



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:58 PM UTC

PDB ID : 9F6Z / pdb_00009f6z
EMDB ID : EMD-17349
Title : Human N-deacetylase/N-sulfotransferase 1 homodimer
Authors : Wild, R.; Lortat-Jacob, H.; Vallet, S.D.
Deposited on : 2024-05-02
Resolution : 4.50 Å(reported)
Based on initial model : .

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

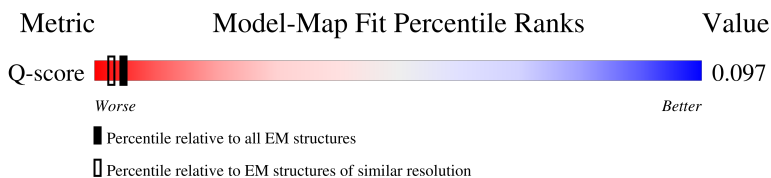
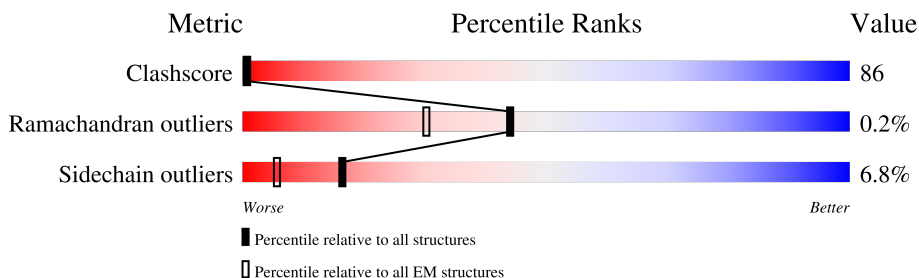
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2937 (4.00 - 5.00)

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	858	42% 31% 53% 9% 6%
1	B	858	34% 28% 54% 10% 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13072 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 Bifunctional heparan sulfate N-deacetylase/N-sulfotransferase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	803	Total	C	N	O	S	0	0
			6526	4225	1111	1168	22		
1	B	806	Total	C	N	O	S	0	0
			6546	4237	1114	1173	22		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	GLY	-	expression tag	UNP P52848
A	41	ALA	-	expression tag	UNP P52848
A	42	SER	-	expression tag	UNP P52848
A	883	ASN	-	expression tag	UNP P52848
A	884	ASN	-	expression tag	UNP P52848
A	885	ASN	-	expression tag	UNP P52848
A	886	ASN	-	expression tag	UNP P52848
A	887	ASN	-	expression tag	UNP P52848
A	888	ASN	-	expression tag	UNP P52848
A	889	GLY	-	expression tag	UNP P52848
A	890	HIS	-	expression tag	UNP P52848
A	891	HIS	-	expression tag	UNP P52848
A	892	HIS	-	expression tag	UNP P52848
A	893	HIS	-	expression tag	UNP P52848
A	894	HIS	-	expression tag	UNP P52848
A	895	HIS	-	expression tag	UNP P52848
A	896	HIS	-	expression tag	UNP P52848
A	897	HIS	-	expression tag	UNP P52848
B	40	GLY	-	expression tag	UNP P52848
B	41	ALA	-	expression tag	UNP P52848
B	42	SER	-	expression tag	UNP P52848
B	883	ASN	-	expression tag	UNP P52848
B	884	ASN	-	expression tag	UNP P52848
B	885	ASN	-	expression tag	UNP P52848
B	886	ASN	-	expression tag	UNP P52848

Continued on next page...

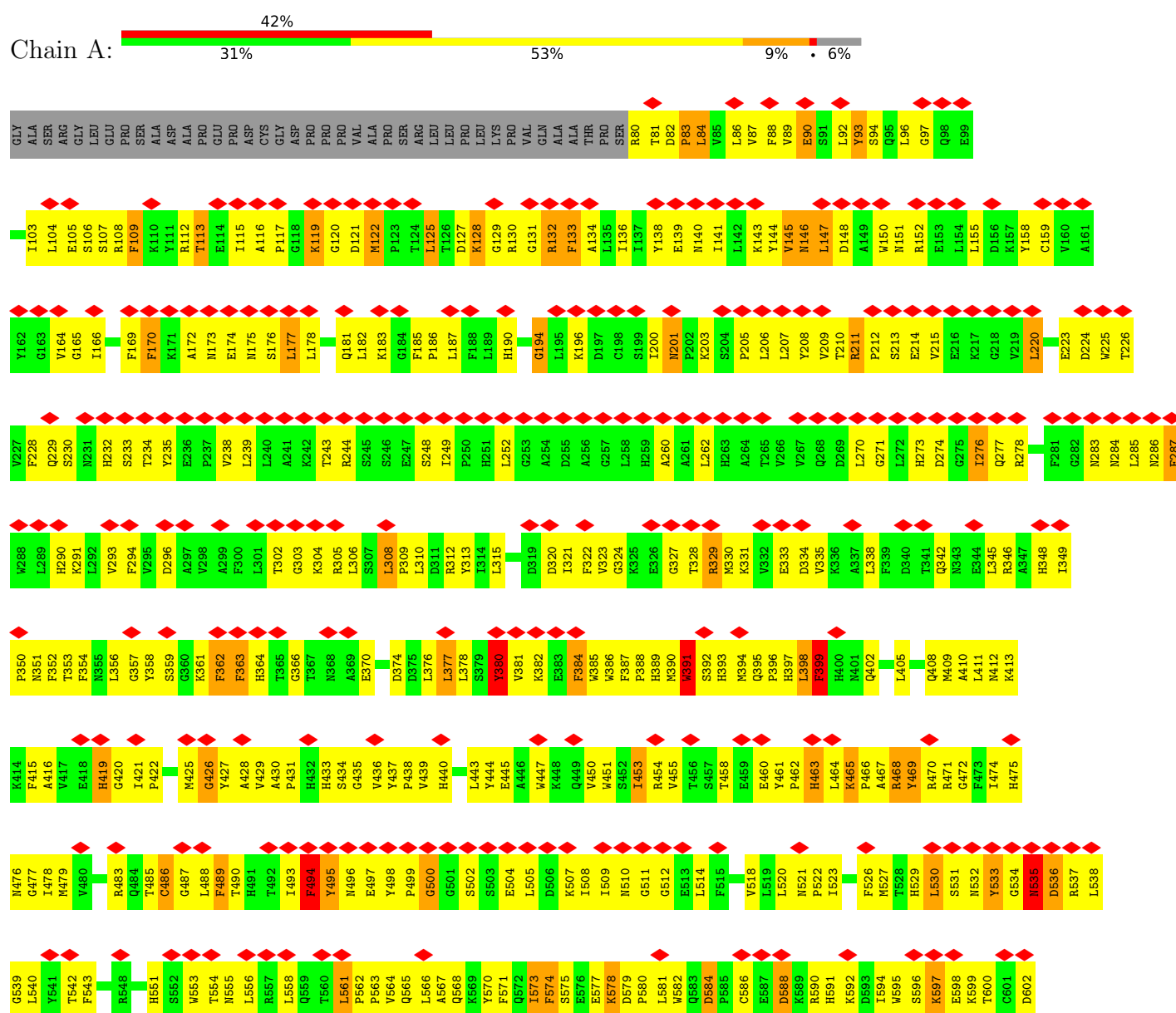
Continued from previous page...

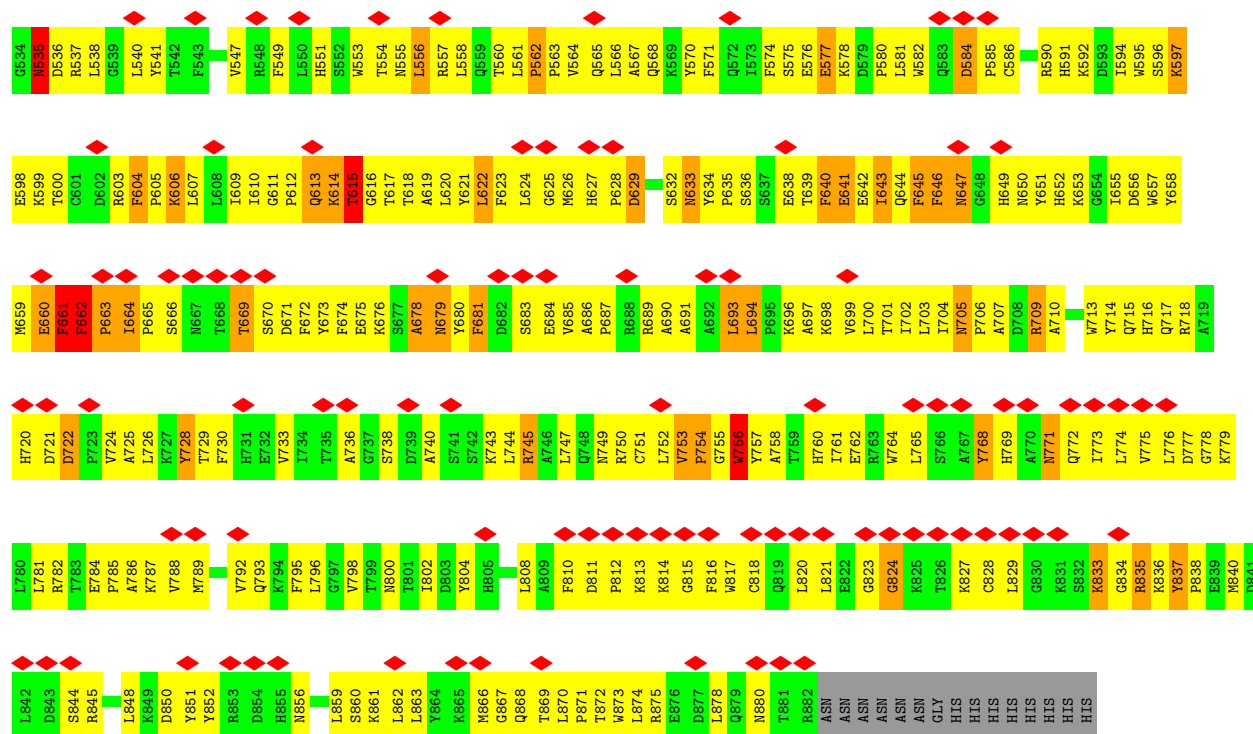
Chain	Residue	Modelled	Actual	Comment	Reference
B	887	ASN	-	expression tag	UNP P52848
B	888	ASN	-	expression tag	UNP P52848
B	889	GLY	-	expression tag	UNP P52848
B	890	HIS	-	expression tag	UNP P52848
B	891	HIS	-	expression tag	UNP P52848
B	892	HIS	-	expression tag	UNP P52848
B	893	HIS	-	expression tag	UNP P52848
B	894	HIS	-	expression tag	UNP P52848
B	895	HIS	-	expression tag	UNP P52848
B	896	HIS	-	expression tag	UNP P52848
B	897	HIS	-	expression tag	UNP P52848

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: Bifunctional heparan sulfate N-deacetylase/N-sulfotransferase 1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	221316	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	38.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	36000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.265	Depositor
Minimum map value	-0.837	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.262	Depositor
Map size (Å)	360.0, 360.0, 360.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.125, 1.125, 1.125	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	1.16	5/6717 (0.1%)	1.59	86/9118 (0.9%)
1	B	1.20	9/6738 (0.1%)	1.62	103/9148 (1.1%)
All	All	1.18	14/13455 (0.1%)	1.60	189/18266 (1.0%)

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	6
1	B	0	6
All	All	0	12

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	753	VAL	CA-CB	-10.02	1.49	1.54
1	A	729	THR	CA-C	-6.65	1.44	1.53
1	B	349	ILE	CA-C	-6.40	1.47	1.52
1	B	753	VAL	CA-CB	-5.89	1.51	1.54
1	B	436	VAL	CA-CB	-5.80	1.47	1.54
1	B	185	PHE	CA-C	-5.58	1.47	1.52
1	B	663	PRO	N-CA	-5.41	1.40	1.47
1	B	768	TYR	CA-C	-5.31	1.46	1.52
1	B	498	TYR	CA-C	-5.31	1.46	1.53
1	A	463	HIS	CA-C	-5.25	1.46	1.52
1	A	399	PHE	CA-C	-5.23	1.46	1.52
1	A	604	PHE	CA-C	-5.22	1.47	1.53
1	B	429	VAL	CA-C	-5.09	1.46	1.52
1	B	664	ILE	CA-C	-5.00	1.48	1.53

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	PHE	CA-CB-CG	-12.35	101.45	113.80
1	A	604	PHE	CA-CB-CG	-12.24	101.56	113.80
1	B	362	PHE	CA-CB-CG	-11.13	102.67	113.80
1	A	510	ASN	CA-CB-CG	-10.22	102.38	112.60
1	A	399	PHE	CA-CB-CG	-9.90	103.90	113.80
1	A	398	LEU	CA-C-N	-9.32	110.13	123.00
1	A	398	LEU	C-N-CA	-9.32	110.13	123.00
1	A	645	PHE	CA-CB-CG	-9.19	104.61	113.80
1	B	419	HIS	CA-CB-CG	-9.08	104.72	113.80
1	B	133	PHE	CA-CB-CG	-9.01	104.79	113.80
1	A	128	LYS	CA-C-N	-8.98	109.74	122.86
1	A	128	LYS	C-N-CA	-8.98	109.74	122.86
1	B	354	PHE	CA-CB-CG	-8.93	104.88	113.80
1	A	815	GLY	N-CA-C	-8.83	103.14	115.32
1	B	349	ILE	CA-C-O	8.55	124.39	119.94
1	A	489	PHE	CA-CB-CG	-8.54	105.26	113.80
1	A	729	THR	N-CA-C	-8.39	98.05	110.46
1	A	573	ILE	CA-C-N	-8.25	111.35	122.99
1	A	573	ILE	C-N-CA	-8.25	111.35	122.99
1	B	498	TYR	CA-CB-CG	-8.23	99.09	113.90
1	A	650	ASN	CA-CB-CG	-8.09	104.52	112.60
1	A	287	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	362	PHE	CA-CB-CG	-8.03	105.77	113.80
1	B	352	PHE	CA-CB-CG	-7.82	105.98	113.80
1	B	109	PHE	CA-CB-CG	-7.76	106.04	113.80
1	B	661	PHE	N-CA-C	-7.66	102.93	111.28
1	B	604	PHE	CA-CB-CG	-7.58	106.22	113.80
1	B	363	PHE	CA-CB-CG	-7.53	106.27	113.80
1	A	170	PHE	CA-CB-CG	-7.46	106.34	113.80
1	B	287	PHE	CA-CB-CG	-7.44	106.36	113.80
1	A	129	GLY	N-CA-C	-7.25	106.06	114.69
1	B	435	GLY	N-CA-C	-7.25	106.07	114.69
1	B	398	LEU	N-CA-C	-7.24	103.39	111.28
1	B	662	PHE	CA-CB-CG	-7.23	106.57	113.80
1	B	640	PHE	CA-CB-CG	-7.17	106.63	113.80
1	B	303	GLY	N-CA-C	-7.06	105.47	115.43
1	A	768	TYR	CA-CB-CG	-6.88	101.52	113.90
1	B	867	GLY	N-CA-C	-6.85	105.87	115.32
1	A	303	GLY	N-CA-C	-6.75	105.32	115.32
1	B	679	ASN	CA-CB-CG	-6.75	105.84	112.60
1	B	562	PRO	N-CA-C	-6.73	102.49	110.70
1	A	616	GLY	N-CA-C	-6.64	105.73	115.63
1	B	487	GLY	N-CA-C	-6.63	105.35	114.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	500	GLY	N-CA-C	-6.62	106.50	113.58
1	A	133	PHE	CA-CB-CG	-6.57	107.23	113.80
1	B	391	TRP	N-CA-C	-6.54	104.08	111.07
1	B	477	GLY	N-CA-C	-6.44	105.88	114.25
1	A	420	GLY	N-CA-C	-6.43	106.36	115.43
1	A	384	PHE	CA-CB-CG	-6.37	107.43	113.80
1	B	532	ASN	N-CA-C	-6.37	104.34	111.28
1	B	231	ASN	CA-CB-CG	-6.31	106.29	112.60
1	B	424	ASP	CA-CB-CG	-6.31	106.29	112.60
1	B	310	LEU	N-CA-C	-6.30	104.49	111.36
1	A	391	TRP	N-CA-C	-6.29	104.34	111.07
1	A	354	PHE	CA-CB-CG	-6.26	107.54	113.80
1	B	140	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	234	THR	N-CA-C	-6.24	104.48	111.28
1	B	146	ASN	CA-CB-CG	-6.22	106.38	112.60
1	A	327	GLY	N-CA-C	-6.20	107.31	114.69
1	A	823	GLY	N-CA-C	-6.19	107.17	115.21
1	B	170	PHE	CA-CB-CG	-6.19	107.61	113.80
1	B	616	GLY	N-CA-C	-6.18	105.85	115.67
1	B	274	ASP	CA-CB-CG	-6.18	106.42	112.60
1	A	645	PHE	CB-CA-C	-6.17	101.19	110.88
1	B	815	GLY	N-CA-C	-6.17	106.72	115.30
1	B	379	SER	CA-C-N	6.15	129.13	120.28
1	B	379	SER	C-N-CA	6.15	129.13	120.28
1	B	753	VAL	N-CA-CB	6.15	115.24	110.45
1	A	588	ASP	CA-CB-CG	-6.14	106.46	112.60
1	B	354	PHE	CA-C-N	-6.10	114.52	123.05
1	B	354	PHE	C-N-CA	-6.10	114.52	123.05
1	A	574	PHE	N-CA-CB	6.08	120.90	110.68
1	A	175	ASN	CA-CB-CG	-6.08	106.52	112.60
1	B	496	ASN	CA-CB-CG	-6.07	106.53	112.60
1	B	489	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	646	PHE	CA-CB-CG	-6.05	107.75	113.80
1	A	486	CYS	N-CA-C	-6.04	105.18	112.54
1	B	322	PHE	N-CA-C	-6.02	105.89	113.23
1	B	615	THR	N-CA-C	-6.00	104.86	111.82
1	A	867	GLY	N-CA-C	-5.99	106.83	115.27
1	A	661	PHE	CA-CB-CG	-5.98	107.82	113.80
1	B	118	GLY	N-CA-C	-5.96	105.57	112.73
1	B	728	TYR	CD1-CG-CD2	5.94	127.02	118.10
1	B	754	PRO	CA-C-N	5.89	127.51	120.14
1	B	754	PRO	C-N-CA	5.89	127.51	120.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	755	GLY	CA-C-N	5.88	132.77	121.54
1	A	755	GLY	C-N-CA	5.88	132.77	121.54
1	B	184	GLY	N-CA-C	-5.83	107.60	115.36
1	B	753	VAL	CB-CA-C	-5.82	106.38	114.00
1	A	194	GLY	N-CA-C	-5.80	104.66	112.14
1	A	270	LEU	N-CA-C	-5.76	105.00	111.28
1	A	640	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	477	GLY	N-CA-C	-5.75	108.24	115.08
1	A	681	PHE	CA-CB-CG	-5.72	108.08	113.80
