-N	21.86	1.60	1.33
2	B	196	ALA	C-N	6.37	1.41	1.33
2	B	364	MET	C-O	-6.26	1.17	1.24
1	A	440	THR	CA-C	-6.14	1.44	1.52
1	A	685	ILE	C-O	-6.14	1.17	1.24
2	B	589	TYR	C-O	-5.86	1.16	1.24
1	A	443	LEU	CA-C	-5.83	1.45	1.52
1	A	269	ALA	CA-C	-5.82	1.45	1.52
1	A	95	GLN	CA-C	-5.74	1.45	1.52
1	A	461	ILE	C-O	-5.70	1.17	1.24
2	B	111	MET	C-O	-5.69	1.16	1.23
1	A	911	TYR	C-O	-5.68	1.17	1.23
1	A	465	VAL	C-O	-5.67	1.17	1.24
1	A	143	SER	CA-C	-5.64	1.45	1.52
1	A	368	VAL	C-O	-5.56	1.18	1.24
1	A	444	MET	C-O	-5.55	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	ALA	C-O	-5.48	1.17	1.24
1	A	625	ARG	C-O	-5.46	1.17	1.24
1	A	143	SER	C-O	-5.39	1.17	1.23
1	A	518	LEU	C-O	-5.34	1.18	1.24
1	A	731	ILE	C-O	-5.33	1.18	1.24
2	B	262	MET	C-O	-5.22	1.17	1.23
2	B	506	PRO	N-CD	5.21	1.55	1.47
1	A	286	ASP	CA-C	-5.21	1.46	1.52
2	B	197	PRO	N-CD	5.18	1.55	1.47
1	A	343	THR	C-O	-5.17	1.17	1.23
1	A	518	LEU	CA-C	-5.16	1.46	1.52
1	A	680	TYR	CA-C	-5.16	1.46	1.52
1	A	729	SER	C-O	-5.16	1.18	1.24
2	B	335	ASP	CA-C	-5.09	1.46	1.52
1	A	330	TYR	C-O	-5.03	1.18	1.24

All (359) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	621	VAL	N-CA-C	16.03	128.65	113.10
1	A	476	GLY	N-CA-C	15.87	131.77	112.73
1	A	433	LYS	N-CA-C	-15.84	93.45	111.82
1	A	747	ILE	CB-CA-C	-13.36	99.30	111.06
1	A	229	TYR	N-CA-C	-13.15	89.43	110.20
1	A	439	ALA	N-CA-C	12.49	124.97	111.36
1	A	623	LEU	N-CA-C	12.41	127.76	112.87
2	B	706	SER	N-CA-C	-12.37	90.70	109.14
2	B	588	PHE	N-CA-C	12.19	128.58	111.52
1	A	591	ALA	N-CA-C	-11.98	98.90	113.15
1	A	307	MET	N-CA-C	11.62	127.45	113.28
1	A	64	GLY	N-CA-C	11.55	130.22	115.21
1	A	936	TYR	N-CA-C	11.55	123.87	111.28
1	A	660	ASN	N-CA-C	11.54	127.55	113.12
1	A	423	GLY	N-CA-C	-11.41	92.46	112.55
1	A	432	THR	N-CA-C	11.38	124.77	111.11
2	B	260	LYS	N-CA-C	11.30	123.34	111.14
1	A	211	VAL	N-CA-C	-11.16	99.44	110.72
1	A	894	ARG	N-CA-C	-11.13	99.52	112.87
2	B	808	GLY	N-CA-C	11.12	131.53	112.51
1	A	697	ASN	N-CA-C	-10.91	96.66	110.19
1	A	42	GLY	N-CA-C	-10.86	95.37	112.85
1	A	414	ASN	N-CA-C	10.81	128.58	113.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	ALA	N-CA-C	-10.80	96.60	110.53
1	A	305	ASP	N-CA-C	-10.66	98.63	108.22
1	A	336	ARG	N-CA-C	-10.56	93.29	109.24
2	B	548	ASN	N-CA-C	-10.54	93.53	109.86
1	A	676	THR	N-CA-C	10.45	126.12	113.16
1	A	888	TYR	N-CA-C	10.24	125.78	113.28
1	A	748	ALA	N-CA-C	-10.20	100.70	113.55
2	B	1003	TYR	N-CA-C	10.19	122.38	111.28
1	A	807	MET	N-CA-C	10.08	122.34	111.36
2	B	652	HIS	N-CA-C	-10.00	97.06	110.55
1	A	92	GLY	N-CA-C	9.91	128.99	115.32
1	A	747	ILE	N-CA-C	9.71	122.67	112.96
2	B	41	ASP	N-CA-C	9.68	121.84	111.28
1	A	601	MET	N-CA-C	9.56	124.77	112.34
2	B	91	LYS	N-CA-C	-9.41	98.39	110.53
2	B	576	TYR	N-CA-C	9.41	124.45	111.74
1	A	229	TYR	CB-CA-C	9.31	125.26	109.53
2	B	466	LEU	N-CA-C	-9.29	93.72	109.24
1	A	889	GLU	N-CA-C	-9.12	100.96	112.90
2	B	1003	TYR	CA-C-N	8.99	138.72	121.54
2	B	1003	TYR	C-N-CA	8.99	138.72	121.54
2	B	389	GLY	N-CA-C	-8.99	98.65	111.42
1	A	741	ALA	N-CA-C	-8.94	100.51	111.33
2	B	806	TYR	N-CA-C	8.93	121.10	111.36
1	A	463	HIS	N-CA-C	8.89	122.14	111.82
1	A	275	ASP	N-CA-C	-8.87	97.52	109.84
1	A	424	ASP	N-CA-C	8.85	120.92	111.28
1	A	718	ARG	N-CA-C	8.80	124.24	112.88
1	A	882	GLY	N-CA-C	-8.78	100.70	112.82
2	B	381	THR	N-CA-C	-8.75	97.60	110.20
1	A	580	GLU	N-CA-C	-8.73	100.74	112.26
2	B	680	LYS	N-CA-C	8.63	125.02	113.97
1	A	450	SER	N-CA-C	8.57	122.96	110.28
1	A	507	VAL	N-CA-C	-8.53	95.72	108.85
1	A	165	LYS	N-CA-C	8.52	120.19	111.07
1	A	253	LEU	N-CA-C	8.49	120.54	111.28
1	A	327	GLY	N-CA-C	-8.49	101.99	112.68
1	A	435	GLN	N-CA-C	8.48	120.61	111.36
1	A	752	LYS	CB-CA-C	-8.47	100.97	111.82
2	B	797	GLY	N-CA-C	-8.46	101.22	112.14
1	A	44	TYR	N-CA-C	8.46	122.96	112.47
1	A	293	ALA	N-CA-C	8.44	123.37	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	685	ILE	N-CA-C	-8.43	96.34	108.48
1	A	571	LEU	N-CA-C	8.43	120.46	111.28
1	A	241	GLY	N-CA-C	-8.41	98.53	112.83
1	A	544	MET	N-CA-C	-8.31	98.78	110.50
1	A	628	SER	N-CA-C	-8.26	96.43	109.23
1	A	240	LYS	N-CA-C	-8.25	96.85	109.14
2	B	569	PHE	N-CA-C	8.21	120.14	111.03
2	B	836	GLU	N-CA-C	8.20	120.00	111.14
1	A	624	ALA	N-CA-C	8.12	122.28	112.38
1	A	899	LEU	N-CA-C	8.12	120.13	111.28
1	A	296	ALA	N-CA-C	8.10	121.62	108.41
1	A	607	ARG	N-CA-C	-8.10	102.53	111.36
1	A	720	GLY	N-CA-C	8.07	132.32	113.18
1	A	259	LEU	N-CA-C	8.07	121.18	110.53
1	A	663	GLY	N-CA-C	8.05	120.78	111.36
1	A	432	THR	CB-CA-C	-8.01	97.99	110.81
1	A	274	VAL	N-CA-C	7.98	123.21	112.04
1	A	438	THR	N-CA-C	-7.96	102.34	112.93
1	A	910	LEU	N-CA-C	7.95	120.03	111.36
1	A	319	ASP	N-CA-C	-7.91	96.97	109.23
1	A	130	HIS	N-CA-C	7.84	119.83	111.28
2	B	564	SER	N-CA-C	7.79	127.40	110.80
1	A	59	GLY	N-CA-C	7.76	126.37	115.43
2	B	314	GLY	N-CA-C	-7.75	100.37	112.85
1	A	794	VAL	CB-CA-C	-7.72	101.97	111.32
1	A	669	ILE	N-CA-CB	-7.67	102.39	111.60
2	B	606	HIS	N-CA-C	7.67	122.26	111.52
1	A	669	ILE	N-CA-C	7.65	118.51	106.88
1	A	572	GLY	N-CA-C	7.64	124.93	110.86
1	A	647	ILE	N-CA-C	7.63	118.42	110.72
1	A	968	MET	N-CA-C	-7.62	102.44	112.34
2	B	329	LEU	N-CA-C	7.60	121.21	110.50
1	A	671	LEU	N-CA-C	7.56	126.52	109.81
1	A	49	LEU	N-CA-C	7.55	119.51	111.28
2	B	664	ASN	N-CA-C	-7.55	98.78	110.17
1	A	151	ASN	N-CA-C	7.53	122.47	113.28
1	A	962	GLY	N-CA-C	-7.53	102.43	112.14
2	B	261	GLY	N-CA-C	7.46	122.31	110.90
1	A	919	LEU	N-CA-C	7.44	121.95	113.02
1	A	745	MET	N-CA-C	7.41	119.14	111.14
1	A	764	GLN	N-CA-C	7.39	122.52	112.68
1	A	324	ARG	N-CA-C	7.37	120.25	111.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	PRO	CA-C-N	-7.34	115.34	126.86
2	B	197	PRO	C-N-CA	-7.34	115.34	126.86
1	A	7	GLN	N-CA-C	7.33	121.53	112.59
2	B	391	GLU	N-CA-C	7.31	119.03	111.14
2	B	187	GLY	N-CA-C	-7.30	96.96	111.34
1	A	606	THR	N-CA-C	-7.30	96.65	109.06
1	A	687	THR	O-C-N	-7.27	114.49	123.36
1	A	840	ALA	N-CA-C	-7.26	102.54	111.33
2	B	327	TYR	N-CA-C	7.23	119.16	111.28
1	A	235	ALA	O-C-N	7.23	132.20	122.59
2	B	214	ARG	N-CA-C	7.21	120.00	111.71
2	B	238	VAL	CA-C-N	7.17	127.89	120.00
2	B	238	VAL	C-N-CA	7.17	127.89	120.00
1	A	415	GLN	N-CA-C	-7.14	98.41	109.76
1	A	576	LEU	N-CA-C	7.13	120.09	111.82
1	A	82	THR	N-CA-C	7.13	122.57	107.67
2	B	319	THR	N-CA-C	7.12	121.55	112.86
1	A	905	GLY	N-CA-C	-7.10	97.47	111.31
1	A	875	THR	N-CA-C	7.09	120.75	108.76
1	A	348	GLN	N-CA-C	7.07	118.98	111.28
2	B	719	GLY	N-CA-C	7.07	125.07	115.32
1	A	602	ALA	N-CA-C	7.06	118.97	111.28
1	A	235	ALA	N-CA-C	-7.05	95.77	110.80
2	B	295	TYR	N-CA-C	-7.05	101.24	110.33
1	A	413	GLN	N-CA-C	-7.04	101.09	110.24
1	A	310	LEU	N-CA-C	7.04	119.82	110.53
2	B	651	GLY	N-CA-C	7.02	121.76	112.77
2	B	196	ALA	CA-C-N	-7.01	112.53	119.90
2	B	196	ALA	C-N-CA	-7.01	112.53	119.90
1	A	543	GLU	N-CA-C	7.01	118.81	111.03
2	B	195	VAL	N-CA-C	6.98	118.85	112.29
1	A	733	SER	N-CA-C	6.96	121.94	112.68
1	A	597	VAL	N-CA-C	6.95	117.74	110.72
1	A	425	ARG	N-CA-CB	-6.95	100.38	110.87
2	B	258	ALA	N-CA-C	6.94	120.03	109.62
1	A	883	LEU	N-CA-C	-6.93	96.03	110.80
1	A	318	ALA	N-CA-C	6.92	121.97	112.90
1	A	704	ILE	N-CA-C	6.91	117.61	110.36
1	A	853	ASP	N-CA-C	6.90	120.00	108.20
2	B	75	MET	N-CA-C	6.89	118.88	111.36
1	A	287	GLY	N-CA-C	6.89	123.53	113.48
1	A	365	ASP	N-CA-C	6.88	123.24	107.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	GLY	N-CA-C	6.88	124.81	115.32
1	A	666	VAL	N-CA-C	-6.85	102.47	110.21
1	A	635	GLY	N-CA-C	6.84	124.85	115.00
2	B	375	VAL	N-CA-C	6.82	123.53	109.34
1	A	900	HIS	N-CA-C	-6.81	103.86	111.28
1	A	827	THR	N-CA-C	-6.80	104.10	112.88
1	A	586	GLN	CB-CA-C	6.80	120.81	109.38
2	B	633	ILE	N-CA-CB	-6.77	104.85	111.89
1	A	145	ILE	N-CA-C	-6.76	102.58	112.04
2	B	633	ILE	N-CA-C	6.74	117.18	106.32
1	A	848	SER	N-CA-CB	-6.74	101.79	111.84
1	A	376	GLY	O-C-N	-6.69	115.85	122.41
1	A	622	GLN	N-CA-C	6.67	125.02	110.80
1	A	555	VAL	N-CA-C	6.67	117.46	110.72
2	B	514	THR	N-CA-C	6.65	118.61	111.36
1	A	589	LEU	N-CA-C	-6.65	101.76	110.53
1	A	357	ALA	N-CA-C	-6.64	98.93	109.23
2	B	429	SER	N-CA-C	-6.64	101.14	110.50
2	B	593	THR	N-CA-C	-6.63	97.70	108.52
2	B	837	ALA	N-CA-C	6.63	120.23	111.28
1	A	629	SER	CA-C-N	-6.60	113.81	123.05
1	A	629	SER	C-N-CA	-6.60	113.81	123.05
1	A	174	ARG	N-CA-C	6.59	118.54	111.36
1	A	461	ILE	CB-CA-C	-6.58	103.26	112.14
1	A	153	THR	N-CA-C	-6.55	101.89	110.53
2	B	10	GLU	N-CA-C	6.53	119.69	110.23
1	A	899	LEU	CA-C-N	-6.52	111.54	120.28
1	A	899	LEU	C-N-CA	-6.52	111.54	120.28
1	A	662	SER	CA-C-N	6.51	126.17	119.92
1	A	662	SER	C-N-CA	6.51	126.17	119.92
1	A	734	SER	N-CA-C	-6.51	98.28	109.15
1	A	334	LYS	N-CA-C	6.51	118.35	109.11
1	A	150	ARG	N-CA-C	-6.50	104.19	111.28
1	A	9	ASP	N-CA-C	-6.49	103.48	111.33
1	A	722	HIS	N-CA-C	-6.47	101.99	110.53
2	B	43	THR	N-CA-C	-6.46	101.40	110.50
1	A	496	GLN	N-CA-C	6.45	117.97	111.07
1	A	391	GLY	N-CA-C	-6.45	104.97	114.90
2	B	748	ASP	N-CA-C	-6.43	105.25	113.23
2	B	116	GLY	CA-C-O	6.41	126.24	119.06
2	B	358	ALA	N-CA-C	-6.41	103.58	111.33
1	A	662	SER	N-CA-C	6.40	118.25	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	31	ASP	N-CA-C	-6.39	99.40	109.50
2	B	310	LEU	N-CA-C	6.39	121.09	113.16
2	B	599	VAL	CB-CA-C	-6.39	101.30	110.83
1	A	340	VAL	N-CA-C	-6.39	99.08	108.54
1	A	829	THR	N-CA-C	6.35	118.97	109.25
1	A	481	LEU	N-CA-C	6.34	118.83	110.08
1	A	56	ILE	N-CA-C	-6.33	104.17	110.62
2	B	368	GLY	N-CA-C	6.31	124.96	114.48
1	A	440	THR	CB-CA-C	-6.26	98.89	109.03
1	A	466	ALA	N-CA-C	6.25	120.74	107.67
2	B	551	VAL	N-CA-C	-6.25	95.37	108.88
2	B	387	VAL	N-CA-C	6.23	115.58	106.55
2	B	665	GLY	N-CA-C	6.23	120.17	112.14
1	A	308	SER	N-CA-C	-6.21	100.31	109.62
2	B	374	GLY	N-CA-C	-6.20	98.88	110.66
1	A	112	MET	N-CA-C	6.19	120.57	112.89
1	A	182	ILE	N-CA-C	-6.18	103.31	110.05
2	B	579	GLY	N-CA-C	6.17	122.11	112.31
2	B	198	MET	N-CA-CB	-6.15	107.95	114.10
1	A	155	ALA	N-CA-C	-6.14	104.59	111.28
2	B	121	GLY	N-CA-C	-6.12	100.13	111.14
2	B	1001	SER	N-CA-C	-6.11	104.81	112.93
2	B	384	ALA	N-CA-C	-6.09	103.96	111.33
1	A	656	ASP	CA-C-N	6.08	131.31	121.83
1	A	656	ASP	C-N-CA	6.08	131.31	121.83
2	B	567	ASP	N-CA-C	6.03	117.93	111.36
1	A	262	ARG	N-CA-C	6.02	117.92	111.36
2	B	681	THR	N-CA-C	-6.02	97.88	108.23
1	A	969	GLU	N-CA-C	5.98	117.88	111.36
1	A	666	VAL	O-C-N	5.96	128.67	122.54
2	B	679	CYS	CB-CA-C	5.92	122.82	110.32
1	A	670	ALA	N-CA-C	-5.92	101.88	110.64
2	B	389	GLY	CA-C-O	-5.91	116.09	121.47
1	A	485	VAL	CB-CA-C	-5.91	101.57	110.55
2	B	664	ASN	CB-CA-C	-5.91	99.78	111.60
2	B	625	THR	N-CA-C	5.88	117.69	111.28
1	A	925	VAL	N-CA-C	-5.87	97.13	109.34
1	A	252	TRP	N-CA-C	-5.86	104.89	111.28
2	B	326	ARG	N-CA-C	-5.85	102.98	110.53
2	B	571	GLY	CA-C-N	-5.85	112.56	119.05
2	B	571	GLY	C-N-CA	-5.85	112.56	119.05
1	A	178	SER	N-CA-C	-5.84	101.63	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	70	SER	N-CA-C	5.83	117.64	111.28
2	B	574	CYS	N-CA-CB	5.82	121.01	110.95
1	A	135	CYS	N-CA-C	5.81	118.39	111.71
2	B	708	GLU	N-CA-C	5.81	117.42	111.14
1	A	329	HIS	N-CA-C	5.80	117.87	108.41
2	B	104	CYS	N-CA-C	5.80	117.40	111.14
1	A	434	ALA	N-CA-C	-5.78	105.33	112.38
2	B	58	GLU	N-CA-C	5.77	118.30	108.90
2	B	807	PHE	N-CA-C	5.76	118.78	109.79
1	A	249	PRO	N-CA-C	-5.76	102.15	111.14
1	A	284	LYS	N-CA-C	-5.76	100.01	109.40
1	A	847	ALA	N-CA-C	5.76	120.31	113.16
1	A	315	GLY	N-CA-C	-5.75	102.63	112.30
1	A	58	GLN	N-CA-C	-5.74	106.12	113.01
2	B	688	ASP	N-CA-C	5.72	119.96	112.92
2	B	200	GLN	N-CA-C	5.72	117.32	111.14
2	B	133	THR	N-CA-C	5.71	118.70	109.40
1	A	813	LEU	CA-C-N	5.71	126.97	119.84
1	A	813	LEU	C-N-CA	5.71	126.97	119.84
2	B	370	GLY	N-CA-C	-5.69	99.70	113.18
2	B	730	ARG	N-CA-C	-5.67	98.71	110.80
1	A	828	ARG	N-CA-C	-5.67	101.46	109.96
1	A	281	VAL	CA-C-N	5.66	130.42	121.99
1	A	281	VAL	C-N-CA	5.66	130.42	121.99
1	A	341	HIS	N-CA-C	-5.66	100.48	109.59
1	A	393	HIS	N-CA-C	-5.66	99.19	108.41
1	A	442	ALA	N-CA-C	-5.65	105.12	111.28
2	B	218	PHE	N-CA-C	5.64	117.41	108.67
1	A	288	VAL	CB-CA-C	-5.63	103.37	111.19
1	A	176	ARG	N-CA-C	-5.62	105.04	112.24
2	B	505	GLY	N-CA-C	-5.61	100.91	112.34
1	A	73	VAL	CB-CA-C	-5.60	102.78	110.96
1	A	933	PRO	O-C-N	5.60	123.89	121.31
2	B	85	ALA	N-CA-C	-5.59	103.16	110.53
1	A	159	ALA	N-CA-C	5.58	117.44	111.36
1	A	885	LEU	N-CA-C	5.58	118.26	108.56
2	B	844	THR	N-CA-C	-5.57	103.34	110.53
1	A	903	LEU	N-CA-C	5.57	117.35	111.28
1	A	305	ASP	CA-C-N	-5.55	112.90	119.84
1	A	305	ASP	C-N-CA	-5.55	112.90	119.84
1	A	461	ILE	N-CA-C	-5.54	104.97	110.62
2	B	328	LEU	N-CA-C	5.50	119.22	111.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	THR	CA-C-N	5.50	128.52	120.71
1	A	710	THR	C-N-CA	5.50	128.52	120.71
2	B	376	ASN	N-CA-C	5.48	122.05	113.72
1	A	227	ASP	N-CA-CB	-5.47	103.56	110.45
2	B	505	GLY	CA-C-N	-5.46	113.02	119.84
2	B	505	GLY	C-N-CA	-5.46	113.02	119.84
1	A	449	ILE	CA-C-N	5.46	128.62	120.87
1	A	449	ILE	C-N-CA	5.46	128.62	120.87
1	A	600	SER	CA-C-N	-5.44	111.87	120.63
1	A	600	SER	C-N-CA	-5.44	111.87	120.63
1	A	65	LEU	N-CA-C	5.44	119.08	111.74
1	A	929	GLN	N-CA-C	-5.44	103.21	110.55
1	A	490	PHE	N-CA-C	5.44	117.29	111.36
1	A	720	GLY	CA-C-N	5.43	129.78	122.93
1	A	720	GLY	C-N-CA	5.43	129.78	122.93
1	A	566	VAL	CA-C-O	-5.43	115.99	121.59
2	B	768	ARG	N-CA-C	5.43	122.36	110.80
2	B	96	GLN	N-CA-C	5.43	117.20	111.28
2	B	33	PRO	N-CA-C	5.42	121.22	113.47
1	A	364	ALA	CB-CA-C	5.39	119.85	110.68
1	A	499	ASP	N-CA-C	5.39	118.10	110.50
2	B	799	ARG	N-CA-C	-5.39	105.41	111.28
1	A	345	GLN	N-CA-C	5.38	118.17	109.40
1	A	235	ALA	CA-C-N	-5.37	112.61	121.80
1	A	235	ALA	C-N-CA	-5.37	112.61	121.80
1	A	876	VAL	CB-CA-C	-5.36	105.45	111.45
2	B	433	TRP	CB-CA-C	-5.35	110.42	116.63
2	B	650	GLU	CA-C-N	5.35	125.88	120.00
2	B	650	GLU	C-N-CA	5.35	125.88	120.00
1	A	88	THR	N-CA-C	-5.32	103.67	110.53
1	A	272	ARG	N-CA-C	-5.30	105.62	111.71
2	B	791	ILE	O-C-N	5.29	127.01	121.87
1	A	810	MET	N-CA-C	-5.28	105.52	111.28
1	A	220	GLU	N-CA-C	-5.28	105.94	112.38
1	A	628	SER	CA-C-O	-5.27	114.95	121.06
2	B	571	GLY	N-CA-C	-5.27	105.85	112.23
2	B	312	SER	N-CA-C	5.26	118.89	111.52
2	B	683	ASP	N-CA-C	5.26	117.07	110.91
2	B	622	LEU	N-CA-C	5.24	117.68	108.56
1	A	354	SER	N-CA-C	-5.24	99.64	110.80
1	A	143	SER	N-CA-C	-5.24	102.64	110.23
2	B	563	GLY	N-CA-C	-5.23	107.29	113.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	662	GLN	N-CA-C	5.23	117.66	108.56
2	B	620	PRO	CA-C-N	-5.23	114.24	119.94
2	B	620	PRO	C-N-CA	-5.23	114.24	119.94
1	A	683	PRO	N-CA-C	5.21	125.65	112.10
1	A	434	ALA	CA-C-N	5.21	127.68	120.29
1	A	434	ALA	C-N-CA	5.21	127.68	120.29
2	B	621	GLY	N-CA-C	5.20	118.78	112.49
2	B	798	GLY	N-CA-C	-5.20	100.86	113.18
1	A	48	GLY	N-CA-C	5.19	123.92	115.46
1	A	315	GLY	O-C-N	5.19	127.93	122.59
1	A	181	ASP	N-CA-C	5.18	119.60	113.28
1	A	390	PHE	N-CA-C	-5.18	105.63	111.28
1	A	350	TYR	N-CA-C	5.17	116.84	109.14
2	B	42	GLY	N-CA-C	5.16	119.80	111.38
2	B	623	ILE	N-CA-C	-5.16	101.20	108.27
1	A	782	GLY	N-CA-C	5.16	125.41	113.18
2	B	725	GLY	N-CA-C	-5.15	100.98	113.18
2	B	134	ALA	CA-C-N	-5.14	115.12	122.68
2	B	134	ALA	C-N-CA	-5.14	115.12	122.68
1	A	157	MET	N-CA-C	5.13	118.80	112.54
1	A	703	VAL	CB-CA-C	-5.13	104.48	111.15
1	A	827	THR	CA-C-N	-5.12	113.77	120.95
1	A	827	THR	C-N-CA	-5.12	113.77	120.95
1	A	161	SER	N-CA-C	-5.11	105.71	111.28
1	A	452	ARG	N-CA-C	5.11	117.58	111.71
1	A	603	GLU	N-CA-C	-5.11	102.72	110.28
1	A	781	ASN	N-CA-C	-5.11	105.84	111.71
1	A	295	ASN	CA-C-N	-5.10	115.80	123.00
1	A	295	ASN	C-N-CA	-5.10	115.80	123.00
1	A	426	MET	O-C-N	5.10	125.81	121.83
1	A	125	MET	N-CA-C	5.07	118.49	112.72
1	A	695	ARG	N-CA-C	5.07	117.64	110.50
1	A	16	ALA	N-CA-C	-5.06	105.85	111.36
2	B	769	ASN	N-CA-C	5.05	117.53	109.96
2	B	32	LYS	CA-C-N	5.04	124.21	118.97
2	B	32	LYS	C-N-CA	5.04	124.21	118.97
1	A	160	VAL	N-CA-CB	5.03	117.39	110.54
2	B	734	LEU	N-CA-C	-5.03	104.22	110.41
2	B	752	HIS	N-CA-C	5.03	120.92	109.81
2	B	469	ILE	N-CA-C	-5.03	101.36	108.65
1	A	712	GLY	N-CA-C	-5.01	101.26	110.83
1	A	820	CYS	N-CA-C	5.01	117.06	108.90

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	GLY	Mainchain
1	A	334	LYS	Peptide
1	A	388	SER	Peptide
1	A	648	LYS	Peptide
1	A	649	HIS	Peptide
1	A	662	SER	Peptide
1	A	701	SER	Peptide
1	A	817	ASP	Peptide
1	A	830	ARG	Peptide
1	A	953	THR	Peptide
1	A	967	GLN	Mainchain
2	B	190	SER	Peptide
2	B	241	SER	Peptide
2	B	348	GLY	Peptide
2	B	354	GLY	Peptide
2	B	424	ARG	Peptide
2	B	666	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7371	0	7232	1923	0
2	B	7592	0	7407	1256	0
All	All	14963	0	14639	2981	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 101.

All (2981) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:LEU:HD11	2:B:284:MET:SD	1.29	1.67
2:B:327:TYR:CE1	2:B:448:MET:HE1	1.31	1.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:THR:HG22	2:B:265:PRO:CD	1.18	1.58
1:A:105:TRP:CD1	1:A:471:ARG:NH1	1.73	1.57
1:A:249:PRO:HG3	1:A:252:TRP:CE2	1.39	1.53
1:A:588:ALA:CB	1:A:592:GLN:HE22	1.18	1.52
2:B:264:THR:CG2	2:B:265:PRO:HD3	1.36	1.51
2:B:673:TRP:CE3	2:B:755:MET:HE1	1.43	1.51
1:A:884:ALA:CB	2:B:506:PRO:HB3	1.41	1.50
1:A:127:PHE:CD2	1:A:189:ARG:CD	1.94	1.50
1:A:371:LEU:HA	1:A:500:MET:CE	1.37	1.49
2:B:673:TRP:CE3	2:B:755:MET:CE	1.92	1.49
1:A:893:VAL:HG23	2:B:503:LEU:CD1	1.41	1.48
2:B:729:ARG:CB	2:B:754:TYR:HE1	1.23	1.48
1:A:55:LEU:CG	1:A:528:MET:CE	1.91	1.47
1:A:713:LEU:CD2	1:A:714:ASN:H	1.27	1.47
2:B:673:TRP:CZ3	2:B:755:MET:CE	1.97	1.46
1:A:208:HIS:HD2	1:A:309:TRP:CH2	1.33	1.46
1:A:380:CYS:SG	1:A:435:GLN:HA	1.54	1.46
2:B:327:TYR:CD1	2:B:448:MET:HE1	1.48	1.45
1:A:894:ARG:CA	1:A:902:MET:CE	1.92	1.45
1:A:79:GLU:CA	1:A:856:THR:HG22	1.45	1.45
1:A:262:ARG:NH2	1:A:401:GLY:CA	1.78	1.44
1:A:79:GLU:CB	1:A:856:THR:CG2	1.94	1.44
1:A:135:CYS:SG	1:A:148:MET:HE2	1.58	1.43
1:A:713:LEU:HD23	1:A:714:ASN:N	1.14	1.43
1:A:671:LEU:HG	1:A:685:ILE:CG2	1.49	1.42
1:A:290:GLN:CB	1:A:413:GLN:HE22	1.29	1.42
1:A:290:GLN:HB2	1:A:413:GLN:NE2	1.10	1.42
2:B:327:TYR:CE1	2:B:448:MET:CE	2.03	1.41
1:A:372:LYS:N	1:A:500:MET:HE3	1.35	1.41
1:A:961:LEU:CD1	2:B:284:MET:SD	2.05	1.41
1:A:367:ILE:CD1	1:A:415:GLN:CD	1.94	1.41
1:A:876:VAL:CG2	2:B:523:HIS:HD2	1.31	1.40
1:A:253:LEU:CD2	1:A:628:SER:HB3	1.48	1.40
1:A:588:ALA:HB1	1:A:592:GLN:NE2	1.08	1.40
1:A:588:ALA:CA	1:A:592:GLN:HE22	1.33	1.39
2:B:256:ASP:HB3	2:B:300:VAL:CG1	1.52	1.39
1:A:532:ALA:HA	1:A:535:CYS:SG	1.61	1.38
1:A:884:ALA:HB2	2:B:506:PRO:CB	1.52	1.38
1:A:79:GLU:CA	1:A:856:THR:CG2	1.98	1.38
1:A:238:HIS:ND1	1:A:334:LYS:HD2	1.27	1.38
1:A:650:ALA:HB3	1:A:796:SER:CB	1.53	1.38

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:MET:CE	2:B:502:VAL:HG21	1.54	1.38
1:A:472:ASP:OD2	1:A:739:ALA:CB	1.68	1.38
1:A:894:ARG:CA	1:A:902:MET:HE3	1.50	1.37
1:A:876:VAL:CG2	2:B:523:HIS:CD2	2.05	1.37
1:A:894:ARG:C	1:A:902:MET:HE1	1.50	1.37
1:A:231:THR:CG2	1:A:343:THR:OG1	1.71	1.37
1:A:262:ARG:NH2	1:A:401:GLY:HA3	1.31	1.37
2:B:43:THR:CG2	2:B:55:LYS:HD3	1.54	1.36
1:A:931:LEU:CD2	2:B:615:MET:SD	2.13	1.36
2:B:576:TYR:CD1	2:B:578:PHE:HE1	1.45	1.34
1:A:127:PHE:HE2	1:A:189:ARG:NE	1.24	1.34
1:A:692:ALA:CB	1:A:722:HIS:O	1.73	1.34
1:A:776:VAL:HG11	1:A:807:MET:CE	1.57	1.34
2:B:523:HIS:CE1	2:B:527:GLN:HE22	1.43	1.34
1:A:105:TRP:HD1	1:A:471:ARG:CZ	1.38	1.33
1:A:79:GLU:HB3	1:A:856:THR:CG2	1.55	1.33
2:B:839:LEU:CD2	2:B:866:LEU:HD23	1.55	1.32
2:B:434:MET:HE2	2:B:502:VAL:CG2	1.61	1.31
1:A:371:LEU:CA	1:A:500:MET:CE	2.07	1.30
2:B:38:LYS:CD	2:B:65:GLU:OE2	1.77	1.30
1:A:314:THR:O	1:A:347:LYS:NZ	1.64	1.29
1:A:657:TRP:CZ2	1:A:662:SER:O	1.84	1.29
1:A:208:HIS:CD2	1:A:309:TRP:HH2	1.50	1.29
1:A:262:ARG:NH2	1:A:401:GLY:C	1.91	1.29
1:A:529:ALA:HA	1:A:594:MET:CE	1.63	1.29
1:A:588:ALA:HB1	1:A:592:GLN:CD	1.55	1.29
1:A:894:ARG:O	1:A:902:MET:HE1	1.12	1.29
1:A:894:ARG:HA	1:A:902:MET:CE	1.51	1.29
1:A:588:ALA:CB	1:A:592:GLN:NE2	1.82	1.28
1:A:247:PRO:HB3	1:A:477:SER:OG	1.15	1.28
2:B:729:ARG:CB	2:B:754:TYR:CE1	2.15	1.28
1:A:472:ASP:OD2	1:A:739:ALA:N	1.65	1.28
2:B:838:ARG:NH2	2:B:932:SER:OG	1.64	1.27
1:A:79:GLU:HA	1:A:856:THR:CG2	1.62	1.27
1:A:316:LEU:HD21	1:A:350:TYR:CZ	1.69	1.27
2:B:502:VAL:CG1	2:B:901:LEU:HD11	1.64	1.27
1:A:249:PRO:HG2	1:A:252:TRP:CG	1.70	1.26
1:A:623:LEU:O	1:A:626:ILE:HG22	1.24	1.26
1:A:55:LEU:CD1	1:A:528:MET:SD	2.22	1.26
1:A:127:PHE:CE2	1:A:189:ARG:NE	2.01	1.26
2:B:589:TYR:CE1	2:B:808:GLY:HA3	1.70	1.26