1	B	693	LEU	CA-C-N	-5.72	115.38	122.42
1	B	693	LEU	C-N-CA	-5.72	115.38	122.42
1	B	362	PHE	CG-CD2-CE2	-5.71	110.99	120.70
1	B	705	ASN	CA-C-N	5.70	125.38	119.56
1	B	705	ASN	C-N-CA	5.70	125.38	119.56
1	A	556	LEU	CA-C-N	-5.69	114.05	122.41
1	A	556	LEU	C-N-CA	-5.69	114.05	122.41
1	B	823	GLY	N-CA-C	-5.68	107.83	115.21
1	B	420	GLY	N-CA-C	-5.67	107.28	115.27
1	B	270	LEU	N-CA-C	-5.65	105.12	111.28
1	A	721	ASP	CA-CB-CG	-5.63	106.97	112.60
1	B	398	LEU	CA-C-N	-5.61	114.16	122.41
1	B	398	LEU	C-N-CA	-5.61	114.16	122.41
1	A	511	GLY	N-CA-C	-5.61	106.26	114.90
1	B	460	GLU	CA-C-N	-5.60	110.66	123.15
1	B	460	GLU	C-N-CA	-5.60	110.66	123.15
1	B	349	ILE	O-C-N	5.60	126.07	120.59
1	A	530	LEU	N-CA-C	-5.59	105.26	111.36
1	B	647	ASN	CA-CB-CG	-5.59	107.01	112.60
1	B	661	PHE	CA-CB-CG	-5.59	108.21	113.80
1	B	467	ALA	N-CA-C	-5.59	105.19	111.28
1	B	437	TYR	CA-CB-CG	-5.58	103.86	113.90
1	B	178	LEU	CA-C-N	-5.55	115.06	122.72
1	B	178	LEU	C-N-CA	-5.55	115.06	122.72
1	B	384	PHE	CA-CB-CG	-5.53	108.27	113.80
1	B	678	ALA	N-CA-C	-5.52	105.26	111.28
1	B	284	ASN	CA-CB-CG	-5.50	107.10	112.60
1	B	662	PHE	CA-C-O	5.44	124.12	119.66
1	A	722	ASP	CA-C-N	5.44	125.26	119.28
1	A	722	ASP	C-N-CA	5.44	125.26	119.28
1	B	305	ARG	N-CA-C	-5.43	105.26	111.07
1	B	381	VAL	CB-CA-C	-5.41	104.95	112.04
1	B	722	ASP	CA-C-N	5.41	125.22	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	722	ASP	C-N-CA	5.41	125.22	119.28
1	B	177	LEU	N-CA-C	-5.40	103.40	110.53
1	A	579	ASP	CA-CB-CG	-5.37	107.23	112.60
1	B	768	TYR	CA-CB-CG	-5.36	104.25	113.90
1	A	309	PRO	N-CA-CB	5.35	108.31	103.33
1	A	536	ASP	CA-CB-CG	-5.35	107.25	112.60
1	B	322	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	835	ARG	CA-C-N	-5.35	114.65	122.19
1	A	835	ARG	C-N-CA	-5.35	114.65	122.19
1	A	584	ASP	CA-C-N	5.34	124.95	119.56
1	A	584	ASP	C-N-CA	5.34	124.95	119.56
1	B	327	GLY	N-CA-C	-5.33	107.31	114.25
1	B	660	GLU	N-CA-C	-5.32	105.59	111.71
1	A	83	PRO	N-CA-C	-5.32	107.49	114.03
1	B	616	GLY	CA-C-N	5.30	127.38	120.28
1	B	616	GLY	C-N-CA	5.30	127.38	120.28
1	B	629	ASP	N-CA-C	-5.27	105.53	111.28
1	A	753	VAL	CB-CA-C	-5.26	107.11	114.00
1	A	837	TYR	CA-C-N	5.26	125.17	119.85
1	A	837	TYR	C-N-CA	5.26	125.17	119.85
1	A	380	TYR	N-CA-CB	5.26	118.31	110.22
1	A	667	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	645	PHE	N-CA-CB	5.25	117.92	110.16
1	B	471	ARG	CD-NE-CZ	-5.24	117.06	124.40
1	A	824	GLY	N-CA-C	-5.23	108.02	115.30
1	A	493	ILE	CB-CA-C	-5.23	105.28	111.97
1	B	418	GLU	CA-C-N	5.22	127.23	120.44
1	B	418	GLU	C-N-CA	5.22	127.23	120.44
1	B	705	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	521	ASN	CA-CB-CG	-5.20	107.41	112.60
1	A	494	PHE	CA-C-N	5.18	127.65	120.29
1	A	494	PHE	C-N-CA	5.18	127.65	120.29
1	B	93	TYR	CA-CB-CG	-5.18	104.57	113.90
1	B	824	GLY	N-CA-C	-5.18	108.10	115.30
1	B	486	CYS	N-CA-C	-5.17	105.82	111.82
1	B	208	TYR	N-CA-C	-5.17	105.73	111.36
1	A	800	ASN	CA-CB-CG	-5.17	107.43	112.60
1	A	755	GLY	N-CA-C	-5.15	107.40	113.99
1	A	145	VAL	CA-C-N	-5.14	115.58	122.42
1	A	145	VAL	C-N-CA	-5.14	115.58	122.42
1	A	533	TYR	CA-CB-CG	-5.14	104.64	113.90
1	A	834	GLY	N-CA-C	-5.14	108.23	115.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	174	GLU	N-CA-C	-5.11	105.71	111.28
1	B	880	ASN	CA-CB-CG	-5.11	107.49	112.60
1	B	584	ASP	CA-C-N	5.10	124.71	119.56
1	B	584	ASP	C-N-CA	5.10	124.71	119.56
1	B	641	GLU	N-CA-C	-5.10	105.72	111.28
1	A	495	TYR	N-CA-C	-5.08	105.83	111.36
1	A	536	ASP	N-CA-C	-5.08	106.19	112.38
1	B	652	HIS	N-CA-C	-5.08	105.75	111.28
1	A	201	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	476	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	426	GLY	N-CA-C	-5.06	106.46	114.10
1	A	233	SER	N-CA-C	-5.06	105.95	111.82
1	B	121	ASP	CA-CB-CG	-5.05	107.55	112.60
1	B	83	PRO	N-CA-C	-5.04	107.82	114.03
1	A	90	GLU	N-CA-C	-5.03	105.71	111.14
1	B	186	PRO	N-CA-C	-5.02	107.85	114.03
1	A	146	ASN	CA-CB-CG	-5.01	107.59	112.60
1	B	109	PHE	CA-C-N	-5.00	113.77	120.87
1	B	109	PHE	C-N-CA	-5.00	113.77	120.87

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLU	Peptide
1	A	380	TYR	Peptide
1	A	694	LEU	Peptide
1	A	709	ARG	Sidechain
1	A	745	ARG	Sidechain
1	A	756	TRP	Peptide
1	B	127	ASP	Peptide
1	B	380	TYR	Peptide
1	B	459	GLU	Peptide
1	B	709	ARG	Sidechain
1	B	745	ARG	Sidechain
1	B	756	TRP	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	6526	0	6429	1064	0
1	B	6546	0	6448	1177	0
All	All	13072	0	12877	2233	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 86.

All (2233) 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:B:329:ARG:HD3	1:B:530:LEU:HD21	1.22	1.19
1:B:615:THR:HB	1:B:617:THR:HG23	1.29	1.14
1:A:455:VAL:HG21	1:A:564:VAL:HA	1.18	1.13
1:A:389:HIS:HB3	1:A:431:PRO:HG3	1.24	1.13
1:A:248:SER:HB2	1:A:252:LEU:HD11	1.28	1.11
1:B:378:LEU:HA	1:B:381:VAL:HG23	1.20	1.11
1:B:451:TRP:HB2	1:B:453:ILE:HD11	1.32	1.11
1:B:715:GLN:HB3	1:B:835:ARG:HD3	1.33	1.10
1:A:159:CYS:HB3	1:A:276:ILE:HG21	1.14	1.09
1:B:694:LEU:HD12	1:B:697:ALA:HB2	1.29	1.09
1:B:99:GLU:HB3	1:B:285:LEU:HD23	1.19	1.09
1:B:508:ILE:HA	1:B:512:GLY:HA3	1.29	1.09
1:A:200:ILE:HD13	1:A:206:LEU:HD22	1.29	1.07
1:B:96:LEU:HB2	1:B:284:ASN:HD21	1.17	1.07
1:A:509:ILE:HD11	1:A:542:THR:HG23	1.35	1.07
1:A:322:PHE:HB3	1:A:363:PHE:HA	1.37	1.06
1:A:730:PHE:HE1	1:A:848:LEU:HD11	1.16	1.05
1:B:775:VAL:HB	1:B:868:GLN:HG2	1.09	1.05
1:A:451:TRP:HB2	1:A:453:ILE:HD11	1.35	1.04
1:B:390:MET:HG3	1:B:408:GLN:HB3	1.39	1.03
1:B:860:SER:HA	1:B:870:LEU:HD21	1.41	1.02
1:B:863:LEU:HD12	1:B:870:LEU:HD23	1.39	1.02
1:A:644:GLN:HG2	1:A:647:ASN:HB3	1.42	1.02
1:B:81:THR:HG22	1:B:131:GLY:HA3	1.42	1.02
1:A:147:LEU:HB2	1:A:152:ARG:HB2	1.38	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:LEU:HD12	1:B:566:LEU:HD12	1.39	1.01
1:A:147:LEU:HD23	1:A:152:ARG:HD3	1.42	1.00
1:B:606:LYS:HE3	1:B:673:TYR:H	1.23	1.00
1:A:694:LEU:HD13	1:A:697:ALA:HB3	1.43	1.00
1:B:322:PHE:HB3	1:B:363:PHE:HA	1.42	1.00
1:B:390:MET:HB3	1:B:393:HIS:H	1.23	0.99
1:A:117:PRO:HB2	1:A:120:GLY:H	1.26	0.99
1:A:703:LEU:HD22	1:A:757:TYR:CG	1.97	0.99
1:B:607:LEU:HD13	1:B:796:LEU:HD21	1.45	0.98
1:B:768:TYR:HD2	1:B:772:GLN:HG2	1.29	0.98
1:A:329:ARG:HB2	1:A:370:GLU:HG2	1.46	0.96
1:B:330:MET:HE3	1:B:335:VAL:HG22	1.47	0.95
1:A:145:VAL:HB	1:A:183:LYS:HD2	1.45	0.95
1:B:117:PRO:HG2	1:B:120:GLY:HA3	1.47	0.95
1:A:597:LYS:HE3	1:A:597:LYS:HA	1.46	0.95
1:A:385:TRP:HB3	1:A:425:MET:HE1	1.47	0.95
1:B:349:ILE:HD11	1:B:558:LEU:HD13	1.46	0.95
1:B:622:LEU:HD21	1:B:827:LYS:HE2	1.48	0.95
1:B:639:THR:HG21	1:B:644:GLN:HB2	1.46	0.95
1:B:313:TYR:CD1	1:B:561:LEU:HG	2.02	0.95
1:B:323:VAL:HG13	1:B:362:PHE:CD2	2.01	0.95
1:A:147:LEU:CD2	1:A:152:ARG:HD3	1.97	0.94
1:A:390:MET:HE1	1:A:409:MET:HG2	1.47	0.94
1:B:378:LEU:HA	1:B:381:VAL:CG2	1.96	0.94
1:A:730:PHE:CE1	1:A:848:LEU:HD11	2.02	0.94
1:A:614:LYS:HE2	1:A:833:LYS:HB3	1.48	0.94
1:A:829:LEU:H	1:A:829:LEU:HD13	1.29	0.94
1:A:210:THR:HG22	1:A:555:ASN:H	1.29	0.94
1:A:716:HIS:CD2	1:A:832:SER:HB2	2.03	0.94
1:B:328:THR:HB	1:B:531:SER:HA	1.48	0.94
1:B:860:SER:HA	1:B:870:LEU:CD2	1.98	0.94
1:A:626:MET:HE2	1:A:819:GLN:HE22	1.30	0.93
1:A:703:LEU:HD11	1:A:761:ILE:CD1	1.97	0.93
1:B:465:LYS:H	1:B:465:LYS:HE3	1.33	0.93
1:A:603:ARG:HH12	1:A:664:ILE:HG22	1.34	0.92
1:A:860:SER:HA	1:A:870:LEU:HD22	1.48	0.92
1:B:613:GLN:HB3	1:B:678:ALA:HB1	1.50	0.92
1:A:561:LEU:HD13	1:A:562:PRO:HD2	1.49	0.92
1:A:239:LEU:HD11	1:A:293:VAL:HG21	1.51	0.92
1:A:659:MET:HA	1:A:662:PHE:CE2	2.05	0.92
1:B:399:PHE:HB2	1:B:405:LEU:HD21	1.51	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:PRO:HG2	1:A:443:LEU:HD22	1.50	0.92
1:B:88:PHE:CD1	1:B:116:ALA:HB2	2.05	0.92
1:B:438:PRO:HB3	1:B:585:PRO:HB3	1.51	0.92
1:B:561:LEU:HB2	1:B:566:LEU:HD13	1.51	0.92
1:A:132:ARG:HG2	1:A:133:PHE:CZ	2.05	0.92
1:B:200:ILE:HD12	1:B:213:SER:HB2	1.50	0.92
1:A:349:ILE:CD1	1:A:558:LEU:HB2	2.00	0.91
1:B:752:LEU:HD22	1:B:851:TYR:CE1	2.05	0.91
1:B:607:LEU:HD22	1:B:796:LEU:HD11	1.52	0.91
1:B:141:ILE:HD13	1:B:168:GLY:HA3	1.52	0.91
1:B:395:GLN:HG2	1:B:434:SER:HB2	1.53	0.91
1:A:866:MET:HG3	1:A:868:GLN:HG2	1.50	0.91
1:A:89:VAL:HG21	1:A:92:LEU:HD23	1.51	0.90
1:A:479:MET:HE1	1:A:568:GLN:HG3	1.54	0.90
1:A:508:ILE:HA	1:A:512:GLY:HA3	1.53	0.90
1:A:705:ASN:HD21	1:A:873:TRP:HB2	1.36	0.90
1:A:509:ILE:CD1	1:A:542:THR:HG23	2.02	0.89
1:A:650:ASN:HA	1:A:653:LYS:HG2	1.52	0.89
1:B:159:CYS:HB3	1:B:276:ILE:HG21	1.52	0.89
1:B:724:VAL:HG21	1:B:743:LYS:HB3	1.53	0.89
1:A:209:VAL:HG12	1:A:555:ASN:HB2	1.53	0.89
1:A:659:MET:HA	1:A:662:PHE:CZ	2.06	0.89
1:B:387:PHE:CD2	1:B:429:VAL:HB	2.07	0.89
1:A:474:ILE:HD12	1:A:578:LYS:HG3	1.55	0.89
1:B:730:PHE:HE2	1:B:751:CYS:HG	0.95	0.89
1:B:635:PRO:HA	1:B:643:ILE:HG23	1.54	0.89
1:B:386:TRP:CD1	1:B:422:PRO:HD2	2.08	0.89
1:A:612:PRO:HG2	1:A:757:TYR:HE1	1.35	0.89
1:B:122:MET:HG2	1:B:155:LEU:HD13	1.55	0.88
1:A:302:THR:HG22	1:A:305:ARG:H	1.36	0.88
1:A:606:LYS:HD2	1:A:672:PHE:CD2	2.07	0.88
1:A:561:LEU:HD11	1:A:565:GLN:HB2	1.52	0.88
1:A:396:PRO:HG3	1:A:443:LEU:HD13	1.56	0.88
1:B:582:TRP:CD1	1:B:655:ILE:HD12	2.08	0.88
1:B:612:PRO:HG2	1:B:757:TYR:CE1	2.08	0.88
1:B:615:THR:HG21	1:B:702:ILE:HD12	1.52	0.88
1:A:612:PRO:HG2	1:A:757:TYR:CE1	2.09	0.88
1:A:611:GLY:HA2	1:A:617:THR:HG21	1.55	0.88
1:A:335:VAL:CG1	1:A:376:LEU:HD23	2.04	0.88
1:A:711:TYR:HB2	1:A:840:MET:HE3	1.53	0.88
1:B:536:ASP:HB2	1:B:538:LEU:HG	1.54	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:LEU:HD21	1:B:792:VAL:CG1	2.04	0.88
1:B:733:VAL:HA	1:B:744:LEU:HD11	1.53	0.88
1:A:455:VAL:CG2	1:A:564:VAL:HA	2.03	0.88
1:A:200:ILE:CD1	1:A:206:LEU:HD22	2.04	0.88
1:B:390:MET:HA	1:B:390:MET:HE3	1.56	0.88
1:A:813:LYS:H	1:A:813:LYS:HD2	1.40	0.87
1:A:863:LEU:HB2	1:A:870:LEU:HD23	1.54	0.87
1:A:328:THR:HG22	1:A:329:ARG:HH21	1.39	0.87
1:B:285:LEU:HD11	1:B:291:LYS:HA	1.55	0.87
1:B:125:LEU:H	1:B:125:LEU:HD12	1.39	0.87
1:A:159:CYS:HB3	1:A:276:ILE:CG2	2.04	0.87
1:B:225:TRP:CE3	1:B:283:ASN:HB2	2.10	0.87
1:B:381:VAL:HG22	1:B:386:TRP:CZ2	2.09	0.87
1:B:466:PRO:HG2	1:B:469:TYR:HD1	1.40	0.87
1:B:440:HIS:CD2	1:B:442:GLN:HB2	2.11	0.86
1:A:200:ILE:HD12	1:A:213:SER:HB2	1.56	0.86
1:B:782:ARG:HD2	1:B:816:PHE:HE1	1.40	0.86
1:A:86:LEU:HB2	1:A:133:PHE:CD2	2.09	0.86
1:B:86:LEU:HD22	1:B:133:PHE:CE1	2.10	0.86
1:A:671:ASP:HB2	1:A:673:TYR:CE1	2.11	0.85
1:A:248:SER:CB	1:A:252:LEU:HD11	2.06	0.85
1:B:117:PRO:HB2	1:B:120:GLY:H	1.39	0.85
1:B:866:MET:HG2	1:B:868:GLN:HB2	1.58	0.85
1:A:323:VAL:HG13	1:A:362:PHE:CD2	2.11	0.85
1:A:329:ARG:HA	1:A:329:ARG:CZ	2.07	0.85
1:B:613:GLN:HB3	1:B:678:ALA:CB	2.06	0.85
1:A:561:LEU:HB3	1:A:566:LEU:HD13	1.58	0.85
1:B:571:PHE:CE1	1:B:577:GLU:HB3	2.12	0.85
1:A:650:ASN:HA	1:A:653:LYS:CG	2.06	0.85
1:A:570:TYR:CE1	1:A:577:GLU:HG3	2.12	0.85
1:A:645:PHE:CZ	1:A:658:TYR:HB2	2.12	0.85
1:B:868:GLN:HE21	1:B:869:THR:HG22	1.41	0.84
1:B:730:PHE:CE1	1:B:848:LEU:HD11	2.12	0.84
1:B:733:VAL:HG11	1:B:747:LEU:HG	1.58	0.84
1:B:181:GLN:HE21	1:B:186:PRO:HA	1.42	0.84
1:B:338:LEU:HD13	1:B:533:TYR:HE2	1.41	0.84
1:A:323:VAL:HG13	1:A:362:PHE:HD2	1.41	0.84
1:A:329:ARG:HH22	1:A:530:LEU:HD22	1.43	0.84
1:A:612:PRO:HD3	1:A:681:PHE:HD1	1.41	0.84
1:B:390:MET:HB3	1:B:393:HIS:N	1.91	0.84
1:A:206:LEU:HD23	1:A:207:LEU:H	1.42	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:PRO:CB	1:B:443:LEU:HD13	2.07	0.84
1:A:388:PRO:HG3	1:A:451:TRP:CZ3	2.13	0.83
1:B:633:ASN:OD1	1:B:643:ILE:HD12	1.78	0.83
1:B:342:GLN:O	1:B:346:ARG:HG3	1.78	0.83
1:B:96:LEU:HG	1:B:139:GLU:HG2	1.59	0.83
1:B:492:THR:HB	1:B:498:TYR:CZ	2.13	0.83
1:A:467:ALA:HA	1:A:470:ARG:HD2	1.61	0.83
1:A:600:THR:O	1:A:603:ARG:HG2	1.79	0.83
1:A:330:MET:HA	1:A:330:MET:HE2	1.60	0.83
1:A:391:TRP:CZ3	1:A:412:ASN:HA	2.14	0.83
1:A:717:GLN:HG3	1:A:747:LEU:HD13	1.59	0.83
1:B:680:TYR:CD2	1:B:686:ALA:HB1	2.14	0.83
1:A:703:LEU:HD11	1:A:761:ILE:HD11	1.60	0.83
1:A:603:ARG:HA	1:A:673:TYR:CE2	2.13	0.82
1:A:436:VAL:HG12	1:A:437:TYR:HD1	1.43	0.82
1:A:753:VAL:HB	1:A:754:PRO:HD3	1.60	0.82
1:B:388:PRO:HD2	1:B:428:ALA:HA	1.60	0.82
1:A:437:TYR:CZ	1:A:439:VAL:HG13	2.14	0.82
1:A:602:ASP:HB3	1:A:671:ASP:O	1.79	0.82
1:B:657:TRP:HA	1:B:660:GLU:CD	2.03	0.82
1:B:102:ALA:HB1	1:B:468:ARG:NH2	1.95	0.82
1:B:607:LEU:HD22	1:B:796:LEU:HD21	1.60	0.82
1:B:716:HIS:HB2	1:B:835:ARG:NH2	1.94	0.82
1:B:863:LEU:CD1	1:B:870:LEU:HD23	2.08	0.82
1:A:146:ASN:O	1:A:147:LEU:HD13	1.79	0.82
1:A:734:ILE:HD12	1:A:847:PHE:CE1	2.15	0.82
1:B:378:LEU:HD23	1:B:381:VAL:HG21	1.62	0.82
1:A:626:MET:HE2	1:A:819:GLN:NE2	1.95	0.82
1:B:409:MET:HB3	1:B:451:TRP:HE1	1.44	0.82
1:B:606:LYS:H	1:B:606:LYS:HD2	1.45	0.82
1:A:243:THR:HG21	1:A:249:ILE:HG23	1.62	0.82
1:A:322:PHE:HB3	1:A:363:PHE:CA	2.10	0.82
1:B:598:GLU:OE2	1:B:599:LYS:HG2	1.80	0.82
1:A:863:LEU:HB2	1:A:870:LEU:CD2	2.10	0.81
1:B:328:THR:HB	1:B:531:SER:CA	2.08	0.81
1:B:416:ALA:HA	1:B:421:ILE:HG12	1.60	0.81
1:A:329:ARG:HB2	1:A:370:GLU:CG	2.10	0.81
1:A:329:ARG:NH2	1:A:530:LEU:HD22	1.95	0.81
1:A:561:LEU:HD13	1:A:562:PRO:CD	2.09	0.81
1:A:602:ASP:HB2	1:A:670:SER:HB3	1.61	0.81
1:A:774:LEU:HD22	1:A:795:PHE:CB	2.10	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:HE1	1:A:409:MET:CG	2.10	0.81
1:A:390:MET:HB2	1:A:393:HIS:H	1.43	0.81
1:B:125:LEU:HD21	1:B:155:LEU:HD12	1.62	0.81
1:A:474:ILE:HD11	1:A:571:PHE:CG	2.15	0.81
1:B:704:ILE:HG12	1:B:778:GLY:HA3	1.60	0.81
1:B:863:LEU:HB2	1:B:870:LEU:CD2	2.11	0.81
1:A:598:GLU:O	1:A:600:THR:HG23	1.79	0.81
1:B:330:MET:CE	1:B:335:VAL:HA	2.10	0.81
1:A:148:ASP:CG	1:B:128:LYS:HG3	2.05	0.81
1:A:486:CYS:SG	1:A:488:LEU:HD22	2.20	0.81
1:A:621:TYR:CZ	1:A:632:SER:HB2	2.16	0.81
1:B:360:GLY:HA3	1:B:391:TRP:CZ3	2.15	0.81
1:B:584:ASP:OD1	1:B:693:LEU:HD11	1.81	0.81
1:B:603:ARG:HD2	1:B:662:PHE:HB3	1.62	0.81
1:B:80:ARG:HB2	1:B:162:TYR:CD1	2.15	0.80
1:B:391:TRP:HH2	1:B:415:PHE:HB2	1.43	0.80
1:A:285:LEU:HD11	1:A:291:LYS:HG2	1.60	0.80
1:A:315:LEU:HD22	1:A:563:PRO:HG3	1.63	0.80
1:A:705:ASN:ND2	1:A:873:TRP:HB2	1.95	0.80
1:B:782:ARG:HD2	1:B:816:PHE:CE1	2.16	0.80
1:B:473:PHE:HB2	1:B:580:PRO:HB3	1.63	0.80
1:A:599:LYS:HA	1:A:603:ARG:HE	1.46	0.80
1:B:338:LEU:HD13	1:B:533:TYR:CE2	2.17	0.80
1:A:690:ALA:O	1:A:694:LEU:HG	1.81	0.80
1:A:860:SER:HA	1:A:870:LEU:CD2	2.10	0.80
1:B:607:LEU:HD22	1:B:796:LEU:CD1	2.10	0.80
1:A:117:PRO:HB2	1:A:120:GLY:N	1.96	0.80
1:A:574:PHE:HB2	1:A:577:GLU:HG2	1.63	0.80
1:B:322:PHE:HB3	1:B:363:PHE:CA	2.11	0.80
1:B:329:ARG:HD3	1:B:530:LEU:CD2	2.09	0.80
1:B:615:THR:HG21	1:B:702:ILE:HB	1.62	0.80
1:B:624:LEU:HG	1:B:789:MET:HE1	1.64	0.80
1:B:109:PHE:CE2	1:B:306:LEU:HD23	2.16	0.80
1:B:610:ILE:O	1:B:681:PHE:HB2	1.81	0.80
1:B:753:VAL:HB	1:B:754:PRO:HD3	1.62	0.80
1:A:603:ARG:HA	1:A:673:TYR:CD2	2.17	0.79
1:A:665:PRO:HG3	1:A:673:TYR:HE2	1.45	0.79
1:B:328:THR:HB	1:B:531:SER:CB	2.11	0.79
1:B:330:MET:HG3	1:B:530:LEU:CD1	2.12	0.79
1:B:109:PHE:HE2	1:B:306:LEU:HD23	1.47	0.79
1:B:170:PHE:CD2	1:B:189:LEU:HD22	2.17	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:LEU:CD2	1:B:702:ILE:HD11	2.12	0.79
1:B:715:GLN:CB	1:B:835:ARG:HD3	2.09	0.79
1:A:145:VAL:HG11	1:A:182:LEU:HD11	1.65	0.79
1:A:733:VAL:HG22	1:A:744:LEU:CD1	2.11	0.79
1:A:836:LYS:H	1:A:836:LYS:HD3	1.48	0.79
1:B:243:THR:HG21	1:B:249:ILE:CD1	2.12	0.79
1:B:367:THR:HG22	1:B:368:ASN:H	1.45	0.79
1:A:86:LEU:HB2	1:A:133:PHE:CG	2.17	0.79
1:A:389:HIS:HD2	1:A:431:PRO:HA	1.47	0.79
1:A:816:PHE:CE2	1:A:834:GLY:HA2	2.17	0.79
1:A:860:SER:HB2	1:A:870:LEU:CD1	2.13	0.79
1:B:360:GLY:HA3	1:B:391:TRP:CH2	2.18	0.79
1:B:381:VAL:CG2	1:B:421:ILE:HG22	2.13	0.79
1:B:607:LEU:HD13	1:B:796:LEU:CD2	2.12	0.79
1:A:145:VAL:HB	1:A:183:LYS:CD	2.13	0.79
1:A:302:THR:HG21	1:A:306:LEU:H	1.47	0.79
1:A:466:PRO:HG2	1:A:468:ARG:HH12	1.45	0.79
1:B:599:LYS:HB3	1:B:659:MET:HE1	1.62	0.79
1:A:523:ILE:HG23	1:A:566:LEU:HD21	1.63	0.79
1:A:816:PHE:CD2	1:A:834:GLY:HA2	2.18	0.79
1:A:335:VAL:HG11	1:A:376:LEU:HD23	1.64	0.78
1:A:694:LEU:CD1	1:A:697:ALA:HB3	2.12	0.78
1:B:133:PHE:HE2	1:B:136:ILE:HD11	1.48	0.78
1:B:508:ILE:CA	1:B:512:GLY:HA3	2.09	0.78
1:B:615:THR:HB	1:B:617:THR:CG2	2.12	0.78
1:A:232:HIS:ND1	1:A:234:THR:HG23	1.97	0.78
1:A:733:VAL:HG22	1:A:744:LEU:HD11	1.66	0.78
1:A:561:LEU:CB	1:A:566:LEU:HD13	2.14	0.78
1:B:409:MET:HB3	1:B:451:TRP:NE1	1.99	0.78
1:B:730:PHE:HE1	1:B:848:LEU:HD11	1.47	0.78
1:B:671:ASP:HB2	1:B:673:TYR:CE1	2.18	0.78
1:A:490:THR:HG23	1:A:527:MET:CE	2.14	0.78
1:A:561:LEU:HD12	1:A:566:LEU:N	1.99	0.78
1:A:603:ARG:HB2	1:A:662:PHE:HE1	1.48	0.78