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:HD2	1:A:189:ARG:CD	1.36	1.26
1:A:275:ASP:OD1	1:A:276:PRO:HD2	1.13	1.26
2:B:332:PRO:HG3	2:B:399:PHE:CZ	1.70	1.26
2:B:332:PRO:CG	2:B:399:PHE:CE2	2.18	1.25
2:B:502:VAL:HG12	2:B:901:LEU:CD1	1.64	1.25
1:A:320:SER:OG	1:A:351:HIS:NE2	1.65	1.25
1:A:529:ALA:CB	1:A:594:MET:CE	2.13	1.25
2:B:597:LEU:HD12	2:B:644:ASP:CG	1.60	1.25
1:A:316:LEU:CD2	1:A:350:TYR:CE1	2.20	1.25
1:A:887:PRO:O	1:A:893:VAL:HG11	1.29	1.25
1:A:86:ASN:HB2	1:A:849:ASP:O	1.36	1.24
1:A:68:PHE:CE1	1:A:71:SER:HB2	1.72	1.24
1:A:598:TRP:O	1:A:600:SER:N	1.70	1.24
1:A:249:PRO:HG3	1:A:252:TRP:CD2	1.72	1.24
1:A:309:TRP:CE3	1:A:343:THR:HG21	1.72	1.24
1:A:671:LEU:CD1	1:A:671:LEU:O	1.85	1.24
2:B:38:LYS:HD2	2:B:65:GLU:OE2	1.12	1.24
1:A:894:ARG:HG3	1:A:902:MET:CE	1.66	1.24
2:B:165:THR:HA	2:B:546:MET:CE	1.68	1.24
2:B:98:PHE:CZ	2:B:496:MET:SD	2.31	1.23
1:A:199:MET:HG3	1:A:440:THR:OG1	1.36	1.23
1:A:652:ASN:ND2	1:A:800:HIS:CE1	2.06	1.22
1:A:931:LEU:HD22	2:B:615:MET:SD	1.74	1.22
2:B:729:ARG:HB3	2:B:754:TYR:CE1	1.73	1.22
1:A:253:LEU:HD22	1:A:628:SER:CB	1.69	1.22
1:A:208:HIS:CD2	1:A:309:TRP:CH2	2.24	1.21
1:A:529:ALA:CA	1:A:594:MET:CE	2.17	1.21
2:B:343:LEU:HD21	2:B:373:THR:CG2	1.68	1.21
2:B:659:ILE:HD11	2:B:788:LEU:CD2	1.70	1.21
1:A:243:VAL:HG21	1:A:473:LEU:O	1.38	1.21
1:A:132:MET:CE	1:A:493:GLN:OE1	1.89	1.21
1:A:231:THR:HG21	1:A:333:TRP:NE1	1.53	1.21
1:A:876:VAL:HG22	2:B:523:HIS:CD2	1.72	1.21
1:A:650:ALA:CB	1:A:796:SER:HB2	1.71	1.20
1:A:428:PRO:O	1:A:430:THR:HG22	1.37	1.20
1:A:776:VAL:CG1	1:A:807:MET:HE1	1.71	1.20
1:A:893:VAL:CG2	2:B:503:LEU:HD12	1.70	1.20
1:A:127:PHE:CD2	1:A:189:ARG:HD2	1.61	1.20
1:A:435:GLN:O	1:A:439:ALA:HB3	1.42	1.20
2:B:247:ARG:CZ	2:B:347:TRP:HE1	1.55	1.20
2:B:597:LEU:HD12	2:B:644:ASP:OD1	1.36	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:MET:N	1:A:426:MET:SD	2.15	1.19
1:A:756:ARG:HH12	1:A:851:HIS:CE1	1.60	1.19
1:A:307:MET:O	1:A:309:TRP:CD1	1.94	1.19
2:B:542:ALA:HA	2:B:572:PRO:O	1.04	1.19
1:A:131:ARG:NH2	1:A:499:ASP:O	1.76	1.19
2:B:550:MET:N	2:B:550:MET:SD	2.15	1.19
1:A:892:CYS:SG	2:B:902:GLN:HG2	1.82	1.18
2:B:332:PRO:HG2	2:B:399:PHE:CE2	1.77	1.18
2:B:794:GLN:OE1	2:B:805:HIS:CE1	1.95	1.18
1:A:887:PRO:O	1:A:893:VAL:CG1	1.91	1.18
1:A:492:VAL:CB	1:A:495:VAL:HG22	1.74	1.18
1:A:231:THR:CG2	1:A:333:TRP:HE1	1.57	1.18
1:A:529:ALA:CA	1:A:594:MET:HE2	1.72	1.18
2:B:38:LYS:NZ	2:B:65:GLU:OE2	1.76	1.18
2:B:659:ILE:CD1	2:B:788:LEU:CD2	2.22	1.18
1:A:492:VAL:HB	1:A:495:VAL:CG2	1.72	1.17
1:A:671:LEU:O	1:A:671:LEU:HD13	1.03	1.17
1:A:964:VAL:HG11	2:B:788:LEU:CD1	1.75	1.17
1:A:973:GLY:O	2:B:791:ILE:HD11	1.42	1.17
2:B:523:HIS:CE1	2:B:527:GLN:NE2	2.11	1.17
2:B:673:TRP:CE3	2:B:755:MET:HE2	1.77	1.17
1:A:671:LEU:CG	1:A:685:ILE:HG22	1.74	1.17
2:B:502:VAL:CG1	2:B:901:LEU:CD1	2.21	1.17
1:A:372:LYS:H	1:A:500:MET:CE	1.56	1.17
1:A:127:PHE:CE2	1:A:189:ARG:CD	2.27	1.16
2:B:493:GLY:CA	2:B:562:LEU:HD23	1.75	1.16
1:A:934:PRO:CB	2:B:613:LEU:HD12	1.75	1.16
1:A:39:ILE:HG23	1:A:507:VAL:CG1	1.74	1.16
1:A:39:ILE:HG23	1:A:507:VAL:HG12	1.23	1.16
1:A:316:LEU:CD2	1:A:350:TYR:CZ	2.29	1.16
1:A:201:MET:HE1	1:A:465:VAL:CG1	1.76	1.16
2:B:261:GLY:O	2:B:299:MET:CG	1.93	1.16
1:A:472:ASP:OD2	1:A:739:ALA:CA	1.93	1.15
1:A:249:PRO:CG	1:A:252:TRP:CD2	2.27	1.15
1:A:894:ARG:CG	1:A:902:MET:HE2	1.76	1.15
1:A:238:HIS:ND1	1:A:334:LYS:CD	2.09	1.15
2:B:261:GLY:O	2:B:299:MET:HG3	0.98	1.15
1:A:275:ASP:OD1	1:A:276:PRO:CD	1.96	1.14
1:A:934:PRO:HB2	2:B:613:LEU:HD12	1.22	1.14
2:B:123:ASN:ND2	2:B:149:GLN:HB3	1.62	1.14
2:B:734:LEU:HD22	2:B:735:HIS:H	1.12	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:CD2	1:A:577:ARG:CD	2.25	1.14
1:A:85:ALA:CB	1:A:910:LEU:HD21	1.78	1.14
2:B:576:TYR:CE1	2:B:578:PHE:CE1	2.35	1.14
1:A:243:VAL:CG2	1:A:473:LEU:O	1.96	1.14
1:A:652:ASN:HD21	1:A:800:HIS:CE1	1.65	1.14
1:A:54:GLU:CD	1:A:600:SER:HG	1.55	1.13
1:A:664:CYS:CB	1:A:737:GLY:HA3	1.78	1.13
1:A:807:MET:O	1:A:810:MET:HB3	1.49	1.13
1:A:868:TYR:OH	2:B:772:PHE:CD2	2.01	1.13
2:B:673:TRP:CZ3	2:B:755:MET:HE1	1.68	1.13
1:A:367:ILE:HD11	1:A:415:GLN:CD	1.62	1.13
1:A:692:ALA:HB1	1:A:722:HIS:O	1.36	1.13
2:B:32:LYS:HE2	2:B:69:GLU:OE1	1.46	1.13
2:B:198:MET:HE2	2:B:458:ASN:O	1.49	1.13
1:A:525:LEU:CD2	1:A:608:LEU:HD12	1.79	1.13
1:A:54:GLU:CD	1:A:600:SER:OG	1.93	1.12
1:A:79:GLU:CB	1:A:856:THR:HG23	1.65	1.12
1:A:367:ILE:CG1	1:A:415:GLN:NE2	2.12	1.12
2:B:659:ILE:HD11	2:B:788:LEU:HD23	1.20	1.12
1:A:68:PHE:CD1	1:A:71:SER:HB2	1.83	1.12
2:B:576:TYR:CD1	2:B:578:PHE:CE1	2.37	1.12
1:A:529:ALA:CB	1:A:594:MET:HE1	1.76	1.12
1:A:542:GLU:OE1	1:A:625:ARG:NH2	1.81	1.12
1:A:127:PHE:CD2	1:A:189:ARG:HD3	1.71	1.12
1:A:231:THR:HG23	1:A:343:THR:OG1	1.40	1.11
1:A:249:PRO:CG	1:A:252:TRP:CG	2.33	1.11
2:B:549:LYS:C	2:B:550:MET:CE	2.23	1.11
2:B:747:ALA:CB	2:B:749:THR:HG23	1.80	1.11
1:A:491:LEU:HD12	1:A:496:GLN:HG2	1.28	1.11
1:A:111:ASN:OD1	1:A:467:GLN:HG3	1.49	1.11
1:A:105:TRP:CD1	1:A:471:ARG:HH12	1.48	1.11
1:A:664:CYS:HB2	1:A:737:GLY:HA3	1.14	1.11
1:A:29:MET:HE2	1:A:135:CYS:SG	1.81	1.11
1:A:247:PRO:CB	1:A:477:SER:OG	1.99	1.11
1:A:268:GLU:OE2	1:A:693:THR:HG21	1.50	1.11
1:A:472:ASP:OD2	1:A:739:ALA:HB2	1.36	1.11
1:A:81:ILE:HD13	1:A:81:ILE:O	1.50	1.10
1:A:232:TRP:HZ3	1:A:344:ILE:HG21	1.16	1.10
1:A:635:GLY:HA2	1:A:640:MET:CE	1.80	1.10
2:B:332:PRO:CG	2:B:399:PHE:CZ	2.33	1.10
1:A:249:PRO:CG	1:A:252:TRP:CE2	2.33	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:N	1:A:500:MET:CE	2.10	1.10
1:A:384:LEU:C	1:A:385:LEU:HD13	1.75	1.10
2:B:263:LEU:HD12	2:B:293:ALA:HB2	1.13	1.10
2:B:729:ARG:HB2	2:B:754:TYR:HE1	1.02	1.10
1:A:132:MET:HE2	1:A:493:GLN:HB3	1.14	1.09
1:A:671:LEU:HG	1:A:685:ILE:HG22	1.11	1.09
1:A:671:LEU:CG	1:A:685:ILE:CG2	2.30	1.09
1:A:46:LEU:HD21	1:A:458:ILE:CD1	1.82	1.09
1:A:893:VAL:HG23	2:B:503:LEU:HD12	1.17	1.09
2:B:737:TYR:HE1	2:B:750:GLU:OE1	1.34	1.09
1:A:893:VAL:CG2	2:B:503:LEU:CD1	2.29	1.09
1:A:894:ARG:CG	1:A:902:MET:CE	2.28	1.09
2:B:502:VAL:HG11	2:B:901:LEU:HD11	1.15	1.09
2:B:623:ILE:HG21	2:B:893:ILE:CD1	1.82	1.09
2:B:433:TRP:CG	2:B:434:MET:H	1.65	1.09
2:B:542:ALA:CA	2:B:572:PRO:O	2.00	1.09
1:A:54:GLU:OE2	1:A:600:SER:OG	1.72	1.08
1:A:205:ALA:HB2	1:A:232:TRP:NE1	1.68	1.08
1:A:380:CYS:SG	1:A:435:GLN:CA	2.40	1.08
2:B:269:SER:CB	2:B:430:ALA:O	2.01	1.08
1:A:109:GLY:HA3	1:A:233:GLU:O	1.51	1.08
1:A:794:VAL:HG23	1:A:794:VAL:O	1.51	1.08
1:A:55:LEU:HD11	1:A:528:MET:SD	1.91	1.08
1:A:433:LYS:CD	1:A:437:ALA:HB2	1.82	1.08
2:B:838:ARG:HH22	2:B:932:SER:CB	1.67	1.08
1:A:58:GLN:CG	1:A:860:ILE:HD12	1.82	1.08
1:A:472:ASP:CG	1:A:739:ALA:HB2	1.78	1.08
2:B:493:GLY:HA2	2:B:562:LEU:HD23	1.17	1.08
2:B:729:ARG:HB3	2:B:754:TYR:HE1	1.09	1.08
1:A:574:LEU:HD21	1:A:577:ARG:HD2	1.27	1.08
1:A:634:ILE:HB	1:A:688:GLU:HG2	1.29	1.08
2:B:673:TRP:CZ3	2:B:755:MET:HE3	1.82	1.08
1:A:371:LEU:CA	1:A:500:MET:HE2	1.75	1.07
1:A:894:ARG:O	1:A:902:MET:CE	2.00	1.07
2:B:434:MET:CE	2:B:502:VAL:CG2	2.25	1.07
2:B:839:LEU:HD23	2:B:866:LEU:CD2	1.82	1.07
1:A:29:MET:CE	1:A:135:CYS:SG	1.18	1.07
1:A:254:ASP:CA	1:A:556:HIS:NE2	1.97	1.07
1:A:894:ARG:CB	1:A:902:MET:CE	2.30	1.07
2:B:332:PRO:HG2	2:B:399:PHE:CD2	1.90	1.07
2:B:722:GLU:HG2	2:B:729:ARG:HH21	1.16	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:HA	1:A:856:THR:HG22	1.10	1.07
1:A:85:ALA:HB2	1:A:910:LEU:CD2	1.84	1.07
1:A:355:THR:O	1:A:418:PHE:HD1	1.38	1.07
1:A:650:ALA:HB3	1:A:796:SER:HB2	1.12	1.07
2:B:194:ILE:HG21	2:B:200:GLN:HA	1.34	1.07
1:A:756:ARG:NH1	1:A:851:HIS:CE1	2.22	1.06
2:B:256:ASP:HB3	2:B:300:VAL:HG11	1.12	1.06
1:A:438:THR:O	1:A:442:ALA:HB3	1.55	1.06
1:A:627:ARG:NH1	1:A:738:CYS:SG	2.27	1.06
1:A:868:TYR:CZ	2:B:772:PHE:CE2	2.42	1.06
2:B:7:GLN:HG2	2:B:29:VAL:HG11	1.36	1.06
1:A:664:CYS:HB2	1:A:737:GLY:CA	1.85	1.06
2:B:576:TYR:CE1	2:B:578:PHE:HE1	1.72	1.06
1:A:876:VAL:HG23	2:B:523:HIS:CD2	1.84	1.06
2:B:197:PRO:O	2:B:198:MET:HB2	1.26	1.06
2:B:84:THR:HG21	2:B:545:ARG:HH11	1.21	1.06
1:A:217:GLU:C	1:A:218:LEU:HD23	1.81	1.05
1:A:650:ALA:CB	1:A:796:SER:CB	2.27	1.05
1:A:52:THR:HG21	1:A:601:MET:HE2	1.09	1.05
1:A:476:GLY:O	1:A:477:SER:HB3	1.53	1.05
1:A:558:VAL:O	1:A:562:LEU:HD23	1.54	1.05
1:A:574:LEU:HD23	1:A:577:ARG:CG	1.86	1.05
1:A:607:ARG:HH11	2:B:4:PRO:HD3	1.21	1.05
1:A:635:GLY:HA2	1:A:640:MET:HE1	1.35	1.05
1:A:966:ALA:O	1:A:969:GLU:HB3	1.55	1.05
1:A:249:PRO:HG3	1:A:252:TRP:NE1	1.70	1.05
1:A:433:LYS:CG	1:A:437:ALA:HB2	1.86	1.05
1:A:660:ASN:ND2	1:A:661:GLU:OE2	1.88	1.05
2:B:729:ARG:HB2	2:B:754:TYR:CE1	1.84	1.05
1:A:55:LEU:CG	1:A:528:MET:HE3	1.70	1.04
1:A:750:GLU:OE2	1:A:751:HIS:N	1.87	1.04
1:A:893:VAL:HG23	2:B:503:LEU:HD11	1.27	1.04
2:B:32:LYS:CE	2:B:69:GLU:OE1	2.05	1.04
2:B:43:THR:HG22	2:B:55:LYS:HD3	1.04	1.04
2:B:498:ILE:HD12	2:B:820:PHE:CE2	1.91	1.04
1:A:367:ILE:CG1	1:A:415:GLN:HE21	1.67	1.04
1:A:957:PHE:O	1:A:958:THR:OG1	1.74	1.04
1:A:973:GLY:O	2:B:791:ILE:CD1	2.04	1.04
1:A:39:ILE:HA	1:A:506:SER:OG	1.56	1.04
1:A:88:THR:HG22	1:A:90:MET:H	1.21	1.04
1:A:272:ARG:HH21	1:A:272:ARG:HB2	1.15	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:747:ALA:HB1	2:B:749:THR:HG23	1.35	1.04
1:A:273:LEU:HD23	1:A:281:VAL:HG23	1.37	1.04
1:A:529:ALA:HB2	1:A:594:MET:CE	1.78	1.04
1:A:957:PHE:CD2	2:B:279:TYR:HE1	1.74	1.04
2:B:549:LYS:C	2:B:550:MET:HE3	1.81	1.04
1:A:249:PRO:CG	1:A:252:TRP:CD1	2.41	1.04
1:A:657:TRP:CE2	1:A:662:SER:O	2.09	1.04
2:B:597:LEU:CG	2:B:644:ASP:OD2	2.05	1.04
1:A:554:ASP:OD1	1:A:672:PRO:HB3	1.57	1.03
1:A:316:LEU:HD22	1:A:350:TYR:CE1	1.92	1.03
1:A:889:GLU:OE1	1:A:889:GLU:N	1.91	1.03
2:B:549:LYS:HA	2:B:550:MET:HE1	1.40	1.03
1:A:105:TRP:CD1	1:A:471:ARG:CZ	2.26	1.03
1:A:231:THR:HG21	1:A:333:TRP:HE1	1.03	1.03
1:A:290:GLN:CB	1:A:413:GLN:NE2	1.99	1.03
1:A:298:VAL:O	1:A:700:GLY:O	1.76	1.03
2:B:433:TRP:NE1	2:B:518:GLN:HG2	1.73	1.03
1:A:85:ALA:CB	1:A:910:LEU:CD2	2.37	1.03
1:A:671:LEU:CB	1:A:685:ILE:HG22	1.88	1.03
1:A:201:MET:HE1	1:A:465:VAL:HG11	1.06	1.03
1:A:477:SER:C	1:A:478:LEU:HD12	1.83	1.03
2:B:679:CYS:O	2:B:741:ILE:O	1.76	1.03
1:A:81:ILE:HD11	1:A:98:GLU:HB2	1.39	1.02
1:A:433:LYS:HG2	1:A:437:ALA:HB2	1.37	1.02
2:B:597:LEU:HD12	2:B:644:ASP:OD2	1.57	1.02
1:A:314:THR:O	1:A:347:LYS:CE	2.07	1.02
1:A:449:ILE:HG13	1:A:453:THR:HG21	1.41	1.02
2:B:330:ALA:N	2:B:450:GLU:OE2	1.91	1.02
1:A:972:GLU:CB	1:A:973:GLY:HA3	1.89	1.02
2:B:36:GLU:OE1	2:B:65:GLU:OE1	1.78	1.02
2:B:163:GLY:HA3	2:B:548:ASN:HB3	1.38	1.02
2:B:618:LEU:HD13	2:B:623:ILE:HD11	1.42	1.02
2:B:794:GLN:CG	2:B:796:ASP:O	2.08	1.02
1:A:79:GLU:N	1:A:856:THR:HG22	1.75	1.02
1:A:85:ALA:HB2	1:A:910:LEU:HD21	1.06	1.02
1:A:231:THR:HG22	1:A:343:THR:OG1	1.55	1.02
1:A:898:THR:HG23	2:B:860:MET:CE	1.89	1.02
1:A:898:THR:CG2	2:B:860:MET:HE1	1.90	1.02
2:B:623:ILE:HG21	2:B:893:ILE:HD11	1.05	1.02
1:A:671:LEU:HG	1:A:685:ILE:HG21	1.39	1.02
1:A:532:ALA:CA	1:A:535:CYS:SG	2.48	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:ILE:HG22	1:A:816:THR:H	1.19	1.01
2:B:722:GLU:CG	2:B:729:ARG:HH21	1.73	1.01
1:A:529:ALA:HB2	1:A:594:MET:HE1	1.03	1.01
2:B:343:LEU:HD21	2:B:373:THR:HG21	1.38	1.01
2:B:498:ILE:HD12	2:B:820:PHE:HE2	1.23	1.01
2:B:546:MET:HA	2:B:546:MET:HE2	1.39	1.01
1:A:650:ALA:HB3	1:A:796:SER:CA	1.89	1.01
2:B:433:TRP:HE1	2:B:518:GLN:HG2	1.26	1.01
1:A:221:ASN:OD1	1:A:431:PHE:CZ	2.14	1.01
1:A:767:ARG:NH2	1:A:821:ASP:OD1	1.92	1.01
2:B:163:GLY:O	2:B:442:PRO:HA	1.58	1.01
2:B:43:THR:CG2	2:B:55:LYS:CD	2.38	1.00
1:A:52:THR:CG2	1:A:601:MET:HE2	1.91	1.00
1:A:127:PHE:HD2	1:A:189:ARG:HD3	0.86	1.00
1:A:316:LEU:HD21	1:A:350:TYR:OH	1.59	1.00
2:B:241:SER:HB3	2:B:390:ARG:HG2	1.40	1.00
2:B:498:ILE:O	2:B:502:VAL:HG23	1.61	1.00
1:A:29:MET:HE1	1:A:135:CYS:SG	0.42	1.00
1:A:432:THR:O	1:A:435:GLN:CB	2.10	1.00
1:A:876:VAL:HA	2:B:520:ASP:OD1	1.61	1.00
2:B:12:ARG:HH12	2:B:991:ASP:CG	1.70	1.00
2:B:343:LEU:HD21	2:B:373:THR:HG23	1.38	1.00
1:A:931:LEU:HD21	2:B:615:MET:SD	1.99	1.00
2:B:747:ALA:HB1	2:B:749:THR:CG2	1.92	1.00
1:A:516:LYS:O	1:A:520:THR:HG22	1.62	1.00
1:A:968:MET:HE1	2:B:659:ILE:HG21	1.40	1.00
2:B:377:GLY:HA3	2:B:451:PRO:HB3	1.42	1.00
2:B:597:LEU:CD1	2:B:644:ASP:OD2	2.08	1.00
2:B:120:LEU:CD1	2:B:152:VAL:HB	1.92	1.00
1:A:79:GLU:HB3	1:A:856:THR:HG21	1.00	0.99
2:B:327:TYR:CZ	2:B:448:MET:CE	2.44	0.99
1:A:232:TRP:HZ3	1:A:344:ILE:CG2	1.73	0.99
1:A:790:PRO:HG3	1:A:819:ASP:HB3	1.43	0.99
2:B:43:THR:HG22	2:B:55:LYS:CD	1.93	0.99
1:A:135:CYS:SG	1:A:148:MET:CE	2.49	0.99
1:A:588:ALA:CA	1:A:592:GLN:NE2	2.16	0.99
2:B:7:GLN:HG2	2:B:29:VAL:CG1	1.92	0.99
1:A:574:LEU:CD2	1:A:577:ARG:HD2	1.87	0.99
2:B:450:GLU:HB3	2:B:451:PRO:HD3	1.45	0.99
1:A:122:SER:OG	1:A:187:ASP:OD2	1.81	0.98
1:A:361:GLU:N	1:A:361:GLU:OE2	1.96	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:NH1	2:B:173:ASP:OD2	1.96	0.98
1:A:309:TRP:H	1:A:309:TRP:HD1	1.06	0.98
1:A:574:LEU:HD23	1:A:577:ARG:HG3	1.45	0.98
2:B:327:TYR:CZ	2:B:448:MET:HE2	1.97	0.98
2:B:373:THR:OG1	2:B:381:THR:HA	1.64	0.98
2:B:623:ILE:CG2	2:B:893:ILE:HD11	1.92	0.98
1:A:29:MET:SD	1:A:135:CYS:SG	2.61	0.98
1:A:231:THR:HG23	1:A:343:THR:HG1	1.25	0.98
1:A:352:ARG:HA	1:A:382:GLU:OE1	1.62	0.98
1:A:671:LEU:HD13	1:A:671:LEU:C	1.89	0.97
1:A:828:ARG:HB3	1:A:828:ARG:HH11	1.29	0.97
1:A:64:GLY:O	1:A:65:LEU:HG	1.62	0.97
1:A:529:ALA:HA	1:A:594:MET:HE2	1.00	0.97
1:A:621:VAL:O	1:A:621:VAL:HG12	1.64	0.97
1:A:668:PHE:HD2	1:A:686:GLY:HA3	1.27	0.97
1:A:19:LYS:HA	1:A:140:LEU:HD21	1.45	0.97
1:A:132:MET:HE2	1:A:493:GLN:CB	1.93	0.97
2:B:673:TRP:HE3	2:B:755:MET:HE2	1.20	0.97
1:A:119:ILE:HG23	1:A:487:LEU:O	1.65	0.97
2:B:509:ILE:O	2:B:632:THR:HA	1.63	0.97
1:A:229:TYR:OH	1:A:311:ASP:OD1	1.81	0.97
1:A:901:SER:OG	2:B:500:GLN:OE1	1.82	0.97
2:B:247:ARG:CZ	2:B:347:TRP:NE1	2.28	0.97
2:B:256:ASP:CB	2:B:300:VAL:HG11	1.93	0.97
2:B:493:GLY:HA2	2:B:562:LEU:CD2	1.94	0.97
1:A:78:ALA:C	1:A:856:THR:HG22	1.87	0.97
1:A:79:GLU:HB2	1:A:856:THR:HG23	1.44	0.97
1:A:607:ARG:NH1	2:B:4:PRO:HD3	1.78	0.97
1:A:876:VAL:HG22	2:B:523:HIS:HD2	0.80	0.97
2:B:227:VAL:HG22	2:B:364:MET:SD	2.05	0.97
1:A:372:LYS:NZ	1:A:499:ASP:OD2	1.98	0.97
2:B:576:TYR:HD1	2:B:578:PHE:HE1	1.10	0.97
1:A:204:SER:OG	1:A:523:TYR:CE1	2.18	0.96
2:B:38:LYS:CE	2:B:65:GLU:OE2	2.12	0.96
2:B:839:LEU:HD23	2:B:866:LEU:HD23	0.98	0.96
1:A:554:ASP:O	1:A:558:VAL:HG23	1.64	0.96
2:B:189:ALA:O	2:B:190:SER:HB3	1.64	0.96
1:A:156:THR:HG23	1:A:157:MET:H	1.27	0.96
2:B:442:PRO:O	2:B:576:TYR:OH	1.81	0.96
2:B:121:GLY:HA2	2:B:150:CYS:O	1.64	0.96
2:B:263:LEU:CD1	2:B:293:ALA:HB2	1.96	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LEU:CD2	1:A:628:SER:CB	2.35	0.96
1:A:756:ARG:NH1	1:A:851:HIS:ND1	2.14	0.96
2:B:676:TRP:CD1	2:B:754:TYR:HB2	2.00	0.96
1:A:232:TRP:CZ3	1:A:344:ILE:HG21	2.00	0.96
1:A:892:CYS:SG	2:B:902:GLN:CG	2.54	0.96
1:A:894:ARG:HG3	1:A:902:MET:HE1	1.40	0.96
1:A:55:LEU:CD2	1:A:528:MET:HE1	1.95	0.96
1:A:127:PHE:HE1	1:A:452:ARG:NE	1.62	0.96
1:A:432:THR:HG23	1:A:433:LYS:N	1.80	0.96
1:A:442:ALA:HA	1:A:509:VAL:CG1	1.95	0.96
2:B:117:ARG:NE	2:B:155:GLU:OE2	1.99	0.96
1:A:549:VAL:HG13	1:A:553:THR:HG21	1.46	0.95
1:A:742:MET:HA	1:A:742:MET:HE3	1.47	0.95
1:A:776:VAL:HG11	1:A:807:MET:HE1	0.96	0.95
1:A:921:ASP:HB2	2:B:626:ALA:HB1	1.46	0.95
2:B:433:TRP:HE1	2:B:518:GLN:CG	1.79	0.95
1:A:634:ILE:HB	1:A:688:GLU:CG	1.95	0.95
1:A:868:TYR:CZ	2:B:772:PHE:CD2	2.54	0.95
1:A:309:TRP:CD1	1:A:309:TRP:H	1.79	0.95
1:A:288:VAL:O	1:A:324:ARG:HD3	1.67	0.95
1:A:35:ALA:O	1:A:42:GLY:HA2	1.65	0.95
1:A:964:VAL:HG11	2:B:788:LEU:HD12	1.48	0.95
2:B:197:PRO:O	2:B:198:MET:CB	2.09	0.95
2:B:589:TYR:CD1	2:B:808:GLY:HA3	2.01	0.95
1:A:262:ARG:HH22	1:A:401:GLY:C	1.59	0.95
1:A:623:LEU:O	1:A:626:ILE:CG2	2.14	0.95
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.28	0.94
1:A:132:MET:HE3	1:A:493:GLN:OE1	1.67	0.94
2:B:98:PHE:HZ	2:B:496:MET:SD	1.86	0.94
2:B:165:THR:HG22	2:B:219:GLN:HE22	1.31	0.94
1:A:621:VAL:O	1:A:621:VAL:CG1	2.13	0.94
1:A:756:ARG:NH1	1:A:851:HIS:CG	2.34	0.94
2:B:269:SER:HB3	2:B:430:ALA:O	1.64	0.94
1:A:29:MET:HE1	1:A:135:CYS:CB	1.96	0.94
1:A:352:ARG:NE	1:A:382:GLU:OE2	1.85	0.94
1:A:58:GLN:HA	1:A:58:GLN:HE21	1.30	0.94
1:A:211:VAL:HG22	1:A:216:GLN:HB2	1.50	0.94
1:A:964:VAL:HG11	2:B:788:LEU:HD13	1.47	0.94
1:A:371:LEU:C	1:A:500:MET:CE	2.39	0.94
1:A:29:MET:HE3	1:A:135:CYS:SG	1.53	0.94
1:A:232:TRP:CZ3	1:A:344:ILE:CG2	2.50	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:ASN:OD1	2:B:115:ALA:N	1.99	0.94
2:B:428:CYS:SG	2:B:818:HIS:CB	2.54	0.94
2:B:434:MET:HE1	2:B:502:VAL:HG11	1.49	0.94
1:A:371:LEU:CA	1:A:500:MET:HE1	1.96	0.94
1:A:634:ILE:H	1:A:634:ILE:HD13	1.32	0.94
2:B:7:GLN:HE22	2:B:76:ASP:HB2	1.29	0.94
1:A:26:LEU:HD11	1:A:144:THR:HG22	1.49	0.94
1:A:68:PHE:CD2	2:B:214:ARG:HD2	2.03	0.94
1:A:180:SER:OG	1:A:181:ASP:OD1	1.85	0.94
1:A:894:ARG:CA	1:A:902:MET:HE1	1.75	0.94
2:B:327:TYR:CD1	2:B:448:MET:CE	2.42	0.94
1:A:815:ILE:HG22	1:A:816:THR:N	1.74	0.93
1:A:68:PHE:CE1	1:A:71:SER:CB	2.52	0.93
2:B:839:LEU:CD2	2:B:866:LEU:CD2	2.39	0.93
1:A:132:MET:HE1	1:A:493:GLN:OE1	1.66	0.93
2:B:123:ASN:HD22	2:B:149:GLN:HB3	1.30	0.93
1:A:103:ARG:HG3	1:A:103:ARG:HH21	1.31	0.93
1:A:29:MET:CE	1:A:135:CYS:HG	0.88	0.93
1:A:634:ILE:HD11	1:A:718:ARG:NH2	1.83	0.93
1:A:932:ARG:NH2	1:A:932:ARG:HB3	1.84	0.93
2:B:722:GLU:CG	2:B:729:ARG:NH2	2.31	0.93
1:A:234:LEU:O	1:A:236:CYS:N	2.01	0.92
1:A:238:HIS:HE2	1:A:338:SER:HA	1.34	0.92
2:B:165:THR:CG2	2:B:219:GLN:HE22	1.80	0.92
1:A:433:LYS:CD	1:A:437:ALA:CB	2.46	0.92
2:B:12:ARG:NH1	2:B:991:ASP:OD2	2.01	0.92
2:B:247:ARG:NH2	2:B:347:TRP:HE1	1.66	0.92
1:A:84:THR:HA	1:A:95:GLN:HB3	1.49	0.92
1:A:352:ARG:HG2	1:A:352:ARG:HH11	1.34	0.92
1:A:704:ILE:HA	1:A:707:ILE:CD1	1.99	0.92
2:B:89:ASP:CG	2:B:410:GLN:OE1	2.13	0.92
1:A:46:LEU:HD21	1:A:458:ILE:HD12	1.49	0.92
2:B:45:ILE:C	2:B:53:ILE:HD11	1.89	0.92
1:A:132:MET:CE	1:A:493:GLN:HB3	1.99	0.92
1:A:574:LEU:HD21	1:A:577:ARG:CD	1.93	0.92
1:A:588:ALA:C	1:A:592:GLN:NE2	2.27	0.92
1:A:525:LEU:HD23	1:A:608:LEU:CD1	2.00	0.92
2:B:673:TRP:HZ3	2:B:755:MET:HE3	1.31	0.92
2:B:363:VAL:HG13	2:B:441:MET:HE2	1.50	0.92
1:A:247:PRO:HB3	1:A:477:SER:HG	1.31	0.91
2:B:165:THR:HA	2:B:546:MET:HE1	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:THR:HG22	2:B:265:PRO:HD2	1.49	0.91
1:A:58:GLN:HG2	1:A:860:ILE:CD1	2.00	0.91
1:A:692:ALA:CA	1:A:722:HIS:O	2.17	0.91
2:B:589:TYR:HE1	2:B:808:GLY:HA3	1.34	0.91
1:A:532:ALA:HB1	1:A:597:VAL:HG21	1.52	0.91
1:A:627:ARG:HG3	1:A:730:THR:O	1.70	0.91
1:A:652:ASN:HD21	1:A:800:HIS:HE1	0.94	0.91
1:A:788:ILE:HD11	1:A:823:VAL:CG2	2.00	0.91
1:A:29:MET:CE	1:A:135:CYS:CB	2.49	0.91
1:A:238:HIS:CE1	1:A:334:LYS:CG	2.54	0.91
1:A:932:ARG:HB3	1:A:932:ARG:CZ	1.99	0.91
2:B:363:VAL:HG13	2:B:441:MET:CE	2.00	0.91
1:A:532:ALA:O	1:A:536:GLU:N	2.04	0.91
2:B:428:CYS:SG	2:B:818:HIS:HB3	2.11	0.91
2:B:7:GLN:CG	2:B:29:VAL:HG11	2.00	0.91
1:A:253:LEU:HD22	1:A:628:SER:HB3	0.92	0.91
1:A:634:ILE:CB	1:A:688:GLU:HG2	2.00	0.91
1:A:238:HIS:NE2	1:A:338:SER:HA	1.86	0.91
2:B:111:MET:SD	2:B:118:PHE:HD2	1.93	0.91
2:B:327:TYR:CE1	2:B:448:MET:HE2	2.05	0.91
1:A:588:ALA:C	1:A:592:GLN:HE22	1.79	0.90
2:B:499:TYR:HE1	2:B:901:LEU:HD22	1.35	0.90
1:A:885:LEU:HD22	1:A:885:LEU:H	1.35	0.90
2:B:32:LYS:CD	2:B:69:GLU:OE1	2.20	0.90
2:B:450:GLU:CB	2:B:451:PRO:HD3	1.95	0.90
1:A:574:LEU:CD2	1:A:577:ARG:CG	2.49	0.90
1:A:908:PRO:HG3	2:B:528:TYR:HE1	1.34	0.90
2:B:549:LYS:C	2:B:550:MET:SD	2.53	0.90
2:B:467:GLN:NE2	2:B:467:GLN:O	2.03	0.90
1:A:68:PHE:HD2	2:B:214:ARG:HD2	1.33	0.90
1:A:431:PHE:O	1:A:434:ALA:HB3	1.70	0.90
2:B:84:THR:CG2	2:B:545:ARG:HD3	2.01	0.90
2:B:737:TYR:CE1	2:B:750:GLU:OE1	2.25	0.90
1:A:529:ALA:CB	1:A:594:MET:HE3	1.99	0.90
1:A:892:CYS:HG	2:B:902:GLN:CD	1.79	0.90
1:A:432:THR:O	1:A:435:GLN:HB2	1.68	0.90
1:A:807:MET:HE2	1:A:810:MET:HE2	1.51	0.90
2:B:264:THR:CG2	2:B:265:PRO:CD	2.13	0.90
1:A:481:LEU:HD22	1:A:481:LEU:H	1.35	0.89
1:A:571:LEU:CD2	1:A:592:GLN:HG3	2.02	0.89
1:A:713:LEU:CD2	1:A:714:ASN:N	2.02	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:ALA:CB	1:A:274:VAL:CG2	2.49	0.89
1:A:316:LEU:CD2	1:A:350:TYR:OH	2.19	0.89
1:A:642:ASP:O	1:A:644:SER:N	2.04	0.89
2:B:78:LEU:HD22	2:B:180:LEU:HD21	1.53	0.89
1:A:77:LEU:HD22	1:A:742:MET:HE2	1.54	0.89
1:A:525:LEU:CD2	1:A:608:LEU:CD1	2.49	0.89
2:B:331:LEU:HD12	2:B:373:THR:HG22	1.54	0.89
2:B:334:CYS:O	2:B:379:ARG:NH1	2.05	0.89
1:A:499:ASP:OD1	1:A:500:MET:N	2.06	0.89
1:A:532:ALA:HB1	1:A:597:VAL:CG2	2.03	0.89
1:A:387:ASN:HD22	1:A:391:GLY:CA	1.86	0.89
1:A:788:ILE:HD11	1:A:823:VAL:HG21	1.55	0.89
2:B:57:GLY:O	2:B:478:HIS:HB2	1.72	0.89
2:B:89:ASP:HA	2:B:410:GLN:NE2	1.88	0.89
1:A:214:ARG:HD3	1:A:214:ARG:H	1.37	0.89
1:A:307:MET:O	1:A:309:TRP:HD1	1.43	0.89
1:A:309:TRP:CE3	1:A:343:THR:CG2	2.55	0.89
2:B:263:LEU:HD12	2:B:293:ALA:CB	2.01	0.89
1:A:830:ARG:NH1	1:A:830:ARG:O	2.06	0.88
1:A:262:ARG:HH22	1:A:401:GLY:CA	1.61	0.88
1:A:932:ARG:HB2	1:A:933:PRO:HD2	1.54	0.88
2:B:247:ARG:NE	2:B:347:TRP:NE1	2.21	0.88
1:A:843:ARG:HB3	1:A:843:ARG:HH11	1.35	0.88
2:B:110:GLN:HA	2:B:110:GLN:HE21	1.37	0.88
1:A:79:GLU:N	1:A:79:GLU:OE1	2.07	0.88
2:B:597:LEU:HG	2:B:644:ASP:OD2	1.70	0.88
1:A:638:ARG:HH21	1:A:638:ARG:HG3	1.36	0.88
2:B:549:LYS:CA	2:B:550:MET:HE1	2.03	0.88
1:A:39:ILE:CA	1:A:506:SER:OG	2.21	0.88
1:A:309:TRP:HE3	1:A:343:THR:HG21	1.20	0.88
1:A:664:CYS:SG	1:A:737:GLY:HA3	2.14	0.88
1:A:199:MET:HG3	1:A:440:THR:HG1	1.26	0.88
1:A:262:ARG:HH21	1:A:401:GLY:CA	1.69	0.88
1:A:525:LEU:HD23	1:A:608:LEU:HD12	1.56	0.88
2:B:165:THR:HG21	2:B:219:GLN:NE2	1.89	0.88
1:A:525:LEU:HD21	1:A:608:LEU:HD12	1.56	0.88
1:A:244:ALA:CB	1:A:274:VAL:HG23	2.03	0.87
1:A:68:PHE:HE1	1:A:71:SER:HB2	1.30	0.87
1:A:78:ALA:O	1:A:856:THR:HG22	1.73	0.87
2:B:734:LEU:CD2	2:B:735:HIS:H	1.86	0.87
1:A:380:CYS:SG	1:A:434:ALA:O	2.31	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:CE1	1:A:452:ARG:NE	2.42	0.87
1:A:205:ALA:HB2	1:A:232:TRP:CE2	2.09	0.87
1:A:117:VAL:CG2	1:A:485:VAL:HG23	2.04	0.87
1:A:894:ARG:HG3	1:A:902:MET:HE2	1.34	0.87
1:A:476:GLY:O	1:A:477:SER:CB	2.22	0.87
1:A:117:VAL:HG22	1:A:485:VAL:HG23	1.56	0.87
1:A:231:THR:HG21	1:A:333:TRP:CE2	2.10	0.87
1:A:478:LEU:HD13	1:A:534:VAL:HG13	1.56	0.87
2:B:165:THR:CG2	2:B:219:GLN:NE2	2.38	0.86
1:A:756:ARG:HH11	1:A:851:HIS:CG	1.94	0.86
2:B:66:ARG:HH11	2:B:66:ARG:HG3	1.40	0.86
1:A:868:TYR:CE1	2:B:772:PHE:CE2	2.63	0.86
2:B:334:CYS:SG	2:B:468:MET:CE	2.63	0.86
1:A:777:LEU:HD22	1:A:834:MET:HE2	1.57	0.86
1:A:957:PHE:HD2	2:B:279:TYR:HE1	1.21	0.86
2:B:549:LYS:CA	2:B:550:MET:CE	2.53	0.86
2:B:839:LEU:HD22	2:B:866:LEU:HD23	1.57	0.86
1:A:298:VAL:C	1:A:299:HIS:CD2	2.53	0.86
1:A:248:VAL:HB	1:A:249:PRO:HD2	1.56	0.86
2:B:26:GLN:O	2:B:27:THR:OG1	1.92	0.86
1:A:55:LEU:HD13	1:A:528:MET:SD	2.05	0.86
1:A:320:SER:OG	1:A:351:HIS:CD2	2.29	0.86
1:A:807:MET:O	1:A:810:MET:CB	2.23	0.86
1:A:957:PHE:CD2	2:B:279:TYR:CE1	2.63	0.86
2:B:433:TRP:NE1	2:B:518:GLN:CG	2.36	0.86
2:B:611:SER:O	2:B:615:MET:HG2	1.76	0.86
1:A:208:HIS:CD2	1:A:309:TRP:CZ2	2.64	0.86
1:A:260:THR:HG22	1:A:263:GLU:OE1	1.75	0.86
1:A:917:MET:HE1	2:B:511:ASP:OD1	1.74	0.86
1:A:961:LEU:HD12	2:B:284:MET:SD	2.16	0.86
2:B:84:THR:HG21	2:B:545:ARG:HD3	1.56	0.86
1:A:794:VAL:O	1:A:794:VAL:CG2	2.24	0.85
1:A:966:ALA:O	1:A:969:GLU:CB	2.24	0.85
2:B:117:ARG:CZ	2:B:155:GLU:OE2	2.23	0.85
2:B:120:LEU:HD11	2:B:152:VAL:HB	1.56	0.85
2:B:257:PHE:CD1	2:B:357:HIS:NE2	2.44	0.85
2:B:240:ASP:O	2:B:241:SER:OG	1.94	0.85
2:B:256:ASP:HB3	2:B:300:VAL:HG13	1.53	0.85
1:A:106:LEU:CD1	1:A:470:VAL:HG12	2.05	0.85
1:A:455:HIS:O	1:A:459:THR:HG22	1.74	0.85
1:A:828:ARG:HH11	1:A:828:ARG:CB	1.88	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:SER:HA	1:A:351:HIS:HD2	1.41	0.85
1:A:127:PHE:CE2	1:A:189:ARG:HD2	2.04	0.85
1:A:492:VAL:HB	1:A:495:VAL:HG22	0.90	0.85
2:B:198:MET:O	2:B:204:GLN:HB3	1.74	0.85
1:A:438:THR:O	1:A:442:ALA:CB	2.23	0.85
1:A:882:GLY:C	1:A:883:LEU:HD23	2.01	0.85
2:B:427:ALA:HA	2:B:432:GLU:OE1	1.76	0.85
1:A:499:ASP:HB2	2:B:1001:SER:OG	1.76	0.85
1:A:940:PRO:HG3	2:B:915:SER:HB3	1.59	0.85
1:A:972:GLU:CB	1:A:973:GLY:CA	2.54	0.85
1:A:507:VAL:CG2	1:A:512:MET:HE3	2.07	0.85
1:A:531:LEU:CD2	1:A:747:ILE:HD11	2.06	0.85
1:A:964:VAL:CG1	2:B:788:LEU:HD13	2.07	0.85
1:A:170:LEU:HD13	1:A:171:ALA:N	1.92	0.84
1:A:861:ARG:NH2	2:B:547:ALA:HB2	1.91	0.84
1:A:957:PHE:HD2	2:B:279:TYR:CE1	1.95	0.84
2:B:117:ARG:HE	2:B:155:GLU:CD	1.83	0.84
1:A:344:ILE:CD1	1:A:396:LEU:HD11	2.06	0.84
1:A:367:ILE:HD13	1:A:415:GLN:HE21	0.69	0.84
1:A:379:ALA:HB2	1:A:427:PRO:O	1.77	0.84
1:A:843:ARG:HH11	1:A:843:ARG:CB	1.90	0.84
1:A:876:VAL:HG21	1:A:909:LEU:HD11	1.59	0.84
2:B:686:HIS:CD2	2:B:786:ALA:CB	2.60	0.84
1:A:898:THR:HG23	2:B:860:MET:HE1	0.94	0.84
1:A:531:LEU:HD21	1:A:747:ILE:HD11	1.57	0.84
1:A:754:VAL:HG12	1:A:855:ALA:HB2	1.58	0.84
1:A:972:GLU:HB2	1:A:973:GLY:HA3	1.56	0.84
2:B:98:PHE:CE1	2:B:496:MET:SD	2.71	0.84
2:B:165:THR:HA	2:B:546:MET:HE3	1.58	0.84
1:A:14:THR:O	1:A:18:ILE:HG12	1.76	0.84
1:A:598:TRP:C	1:A:600:SER:H	1.84	0.84
2:B:83:PHE:CE1	2:B:169:GLN:HG3	2.13	0.84
2:B:524:HIS:O	2:B:528:TYR:HD1	1.59	0.84
2:B:799:ARG:HH11	2:B:799:ARG:HG3	1.40	0.84
1:A:574:LEU:CD2	1:A:577:ARG:HG3	2.07	0.84
2:B:330:ALA:H	2:B:450:GLU:CD	1.82	0.84
2:B:680:LYS:NZ	2:B:737:TYR:OH	2.10	0.84
2:B:838:ARG:NH2	2:B:932:SER:CB	2.33	0.84
2:B:7:GLN:NE2	2:B:76:ASP:OD2	2.11	0.84
2:B:117:ARG:NH2	2:B:155:GLU:OE2	2.11	0.84
1:A:421:GLY:O	1:A:422:ILE:HD12	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:HIS:CD2	1:A:617:PRO:HG2	2.12	0.84
1:A:79:GLU:HA	1:A:856:THR:HG23	1.55	0.84
1:A:442:ALA:HA	1:A:509:VAL:HG11	1.58	0.84
2:B:332:PRO:HG3	2:B:399:PHE:CE2	1.99	0.84
1:A:290:GLN:HB2	1:A:413:GLN:HE21	1.40	0.83
1:A:584:SER:O	1:A:585:SER:OG	1.96	0.83
1:A:877:SER:O	1:A:881:SER:OG	1.96	0.83
2:B:523:HIS:HE1	2:B:527:GLN:HE22	0.86	0.83
1:A:950:MET:HE1	2:B:112:THR:CG2	2.08	0.83
2:B:729:ARG:HB3	2:B:754:TYR:CD1	2.13	0.83
1:A:156:THR:HG23	1:A:157:MET:N	1.92	0.83
1:A:690:TRP:HZ3	1:A:721:VAL:CG2	1.91	0.83
1:A:553:THR:HG22	1:A:558:VAL:HG22	1.60	0.83
1:A:973:GLY:H	2:B:791:ILE:HD12	1.41	0.83
1:A:231:THR:CG2	1:A:333:TRP:NE1	2.29	0.83
1:A:316:LEU:HD22	1:A:350:TYR:HE1	1.38	0.83
1:A:380:CYS:HG	1:A:435:GLN:HA	1.44	0.83
1:A:788:ILE:O	1:A:820:CYS:HB2	1.77	0.83
2:B:499:TYR:CE1	2:B:901:LEU:HD22	2.13	0.83
1:A:900:HIS:O	1:A:903:LEU:N	2.11	0.83
1:A:273:LEU:HD23	1:A:281:VAL:CG2	2.07	0.83
1:A:622:GLN:HB2	1:A:623:LEU:HD22	1.57	0.83
2:B:5:SER:HB3	2:B:76:ASP:O	1.78	0.83
2:B:446:ARG:HH11	2:B:446:ARG:HG3	1.43	0.83
2:B:1003:TYR:CE2	2:B:1005:LYS:NZ	2.47	0.83
1:A:230:LEU:HD12	1:A:232:TRP:CH2	2.14	0.83
1:A:249:PRO:HG2	1:A:252:TRP:CD1	2.09	0.83
1:A:690:TRP:CZ3	1:A:721:VAL:HG21	2.14	0.83
2:B:198:MET:HA	2:B:204:GLN:HE21	1.44	0.83
2:B:606:HIS:CG	2:B:606:HIS:O	2.32	0.83
2:B:623:ILE:HB	2:B:893:ILE:HG13	1.61	0.83
1:A:231:THR:HA	1:A:342:LEU:O	1.77	0.82
1:A:371:LEU:C	1:A:500:MET:HE3	2.03	0.82
1:A:444:MET:O	1:A:449:ILE:HG22	1.78	0.82
1:A:463:HIS:O	1:A:463:HIS:ND1	2.09	0.82
2:B:467:GLN:HE21	2:B:467:GLN:C	1.87	0.82
1:A:249:PRO:HG3	1:A:252:TRP:CD1	2.12	0.82
1:A:934:PRO:HB3	2:B:613:LEU:HD12	1.61	0.82
1:A:58:GLN:CG	1:A:860:ILE:CD1	2.57	0.82
1:A:68:PHE:HE1	1:A:71:SER:CB	1.88	0.82
1:A:494:GLY:O	1:A:498:TRP:HB2	1.78	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ALA:CB	2:B:557:LEU:CD2	2.58	0.82
1:A:652:ASN:HD22	1:A:800:HIS:CE1	1.93	0.82
1:A:873:ILE:HD13	1:A:873:ILE:H	1.42	0.82
2:B:214:ARG:HB3	2:B:214:ARG:CZ	2.07	0.82
2:B:673:TRP:CH2	2:B:759:TYR:HD2	1.96	0.82
1:A:368:VAL:HG22	1:A:418:PHE:HB2	1.60	0.82
1:A:507:VAL:HG21	1:A:512:MET:HE3	1.60	0.82
1:A:783:ASP:OD2	1:A:838:PRO:HB3	1.79	0.82
1:A:972:GLU:O	2:B:797:GLY:CA	2.27	0.82
1:A:428:PRO:O	1:A:430:THR:CG2	2.25	0.82
2:B:606:HIS:O	2:B:606:HIS:ND1	2.12	0.82
1:A:192:ALA:O	1:A:196:LEU:HB2	1.80	0.81
1:A:244:ALA:HB3	1:A:274:VAL:CG2	2.09	0.81
1:A:272:ARG:HH21	1:A:272:ARG:CB	1.93	0.81
2:B:794:GLN:HG3	2:B:796:ASP:O	1.79	0.81
1:A:105:TRP:HD1	1:A:471:ARG:NH2	1.78	0.81
1:A:635:GLY:HA2	1:A:640:MET:HE3	1.63	0.81
1:A:892:CYS:SG	2:B:902:GLN:OE1	2.37	0.81
1:A:921:ASP:CB	2:B:626:ALA:HB1	2.10	0.81
2:B:257:PHE:CE1	2:B:357:HIS:NE2	2.48	0.81
2:B:433:TRP:CD1	2:B:518:GLN:CG	2.64	0.81
2:B:502:VAL:HG12	2:B:901:LEU:HD12	1.60	0.81
2:B:549:LYS:HA	2:B:550:MET:CE	2.08	0.81
2:B:576:TYR:HE1	2:B:578:PHE:CE1	1.89	0.81
1:A:39:ILE:CG2	1:A:507:VAL:CG1	2.56	0.81
1:A:807:MET:CE	1:A:810:MET:HE2	2.10	0.81
1:A:36:GLY:O	1:A:505:GLY:HA3	1.80	0.81
1:A:677:ILE:HG13	1:A:678:THR:H	1.44	0.81
1:A:972:GLU:HB3	1:A:973:GLY:HA3	1.61	0.81
1:A:221:ASN:OD1	1:A:431:PHE:HZ	1.62	0.81
1:A:384:LEU:C	1:A:385:LEU:CD1	2.53	0.81
2:B:198:MET:CA	2:B:204:GLN:HE21	1.93	0.81
2:B:231:ILE:HD12	2:B:397:LEU:HD12	1.60	0.81
2:B:343:LEU:CD2	2:B:373:THR:CG2	2.57	0.81
2:B:120:LEU:HD12	2:B:152:VAL:HB	1.61	0.81
2:B:622:LEU:H	2:B:622:LEU:HD12	1.46	0.81
1:A:58:GLN:HG3	1:A:860:ILE:HD12	1.63	0.81
1:A:201:MET:CE	1:A:465:VAL:HG11	2.02	0.81
1:A:512:MET:C	2:B:188:GLY:HA3	2.06	0.81
2:B:224:LEU:HD21	2:B:401:LEU:HD23	1.63	0.81
2:B:729:ARG:HG2	2:B:729:ARG:HH11	1.45	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:LEU:HD22	2:B:735:HIS:N	1.94	0.81
1:A:433:LYS:HD2	1:A:437:ALA:CB	2.11	0.81
1:A:39:ILE:HD11	2:B:988:VAL:O	1.81	0.80
2:B:114:ASN:HB3	2:B:119:TYR:CE2	2.16	0.80
2:B:546:MET:CE	2:B:546:MET:HA	2.11	0.80
2:B:623:ILE:CD1	2:B:893:ILE:HD11	2.11	0.80
2:B:659:ILE:CD1	2:B:788:LEU:HD22	2.11	0.80
1:A:650:ALA:HB3	1:A:796:SER:HA	1.63	0.80
1:A:728:ARG:HD3	1:A:730:THR:HG22	1.61	0.80
2:B:198:MET:HG3	2:B:204:GLN:HE22	1.45	0.80
1:A:355:THR:O	1:A:418:PHE:CD1	2.30	0.80
1:A:372:LYS:H	1:A:500:MET:HE3	0.68	0.80
2:B:12:ARG:NH1	2:B:991:ASP:OD1	2.15	0.80
2:B:433:TRP:CG	2:B:434:MET:N	2.36	0.80
2:B:673:TRP:N	2:B:754:TYR:HE2	1.79	0.80
2:B:7:GLN:HE22	2:B:76:ASP:CB	1.95	0.80
2:B:89:ASP:CB	2:B:410:GLN:OE1	2.29	0.80
2:B:202:VAL:O	2:B:205:GLU:N	2.15	0.80
2:B:265:PRO:HD2	2:B:266:HIS:H	1.47	0.80
2:B:549:LYS:O	2:B:550:MET:HE3	1.80	0.80
1:A:105:TRP:NE1	1:A:471:ARG:HH12	1.78	0.80
1:A:634:ILE:HD11	1:A:718:ARG:HH21	1.46	0.80
1:A:669:ILE:O	1:A:670:ALA:C	2.25	0.80
1:A:777:LEU:HD22	1:A:834:MET:CE	2.10	0.80
1:A:697:ASN:HB2	1:A:701:SER:HB2	1.63	0.80
1:A:865:ARG:HH11	2:B:447:PRO:CG	1.94	0.80
1:A:932:ARG:HB2	1:A:933:PRO:CD	2.11	0.80
1:A:314:THR:O	1:A:347:LYS:HE3	1.80	0.79
1:A:399:VAL:HG13	1:A:464:MET:HE3	1.64	0.79
1:A:948:PHE:CZ	1:A:950:MET:HE3	2.17	0.79
1:A:972:GLU:O	2:B:798:GLY:N	2.15	0.79
2:B:647:LEU:H	2:B:647:LEU:HD12	1.46	0.79
1:A:29:MET:HE2	1:A:135:CYS:HG	1.27	0.79
1:A:88:THR:HG22	1:A:90:MET:N	1.97	0.79
1:A:776:VAL:CG1	1:A:807:MET:CE	2.44	0.79
2:B:509:ILE:CG2	2:B:512:GLY:HA2	2.12	0.79
1:A:185:ASN:OD1	1:A:187:ASP:N	2.15	0.79
1:A:220:GLU:HG3	2:B:186:TRP:CZ2	2.17	0.79
1:A:238:HIS:CE1	1:A:334:LYS:HG2	2.18	0.79
1:A:55:LEU:CG	1:A:528:MET:HE1	1.83	0.79
1:A:455:HIS:HA	1:A:458:ILE:CG2	2.12	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:GLY:O	1:A:735:PRO:HG2	1.82	0.79
1:A:598:TRP:C	1:A:600:SER:N	2.39	0.79
1:A:713:LEU:CG	1:A:714:ASN:H	1.95	0.79
2:B:550:MET:O	2:B:551:VAL:C	2.23	0.79
1:A:961:LEU:HD11	2:B:284:MET:CG	2.12	0.79
1:A:371:LEU:HA	1:A:500:MET:HE2	0.79	0.79
2:B:658:THR:CG2	2:B:695:VAL:HG21	2.12	0.79
1:A:244:ALA:HB3	1:A:274:VAL:HG23	1.63	0.79
1:A:508:SER:O	1:A:510:HIS:N	2.15	0.79
1:A:532:ALA:CB	1:A:597:VAL:HG21	2.12	0.79
1:A:652:ASN:ND2	1:A:800:HIS:HE1	1.58	0.79
2:B:260:LYS:HD2	2:B:260:LYS:O	1.82	0.79
1:A:58:GLN:HA	1:A:58:GLN:NE2	1.96	0.79
2:B:318:THR:HG22	2:B:319:THR:OG1	1.83	0.79
1:A:286:ASP:OD1	1:A:287:GLY:N	2.16	0.79
1:A:65:LEU:HD12	1:A:65:LEU:O	1.83	0.78
1:A:790:PRO:HG3	1:A:819:ASP:CB	2.14	0.78
2:B:708:GLU:OE1	2:B:770:ASP:OD1	2.00	0.78
1:A:55:LEU:O	1:A:55:LEU:HD23	1.82	0.78
1:A:217:GLU:O	1:A:218:LEU:HD23	1.83	0.78
1:A:740:GLU:O	1:A:741:ALA:C	2.23	0.78
2:B:7:GLN:NE2	2:B:76:ASP:CB	2.46	0.78
2:B:400:ALA:O	2:B:404:MET:HB2	1.82	0.78