1:B:345:LEU:HB3	1:B:352:PHE:CD2	2.18	0.78
1:A:361:LYS:HB2	1:A:391:TRP:HD1	1.49	0.78
1:A:831:LYS:HE2	1:A:832:SER:HB3	1.66	0.78
1:B:84:LEU:HD22	1:B:132:ARG:HE	1.48	0.78
1:B:607:LEU:HD22	1:B:796:LEU:CD2	2.14	0.78
1:B:561:LEU:HB2	1:B:566:LEU:HB2	1.66	0.77
1:A:243:THR:HG21	1:A:249:ILE:CG2	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:724:VAL:HG21	1:A:743:LYS:HB3	1.66	0.77
1:B:216:GLU:HB2	1:B:553:TRP:CZ2	2.19	0.77
1:B:451:TRP:HB2	1:B:453:ILE:CD1	2.13	0.77
1:B:330:MET:HG3	1:B:530:LEU:HD11	1.65	0.77
1:B:378:LEU:HD21	1:B:419:HIS:CD2	2.19	0.77
1:B:639:THR:CG2	1:B:644:GLN:HB2	2.14	0.77
1:B:657:TRP:HA	1:B:660:GLU:OE1	1.83	0.77
1:B:755:GLY:HA3	1:B:852:TYR:CE1	2.18	0.77
1:B:633:ASN:HA	1:B:662:PHE:HZ	1.49	0.77
1:A:315:LEU:CD2	1:A:563:PRO:HG3	2.15	0.77
1:B:586:CYS:HA	1:B:592:LYS:CG	2.15	0.77
1:A:665:PRO:HG3	1:A:673:TYR:CE2	2.19	0.77
1:A:599:LYS:HA	1:A:603:ARG:NE	1.99	0.77
1:B:133:PHE:CE2	1:B:136:ILE:HD11	2.20	0.77
1:B:313:TYR:CB	1:B:566:LEU:HD11	2.14	0.77
1:B:335:VAL:CG1	1:B:376:LEU:HD23	2.13	0.77
1:B:586:CYS:HA	1:B:592:LYS:HG3	1.65	0.77
1:B:768:TYR:CD2	1:B:772:GLN:HG2	2.19	0.77
1:A:561:LEU:CD1	1:A:565:GLN:HB2	2.15	0.77
1:A:613:GLN:HB3	1:A:678:ALA:CB	2.14	0.77
1:B:492:THR:HG23	1:B:497:GLU:OE1	1.85	0.77
1:B:627:HIS:NE2	1:B:800:ASN:HB2	2.00	0.77
1:B:863:LEU:HB2	1:B:870:LEU:HD23	1.67	0.77
1:A:604:PHE:HE1	1:A:693:LEU:HD11	1.49	0.77
1:A:620:LEU:HD11	1:A:792:VAL:HG21	1.65	0.77
1:A:366:GLY:HA3	1:A:370:GLU:CB	2.15	0.76
1:A:612:PRO:HD3	1:A:681:PHE:CD1	2.19	0.76
1:A:158:TYR:CE1	1:A:164:VAL:HG21	2.21	0.76
1:B:345:LEU:HB3	1:B:352:PHE:HD2	1.50	0.76
1:B:381:VAL:HG22	1:B:421:ILE:HG22	1.65	0.76
1:A:117:PRO:HB3	1:A:119:LYS:HE2	1.67	0.76
1:B:473:PHE:HB2	1:B:580:PRO:CG	2.16	0.76
1:B:492:THR:HB	1:B:498:TYR:OH	1.84	0.76
1:B:694:LEU:CD1	1:B:697:ALA:HB2	2.11	0.76
1:B:840:MET:HE2	1:B:845:ARG:N	1.99	0.76
1:A:397:HIS:NE2	1:A:594:ILE:HG22	2.00	0.76
1:A:866:MET:CG	1:A:868:GLN:HG2	2.15	0.76
1:A:774:LEU:HB2	1:A:795:PHE:CE2	2.21	0.76
1:B:249:ILE:O	1:B:252:LEU:HG	1.86	0.76
1:B:329:ARG:NH2	1:B:365:THR:HG22	2.01	0.76
1:B:391:TRP:CH2	1:B:415:PHE:HB2	2.20	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:HH12	1:A:530:LEU:HD13	1.50	0.76
1:A:213:SER:HB3	1:A:553:TRP:CZ3	2.20	0.76
1:B:96:LEU:CG	1:B:139:GLU:HG2	2.14	0.76
1:B:683:SER:HB3	1:B:685:VAL:HG22	1.68	0.76
1:B:615:THR:CG2	1:B:702:ILE:HB	2.16	0.76
1:A:392:SER:HB3	1:A:408:GLN:CG	2.15	0.75
1:A:775:VAL:HG11	1:A:863:LEU:HD21	1.66	0.75
1:B:132:ARG:HB3	1:B:133:PHE:CD1	2.22	0.75
1:B:716:HIS:HB2	1:B:835:ARG:HH21	1.49	0.75
1:A:615:THR:OG1	1:A:617:THR:HG23	1.85	0.75
1:A:621:TYR:OH	1:A:632:SER:HB2	1.86	0.75
1:B:335:VAL:HG12	1:B:376:LEU:HD23	1.68	0.75
1:B:570:TYR:HE1	1:B:577:GLU:HG3	1.49	0.75
1:A:150:TRP:CD1	1:B:126:THR:HG1	2.04	0.75
1:A:636:SER:HB2	1:A:639:THR:OG1	1.86	0.75
1:A:644:GLN:CG	1:A:647:ASN:HB3	2.16	0.75
1:A:338:LEU:HD13	1:A:533:TYR:CE1	2.21	0.75
1:B:378:LEU:HD11	1:B:419:HIS:CD2	2.21	0.75
1:A:122:MET:SD	1:A:155:LEU:HD13	2.27	0.75
1:B:331:LYS:N	1:B:331:LYS:HD2	2.01	0.75
1:B:330:MET:HE3	1:B:335:VAL:CG2	2.17	0.75
1:B:607:LEU:CD1	1:B:796:LEU:HD21	2.15	0.75
1:B:775:VAL:HG11	1:B:863:LEU:HD21	1.66	0.75
1:A:392:SER:HB3	1:A:408:GLN:HG3	1.69	0.75
1:A:781:LEU:CA	1:A:788:VAL:HG21	2.16	0.75
1:A:561:LEU:HD11	1:A:565:GLN:CB	2.17	0.75
1:A:684:GLU:O	1:A:687:PRO:HD2	1.87	0.75
1:B:99:GLU:CB	1:B:285:LEU:HD23	2.09	0.75
1:B:619:ALA:HB2	1:B:829:LEU:HB3	1.68	0.75
1:B:684:GLU:O	1:B:687:PRO:HD2	1.86	0.75
1:B:774:LEU:HD22	1:B:795:PHE:CB	2.17	0.75
1:A:361:LYS:HB2	1:A:391:TRP:CD1	2.22	0.74
1:A:724:VAL:HG11	1:A:744:LEU:HA	1.68	0.74
1:B:775:VAL:CB	1:B:868:GLN:HG2	2.04	0.74
1:A:87:VAL:HG21	1:A:104:LEU:CD1	2.16	0.74
1:A:627:HIS:NE2	1:A:629:ASP:HB2	2.02	0.74
1:B:346:ARG:HA	1:B:352:PHE:HB2	1.68	0.74
1:B:394:MET:SD	1:B:398:LEU:HB2	2.27	0.74
1:B:789:MET:HB3	1:B:804:TYR:CE2	2.21	0.74
1:A:328:THR:HG23	1:A:531:SER:HA	1.69	0.74
1:A:694:LEU:HB3	1:A:697:ALA:H	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:SER:HB2	1:A:870:LEU:HD13	1.67	0.74
1:B:473:PHE:HB2	1:B:580:PRO:CB	2.17	0.74
1:B:624:LEU:HD21	1:B:792:VAL:HG12	1.68	0.74
1:B:201:ASN:CG	1:B:203:LYS:HD3	2.12	0.74
1:B:613:GLN:HG3	1:B:750:ARG:HH22	1.52	0.74
1:B:768:TYR:HB2	1:B:773:ILE:HD11	1.68	0.74
1:B:793:GLN:HE22	1:B:802:ILE:H	1.35	0.74
1:A:122:MET:SD	1:A:155:LEU:HB2	2.27	0.74
1:A:165:GLY:HA2	1:A:277:GLN:HE21	1.53	0.74
1:B:596:SER:HB2	1:B:598:GLU:OE2	1.87	0.74
1:B:310:LEU:HD13	1:B:556:LEU:HA	1.70	0.74
1:B:777:ASP:OD2	1:B:872:THR:HG23	1.88	0.74
1:A:453:ILE:H	1:A:453:ILE:HD12	1.52	0.74
1:B:599:LYS:HB3	1:B:659:MET:CE	2.17	0.74
1:A:626:MET:HA	1:A:626:MET:HE3	1.70	0.74
1:A:687:PRO:HA	1:A:764:TRP:CZ2	2.23	0.74
1:B:455:VAL:HG21	1:B:564:VAL:HA	1.70	0.74
1:A:462:PRO:HD2	1:A:470:ARG:HA	1.70	0.74
1:B:578:LYS:O	1:B:580:PRO:HD3	1.87	0.74
1:B:785:PRO:HG3	1:B:817:TRP:CB	2.18	0.74
1:A:603:ARG:CZ	1:A:665:PRO:HD2	2.18	0.73
1:B:645:PHE:HB2	1:B:650:ASN:HD22	1.52	0.73
1:B:144:TYR:O	1:B:147:LEU:HD23	1.87	0.73
1:A:627:HIS:CD2	1:A:629:ASP:HB2	2.23	0.73
1:A:711:TYR:HB2	1:A:840:MET:CE	2.18	0.73
1:B:271:GLY:HA3	1:B:276:ILE:O	1.87	0.73
1:A:774:LEU:HB2	1:A:795:PHE:CD2	2.23	0.73
1:B:356:LEU:HD13	1:B:377:LEU:CD2	2.17	0.73
1:A:468:ARG:NH1	1:A:468:ARG:HB3	2.02	0.73
1:A:412:ASN:HB3	1:A:451:TRP:HZ2	1.53	0.73
1:A:863:LEU:CD1	1:A:871:PRO:HD3	2.19	0.73
1:B:394:MET:HE1	1:B:399:PHE:CE1	2.24	0.73
1:B:470:ARG:HD2	1:B:482:PRO:CB	2.18	0.73
1:B:703:LEU:HD11	1:B:761:ILE:CD1	2.19	0.73
1:B:863:LEU:HD12	1:B:870:LEU:CD2	2.18	0.73
1:A:623:PHE:HA	1:A:626:MET:HG2	1.70	0.73
1:A:680:TYR:HA	1:A:686:ALA:CB	2.19	0.73
1:A:699:VAL:HG21	1:A:764:TRP:CZ3	2.23	0.73
1:A:779:LYS:HD2	1:A:873:TRP:HB3	1.70	0.73
1:B:358:TYR:OH	1:B:416:ALA:HB2	1.89	0.73
1:B:474:ILE:H	1:B:580:PRO:HG3	1.52	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:785:PRO:HG3	1:A:817:TRP:CB	2.19	0.73
1:B:276:ILE:HD11	1:B:278:ARG:NE	2.04	0.73
1:A:644:GLN:HG3	1:A:679:ASN:OD1	1.88	0.73
1:B:715:GLN:NE2	1:B:838:PRO:HD2	2.04	0.73
1:A:366:GLY:HA3	1:A:370:GLU:HB2	1.71	0.72
1:B:243:THR:HG21	1:B:249:ILE:HD11	1.70	0.72
1:B:395:GLN:CG	1:B:434:SER:HB2	2.19	0.72
1:B:438:PRO:HD3	1:B:594:ILE:HB	1.71	0.72
1:B:453:ILE:HD12	1:B:453:ILE:H	1.54	0.72
1:B:774:LEU:HB2	1:B:795:PHE:CD2	2.24	0.72
1:B:378:LEU:HD23	1:B:381:VAL:CG2	2.18	0.72
1:B:733:VAL:HG21	1:B:747:LEU:HD23	1.70	0.72
1:B:775:VAL:HB	1:B:868:GLN:CG	2.04	0.72
1:A:93:TYR:HB3	1:B:878:LEU:O	1.89	0.72
1:A:187:LEU:HD12	1:A:229:GLN:O	1.88	0.72
1:A:603:ARG:HD2	1:A:659:MET:CE	2.19	0.72
1:A:703:LEU:HD22	1:A:757:TYR:HB3	1.72	0.72
1:B:93:TYR:HA	1:B:98:GLN:HE21	1.54	0.72
1:B:473:PHE:HB2	1:B:580:PRO:HG3	1.71	0.72
1:A:471:ARG:HD3	1:A:577:GLU:OE2	1.89	0.72
1:B:159:CYS:CB	1:B:276:ILE:HG21	2.19	0.72
1:A:706:PRO:HD3	1:A:873:TRP:CH2	2.25	0.72
1:A:187:LEU:HD21	1:A:228:PHE:CD1	2.24	0.72
1:A:774:LEU:HD22	1:A:795:PHE:CG	2.24	0.72
1:A:330:MET:HE3	1:A:533:TYR:HB2	1.72	0.72
1:A:451:TRP:HB2	1:A:453:ILE:CD1	2.18	0.72
1:A:486:CYS:HB3	1:A:543:PHE:CZ	2.25	0.72
1:B:87:VAL:HG21	1:B:104:LEU:CD1	2.19	0.72
1:B:125:LEU:HD22	1:B:158:TYR:CG	2.25	0.72
1:B:388:PRO:HG3	1:B:451:TRP:CE2	2.25	0.72
1:B:705:ASN:HD21	1:B:707:ALA:HB3	1.54	0.72
1:A:210:THR:HG22	1:A:555:ASN:N	2.05	0.72
1:A:537:ARG:HH11	1:A:540:LEU:HD12	1.55	0.72
1:B:698:LYS:HD3	1:B:772:GLN:NE2	2.04	0.72
1:A:494:PHE:HB2	1:A:497:GLU:OE2	1.90	0.71
1:A:602:ASP:HB2	1:A:670:SER:CB	2.19	0.71
1:A:610:ILE:HD12	1:A:681:PHE:CD2	2.24	0.71
1:B:159:CYS:HB3	1:B:276:ILE:CG2	2.19	0.71
1:B:599:LYS:HA	1:B:603:ARG:NH2	2.05	0.71
1:B:622:LEU:HD21	1:B:827:LYS:CE	2.20	0.71
1:B:96:LEU:HB2	1:B:284:ASN:ND2	2.01	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ILE:HD11	1:A:542:THR:CG2	2.16	0.71
1:A:613:GLN:HB3	1:A:678:ALA:HB1	1.73	0.71
1:B:863:LEU:CD1	1:B:871:PRO:HD3	2.20	0.71
1:A:381:VAL:HA	1:A:386:TRP:HE1	1.55	0.71
1:A:829:LEU:HD23	1:A:833:LYS:O	1.91	0.71
1:A:127:ASP:O	1:A:128:LYS:HG2	1.91	0.71
1:A:433:HIS:CE1	1:A:458:THR:HA	2.25	0.71
1:A:859:LEU:HD23	1:A:874:LEU:HD22	1.71	0.71
1:B:724:VAL:CG2	1:B:743:LYS:HB3	2.20	0.71
1:A:144:TYR:O	1:A:147:LEU:HD21	1.90	0.71
1:A:703:LEU:HD22	1:A:757:TYR:CB	2.21	0.71
1:B:145:VAL:HB	1:B:183:LYS:HB2	1.72	0.71
1:B:624:LEU:HD21	1:B:792:VAL:HG11	1.70	0.71
1:B:733:VAL:CG2	1:B:747:LEU:HD23	2.21	0.71
1:A:122:MET:SD	1:A:155:LEU:HD22	2.31	0.71
1:A:397:HIS:CE1	1:A:594:ILE:HG22	2.25	0.71
1:B:687:PRO:HA	1:B:764:TRP:CH2	2.25	0.71
1:B:784:GLU:OE2	1:B:786:ALA:HB3	1.91	0.71
1:B:561:LEU:HD12	1:B:566:LEU:HA	1.72	0.71
1:B:276:ILE:HD11	1:B:278:ARG:CZ	2.21	0.70
1:A:274:ASP:HB3	1:A:276:ILE:CD1	2.21	0.70
1:A:714:TYR:OH	1:A:729:THR:HA	1.91	0.70
1:B:213:SER:OG	1:B:553:TRP:HA	1.90	0.70
1:B:310:LEU:HD12	1:B:557:ARG:HG3	1.73	0.70
1:B:597:LYS:HE3	1:B:597:LYS:H	1.55	0.70
1:B:606:LYS:HG3	1:B:696:LYS:NZ	2.06	0.70
1:B:615:THR:HG21	1:B:702:ILE:CD1	2.21	0.70
1:B:779:LYS:HD3	1:B:872:THR:OG1	1.92	0.70
1:A:620:LEU:HD12	1:A:789:MET:SD	2.31	0.70
1:A:655:ILE:HD13	1:A:693:LEU:HD13	1.73	0.70
1:A:793:GLN:OE1	1:A:802:ILE:HG22	1.91	0.70
1:A:328:THR:HG22	1:A:329:ARG:NH2	2.05	0.70
1:B:349:ILE:HG12	1:B:558:LEU:HB2	1.73	0.70
1:B:360:GLY:HA3	1:B:391:TRP:CE3	2.25	0.70
1:B:387:PHE:CE2	1:B:429:VAL:HB	2.25	0.70
1:B:613:GLN:HG3	1:B:750:ARG:NH2	2.06	0.70
1:B:740:ALA:HB1	1:B:744:LEU:HB3	1.71	0.70
1:A:116:ALA:CB	1:A:143:LYS:HB3	2.21	0.70
1:A:427:TYR:HE2	1:A:455:VAL:HG12	1.57	0.70
1:A:615:THR:HG1	1:A:617:THR:HG23	1.55	0.70
1:B:390:MET:HA	1:B:390:MET:CE	2.21	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:LYS:HA	1:B:835:ARG:NH2	2.07	0.70
1:A:396:PRO:CG	1:A:443:LEU:HD22	2.21	0.70
1:B:225:TRP:HH2	1:B:287:PHE:CD2	2.10	0.70
1:B:390:MET:HE1	1:B:409:MET:CG	2.22	0.70
1:B:571:PHE:CD1	1:B:577:GLU:HB3	2.26	0.70
1:A:274:ASP:HB3	1:A:276:ILE:HD11	1.73	0.70
1:A:721:ASP:HB3	1:A:726:LEU:HD11	1.72	0.70
1:A:182:LEU:HD23	1:A:185:PHE:HD2	1.57	0.69
1:A:389:HIS:HB3	1:A:431:PRO:CG	2.15	0.69
1:A:427:TYR:HE2	1:A:455:VAL:CG1	2.05	0.69
1:B:99:GLU:OE2	1:B:285:LEU:HB3	1.91	0.69
1:B:146:ASN:O	1:B:147:LEU:HD22	1.92	0.69
1:B:687:PRO:HA	1:B:764:TRP:CZ2	2.27	0.69
1:B:597:LYS:H	1:B:597:LYS:CE	2.05	0.69
1:B:705:ASN:HA	1:B:873:TRP:CZ2	2.27	0.69
1:A:570:TYR:HE1	1:A:577:GLU:HG3	1.55	0.69
1:B:330:MET:HE1	1:B:335:VAL:HA	1.74	0.69
1:B:703:LEU:HD21	1:B:761:ILE:HD11	1.74	0.69
1:A:335:VAL:HG12	1:A:376:LEU:HD23	1.73	0.69
1:B:605:PRO:HB3	1:B:674:PHE:CA	2.22	0.69
1:A:207:LEU:HD13	1:A:210:THR:CG2	2.23	0.69
1:A:437:TYR:CE1	1:A:439:VAL:HG13	2.27	0.69
1:A:860:SER:O	1:A:870:LEU:HD21	1.91	0.69
1:B:360:GLY:O	1:B:363:PHE:HB3	1.92	0.69
1:B:605:PRO:HB3	1:B:674:PHE:HA	1.73	0.69
1:B:234:THR:HG23	1:B:269:ASP:OD1	1.92	0.69
1:B:394:MET:HG2	1:B:395:GLN:N	2.06	0.69
1:B:624:LEU:HD11	1:B:792:VAL:HG11	1.74	0.69
1:B:391:TRP:CZ3	1:B:412:ASN:HA	2.26	0.69
1:B:611:GLY:HA2	1:B:617:THR:HG21	1.72	0.69
1:B:786:ALA:HA	1:B:804:TYR:HB2	1.75	0.69
1:A:329:ARG:HH12	1:A:530:LEU:CD1	2.04	0.69
1:A:349:ILE:HD12	1:A:558:LEU:HB2	1.75	0.69
1:A:665:PRO:HB3	1:A:670:SER:HA	1.73	0.69
1:B:109:PHE:CE2	1:B:306:LEU:HB3	2.27	0.69
1:B:200:ILE:HD12	1:B:213:SER:CB	2.21	0.69
1:B:283:ASN:H	1:B:290:HIS:HE1	1.39	0.69
1:B:323:VAL:HG22	1:B:362:PHE:CB	2.23	0.69
1:A:603:ARG:HB2	1:A:662:PHE:CE1	2.27	0.69
1:A:694:LEU:HD22	1:A:697:ALA:CB	2.23	0.69
1:B:288:TRP:HB2	1:B:511:GLY:CA	2.23	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:SER:HB3	1:A:408:GLN:CD	2.18	0.69
1:B:134:ALA:O	1:B:164:VAL:HG13	1.93	0.69
1:B:561:LEU:HD12	1:B:566:LEU:CD1	2.22	0.69
1:A:590:ARG:O	1:A:594:ILE:HG13	1.92	0.68
1:A:603:ARG:NH2	1:A:665:PRO:HD2	2.08	0.68
1:B:390:MET:CG	1:B:408:GLN:HB3	2.19	0.68
1:A:331:LYS:HA	1:A:331:LYS:HE2	1.75	0.68
1:A:381:VAL:HG23	1:A:386:TRP:NE1	2.09	0.68
1:A:785:PRO:HG3	1:A:817:TRP:HB3	1.75	0.68
1:A:860:SER:HB3	1:A:878:LEU:CD1	2.23	0.68
1:B:814:LYS:NZ	1:B:828:CYS:HB3	2.08	0.68
1:A:378:LEU:HD21	1:A:419:HIS:NE2	2.07	0.68
1:A:603:ARG:HH22	1:A:664:ILE:HB	1.59	0.68
1:A:704:ILE:HG12	1:A:705:ASN:H	1.58	0.68
1:B:96:LEU:HD23	1:B:139:GLU:OE1	1.94	0.68
1:B:117:PRO:CG	1:B:120:GLY:HA3	2.24	0.68
1:B:338:LEU:CD1	1:B:533:TYR:HE2	2.06	0.68
1:B:620:LEU:HD22	1:B:702:ILE:HD11	1.74	0.68
1:A:211:ARG:HD2	1:A:555:ASN:OD1	1.93	0.68
1:A:479:MET:HB3	1:A:567:ALA:HB1	1.75	0.68
1:A:614:LYS:CE	1:A:833:LYS:HB3	2.21	0.68
1:B:135:LEU:HD13	1:B:301:LEU:HB2	1.75	0.68
1:B:388:PRO:HG3	1:B:451:TRP:CZ2	2.29	0.68
1:B:633:ASN:O	1:B:635:PRO:HD3	1.93	0.68
1:B:733:VAL:HG21	1:B:747:LEU:CD2	2.23	0.68
1:A:147:LEU:CB	1:A:152:ARG:HB2	2.20	0.68
1:A:681:PHE:HZ	1:A:761:ILE:HG13	1.58	0.68
1:A:770:ALA:O	1:A:866:MET:HE1	1.93	0.68
1:B:486:CYS:O	1:B:514:LEU:HD22	1.94	0.68
1:B:680:TYR:CE2	1:B:690:ALA:HB2	2.29	0.68
1:A:586:CYS:HA	1:A:592:LYS:HD2	1.76	0.68
1:B:288:TRP:HB2	1:B:511:GLY:HA3	1.74	0.68
1:A:608:LEU:HD11	1:A:694:LEU:HD21	1.75	0.68
1:A:740:ALA:CB	1:A:744:LEU:HD23	2.23	0.68
1:B:361:LYS:HE2	1:B:391:TRP:CD1	2.28	0.68
1:B:402:GLN:NE2	1:B:445:GLU:HB3	2.08	0.68
1:A:769:HIS:CD2	1:A:771:ASN:H	2.12	0.68
1:A:871:PRO:HD2	1:A:874:LEU:HD23	1.76	0.68
1:B:187:LEU:HD22	1:B:229:GLN:O	1.94	0.68
1:B:339:PHE:HB2	1:B:380:TYR:CE2	2.28	0.68
1:B:391:TRP:HZ3	1:B:412:ASN:HA	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:PHE:HD1	1:B:577:GLU:HG2	1.59	0.68
1:B:752:LEU:HB3	1:B:851:TYR:OH	1.94	0.68
1:A:330:MET:HE2	1:A:330:MET:CA	2.22	0.68
1:B:165:GLY:HA3	1:B:301:LEU:HD22	1.76	0.68
1:B:349:ILE:HG12	1:B:558:LEU:CB	2.23	0.68
1:A:115:ILE:HD13	1:B:861:LYS:HE2	1.75	0.67
1:A:645:PHE:HE2	1:A:657:TRP:CE3	2.13	0.67
1:B:561:LEU:HB2	1:B:566:LEU:CD1	2.22	0.67
1:A:438:PRO:HD3	1:A:594:ILE:HD12	1.75	0.67
1:B:454:ARG:NH2	1:B:479:MET:HE2	2.08	0.67
1:B:639:THR:HG22	1:B:644:GLN:OE1	1.94	0.67
1:A:345:LEU:HA	1:A:348:HIS:HD2	1.58	0.67
1:A:122:MET:CE	1:A:122:MET:H	2.08	0.67
1:A:614:LYS:HE2	1:A:833:LYS:CB	2.24	0.67
1:A:620:LEU:CD1	1:A:792:VAL:HG21	2.24	0.67
1:A:813:LYS:HD2	1:A:813:LYS:N	2.08	0.67
1:B:703:LEU:CD1	1:B:859:LEU:HD11	2.24	0.67
1:A:210:THR:CG2	1:A:554:THR:HA	2.24	0.67
1:A:646:PHE:HB2	1:A:680:TYR:CE1	2.29	0.67
1:A:789:MET:HB3	1:A:804:TYR:CD2	2.29	0.67
1:B:623:PHE:O	1:B:626:MET:HG2	1.95	0.67
1:B:785:PRO:HG2	1:B:808:LEU:HD13	1.75	0.67
1:A:588:ASP:HB3	1:A:591:HIS:HB2	1.76	0.67
1:B:439:VAL:HG13	1:B:444:TYR:CE2	2.29	0.67
1:B:454:ARG:HB3	1:B:454:ARG:CZ	2.25	0.67
1:A:134:ALA:O	1:A:164:VAL:HG13	1.95	0.67
1:A:683:SER:HB3	1:A:685:VAL:HG22	1.76	0.67
1:B:201:ASN:ND2	1:B:203:LYS:HD3	2.09	0.67
1:B:397:HIS:NE2	1:B:595:TRP:HA	2.09	0.67
1:B:454:ARG:O	1:B:478:ILE:HG23	1.94	0.67
1:B:700:LEU:HD11	1:B:792:VAL:HG22	1.77	0.67
1:B:81:THR:OG1	1:B:134:ALA:HA	1.93	0.67
1:B:382:LYS:HD2	1:B:383:GLU:N	2.10	0.67
1:A:209:VAL:HG21	1:A:310:LEU:HD12	1.77	0.67
1:A:388:PRO:HG2	1:A:428:ALA:HB2	1.74	0.67
1:A:426:GLY:O	1:A:453:ILE:HG23	1.95	0.67
1:A:532:ASN:O	1:A:535:ASN:HB2	1.95	0.67
1:A:680:TYR:O	1:A:686:ALA:HB3	1.93	0.67
1:B:360:GLY:HA3	1:B:391:TRP:CD2	2.30	0.67
1:B:479:MET:HB3	1:B:567:ALA:HB1	1.77	0.67
1:B:856:ASN:HB3	1:B:874:LEU:CD1	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:PRO:CG	1:B:469:TYR:HB2	2.25	0.66
1:B:561:LEU:CB	1:B:566:LEU:HB2	2.24	0.66
1:B:356:LEU:HD11	1:B:384:PHE:CD1	2.29	0.66
1:B:419:HIS:HB3	1:B:421:ILE:HG23	1.77	0.66
1:B:814:LYS:HD3	1:B:828:CYS:SG	2.35	0.66
1:A:615:THR:HG21	1:A:702:ILE:O	1.95	0.66
1:B:108:ARG:HH12	1:B:471:ARG:HG2	1.60	0.66
1:B:201:ASN:OD1	1:B:203:LYS:HD3	1.94	0.66
1:B:409:MET:CB	1:B:451:TRP:HE1	2.08	0.66
1:B:740:ALA:CB	1:B:744:LEU:HD23	2.25	0.66
1:A:210:THR:HA	1:A:555:ASN:CG	2.20	0.66
1:B:335:VAL:HB	1:B:376:LEU:HD23	1.77	0.66
1:B:769:HIS:HD2	1:B:771:ASN:HB3	1.59	0.66
1:B:776:LEU:HD11	1:B:792:VAL:CG2	2.26	0.66
1:A:703:LEU:CD1	1:A:859:LEU:HD11	2.26	0.66
1:B:451:TRP:CB	1:B:453:ILE:HD11	2.18	0.66
1:A:596:SER:HB2	1:A:599:LYS:HZ3	1.61	0.66
1:B:378:LEU:CA	1:B:381:VAL:HG23	2.12	0.66
1:B:607:LEU:CD2	1:B:796:LEU:HD21	2.25	0.66
1:B:620:LEU:HD23	1:B:702:ILE:HD11	1.77	0.66
1:B:642:GLU:O	1:B:644:GLN:HG3	1.95	0.66
1:B:207:LEU:HB2	1:B:210:THR:OG1	1.95	0.66
1:B:356:LEU:HD11	1:B:384:PHE:HD1	1.60	0.66
1:B:705:ASN:OD1	1:B:706:PRO:HD2	1.96	0.66
1:A:465:LYS:HB2	1:A:466:PRO:HA	1.78	0.66
1:A:728:TYR:CD2	1:A:732:GLU:HB3	2.31	0.66
1:A:740:ALA:HB1	1:A:744:LEU:HB3	1.78	0.66
1:B:325:LYS:H	1:B:328:THR:HG21	1.58	0.66
1:A:147:LEU:N	1:A:147:LEU:HD22	2.10	0.66
1:A:165:GLY:CA	1:A:277:GLN:HE21	2.09	0.66
1:A:694:LEU:HB3	1:A:697:ALA:CB	2.26	0.66
1:B:181:GLN:NE2	1:B:186:PRO:HA	2.11	0.66
1:B:322:PHE:O	1:B:362:PHE:HB3	1.96	0.66