2:B:645:GLY:N	2:B:809:GLU:O	2.14	0.78
2:B:729:ARG:O	2:B:730:ARG:HG2	1.83	0.78
1:A:690:TRP:HZ3	1:A:721:VAL:HG21	1.45	0.78
1:A:81:ILE:CD1	1:A:98:GLU:HB2	2.12	0.78
1:A:111:ASN:CG	1:A:467:GLN:HG3	2.09	0.78
1:A:519:LEU:C	1:A:519:LEU:HD23	2.08	0.78
2:B:12:ARG:NH1	2:B:991:ASP:CG	2.38	0.78
2:B:186:TRP:HH2	2:B:212:VAL:O	1.66	0.78
1:A:316:LEU:HD23	1:A:350:TYR:CE1	2.19	0.78
1:A:702:LYS:HZ1	1:A:707:ILE:HG12	1.49	0.78
1:A:815:ILE:O	1:A:816:THR:OG1	2.00	0.78
2:B:163:GLY:O	2:B:442:PRO:CA	2.31	0.78
2:B:648:VAL:HG11	2:B:653:VAL:HG21	1.64	0.78
1:A:353:MET:HG3	1:A:354:SER:N	1.97	0.78
1:A:906:ALA:O	1:A:907:VAL:HG13	1.84	0.78
2:B:241:SER:CB	2:B:390:ARG:HG2	2.14	0.78
1:A:238:HIS:ND1	1:A:334:LYS:CG	2.46	0.78
1:A:353:MET:O	1:A:355:THR:HG23	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:ASP:CG	1:A:739:ALA:CB	2.49	0.78
1:A:546:ALA:HB1	1:A:681:ALA:O	1.83	0.78
1:A:752:LYS:CE	1:A:857:ASP:OD2	2.32	0.78
2:B:990:HIS:HB3	2:B:992:TYR:CE1	2.19	0.78
1:A:756:ARG:NH1	1:A:851:HIS:CD2	2.52	0.78
1:A:802:ARG:HG3	1:A:802:ARG:HH21	1.49	0.78
2:B:189:ALA:O	2:B:190:SER:CB	2.31	0.78
2:B:257:PHE:HE1	2:B:357:HIS:CE1	2.02	0.78
2:B:263:LEU:O	2:B:263:LEU:HD13	1.84	0.78
2:B:558:ALA:O	2:B:562:LEU:HB2	1.84	0.78
1:A:425:ARG:C	1:A:426:MET:SD	2.67	0.77
1:A:692:ALA:HB2	1:A:722:HIS:O	1.80	0.77
1:A:713:LEU:HD23	1:A:714:ASN:CA	2.13	0.77
1:A:802:ARG:HG2	1:A:803:GLY:N	1.99	0.77
2:B:523:HIS:HE1	2:B:527:GLN:NE2	1.62	0.77
1:A:435:GLN:HE21	1:A:435:GLN:C	1.93	0.77
1:A:106:LEU:HD12	1:A:470:VAL:HG12	1.65	0.77
1:A:344:ILE:HD11	1:A:396:LEU:HD11	1.66	0.77
1:A:455:HIS:O	1:A:458:ILE:HG22	1.85	0.77
1:A:704:ILE:C	1:A:707:ILE:HD12	2.10	0.77
1:A:807:MET:O	1:A:810:MET:N	2.17	0.77
1:A:449:ILE:HG23	1:A:449:ILE:O	1.85	0.77
2:B:263:LEU:HD22	2:B:264:THR:N	1.98	0.77
2:B:673:TRP:HZ3	2:B:755:MET:CE	1.82	0.77
1:A:125:MET:HE1	1:A:186:ASN:ND2	1.98	0.77
1:A:127:PHE:HE1	1:A:452:ARG:HE	1.32	0.77
1:A:253:LEU:HD21	1:A:628:SER:HB3	1.63	0.77
2:B:722:GLU:HG3	2:B:729:ARG:NH2	1.99	0.77
1:A:75:LEU:CD1	1:A:106:LEU:HD22	2.15	0.77
1:A:248:VAL:HG11	1:A:630:PHE:CE1	2.20	0.77
1:A:463:HIS:CD2	1:A:617:PRO:CG	2.68	0.77
1:A:776:VAL:HG11	1:A:807:MET:HE3	1.66	0.77
2:B:618:LEU:CD1	2:B:623:ILE:HD11	2.14	0.77
2:B:753:PRO:HG2	2:B:756:ARG:HH12	1.49	0.77
1:A:154:THR:O	1:A:158:ASN:N	2.11	0.76
1:A:309:TRP:CD1	1:A:309:TRP:N	2.53	0.76
1:A:704:ILE:O	1:A:707:ILE:HD12	1.84	0.76
1:A:964:VAL:CG1	2:B:788:LEU:CD1	2.59	0.76
2:B:500:GLN:HG3	2:B:560:TRP:CZ2	2.20	0.76
1:A:455:HIS:HA	1:A:458:ILE:HG22	1.65	0.76
1:A:692:ALA:HA	1:A:722:HIS:O	1.84	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:ALA:HB1	2:B:557:LEU:CD2	2.15	0.76
2:B:48:ALA:O	2:B:49:THR:OG1	2.03	0.76
2:B:533:TYR:O	2:B:534:ALA:HB3	1.85	0.76
1:A:368:VAL:CG2	1:A:418:PHE:HB2	2.14	0.76
1:A:558:VAL:O	1:A:562:LEU:CD2	2.32	0.76
1:A:844:GLY:O	1:A:849:ASP:OD1	2.02	0.76
2:B:454:ARG:HD3	2:B:466:LEU:HD11	1.67	0.76
1:A:234:LEU:HD21	1:A:266:PHE:HZ	1.50	0.76
1:A:268:GLU:OE2	1:A:693:THR:CG2	2.31	0.76
1:A:387:ASN:HD22	1:A:391:GLY:HA2	1.49	0.76
1:A:894:ARG:NE	1:A:902:MET:HE2	1.99	0.76
2:B:838:ARG:HH11	2:B:838:ARG:HG3	1.50	0.76
1:A:254:ASP:HA	1:A:556:HIS:NE2	1.53	0.76
1:A:589:LEU:CD1	1:A:589:LEU:H	1.98	0.76
1:A:262:ARG:CZ	1:A:401:GLY:HA3	2.16	0.76
1:A:477:SER:O	1:A:478:LEU:HD12	1.85	0.76
2:B:51:LEU:HD22	2:B:52:PRO:HD2	1.68	0.76
2:B:194:ILE:HG21	2:B:200:GLN:CA	2.13	0.76
2:B:293:ALA:CB	2:B:298:ARG:O	2.33	0.76
1:A:801:LEU:HD21	1:A:813:LEU:CD2	2.17	0.76
1:A:352:ARG:HG2	1:A:352:ARG:NH1	1.95	0.75
1:A:788:ILE:CD1	1:A:823:VAL:HG21	2.15	0.75
2:B:433:TRP:CD1	2:B:518:GLN:HG2	2.20	0.75
1:A:894:ARG:HE	1:A:902:MET:HE2	1.50	0.75
1:A:934:PRO:HB2	2:B:613:LEU:CD1	2.10	0.75
2:B:224:LEU:HD23	2:B:404:MET:SD	2.27	0.75
1:A:367:ILE:CD1	1:A:415:GLN:HE21	0.31	0.75
1:A:380:CYS:SG	1:A:434:ALA:C	2.70	0.75
1:A:660:ASN:HD22	1:A:661:GLU:N	1.84	0.75
1:A:109:GLY:CA	1:A:233:GLU:O	2.32	0.75
1:A:435:GLN:C	1:A:439:ALA:HB3	2.11	0.75
1:A:740:GLU:OE1	1:A:740:GLU:N	2.19	0.75
1:A:836:THR:O	1:A:837:SER:OG	2.04	0.75
2:B:546:MET:HE2	2:B:546:MET:CA	2.16	0.75
2:B:658:THR:HG22	2:B:695:VAL:HG21	1.68	0.75
1:A:222:ASP:OD1	1:A:223:ALA:N	2.20	0.75
1:A:555:VAL:HG12	1:A:687:THR:CG2	2.17	0.75
1:A:668:PHE:CD2	1:A:686:GLY:HA3	2.17	0.75
2:B:458:ASN:ND2	2:B:463:SER:O	2.20	0.75
2:B:764:LEU:O	2:B:769:ASN:ND2	2.20	0.75
2:B:832:HIS:O	2:B:937:VAL:HB	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:VAL:H	1:A:687:THR:HG21	1.51	0.75
2:B:211:ARG:O	2:B:323:ASN:OD1	2.04	0.75
2:B:749:THR:O	2:B:750:GLU:C	2.29	0.75
1:A:19:LYS:HG2	1:A:140:LEU:HD23	1.67	0.75
1:A:81:ILE:HD13	1:A:81:ILE:C	2.12	0.75
1:A:690:TRP:NE1	1:A:712:GLY:C	2.44	0.75
2:B:846:THR:HB	2:B:847:PRO:HD2	1.69	0.75
1:A:262:ARG:HH21	1:A:401:GLY:C	1.73	0.75
1:A:472:ASP:OD2	1:A:739:ALA:HB3	1.85	0.75
1:A:948:PHE:HB3	2:B:149:GLN:HE22	1.49	0.75
2:B:7:GLN:NE2	2:B:76:ASP:HB2	2.00	0.75
1:A:39:ILE:CD1	2:B:988:VAL:O	2.35	0.74
1:A:943:ARG:HH11	1:A:943:ARG:HG3	1.49	0.74
2:B:794:GLN:HG2	2:B:796:ASP:O	1.85	0.74
1:A:81:ILE:HD11	1:A:98:GLU:CB	2.17	0.74
1:A:853:ASP:N	1:A:853:ASP:OD1	2.19	0.74
1:A:892:CYS:SG	2:B:902:GLN:CD	2.70	0.74
2:B:493:GLY:CA	2:B:562:LEU:CD2	2.60	0.74
1:A:894:ARG:CG	1:A:902:MET:HE1	2.04	0.74
2:B:293:ALA:HB1	2:B:298:ARG:O	1.88	0.74
2:B:597:LEU:CD1	2:B:644:ASP:OD1	2.28	0.74
1:A:248:VAL:HG23	1:A:628:SER:HB2	1.70	0.74
1:A:298:VAL:C	1:A:299:HIS:HD2	1.91	0.74
1:A:314:THR:C	1:A:347:LYS:HZ1	1.93	0.74
1:A:367:ILE:HD13	1:A:415:GLN:NE2	1.39	0.74
1:A:690:TRP:HE1	1:A:712:GLY:C	1.95	0.74
2:B:551:VAL:HG13	2:B:579:GLY:HA3	1.68	0.74
1:A:367:ILE:CD1	1:A:415:GLN:NE2	0.72	0.74
1:A:444:MET:HB3	1:A:449:ILE:HG21	1.67	0.74
1:A:887:PRO:C	1:A:893:VAL:HG11	2.11	0.74
2:B:198:MET:CE	2:B:458:ASN:O	2.34	0.74
2:B:216:SER:HB3	2:B:447:PRO:O	1.86	0.74
2:B:216:SER:C	2:B:448:MET:HB3	2.11	0.74
2:B:618:LEU:HD13	2:B:623:ILE:CD1	2.16	0.74
1:A:508:SER:CB	2:B:992:TYR:CE2	2.70	0.74
1:A:704:ILE:O	1:A:707:ILE:CD1	2.36	0.74
2:B:354:GLY:O	2:B:687:ALA:HB1	1.88	0.74
2:B:647:LEU:HD12	2:B:647:LEU:N	2.02	0.74
1:A:290:GLN:HB3	1:A:413:GLN:HE22	1.49	0.74
2:B:659:ILE:CD1	2:B:788:LEU:HD23	2.00	0.74
1:A:117:VAL:HG23	1:A:485:VAL:CG2	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:PRO:HG3	2:B:610:ASP:HB3	1.70	0.74
1:A:8:ARG:O	1:A:11:GLY:N	2.18	0.74
1:A:82:THR:HG23	1:A:82:THR:O	1.87	0.74
1:A:111:ASN:HB2	1:A:467:GLN:HB2	1.69	0.74
2:B:794:GLN:OE1	2:B:805:HIS:ND1	2.20	0.74
2:B:673:TRP:CH2	2:B:677:HIS:HE1	2.06	0.73
1:A:639:GLN:CA	1:A:639:GLN:HE21	2.01	0.73
1:A:788:ILE:CD1	1:A:823:VAL:CG2	2.64	0.73
1:A:885:LEU:HD22	1:A:885:LEU:N	2.02	0.73
2:B:78:LEU:HD22	2:B:180:LEU:CD2	2.17	0.73
2:B:329:LEU:HD12	2:B:450:GLU:HG2	1.68	0.73
2:B:331:LEU:CD1	2:B:373:THR:HG22	2.17	0.73
1:A:202:HIS:ND1	1:A:202:HIS:O	2.21	0.73
2:B:32:LYS:HG2	2:B:69:GLU:OE1	1.88	0.73
1:A:72:ARG:O	1:A:863:VAL:HG12	1.87	0.73
1:A:249:PRO:HG2	1:A:252:TRP:CD2	2.11	0.73
1:A:202:HIS:HD2	1:A:346:LEU:HD21	1.51	0.73
1:A:541:GLY:HA3	1:A:733:SER:O	1.88	0.73
1:A:671:LEU:O	1:A:671:LEU:CG	2.34	0.73
2:B:263:LEU:HD22	2:B:263:LEU:C	2.14	0.73
1:A:51:LEU:HD21	1:A:62:ASN:HB2	1.69	0.73
1:A:55:LEU:HD12	1:A:528:MET:CE	1.22	0.73
1:A:214:ARG:HD3	1:A:214:ARG:N	1.97	0.73
1:A:577:ARG:NE	1:A:614:ALA:O	2.21	0.73
2:B:293:ALA:HA	2:B:298:ARG:O	1.87	0.73
2:B:310:LEU:O	2:B:310:LEU:HD23	1.88	0.73
1:A:868:TYR:OH	2:B:772:PHE:HD2	1.68	0.73
2:B:708:GLU:HA	2:B:708:GLU:OE2	1.87	0.73
2:B:838:ARG:NH2	2:B:932:SER:HG	1.86	0.73
1:A:833:ARG:HH11	1:A:833:ARG:HG3	1.51	0.73
2:B:84:THR:HG21	2:B:545:ARG:NH1	2.03	0.73
1:A:19:LYS:HA	1:A:140:LEU:CD2	2.17	0.73
1:A:39:ILE:HG12	1:A:506:SER:OG	1.89	0.73
1:A:211:VAL:CG2	1:A:216:GLN:HG3	2.18	0.73
1:A:598:TRP:O	1:A:599:SER:C	2.32	0.73
2:B:500:GLN:HA	2:B:500:GLN:NE2	2.02	0.73
1:A:170:LEU:HD13	1:A:170:LEU:C	2.12	0.73
1:A:948:PHE:CB	2:B:149:GLN:HE22	2.01	0.73
2:B:165:THR:CA	2:B:546:MET:CE	2.61	0.73
2:B:198:MET:O	2:B:204:GLN:CB	2.36	0.73
1:A:309:TRP:HE3	1:A:343:THR:CG2	1.98	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:TYR:CE2	2:B:860:MET:HG2	2.23	0.72
2:B:524:HIS:O	2:B:528:TYR:CD1	2.42	0.72
1:A:342:LEU:HD23	1:A:343:THR:N	2.04	0.72
1:A:477:SER:O	1:A:478:LEU:CD1	2.37	0.72
1:A:668:PHE:CZ	1:A:728:ARG:NH1	2.57	0.72
1:A:854:ILE:H	1:A:854:ILE:HD12	1.53	0.72
2:B:141:TYR:HB2	2:B:922:GLY:HA3	1.70	0.72
2:B:293:ALA:CA	2:B:298:ARG:O	2.37	0.72
2:B:307:LYS:HG2	2:B:311:ARG:NH2	2.04	0.72
1:A:455:HIS:CA	1:A:458:ILE:HG22	2.20	0.72
1:A:740:GLU:O	1:A:743:ALA:N	2.22	0.72
1:A:702:LYS:NZ	1:A:707:ILE:HG12	2.05	0.72
1:A:238:HIS:CD2	1:A:338:SER:HA	2.24	0.72
1:A:702:LYS:NZ	1:A:707:ILE:CG1	2.53	0.72
2:B:515:THR:HG21	2:B:656:TYR:HE2	1.55	0.72
2:B:659:ILE:HD12	2:B:788:LEU:HD22	1.72	0.72
1:A:107:HIS:HD2	1:A:236:CYS:O	1.71	0.72
1:A:254:ASP:N	1:A:556:HIS:NE2	2.36	0.72
1:A:574:LEU:CD2	1:A:577:ARG:HD3	2.20	0.72
1:A:634:ILE:HB	1:A:688:GLU:CB	2.19	0.72
1:A:894:ARG:CB	1:A:902:MET:HE2	2.06	0.72
1:A:352:ARG:CA	1:A:382:GLU:OE1	2.36	0.72
1:A:444:MET:HB3	1:A:449:ILE:CG2	2.18	0.72
1:A:634:ILE:CG2	1:A:688:GLU:CG	2.68	0.72
1:A:23:ARG:HH11	1:A:23:ARG:HG3	1.54	0.71
2:B:493:GLY:HA3	2:B:562:LEU:HD23	1.72	0.71
2:B:797:GLY:O	2:B:799:ARG:N	2.23	0.71
1:A:606:THR:HG23	1:A:609:TYR:H	1.54	0.71
2:B:89:ASP:OD1	2:B:89:ASP:N	2.22	0.71
2:B:114:ASN:HB3	2:B:119:TYR:CD2	2.25	0.71
1:A:280:CYS:HA	1:A:332:LEU:O	1.90	0.71
1:A:646:LEU:HD23	1:A:646:LEU:C	2.15	0.71
1:A:802:ARG:HG3	1:A:802:ARG:NH2	2.04	0.71
2:B:121:GLY:CA	2:B:150:CYS:O	2.38	0.71
2:B:747:ALA:HB3	2:B:749:THR:HG23	1.71	0.71
1:A:934:PRO:CB	2:B:613:LEU:CD1	2.64	0.71
1:A:23:ARG:HG3	1:A:23:ARG:NH1	2.04	0.71
2:B:327:TYR:HB2	2:B:368:GLY:O	1.89	0.71
2:B:726:SER:HB2	2:B:727:PRO:HD3	1.71	0.71
2:B:355:ALA:HB3	2:B:358:ALA:HB2	1.72	0.71
1:A:380:CYS:SG	1:A:439:ALA:HB2	2.30	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:490:PHE:O	1:A:492:VAL:HG23	1.90	0.71
1:A:646:LEU:HD12	1:A:681:ALA:HB2	1.72	0.71
2:B:735:HIS:ND1	2:B:735:HIS:O	2.24	0.71
1:A:6:GLN:HE21	1:A:6:GLN:CA	2.00	0.71
1:A:664:CYS:HB2	1:A:737:GLY:C	2.15	0.71
2:B:329:LEU:HG	2:B:450:GLU:OE2	1.90	0.71
1:A:280:CYS:HB3	1:A:333:TRP:HB3	1.72	0.71
1:A:273:LEU:O	1:A:273:LEU:HD13	1.90	0.71
1:A:371:LEU:CD1	1:A:419:LEU:HD13	2.21	0.71
2:B:84:THR:CG2	2:B:545:ARG:HH11	2.02	0.71
2:B:497:ALA:HB1	2:B:557:LEU:HD21	1.72	0.71
1:A:117:VAL:CG2	1:A:485:VAL:CG2	2.69	0.70
2:B:165:THR:CA	2:B:546:MET:HE1	2.21	0.70
2:B:322:GLU:HA	2:B:328:LEU:HD11	1.73	0.70
2:B:332:PRO:HG2	2:B:399:PHE:CZ	2.15	0.70
2:B:555:ASN:ND2	2:B:569:PHE:HB3	2.05	0.70
1:A:367:ILE:CD1	1:A:415:GLN:CG	2.69	0.70
1:A:455:HIS:C	1:A:458:ILE:HG22	2.16	0.70
2:B:104:CYS:HB3	2:B:830:THR:HB	1.73	0.70
2:B:445:SER:O	2:B:447:PRO:HD3	1.91	0.70
1:A:81:ILE:CD1	1:A:98:GLU:CB	2.69	0.70
1:A:193:PHE:HZ	1:A:464:MET:CE	2.04	0.70
2:B:713:ARG:O	2:B:716:ALA:O	2.08	0.70
1:A:35:ALA:O	1:A:42:GLY:CA	2.40	0.70
1:A:481:LEU:HD22	1:A:481:LEU:N	2.03	0.70
1:A:898:THR:HG22	2:B:858:PRO:HB3	1.74	0.70
1:A:901:SER:OG	2:B:500:GLN:CD	2.34	0.70
2:B:556:ALA:HA	2:B:566:MET:HE1	1.73	0.70
1:A:367:ILE:HD13	1:A:415:GLN:CG	2.20	0.70
2:B:559:ALA:O	2:B:564:SER:HA	1.90	0.70
2:B:708:GLU:OE2	2:B:711:ARG:NH1	2.24	0.70
1:A:518:LEU:O	1:A:518:LEU:HD23	1.91	0.70
1:A:576:LEU:HB2	1:A:614:ALA:HB1	1.72	0.70
1:A:646:LEU:HB2	1:A:669:ILE:HD13	1.73	0.70
1:A:833:ARG:HG2	1:A:833:ARG:O	1.90	0.70
2:B:257:PHE:HD1	2:B:357:HIS:NE2	1.88	0.70
2:B:343:LEU:CD2	2:B:373:THR:HG23	2.16	0.70
2:B:354:GLY:O	2:B:687:ALA:CB	2.39	0.70
2:B:673:TRP:CH2	2:B:759:TYR:CD2	2.79	0.70
1:A:328:GLU:HB3	1:A:390:PHE:CE2	2.26	0.70
1:A:507:VAL:HG21	1:A:512:MET:CE	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ALA:HA	1:A:594:MET:HE3	1.72	0.70
1:A:639:GLN:HE21	1:A:639:GLN:C	2.00	0.70
1:A:650:ALA:CB	1:A:796:SER:OG	2.40	0.70
2:B:623:ILE:HD13	2:B:893:ILE:HD11	1.72	0.70
2:B:794:GLN:NE2	2:B:796:ASP:O	2.24	0.70
1:A:623:LEU:HD22	1:A:623:LEU:N	2.07	0.70
2:B:659:ILE:CD1	2:B:788:LEU:HD21	2.20	0.70
2:B:510:THR:HG22	2:B:632:THR:CG2	2.22	0.70
1:A:111:ASN:OD1	1:A:467:GLN:CG	2.34	0.69
1:A:211:VAL:HG22	1:A:216:GLN:CB	2.22	0.69
1:A:742:MET:HA	1:A:742:MET:CE	2.21	0.69
2:B:442:PRO:O	2:B:576:TYR:CZ	2.45	0.69
1:A:432:THR:CG2	1:A:433:LYS:N	2.52	0.69
1:A:892:CYS:HB2	2:B:905:PRO:HG3	1.73	0.69
2:B:32:LYS:CG	2:B:69:GLU:OE1	2.40	0.69
2:B:83:PHE:HE1	2:B:169:GLN:HG3	1.57	0.69
1:A:690:TRP:CD1	1:A:690:TRP:H	2.09	0.69
1:A:752:LYS:NZ	1:A:857:ASP:OD2	2.24	0.69
2:B:36:GLU:O	2:B:65:GLU:HG2	1.91	0.69
1:A:639:GLN:HE21	1:A:639:GLN:H	1.41	0.69
2:B:163:GLY:CA	2:B:548:ASN:HB3	2.18	0.69
2:B:433:TRP:CD1	2:B:518:GLN:HE21	2.11	0.69
1:A:442:ALA:CA	1:A:509:VAL:CG1	2.70	0.69
2:B:7:GLN:CG	2:B:29:VAL:CG1	2.67	0.69
2:B:66:ARG:NH1	2:B:66:ARG:HG3	2.03	0.69
2:B:673:TRP:HE3	2:B:755:MET:CE	1.75	0.69
2:B:3:ALA:O	2:B:79:ARG:HG3	1.92	0.69
2:B:219:GLN:O	2:B:327:TYR:OH	2.11	0.69
2:B:767:ALA:C	2:B:768:ARG:HG3	2.17	0.69
1:A:232:TRP:CZ3	1:A:344:ILE:HG22	2.27	0.69
1:A:240:LYS:HD3	1:A:240:LYS:N	2.08	0.69
1:A:260:THR:CG2	1:A:263:GLU:OE1	2.41	0.69
1:A:307:MET:C	1:A:309:TRP:CD1	2.71	0.69
1:A:320:SER:HA	1:A:351:HIS:CD2	2.27	0.69
1:A:371:LEU:HD12	1:A:419:LEU:HD13	1.75	0.69
1:A:380:CYS:SG	1:A:435:GLN:N	2.65	0.69
1:A:486:ASN:OD1	1:A:486:ASN:N	2.22	0.69
1:A:873:ILE:HD13	1:A:873:ILE:N	2.07	0.69
2:B:34:THR:HG23	2:B:980:ASN:OD1	1.91	0.69
2:B:405:ALA:O	2:B:406:ASP:C	2.34	0.69
1:A:239:GLY:C	1:A:240:LYS:HD3	2.18	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:CG1	1:A:553:THR:HG21	2.20	0.69
1:A:555:VAL:HG12	1:A:687:THR:HG21	1.75	0.69
1:A:690:TRP:HE1	1:A:713:LEU:N	1.91	0.69
1:A:244:ALA:HB1	1:A:274:VAL:HG23	1.74	0.69
1:A:529:ALA:HB1	1:A:594:MET:HE3	1.73	0.69
1:A:888:TYR:O	1:A:894:ARG:CZ	2.40	0.69
2:B:161:LEU:O	2:B:161:LEU:HD13	1.93	0.69
2:B:198:MET:HA	2:B:204:GLN:NE2	2.07	0.69
2:B:428:CYS:SG	2:B:818:HIS:CD2	2.86	0.69
1:A:634:ILE:HG22	1:A:688:GLU:HG3	1.73	0.68
2:B:112:THR:O	2:B:119:TYR:HB2	1.93	0.68
1:A:957:PHE:CE2	2:B:279:TYR:HE1	2.11	0.68
1:A:967:GLN:O	1:A:968:MET:C	2.36	0.68
2:B:673:TRP:CH2	2:B:677:HIS:CE1	2.81	0.68
2:B:999:LEU:O	2:B:1000:ALA:HB2	1.92	0.68
1:A:309:TRP:CZ3	1:A:343:THR:HG21	2.28	0.68
1:A:449:ILE:CG1	1:A:453:THR:HG21	2.22	0.68
1:A:639:GLN:HE21	1:A:639:GLN:N	1.91	0.68
2:B:502:VAL:HG12	2:B:901:LEU:HD13	1.68	0.68
2:B:576:TYR:HD1	2:B:578:PHE:CE1	1.92	0.68
2:B:600:TYR:CE2	2:B:618:LEU:HD11	2.28	0.68
2:B:665:GLY:C	2:B:667:GLN:H	2.00	0.68
1:A:329:HIS:CD2	1:A:348:GLN:NE2	2.61	0.68
1:A:55:LEU:CD1	1:A:528:MET:HE1	1.16	0.68
1:A:79:GLU:CA	1:A:856:THR:HG23	1.92	0.68
2:B:442:PRO:HD2	2:B:576:TYR:CE1	2.29	0.68
2:B:589:TYR:CE1	2:B:808:GLY:CA	2.64	0.68
1:A:655:TYR:CE1	1:A:666:VAL:HG12	2.29	0.68
1:A:925:VAL:HG12	1:A:926:THR:N	2.08	0.68
1:A:42:GLY:CA	1:A:445:ARG:HH22	2.06	0.68
1:A:399:VAL:O	1:A:403:THR:HG23	1.92	0.68
1:A:650:ALA:O	1:A:796:SER:OG	2.09	0.68
2:B:89:ASP:HB3	2:B:410:GLN:OE1	1.94	0.68
2:B:726:SER:CB	2:B:727:PRO:HD3	2.24	0.68
1:A:618:PHE:C	1:A:619:VAL:HG13	2.19	0.68
1:A:865:ARG:NH1	2:B:447:PRO:CG	2.56	0.68
1:A:27:LYS:CG	1:A:28:ASP:OD1	2.42	0.68
1:A:307:MET:O	1:A:309:TRP:NE1	2.26	0.68
1:A:533:HIS:O	1:A:537:GLN:HG2	1.93	0.68
1:A:619:VAL:HG23	1:A:620:ASP:N	2.09	0.68
2:B:199:LEU:HG	2:B:456:VAL:CG2	2.24	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ALA:HB1	1:A:137:PRO:HB3	1.74	0.67
1:A:258:GLN:HG2	1:A:258:GLN:O	1.94	0.67
1:A:671:LEU:HB2	1:A:685:ILE:HG22	1.75	0.67
2:B:510:THR:O	2:B:511:ASP:HB2	1.92	0.67
1:A:273:LEU:CD2	1:A:281:VAL:HG23	2.20	0.67
1:A:275:ASP:CG	1:A:276:PRO:HD2	2.14	0.67
1:A:452:ARG:NH2	1:A:452:ARG:HG3	2.07	0.67
1:A:481:LEU:CD1	1:A:624:ALA:HB2	2.24	0.67
1:A:588:ALA:HB1	1:A:592:GLN:OE1	1.94	0.67
1:A:355:THR:OG1	1:A:417:LEU:O	2.12	0.67
1:A:861:ARG:HH21	2:B:547:ALA:HB2	1.59	0.67
1:A:562:LEU:HD22	1:A:562:LEU:N	2.09	0.67
1:A:634:ILE:CB	1:A:688:GLU:CG	2.65	0.67
2:B:118:PHE:HE2	2:B:950:LEU:HD22	1.58	0.67
2:B:201:THR:OG1	2:B:204:GLN:HG3	1.94	0.67
2:B:256:ASP:CB	2:B:300:VAL:CG1	2.49	0.67
2:B:257:PHE:CE1	2:B:357:HIS:CE1	2.82	0.67
2:B:729:ARG:HG2	2:B:729:ARG:NH1	2.05	0.67
1:A:26:LEU:CD1	1:A:144:THR:HG22	2.24	0.67
1:A:452:ARG:HG3	1:A:452:ARG:HH21	1.58	0.67
2:B:842:ASN:O	2:B:844:THR:O	2.12	0.67
1:A:105:TRP:CD1	1:A:471:ARG:NH2	2.57	0.67
1:A:248:VAL:HG23	1:A:628:SER:CB	2.24	0.67
1:A:352:ARG:NH2	1:A:426:MET:O	2.28	0.67
1:A:664:CYS:HB2	1:A:737:GLY:O	1.94	0.67
1:A:899:LEU:O	1:A:900:HIS:C	2.33	0.67
2:B:263:LEU:CD1	2:B:293:ALA:CB	2.66	0.67
2:B:648:VAL:HG11	2:B:653:VAL:CG2	2.25	0.67
1:A:249:PRO:CG	1:A:252:TRP:NE1	2.43	0.67
1:A:388:SER:O	1:A:391:GLY:N	2.28	0.67
2:B:134:ALA:O	2:B:135:ASP:C	2.33	0.67
1:A:512:MET:HA	2:B:188:GLY:HA3	1.77	0.67
1:A:868:TYR:HH	2:B:772:PHE:HD2	1.31	0.67
2:B:623:ILE:HB	2:B:893:ILE:CG1	2.25	0.67
1:A:553:THR:CG2	1:A:558:VAL:HG22	2.24	0.67
1:A:588:ALA:CB	1:A:592:GLN:CD	2.44	0.67
2:B:78:LEU:HD11	2:B:81:GLU:OE2	1.94	0.67
2:B:194:ILE:HG23	2:B:199:LEU:O	1.95	0.67
1:A:8:ARG:O	1:A:9:ASP:C	2.36	0.66
1:A:760:ILE:HG23	1:A:810:MET:HG2	1.78	0.66
2:B:332:PRO:CD	2:B:399:PHE:CE2	2.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:450:GLU:OE1	2:B:450:GLU:HA	1.95	0.66
1:A:435:GLN:O	1:A:439:ALA:CB	2.35	0.66
1:A:455:HIS:HB2	1:A:615:TYR:HE2	1.59	0.66
1:A:788:ILE:O	1:A:820:CYS:CB	2.43	0.66
2:B:43:THR:HG23	2:B:55:LYS:HD3	1.69	0.66
2:B:45:ILE:C	2:B:53:ILE:CD1	2.67	0.66
2:B:162:SER:OG	2:B:440:LEU:HD11	1.94	0.66
2:B:194:ILE:CG2	2:B:199:LEU:O	2.43	0.66
1:A:690:TRP:CZ3	1:A:721:VAL:CG2	2.75	0.66
1:A:68:PHE:HD1	1:A:71:SER:HB2	1.54	0.66
1:A:894:ARG:C	1:A:902:MET:CE	2.26	0.66
2:B:428:CYS:SG	2:B:818:HIS:HB2	2.36	0.66
1:A:253:LEU:HD11	1:A:630:PHE:HE1	1.61	0.66
1:A:371:LEU:HB3	1:A:500:MET:HE1	1.78	0.66
1:A:380:CYS:HG	1:A:434:ALA:C	2.02	0.66
1:A:514:ILE:HG13	1:A:514:ILE:O	1.94	0.66
1:A:943:ARG:NH1	2:B:616:ALA:O	2.28	0.66
2:B:264:THR:O	2:B:265:PRO:C	2.32	0.66
1:A:103:ARG:HG3	1:A:103:ARG:NH2	2.04	0.66
1:A:191:PHE:O	1:A:192:ALA:C	2.37	0.66
1:A:876:VAL:HG21	1:A:909:LEU:CD1	2.25	0.66
2:B:130:ALA:O	2:B:140:GLU:HA	1.96	0.66
2:B:214:ARG:HB3	2:B:214:ARG:NH1	2.10	0.66
2:B:330:ALA:N	2:B:450:GLU:CD	2.41	0.66
2:B:383:HIS:O	2:B:384:ALA:C	2.39	0.66
2:B:442:PRO:HG2	2:B:576:TYR:CZ	2.30	0.66
1:A:68:PHE:CD1	1:A:71:SER:CB	2.71	0.66
1:A:316:LEU:HD21	1:A:350:TYR:HH	1.59	0.66
1:A:330:TYR:CE2	1:A:397:PRO:HG3	2.30	0.66
1:A:429:ALA:O	1:A:430:THR:HG23	1.95	0.66
2:B:57:GLY:O	2:B:478:HIS:CB	2.42	0.66
2:B:78:LEU:CD1	2:B:81:GLU:OE2	2.44	0.66
1:A:127:PHE:HE2	1:A:189:ARG:HE	0.68	0.66
1:A:205:ALA:HB2	1:A:232:TRP:HE1	1.57	0.66
1:A:525:LEU:HD23	1:A:608:LEU:HD11	1.78	0.66
1:A:908:PRO:HG3	2:B:528:TYR:CE1	2.25	0.66
1:A:921:ASP:OD1	2:B:638:GLU:OE1	2.13	0.66
2:B:38:LYS:NZ	2:B:65:GLU:CD	2.52	0.66
2:B:343:LEU:CD2	2:B:373:THR:HG21	2.23	0.66
1:A:39:ILE:CG2	1:A:507:VAL:HG12	2.15	0.66
1:A:79:GLU:CB	1:A:856:THR:HG21	1.82	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LEU:HG	1:A:311:ASP:H	1.59	0.66
1:A:371:LEU:CB	1:A:500:MET:HE1	2.26	0.66
1:A:529:ALA:CA	1:A:594:MET:HE3	2.19	0.66
1:A:635:GLY:CA	1:A:640:MET:CE	2.68	0.66
1:A:838:PRO:O	1:A:841:HIS:HB3	1.96	0.66
2:B:562:LEU:O	2:B:564:SER:N	2.29	0.66
1:A:333:TRP:NE1	1:A:343:THR:OG1	2.29	0.66
1:A:464:MET:HB3	1:A:483:PHE:CZ	2.31	0.65
1:A:639:GLN:NE2	1:A:639:GLN:O	2.28	0.65
2:B:111:MET:SD	2:B:118:PHE:CD2	2.84	0.65
2:B:499:TYR:HE1	2:B:901:LEU:CD2	2.07	0.65
1:A:209:GLY:HA3	1:A:218:LEU:HD11	1.77	0.65
1:A:607:ARG:HH11	2:B:4:PRO:CD	2.03	0.65
1:A:865:ARG:NH1	2:B:447:PRO:HG2	2.11	0.65
1:A:892:CYS:HG	2:B:902:GLN:CG	2.03	0.65
2:B:288:THR:OG1	2:B:683:ASP:OD1	2.14	0.65
2:B:622:LEU:HD12	2:B:622:LEU:N	2.10	0.65
1:A:50:SER:C	1:A:51:LEU:HD13	2.19	0.65
1:A:595:LYS:O	1:A:599:SER:HA	1.96	0.65
2:B:117:ARG:NH2	2:B:299:MET:O	2.27	0.65
1:A:214:ARG:H	1:A:214:ARG:CD	2.06	0.65
1:A:607:ARG:NH1	2:B:4:PRO:CD	2.57	0.65
1:A:648:LYS:O	1:A:649:HIS:HB3	1.96	0.65
1:A:756:ARG:HH11	1:A:851:HIS:CD2	2.12	0.65
1:A:972:GLU:O	2:B:797:GLY:C	2.39	0.65
2:B:434:MET:CE	2:B:502:VAL:HG11	2.24	0.65
2:B:434:MET:HE2	2:B:502:VAL:HG21	0.72	0.65
1:A:164:MET:HG2	1:A:184:ASP:HB2	1.77	0.65
1:A:478:LEU:HD12	1:A:478:LEU:N	2.12	0.65
1:A:613:GLN:OE1	1:A:614:ALA:N	2.29	0.65
1:A:815:ILE:CG2	1:A:816:THR:H	1.88	0.65
1:A:839:GLU:O	1:A:840:ALA:C	2.38	0.65
1:A:704:ILE:CA	1:A:707:ILE:CD1	2.74	0.65
1:A:272:ARG:HB2	1:A:272:ARG:NH2	2.01	0.65
1:A:310:LEU:HG	1:A:311:ASP:N	2.11	0.65
1:A:894:ARG:HA	1:A:902:MET:HE3	0.70	0.65
2:B:110:GLN:NE2	2:B:951:TYR:CE1	2.64	0.65
2:B:587:CYS:N	2:B:588:PHE:HD1	1.95	0.65
2:B:673:TRP:HH2	2:B:759:TYR:CD2	2.15	0.65
2:B:838:ARG:HA	2:B:934:SER:HA	1.77	0.65
1:A:309:TRP:CZ3	1:A:343:THR:CG2	2.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ILE:CD1	1:A:396:LEU:CD1	2.74	0.65
1:A:940:PRO:HG3	2:B:915:SER:CB	2.25	0.65
1:A:950:MET:CE	2:B:112:THR:HG22	2.27	0.65
2:B:38:LYS:HZ3	2:B:65:GLU:CD	2.05	0.65
1:A:117:VAL:HA	1:A:485:VAL:O	1.96	0.65
1:A:507:VAL:CG2	1:A:512:MET:CE	2.75	0.65
1:A:639:GLN:H	1:A:639:GLN:NE2	1.95	0.65
1:A:26:LEU:HD11	1:A:144:THR:CG2	2.24	0.65
1:A:525:LEU:HA	1:A:608:LEU:HD11	1.78	0.65
1:A:968:MET:HG3	2:B:734:LEU:HD13	1.79	0.65
2:B:340:ALA:HB2	2:B:386:THR:HB	1.78	0.65
1:A:153:THR:HB	2:B:1001:SER:O	1.96	0.64
1:A:280:CYS:SG	1:A:308:SER:O	2.53	0.64
1:A:433:LYS:HD3	1:A:437:ALA:CB	2.25	0.64
1:A:638:ARG:HG3	1:A:638:ARG:NH2	2.04	0.64
1:A:677:ILE:HG13	1:A:678:THR:N	2.12	0.64
1:A:883:LEU:HD23	1:A:883:LEU:N	2.12	0.64
2:B:676:TRP:CZ3	2:B:680:LYS:HE2	2.31	0.64
2:B:990:HIS:CB	2:B:992:TYR:HE1	2.10	0.64
1:A:649:HIS:O	1:A:651:GLN:N	2.29	0.64
2:B:26:GLN:C	2:B:27:THR:HG23	2.21	0.64
2:B:262:MET:HE3	2:B:430:ALA:HB2	1.79	0.64
2:B:600:TYR:HE2	2:B:618:LEU:HD11	1.62	0.64
2:B:799:ARG:HG3	2:B:799:ARG:NH1	2.08	0.64
1:A:750:GLU:C	1:A:751:HIS:HD1	2.06	0.64
2:B:245:ARG:C	2:B:387:VAL:HG12	2.22	0.64
2:B:498:ILE:HD12	2:B:820:PHE:CZ	2.32	0.64
1:A:105:TRP:HA	1:A:105:TRP:CE3	2.31	0.64
1:A:432:THR:O	1:A:435:GLN:CA	2.46	0.64
1:A:88:THR:HG22	1:A:89:ASP:N	2.11	0.64
2:B:110:GLN:HA	2:B:110:GLN:NE2	2.09	0.64
2:B:199:LEU:HG	2:B:456:VAL:HG21	1.79	0.64
1:A:421:GLY:C	1:A:422:ILE:CD1	2.71	0.64
1:A:807:MET:SD	1:A:810:MET:CE	2.85	0.64
1:A:865:ARG:HD3	2:B:447:PRO:HG3	1.79	0.64
1:A:298:VAL:O	1:A:299:HIS:CD2	2.51	0.64
1:A:317:SER:HB3	1:A:323:GLY:HA2	1.80	0.64
1:A:385:LEU:HD13	1:A:385:LEU:N	2.11	0.64
1:A:429:ALA:C	1:A:430:THR:CG2	2.70	0.64
1:A:623:LEU:HD22	1:A:623:LEU:H	1.63	0.64
1:A:704:ILE:HA	1:A:707:ILE:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD12	1:A:140:LEU:O	1.98	0.64
1:A:972:GLU:HB3	1:A:973:GLY:CA	2.23	0.64
1:A:635:GLY:CA	1:A:640:MET:HE3	2.27	0.64
2:B:81:GLU:OE2	2:B:179:ALA:HB1	1.97	0.64
1:A:190:GLY:HA3	1:A:488:SER:O	1.98	0.64
1:A:921:ASP:HB2	2:B:626:ALA:CB	2.26	0.64
2:B:38:LYS:O	2:B:38:LYS:HG3	1.97	0.64
1:A:72:ARG:O	1:A:863:VAL:CG1	2.46	0.63
1:A:152:VAL:HG12	1:A:156:THR:HG21	1.80	0.63
1:A:958:THR:HG22	1:A:959:LYS:N	2.13	0.63
1:A:221:ASN:HB2	2:B:209:ARG:HD2	1.79	0.63
1:A:519:LEU:O	1:A:522:THR:HG22	1.96	0.63
1:A:865:ARG:HH11	2:B:447:PRO:HG3	1.62	0.63
1:A:38:ASN:C	1:A:38:ASN:HD22	2.06	0.63
1:A:650:ALA:O	1:A:796:SER:CA	2.46	0.63
1:A:650:ALA:O	1:A:796:SER:HA	1.98	0.63
1:A:807:MET:HE2	1:A:807:MET:HA	1.81	0.63
2:B:769:ASN:H	2:B:769:ASN:HD22	1.47	0.63
1:A:60:LEU:HD12	1:A:860:ILE:CG2	2.27	0.63
1:A:618:PHE:O	1:A:619:VAL:HG22	1.99	0.63
1:A:643:ALA:HA	1:A:669:ILE:HG23	1.80	0.63
1:A:689:ARG:HH11	1:A:689:ARG:HG3	1.63	0.63
2:B:549:LYS:HD2	2:B:549:LYS:N	2.13	0.63
1:A:83:VAL:O	1:A:95:GLN:HA	1.98	0.63
1:A:125:MET:CE	1:A:186:ASN:HD22	2.12	0.63
1:A:188:CYS:SG	1:A:492:VAL:HG11	2.37	0.63
1:A:433:LYS:HD2	1:A:437:ALA:HB2	1.75	0.63
2:B:162:SER:OG	2:B:163:GLY:N	2.31	0.63
1:A:367:ILE:HD12	1:A:415:GLN:CD	1.90	0.63
1:A:571:LEU:CD2	1:A:592:GLN:CG	2.76	0.63
2:B:597:LEU:CB	2:B:644:ASP:OD2	2.47	0.63
2:B:599:VAL:HG13	2:B:624:ALA:O	1.97	0.63
1:A:58:GLN:HG2	1:A:860:ILE:HD11	1.80	0.63
1:A:193:PHE:CZ	1:A:464:MET:CE	2.81	0.63
1:A:512:MET:CA	2:B:188:GLY:HA3	2.29	0.63
1:A:795:ALA:O	1:A:796:SER:HB3	1.97	0.63
2:B:676:TRP:NE1	2:B:754:TYR:H	1.97	0.63
1:A:807:MET:CE	1:A:810:MET:CE	2.77	0.63
1:A:634:ILE:CG2	1:A:688:GLU:HG3	2.28	0.62
2:B:335:ASP:N	2:B:335:ASP:OD1	2.29	0.62
1:A:756:ARG:NH1	1:A:851:HIS:NE2	2.44	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ARG:CB	1:A:933:PRO:CD	2.74	0.62
1:A:973:GLY:N	2:B:791:ILE:HD12	2.12	0.62
2:B:563:GLY:C	2:B:564:SER:OG	2.38	0.62
1:A:432:THR:O	1:A:435:GLN:N	2.32	0.62
1:A:481:LEU:HD11	1:A:624:ALA:HB2	1.81	0.62
1:A:503:THR:C	1:A:504:GLU:OE1	2.42	0.62
1:A:525:LEU:HG	1:A:608:LEU:CD1	2.28	0.62
1:A:552:PHE:HE1	1:A:674:PRO:HB3	1.64	0.62
1:A:650:ALA:HB1	1:A:796:SER:OG	1.98	0.62
1:A:843:ARG:HB3	1:A:843:ARG:NH1	2.11	0.62
2:B:198:MET:CA	2:B:204:GLN:NE2	2.61	0.62
2:B:442:PRO:HG2	2:B:576:TYR:CE1	2.34	0.62
1:A:218:LEU:HD23	1:A:218:LEU:N	2.12	0.62
1:A:551:ARG:HG2	1:A:551:ARG:HH11	1.65	0.62
1:A:650:ALA:HB1	1:A:796:SER:CB	2.26	0.62
2:B:214:ARG:CG	2:B:214:ARG:HH11	2.13	0.62
2:B:734:LEU:O	2:B:735:HIS:CD2	2.52	0.62
2:B:797:GLY:C	2:B:799:ARG:H	2.07	0.62
1:A:238:HIS:CE1	1:A:334:LYS:HG3	2.33	0.62
1:A:380:CYS:SG	1:A:439:ALA:CB	2.87	0.62
1:A:801:LEU:HD21	1:A:813:LEU:HD21	1.80	0.62
1:A:841:HIS:O	1:A:844:GLY:N	2.32	0.62
1:A:78:ALA:O	1:A:856:THR:CG2	2.47	0.62
1:A:421:GLY:C	1:A:422:ILE:HD12	2.24	0.62
1:A:508:SER:CB	2:B:992:TYR:CD2	2.83	0.62
1:A:508:SER:OG	2:B:992:TYR:CD2	2.53	0.62
1:A:563:PHE:HA	1:A:566:VAL:HG23	1.81	0.62
1:A:39:ILE:HG12	1:A:506:SER:HG	1.64	0.62
1:A:225:THR:O	1:A:226:ALA:C	2.41	0.62
1:A:906:ALA:O	1:A:907:VAL:CG1	2.47	0.62
1:A:319:ASP:N	1:A:319:ASP:OD1	2.29	0.62
1:A:532:ALA:O	1:A:536:GLU:HB2	2.00	0.62
1:A:943:ARG:HG3	1:A:943:ARG:NH1	2.11	0.62
1:A:952:THR:HG21	2:B:256:ASP:OD2	2.00	0.62
2:B:434:MET:HE3	2:B:502:VAL:CG2	2.29	0.62
1:A:950:MET:HE1	2:B:112:THR:HG21	1.82	0.62
2:B:434:MET:HE1	2:B:502:VAL:CG1	2.27	0.62
1:A:125:MET:HE3	1:A:132:MET:HG3	1.82	0.62
1:A:231:THR:CG2	1:A:343:THR:HG1	1.84	0.62
1:A:333:TRP:HE1	1:A:343:THR:HG1	1.46	0.62
1:A:752:LYS:HE3	1:A:857:ASP:OD2	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:214:ARG:HH11	2:B:214:ARG:HG2	1.65	0.62
2:B:434:MET:CE	2:B:502:VAL:CG1	2.78	0.62
2:B:549:LYS:CA	2:B:550:MET:SD	2.88	0.62
2:B:623:ILE:HD12	2:B:893:ILE:CD1	2.30	0.62
2:B:666:LEU:O	2:B:666:LEU:HD22	2.00	0.62
2:B:769:ASN:O	2:B:770:ASP:C	2.42	0.61
1:A:273:LEU:HD11	1:A:334:LYS:HB2	1.81	0.61
1:A:492:VAL:CB	1:A:495:VAL:CG2	2.53	0.61
1:A:713:LEU:CG	1:A:714:ASN:N	2.55	0.61
2:B:498:ILE:CD1	2:B:820:PHE:CE2	2.76	0.61
2:B:589:TYR:HE1	2:B:808:GLY:CA	2.09	0.61
1:A:105:TRP:HA	1:A:105:TRP:HE3	1.65	0.61
1:A:163:GLU:HA	1:A:163:GLU:OE2	2.00	0.61
1:A:265:VAL:HG22	1:A:265:VAL:O	2.00	0.61
1:A:532:ALA:C	1:A:535:CYS:HG	2.06	0.61
1:A:551:ARG:HG2	1:A:551:ARG:NH1	2.14	0.61
1:A:551:ARG:O	1:A:553:THR:OG1	2.17	0.61
1:A:750:GLU:O	1:A:751:HIS:ND1	2.23	0.61
2:B:1:MET:SD	2:B:2:SER:N	2.72	0.61
2:B:262:MET:HE2	2:B:428:CYS:O	2.00	0.61
2:B:349:LYS:H	2:B:349:LYS:HD3	1.64	0.61
2:B:428:CYS:SG	2:B:818:HIS:CG	2.93	0.61
2:B:442:PRO:HG2	2:B:576:TYR:CE2	2.36	0.61
1:A:58:GLN:CB	1:A:860:ILE:HD12	2.30	0.61
1:A:152:VAL:CG1	1:A:156:THR:HG21	2.31	0.61
1:A:350:TYR:CD2	1:A:383:PHE:HD1	2.19	0.61
1:A:455:HIS:O	1:A:458:ILE:CG2	2.48	0.61
2:B:170:ASP:OD1	2:B:171:ASN:N	2.33	0.61
2:B:294:ASP:O	2:B:295:TYR:O	2.18	0.61
1:A:64:GLY:C	1:A:65:LEU:HG	2.25	0.61
1:A:435:GLN:O	1:A:435:GLN:NE2	2.33	0.61
1:A:449:ILE:O	1:A:449:ILE:CG2	2.48	0.61
2:B:197:PRO:CG	2:B:457:TRP:HA	2.30	0.61
2:B:230:THR:HG21	2:B:364:MET:HB2	1.82	0.61
2:B:327:TYR:CD1	2:B:329:LEU:HD13	2.35	0.61
2:B:659:ILE:HD11	2:B:788:LEU:HD21	1.78	0.61
1:A:55:LEU:CB	1:A:528:MET:HE2	2.31	0.61
1:A:371:LEU:C	1:A:500:MET:HE1	2.17	0.61
2:B:509:ILE:HG21	2:B:512:GLY:HA2	1.81	0.61
1:A:437:ALA:O	1:A:509:VAL:O	2.18	0.61
1:A:495:VAL:HG23	1:A:496:GLN:N	2.13	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:THR:HG22	1:A:676:THR:O	2.00	0.61
2:B:161:LEU:CD1	2:B:161:LEU:H	2.14	0.61
1:A:51:LEU:HD21	1:A:62:ASN:CB	2.30	0.61
1:A:558:VAL:O	1:A:558:VAL:HG12	2.00	0.61
1:A:742:MET:O	1:A:746:VAL:HG23	2.01	0.61
1:A:790:PRO:CD	1:A:819:ASP:HB2	2.30	0.61
1:A:893:VAL:C	1:A:895:ASP:N	2.54	0.61
2:B:227:VAL:CG2	2:B:364:MET:SD	2.86	0.61
2:B:672:ASN:HB2	2:B:754:TYR:CZ	2.35	0.61
1:A:72:ARG:HB2	1:A:863:VAL:CG1	2.31	0.61
1:A:385:LEU:HD21	1:A:443:LEU:HD11	1.82	0.61
2:B:672:ASN:C	2:B:754:TYR:CE2	2.79	0.61
1:A:55:LEU:HD12	1:A:528:MET:HE2	1.01	0.61
2:B:421:SER:HB2	2:B:554:VAL:HG23	1.82	0.61
2:B:684:SER:OG	2:B:785:ARG:HD3	2.00	0.61
1:A:125:MET:HE1	1:A:186:ASN:HD22	1.65	0.60
1:A:471:ARG:O	1:A:471:ARG:HG2	1.99	0.60
1:A:645:ALA:O	1:A:649:HIS:HA	2.01	0.60
1:A:925:VAL:O	1:A:926:THR:HG22	2.01	0.60
2:B:120:LEU:O	2:B:151:VAL:HA	2.01	0.60
2:B:241:SER:CB	2:B:390:ARG:CG	2.79	0.60
2:B:666:LEU:O	2:B:666:LEU:HD13	2.01	0.60
1:A:69:GLU:CD	1:A:217:GLU:OE1	2.43	0.60
1:A:125:MET:CE	1:A:132:MET:HG3	2.31	0.60
1:A:589:LEU:H	1:A:589:LEU:HD12	1.67	0.60
1:A:788:ILE:HD11	1:A:823:VAL:HG23	1.83	0.60
2:B:259:VAL:HG13	2:B:260:LYS:H	1.66	0.60
1:A:452:ARG:HH21	1:A:452:ARG:CG	2.13	0.60
1:A:801:LEU:CD2	1:A:813:LEU:HD21	2.31	0.60
1:A:919:LEU:O	1:A:919:LEU:HD23	2.01	0.60
1:A:335:GLY:HA2	1:A:341:HIS:HD2	1.66	0.60
1:A:637:SER:O	1:A:638:ARG:C	2.44	0.60
1:A:696:LEU:HA	1:A:701:SER:O	2.00	0.60
1:A:888:TYR:C	1:A:889:GLU:OE1	2.43	0.60
2:B:186:TRP:CH2	2:B:212:VAL:O	2.52	0.60
2:B:647:LEU:H	2:B:647:LEU:CD1	2.14	0.60
1:A:90:MET:O	1:A:90:MET:HE3	2.02	0.60
1:A:238:HIS:CG	1:A:334:LYS:HD2	2.27	0.60
1:A:51:LEU:O	2:B:1:MET:HA	2.02	0.60
1:A:127:PHE:CD1	1:A:452:ARG:HD2	2.37	0.60
1:A:201:MET:HG3	1:A:400:PHE:CE1	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:HIS:HD2	1:A:348:GLN:NE2	1.99	0.60
1:A:702:LYS:NZ	1:A:707:ILE:HG13	2.16	0.60
1:A:900:HIS:O	1:A:901:SER:C	2.44	0.60
2:B:208:PHE:CE2	2:B:452:ALA:HB1	2.36	0.60
2:B:648:VAL:CG1	2:B:653:VAL:HG21	2.30	0.60
1:A:113:ALA:HB2	1:A:480:PRO:O	2.00	0.60
1:A:702:LYS:HZ1	1:A:707:ILE:CG1	2.13	0.60
1:A:893:VAL:C	1:A:895:ASP:H	2.08	0.60
1:A:943:ARG:O	1:A:943:ARG:HD3	2.02	0.60
2:B:688:ASP:O	2:B:689:ILE:C	2.44	0.60
2:B:734:LEU:O	2:B:735:HIS:CG	2.55	0.60
1:A:477:SER:OG	1:A:478:LEU:N	2.34	0.60
1:A:656:ASP:OD2	1:A:802:ARG:HD2	2.02	0.60
1:A:788:ILE:CD1	1:A:823:VAL:HG23	2.31	0.60
2:B:56:ARG:HH22	2:B:485:GLN:HE22	1.48	0.60
2:B:265:PRO:CD	2:B:266:HIS:H	2.13	0.60
2:B:446:ARG:HG3	2:B:446:ARG:NH1	2.14	0.60
2:B:623:ILE:CG2	2:B:893:ILE:CG1	2.79	0.60
2:B:990:HIS:CB	2:B:992:TYR:CE1	2.85	0.60
1:A:880:VAL:O	1:A:880:VAL:HG22	2.01	0.60
2:B:74:MET:HE2	2:B:984:ILE:CD1	2.32	0.60
2:B:212:VAL:HG22	2:B:449:ASN:HB2	1.84	0.60
2:B:221:HIS:CD2	2:B:411:VAL:HG21	2.37	0.60
2:B:224:LEU:HB2	2:B:404:MET:HG2	1.82	0.60
2:B:374:GLY:O	2:B:375:VAL:HG22	2.01	0.60
2:B:553:PRO:HA	2:B:579:GLY:HA2	1.84	0.60
2:B:623:ILE:CG2	2:B:893:ILE:CD1	2.64	0.60
2:B:707:VAL:O	2:B:707:VAL:HG12	2.02	0.60
2:B:733:ARG:O	2:B:736:HIS:ND1	2.27	0.60
1:A:49:LEU:HG	1:A:607:ARG:HG3	1.84	0.60
1:A:262:ARG:HH22	1:A:401:GLY:HA3	1.23	0.60
1:A:584:SER:C	1:A:585:SER:HG	2.02	0.60
1:A:618:PHE:O	1:A:619:VAL:HG13	2.00	0.60
1:A:807:MET:SD	1:A:810:MET:HE1	2.41	0.60
1:A:819:ASP:OD1	1:A:819:ASP:N	2.35	0.60
1:A:894:ARG:CD	1:A:902:MET:HE2	2.30	0.60
1:A:42:GLY:CA	1:A:445:ARG:NH2	2.65	0.59
1:A:238:HIS:CD2	1:A:338:SER:CA	2.85	0.59
1:A:305:ASP:OD1	1:A:306:PRO:HD2	2.02	0.59
2:B:794:GLN:HG3	2:B:796:ASP:H	1.66	0.59
1:A:55:LEU:HD22	1:A:528:MET:HE1	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:ASN:OD1	1:A:475:ASN:N	2.33	0.59
1:A:923:THR:CG2	2:B:627:THR:OG1	2.49	0.59
1:A:951:GLY:H	2:B:114:ASN:HD21	1.50	0.59
2:B:170:ASP:HB2	2:B:545:ARG:HH22	1.67	0.59
2:B:431:HIS:O	2:B:812:ALA:HB3	2.02	0.59
2:B:559:ALA:HB2	2:B:569:PHE:CD2	2.36	0.59
2:B:640:ALA:HB1	2:B:887:THR:HG21	1.85	0.59
2:B:695:VAL:HG22	2:B:780:ILE:HG23	1.84	0.59
2:B:751:ARG:O	2:B:752:HIS:HB2	2.02	0.59
1:A:60:LEU:HD12	1:A:860:ILE:HG21	1.84	0.59
1:A:433:LYS:O	1:A:437:ALA:N	2.26	0.59
2:B:25:VAL:HG12	2:B:25:VAL:O	2.01	0.59
2:B:95:GLN:HA	2:B:95:GLN:HE21	1.67	0.59
2:B:195:VAL:HG22	2:B:984:ILE:CG2	2.31	0.59
2:B:241:SER:HB3	2:B:390:ARG:CG	2.26	0.59
1:A:125:MET:HG2	1:A:136:ASP:OD2	2.02	0.59
1:A:353:MET:CE	1:A:385:LEU:HB2	2.31	0.59
1:A:450:SER:O	1:A:453:THR:HG22	2.01	0.59
1:A:654:THR:OG1	1:A:667:GLN:NE2	2.36	0.59
2:B:238:VAL:O	2:B:238:VAL:HG23	2.02	0.59
2:B:329:LEU:HD12	2:B:450:GLU:CG	2.32	0.59
2:B:500:GLN:HG3	2:B:560:TRP:CH2	2.37	0.59
2:B:761:PRO:HG3	2:B:778:TRP:CD1	2.38	0.59
1:A:200:VAL:O	1:A:200:VAL:HG12	2.03	0.59
1:A:837:SER:OG	1:A:837:SER:O	2.14	0.59
2:B:113:VAL:O	2:B:113:VAL:HG12	2.00	0.59
2:B:334:CYS:CB	2:B:468:MET:HE3	2.32	0.59
1:A:77:LEU:HD22	1:A:742:MET:CE	2.30	0.59
1:A:590:PHE:C	1:A:592:GLN:N	2.60	0.59
1:A:828:ARG:HH11	1:A:828:ARG:CG	2.15	0.59
1:A:970:LEU:N	1:A:970:LEU:HD12	2.17	0.59
2:B:332:PRO:HG2	2:B:399:PHE:CG	2.36	0.59
2:B:373:THR:OG1	2:B:381:THR:CA	2.46	0.59
2:B:433:TRP:CH2	2:B:521:LEU:HD23	2.37	0.59
2:B:830:THR:HA	2:B:939:MET:SD	2.43	0.59
1:A:156:THR:CG2	1:A:157:MET:H	2.09	0.59
1:A:185:ASN:OD1	1:A:186:ASN:N	2.35	0.59
1:A:195:VAL:HG23	1:A:384:LEU:HB3	1.84	0.59
1:A:367:ILE:HD12	1:A:415:GLN:NE2	0.93	0.59
1:A:589:LEU:N	1:A:592:GLN:NE2	2.50	0.59
1:A:696:LEU:C	1:A:697:ASN:O	2.40	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:197:PRO:O	2:B:456:VAL:O	2.20	0.59
2:B:761:PRO:HG3	2:B:778:TRP:NE1	2.17	0.59
1:A:320:SER:CA	1:A:351:HIS:CD2	2.86	0.59
1:A:387:ASN:ND2	1:A:391:GLY:CA	2.64	0.59
2:B:57:GLY:O	2:B:478:HIS:CG	2.55	0.59
2:B:484:ALA:HB2	2:B:950:LEU:HD23	1.84	0.59
1:A:243:VAL:HG23	1:A:473:LEU:O	1.98	0.59
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.67	0.59
1:A:833:ARG:HH11	1:A:833:ARG:CG	2.13	0.59
1:A:925:VAL:HG12	1:A:926:THR:H	1.67	0.59
2:B:587:CYS:N	2:B:588:PHE:CD1	2.71	0.59
2:B:623:ILE:CD1	2:B:893:ILE:CD1	2.80	0.59
2:B:672:ASN:CB	2:B:754:TYR:CE2	2.86	0.59
1:A:107:HIS:CD2	1:A:236:CYS:O	2.55	0.59
1:A:407:HIS:HE1	1:A:490:PHE:CE2	2.20	0.59
1:A:632:ARG:O	1:A:726:TYR:CE1	2.56	0.59
1:A:958:THR:C	1:A:959:LYS:HG2	2.27	0.59
2:B:327:TYR:CD1	2:B:329:LEU:CD1	2.86	0.59
2:B:514:THR:HG21	2:B:587:CYS:HB2	1.85	0.59
2:B:658:THR:CG2	2:B:695:VAL:CG2	2.81	0.59
2:B:658:THR:HG21	2:B:695:VAL:HG21	1.84	0.59
1:A:27:LYS:HG3	1:A:28:ASP:OD1	2.03	0.58
1:A:264:ARG:HG2	1:A:707:ILE:CG2	2.32	0.58
1:A:822:LEU:C	1:A:822:LEU:HD12	2.28	0.58
1:A:898:THR:HG22	2:B:858:PRO:HG3	1.85	0.58
1:A:950:MET:HG3	2:B:114:ASN:HD22	1.67	0.58
2:B:832:HIS:CE1	2:B:837:ALA:HB1	2.37	0.58
1:A:23:ARG:HH11	1:A:23:ARG:CG	2.15	0.58
1:A:468:THR:HG23	1:A:468:THR:O	2.01	0.58
1:A:481:LEU:N	1:A:481:LEU:HD13	2.18	0.58
2:B:257:PHE:HB3	2:B:355:ALA:HB1	1.85	0.58
2:B:375:VAL:HG23	2:B:375:VAL:O	2.01	0.58
2:B:433:TRP:HD1	2:B:518:GLN:HE21	1.49	0.58
2:B:442:PRO:HD2	2:B:576:TYR:CZ	2.38	0.58
1:A:31:VAL:HG12	1:A:31:VAL:O	2.03	0.58
1:A:203:ASN:HB3	1:A:519:LEU:CD1	2.32	0.58
1:A:262:ARG:NH2	1:A:401:GLY:O	2.32	0.58
1:A:611:LEU:O	1:A:611:LEU:HD22	2.03	0.58
1:A:961:LEU:CD1	2:B:284:MET:CG	2.79	0.58
2:B:269:SER:HB2	2:B:430:ALA:O	2.01	0.58
2:B:440:LEU:O	2:B:578:PHE:HB3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ALA:HB1	1:A:910:LEU:CD2	2.28	0.58
1:A:131:ARG:CG	1:A:131:ARG:HH11	2.16	0.58
1:A:432:THR:HG23	1:A:433:LYS:H	1.63	0.58
1:A:852:VAL:O	1:A:852:VAL:HG13	2.03	0.58
1:A:264:ARG:HG2	1:A:707:ILE:HG21	1.86	0.58
1:A:436:LEU:O	1:A:436:LEU:HD13	2.03	0.58
1:A:455:HIS:HB3	1:A:611:LEU:HD21	1.86	0.58
1:A:886:ARG:CZ	1:A:889:GLU:HG2	2.34	0.58
2:B:434:MET:CE	2:B:502:VAL:HG22	2.32	0.58
2:B:497:ALA:CB	2:B:557:LEU:HD22	2.33	0.58
1:A:78:ALA:C	1:A:856:THR:CG2	2.72	0.58
1:A:189:ARG:HG3	1:A:189:ARG:NH2	2.18	0.58
1:A:199:MET:SD	1:A:203:ASN:OD1	2.62	0.58
1:A:359:THR:HB	2:B:999:LEU:O	2.03	0.58
1:A:570:GLU:O	1:A:570:GLU:HG3	2.02	0.58
1:A:667:GLN:O	1:A:684:ALA:HB3	2.02	0.58
1:A:843:ARG:HH11	1:A:843:ARG:CG	2.17	0.58
2:B:195:VAL:HG22	2:B:984:ILE:HG22	1.85	0.58
2:B:525:LEU:HD13	2:B:557:LEU:HD11	1.86	0.58
2:B:602:VAL:HG11	2:B:615:MET:HE1	1.84	0.58
1:A:39:ILE:N	1:A:506:SER:OG	2.35	0.58
1:A:193:PHE:CZ	1:A:464:MET:HE2	2.38	0.58
1:A:211:VAL:HG23	1:A:216:GLN:HG3	1.85	0.58
1:A:525:LEU:CG	1:A:608:LEU:CD1	2.81	0.58
1:A:532:ALA:O	1:A:535:CYS:SG	2.60	0.58
1:A:590:PHE:C	1:A:592:GLN:H	2.11	0.58
2:B:347:TRP:O	2:B:348:GLY:C	2.46	0.58
1:A:376:GLY:C	1:A:377:LEU:HD23	2.28	0.58
1:A:967:GLN:O	1:A:969:GLU:N	2.37	0.58
2:B:307:LYS:CG	2:B:311:ARG:NH2	2.67	0.58
2:B:433:TRP:CD1	2:B:518:GLN:HG3	2.38	0.58
2:B:576:TYR:HE1	2:B:578:PHE:CZ	2.22	0.58
2:B:597:LEU:HB2	2:B:644:ASP:OD2	2.04	0.58
1:A:10:ASN:O	1:A:10:ASN:ND2	2.36	0.58
1:A:65:LEU:O	1:A:65:LEU:CD1	2.51	0.58
1:A:145:ILE:HD11	1:A:157:MET:CE	2.34	0.58
1:A:757:HIS:CD2	1:A:758:THR:N	2.72	0.58
1:A:777:LEU:CD2	1:A:834:MET:HE2	2.32	0.58
1:A:958:THR:O	1:A:959:LYS:HD2	2.04	0.58
1:A:556:HIS:CE1	1:A:626:ILE:CD1	2.87	0.57
2:B:101:ILE:HD11	2:B:857:VAL:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:433:TRP:HD1	2:B:518:GLN:NE2	2.01	0.57
2:B:597:LEU:HD22	2:B:622:LEU:HB3	1.86	0.57
2:B:607:THR:HG21	2:B:909:ASN:ND2	2.19	0.57
2:B:747:ALA:HB1	2:B:749:THR:HG22	1.83	0.57
2:B:247:ARG:NE	2:B:347:TRP:CD1	2.71	0.57
1:A:248:VAL:CB	1:A:249:PRO:HD2	2.28	0.57
1:A:275:ASP:CG	1:A:276:PRO:CD	2.75	0.57
1:A:305:ASP:OD1	1:A:306:PRO:N	2.37	0.57
1:A:478:LEU:O	1:A:480:PRO:HD3	2.04	0.57
1:A:615:TYR:CD1	1:A:615:TYR:N	2.72	0.57
1:A:790:PRO:CG	1:A:819:ASP:CB	2.82	0.57
2:B:405:ALA:O	2:B:407:ALA:N	2.36	0.57
2:B:653:VAL:O	2:B:653:VAL:HG12	2.04	0.57
2:B:837:ALA:O	2:B:839:LEU:HD12	2.04	0.57
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.19	0.57
1:A:149:SER:O	1:A:150:ARG:C	2.45	0.57
1:A:783:ASP:OD2	1:A:838:PRO:CB	2.51	0.57
2:B:748:ASP:N	2:B:748:ASP:OD1	2.37	0.57
2:B:838:ARG:NH1	2:B:841:SER:OG	2.38	0.57
1:A:446:ARG:HH11	1:A:446:ARG:CG	2.17	0.57
1:A:556:HIS:O	1:A:559:ALA:HB3	2.05	0.57
1:A:597:VAL:CG1	1:A:748:ALA:HB2	2.34	0.57
2:B:38:LYS:HD2	2:B:65:GLU:CD	2.15	0.57
2:B:648:VAL:CG1	2:B:653:VAL:CG2	2.82	0.57
2:B:673:TRP:N	2:B:754:TYR:CE2	2.69	0.57
1:A:153:THR:O	1:A:156:THR:HG22	2.05	0.57
1:A:189:ARG:HH21	1:A:189:ARG:CG	2.17	0.57
1:A:924:PRO:C	1:A:925:VAL:O	2.39	0.57
2:B:45:ILE:O	2:B:53:ILE:HD11	2.04	0.57
1:A:945:PRO:HB3	2:B:896:ASP:OD1	2.05	0.57
1:A:961:LEU:CD2	2:B:286:THR:HG21	2.34	0.57
2:B:89:ASP:HA	2:B:410:GLN:HE22	1.69	0.57
2:B:509:ILE:HG23	2:B:512:GLY:HA2	1.85	0.57
2:B:510:THR:HG22	2:B:632:THR:HG22	1.87	0.57
2:B:735:HIS:ND1	2:B:735:HIS:C	2.63	0.57
2:B:769:ASN:ND2	2:B:769:ASN:H	2.01	0.57
2:B:807:PHE:CD1	2:B:807:PHE:N	2.73	0.57
1:A:117:VAL:HG23	1:A:485:VAL:HG23	1.79	0.57
1:A:350:TYR:CE2	1:A:383:PHE:HD1	2.23	0.57
1:A:411:TYR:N	1:A:411:TYR:CD1	2.72	0.57
1:A:704:ILE:C	1:A:707:ILE:CD1	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ARG:HD3	1:A:730:THR:CG2	2.33	0.57
1:A:943:ARG:HD3	1:A:943:ARG:C	2.30	0.57
2:B:77:LEU:HD23	2:B:192:VAL:HG13	1.85	0.57
2:B:198:MET:HE1	2:B:459:VAL:HA	1.87	0.57
2:B:839:LEU:HD22	2:B:935:VAL:HG21	1.87	0.57
1:A:507:VAL:HG23	1:A:512:MET:HE3	1.85	0.57
1:A:691:PHE:N	1:A:691:PHE:CD1	2.73	0.57
1:A:757:HIS:CD2	1:A:758:THR:HG23	2.40	0.57
1:A:789:ARG:HA	1:A:820:CYS:HB3	1.85	0.57
2:B:26:GLN:O	2:B:27:THR:CB	2.51	0.57
2:B:790:LEU:O	2:B:794:GLN:HB3	2.05	0.57
1:A:243:VAL:HA	1:A:631:VAL:HG12	1.87	0.57
1:A:305:ASP:OD1	1:A:306:PRO:CD	2.52	0.57
1:A:342:LEU:HD23	1:A:343:THR:H	1.70	0.57
1:A:508:SER:HB3	2:B:992:TYR:CE2	2.39	0.57
2:B:383:HIS:HD2	2:B:385:ASP:OD1	1.87	0.57
1:A:792:THR:O	1:A:793:SER:HB2	2.04	0.56
2:B:607:THR:HG21	2:B:909:ASN:CG	2.30	0.56
2:B:737:TYR:CD1	2:B:738:ASP:N	2.72	0.56
1:A:384:LEU:O	1:A:385:LEU:CD1	2.52	0.56
2:B:348:GLY:O	2:B:349:LYS:C	2.47	0.56
1:A:83:VAL:O	1:A:95:GLN:CA	2.54	0.56
1:A:299:HIS:CD2	1:A:299:HIS:N	2.73	0.56
1:A:634:ILE:HG22	1:A:688:GLU:CG	2.35	0.56
1:A:634:ILE:HD12	1:A:726:TYR:CD2	2.40	0.56
2:B:165:THR:HG22	2:B:219:GLN:NE2	2.08	0.56
2:B:433:TRP:NE1	2:B:518:GLN:HG3	2.17	0.56
2:B:510:THR:O	2:B:511:ASP:CB	2.51	0.56
2:B:588:PHE:CD1	2:B:588:PHE:N	2.73	0.56
1:A:367:ILE:CD1	1:A:415:GLN:HE22	1.22	0.56
1:A:549:VAL:HG13	1:A:553:THR:CG2	2.29	0.56
1:A:690:TRP:CD1	1:A:690:TRP:N	2.73	0.56
1:A:923:THR:HG23	2:B:627:THR:OG1	2.05	0.56
2:B:269:SER:OG	2:B:430:ALA:O	2.23	0.56
2:B:838:ARG:NH1	2:B:932:SER:HB2	2.21	0.56
1:A:39:ILE:CG2	1:A:507:VAL:HG11	2.36	0.56
1:A:231:THR:HG21	1:A:333:TRP:CZ2	2.41	0.56
1:A:231:THR:CA	1:A:342:LEU:O	2.52	0.56
1:A:940:PRO:HB3	2:B:914:LEU:HD22	1.87	0.56
2:B:7:GLN:NE2	2:B:76:ASP:CG	2.63	0.56
2:B:122:CYS:CB	2:B:939:MET:HE2	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:H	2:B:378:THR:CG2	2.18	0.56
2:B:673:TRP:HH2	2:B:759:TYR:HD2	1.44	0.56
2:B:739:GLY:HA3	2:B:750:GLU:OE2	2.05	0.56
1:A:199:MET:CG	1:A:440:THR:OG1	2.30	0.56
1:A:697:ASN:CB	1:A:701:SER:HB2	2.34	0.56
2:B:548:ASN:O	2:B:550:MET:HE1	2.06	0.56
1:A:238:HIS:CD2	1:A:338:SER:CB	2.88	0.56
1:A:690:TRP:CZ2	1:A:712:GLY:HA3	2.41	0.56
2:B:128:ILE:O	2:B:129:ILE:HD13	2.05	0.56
2:B:135:ASP:N	2:B:135:ASP:OD1	2.37	0.56
2:B:141:TYR:CD1	2:B:141:TYR:N	2.73	0.56
2:B:838:ARG:HG3	2:B:838:ARG:NH1	2.19	0.56
1:A:433:LYS:HD3	1:A:437:ALA:HB2	1.77	0.56
1:A:542:GLU:HB2	1:A:733:SER:CB	2.36	0.56
1:A:674:PRO:C	1:A:675:SER:OG	2.48	0.56
1:A:915:GLU:O	1:A:915:GLU:HG2	2.06	0.56
1:A:968:MET:O	1:A:971:ARG:HA	2.06	0.56
2:B:427:ALA:CA	2:B:432:GLU:OE1	2.53	0.56
2:B:992:TYR:N	2:B:992:TYR:CD1	2.72	0.56
1:A:68:PHE:CD1	1:A:68:PHE:N	2.73	0.56
1:A:412:ALA:O	1:A:413:GLN:C	2.48	0.56
1:A:571:LEU:HD22	1:A:592:GLN:HG3	1.82	0.56
2:B:153:ALA:HB3	2:B:426:ALA:HB3	1.86	0.56
2:B:230:THR:CG2	2:B:364:MET:HB2	2.36	0.56
2:B:329:LEU:HD21	2:B:404:MET:HE2	1.86	0.56
2:B:992:TYR:N	2:B:992:TYR:HD1	2.04	0.56
1:A:201:MET:CG	1:A:400:PHE:CE1	2.89	0.56
1:A:211:VAL:CG2	1:A:216:GLN:CB	2.84	0.56
1:A:367:ILE:HD12	1:A:367:ILE:N	2.20	0.56
1:A:481:LEU:H	1:A:481:LEU:CD2	2.04	0.56
1:A:555:VAL:CG1	1:A:687:THR:HG23	2.36	0.56
2:B:334:CYS:SG	2:B:468:MET:HE1	2.43	0.56
2:B:586:GLY:HA3	2:B:588:PHE:CE1	2.41	0.56
2:B:797:GLY:C	2:B:799:ARG:N	2.60	0.56
1:A:153:THR:O	1:A:156:THR:CG2	2.54	0.55
1:A:153:THR:CB	2:B:1001:SER:O	2.54	0.55
1:A:195:VAL:CG2	1:A:384:LEU:HD13	2.36	0.55
1:A:198:ARG:HG2	1:A:198:ARG:NH1	2.21	0.55
1:A:879:ARG:NH2	1:A:915:GLU:OE1	2.38	0.55
1:A:917:MET:O	1:A:918:LYS:C	2.48	0.55
2:B:664:ASN:O	2:B:668:ARG:HG3	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:O	1:A:90:MET:HG3	2.07	0.55
1:A:268:GLU:OE1	1:A:702:LYS:HE2	2.07	0.55
1:A:356:THR:OG1	1:A:424:ASP:O	2.23	0.55
1:A:785:MET:SD	1:A:824:VAL:HG22	2.47	0.55
1:A:801:LEU:CD2	1:A:813:LEU:CD2	2.84	0.55
2:B:43:THR:CG2	2:B:55:LYS:CG	2.85	0.55
2:B:253:HIS:C	2:B:253:HIS:CD2	2.85	0.55
1:A:27:LYS:HG2	1:A:28:ASP:OD1	2.06	0.55
1:A:188:CYS:HB3	1:A:449:ILE:HD11	1.89	0.55
1:A:372:LYS:N	1:A:500:MET:HE1	2.15	0.55
1:A:634:ILE:HB	1:A:688:GLU:HB3	1.87	0.55
1:A:673:VAL:HG13	1:A:673:VAL:O	2.06	0.55
2:B:118:PHE:CE2	2:B:950:LEU:HD22	2.42	0.55
1:A:112:MET:HG2	1:A:266:PHE:HE2	1.70	0.55
1:A:455:HIS:HA	1:A:458:ILE:HG21	1.89	0.55
1:A:940:PRO:CG	2:B:915:SER:HB3	2.35	0.55
1:A:968:MET:HE3	2:B:659:ILE:HD13	1.89	0.55
2:B:247:ARG:HD2	2:B:347:TRP:CD1	2.41	0.55
1:A:284:LYS:HA	1:A:329:HIS:HB3	1.87	0.55
1:A:289:THR:HG22	1:A:290:GLN:H	1.72	0.55
1:A:329:HIS:CD2	1:A:329:HIS:H	2.25	0.55
1:A:929:GLN:HG3	2:B:600:TYR:CE1	2.42	0.55
2:B:146:ILE:HD11	2:B:921:HIS:CE1	2.41	0.55
2:B:555:ASN:HD22	2:B:569:PHE:HB3	1.72	0.55
1:A:19:LYS:HB3	1:A:23:ARG:HH12	1.72	0.55
1:A:352:ARG:HH11	1:A:352:ARG:CG	2.14	0.55
1:A:483:PHE:HB2	1:A:617:PRO:HB2	1.89	0.55
1:A:898:THR:HG22	2:B:858:PRO:CB	2.37	0.55
1:A:121:SER:HB2	1:A:183:ALA:O	2.07	0.55
1:A:477:SER:O	1:A:478:LEU:CG	2.55	0.55
1:A:671:LEU:CD2	1:A:685:ILE:CG2	2.85	0.55
1:A:782:GLY:O	1:A:802:ARG:NH2	2.40	0.55
1:A:963:ASP:OD1	1:A:963:ASP:N	2.39	0.55
2:B:161:LEU:H	2:B:161:LEU:HD12	1.72	0.55
2:B:363:VAL:HG13	2:B:441:MET:SD	2.47	0.55
1:A:210:VAL:O	1:A:210:VAL:HG22	2.07	0.55
1:A:464:MET:SD	1:A:483:PHE:CZ	3.00	0.55
1:A:952:THR:CG2	2:B:115:ALA:CB	2.85	0.55
2:B:198:MET:N	2:B:198:MET:SD	2.79	0.55
1:A:245:ILE:HD12	1:A:274:VAL:HG23	1.88	0.55
1:A:459:THR:HB	1:A:611:LEU:HD11	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ARG:HD3	2:B:510:THR:HG21	1.88	0.55
2:B:794:GLN:OE1	2:B:805:HIS:HE1	1.78	0.55
1:A:55:LEU:HD12	1:A:528:MET:HE3	1.15	0.54
2:B:114:ASN:CB	2:B:119:TYR:CE2	2.88	0.54
1:A:574:LEU:HD23	1:A:577:ARG:CD	2.15	0.54
1:A:688:GLU:OE1	1:A:688:GLU:N	2.40	0.54
1:A:861:ARG:CZ	2:B:547:ALA:HB2	2.36	0.54
2:B:129:ILE:O	2:B:933:VAL:HA	2.08	0.54
2:B:170:ASP:HB2	2:B:545:ARG:NH2	2.21	0.54
2:B:1003:TYR:HE2	2:B:1005:LYS:NZ	1.99	0.54
1:A:125:MET:CE	1:A:186:ASN:ND2	2.68	0.54
1:A:260:THR:OG1	1:A:261:GLY:N	2.40	0.54
1:A:442:ALA:CA	1:A:509:VAL:HG11	2.33	0.54
1:A:477:SER:C	1:A:478:LEU:CD1	2.69	0.54
1:A:607:ARG:HG3	1:A:607:ARG:HH21	1.72	0.54
1:A:646:LEU:HD23	1:A:647:ILE:N	2.22	0.54
1:A:849:ASP:OD1	1:A:849:ASP:N	2.34	0.54
1:A:972:GLU:O	2:B:797:GLY:HA3	2.06	0.54
2:B:168:THR:OG1	2:B:545:ARG:CD	2.55	0.54
2:B:514:THR:HG21	2:B:587:CYS:SG	2.48	0.54
2:B:1003:TYR:O	2:B:1004:ASP:O	2.25	0.54
1:A:297:ARG:HG2	1:A:297:ARG:NH1	2.21	0.54
1:A:556:HIS:HD1	1:A:626:ILE:HD12	1.73	0.54
1:A:884:ALA:CB	2:B:506:PRO:CB	2.38	0.54
2:B:43:THR:HG21	2:B:55:LYS:CD	2.35	0.54
2:B:66:ARG:CZ	2:B:173:ASP:OD2	2.54	0.54
2:B:653:VAL:O	2:B:657:THR:HG23	2.07	0.54
2:B:846:THR:HB	2:B:847:PRO:CD	2.37	0.54
1:A:268:GLU:OE1	1:A:702:LYS:CE	2.56	0.54
1:A:350:TYR:CD1	1:A:350:TYR:C	2.85	0.54
1:A:650:ALA:O	1:A:797:SER:N	2.41	0.54
1:A:931:LEU:HD23	2:B:615:MET:SD	2.39	0.54
2:B:194:ILE:CG2	2:B:199:LEU:C	2.81	0.54
1:A:502:ASP:OD1	1:A:502:ASP:O	2.25	0.54
1:A:657:TRP:CE3	1:A:664:CYS:SG	3.01	0.54
1:A:779:ALA:O	1:A:803:GLY:O	2.26	0.54
1:A:815:ILE:O	1:A:816:THR:HG23	2.07	0.54
1:A:898:THR:HG22	2:B:858:PRO:CG	2.37	0.54
1:A:939:ASN:HD22	1:A:939:ASN:N	2.05	0.54
2:B:219:GLN:C	2:B:327:TYR:OH	2.51	0.54
2:B:450:GLU:CB	2:B:451:PRO:CD	2.78	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:HIS:CD2	1:A:20:HIS:C	2.86	0.54
1:A:431:PHE:CD1	1:A:432:THR:N	2.76	0.54
1:A:546:ALA:CB	1:A:681:ALA:O	2.56	0.54
1:A:588:ALA:CB	1:A:592:GLN:OE1	2.53	0.54
1:A:634:ILE:HD13	1:A:634:ILE:N	2.09	0.54
1:A:532:ALA:C	1:A:535:CYS:SG	2.90	0.54
2:B:611:SER:O	2:B:615:MET:CG	2.53	0.54
2:B:633:ILE:HD13	2:B:643:VAL:HG11	1.89	0.54
2:B:672:ASN:HB3	2:B:754:TYR:CE2	2.42	0.54
1:A:52:THR:HG21	1:A:601:MET:CE	2.06	0.54
1:A:298:VAL:HG12	1:A:299:HIS:N	2.23	0.54
1:A:350:TYR:CD2	1:A:383:PHE:CD1	2.96	0.54
1:A:387:ASN:ND2	1:A:391:GLY:HA2	2.21	0.54
2:B:271:MET:HE3	2:B:299:MET:HE2	1.90	0.54
2:B:502:VAL:CG1	2:B:901:LEU:HD12	2.28	0.54
2:B:563:GLY:O	2:B:564:SER:OG	2.22	0.54
2:B:576:TYR:CE1	2:B:578:PHE:CZ	2.94	0.54
2:B:607:THR:HG22	2:B:612:TYR:OH	2.08	0.54
2:B:806:TYR:CD1	2:B:806:TYR:C	2.86	0.54
2:B:26:GLN:HG3	2:B:27:THR:HG23	1.90	0.54
2:B:231:ILE:C	2:B:231:ILE:HD13	2.33	0.54
2:B:597:LEU:CD1	2:B:644:ASP:CG	2.51	0.54
1:A:72:ARG:HH22	1:A:863:VAL:CG2	2.20	0.53
1:A:211:VAL:CG2	1:A:216:GLN:CG	2.86	0.53
1:A:279:GLY:O	1:A:333:TRP:HA	2.08	0.53
1:A:833:ARG:HH12	1:A:874:PRO:HG2	1.74	0.53
1:A:950:MET:HG3	2:B:114:ASN:ND2	2.22	0.53
2:B:442:PRO:HG2	2:B:576:TYR:CD1	2.43	0.53
2:B:498:ILE:CD1	2:B:820:PHE:CZ	2.91	0.53
1:A:442:ALA:HA	1:A:509:VAL:HG13	1.87	0.53
1:A:554:ASP:OD1	1:A:672:PRO:CB	2.45	0.53
1:A:619:VAL:HG23	1:A:620:ASP:H	1.72	0.53
1:A:940:PRO:HB2	1:A:944:MET:HE2	1.90	0.53
2:B:56:ARG:HH22	2:B:485:GLN:NE2	2.07	0.53
2:B:114:ASN:CB	2:B:119:TYR:CD2	2.91	0.53
2:B:585:ASP:OD2	2:B:689:ILE:HD13	2.08	0.53
1:A:349:LEU:HD21	1:A:400:PHE:CE1	2.42	0.53
1:A:950:MET:CE	2:B:112:THR:CG2	2.81	0.53
2:B:130:ALA:HB2	2:B:922:GLY:O	2.08	0.53
2:B:223:ALA:HB2	2:B:327:TYR:CE2	2.42	0.53
1:A:52:THR:HG23	1:A:606:THR:OG1	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:PHE:HE1	1:A:71:SER:OG	1.91	0.53
1:A:83:VAL:O	1:A:95:GLN:CB	2.56	0.53
1:A:240:LYS:HA	1:A:632:ARG:HH12	1.73	0.53
2:B:56:ARG:O	2:B:481:ARG:NH2	2.41	0.53
2:B:433:TRP:CD2	2:B:434:MET:N	2.68	0.53
2:B:577:TYR:CD1	2:B:577:TYR:C	2.85	0.53
2:B:752:HIS:N	2:B:753:PRO:HD2	2.23	0.53
2:B:794:GLN:CD	2:B:796:ASP:O	2.51	0.53
1:A:66:LEU:HD13	1:A:519:LEU:HD22	1.90	0.53
2:B:34:THR:HG22	2:B:980:ASN:HA	1.89	0.53
2:B:556:ALA:CA	2:B:566:MET:HE1	2.39	0.53
2:B:751:ARG:C	2:B:753:PRO:HD2	2.33	0.53
1:A:204:SER:OG	1:A:523:TYR:CZ	2.50	0.53
1:A:481:LEU:H	1:A:481:LEU:HD13	1.73	0.53
1:A:736:LEU:HD23	1:A:737:GLY:N	2.23	0.53
1:A:789:ARG:NH2	1:A:799:VAL:HG23	2.24	0.53
1:A:833:ARG:NH1	1:A:874:PRO:HG2	2.23	0.53
2:B:129:ILE:HB	2:B:934:SER:OG	2.09	0.53
2:B:411:VAL:O	2:B:415:VAL:HG23	2.07	0.53
2:B:442:PRO:HG2	2:B:576:TYR:CD2	2.44	0.53
2:B:510:THR:HG22	2:B:632:THR:HB	1.90	0.53
2:B:593:THR:O	2:B:595:ARG:HB2	2.08	0.53
1:A:446:ARG:O	1:A:501:ASN:HB3	2.08	0.53
1:A:967:GLN:C	1:A:969:GLU:N	2.58	0.53
2:B:533:TYR:O	2:B:534:ALA:CB	2.52	0.53
1:A:671:LEU:O	1:A:671:LEU:CD2	2.57	0.53
2:B:340:ALA:CB	2:B:386:THR:HB	2.39	0.53
1:A:336:ARG:O	1:A:337:HIS:HB2	2.06	0.53
1:A:562:LEU:O	1:A:563:PHE:C	2.51	0.53
1:A:767:ARG:HH21	1:A:771:ILE:HD11	1.74	0.53
2:B:295:TYR:CE2	2:B:296:ALA:HB2	2.44	0.53
2:B:334:CYS:SG	2:B:468:MET:HE3	2.47	0.53
2:B:732:TRP:HE3	2:B:732:TRP:O	1.91	0.53
2:B:838:ARG:HH11	2:B:838:ARG:CG	2.18	0.53
1:A:255:PRO:HD3	1:A:556:HIS:HD2	1.74	0.53
1:A:492:VAL:CG1	1:A:495:VAL:HG22	2.37	0.53
1:A:555:VAL:HG12	1:A:687:THR:HG23	1.88	0.53
1:A:634:ILE:CB	1:A:688:GLU:HB3	2.39	0.53
1:A:950:MET:HE1	2:B:112:THR:HG22	1.82	0.53
2:B:254:GLN:CD	2:B:254:GLN:H	2.16	0.53
2:B:373:THR:O	2:B:381:THR:HB	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:CD1	1:A:439:ALA:O	2.57	0.52
1:A:948:PHE:HB3	2:B:149:GLN:NE2	2.22	0.52
2:B:128:ILE:O	2:B:142:SER:HB3	2.09	0.52
2:B:349:LYS:H	2:B:349:LYS:CD	2.22	0.52
2:B:648:VAL:HG22	2:B:809:GLU:CD	2.33	0.52
2:B:729:ARG:HD3	2:B:754:TYR:CE1	2.44	0.52
2:B:734:LEU:CD2	2:B:735:HIS:N	2.65	0.52
1:A:238:HIS:HA	1:A:244:ALA:O	2.10	0.52
1:A:490:PHE:O	1:A:491:LEU:C	2.49	0.52
1:A:589:LEU:H	1:A:589:LEU:HD13	1.70	0.52
1:A:621:VAL:O	1:A:621:VAL:HG13	2.08	0.52
2:B:294:ASP:O	2:B:295:TYR:C	2.52	0.52
2:B:640:ALA:CB	2:B:887:THR:HG21	2.40	0.52
2:B:838:ARG:CZ	2:B:932:SER:CB	2.87	0.52
1:A:899:LEU:O	1:A:899:LEU:HD12	2.09	0.52
1:A:88:THR:CG2	1:A:89:ASP:N	2.73	0.52
1:A:145:ILE:HD11	1:A:157:MET:HE3	1.91	0.52
1:A:288:VAL:HG22	1:A:296:ALA:HB2	1.90	0.52
1:A:531:LEU:CD2	1:A:747:ILE:CD1	2.82	0.52
1:A:920:GLY:O	1:A:922:ASN:N	2.41	0.52
2:B:227:VAL:O	2:B:231:ILE:HG22	2.09	0.52
2:B:662:GLN:HG3	2:B:662:GLN:O	2.09	0.52
1:A:49:LEU:HD21	1:A:608:LEU:HA	1.92	0.52
1:A:233:GLU:CG	1:A:339:LYS:HB3	2.39	0.52
1:A:249:PRO:CB	1:A:252:TRP:CD1	2.92	0.52
1:A:452:ARG:NH2	1:A:452:ARG:CG	2.73	0.52
1:A:887:PRO:HG2	2:B:504:ALA:O	2.09	0.52
1:A:958:THR:CG2	1:A:959:LYS:N	2.73	0.52
2:B:262:MET:SD	2:B:262:MET:C	2.92	0.52
2:B:589:TYR:CD1	2:B:589:TYR:N	2.76	0.52
2:B:672:ASN:C	2:B:754:TYR:HE2	2.17	0.52
2:B:672:ASN:CB	2:B:754:TYR:CZ	2.92	0.52
1:A:591:ALA:HB3	1:A:613:GLN:HB2	1.91	0.52
1:A:805:ILE:HG23	1:A:806:PRO:HD2	1.91	0.52
1:A:884:ALA:HB2	2:B:506:PRO:HB3	0.59	0.52
2:B:528:TYR:HD2	2:B:560:TRP:CZ2	2.28	0.52
2:B:686:HIS:HD2	2:B:786:ALA:CB	2.19	0.52
1:A:44:TYR:O	1:A:45:ASP:HB3	2.10	0.52
1:A:55:LEU:HD13	1:A:528:MET:HE1	0.98	0.52
1:A:189:ARG:NH2	1:A:189:ARG:CG	2.72	0.52
1:A:347:LYS:NZ	1:A:347:LYS:CB	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:TRP:CE2	1:A:712:GLY:HA3	2.45	0.52
1:A:883:LEU:N	1:A:883:LEU:CD2	2.72	0.52
2:B:161:LEU:O	2:B:161:LEU:HD22	2.09	0.52
2:B:257:PHE:N	2:B:301:VAL:O	2.37	0.52
2:B:264:THR:CB	2:B:265:PRO:CD	2.84	0.52
2:B:615:MET:O	2:B:618:LEU:HB2	2.10	0.52
1:A:244:ALA:HB1	1:A:274:VAL:CG2	2.30	0.52
1:A:627:ARG:O	1:A:729:SER:HA	2.10	0.52
1:A:713:LEU:HD23	1:A:713:LEU:C	2.15	0.52
1:A:970:LEU:N	1:A:970:LEU:CD1	2.73	0.52
2:B:64:LEU:N	2:B:64:LEU:CD1	2.73	0.52
2:B:74:MET:HE2	2:B:984:ILE:HD13	1.91	0.52
2:B:89:ASP:HA	2:B:410:GLN:CD	2.34	0.52
2:B:102:VAL:O	2:B:106:LYS:HG3	2.10	0.52
2:B:268:ALA:O	2:B:589:TYR:HB2	2.10	0.52
2:B:329:LEU:HG	2:B:450:GLU:CD	2.35	0.52
2:B:374:GLY:C	2:B:375:VAL:HG22	2.34	0.52
1:A:253:LEU:HD22	1:A:628:SER:OG	2.09	0.52
1:A:345:GLN:O	1:A:346:LEU:C	2.50	0.52
1:A:380:CYS:HG	1:A:435:GLN:CA	2.11	0.52
1:A:671:LEU:O	1:A:671:LEU:HD22	2.10	0.52
1:A:844:GLY:O	1:A:849:ASP:CG	2.53	0.52
1:A:936:TYR:OH	2:B:610:ASP:CG	2.53	0.52
2:B:363:VAL:CG1	2:B:441:MET:HE2	2.33	0.52
1:A:127:PHE:CE1	1:A:452:ARG:CD	2.93	0.52
1:A:200:VAL:HG11	1:A:522:THR:HG21	1.92	0.52
1:A:297:ARG:NE	1:A:701:SER:OG	2.39	0.52
1:A:407:HIS:CE1	1:A:490:PHE:CE2	2.98	0.52
1:A:562:LEU:CD2	1:A:562:LEU:N	2.73	0.52
1:A:676:THR:O	1:A:676:THR:CG2	2.58	0.52
1:A:952:THR:HG21	2:B:115:ALA:CB	2.40	0.52
2:B:1:MET:CG	2:B:2:SER:H	2.22	0.52
1:A:253:LEU:N	1:A:253:LEU:CD1	2.73	0.51
1:A:329:HIS:CD2	1:A:348:GLN:HE22	2.28	0.51
1:A:969:GLU:C	1:A:971:ARG:H	2.17	0.51
2:B:48:ALA:C	2:B:49:THR:HG23	2.36	0.51
2:B:257:PHE:HD1	2:B:357:HIS:CD2	2.28	0.51
2:B:467:GLN:HE21	2:B:467:GLN:CA	2.17	0.51
1:A:26:LEU:O	1:A:27:LYS:C	2.54	0.51
1:A:815:ILE:O	1:A:816:THR:CB	2.58	0.51
1:A:865:ARG:NH1	2:B:447:PRO:HG3	2.22	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:ARG:NE	2:B:155:GLU:CD	2.56	0.51
2:B:214:ARG:NH1	2:B:214:ARG:CB	2.73	0.51
2:B:230:THR:HG21	2:B:364:MET:CB	2.40	0.51
2:B:234:TRP:O	2:B:237:HIS:O	2.29	0.51
2:B:349:LYS:CD	2:B:349:LYS:N	2.73	0.51
1:A:198:ARG:HH11	1:A:198:ARG:CG	2.22	0.51
1:A:754:VAL:HG23	1:A:754:VAL:O	2.09	0.51
2:B:139:ILE:C	2:B:140:GLU:HG2	2.35	0.51
2:B:219:GLN:C	2:B:327:TYR:HH	2.17	0.51
2:B:251:LEU:CD2	2:B:305:LEU:HD12	2.40	0.51
2:B:259:VAL:CG1	2:B:260:LYS:N	2.73	0.51
2:B:373:THR:OG1	2:B:373:THR:O	2.24	0.51
2:B:549:LYS:N	2:B:549:LYS:CD	2.73	0.51
1:A:203:ASN:ND2	1:A:432:THR:OG1	2.43	0.51
1:A:208:HIS:HE1	1:A:217:GLU:OE1	1.94	0.51
1:A:455:HIS:HB3	1:A:611:LEU:CD2	2.40	0.51
2:B:162:SER:OG	2:B:440:LEU:CD1	2.57	0.51
1:A:297:ARG:HG2	1:A:297:ARG:HH11	1.75	0.51
1:A:298:VAL:CG1	1:A:300:TYR:CE1	2.94	0.51
1:A:422:ILE:CD1	1:A:422:ILE:N	2.74	0.51
1:A:455:HIS:CB	1:A:615:TYR:HE2	2.22	0.51
1:A:690:TRP:CH2	1:A:721:VAL:HG21	2.46	0.51
2:B:216:SER:CB	2:B:447:PRO:O	2.55	0.51
2:B:262:MET:SD	2:B:263:LEU:N	2.83	0.51
2:B:359:ASN:O	2:B:363:VAL:HG23	2.09	0.51
2:B:618:LEU:CD1	2:B:623:ILE:CD1	2.82	0.51
2:B:652:HIS:O	2:B:653:VAL:HB	2.11	0.51
1:A:6:GLN:HA	1:A:6:GLN:NE2	2.11	0.51
1:A:55:LEU:CG	1:A:528:MET:HE2	1.96	0.51
1:A:185:ASN:ND2	1:A:488:SER:OG	2.42	0.51
1:A:450:SER:O	1:A:451:GLU:C	2.52	0.51
1:A:786:THR:OG1	1:A:823:VAL:O	2.18	0.51
1:A:925:VAL:CG1	1:A:926:THR:N	2.73	0.51
1:A:928:ARG:HB3	2:B:601:ALA:HB2	1.92	0.51
2:B:102:VAL:HG12	2:B:106:LYS:HD2	1.93	0.51
2:B:747:ALA:CB	2:B:749:THR:CG2	2.63	0.51
1:A:66:LEU:O	1:A:67:PRO:C	2.53	0.51
1:A:477:SER:O	1:A:478:LEU:HG	2.11	0.51
1:A:502:ASP:HB2	2:B:994:LEU:HB2	1.91	0.51
1:A:868:TYR:CE1	2:B:772:PHE:HE2	2.26	0.51
2:B:224:LEU:HG	2:B:404:MET:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:ALA:O	2:B:564:SER:CA	2.59	0.51
1:A:260:THR:CG2	1:A:263:GLU:CD	2.84	0.51
1:A:290:GLN:CG	1:A:413:GLN:NE2	2.70	0.51
1:A:479:SER:O	1:A:481:LEU:HD13	2.10	0.51
1:A:607:ARG:NH2	1:A:607:ARG:CG	2.73	0.51
2:B:168:THR:OG1	2:B:545:ARG:HD2	2.11	0.51
2:B:585:ASP:HA	2:B:656:TYR:OH	2.11	0.51
2:B:838:ARG:HH12	2:B:932:SER:CB	2.24	0.51
1:A:219:GLY:O	1:A:220:GLU:C	2.51	0.51
1:A:268:GLU:CD	1:A:693:THR:HG21	2.31	0.51
1:A:384:LEU:CB	1:A:385:LEU:HD13	2.39	0.51
1:A:446:ARG:CG	1:A:446:ARG:NH1	2.73	0.51
1:A:607:ARG:HH21	1:A:607:ARG:CG	2.23	0.51
1:A:704:ILE:O	1:A:707:ILE:HD13	2.10	0.51
1:A:839:GLU:O	1:A:842:ARG:N	2.44	0.51
1:A:921:ASP:CB	2:B:626:ALA:CB	2.86	0.51
1:A:238:HIS:CD2	1:A:338:SER:HB3	2.45	0.51
1:A:353:MET:HE3	1:A:385:LEU:HB2	1.92	0.51
1:A:377:LEU:O	1:A:378:GLY:C	2.53	0.51
1:A:574:LEU:HD22	1:A:577:ARG:HD3	1.93	0.51
1:A:655:TYR:OH	1:A:683:PRO:HG3	2.10	0.51
1:A:672:PRO:HG3	1:A:713:LEU:CD1	2.40	0.51
1:A:783:ASP:OD1	1:A:783:ASP:N	2.44	0.51
2:B:117:ARG:NH2	2:B:259:VAL:O	2.44	0.51
2:B:197:PRO:HD2	2:B:457:TRP:CE3	2.46	0.51
2:B:509:ILE:CD1	2:B:813:ILE:HD11	2.41	0.51
1:A:833:ARG:NH2	2:B:527:GLN:OE1	2.44	0.50
2:B:198:MET:CB	2:B:204:GLN:NE2	2.74	0.50
2:B:549:LYS:HA	2:B:550:MET:SD	2.51	0.50
2:B:665:GLY:C	2:B:667:GLN:N	2.67	0.50
1:A:271:ALA:O	1:A:274:VAL:HG12	2.11	0.50
1:A:421:GLY:C	1:A:422:ILE:HD13	2.37	0.50
2:B:96:GLN:OE1	2:B:96:GLN:HA	2.10	0.50
2:B:480:LEU:HD23	2:B:950:LEU:O	2.11	0.50
2:B:673:TRP:CZ3	2:B:677:HIS:CE1	2.99	0.50
1:A:52:THR:CB	1:A:601:MET:HE2	2.39	0.50
1:A:562:LEU:HD22	1:A:562:LEU:H	1.76	0.50
1:A:736:LEU:HD23	1:A:737:GLY:H	1.76	0.50
1:A:843:ARG:NH1	1:A:843:ARG:CG	2.73	0.50
2:B:128:ILE:C	2:B:129:ILE:HD13	2.36	0.50
2:B:383:HIS:CD2	2:B:384:ALA:H	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:680:LYS:HG3	2:B:758:LEU:HD11	1.94	0.50
1:A:46:LEU:HD21	1:A:458:ILE:HD13	1.82	0.50
1:A:508:SER:CB	2:B:992:TYR:CZ	2.95	0.50
1:A:648:LYS:O	1:A:649:HIS:CB	2.58	0.50
1:A:833:ARG:CG	1:A:833:ARG:NH1	2.73	0.50
2:B:13:SER:HA	2:B:14:PRO:C	2.36	0.50
2:B:43:THR:HG21	2:B:55:LYS:HG2	1.94	0.50
2:B:260:LYS:NZ	2:B:272:ASP:OD1	2.43	0.50
2:B:265:PRO:CD	2:B:266:HIS:N	2.74	0.50
2:B:334:CYS:HB3	2:B:468:MET:HE3	1.93	0.50
2:B:838:ARG:CZ	2:B:932:SER:HB2	2.42	0.50
1:A:316:LEU:HD22	1:A:350:TYR:OH	2.07	0.50
1:A:344:ILE:HG13	1:A:345:GLN:H	1.77	0.50
1:A:961:LEU:HD11	2:B:284:MET:CB	2.41	0.50
1:A:968:MET:CE	2:B:659:ILE:HG21	2.27	0.50
2:B:122:CYS:CB	2:B:939:MET:CE	2.88	0.50
2:B:216:SER:HB2	2:B:448:MET:HA	1.94	0.50
2:B:271:MET:HE1	2:B:279:TYR:HD2	1.76	0.50
2:B:589:TYR:N	2:B:589:TYR:HD1	2.09	0.50
2:B:623:ILE:CG2	2:B:893:ILE:HG12	2.41	0.50
2:B:676:TRP:CD1	2:B:754:TYR:CB	2.87	0.50
2:B:801:GLN:HG3	2:B:801:GLN:O	2.10	0.50
2:B:832:HIS:CE1	2:B:837:ALA:CB	2.95	0.50
1:A:68:PHE:O	1:A:69:GLU:C	2.54	0.50
1:A:215:LEU:N	1:A:215:LEU:CD1	2.75	0.50
1:A:305:ASP:HA	2:B:710:HIS:CD2	2.46	0.50
1:A:432:THR:C	1:A:435:GLN:HB2	2.36	0.50
1:A:542:GLU:HB2	1:A:733:SER:HB3	1.93	0.50
1:A:634:ILE:H	1:A:634:ILE:CD1	2.14	0.50
2:B:409:GLU:HA	2:B:409:GLU:OE2	2.11	0.50
1:A:478:LEU:HD11	1:A:740:GLU:OE2	2.11	0.50
1:A:492:VAL:CG2	1:A:495:VAL:CG2	2.89	0.50
1:A:513:GLY:N	2:B:188:GLY:HA3	2.27	0.50
1:A:518:LEU:CD2	1:A:518:LEU:C	2.84	0.50
1:A:690:TRP:HZ3	1:A:721:VAL:HG23	1.74	0.50
1:A:789:ARG:HH21	1:A:799:VAL:HG23	1.76	0.50
1:A:830:ARG:O	1:A:836:THR:CG2	2.60	0.50
2:B:198:MET:CG	2:B:204:GLN:HE22	2.20	0.50
2:B:355:ALA:HB3	2:B:358:ALA:CB	2.41	0.50
1:A:238:HIS:HD2	1:A:338:SER:CB	2.24	0.50
1:A:285:ILE:CD1	1:A:395:PHE:HB3	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:MET:CE	1:A:135:CYS:CA	2.90	0.50
1:A:511:ASP:O	2:B:189:ALA:O	2.30	0.50
1:A:619:VAL:CG2	1:A:620:ASP:N	2.73	0.50
1:A:655:TYR:HE1	1:A:666:VAL:HG12	1.77	0.50
2:B:717:GLY:O	2:B:722:GLU:OE2	2.30	0.50
2:B:752:HIS:N	2:B:753:PRO:CD	2.74	0.50
1:A:54:GLU:OE2	1:A:600:SER:CB	2.60	0.49
1:A:76:GLU:HB3	1:A:103:ARG:HG3	1.92	0.49
1:A:492:VAL:CG2	1:A:495:VAL:HG21	2.42	0.49
1:A:777:LEU:HD22	1:A:834:MET:HE1	1.92	0.49
2:B:409:GLU:HG3	2:B:409:GLU:O	2.12	0.49
2:B:1002:THR:HG23	2:B:1004:ASP:OD2	2.12	0.49
1:A:75:LEU:HD11	1:A:106:LEU:HD22	1.94	0.49
1:A:886:ARG:NH1	1:A:889:GLU:HG2	2.27	0.49
2:B:216:SER:HA	2:B:447:PRO:O	2.12	0.49
2:B:330:ALA:HA	2:B:378:THR:CG2	2.42	0.49
2:B:378:THR:HG23	2:B:451:PRO:HG3	1.94	0.49
2:B:633:ILE:O	2:B:633:ILE:HG22	2.12	0.49
1:A:160:VAL:HG23	1:A:497:PHE:HB2	1.94	0.49
1:A:885:LEU:C	1:A:886:ARG:CG	2.85	0.49
2:B:84:THR:HG21	2:B:545:ARG:CD	2.36	0.49
2:B:219:GLN:OE1	2:B:444:VAL:HG13	2.13	0.49
2:B:604:VAL:HG13	2:B:880:VAL:CG1	2.42	0.49
2:B:671:TYR:CE2	2:B:675:LEU:HD11	2.46	0.49
1:A:131:ARG:HH11	1:A:131:ARG:HG3	1.77	0.49
1:A:145:ILE:HD11	1:A:157:MET:SD	2.52	0.49
1:A:212:ASN:OD1	1:A:213:GLY:N	2.45	0.49
1:A:244:ALA:CB	1:A:632:ARG:NH2	2.75	0.49
1:A:392:HIS:O	1:A:408:GLU:HG3	2.12	0.49
1:A:939:ASN:O	1:A:939:ASN:ND2	2.45	0.49
2:B:130:ALA:HB3	2:B:141:TYR:HD1	1.77	0.49
2:B:547:ALA:C	2:B:548:ASN:O	2.52	0.49
1:A:342:LEU:C	1:A:342:LEU:CD2	2.85	0.49
1:A:968:MET:CE	2:B:659:ILE:HD13	2.42	0.49
2:B:7:GLN:HG2	2:B:29:VAL:HG13	1.88	0.49
2:B:32:LYS:HD2	2:B:69:GLU:OE1	2.10	0.49
2:B:329:LEU:HD12	2:B:450:GLU:CD	2.37	0.49
2:B:543:ASN:O	2:B:545:ARG:N	2.46	0.49
2:B:633:ILE:HD13	2:B:643:VAL:CG1	2.42	0.49
2:B:647:LEU:HA	2:B:807:PHE:O	2.12	0.49
2:B:676:TRP:HE1	2:B:754:TYR:H	1.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:839:LEU:HD22	2:B:866:LEU:CD2	2.27	0.49
1:A:19:LYS:HG2	1:A:140:LEU:CD2	2.39	0.49
1:A:472:ASP:O	1:A:475:ASN:O	2.30	0.49
1:A:508:SER:HB2	2:B:992:TYR:CD2	2.48	0.49
1:A:555:VAL:H	1:A:687:THR:CG2	2.23	0.49
1:A:650:ALA:CB	1:A:796:SER:HA	2.39	0.49
1:A:961:LEU:CD1	2:B:284:MET:HB3	2.42	0.49
1:A:971:ARG:HH11	2:B:735:HIS:CD2	2.31	0.49
2:B:224:LEU:HB2	2:B:404:MET:CG	2.42	0.49
2:B:399:PHE:HZ	2:B:466:LEU:HD22	1.76	0.49
2:B:799:ARG:NH1	2:B:799:ARG:CG	2.73	0.49
1:A:551:ARG:HH11	1:A:551:ARG:CG	2.26	0.49
1:A:828:ARG:CG	1:A:828:ARG:NH1	2.74	0.49
1:A:965:ARG:HD2	1:A:965:ARG:C	2.38	0.49
1:A:973:GLY:O	2:B:791:ILE:HD12	2.05	0.49
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.15	0.49
2:B:78:LEU:CD2	2:B:180:LEU:CD2	2.89	0.49
2:B:619:GLU:HB2	2:B:622:LEU:HD11	1.95	0.49
1:A:232:TRP:N	1:A:342:LEU:O	2.41	0.49
1:A:371:LEU:HD11	1:A:419:LEU:HD13	1.95	0.49
1:A:589:LEU:CD1	1:A:589:LEU:N	2.73	0.49
1:A:644:SER:O	1:A:647:ILE:N	2.46	0.49
1:A:925:VAL:CG1	1:A:926:THR:H	2.25	0.49
2:B:214:ARG:NH1	2:B:214:ARG:CG	2.73	0.49
2:B:259:VAL:HG12	2:B:299:MET:HE3	1.95	0.49
1:A:247:PRO:HB3	1:A:477:SER:CB	2.29	0.49
1:A:353:MET:HE1	1:A:385:LEU:HB2	1.93	0.49
1:A:534:VAL:HG12	1:A:740:GLU:HG3	1.94	0.49
2:B:114:ASN:O	2:B:116:GLY:N	2.45	0.49
2:B:387:VAL:HG23	2:B:387:VAL:O	2.13	0.49
2:B:672:ASN:HB2	2:B:754:TYR:OH	2.13	0.49
2:B:681:THR:O	2:B:785:ARG:NE	2.46	0.49
1:A:55:LEU:HD23	1:A:55:LEU:C	2.38	0.49
1:A:72:ARG:HH22	1:A:863:VAL:HG21	1.77	0.49
1:A:152:VAL:HG12	1:A:156:THR:CG2	2.43	0.49
1:A:230:LEU:O	1:A:343:THR:HA	2.13	0.49
1:A:289:THR:HG22	1:A:290:GLN:N	2.28	0.49
1:A:454:CYS:O	1:A:458:ILE:HG22	2.13	0.49
1:A:508:SER:HB2	2:B:992:TYR:CD1	2.48	0.49
1:A:544:MET:O	1:A:544:MET:HG2	2.12	0.49
1:A:646:LEU:CB	1:A:669:ILE:HD13	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:ARG:O	1:A:938:ARG:HG3	2.13	0.49
2:B:626:ALA:O	2:B:643:VAL:HA	2.13	0.49
2:B:846:THR:CB	2:B:847:PRO:HD2	2.40	0.49
1:A:75:LEU:HB2	1:A:104:ALA:HB3	1.94	0.48
1:A:519:LEU:C	1:A:519:LEU:CD2	2.85	0.48
2:B:48:ALA:O	2:B:49:THR:CB	2.61	0.48
2:B:331:LEU:HB2	2:B:378:THR:HB	1.94	0.48
1:A:58:GLN:HB3	1:A:860:ILE:HD12	1.94	0.48
1:A:335:GLY:HA2	1:A:341:HIS:CD2	2.46	0.48
1:A:339:LYS:O	1:A:341:HIS:CD2	2.66	0.48
1:A:464:MET:SD	1:A:483:PHE:HZ	2.36	0.48
1:A:492:VAL:HG21	1:A:495:VAL:HG21	1.95	0.48
2:B:110:GLN:NE2	2:B:110:GLN:CA	2.73	0.48
2:B:117:ARG:HG2	2:B:155:GLU:HG3	1.95	0.48
2:B:265:PRO:HD2	2:B:266:HIS:N	2.24	0.48
2:B:311:ARG:O	2:B:312:SER:OG	2.19	0.48
2:B:509:ILE:HD11	2:B:811:ALA:HB3	1.95	0.48
2:B:510:THR:HG22	2:B:632:THR:CB	2.42	0.48
2:B:551:VAL:CG1	2:B:579:GLY:HA3	2.40	0.48
2:B:659:ILE:HD12	2:B:788:LEU:CD2	2.22	0.48
1:A:129:THR:HG21	1:A:447:TYR:O	2.12	0.48
1:A:238:HIS:CE1	1:A:334:LYS:CD	2.85	0.48
1:A:317:SER:CB	1:A:323:GLY:HA2	2.42	0.48
1:A:330:TYR:HE2	1:A:397:PRO:HG3	1.77	0.48
1:A:374:PHE:CZ	1:A:442:ALA:HB3	2.49	0.48
1:A:522:THR:HG23	1:A:523:TYR:N	2.28	0.48
1:A:553:THR:HG22	1:A:558:VAL:CG2	2.36	0.48
1:A:634:ILE:N	1:A:634:ILE:CD1	2.74	0.48
1:A:634:ILE:HG23	1:A:726:TYR:HB3	1.95	0.48
1:A:672:PRO:HG3	1:A:713:LEU:HD11	1.95	0.48
1:A:838:PRO:O	1:A:841:HIS:CB	2.61	0.48
1:A:940:PRO:HB2	1:A:944:MET:CE	2.43	0.48
2:B:156:PRO:HG2	2:B:356:GLY:O	2.14	0.48
2:B:556:ALA:CB	2:B:566:MET:HE1	2.43	0.48
2:B:686:HIS:ND1	2:B:686:HIS:N	2.60	0.48
2:B:734:LEU:O	2:B:735:HIS:CB	2.61	0.48
2:B:838:ARG:NH1	2:B:932:SER:CB	2.77	0.48
1:A:248:VAL:HG11	1:A:630:PHE:CD1	2.47	0.48
1:A:299:HIS:HA	1:A:700:GLY:O	2.13	0.48
1:A:703:VAL:O	1:A:707:ILE:HD12	2.13	0.48