1:B:866:MET:HG3	1:B:868:GLN:N	2.11	0.66
1:B:436:VAL:HG23	1:B:437:TYR:N	2.11	0.66
1:B:635:PRO:CB	1:B:643:ILE:HD13	2.26	0.66
1:B:704:ILE:CG1	1:B:778:GLY:HA3	2.26	0.66
1:A:248:SER:HB3	1:A:252:LEU:HD21	1.78	0.65
1:B:174:GLU:HG2	1:B:175:ASN:N	2.10	0.65
1:B:211:ARG:HD2	1:B:551:HIS:O	1.96	0.65
1:B:335:VAL:CB	1:B:376:LEU:HD23	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:LEU:CD2	1:B:796:LEU:HD11	2.24	0.65
1:B:714:TYR:OH	1:B:729:THR:HA	1.95	0.65
1:B:793:GLN:NE2	1:B:802:ILE:H	1.95	0.65
1:A:132:ARG:HG2	1:A:133:PHE:CE2	2.31	0.65
1:A:444:TYR:CE1	1:A:475:HIS:HD2	2.13	0.65
1:A:829:LEU:H	1:A:829:LEU:CD1	2.07	0.65
1:B:680:TYR:HE2	1:B:690:ALA:HB2	1.61	0.65
1:A:119:LYS:HD2	1:A:120:GLY:N	2.12	0.65
1:A:419:HIS:HB3	1:A:421:ILE:HG13	1.77	0.65
1:A:623:PHE:HB3	1:A:804:TYR:CE1	2.31	0.65
1:B:339:PHE:HB2	1:B:380:TYR:CZ	2.31	0.65
1:A:285:LEU:CD1	1:A:291:LYS:HG2	2.26	0.65
1:A:606:LYS:O	1:A:697:ALA:HB1	1.96	0.65
1:A:789:MET:HE2	1:A:804:TYR:CZ	2.32	0.65
1:A:205:PRO:HB2	1:A:207:LEU:C	2.22	0.65
1:B:81:THR:HA	1:B:131:GLY:O	1.97	0.65
1:B:204:SER:OG	1:B:238:VAL:HG22	1.96	0.65
1:B:239:LEU:HD13	1:B:289:LEU:HD23	1.79	0.65
1:B:378:LEU:HD11	1:B:419:HIS:CE1	2.31	0.65
1:A:321:ILE:CD1	1:A:530:LEU:HD12	2.27	0.65
1:B:586:CYS:SG	1:B:600:THR:HA	2.36	0.65
1:A:523:ILE:HD13	1:A:566:LEU:HG	1.79	0.65
1:A:724:VAL:HG21	1:A:743:LYS:CB	2.26	0.65
1:A:321:ILE:HD13	1:A:530:LEU:HD12	1.79	0.65
1:A:509:ILE:CG1	1:A:542:THR:HG23	2.27	0.65
1:A:694:LEU:CG	1:A:697:ALA:HB3	2.27	0.65
1:B:187:LEU:HD13	1:B:188:PHE:C	2.22	0.65
1:B:704:ILE:HG12	1:B:778:GLY:CA	2.27	0.65
1:B:717:GLN:HB3	1:B:725:ALA:HB2	1.79	0.65
1:A:276:ILE:H	1:A:276:ILE:HD13	1.62	0.65
1:A:330:MET:CE	1:A:533:TYR:HB2	2.26	0.65
1:A:391:TRP:HH2	1:A:415:PHE:HB2	1.63	0.65
1:A:721:ASP:CB	1:A:726:LEU:HD11	2.26	0.65
1:A:781:LEU:N	1:A:788:VAL:HG21	2.12	0.65
1:B:313:TYR:CE1	1:B:561:LEU:HG	2.32	0.65
1:B:389:HIS:HB3	1:B:393:HIS:HD2	1.60	0.65
1:B:80:ARG:HB2	1:B:162:TYR:HD1	1.59	0.64
1:B:863:LEU:CB	1:B:870:LEU:HD23	2.27	0.64
1:A:181:GLN:HE21	1:A:186:PRO:HA	1.62	0.64
1:B:605:PRO:HB3	1:B:673:TYR:C	2.22	0.64
1:B:736:ALA:HB1	1:B:740:ALA:HB2	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:HB2	1:A:176:SER:OG	1.98	0.64
1:A:271:GLY:HA3	1:A:276:ILE:O	1.97	0.64
1:A:571:PHE:CD1	1:A:578:LYS:HA	2.31	0.64
1:B:479:MET:HE1	1:B:568:GLN:HG3	1.80	0.64
1:B:288:TRP:CB	1:B:511:GLY:HA3	2.27	0.64
1:B:532:ASN:O	1:B:535:ASN:HB2	1.98	0.64
1:B:740:ALA:HB1	1:B:744:LEU:CG	2.27	0.64
1:A:330:MET:HA	1:A:330:MET:CE	2.26	0.64
1:A:397:HIS:HA	1:A:440:HIS:NE2	2.13	0.64
1:A:468:ARG:HB3	1:A:468:ARG:CZ	2.25	0.64
1:B:599:LYS:HD3	1:B:603:ARG:HH22	1.62	0.64
1:B:752:LEU:HD13	1:B:851:TYR:CZ	2.32	0.64
1:A:419:HIS:CB	1:A:421:ILE:HG13	2.28	0.64
1:A:584:ASP:OD2	1:A:693:LEU:HD12	1.97	0.64
1:B:361:LYS:HE2	1:B:361:LYS:HA	1.80	0.64
1:B:585:PRO:HG2	1:B:595:TRP:CD2	2.32	0.64
1:B:704:ILE:HG22	1:B:705:ASN:N	2.13	0.64
1:B:738:SER:CA	1:B:745:ARG:HH21	2.11	0.64
1:B:125:LEU:HD12	1:B:125:LEU:N	2.12	0.64
1:B:606:LYS:HD3	1:B:672:PHE:CG	2.32	0.64
1:B:785:PRO:HG3	1:B:817:TRP:HB3	1.79	0.64
1:A:433:HIS:HE1	1:A:483:ARG:HD2	1.62	0.64
1:B:633:ASN:HA	1:B:662:PHE:CZ	2.32	0.64
1:A:645:PHE:HE2	1:A:657:TRP:CZ3	2.15	0.64
1:B:576:GLU:HG2	1:B:577:GLU:OE2	1.98	0.64
1:B:204:SER:HB2	1:B:237:PRO:O	1.98	0.64
1:B:399:PHE:HB2	1:B:405:LEU:CD2	2.25	0.64
1:A:391:TRP:HZ3	1:A:412:ASN:HA	1.63	0.63
1:B:627:HIS:CE1	1:B:629:ASP:HB3	2.32	0.63
1:B:634:TYR:CD2	1:B:635:PRO:HD2	2.33	0.63
1:A:561:LEU:HD13	1:A:562:PRO:N	2.14	0.63
1:A:606:LYS:HD2	1:A:672:PHE:CE2	2.33	0.63
1:A:704:ILE:HG12	1:A:705:ASN:N	2.12	0.63
1:B:866:MET:CG	1:B:868:GLN:HB2	2.27	0.63
1:B:270:LEU:HA	1:B:277:GLN:OE1	1.98	0.63
1:B:285:LEU:HG	1:B:291:LYS:HG2	1.79	0.63
1:B:390:MET:HE1	1:B:409:MET:HG3	1.79	0.63
1:B:495:TYR:OH	1:B:505:LEU:HD13	1.98	0.63
1:B:730:PHE:HE1	1:B:848:LEU:CD1	2.12	0.63
1:B:774:LEU:HB2	1:B:795:PHE:CE2	2.33	0.63
1:B:835:ARG:HD2	1:B:835:ARG:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:CYS:CB	1:A:276:ILE:HG21	2.09	0.63
1:A:196:LYS:HA	1:A:220:LEU:CD2	2.28	0.63
1:A:349:ILE:CG1	1:A:558:LEU:HB2	2.29	0.63
1:A:485:THR:O	1:A:514:LEU:HD13	1.98	0.63
1:B:329:ARG:HH11	1:B:329:ARG:HG2	1.63	0.63
1:A:508:ILE:CA	1:A:512:GLY:HA3	2.25	0.63
1:A:624:LEU:HD11	1:A:792:VAL:HG11	1.80	0.63
1:A:768:TYR:HB3	1:A:772:GLN:HB2	1.79	0.63
1:A:322:PHE:CE1	1:A:377:LEU:HD13	2.34	0.63
1:A:488:LEU:HD23	1:A:488:LEU:O	1.98	0.63
1:B:96:LEU:CD2	1:B:139:GLU:HG2	2.28	0.63
1:B:574:PHE:CD1	1:B:577:GLU:HG2	2.34	0.63
1:A:530:LEU:O	1:A:530:LEU:HD23	1.99	0.63
1:B:178:LEU:HD23	1:B:178:LEU:H	1.63	0.63
1:B:390:MET:HE3	1:B:390:MET:CA	2.28	0.63
1:B:705:ASN:HA	1:B:873:TRP:CE2	2.33	0.63
1:A:136:ILE:HG13	1:A:164:VAL:HG11	1.80	0.63
1:A:209:VAL:HG21	1:A:310:LEU:CD1	2.29	0.63
1:A:490:THR:HG23	1:A:527:MET:HE3	1.81	0.63
1:A:494:PHE:CB	1:A:497:GLU:HG3	2.28	0.63
1:A:859:LEU:CD2	1:A:874:LEU:HD22	2.28	0.63
1:B:93:TYR:HA	1:B:98:GLN:NE2	2.13	0.63
1:B:381:VAL:CG1	1:B:422:PRO:HD3	2.28	0.63
1:B:436:VAL:HG23	1:B:437:TYR:H	1.61	0.63
1:B:378:LEU:HD11	1:B:419:HIS:NE2	2.14	0.63
1:B:705:ASN:ND2	1:B:707:ALA:HB3	2.13	0.63
1:A:711:TYR:CB	1:A:840:MET:HE3	2.27	0.62
1:A:785:PRO:HB2	1:A:808:LEU:HD13	1.80	0.62
1:A:825:LYS:H	1:A:825:LYS:HD2	1.63	0.62
1:A:125:LEU:HD22	1:A:125:LEU:H	1.63	0.62
1:A:381:VAL:HG23	1:A:386:TRP:CE2	2.33	0.62
1:A:624:LEU:HD22	1:A:630:LEU:HD13	1.81	0.62
1:B:733:VAL:HG11	1:B:747:LEU:CG	2.28	0.62
1:B:786:ALA:HA	1:B:804:TYR:CB	2.28	0.62
1:B:703:LEU:HD22	1:B:757:TYR:HB3	1.81	0.62
1:A:466:PRO:CG	1:A:468:ARG:HH12	2.12	0.62
1:A:623:PHE:CZ	1:A:808:LEU:HD22	2.35	0.62
1:B:386:TRP:CD2	1:B:421:ILE:HB	2.35	0.62
1:B:394:MET:CG	1:B:398:LEU:HD12	2.29	0.62
1:B:438:PRO:HB3	1:B:585:PRO:CB	2.28	0.62
1:B:465:LYS:H	1:B:465:LYS:CE	2.11	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HD11	1:A:384:PHE:CD2	2.35	0.62
1:A:412:ASN:HB3	1:A:451:TRP:CZ2	2.32	0.62
1:B:77:THR:HG21	1:B:80:ARG:NH2	2.13	0.62
1:B:704:ILE:HG22	1:B:705:ASN:H	1.64	0.62
1:A:302:THR:HG22	1:A:305:ARG:N	2.13	0.62
1:A:328:THR:CG2	1:A:329:ARG:HH21	2.12	0.62
1:A:392:SER:HB3	1:A:408:GLN:OE1	2.00	0.62
1:A:451:TRP:CB	1:A:453:ILE:HD11	2.20	0.62
1:A:479:MET:HE1	1:A:568:GLN:CG	2.29	0.62
1:A:357:GLY:HA3	1:A:389:HIS:HE1	1.65	0.62
1:A:387:PHE:CE2	1:A:429:VAL:HG12	2.33	0.62
1:A:603:ARG:NH1	1:A:664:ILE:HG22	2.10	0.62
1:A:613:GLN:HB3	1:A:678:ALA:HB2	1.81	0.62
1:B:729:THR:HG22	1:B:730:PHE:N	2.15	0.62
1:A:330:MET:HE1	1:A:534:GLY:N	2.15	0.62
1:A:366:GLY:HA3	1:A:370:GLU:HB3	1.80	0.62
1:B:87:VAL:HG21	1:B:104:LEU:HD11	1.82	0.62
1:B:360:GLY:HA3	1:B:391:TRP:CZ2	2.35	0.62
1:A:276:ILE:HD13	1:A:276:ILE:N	2.15	0.62
1:A:390:MET:HB2	1:A:393:HIS:N	2.13	0.62
1:A:433:HIS:O	1:A:436:VAL:HG23	1.99	0.62
1:A:437:TYR:HA	1:A:438:PRO:C	2.25	0.62
1:A:624:LEU:O	1:A:630:LEU:HB2	1.99	0.62
1:A:649:HIS:HA	1:A:652:HIS:HD2	1.65	0.62
1:A:799:THR:HG23	1:A:800:ASN:N	2.15	0.62
1:B:612:PRO:HG3	1:B:681:PHE:CE2	2.34	0.62
1:B:802:ILE:HB	1:B:804:TYR:CE2	2.35	0.62
1:B:561:LEU:CD1	1:B:566:LEU:HA	2.30	0.61
1:B:595:TRP:CH2	1:B:599:LYS:HB3	2.35	0.61
1:A:358:TYR:OH	1:A:416:ALA:HB2	2.01	0.61
1:A:381:VAL:HG21	1:A:421:ILE:HG12	1.81	0.61
1:A:602:ASP:CG	1:A:606:LYS:HE3	2.25	0.61
1:A:205:PRO:N	1:A:206:LEU:HA	2.16	0.61
1:B:298:VAL:O	1:B:302:THR:HG23	2.01	0.61
1:B:366:GLY:HA2	1:B:370:GLU:OE2	2.00	0.61
1:A:704:ILE:O	1:A:757:TYR:HE2	1.84	0.61
1:A:863:LEU:CB	1:A:870:LEU:HD23	2.27	0.61
1:B:115:ILE:O	1:B:117:PRO:HD3	2.00	0.61
1:B:135:LEU:HD13	1:B:301:LEU:CB	2.30	0.61
1:A:81:THR:HG22	1:A:131:GLY:HA3	1.82	0.61
1:A:119:LYS:HD2	1:A:120:GLY:CA	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD22	1:A:308:LEU:N	2.16	0.61
1:B:281:PHE:CZ	1:B:293:VAL:HG12	2.35	0.61
1:B:635:PRO:HB3	1:B:643:ILE:HD13	1.82	0.61
1:A:103:ILE:HG21	1:A:294:PHE:CD1	2.36	0.61
1:A:633:ASN:OD1	1:A:662:PHE:HB3	1.99	0.61
1:A:694:LEU:HB2	1:A:695:PRO:CA	2.31	0.61
1:B:86:LEU:HB2	1:B:133:PHE:CD1	2.36	0.61
1:B:346:ARG:HG2	1:B:352:PHE:CB	2.30	0.61
1:B:381:VAL:HG13	1:B:422:PRO:HD3	1.82	0.61
1:B:117:PRO:HB2	1:B:120:GLY:N	2.14	0.61
1:A:462:PRO:HD2	1:A:470:ARG:CA	2.31	0.61
1:A:612:PRO:O	1:A:615:THR:HG23	2.00	0.61
1:B:80:ARG:HB2	1:B:162:TYR:CE1	2.35	0.61