1:A:757:HIS:HD2	1:A:758:THR:H	1.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:TYR:OH	2:B:610:ASP:OD1	2.32	0.48
2:B:161:LEU:CD1	2:B:161:LEU:N	2.75	0.48
2:B:433:TRP:CD1	2:B:434:MET:H	2.23	0.48
1:A:229:TYR:HB3	1:A:343:THR:CG2	2.43	0.48
1:A:244:ALA:CB	1:A:274:VAL:HG22	2.38	0.48
1:A:244:ALA:HB2	1:A:632:ARG:NH2	2.29	0.48
1:A:972:GLU:C	2:B:798:GLY:H	2.20	0.48
2:B:307:LYS:HG2	2:B:311:ARG:HH21	1.76	0.48
2:B:322:GLU:OE2	2:B:375:VAL:HG21	2.13	0.48
2:B:559:ALA:O	2:B:562:LEU:O	2.31	0.48
1:A:495:VAL:CG2	1:A:496:GLN:N	2.75	0.48
1:A:644:SER:O	1:A:647:ILE:HB	2.13	0.48
2:B:311:ARG:HD2	2:B:782:MET:SD	2.54	0.48
1:A:458:ILE:HG23	1:A:459:THR:N	2.29	0.48
1:A:504:GLU:OE1	1:A:504:GLU:N	2.46	0.48
1:A:815:ILE:CG2	1:A:816:THR:N	2.46	0.48
2:B:397:LEU:HD23	2:B:397:LEU:C	2.38	0.48
2:B:930:ASN:N	2:B:930:ASN:OD1	2.47	0.48
1:A:264:ARG:O	1:A:268:GLU:HG3	2.14	0.48
1:A:286:ASP:CG	1:A:287:GLY:N	2.71	0.48
1:A:326:SER:HB2	1:A:389:ARG:NH2	2.29	0.48
1:A:353:MET:O	1:A:354:SER:C	2.56	0.48
1:A:429:ALA:O	1:A:430:THR:C	2.55	0.48
1:A:692:ALA:HB3	1:A:721:VAL:HB	1.95	0.48
1:A:885:LEU:CD2	2:B:636:ASN:ND2	2.77	0.48
2:B:36:GLU:HG2	2:B:65:GLU:CG	2.44	0.48
2:B:267:ILE:HG13	2:B:268:ALA:N	2.28	0.48
1:A:262:ARG:HH22	1:A:402:VAL:N	2.07	0.48
1:A:367:ILE:HD11	1:A:415:GLN:NE2	0.72	0.48
1:A:508:SER:HB2	2:B:992:TYR:CG	2.48	0.48
1:A:892:CYS:O	2:B:902:GLN:OE1	2.32	0.48
2:B:586:GLY:CA	2:B:588:PHE:CE1	2.97	0.48
1:A:38:ASN:C	1:A:38:ASN:ND2	2.72	0.48
1:A:167:MET:C	1:A:167:MET:SD	2.97	0.48
1:A:317:SER:OG	1:A:389:ARG:HD2	2.14	0.48
1:A:351:HIS:ND1	1:A:351:HIS:C	2.72	0.48
1:A:517:GLU:O	1:A:521:ALA:HB2	2.13	0.48
1:A:518:LEU:HD23	1:A:518:LEU:C	2.39	0.48
1:A:556:HIS:HD1	1:A:626:ILE:CD1	2.27	0.48
1:A:562:LEU:CD2	1:A:562:LEU:H	2.26	0.48
1:A:969:GLU:C	1:A:971:ARG:N	2.71	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:GLN:O	2:B:254:GLN:HG2	2.13	0.48
2:B:260:LYS:HD2	2:B:260:LYS:C	2.38	0.48
2:B:722:GLU:HG3	2:B:729:ARG:HH22	1.78	0.48
2:B:926:ILE:HD13	2:B:933:VAL:HG22	1.95	0.48
1:A:54:GLU:OE1	1:A:600:SER:OG	2.27	0.47
1:A:81:ILE:HD12	1:A:98:GLU:HB3	1.95	0.47
1:A:288:VAL:O	1:A:324:ARG:CD	2.50	0.47
1:A:432:THR:O	1:A:435:GLN:HB3	2.07	0.47
1:A:692:ALA:HB1	1:A:722:HIS:N	2.29	0.47
1:A:829:THR:HG23	1:A:829:THR:O	2.12	0.47
1:A:906:ALA:C	1:A:907:VAL:HG13	2.39	0.47
2:B:195:VAL:HG13	2:B:195:VAL:O	2.13	0.47
2:B:751:ARG:C	2:B:753:PRO:CD	2.86	0.47
1:A:201:MET:HG3	1:A:400:PHE:CZ	2.49	0.47
1:A:351:HIS:C	1:A:351:HIS:HD1	2.22	0.47
1:A:387:ASN:HD22	1:A:391:GLY:HA3	1.74	0.47
1:A:828:ARG:HB3	1:A:828:ARG:NH1	2.12	0.47
2:B:432:GLU:HG2	2:B:817:GLY:HA3	1.96	0.47
2:B:442:PRO:HG2	2:B:576:TYR:CG	2.49	0.47
1:A:211:VAL:CG2	1:A:216:GLN:HB2	2.32	0.47
1:A:696:LEU:HD12	1:A:696:LEU:N	2.29	0.47
1:A:762:ARG:NE	1:A:815:ILE:HD13	2.30	0.47
2:B:173:ASP:O	2:B:177:LEU:HD12	2.13	0.47
2:B:329:LEU:CG	2:B:450:GLU:CD	2.88	0.47
2:B:753:PRO:HG2	2:B:756:ARG:NH1	2.24	0.47
1:A:111:ASN:HB2	1:A:467:GLN:CB	2.41	0.47
1:A:257:ALA:HB1	1:A:259:LEU:HG	1.96	0.47
2:B:877:CYS:SG	2:B:911:ILE:HD12	2.55	0.47
1:A:42:GLY:HA3	1:A:445:ARG:NH2	2.29	0.47
1:A:298:VAL:HG12	1:A:300:TYR:CE1	2.50	0.47
1:A:384:LEU:O	1:A:385:LEU:HD12	2.13	0.47
1:A:657:TRP:NE1	1:A:661:GLU:O	2.36	0.47
1:A:690:TRP:NE1	1:A:712:GLY:CA	2.77	0.47
1:A:849:ASP:OD2	1:A:911:TYR:OH	2.33	0.47
2:B:131:GLY:O	2:B:931:GLY:HA3	2.14	0.47
2:B:197:PRO:HG2	2:B:457:TRP:HA	1.96	0.47
1:A:44:TYR:HE2	1:A:444:MET:HE3	1.80	0.47
1:A:432:THR:C	1:A:435:GLN:H	2.22	0.47
1:A:650:ALA:HB1	1:A:796:SER:HB2	1.82	0.47
1:A:923:THR:HG21	2:B:627:THR:OG1	2.14	0.47
2:B:43:THR:HG21	2:B:55:LYS:CG	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:THR:HG22	2:B:823:LEU:HD21	1.95	0.47
2:B:499:TYR:CE2	2:B:860:MET:CG	2.95	0.47
2:B:836:GLU:HG2	2:B:936:LYS:HG2	1.97	0.47
2:B:867:SER:O	2:B:890:GLY:HA2	2.14	0.47
1:A:42:GLY:O	1:A:43:GLY:C	2.57	0.47
1:A:55:LEU:CD1	1:A:528:MET:CE	0.48	0.47
1:A:72:ARG:HG3	1:A:72:ARG:HH21	1.80	0.47
1:A:82:THR:O	1:A:82:THR:CG2	2.59	0.47
1:A:106:LEU:HD11	1:A:470:VAL:HG12	1.92	0.47
1:A:110:LEU:HD22	1:A:465:VAL:HG12	1.97	0.47
1:A:115:HIS:ND1	1:A:483:PHE:CZ	2.82	0.47
1:A:131:ARG:CG	1:A:131:ARG:NH1	2.74	0.47
1:A:153:THR:HG22	1:A:154:THR:N	2.29	0.47
1:A:202:HIS:ND1	1:A:202:HIS:C	2.72	0.47
1:A:246:THR:HG23	1:A:246:THR:O	2.14	0.47
1:A:307:MET:C	1:A:309:TRP:HD1	2.14	0.47
1:A:377:LEU:HD23	1:A:377:LEU:N	2.30	0.47
1:A:646:LEU:C	1:A:646:LEU:CD2	2.86	0.47
1:A:754:VAL:HA	1:A:854:ILE:O	2.14	0.47
1:A:934:PRO:HG3	2:B:610:ASP:CB	2.44	0.47
1:A:958:THR:CG2	1:A:959:LYS:H	2.28	0.47
1:A:961:LEU:CG	2:B:284:MET:SD	2.95	0.47
1:A:967:GLN:O	1:A:970:LEU:N	2.48	0.47
2:B:207:THR:O	2:B:211:ARG:HG3	2.14	0.47
2:B:327:TYR:HD1	2:B:329:LEU:CD1	2.28	0.47
2:B:355:ALA:H	2:B:358:ALA:HB3	1.79	0.47
2:B:514:THR:HG21	2:B:587:CYS:CB	2.43	0.47
2:B:623:ILE:CB	2:B:893:ILE:CG1	2.92	0.47
2:B:729:ARG:CG	2:B:754:TYR:CE1	2.94	0.47
1:A:81:ILE:CD1	1:A:98:GLU:HB3	2.42	0.47
1:A:214:ARG:NH1	1:A:216:GLN:NE2	2.63	0.47
1:A:472:ASP:CB	1:A:739:ALA:HB2	2.43	0.47
1:A:532:ALA:HB1	1:A:597:VAL:HG23	1.93	0.47
1:A:535:CYS:HG	1:A:536:GLU:N	2.13	0.47
1:A:702:LYS:NZ	1:A:702:LYS:CB	2.78	0.47
2:B:122:CYS:SG	2:B:826:TYR:HA	2.54	0.47
2:B:164:SER:HA	2:B:443:LYS:O	2.15	0.47
2:B:676:TRP:CZ3	2:B:680:LYS:HG3	2.50	0.47
1:A:64:GLY:O	1:A:65:LEU:CG	2.50	0.47
1:A:464:MET:HB3	1:A:483:PHE:HZ	1.77	0.47
1:A:792:THR:O	1:A:792:THR:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:LEU:H	1:A:931:LEU:HD12	1.78	0.47
2:B:122:CYS:HB3	2:B:939:MET:HE2	1.97	0.47
1:A:103:ARG:NH2	1:A:103:ARG:CG	2.73	0.47
1:A:125:MET:CG	1:A:136:ASP:OD2	2.63	0.47
1:A:215:LEU:CD1	1:A:215:LEU:H	2.28	0.47
1:A:529:ALA:HB2	1:A:612:ASN:ND2	2.29	0.47
1:A:714:ASN:O	1:A:714:ASN:ND2	2.48	0.47
1:A:750:GLU:C	1:A:751:HIS:ND1	2.73	0.47
1:A:830:ARG:HG2	1:A:831:PRO:HD2	1.97	0.47
1:A:888:TYR:O	1:A:894:ARG:NH2	2.46	0.47
2:B:77:LEU:CD2	2:B:192:VAL:HG13	2.45	0.47
2:B:247:ARG:CD	2:B:347:TRP:CD1	2.99	0.47
1:A:6:GLN:HB2	1:A:7:GLN:HG2	1.97	0.46
1:A:242:GLU:O	1:A:631:VAL:HA	2.15	0.46
1:A:388:SER:O	1:A:391:GLY:CA	2.62	0.46
1:A:542:GLU:HB2	1:A:733:SER:HB2	1.96	0.46
1:A:822:LEU:HD12	1:A:822:LEU:O	2.15	0.46
1:A:830:ARG:CG	1:A:831:PRO:HD2	2.45	0.46
1:A:886:ARG:N	1:A:887:PRO:HD3	2.30	0.46
1:A:372:LYS:HD2	2:B:999:LEU:HD11	1.95	0.46
1:A:508:SER:HB3	2:B:992:TYR:CZ	2.50	0.46
1:A:784:MET:O	1:A:785:MET:HG2	2.16	0.46
1:A:876:VAL:HG23	2:B:523:HIS:NE2	2.28	0.46
1:A:876:VAL:HG13	2:B:520:ASP:OD1	2.15	0.46
2:B:191:THR:O	2:B:192:VAL:CG2	2.63	0.46
2:B:418:GLN:OE1	2:B:418:GLN:N	2.48	0.46
1:A:39:ILE:CG1	1:A:506:SER:OG	2.62	0.46
1:A:170:LEU:C	1:A:170:LEU:CD1	2.85	0.46
1:A:499:ASP:CB	2:B:1001:SER:OG	2.57	0.46
1:A:704:ILE:CA	1:A:707:ILE:HD12	2.42	0.46
2:B:294:ASP:CG	2:B:295:TYR:H	2.22	0.46
2:B:307:LYS:HG2	2:B:311:ARG:HH22	1.79	0.46
1:A:198:ARG:NH1	1:A:198:ARG:CG	2.73	0.46
1:A:240:LYS:HE2	1:A:240:LYS:HB2	1.71	0.46
1:A:367:ILE:HD11	1:A:415:GLN:HE22	0.96	0.46
1:A:607:ARG:O	1:A:608:LEU:C	2.57	0.46
1:A:649:HIS:CD2	1:A:651:GLN:OE1	2.68	0.46
1:A:751:HIS:CD2	1:A:858:GLY:H	2.33	0.46
2:B:36:GLU:CD	2:B:65:GLU:OE1	2.56	0.46
2:B:156:PRO:HG2	2:B:356:GLY:C	2.40	0.46
2:B:197:PRO:HD2	2:B:457:TRP:HA	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ALA:HB1	2:B:250:TRP:CZ2	2.50	0.46
2:B:346:THR:CG2	2:B:364:MET:HG2	2.45	0.46
2:B:433:TRP:CD1	2:B:518:GLN:NE2	2.78	0.46
2:B:436:VAL:HG12	2:B:584:ALA:CB	2.46	0.46
1:A:39:ILE:HD11	2:B:988:VAL:C	2.41	0.46
1:A:55:LEU:HG	1:A:528:MET:HE3	1.86	0.46
1:A:961:LEU:HD22	2:B:286:THR:HG21	1.96	0.46
2:B:219:GLN:OE1	2:B:444:VAL:CG1	2.64	0.46
1:A:353:MET:CE	1:A:385:LEU:CB	2.94	0.46
1:A:368:VAL:HG23	1:A:418:PHE:HB2	1.96	0.46
1:A:571:LEU:HD23	1:A:592:GLN:HG3	1.95	0.46
2:B:263:LEU:HD13	2:B:263:LEU:C	2.41	0.46
2:B:562:LEU:C	2:B:564:SER:N	2.73	0.46
2:B:589:TYR:HD1	2:B:589:TYR:H	1.64	0.46
1:A:17:ASN:ND2	1:A:17:ASN:C	2.72	0.46
1:A:68:PHE:CE1	1:A:862:HIS:HE1	2.33	0.46
1:A:485:VAL:CG1	1:A:617:PRO:HB3	2.45	0.46
1:A:677:ILE:CG1	1:A:678:THR:N	2.77	0.46
2:B:340:ALA:HB2	2:B:386:THR:CB	2.46	0.46
2:B:633:ILE:CG2	2:B:638:GLU:HB3	2.45	0.46
2:B:655:LEU:O	2:B:656:TYR:CG	2.69	0.46
2:B:833:GLY:O	2:B:937:VAL:O	2.34	0.46
1:A:10:ASN:ND2	1:A:10:ASN:C	2.73	0.46
1:A:230:LEU:HD12	1:A:232:TRP:CZ2	2.50	0.46
1:A:255:PRO:HD2	1:A:256:GLU:H	1.80	0.46
1:A:300:TYR:N	1:A:300:TYR:CD1	2.84	0.46
1:A:331:THR:HG23	1:A:343:THR:HB	1.97	0.46
1:A:563:PHE:HA	1:A:566:VAL:CG2	2.45	0.46
1:A:682:THR:HA	1:A:683:PRO:HA	1.56	0.46
1:A:885:LEU:O	1:A:886:ARG:HG3	2.15	0.46
2:B:266:HIS:CE1	2:B:619:GLU:HG2	2.51	0.46
1:A:55:LEU:CD2	1:A:60:LEU:HB2	2.45	0.46
1:A:330:TYR:CE2	1:A:397:PRO:CG	2.99	0.46
1:A:356:THR:HA	1:A:419:LEU:O	2.16	0.46
1:A:463:HIS:HD2	1:A:617:PRO:CG	2.24	0.46
1:A:519:LEU:HD23	1:A:519:LEU:O	2.16	0.46
1:A:556:HIS:ND1	1:A:626:ILE:CD1	2.79	0.46
1:A:762:ARG:HE	1:A:815:ILE:HD13	1.81	0.46
1:A:934:PRO:HB3	2:B:613:LEU:CD1	2.36	0.46
2:B:264:THR:HG22	2:B:265:PRO:HD3	0.49	0.46
2:B:273:TRP:HZ2	2:B:653:VAL:CG1	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LEU:H	2:B:378:THR:HG22	1.81	0.46
1:A:220:GLU:OE2	2:B:214:ARG:NH2	2.49	0.46
1:A:247:PRO:CG	1:A:477:SER:OG	2.60	0.46
1:A:380:CYS:HG	1:A:439:ALA:HB2	1.79	0.46
1:A:535:CYS:SG	1:A:597:VAL:HG21	2.56	0.46
1:A:738:CYS:O	1:A:739:ALA:C	2.56	0.46
1:A:879:ARG:CD	2:B:510:THR:HG21	2.46	0.46
1:A:894:ARG:CB	1:A:902:MET:HE1	2.19	0.46
1:A:943:ARG:NH1	1:A:943:ARG:CG	2.73	0.46
2:B:197:PRO:CD	2:B:457:TRP:CE3	2.99	0.46
2:B:198:MET:C	2:B:204:GLN:HE21	2.24	0.46
2:B:383:HIS:CD2	2:B:385:ASP:OD1	2.67	0.46
2:B:515:THR:HG21	2:B:656:TYR:CE2	2.44	0.46
2:B:526:PHE:O	2:B:526:PHE:HD1	1.99	0.46
2:B:263:LEU:C	2:B:263:LEU:CD2	2.85	0.45
2:B:548:ASN:O	2:B:550:MET:CE	2.63	0.45
2:B:586:GLY:CA	2:B:588:PHE:HE1	2.28	0.45
2:B:796:ASP:OD1	2:B:797:GLY:N	2.49	0.45
1:A:193:PHE:HE2	1:A:460:THR:HG22	1.80	0.45
1:A:433:LYS:HD2	1:A:437:ALA:HB3	1.94	0.45
1:A:531:LEU:HD23	1:A:747:ILE:HD11	1.95	0.45
1:A:574:LEU:HD22	1:A:577:ARG:CD	2.34	0.45
1:A:690:TRP:NE1	1:A:712:GLY:HA3	2.30	0.45
1:A:807:MET:SD	1:A:810:MET:HE2	2.56	0.45
2:B:26:GLN:O	2:B:27:THR:HG23	2.16	0.45
2:B:383:HIS:CD2	2:B:384:ALA:N	2.84	0.45
2:B:758:LEU:HA	2:B:758:LEU:HD23	1.74	0.45
1:A:96:TYR:CD2	1:A:96:TYR:O	2.69	0.45
1:A:104:ALA:O	1:A:105:TRP:CE3	2.69	0.45
1:A:188:CYS:SG	1:A:495:VAL:HG11	2.57	0.45
1:A:246:THR:HB	1:A:629:SER:HB3	1.99	0.45
1:A:290:GLN:OE1	1:A:291:ASN:OD1	2.34	0.45
2:B:442:PRO:O	2:B:576:TYR:CE2	2.69	0.45
2:B:695:VAL:HG22	2:B:780:ILE:CG2	2.46	0.45
2:B:832:HIS:CD2	2:B:837:ALA:HB2	2.51	0.45
1:A:36:GLY:O	1:A:505:GLY:CA	2.59	0.45
1:A:148:MET:HE3	1:A:148:MET:HB2	1.81	0.45
1:A:231:THR:HB	1:A:341:HIS:HB3	1.98	0.45
1:A:429:ALA:C	1:A:430:THR:HG23	2.39	0.45
1:A:531:LEU:O	1:A:535:CYS:HB3	2.16	0.45
1:A:553:THR:HB	1:A:554:ASP:H	1.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:VAL:HG13	1:A:894:ARG:N	2.32	0.45
2:B:623:ILE:HD12	2:B:893:ILE:HD12	1.99	0.45
2:B:702:LEU:HD11	2:B:777:ILE:HG12	1.98	0.45
1:A:202:HIS:O	1:A:202:HIS:CG	2.69	0.45
1:A:319:ASP:OD1	1:A:322:ALA:HB3	2.17	0.45
1:A:690:TRP:O	1:A:690:TRP:CD2	2.70	0.45
1:A:886:ARG:O	1:A:888:TYR:N	2.49	0.45
2:B:117:ARG:NH1	2:B:299:MET:O	2.50	0.45
2:B:123:ASN:O	2:B:939:MET:HA	2.16	0.45
2:B:294:ASP:CG	2:B:295:TYR:N	2.74	0.45
2:B:807:PHE:H	2:B:807:PHE:HD1	1.57	0.45
1:A:309:TRP:HB2	1:A:331:THR:HG21	1.99	0.45
1:A:330:TYR:CG	1:A:330:TYR:O	2.69	0.45
1:A:372:LYS:NZ	1:A:499:ASP:CG	2.73	0.45
1:A:807:MET:C	1:A:810:MET:H	2.17	0.45
1:A:894:ARG:O	1:A:894:ARG:HG3	2.15	0.45
1:A:928:ARG:CB	2:B:601:ALA:HB2	2.46	0.45
1:A:958:THR:HG22	1:A:959:LYS:H	1.78	0.45
2:B:796:ASP:HB3	2:B:797:GLY:O	2.17	0.45
2:B:870:LEU:HB3	2:B:875:ALA:HB3	1.98	0.45
1:A:129:THR:CG2	1:A:447:TYR:O	2.65	0.45
1:A:204:SER:OG	1:A:523:TYR:HE1	1.90	0.45
1:A:215:LEU:H	1:A:215:LEU:HD13	1.82	0.45
1:A:220:GLU:HG3	2:B:186:TRP:HZ2	1.75	0.45
2:B:347:TRP:O	2:B:348:GLY:O	2.33	0.45
1:A:55:LEU:HD12	1:A:528:MET:CG	2.47	0.45
1:A:334:LYS:HG2	1:A:334:LYS:O	2.16	0.45
1:A:481:LEU:HD12	1:A:624:ALA:HB2	1.99	0.45
1:A:634:ILE:CB	1:A:688:GLU:CB	2.93	0.45
1:A:889:GLU:N	1:A:889:GLU:CD	2.72	0.45
1:A:910:LEU:O	1:A:911:TYR:CG	2.70	0.45
2:B:165:THR:HA	2:B:546:MET:HE2	1.82	0.45
2:B:251:LEU:HD23	2:B:305:LEU:HD12	1.98	0.45
2:B:434:MET:HE3	2:B:502:VAL:HG22	1.96	0.45
2:B:449:ASN:HB3	2:B:452:ALA:HB2	1.98	0.45
2:B:468:MET:HE2	2:B:468:MET:HB2	1.63	0.45
2:B:648:VAL:O	2:B:805:HIS:HB2	2.17	0.45
2:B:658:THR:HG21	2:B:695:VAL:CG2	2.44	0.45
2:B:737:TYR:HD1	2:B:738:ASP:H	1.64	0.45
1:A:22:ALA:CB	1:A:140:LEU:HD11	2.47	0.45
1:A:108:VAL:HG12	1:A:468:THR:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:CE1	1:A:217:GLU:OE1	2.69	0.45
1:A:461:ILE:HG22	1:A:465:VAL:HG22	1.97	0.45
1:A:910:LEU:O	1:A:911:TYR:CD1	2.70	0.45
2:B:39:GLY:H	2:B:62:VAL:HG23	1.82	0.45
2:B:336:ALA:O	2:B:337:GLY:C	2.58	0.45
2:B:346:THR:HG22	2:B:364:MET:HG2	1.97	0.45
2:B:526:PHE:O	2:B:526:PHE:CD1	2.70	0.45
1:A:105:TRP:CG	1:A:471:ARG:NH1	2.63	0.45
1:A:526:GLY:O	1:A:530:SER:HB3	2.17	0.45
1:A:623:LEU:N	1:A:623:LEU:CD2	2.77	0.45
1:A:805:ILE:CG2	1:A:806:PRO:N	2.80	0.45
1:A:961:LEU:HD21	2:B:286:THR:HG21	1.99	0.45
2:B:195:VAL:HG22	2:B:984:ILE:HG21	1.98	0.45
2:B:349:LYS:HA	2:B:350:PRO:HD3	1.77	0.45
2:B:518:GLN:HB3	2:B:584:ALA:HB1	1.98	0.45
2:B:844:THR:HG22	2:B:908:VAL:O	2.16	0.45
1:A:576:LEU:HB2	1:A:614:ALA:CB	2.42	0.44
2:B:122:CYS:HB2	2:B:939:MET:CE	2.47	0.44
2:B:729:ARG:CD	2:B:754:TYR:CE1	2.99	0.44
1:A:102:TRP:CZ2	1:A:804:TYR:CE2	3.05	0.44
1:A:170:LEU:CD1	1:A:171:ALA:N	2.73	0.44
1:A:297:ARG:HH11	1:A:297:ARG:CG	2.31	0.44
1:A:371:LEU:HD11	1:A:419:LEU:CD1	2.47	0.44
1:A:490:PHE:C	1:A:491:LEU:O	2.59	0.44
1:A:689:ARG:HG3	1:A:689:ARG:NH1	2.32	0.44
1:A:944:MET:HG2	1:A:945:PRO:HD2	1.99	0.44
2:B:112:THR:N	2:B:119:TYR:O	2.50	0.44
2:B:253:HIS:CD2	2:B:253:HIS:O	2.70	0.44
2:B:436:VAL:HG12	2:B:584:ALA:HB2	1.98	0.44
2:B:741:ILE:O	2:B:741:ILE:HG22	2.17	0.44
2:B:769:ASN:ND2	2:B:769:ASN:N	2.65	0.44
2:B:830:THR:HG23	2:B:939:MET:HE1	1.99	0.44
1:A:78:ALA:O	1:A:856:THR:CB	2.65	0.44
1:A:193:PHE:CE2	1:A:464:MET:HE2	2.52	0.44
1:A:310:LEU:HD22	1:A:329:HIS:HB2	1.99	0.44
1:A:432:THR:CG2	1:A:433:LYS:H	2.24	0.44
1:A:448:ASP:OD2	1:A:501:ASN:CG	2.60	0.44
1:A:453:THR:HG23	1:A:454:CYS:N	2.31	0.44
1:A:588:ALA:C	1:A:592:GLN:HE21	2.21	0.44
1:A:645:ALA:O	1:A:649:HIS:CA	2.66	0.44
1:A:762:ARG:HG3	1:A:762:ARG:NH1	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:788:ILE:HG22	1:A:798:ALA:HB2	1.98	0.44
1:A:830:ARG:NH1	1:A:830:ARG:C	2.73	0.44
1:A:892:CYS:HG	2:B:902:GLN:HG2	1.60	0.44
2:B:78:LEU:CD2	2:B:180:LEU:HD21	2.34	0.44
2:B:263:LEU:HA	2:B:268:ALA:HA	1.99	0.44
2:B:319:THR:CG2	2:B:343:LEU:HD13	2.47	0.44
2:B:334:CYS:SG	2:B:468:MET:HE2	2.55	0.44
2:B:585:ASP:HA	2:B:656:TYR:HH	1.82	0.44
1:A:189:ARG:HG3	1:A:189:ARG:HH21	1.82	0.44
1:A:237:ALA:O	1:A:245:ILE:HA	2.17	0.44
1:A:408:GLU:C	1:A:408:GLU:CD	2.86	0.44
1:A:422:ILE:HG22	1:A:423:GLY:N	2.32	0.44
2:B:284:MET:O	2:B:285:GLU:HG3	2.17	0.44
2:B:292:ARG:O	2:B:300:VAL:N	2.50	0.44
2:B:294:ASP:C	2:B:295:TYR:O	2.56	0.44
2:B:442:PRO:CD	2:B:576:TYR:CE1	2.98	0.44
1:A:20:HIS:CD2	1:A:20:HIS:O	2.70	0.44
1:A:433:LYS:CG	1:A:513:GLY:O	2.65	0.44
1:A:795:ALA:O	1:A:796:SER:CB	2.62	0.44
1:A:843:ARG:HD2	1:A:843:ARG:HA	1.75	0.44
1:A:876:VAL:CG2	2:B:523:HIS:NE2	2.73	0.44
1:A:957:PHE:CD1	1:A:958:THR:N	2.85	0.44
2:B:506:PRO:HG2	2:B:506:PRO:O	2.17	0.44
2:B:669:GLU:HG3	2:B:730:ARG:HE	1.83	0.44
2:B:838:ARG:NH1	2:B:838:ARG:CG	2.73	0.44
1:A:77:LEU:HA	1:A:858:GLY:HA2	1.98	0.44
1:A:79:GLU:N	1:A:856:THR:CG2	2.54	0.44
1:A:110:LEU:CD2	1:A:465:VAL:HG12	2.48	0.44
1:A:119:ILE:HD13	1:A:406:VAL:HG22	1.98	0.44
1:A:492:VAL:HG11	1:A:495:VAL:HG13	2.00	0.44
1:A:508:SER:HB2	2:B:992:TYR:CE1	2.53	0.44
1:A:660:ASN:ND2	1:A:661:GLU:N	2.60	0.44
1:A:740:GLU:C	1:A:742:MET:N	2.69	0.44
2:B:221:HIS:CE1	2:B:405:ALA:HA	2.53	0.44
2:B:732:TRP:O	2:B:732:TRP:CE3	2.70	0.44
2:B:990:HIS:HB2	2:B:992:TYR:HE1	1.80	0.44
1:A:298:VAL:HG11	1:A:300:TYR:CE1	2.53	0.44
1:A:367:ILE:CG1	1:A:415:GLN:HE22	2.05	0.44
1:A:367:ILE:HD13	1:A:415:GLN:HG2	1.97	0.44
1:A:411:TYR:CE2	1:A:417:LEU:HD11	2.53	0.44
1:A:481:LEU:H	1:A:481:LEU:CD1	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:CG	1:A:608:LEU:HD12	2.42	0.44
1:A:634:ILE:HD11	1:A:718:ARG:HH22	1.73	0.44
1:A:810:MET:HE2	1:A:810:MET:HB2	1.70	0.44
2:B:74:MET:HE2	2:B:984:ILE:HD11	1.99	0.44
2:B:623:ILE:CB	2:B:893:ILE:HD11	2.47	0.44
1:A:240:LYS:N	1:A:240:LYS:CD	2.73	0.44
1:A:367:ILE:HG21	1:A:496:GLN:HE21	1.82	0.44
1:A:535:CYS:SG	1:A:536:GLU:N	2.91	0.44
1:A:593:LYS:O	1:A:596:ALA:HB3	2.16	0.44
1:A:637:SER:O	1:A:639:GLN:N	2.51	0.44
1:A:762:ARG:HH11	1:A:762:ARG:CG	2.31	0.44
1:A:878:GLU:O	1:A:914:GLY:O	2.36	0.44
1:A:957:PHE:CE2	2:B:279:TYR:CE1	3.00	0.44
2:B:577:TYR:CD1	2:B:577:TYR:O	2.70	0.44
2:B:602:VAL:HG11	2:B:615:MET:CE	2.47	0.44
1:A:429:ALA:C	1:A:430:THR:HG22	2.43	0.43
1:A:639:GLN:CA	1:A:639:GLN:NE2	2.74	0.43
1:A:668:PHE:HD1	1:A:668:PHE:H	1.66	0.43
1:A:690:TRP:O	1:A:690:TRP:CG	2.70	0.43
2:B:706:SER:O	2:B:710:HIS:HB2	2.18	0.43
2:B:875:ALA:HB1	2:B:911:ILE:HD11	2.00	0.43
1:A:88:THR:CG2	1:A:90:MET:H	2.09	0.43
1:A:248:VAL:HB	1:A:249:PRO:CD	2.35	0.43
1:A:556:HIS:CE1	1:A:626:ILE:HD11	2.53	0.43
1:A:888:TYR:OH	2:B:504:ALA:CB	2.66	0.43
2:B:102:VAL:HG13	2:B:489:VAL:HG22	2.00	0.43
2:B:588:PHE:HA	2:B:808:GLY:O	2.18	0.43
1:A:51:LEU:HD13	1:A:51:LEU:N	2.32	0.43
1:A:463:HIS:ND1	1:A:463:HIS:C	2.73	0.43
1:A:532:ALA:CB	1:A:597:VAL:CG2	2.81	0.43
1:A:806:PRO:O	1:A:809:ALA:HB3	2.17	0.43
1:A:943:ARG:HH21	2:B:895:GLY:HA2	1.83	0.43
2:B:114:ASN:CG	2:B:115:ALA:H	2.24	0.43
2:B:120:LEU:HD12	2:B:152:VAL:CB	2.42	0.43
2:B:197:PRO:HG2	2:B:456:VAL:O	2.18	0.43
2:B:197:PRO:CD	2:B:457:TRP:HA	2.48	0.43
2:B:197:PRO:C	2:B:198:MET:SD	3.01	0.43
2:B:198:MET:CE	2:B:459:VAL:HA	2.48	0.43
2:B:446:ARG:NH1	2:B:446:ARG:CG	2.73	0.43
2:B:515:THR:OG1	2:B:516:ARG:N	2.50	0.43
2:B:576:TYR:CD1	2:B:576:TYR:O	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:PHE:CE2	2:B:777:ILE:HD13	2.53	0.43
1:A:72:ARG:CZ	1:A:863:VAL:HG11	2.47	0.43
1:A:111:ASN:ND2	1:A:111:ASN:C	2.77	0.43
1:A:203:ASN:HB3	1:A:519:LEU:HD12	2.00	0.43
1:A:238:HIS:HE1	1:A:334:LYS:HG2	1.78	0.43
1:A:558:VAL:HG12	1:A:562:LEU:HD21	2.00	0.43
1:A:876:VAL:HG12	1:A:877:SER:N	2.32	0.43
1:A:968:MET:O	1:A:971:ARG:CA	2.67	0.43
2:B:281:ALA:HB1	2:B:287:THR:OG1	2.19	0.43
2:B:497:ALA:HB3	2:B:557:LEU:HD22	2.01	0.43
1:A:274:VAL:HG22	1:A:274:VAL:O	2.18	0.43
1:A:353:MET:HE1	1:A:385:LEU:CB	2.48	0.43
1:A:551:ARG:HB3	1:A:552:PHE:H	1.59	0.43
1:A:587:GLU:HB3	1:A:618:PHE:HB3	2.01	0.43
1:A:608:LEU:HG	1:A:608:LEU:O	2.19	0.43
1:A:639:GLN:N	1:A:639:GLN:NE2	2.60	0.43
1:A:687:THR:C	1:A:688:GLU:OE1	2.61	0.43
2:B:351:LYS:HD2	2:B:366:GLU:OE1	2.18	0.43
2:B:500:GLN:HA	2:B:500:GLN:HE21	1.78	0.43
2:B:578:PHE:CD1	2:B:578:PHE:N	2.85	0.43
2:B:597:LEU:HD22	2:B:622:LEU:CB	2.47	0.43
2:B:702:LEU:HD22	2:B:712:PHE:CE1	2.54	0.43
1:A:56:ILE:HD13	1:A:56:ILE:HA	1.64	0.43
1:A:290:GLN:OE1	1:A:291:ASN:N	2.52	0.43
1:A:305:ASP:HB2	2:B:710:HIS:NE2	2.33	0.43
1:A:372:LYS:HZ2	1:A:499:ASP:CG	2.26	0.43
1:A:520:THR:HG23	1:A:521:ALA:N	2.34	0.43
1:A:704:ILE:HA	1:A:707:ILE:HD13	1.93	0.43
1:A:832:GLY:O	1:A:875:THR:HB	2.18	0.43
2:B:332:PRO:CG	2:B:399:PHE:CE1	2.97	0.43
2:B:526:PHE:O	2:B:530:THR:HG23	2.18	0.43
2:B:622:LEU:O	2:B:623:ILE:HG13	2.19	0.43
1:A:236:CYS:HB2	1:A:340:VAL:CG2	2.49	0.43
1:A:268:GLU:OE1	1:A:702:LYS:HE3	2.19	0.43
1:A:507:VAL:HG23	1:A:512:MET:CE	2.44	0.43
1:A:583:HIS:CE1	1:A:618:PHE:HE2	2.37	0.43
2:B:74:MET:CE	2:B:984:ILE:CD1	2.97	0.43
2:B:428:CYS:SG	2:B:818:HIS:HD2	2.39	0.43
1:A:39:ILE:HA	1:A:507:VAL:HG13	2.00	0.43
1:A:96:TYR:CE2	1:A:834:MET:HB2	2.53	0.43
1:A:342:LEU:CD2	1:A:343:THR:N	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:CB	1:A:449:ILE:HG21	2.43	0.43
1:A:638:ARG:NH2	1:A:638:ARG:CG	2.73	0.43
1:A:671:LEU:N	1:A:672:PRO:CD	2.82	0.43
1:A:926:THR:O	1:A:926:THR:HG23	2.19	0.43
2:B:123:ASN:HD21	2:B:149:GLN:HB3	1.67	0.43
1:A:217:GLU:O	1:A:218:LEU:CD2	2.63	0.43
1:A:440:THR:O	1:A:440:THR:HG22	2.18	0.43
1:A:664:CYS:N	1:A:737:GLY:O	2.49	0.43
1:A:757:HIS:CD2	1:A:758:THR:H	2.35	0.43
1:A:883:LEU:HD12	2:B:634:THR:OG1	2.19	0.43
2:B:32:LYS:HG3	2:B:32:LYS:O	2.19	0.43
2:B:129:ILE:HB	2:B:934:SER:O	2.19	0.43
2:B:198:MET:HG3	2:B:204:GLN:NE2	2.25	0.43
2:B:357:HIS:O	2:B:358:ALA:C	2.59	0.43
2:B:726:SER:CB	2:B:727:PRO:CD	2.96	0.43
1:A:35:ALA:O	1:A:41:ALA:O	2.37	0.43
1:A:58:GLN:NE2	1:A:58:GLN:CA	2.72	0.43
1:A:191:PHE:O	1:A:194:GLY:N	2.52	0.43
1:A:211:VAL:HG23	1:A:212:ASN:N	2.34	0.43
1:A:433:LYS:C	1:A:435:GLN:N	2.73	0.43
1:A:442:ALA:CB	1:A:509:VAL:HG11	2.49	0.43
1:A:481:LEU:HD11	1:A:624:ALA:CB	2.46	0.43
1:A:490:PHE:O	1:A:491:LEU:O	2.37	0.43
1:A:511:ASP:O	1:A:512:MET:HG3	2.19	0.43
1:A:669:ILE:O	1:A:669:ILE:HG22	2.19	0.43
1:A:674:PRO:C	1:A:675:SER:HG	2.25	0.43
1:A:948:PHE:HB2	2:B:149:GLN:HE22	1.80	0.43
2:B:838:ARG:NH2	2:B:932:SER:HB2	2.28	0.43
1:A:51:LEU:N	1:A:51:LEU:HD22	2.33	0.42
1:A:209:GLY:HA3	1:A:218:LEU:HD21	2.00	0.42
1:A:262:ARG:HH21	1:A:401:GLY:HA2	1.73	0.42
1:A:445:ARG:NH1	1:A:445:ARG:HG3	2.34	0.42
1:A:532:ALA:CA	1:A:535:CYS:HG	2.23	0.42
1:A:587:GLU:HG2	1:A:619:VAL:O	2.18	0.42
1:A:607:ARG:H	1:A:607:ARG:HG2	1.55	0.42
1:A:948:PHE:CZ	1:A:950:MET:CE	2.94	0.42
2:B:620:PRO:O	2:B:893:ILE:O	2.37	0.42
1:A:69:GLU:OE2	1:A:206:ARG:HG3	2.19	0.42
1:A:467:GLN:HA	1:A:467:GLN:NE2	2.34	0.42
1:A:576:LEU:HA	1:A:576:LEU:HD23	1.83	0.42
1:A:627:ARG:CZ	1:A:738:CYS:SG	3.03	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:THR:O	1:A:728:ARG:HA	2.19	0.42
1:A:847:ALA:O	1:A:848:SER:HB2	2.18	0.42
1:A:929:GLN:H	1:A:929:GLN:HG2	1.50	0.42
1:A:951:GLY:C	1:A:952:THR:CG2	2.92	0.42
1:A:970:LEU:O	1:A:971:ARG:CB	2.66	0.42
2:B:245:ARG:O	2:B:387:VAL:HG12	2.19	0.42
2:B:266:HIS:NE2	2:B:619:GLU:HG2	2.34	0.42
2:B:383:HIS:O	2:B:385:ASP:N	2.51	0.42
2:B:442:PRO:CG	2:B:576:TYR:CZ	3.00	0.42
2:B:514:THR:O	2:B:517:LEU:HB3	2.19	0.42
1:A:42:GLY:HA2	1:A:445:ARG:NH2	2.35	0.42
1:A:42:GLY:HA3	1:A:445:ARG:HH22	1.81	0.42
1:A:66:LEU:HD13	1:A:519:LEU:CD2	2.49	0.42
1:A:68:PHE:CZ	1:A:862:HIS:CE1	3.08	0.42
1:A:299:HIS:C	1:A:300:TYR:CD1	2.98	0.42
1:A:368:VAL:HG22	1:A:418:PHE:CB	2.38	0.42
1:A:508:SER:HB2	2:B:992:TYR:CE2	2.53	0.42
1:A:590:PHE:CE2	1:A:619:VAL:HG11	2.55	0.42
1:A:961:LEU:HD13	2:B:284:MET:HB3	2.00	0.42
1:A:96:TYR:CZ	1:A:834:MET:HB2	2.55	0.42
1:A:234:LEU:HD21	1:A:266:PHE:CZ	2.42	0.42
1:A:671:LEU:N	1:A:686:GLY:O	2.48	0.42
2:B:433:TRP:CZ2	2:B:517:LEU:HD22	2.54	0.42
2:B:676:TRP:CH2	2:B:680:LYS:HE2	2.54	0.42
2:B:828:ALA:HB1	2:B:865:GLN:HE21	1.84	0.42
1:A:199:MET:HG2	1:A:435:GLN:NE2	2.34	0.42
1:A:347:LYS:HB2	1:A:347:LYS:HZ2	1.84	0.42
1:A:447:TYR:O	1:A:448:ASP:HB2	2.19	0.42
2:B:56:ARG:NH2	2:B:485:GLN:NE2	2.68	0.42
2:B:172:SER:H	2:B:175:ALA:HB3	1.85	0.42
1:A:55:LEU:CD1	1:A:528:MET:CG	2.97	0.42
1:A:193:PHE:HZ	1:A:464:MET:HE3	1.84	0.42
1:A:206:ARG:NH1	1:A:217:GLU:OE1	2.53	0.42
1:A:488:SER:HB2	1:A:489:PRO:HD2	2.02	0.42
1:A:611:LEU:HD13	1:A:611:LEU:C	2.45	0.42
1:A:618:PHE:C	1:A:619:VAL:CG1	2.87	0.42
1:A:752:LYS:O	1:A:753:VAL:CG1	2.68	0.42
1:A:784:MET:C	1:A:785:MET:HG2	2.44	0.42
2:B:307:LYS:CG	2:B:311:ARG:HH22	2.32	0.42
2:B:312:SER:HB3	2:B:778:TRP:CD1	2.55	0.42
2:B:320:GLU:HG2	2:B:370:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:346:THR:O	2:B:346:THR:OG1	2.35	0.42
1:A:43:GLY:N	1:A:445:ARG:HH22	2.17	0.42
1:A:432:THR:HA	1:A:435:GLN:HB2	2.02	0.42
1:A:508:SER:HB2	2:B:992:TYR:CZ	2.55	0.42
1:A:543:GLU:CD	1:A:543:GLU:C	2.86	0.42
1:A:597:VAL:HG12	1:A:748:ALA:HB2	2.01	0.42
1:A:861:ARG:CZ	2:B:547:ALA:CB	2.97	0.42
1:A:972:GLU:H	1:A:972:GLU:HG3	1.49	0.42
2:B:217:GLY:N	2:B:448:MET:HB3	2.34	0.42
2:B:855:ASP:O	2:B:856:LEU:HB2	2.19	0.42
1:A:555:VAL:HG22	1:A:555:VAL:O	2.19	0.42
1:A:581:VAL:O	1:A:581:VAL:HG22	2.19	0.42
1:A:668:PHE:N	1:A:668:PHE:CD1	2.88	0.42
1:A:757:HIS:HD2	1:A:758:THR:HG23	1.84	0.42
1:A:789:ARG:HH12	1:A:816:THR:HG22	1.85	0.42
2:B:89:ASP:CA	2:B:410:GLN:NE2	2.71	0.42
2:B:253:HIS:O	2:B:253:HIS:HD2	2.03	0.42
2:B:347:TRP:O	2:B:350:PRO:HD3	2.19	0.42
1:A:18:ILE:HG12	1:A:18:ILE:H	1.65	0.42
1:A:77:LEU:CD2	1:A:742:MET:HE2	2.39	0.42
1:A:111:ASN:HB2	1:A:467:GLN:CG	2.50	0.42
1:A:218:LEU:N	1:A:218:LEU:CD2	2.81	0.42
1:A:219:GLY:O	1:A:221:ASN:N	2.53	0.42
1:A:375:GLU:O	1:A:377:LEU:HD23	2.20	0.42
1:A:453:THR:CG2	1:A:454:CYS:N	2.83	0.42
1:A:529:ALA:N	1:A:594:MET:HE2	2.30	0.42
1:A:589:LEU:N	1:A:592:GLN:HE21	2.17	0.42
2:B:7:GLN:CD	2:B:29:VAL:HG11	2.43	0.42
2:B:94:LEU:HD13	2:B:102:VAL:HG21	2.01	0.42
1:A:72:ARG:C	1:A:863:VAL:HG12	2.44	0.42
1:A:96:TYR:O	1:A:96:TYR:CG	2.70	0.42
1:A:128:GLY:HA2	1:A:188:CYS:HB2	2.02	0.42
1:A:201:MET:HG2	1:A:400:PHE:CE1	2.55	0.42
2:B:881:ASN:O	2:B:882:MET:C	2.63	0.42
1:A:20:HIS:O	1:A:20:HIS:HD2	2.03	0.41
1:A:63:VAL:CG2	1:A:68:PHE:HE2	2.33	0.41
1:A:68:PHE:CZ	1:A:862:HIS:HE1	2.38	0.41
1:A:285:ILE:HG21	1:A:395:PHE:CD2	2.55	0.41
1:A:481:LEU:HD21	1:A:533:HIS:CE1	2.55	0.41
1:A:589:LEU:O	1:A:592:GLN:HB2	2.20	0.41
1:A:601:MET:HB3	1:A:609:TYR:HB2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:671:LEU:HB2	1:A:685:ILE:CG2	2.46	0.41
1:A:692:ALA:CB	1:A:721:VAL:HB	2.50	0.41
1:A:806:PRO:HG2	1:A:809:ALA:HB2	2.02	0.41
2:B:89:ASP:OD2	2:B:410:GLN:OE1	2.34	0.41
2:B:191:THR:O	2:B:192:VAL:HG23	2.19	0.41
2:B:254:GLN:CD	2:B:254:GLN:N	2.78	0.41
2:B:509:ILE:CG2	2:B:512:GLY:CA	2.90	0.41
2:B:857:VAL:O	2:B:858:PRO:O	2.38	0.41
1:A:225:THR:O	1:A:227:ASP:N	2.53	0.41
1:A:815:ILE:O	1:A:816:THR:CG2	2.68	0.41
1:A:883:LEU:O	1:A:884:ALA:HB3	2.20	0.41
1:A:890:ARG:NH1	2:B:903:THR:O	2.51	0.41
1:A:950:MET:HE2	2:B:112:THR:HG22	1.98	0.41
2:B:77:LEU:N	2:B:77:LEU:CD1	2.82	0.41
2:B:231:ILE:HG12	2:B:393:LEU:CD2	2.50	0.41
2:B:509:ILE:HD12	2:B:813:ILE:HD11	2.02	0.41
2:B:576:TYR:HD1	2:B:576:TYR:O	2.04	0.41
2:B:596:THR:HG22	2:B:647:LEU:CD1	2.50	0.41
1:A:14:THR:O	1:A:18:ILE:CG1	2.59	0.41
1:A:69:GLU:OE2	1:A:206:ARG:CD	2.68	0.41
1:A:125:MET:HE1	1:A:132:MET:HG3	2.02	0.41
1:A:202:HIS:CE1	1:A:224:SER:HG	2.38	0.41
1:A:211:VAL:O	1:A:212:ASN:HB2	2.20	0.41
1:A:445:ARG:CG	1:A:445:ARG:HH11	2.33	0.41
1:A:693:THR:O	1:A:694:THR:C	2.64	0.41
1:A:785:MET:HE3	1:A:822:LEU:HD13	2.02	0.41
1:A:908:PRO:HB3	2:B:524:HIS:ND1	2.35	0.41
1:A:952:THR:HG21	2:B:115:ALA:HB1	2.01	0.41
2:B:89:ASP:HB3	2:B:410:GLN:HE22	1.85	0.41
2:B:638:GLU:HA	2:B:885:ASN:HD21	1.85	0.41
1:A:38:ASN:C	1:A:506:SER:CB	2.93	0.41
1:A:128:GLY:O	1:A:449:ILE:HD12	2.20	0.41
1:A:445:ARG:NH1	1:A:445:ARG:CG	2.79	0.41
1:A:637:SER:C	1:A:639:GLN:N	2.76	0.41
1:A:830:ARG:C	1:A:830:ARG:HH11	2.28	0.41
2:B:262:MET:HG2	2:B:430:ALA:HA	2.02	0.41
2:B:672:ASN:HB2	2:B:754:TYR:CE2	2.55	0.41
1:A:40:GLN:HG2	1:A:45:ASP:HA	2.02	0.41
1:A:121:SER:HB3	1:A:185:ASN:HB2	2.02	0.41
1:A:284:LYS:HD2	1:A:329:HIS:HD1	1.85	0.41
1:A:402:VAL:O	1:A:406:VAL:HG23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:HIS:CB	1:A:615:TYR:CE2	3.04	0.41
1:A:664:CYS:SG	1:A:737:GLY:CA	2.97	0.41
1:A:882:GLY:O	1:A:883:LEU:HD23	2.17	0.41
1:A:917:MET:HB2	2:B:632:THR:CG2	2.50	0.41
2:B:247:ARG:NH2	2:B:347:TRP:NE1	2.48	0.41
2:B:652:HIS:C	2:B:653:VAL:HG23	2.45	0.41
1:A:119:ILE:HD13	1:A:406:VAL:HA	2.02	0.41
1:A:392:HIS:HB3	1:A:393:HIS:H	1.69	0.41
1:A:762:ARG:CD	1:A:815:ILE:HD13	2.50	0.41
1:A:807:MET:O	1:A:810:MET:CA	2.69	0.41
1:A:873:ILE:H	1:A:873:ILE:CD1	2.15	0.41
2:B:375:VAL:O	2:B:376:ASN:HB2	2.18	0.41
2:B:566:MET:O	2:B:566:MET:SD	2.79	0.41
1:A:55:LEU:CD1	1:A:528:MET:HE2	0.89	0.41
1:A:68:PHE:HZ	1:A:862:HIS:CE1	2.39	0.41
1:A:208:HIS:CE1	1:A:217:GLU:OE2	2.74	0.41
1:A:309:TRP:CZ3	1:A:343:THR:HG23	2.55	0.41
1:A:371:LEU:CB	1:A:500:MET:CE	2.83	0.41
1:A:386:ALA:O	1:A:407:HIS:CD2	2.74	0.41
1:A:472:ASP:CB	1:A:739:ALA:CB	2.99	0.41
1:A:598:TRP:O	1:A:600:SER:CA	2.62	0.41
1:A:944:MET:HE3	1:A:944:MET:HB2	1.68	0.41
2:B:89:ASP:CB	2:B:410:GLN:CD	2.92	0.41
2:B:155:GLU:CG	2:B:156:PRO:HD2	2.50	0.41
2:B:385:ASP:OD1	2:B:385:ASP:N	2.53	0.41
2:B:648:VAL:HG22	2:B:809:GLU:CG	2.51	0.41
2:B:648:VAL:HG22	2:B:809:GLU:HG3	2.02	0.41
1:A:43:GLY:H	1:A:445:ARG:HH12	1.68	0.41
1:A:527:ALA:O	1:A:531:LEU:HB2	2.20	0.41
1:A:820:CYS:O	1:A:820:CYS:SG	2.78	0.41
1:A:843:ARG:O	1:A:844:GLY:C	2.59	0.41
2:B:89:ASP:HB3	2:B:410:GLN:CD	2.45	0.41
2:B:111:MET:HE1	2:B:487:ILE:HG21	2.02	0.41
2:B:305:LEU:C	2:B:305:LEU:HD13	2.45	0.41
2:B:397:LEU:HD13	2:B:480:LEU:CD1	2.50	0.41
1:A:114:LYS:HE3	1:A:116:HIS:CE1	2.55	0.41
1:A:231:THR:HG23	1:A:309:TRP:HZ3	1.85	0.41
1:A:353:MET:O	1:A:355:THR:N	2.53	0.41
1:A:384:LEU:HD12	1:A:439:ALA:O	2.20	0.41
1:A:452:ARG:O	1:A:452:ARG:HD3	2.21	0.41
1:A:584:SER:C	1:A:586:GLN:H	2.29	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:ILE:HG23	1:A:822:LEU:HB3	2.03	0.41
1:A:830:ARG:O	1:A:836:THR:HG23	2.21	0.41
1:A:880:VAL:HG21	2:B:508:GLY:HA3	2.01	0.41
1:A:951:GLY:O	1:A:952:THR:HG22	2.21	0.41
2:B:129:ILE:O	2:B:933:VAL:HG13	2.19	0.41
2:B:247:ARG:HD2	2:B:344:ALA:HA	2.03	0.41
2:B:314:GLY:HA2	2:B:762:SER:OG	2.21	0.41
2:B:615:MET:HG2	2:B:615:MET:H	1.59	0.41
2:B:648:VAL:CG1	2:B:653:VAL:HG23	2.51	0.41
1:A:44:TYR:CE2	1:A:444:MET:HE3	2.56	0.41
1:A:193:PHE:CD1	1:A:193:PHE:C	2.99	0.41
1:A:632:ARG:O	1:A:726:TYR:HE1	2.04	0.41
2:B:7:GLN:OE1	2:B:77:LEU:HD11	2.21	0.41
2:B:999:LEU:O	2:B:1000:ALA:CB	2.59	0.41
1:A:334:LYS:CG	1:A:334:LYS:O	2.69	0.40
1:A:369:TYR:HE1	1:A:417:LEU:HD23	1.86	0.40
1:A:430:THR:O	1:A:430:THR:OG1	2.21	0.40
1:A:789:ARG:NH1	1:A:816:THR:HG22	2.36	0.40
2:B:155:GLU:HG2	2:B:156:PRO:HD2	2.04	0.40
2:B:815:VAL:HG11	2:B:894:LEU:HD21	2.03	0.40
1:A:208:HIS:CE1	1:A:217:GLU:CD	2.99	0.40
1:A:337:HIS:C	1:A:338:SER:OG	2.64	0.40
1:A:347:LYS:NZ	1:A:347:LYS:HB2	2.37	0.40
1:A:562:LEU:HD13	1:A:562:LEU:HA	1.88	0.40
1:A:723:VAL:HG12	1:A:724:PHE:N	2.37	0.40
1:A:752:LYS:C	1:A:753:VAL:HG13	2.46	0.40
1:A:885:LEU:HD22	2:B:636:ASN:ND2	2.36	0.40
1:A:886:ARG:C	1:A:888:TYR:N	2.77	0.40
2:B:194:ILE:HG21	2:B:200:GLN:N	2.36	0.40
1:A:49:LEU:HD23	1:A:608:LEU:HD13	2.03	0.40
1:A:56:ILE:HG23	1:A:56:ILE:HD12	1.83	0.40
1:A:79:GLU:CA	1:A:79:GLU:OE1	2.69	0.40
1:A:106:LEU:HD12	1:A:106:LEU:HA	1.85	0.40
1:A:119:ILE:CD1	1:A:406:VAL:HG22	2.52	0.40
1:A:153:THR:OG1	2:B:1001:SER:O	2.40	0.40
1:A:249:PRO:HG2	1:A:252:TRP:CB	2.38	0.40
1:A:702:LYS:NZ	1:A:702:LYS:HB3	2.35	0.40
1:A:886:ARG:O	1:A:887:PRO:C	2.63	0.40
1:A:921:ASP:HB3	2:B:626:ALA:HB1	1.97	0.40
1:A:925:VAL:O	1:A:926:THR:CB	2.69	0.40
2:B:254:GLN:H	2:B:254:GLN:NE2	2.18	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ALA:CB	2:B:358:ALA:HB2	2.47	0.40
2:B:512:GLY:O	2:B:809:GLU:OE1	2.39	0.40
2:B:674:LEU:HB3	2:B:784:MET:HE2	2.04	0.40
1:A:43:GLY:H	1:A:445:ARG:HH22	1.67	0.40
1:A:201:MET:CG	1:A:400:PHE:HE1	2.33	0.40
1:A:342:LEU:HD23	1:A:342:LEU:C	2.46	0.40
1:A:433:LYS:HG3	1:A:513:GLY:O	2.21	0.40
1:A:464:MET:SD	1:A:483:PHE:CE2	3.15	0.40
1:A:553:THR:O	1:A:554:ASP:CB	2.70	0.40
1:A:736:LEU:O	1:A:737:GLY:C	2.63	0.40
2:B:320:GLU:HG2	2:B:326:ARG:HG2	1.78	0.40
2:B:528:TYR:CD2	2:B:560:TRP:CZ2	3.08	0.40
2:B:676:TRP:HD1	2:B:754:TYR:HB2	1.73	0.40
2:B:701:TRP:CZ2	2:B:773:VAL:HG22	2.57	0.40
1:A:10:ASN:ND2	1:A:14:THR:OG1	2.53	0.40
1:A:127:PHE:CD1	1:A:452:ARG:CD	3.03	0.40
1:A:209:GLY:CA	1:A:218:LEU:HD21	2.51	0.40
1:A:577:ARG:CD	1:A:614:ALA:O	2.69	0.40
1:A:650:ALA:O	1:A:796:SER:C	2.64	0.40
1:A:650:ALA:C	1:A:796:SER:HA	2.47	0.40
1:A:697:ASN:CG	1:A:701:SER:HB2	2.46	0.40
2:B:165:THR:HG22	2:B:166:SER:O	2.21	0.40
2:B:216:SER:CB	2:B:448:MET:HA	2.52	0.40
2:B:287:THR:O	2:B:290:ARG:NH2	2.54	0.40
2:B:357:HIS:C	2:B:359:ASN:N	2.73	0.40
2:B:506:PRO:O	2:B:506:PRO:CG	2.70	0.40
2:B:563:GLY:O	2:B:564:SER:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	970/1357 (72%)	894 (92%)	60 (6%)	16 (2%)	7	35
2	B	1001/1059 (94%)	874 (87%)	94 (9%)	33 (3%)	3	25
All	All	1971/2416 (82%)	1768 (90%)	154 (8%)	49 (2%)	6	29

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	477	SER
1	A	509	VAL
1	A	554	ASP
1	A	599	SER
1	A	619	VAL
1	A	649	HIS
1	A	793	SER
1	A	816	THR
2	B	109	PRO
2	B	115	ALA
2	B	750	GLU
2	B	752	HIS
2	B	853	ALA
2	B	858	PRO
2	B	859	PRO
2	B	918	GLY
2	B	973	LEU
2	B	984	ILE
2	B	988	VAL
2	B	1000	ALA
2	B	1004	ASP
1	A	971	ARG
2	B	190	SER
2	B	656	TYR
2	B	882	MET
2	B	963	GLN
2	B	60	PRO
2	B	727	PRO
2	B	883	GLY
1	A	501	ASN
1	A	643	ALA
1	A	815	ILE
1	A	883	LEU
2	B	382	PRO
2	B	447	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	884	GLY
2	B	982	ASN
2	B	544	THR
2	B	730	ARG
2	B	749	THR
2	B	954	ASN
2	B	983	THR
1	A	814	PRO
2	B	350	PRO
1	A	671	LEU
2	B	620	PRO
1	A	247	PRO
2	B	653	VAL
2	B	689	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	774/1083 (72%)	478 (62%)	296 (38%)	0	0
2	B	800/833 (96%)	583 (73%)	217 (27%)	0	3
All	All	1574/1916 (82%)	1061 (67%)	513 (33%)	1	1