1:A:409:MET:C	1:A:450:VAL:HG11	2.25	0.61
1:A:436:VAL:HG12	1:A:437:TYR:CD1	2.31	0.61
1:B:360:GLY:HA3	1:B:391:TRP:CE2	2.35	0.61
1:B:715:GLN:HB3	1:B:835:ARG:CD	2.21	0.61
1:B:738:SER:HA	1:B:745:ARG:HH21	1.65	0.61
1:B:836:LYS:HE3	1:B:837:TYR:O	1.99	0.61
1:A:643:ILE:H	1:A:643:ILE:HD12	1.65	0.61
1:B:430:ALA:HB1	1:B:434:SER:O	2.00	0.61
1:B:328:THR:CB	1:B:531:SER:HA	2.27	0.60
1:B:687:PRO:HG3	1:B:764:TRP:NE1	2.16	0.60
1:A:132:ARG:HG2	1:A:133:PHE:CE1	2.36	0.60
1:A:220:LEU:HD22	1:A:220:LEU:N	2.16	0.60
1:A:494:PHE:HB3	1:A:497:GLU:HG3	1.83	0.60
1:B:361:LYS:HE2	1:B:391:TRP:NE1	2.15	0.60
1:A:122:MET:H	1:A:122:MET:HE2	1.67	0.60
1:A:283:ASN:HB3	1:A:290:HIS:CE1	2.36	0.60
1:A:764:TRP:HB3	1:A:773:ILE:HD13	1.83	0.60
1:B:561:LEU:CB	1:B:566:LEU:HD13	2.28	0.60
1:A:391:TRP:CH2	1:A:415:PHE:HB2	2.37	0.60
1:A:691:ALA:HB2	1:A:768:TYR:HE2	1.67	0.60
1:B:322:PHE:HA	1:B:329:ARG:NE	2.16	0.60
1:B:386:TRP:CG	1:B:421:ILE:HB	2.37	0.60
1:B:607:LEU:HB2	1:B:796:LEU:HD22	1.82	0.60
1:A:84:LEU:HD23	1:A:133:PHE:CE1	2.36	0.60
1:A:389:HIS:CD2	1:A:431:PRO:HA	2.33	0.60
1:A:645:PHE:O	1:A:651:TYR:HB2	2.02	0.60
1:A:768:TYR:HD1	1:A:772:GLN:HG3	1.66	0.60
1:B:348:HIS:CG	1:B:547:VAL:HG11	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ILE:CD1	1:B:558:LEU:HB3	2.32	0.60
1:B:390:MET:HG3	1:B:408:GLN:CB	2.24	0.60
1:B:604:PHE:CZ	1:B:659:MET:HG3	2.36	0.60
1:A:211:ARG:HD3	1:A:551:HIS:O	2.01	0.60
1:B:84:LEU:CD2	1:B:132:ARG:HE	2.12	0.60
1:B:167:ILE:HG13	1:B:301:LEU:HD12	1.84	0.60
1:B:536:ASP:O	1:B:537:ARG:HB2	2.01	0.60
1:A:349:ILE:HG13	1:A:558:LEU:HB2	1.83	0.60
1:A:681:PHE:CE2	1:A:760:HIS:HB3	2.37	0.60
1:B:554:THR:HG22	1:B:555:ASN:N	2.16	0.60
1:B:738:SER:CB	1:B:745:ARG:HH21	2.14	0.60
1:A:86:LEU:HD13	1:A:133:PHE:CZ	2.36	0.60
1:A:328:THR:CG2	1:A:531:SER:HA	2.31	0.60
1:A:649:HIS:O	1:A:652:HIS:HB2	2.02	0.60
1:A:715:GLN:HG3	1:A:837:TYR:CD2	2.36	0.60
1:B:201:ASN:OD1	1:B:203:LYS:HB2	2.02	0.60
1:B:335:VAL:HG11	1:B:376:LEU:HB3	1.84	0.60
1:B:467:ALA:HB1	1:B:484:GLN:OE1	2.01	0.60
1:A:356:LEU:HD11	1:A:384:PHE:HD2	1.67	0.60
1:A:831:LYS:HE2	1:A:832:SER:CB	2.32	0.60
1:B:321:ILE:HD13	1:B:530:LEU:HB2	1.83	0.60
1:A:116:ALA:O	1:A:143:LYS:HD2	2.01	0.59
1:A:285:LEU:CD1	1:A:291:LYS:HE2	2.31	0.59
1:A:321:ILE:HD13	1:A:530:LEU:HB2	1.84	0.59
1:A:385:TRP:CB	1:A:425:MET:HE1	2.26	0.59
1:A:394:MET:SD	1:A:399:PHE:HB2	2.42	0.59
1:B:378:LEU:HD21	1:B:419:HIS:CG	2.37	0.59
1:B:840:MET:HE1	1:B:848:LEU:HD12	1.82	0.59
1:A:276:ILE:HD11	1:A:278:ARG:HH22	1.67	0.59
1:A:386:TRP:HB2	1:A:421:ILE:CG2	2.32	0.59
1:A:396:PRO:HD2	1:A:435:GLY:HA3	1.84	0.59
1:A:413:LYS:HD2	1:A:450:VAL:O	2.01	0.59
1:A:776:LEU:HD11	1:A:792:VAL:CG2	2.32	0.59
1:A:785:PRO:HB2	1:A:808:LEU:CD1	2.32	0.59
1:A:829:LEU:HD21	1:A:834:GLY:HA3	1.83	0.59
1:A:860:SER:HB3	1:A:878:LEU:HD11	1.84	0.59
1:A:285:LEU:O	1:A:285:LEU:HD13	2.02	0.59
1:A:860:SER:HB2	1:A:870:LEU:HD11	1.84	0.59
1:B:182:LEU:HB3	1:B:185:PHE:HB2	1.84	0.59
1:B:322:PHE:HA	1:B:329:ARG:NH2	2.17	0.59
1:B:396:PRO:HB2	1:B:443:LEU:HD13	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:717:GLN:O	1:B:720:HIS:HB2	2.02	0.59
1:A:121:ASP:HB3	1:A:151:ASN:HD21	1.67	0.59
1:A:322:PHE:HB3	1:A:363:PHE:HB2	1.84	0.59
1:B:243:THR:CG2	1:B:249:ILE:HD11	2.32	0.59
1:B:793:GLN:HB3	1:B:798:VAL:CG1	2.31	0.59
1:B:821:LEU:HD12	1:B:821:LEU:N	2.17	0.59
1:A:116:ALA:HB3	1:A:143:LYS:HB3	1.84	0.59
1:A:200:ILE:CD1	1:A:213:SER:HB2	2.32	0.59
1:A:724:VAL:HG11	1:A:744:LEU:CA	2.33	0.59
1:B:117:PRO:HG2	1:B:120:GLY:CA	2.28	0.59
1:B:341:THR:HG21	1:B:540:LEU:HD22	1.83	0.59
1:B:492:THR:HG21	1:B:497:GLU:HB3	1.83	0.59
1:B:585:PRO:HD2	1:B:595:TRP:CZ3	2.37	0.59
1:A:206:LEU:CD2	1:A:207:LEU:H	2.14	0.59
1:A:213:SER:HB3	1:A:553:TRP:CE3	2.37	0.59
1:A:322:PHE:HB3	1:A:363:PHE:CB	2.32	0.59
1:A:322:PHE:CB	1:A:363:PHE:HB2	2.32	0.59
1:B:125:LEU:HD22	1:B:158:TYR:CB	2.33	0.59
1:B:603:ARG:HG2	1:B:603:ARG:HH11	1.68	0.59
1:B:859:LEU:HD23	1:B:874:LEU:HD22	1.83	0.59
1:A:486:CYS:O	1:A:514:LEU:HD22	2.03	0.59
1:B:272:LEU:HD23	1:B:272:LEU:O	2.03	0.59
1:B:453:ILE:HD12	1:B:453:ILE:N	2.17	0.59
1:B:694:LEU:HG	1:B:694:LEU:O	2.01	0.59
1:B:694:LEU:HD23	1:B:694:LEU:N	2.18	0.59
1:A:761:ILE:HG22	1:A:862:LEU:HD21	1.85	0.59
1:B:207:LEU:HD12	1:B:207:LEU:H	1.68	0.59
1:B:470:ARG:HD2	1:B:482:PRO:HB3	1.84	0.59
1:B:618:THR:HB	1:B:833:LYS:HD2	1.85	0.59
1:B:625:GLY:HA2	1:B:674:PHE:CZ	2.37	0.59
1:B:774:LEU:HD22	1:B:795:PHE:HB2	1.84	0.59
1:A:117:PRO:CB	1:A:119:LYS:HE2	2.32	0.59
1:A:200:ILE:HG21	1:A:206:LEU:HB3	1.85	0.59
1:A:485:THR:HG21	1:A:489:PHE:CE2	2.38	0.59
1:A:740:ALA:HB1	1:A:744:LEU:CG	2.33	0.59
1:B:577:GLU:OE1	1:B:577:GLU:HA	2.03	0.59
1:B:612:PRO:HG2	1:B:757:TYR:CD1	2.38	0.59
1:B:715:GLN:CG	1:B:837:TYR:HB3	2.33	0.59
1:A:462:PRO:HB2	1:A:463:HIS:CD2	2.38	0.59
1:A:734:ILE:HD12	1:A:847:PHE:HE1	1.66	0.59
1:B:102:ALA:HB1	1:B:468:ARG:CZ	2.33	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:O	1:B:380:TYR:HB2	2.02	0.58
1:B:625:GLY:CA	1:B:674:PHE:HZ	2.15	0.58
1:A:617:THR:HA	1:A:702:ILE:CD1	2.32	0.58
1:B:283:ASN:HB3	1:B:290:HIS:CE1	2.37	0.58
1:B:793:GLN:HB3	1:B:798:VAL:HG11	1.84	0.58
1:A:284:ASN:ND2	1:A:286:ASN:HB2	2.18	0.58
1:A:321:ILE:HG21	1:A:377:LEU:HD22	1.85	0.58
1:A:529:HIS:O	1:A:532:ASN:HB3	2.03	0.58
1:A:774:LEU:HB2	1:A:795:PHE:CZ	2.38	0.58
1:B:216:GLU:HB2	1:B:553:TRP:CH2	2.38	0.58
1:B:581:LEU:N	1:B:581:LEU:HD12	2.18	0.58
1:B:740:ALA:HB1	1:B:744:LEU:CB	2.32	0.58
1:A:596:SER:CB	1:A:599:LYS:HZ3	2.16	0.58
1:B:84:LEU:HD22	1:B:132:ARG:NE	2.19	0.58
1:B:455:VAL:CG2	1:B:564:VAL:HA	2.33	0.58
1:B:474:ILE:HD11	1:B:571:PHE:CG	2.38	0.58
1:A:125:LEU:HD22	1:A:125:LEU:N	2.18	0.58
1:A:366:GLY:HA2	1:A:370:GLU:OE2	2.03	0.58
1:A:433:HIS:ND1	1:A:458:THR:HA	2.19	0.58
1:A:523:ILE:CG2	1:A:566:LEU:HD21	2.33	0.58
1:A:716:HIS:NE2	1:A:832:SER:HB2	2.19	0.58
1:B:313:TYR:HD1	1:B:561:LEU:HG	1.63	0.58
1:B:349:ILE:HD13	1:B:558:LEU:HB3	1.85	0.58
1:B:466:PRO:CB	1:B:469:TYR:HB2	2.34	0.58
1:B:603:ARG:HE	1:B:665:PRO:HD3	1.69	0.58
1:B:789:MET:HB3	1:B:804:TYR:CD2	2.39	0.58
1:A:786:ALA:HA	1:A:804:TYR:HB2	1.85	0.58
1:A:825:LYS:HD2	1:A:825:LYS:N	2.18	0.58
1:B:322:PHE:HB3	1:B:363:PHE:CB	2.33	0.58
1:B:781:LEU:CA	1:B:788:VAL:HG21	2.33	0.58
1:A:603:ARG:HA	1:A:673:TYR:HE2	1.65	0.58
1:A:691:ALA:O	1:A:695:PRO:HB3	2.04	0.58
1:B:866:MET:HG2	1:B:868:GLN:CB	2.32	0.58
1:A:139:GLU:O	1:A:169:PHE:HB2	2.04	0.58
1:A:756:TRP:HB2	1:A:760:HIS:CD2	2.39	0.58
1:B:658:TYR:O	1:B:661:PHE:HB2	2.04	0.58
1:A:649:HIS:HA	1:A:652:HIS:CD2	2.39	0.57
1:B:536:ASP:CB	1:B:538:LEU:HG	2.29	0.57
1:B:597:LYS:H	1:B:597:LYS:CD	2.17	0.57
1:B:715:GLN:HG3	1:B:837:TYR:HB3	1.86	0.57
1:A:378:LEU:HD21	1:A:419:HIS:CD2	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASP:OD1	1:B:276:ILE:HG12	2.04	0.57
1:B:356:LEU:HD13	1:B:377:LEU:HD21	1.86	0.57
1:B:466:PRO:HG2	1:B:469:TYR:CD1	2.30	0.57
1:B:829:LEU:C	1:B:829:LEU:HD12	2.30	0.57
1:A:80:ARG:O	1:A:130:ARG:HA	2.03	0.57
1:A:207:LEU:HB3	1:A:210:THR:OG1	2.05	0.57
1:A:485:THR:HG21	1:A:489:PHE:HE2	1.69	0.57
1:A:536:ASP:HB2	1:A:538:LEU:HG	1.87	0.57
1:B:322:PHE:CB	1:B:363:PHE:HB2	2.35	0.57
1:B:330:MET:HE3	1:B:335:VAL:HA	1.86	0.57
1:B:454:ARG:O	1:B:478:ILE:HA	2.05	0.57
1:B:556:LEU:HD22	1:B:556:LEU:N	2.20	0.57
1:A:207:LEU:HB3	1:A:210:THR:HG23	1.85	0.57
1:B:125:LEU:H	1:B:125:LEU:CD1	2.14	0.57
1:B:138:TYR:CG	1:B:144:TYR:HB2	2.39	0.57
1:B:248:SER:HB2	1:B:252:LEU:HD12	1.86	0.57
1:B:313:TYR:HB3	1:B:566:LEU:HD11	1.83	0.57
1:B:514:LEU:HD11	1:B:526:PHE:CE1	2.40	0.57
1:B:325:LYS:O	1:B:328:THR:HG23	2.04	0.57
1:B:753:VAL:HG12	1:B:760:HIS:HE2	1.69	0.57
1:A:138:TYR:CG	1:A:144:TYR:HB2	2.39	0.57
1:A:433:HIS:HB3	1:A:436:VAL:HG21	1.85	0.57
1:A:755:GLY:HA3	1:A:852:TYR:CE1	2.40	0.57
1:B:465:LYS:HB2	1:B:466:PRO:HA	1.86	0.57
1:B:474:ILE:N	1:B:580:PRO:HG3	2.18	0.57
1:A:388:PRO:HG2	1:A:428:ALA:CB	2.35	0.57
1:A:427:TYR:HA	1:A:453:ILE:HG23	1.86	0.57
1:A:582:TRP:CG	1:A:651:TYR:HH	2.23	0.57
1:B:322:PHE:HB3	1:B:363:PHE:HB2	1.86	0.57
1:B:378:LEU:CD2	1:B:419:HIS:HB3	2.34	0.57
1:B:755:GLY:HA3	1:B:852:TYR:HE1	1.68	0.57
1:A:328:THR:HG23	1:A:531:SER:CB	2.34	0.57
1:A:665:PRO:CB	1:A:670:SER:HA	2.34	0.57
1:B:133:PHE:CD2	1:B:136:ILE:HG12	2.40	0.57
1:B:169:PHE:HZ	1:B:294:PHE:CD2	2.23	0.57