All (513) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	7	GLN
1	A	8	ARG
1	A	9	ASP
1	A	10	ASN
1	A	12	GLU
1	A	18	ILE
1	A	23	ARG
1	A	24	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	LYS
1	A	34	LEU
1	A	37	ILE
1	A	38	ASN
1	A	39	ILE
1	A	46	LEU
1	A	49	LEU
1	A	51	LEU
1	A	52	THR
1	A	54	GLU
1	A	55	LEU
1	A	56	ILE
1	A	58	GLN
1	A	60	LEU
1	A	63	VAL
1	A	66	LEU
1	A	68	PHE
1	A	69	GLU
1	A	70	HIS
1	A	75	LEU
1	A	77	LEU
1	A	79	GLU
1	A	81	ILE
1	A	83	VAL
1	A	86	ASN
1	A	89	ASP
1	A	90	MET
1	A	93	SER
1	A	95	GLN
1	A	103	ARG
1	A	105	TRP
1	A	106	LEU
1	A	111	ASN
1	A	112	MET
1	A	114	LYS
1	A	116	HIS
1	A	117	VAL
1	A	118	ARG
1	A	120	ARG
1	A	121	SER
1	A	125	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	131	ARG
1	A	132	MET
1	A	133	MET
1	A	135	CYS
1	A	136	ASP
1	A	140	LEU
1	A	143	SER
1	A	144	THR
1	A	145	ILE
1	A	149	SER
1	A	150	ARG
1	A	156	THR
1	A	157	MET
1	A	160	VAL
1	A	162	ARG
1	A	163	GLU
1	A	164	MET
1	A	167	MET
1	A	170	LEU
1	A	175	SER
1	A	176	ARG
1	A	178	SER
1	A	179	GLN
1	A	188	CYS
1	A	189	ARG
1	A	196	LEU
1	A	198	ARG
1	A	199	MET
1	A	201	MET
1	A	211	VAL
1	A	214	ARG
1	A	217	GLU
1	A	218	LEU
1	A	220	GLU
1	A	228	THR
1	A	230	LEU
1	A	231	THR
1	A	240	LYS
1	A	243	VAL
1	A	246	THR
1	A	248	VAL
1	A	253	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	256	GLU
1	A	260	THR
1	A	262	ARG
1	A	264	ARG
1	A	267	SER
1	A	270	LEU
1	A	272	ARG
1	A	273	LEU
1	A	278	VAL
1	A	290	GLN
1	A	291	ASN
1	A	295	ASN
1	A	297	ARG
1	A	299	HIS
1	A	300	TYR
1	A	303	ARG
1	A	305	ASP
1	A	309	TRP
1	A	310	LEU
1	A	311	ASP
1	A	316	LEU
1	A	317	SER
1	A	319	ASP
1	A	328	GLU
1	A	329	HIS
1	A	332	LEU
1	A	338	SER
1	A	339	LYS
1	A	342	LEU
1	A	344	ILE
1	A	346	LEU
1	A	347	LYS
1	A	348	GLN
1	A	349	LEU
1	A	351	HIS
1	A	352	ARG
1	A	359	THR
1	A	361	GLU
1	A	363	ARG
1	A	368	VAL
1	A	372	LYS
1	A	377	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	CYS
1	A	385	LEU
1	A	387	ASN
1	A	388	SER
1	A	389	ARG
1	A	405	ASP
1	A	407	HIS
1	A	411	TYR
1	A	414	ASN
1	A	415	GLN
1	A	419	LEU
1	A	422	ILE
1	A	425	ARG
1	A	426	MET
1	A	430	THR
1	A	435	GLN
1	A	436	LEU
1	A	438	THR
1	A	443	LEU
1	A	445	ARG
1	A	446	ARG
1	A	452	ARG
1	A	454	CYS
1	A	459	THR
1	A	460	THR
1	A	464	MET
1	A	472	ASP
1	A	475	ASN
1	A	481	LEU
1	A	486	ASN
1	A	487	LEU
1	A	490	PHE
1	A	491	LEU
1	A	493	GLN
1	A	504	GLU
1	A	509	VAL
1	A	514	ILE
1	A	516	LYS
1	A	517	GLU
1	A	518	LEU
1	A	525	LEU
1	A	528	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	536	GLU
1	A	542	GLU
1	A	544	MET
1	A	547	ILE
1	A	551	ARG
1	A	552	PHE
1	A	553	THR
1	A	564	ARG
1	A	565	LYS
1	A	568	MET
1	A	569	THR
1	A	571	LEU
1	A	574	LEU
1	A	575	LYS
1	A	577	ARG
1	A	589	LEU
1	A	592	GLN
1	A	593	LYS
1	A	597	VAL
1	A	603	GLU
1	A	607	ARG
1	A	611	LEU
1	A	613	GLN
1	A	615	TYR
1	A	619	VAL
1	A	622	GLN
1	A	623	LEU
1	A	625	ARG
1	A	627	ARG
1	A	629	SER
1	A	632	ARG
1	A	633	ASP
1	A	634	ILE
1	A	638	ARG
1	A	639	GLN
1	A	641	MET
1	A	642	ASP
1	A	646	LEU
1	A	648	LYS
1	A	651	GLN
1	A	652	ASN
1	A	653	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	660	ASN
1	A	662	SER
1	A	668	PHE
1	A	671	LEU
1	A	675	SER
1	A	677	ILE
1	A	688	GLU
1	A	689	ARG
1	A	691	PHE
1	A	702	LYS
1	A	706	GLU
1	A	708	ARG
1	A	710	THR
1	A	715	SER
1	A	716	ASP
1	A	718	ARG
1	A	729	SER
1	A	730	THR
1	A	734	SER
1	A	740	GLU
1	A	742	MET
1	A	745	MET
1	A	762	ARG
1	A	764	GLN
1	A	765	SER
1	A	768	THR
1	A	776	VAL
1	A	781	ASN
1	A	784	MET
1	A	788	ILE
1	A	800	HIS
1	A	801	LEU
1	A	802	ARG
1	A	807	MET
1	A	810	MET
1	A	812	MET
1	A	819	ASP
1	A	828	ARG
1	A	830	ARG
1	A	833	ARG
1	A	834	MET
1	A	836	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	842	ARG
1	A	843	ARG
1	A	846	LEU
1	A	849	ASP
1	A	853	ASP
1	A	856	THR
1	A	865	ARG
1	A	866	GLU
1	A	869	THR
1	A	873	ILE
1	A	878	GLU
1	A	879	ARG
1	A	881	SER
1	A	883	LEU
1	A	885	LEU
1	A	886	ARG
1	A	889	GLU
1	A	901	SER
1	A	902	MET
1	A	903	LEU
1	A	918	LYS
1	A	919	LEU
1	A	923	THR
1	A	926	THR
1	A	927	ASN
1	A	928	ARG
1	A	929	GLN
1	A	931	LEU
1	A	932	ARG
1	A	938	ARG
1	A	939	ASN
1	A	950	MET
1	A	965	ARG
1	A	968	MET
1	A	972	GLU
2	B	2	SER
2	B	5	SER
2	B	7	GLN
2	B	10	GLU
2	B	11	THR
2	B	15	THR
2	B	16	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	29	VAL
2	B	32	LYS
2	B	34	THR
2	B	37	LEU
2	B	38	LYS
2	B	43	THR
2	B	47	GLU
2	B	51	LEU
2	B	53	ILE
2	B	55	LYS
2	B	56	ARG
2	B	58	GLU
2	B	59	VAL
2	B	64	LEU
2	B	66	ARG
2	B	74	MET
2	B	75	MET
2	B	77	LEU
2	B	78	LEU
2	B	79	ARG
2	B	81	GLU
2	B	82	LYS
2	B	89	ASP
2	B	91	LYS
2	B	92	LEU
2	B	93	MET
2	B	95	GLN
2	B	120	LEU
2	B	123	ASN
2	B	135	ASP
2	B	138	GLU
2	B	140	GLU
2	B	141	TYR
2	B	149	GLN
2	B	161	LEU
2	B	167	SER
2	B	169	GLN
2	B	172	SER
2	B	173	ASP
2	B	177	LEU
2	B	191	THR
2	B	194	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	195	VAL
2	B	198	MET
2	B	201	THR
2	B	202	VAL
2	B	214	ARG
2	B	216	SER
2	B	218	PHE
2	B	220	HIS
2	B	224	LEU
2	B	227	VAL
2	B	231	ILE
2	B	237	HIS
2	B	240	ASP
2	B	246	SER
2	B	248	ASP
2	B	253	HIS
2	B	255	THR
2	B	259	VAL
2	B	262	MET
2	B	263	LEU
2	B	267	ILE
2	B	273	TRP
2	B	278	THR
2	B	285	GLU
2	B	288	THR
2	B	310	LEU
2	B	313	ARG
2	B	315	THR
2	B	319	THR
2	B	326	ARG
2	B	327	TYR
2	B	328	LEU
2	B	329	LEU
2	B	334	CYS
2	B	343	LEU
2	B	347	TRP
2	B	349	LYS
2	B	351	LYS
2	B	364	MET
2	B	365	SER
2	B	366	GLU
2	B	373	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	381	THR
2	B	390	ARG
2	B	391	GLU
2	B	393	LEU
2	B	403	HIS
2	B	404	MET
2	B	406	ASP
2	B	428	CYS
2	B	432	GLU
2	B	434	MET
2	B	435	ASN
2	B	440	LEU
2	B	443	LYS
2	B	446	ARG
2	B	448	MET
2	B	450	GLU
2	B	454	ARG
2	B	455	GLU
2	B	456	VAL
2	B	464	SER
2	B	467	GLN
2	B	468	MET
2	B	469	ILE
2	B	475	ASN
2	B	496	MET
2	B	500	GLN
2	B	503	LEU
2	B	511	ASP
2	B	513	ASP
2	B	514	THR
2	B	517	LEU
2	B	520	ASP
2	B	521	LEU
2	B	527	GLN
2	B	532	THR
2	B	535	ASP
2	B	543	ASN
2	B	546	MET
2	B	549	LYS
2	B	550	MET
2	B	551	VAL
2	B	554	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	557	LEU
2	B	560	TRP
2	B	564	SER
2	B	568	SER
2	B	570	THR
2	B	588	PHE
2	B	589	TYR
2	B	591	THR
2	B	593	THR
2	B	595	ARG
2	B	603	ASP
2	B	606	HIS
2	B	615	MET
2	B	622	LEU
2	B	627	THR
2	B	631	SER
2	B	632	THR
2	B	644	ASP
2	B	655	LEU
2	B	658	THR
2	B	666	LEU
2	B	676	TRP
2	B	681	THR
2	B	684	SER
2	B	686	HIS
2	B	688	ASP
2	B	694	GLU
2	B	706	SER
2	B	708	GLU
2	B	710	HIS
2	B	722	GLU
2	B	729	ARG
2	B	734	LEU
2	B	735	HIS
2	B	748	ASP
2	B	749	THR
2	B	757	ARG
2	B	760	THR
2	B	762	SER
2	B	763	GLU
2	B	765	ARG
2	B	769	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	771	LEU
2	B	776	ARG
2	B	779	LYS
2	B	787	GLN
2	B	788	LEU
2	B	794	GLN
2	B	795	GLU
2	B	799	ARG
2	B	801	GLN
2	B	805	HIS
2	B	806	TYR
2	B	807	PHE
2	B	813	ILE
2	B	815	VAL
2	B	818	HIS
2	B	831	VAL
2	B	835	ARG
2	B	838	ARG
2	B	843	CYS
2	B	844	THR
2	B	846	THR
2	B	852	GLU
2	B	856	LEU
2	B	860	MET
2	B	866	LEU
2	B	891	LEU
2	B	914	LEU
2	B	921	HIS
2	B	924	GLU
2	B	926	ILE
2	B	929	THR
2	B	930	ASN
2	B	943	GLU
2	B	948	PHE
2	B	963	GLN
2	B	970	TYR
2	B	979	LYS
2	B	988	VAL
2	B	992	TYR
2	B	993	LYS
2	B	999	LEU
2	B	1005	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	6	GLN
1	A	7	GLN
1	A	10	ASN
1	A	17	ASN
1	A	20	HIS
1	A	38	ASN
1	A	58	GLN
1	A	107	HIS
1	A	116	HIS
1	A	179	GLN
1	A	203	ASN
1	A	208	HIS
1	A	216	GLN
1	A	238	HIS
1	A	299	HIS
1	A	337	HIS
1	A	341	HIS
1	A	348	GLN
1	A	387	ASN
1	A	407	HIS
1	A	435	GLN
1	A	455	HIS
1	A	467	GLN
1	A	592	GLN
1	A	639	GLN
1	A	649	HIS
1	A	652	ASN
1	A	660	ASN
1	A	667	GLN
1	A	714	ASN
1	A	722	HIS
1	A	757	HIS
1	A	800	HIS
1	A	851	HIS
1	A	862	HIS
1	A	939	ASN
2	B	7	GLN
2	B	95	GLN
2	B	110	GLN
2	B	123	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	149	GLN
2	B	169	GLN
2	B	184	GLN
2	B	204	GLN
2	B	219	GLN
2	B	221	HIS
2	B	253	HIS
2	B	254	GLN
2	B	302	HIS
2	B	383	HIS
2	B	431	HIS
2	B	437	HIS
2	B	449	ASN
2	B	467	GLN
2	B	475	ASN
2	B	485	GLN
2	B	523	HIS
2	B	527	GLN
2	B	538	GLN
2	B	555	ASN
2	B	636	ASN
2	B	667	GLN
2	B	677	HIS
2	B	705	ASN
2	B	744	ASN
2	B	769	ASN
2	B	801	GLN
2	B	805	HIS
2	B	818	HIS
2	B	832	HIS
2	B	865	GLN
2	B	881	ASN
2	B	885	ASN
2	B	963	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	235:ALA	C	236:CYS	N	1.61

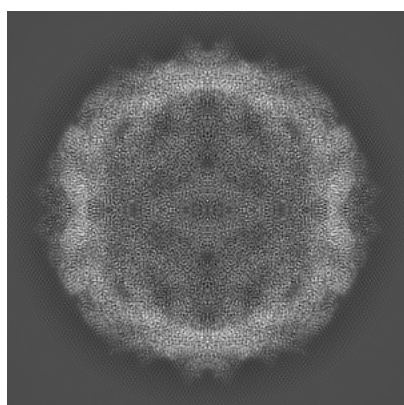
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3619. These allow visual inspection of the internal detail of the map and identification of artifacts.

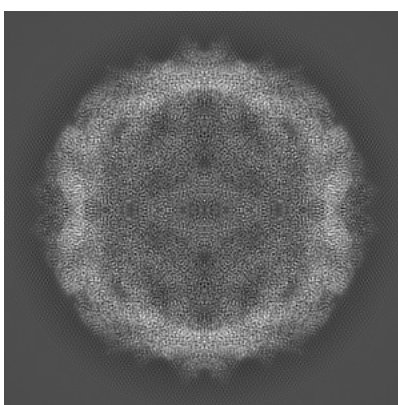
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

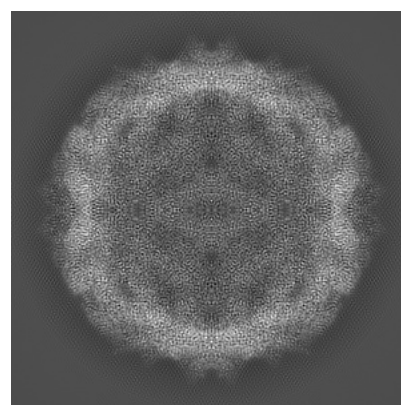
6.1.1 Primary map



X



Y

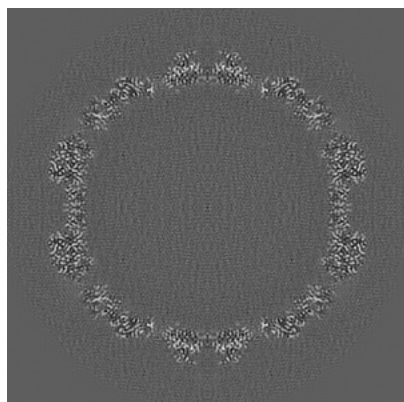


Z

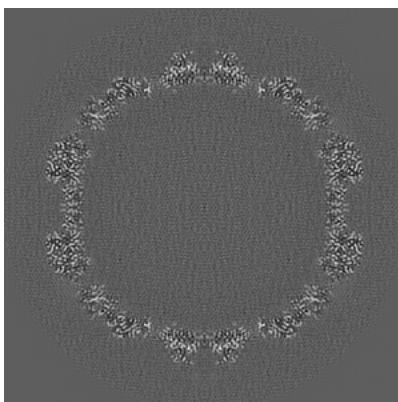
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

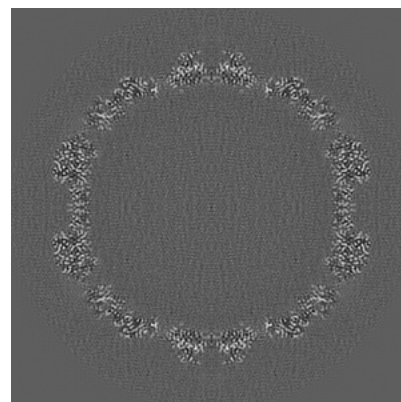
6.2.1 Primary map



X Index: 200



Y Index: 200

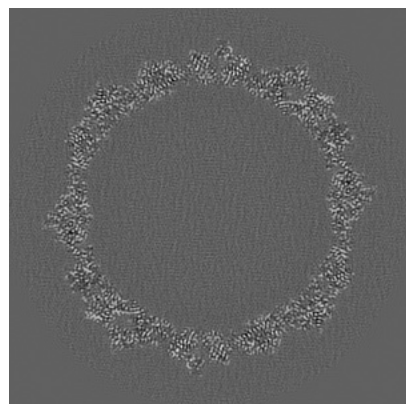


Z Index: 200

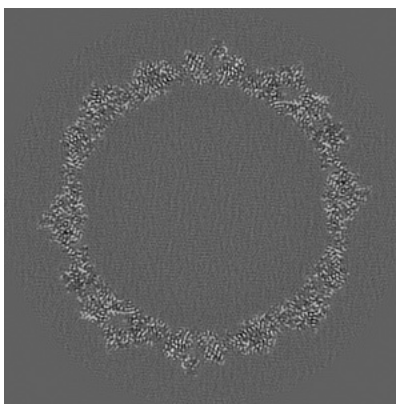
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

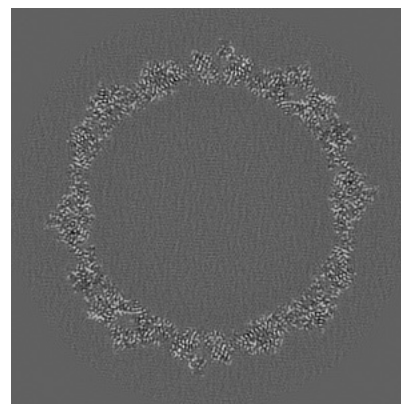
6.3.1 Primary map



X Index: 226



Y Index: 226

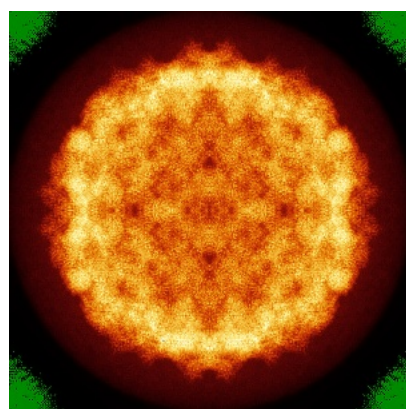


Z Index: 226

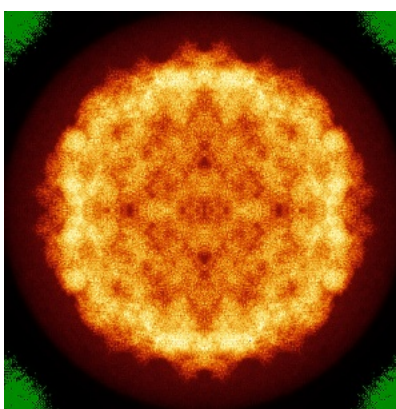
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

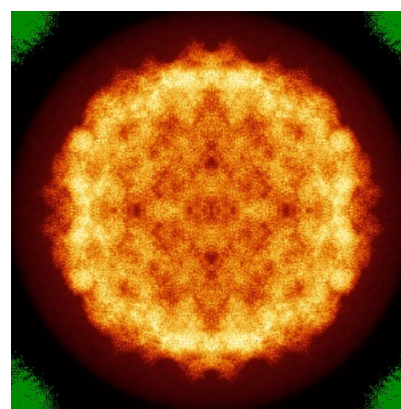
6.4.1 Primary map



X



Y

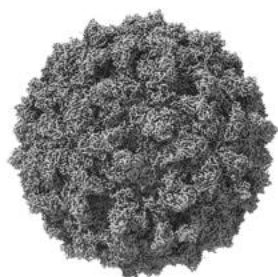


Z

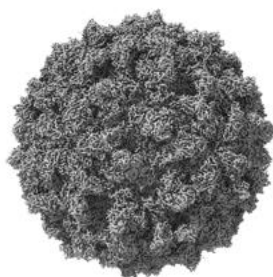
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

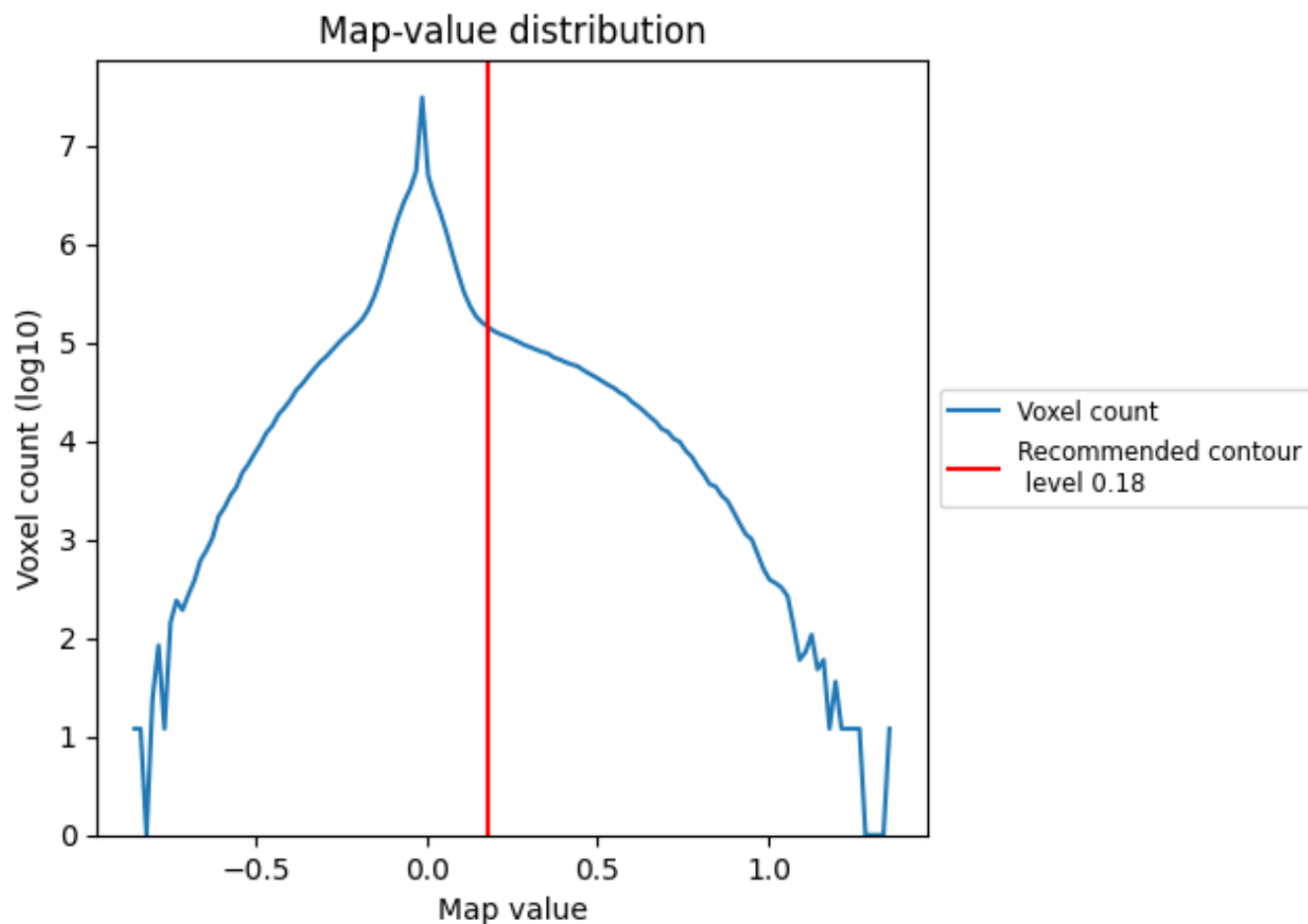
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

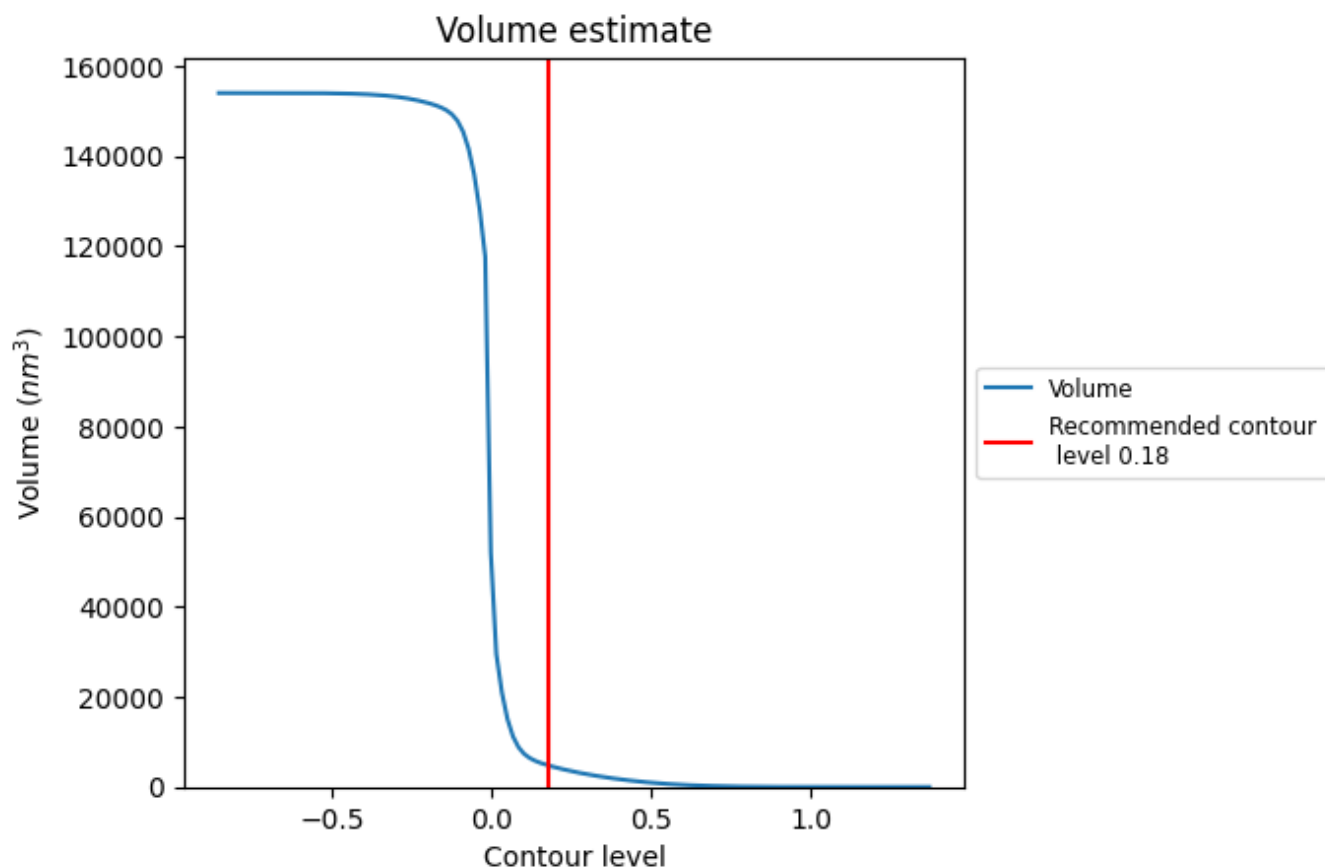
This section contains the results of statistical analysis of the map.

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.

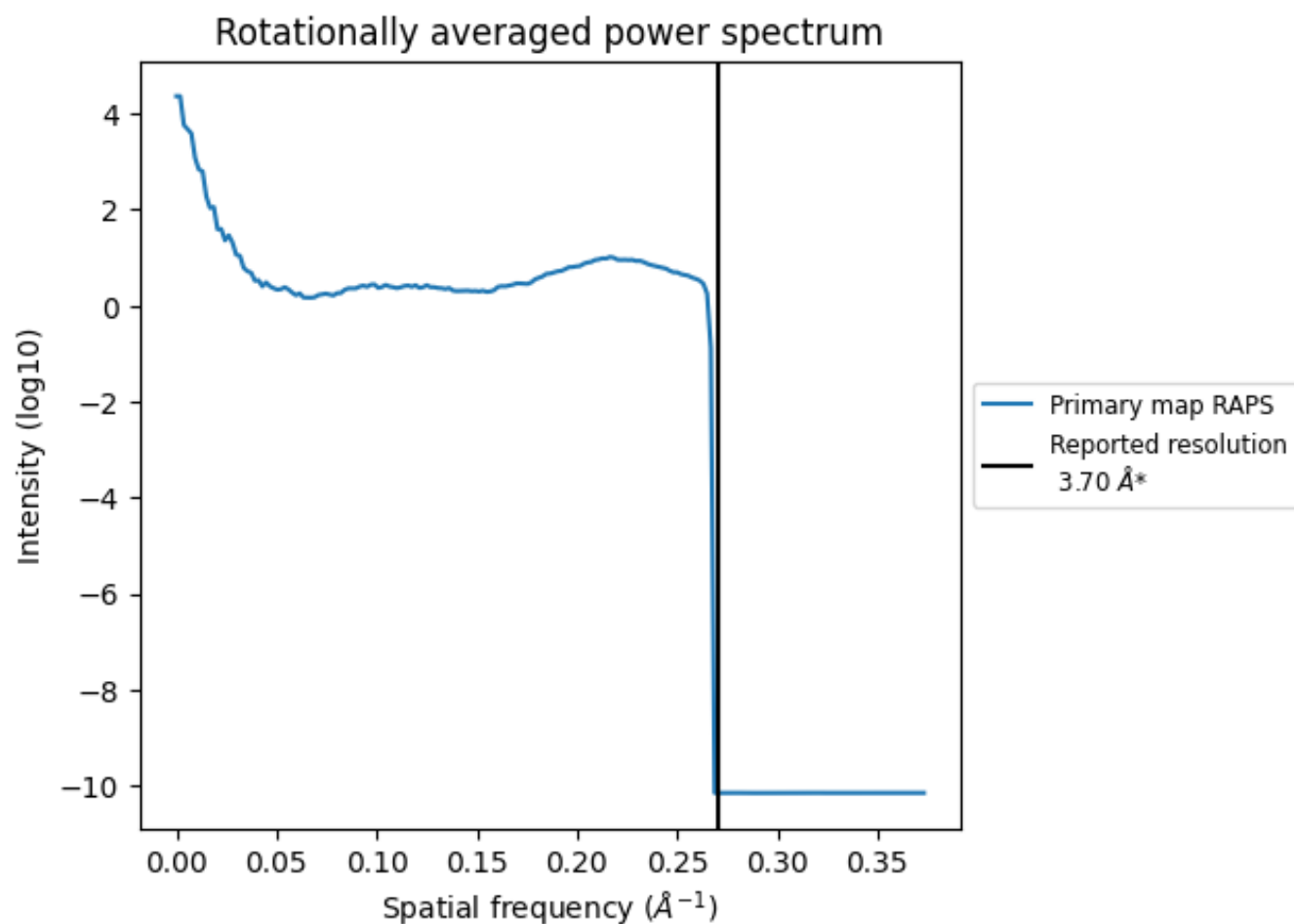
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4755 nm³; this corresponds to an approximate mass of 4296 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

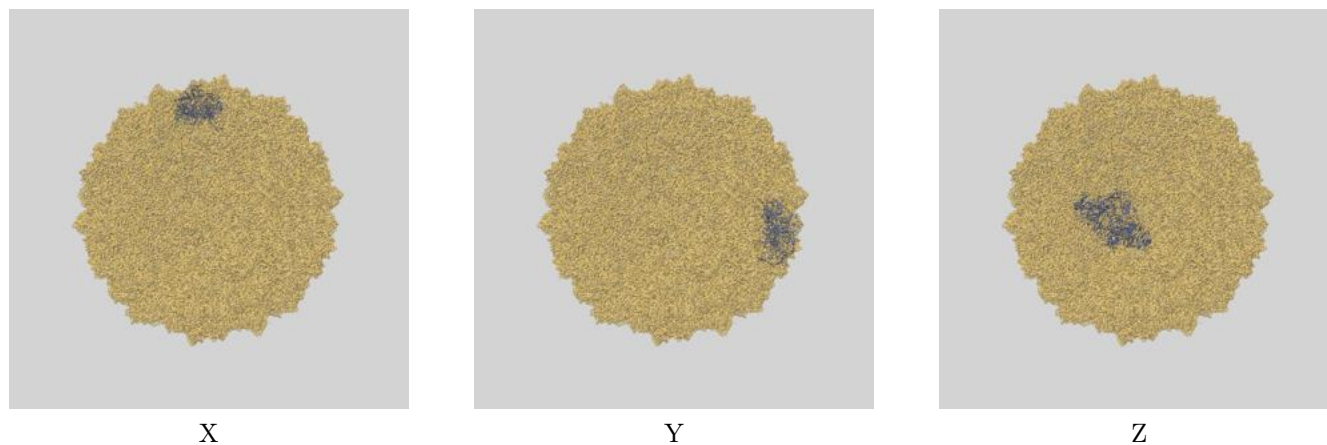
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

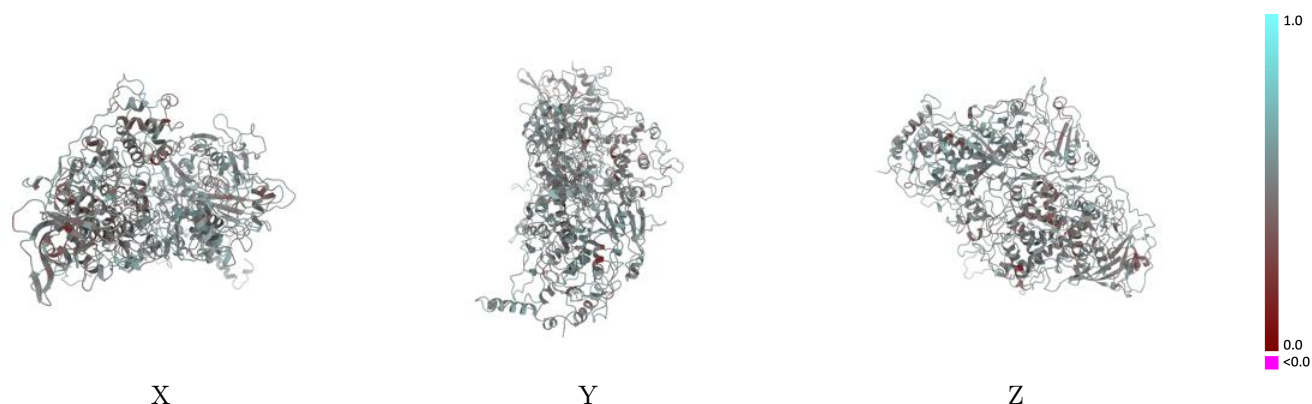
This section contains information regarding the fit between EMDB map EMD-3619 and PDB model 5ND1. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.18 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](#)



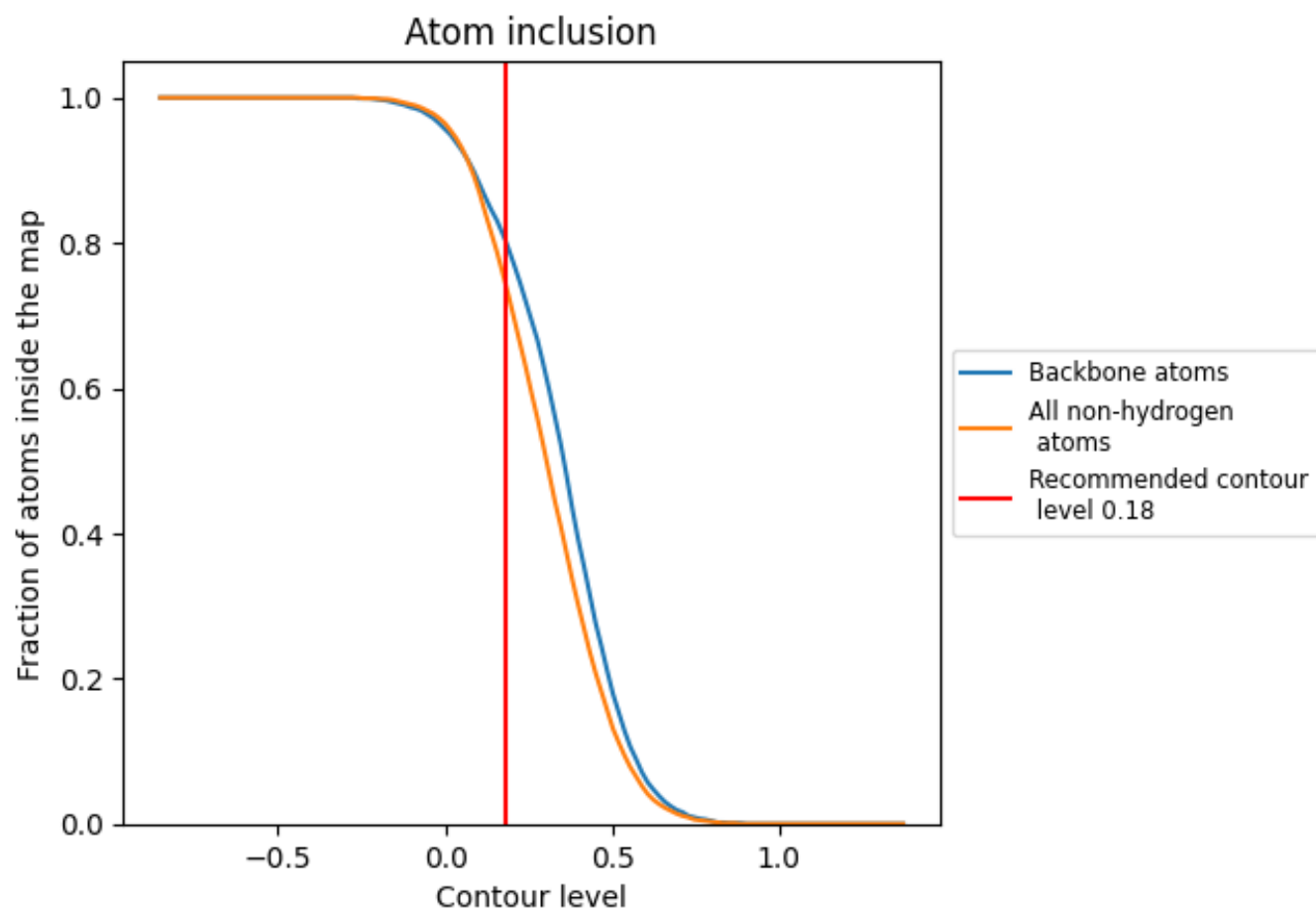
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.18).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7450	0.5060
A	0.7630	0.5210
B	0.7270	0.4910