1:A:353:THR:HG21	1:A:385:TRP:CD2	2.40	0.57
1:A:500:GLY:O	1:A:504:GLU:HB2	2.04	0.57
1:B:182:LEU:HD13	1:B:189:LEU:HD11	1.85	0.57
1:A:356:LEU:HD13	1:A:377:LEU:HD23	1.87	0.57
1:A:214:GLU:HG3	1:A:215:VAL:N	2.20	0.56
1:A:330:MET:HE1	1:A:534:GLY:H	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:GLU:HG3	1:A:464:LEU:HD11	1.86	0.56
1:A:603:ARG:HD2	1:A:659:MET:HE2	1.87	0.56
1:B:394:MET:O	1:B:431:PRO:HB2	2.04	0.56
1:B:473:PHE:CB	1:B:580:PRO:HB3	2.33	0.56
1:B:576:GLU:CD	1:B:576:GLU:H	2.13	0.56
1:B:606:LYS:HE3	1:B:673:TYR:N	2.06	0.56
1:B:606:LYS:HG3	1:B:696:LYS:HZ1	1.68	0.56
1:A:532:ASN:HD21	1:A:539:GLY:HA3	1.69	0.56
1:B:283:ASN:H	1:B:290:HIS:CE1	2.21	0.56
1:A:338:LEU:HD13	1:A:533:TYR:HE1	1.69	0.56
1:A:388:PRO:CG	1:A:428:ALA:HB2	2.35	0.56
1:A:433:HIS:C	1:A:436:VAL:HG23	2.30	0.56
1:A:836:LYS:H	1:A:836:LYS:CD	2.17	0.56
1:B:329:ARG:HG2	1:B:329:ARG:NH1	2.20	0.56
1:B:495:TYR:O	1:B:498:TYR:HB2	2.05	0.56
1:B:829:LEU:HD13	1:B:833:LYS:HG3	1.87	0.56
1:A:310:LEU:H	1:A:310:LEU:HD22	1.71	0.56
1:B:323:VAL:HG22	1:B:362:PHE:HB2	1.86	0.56
1:B:335:VAL:HG12	1:B:376:LEU:CD2	2.35	0.56
1:B:636:SER:HB3	1:B:650:ASN:HD21	1.69	0.56
1:B:691:ALA:HA	1:B:768:TYR:OH	2.05	0.56
1:B:698:LYS:HA	1:B:772:GLN:HE21	1.71	0.56
1:A:105:GLU:O	1:A:108:ARG:HD3	2.05	0.56
1:A:485:THR:HB	1:A:487:GLY:H	1.70	0.56
1:A:643:ILE:HD12	1:A:643:ILE:N	2.20	0.56
1:B:274:ASP:CG	1:B:278:ARG:HH22	2.13	0.56
1:B:570:TYR:HE1	1:B:577:GLU:CG	2.16	0.56
1:B:837:TYR:O	1:B:837:TYR:HD2	1.89	0.56
1:A:206:LEU:HD23	1:A:207:LEU:N	2.19	0.56
1:A:596:SER:H	1:A:599:LYS:NZ	2.02	0.56
1:A:694:LEU:HB3	1:A:697:ALA:HB3	1.88	0.56
1:A:729:THR:HG22	1:A:730:PHE:H	1.71	0.56
1:B:537:ARG:NH1	1:B:537:ARG:HG2	2.19	0.56
1:A:90:GLU:O	1:A:115:ILE:HG23	2.06	0.56
1:A:749:ASN:OD1	1:A:753:VAL:HG21	2.05	0.56
1:B:108:ARG:NH1	1:B:471:ARG:HG2	2.21	0.56
1:B:109:PHE:HE2	1:B:306:LEU:CD2	2.18	0.56
1:B:396:PRO:CG	1:B:431:PRO:HD2	2.36	0.56
1:B:605:PRO:HB3	1:B:674:PHE:N	2.21	0.56
1:B:785:PRO:CG	1:B:808:LEU:HD13	2.36	0.56
1:A:363:PHE:CE1	1:A:364:HIS:HB2	2.41	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:LEU:CD2	1:B:381:VAL:HG21	2.35	0.56
1:B:468:ARG:HG3	1:B:469:TYR:N	2.19	0.56
1:B:633:ASN:CG	1:B:643:ILE:HD12	2.31	0.56
1:A:207:LEU:HG	1:A:296:ASP:OD1	2.06	0.56
1:B:367:THR:HG22	1:B:368:ASN:N	2.18	0.56
1:B:765:LEU:HA	1:B:773:ILE:CD1	2.36	0.56
1:A:386:TRP:HB2	1:A:421:ILE:HG21	1.88	0.56
1:A:537:ARG:NH1	1:A:537:ARG:HB3	2.21	0.56
1:A:716:HIS:HD2	1:A:832:SER:HB2	1.64	0.56
1:A:769:HIS:HB3	1:A:772:GLN:HG2	1.88	0.56
1:B:440:HIS:NE2	1:B:442:GLN:HB2	2.20	0.56
1:B:615:THR:HG21	1:B:702:ILE:CB	2.36	0.56
1:B:740:ALA:HB1	1:B:744:LEU:HD23	1.87	0.56
1:B:781:LEU:N	1:B:788:VAL:HG21	2.21	0.56
1:B:860:SER:HA	1:B:870:LEU:HD22	1.87	0.56
1:A:366:GLY:CA	1:A:370:GLU:HB2	2.36	0.55
1:A:381:VAL:CG2	1:A:421:ILE:HG12	2.36	0.55
1:A:694:LEU:HB2	1:A:695:PRO:HA	1.88	0.55
1:B:283:ASN:N	1:B:290:HIS:HE1	2.04	0.55
1:B:440:HIS:HD2	1:B:442:GLN:HB2	1.70	0.55
1:A:88:PHE:HB3	1:A:116:ALA:HB2	1.89	0.55
1:A:109:PHE:CE1	1:A:308:LEU:HD21	2.41	0.55
1:A:471:ARG:HB2	1:A:577:GLU:CD	2.31	0.55
1:A:494:PHE:HB2	1:A:497:GLU:CD	2.30	0.55
1:B:288:TRP:CD1	1:B:510:ASN:HB3	2.41	0.55
1:B:728:TYR:HB3	1:B:733:VAL:HG23	1.88	0.55
1:B:769:HIS:CD2	1:B:771:ASN:H	2.23	0.55
1:A:322:PHE:HE1	1:A:377:LEU:HD13	1.71	0.55
1:A:562:PRO:HB2	1:A:565:GLN:OE1	2.06	0.55
1:A:781:LEU:HD13	1:A:788:VAL:HG11	1.88	0.55
1:B:509:ILE:O	1:B:515:PHE:HB2	2.06	0.55
1:B:785:PRO:HG3	1:B:817:TRP:HB2	1.88	0.55
1:A:201:ASN:ND2	1:A:203:LYS:HB2	2.22	0.55
1:A:410:ALA:N	1:A:450:VAL:HG11	2.20	0.55
1:B:649:HIS:HB3	1:B:653:LYS:NZ	2.21	0.55
1:B:863:LEU:HB2	1:B:870:LEU:HD21	1.86	0.55
1:A:87:VAL:HG21	1:A:104:LEU:HD11	1.86	0.55
1:A:277:GLN:H	1:A:277:GLN:CD	2.14	0.55
1:A:330:MET:HB3	1:A:335:VAL:CG2	2.36	0.55
1:B:125:LEU:HD23	1:B:158:TYR:CD1	2.41	0.55
1:B:272:LEU:HD23	1:B:272:LEU:C	2.32	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:CB	1:B:352:PHE:HD2	2.17	0.55
1:B:381:VAL:HG21	1:B:421:ILE:HG22	1.87	0.55
1:B:416:ALA:HA	1:B:421:ILE:CG1	2.33	0.55
1:A:389:HIS:CB	1:A:431:PRO:HG3	2.16	0.55
1:B:866:MET:HG3	1:B:868:GLN:H	1.69	0.55
1:A:117:PRO:HB2	1:A:120:GLY:CA	2.37	0.55
1:B:106:SER:HB2	1:B:520:LEU:HD13	1.88	0.55
1:B:322:PHE:HA	1:B:329:ARG:CZ	2.36	0.55
1:B:396:PRO:HA	1:B:405:LEU:CD2	2.36	0.55
1:B:657:TRP:CH2	1:B:661:PHE:HE2	2.25	0.55
1:B:738:SER:HB3	1:B:745:ARG:NH2	2.22	0.55
1:B:814:LYS:HZ3	1:B:828:CYS:HB3	1.72	0.55
1:A:427:TYR:CE2	1:A:455:VAL:HB	2.42	0.55
1:A:597:LYS:HA	1:A:597:LYS:CE	2.29	0.55
1:A:694:LEU:HD22	1:A:697:ALA:HB3	1.88	0.55
1:B:178:LEU:HG	1:B:179:SER:N	2.22	0.55
1:B:331:LYS:HD2	1:B:331:LYS:H	1.72	0.55
1:B:361:LYS:HA	1:B:361:LYS:CE	2.35	0.55
1:B:361:LYS:HB2	1:B:391:TRP:CD1	2.41	0.55
1:B:704:ILE:O	1:B:757:TYR:HE2	1.89	0.55
1:B:784:GLU:HG3	1:B:787:LYS:H	1.72	0.55
1:B:840:MET:HE2	1:B:844:SER:C	2.30	0.55
1:A:107:SER:O	1:A:308:LEU:HD11	2.07	0.55
1:A:141:ILE:CG2	1:A:170:PHE:HD1	2.20	0.55
1:A:409:MET:HB3	1:A:451:TRP:NE1	2.22	0.55
1:A:703:LEU:HD11	1:A:761:ILE:HD12	1.83	0.55
1:A:818:CYS:SG	1:A:828:CYS:HA	2.47	0.55
1:B:349:ILE:CD1	1:B:558:LEU:HD13	2.28	0.55
1:B:396:PRO:HA	1:B:405:LEU:HD21	1.88	0.55
1:B:614:LYS:CG	1:B:713:TRP:HE3	2.19	0.55
1:B:615:THR:CG2	1:B:702:ILE:HD12	2.31	0.55
1:A:207:LEU:HD23	1:A:208:TYR:N	2.22	0.55
1:A:472:GLY:O	1:A:577:GLU:HB3	2.07	0.55
1:B:92:LEU:O	1:B:98:GLN:HG3	2.07	0.55
1:B:132:ARG:HB3	1:B:133:PHE:CE1	2.41	0.55
1:B:207:LEU:HD23	1:B:293:VAL:HG22	1.89	0.55
1:B:346:ARG:HG2	1:B:352:PHE:HB2	1.88	0.55
1:B:381:VAL:HG22	1:B:386:TRP:HZ2	1.70	0.55
1:B:664:ILE:HG13	1:B:664:ILE:O	2.06	0.55
1:B:835:ARG:H	1:B:835:ARG:CZ	2.20	0.55
1:B:656:ASP:O	1:B:660:GLU:HG3	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD22	1:A:210:THR:HG23	1.90	0.54
1:A:381:VAL:HG13	1:A:382:LYS:N	2.21	0.54
1:B:603:ARG:HG2	1:B:603:ARG:NH1	2.22	0.54
1:B:775:VAL:HG11	1:B:863:LEU:CD2	2.34	0.54
1:A:328:THR:HG23	1:A:531:SER:CA	2.36	0.54
1:B:106:SER:CB	1:B:520:LEU:HD13	2.38	0.54
1:B:114:GLU:HG3	1:B:123:PRO:CG	2.37	0.54
1:B:133:PHE:CE2	1:B:158:TYR:CE1	2.95	0.54
1:B:178:LEU:HD23	1:B:178:LEU:N	2.22	0.54
1:B:399:PHE:CE2	1:B:404:VAL:HG12	2.43	0.54
1:B:466:PRO:HB3	1:B:468:ARG:NH1	2.23	0.54
1:B:698:LYS:HD3	1:B:772:GLN:HE21	1.71	0.54
1:A:391:TRP:CE3	1:A:412:ASN:HA	2.41	0.54
1:A:831:LYS:HE2	1:A:832:SER:CA	2.37	0.54
1:B:338:LEU:CD1	1:B:354:PHE:HE2	2.21	0.54
1:B:388:PRO:CB	1:B:412:ASN:HD22	2.20	0.54
1:B:596:SER:HB3	1:B:598:GLU:OE1	2.07	0.54
1:B:793:GLN:OE1	1:B:802:ILE:HG12	2.07	0.54
1:A:388:PRO:HG3	1:A:451:TRP:CH2	2.43	0.54
1:A:694:LEU:HB2	1:A:695:PRO:C	2.31	0.54
1:A:731:HIS:O	1:A:735:THR:HG23	2.06	0.54
1:B:136:ILE:HG13	1:B:164:VAL:HG11	1.88	0.54
1:B:687:PRO:HG3	1:B:764:TRP:CE2	2.42	0.54
1:B:793:GLN:NE2	1:B:804:TYR:HE2	2.05	0.54
1:A:758:ALA:HB2	1:A:859:LEU:CA	2.37	0.54
1:A:857:ILE:HG13	1:A:878:LEU:CD2	2.38	0.54
1:B:125:LEU:O	1:B:132:ARG:HB2	2.07	0.54
1:B:402:GLN:HE22	1:B:445:GLU:HB3	1.73	0.54
1:B:610:ILE:HD12	1:B:681:PHE:CD1	2.43	0.54
1:B:753:VAL:O	1:B:756:TRP:HB2	2.08	0.54
1:A:207:LEU:HB3	1:A:210:THR:CG2	2.37	0.54
1:A:276:ILE:HD11	1:A:278:ARG:NH2	2.23	0.54
1:A:466:PRO:HD2	1:A:469:TYR:CD2	2.43	0.54
1:A:703:LEU:HD22	1:A:757:TYR:CD1	2.41	0.54
1:A:813:LYS:H	1:A:813:LYS:CD	2.18	0.54
1:A:857:ILE:N	1:A:878:LEU:HD21	2.23	0.54
1:B:244:ARG:HG3	1:B:244:ARG:NH1	2.22	0.54
1:B:346:ARG:HA	1:B:349:ILE:O	2.08	0.54
1:B:574:PHE:HB2	1:B:577:GLU:HG2	1.89	0.54
1:A:274:ASP:CG	1:A:278:ARG:HH12	2.16	0.54
1:A:765:LEU:HD22	1:A:862:LEU:HD11	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:VAL:CG2	1:A:526:PHE:HZ	2.21	0.54
1:B:582:TRP:NE1	1:B:655:ILE:HD12	2.23	0.54
1:B:782:ARG:HG3	1:B:816:PHE:CD1	2.42	0.54
1:A:232:HIS:CE1	1:A:234:THR:HG23	2.42	0.54
1:A:622:LEU:O	1:A:626:MET:HG2	2.08	0.54
1:A:829:LEU:O	1:A:829:LEU:HD22	2.08	0.54
1:A:831:LYS:HD2	1:A:831:LYS:C	2.33	0.54
1:B:109:PHE:HE2	1:B:306:LEU:HB3	1.70	0.54
1:B:646:PHE:CZ	1:B:689:ARG:HB3	2.43	0.54
1:B:786:ALA:CA	1:B:804:TYR:HB2	2.38	0.54
1:A:717:GLN:HG3	1:A:747:LEU:CD1	2.32	0.53
1:B:390:MET:HE1	1:B:409:MET:HG2	1.88	0.53
1:B:436:VAL:HG21	1:B:458:THR:OG1	2.08	0.53
1:A:518:VAL:HG22	1:A:526:PHE:HZ	1.73	0.53
1:A:561:LEU:HB3	1:A:566:LEU:CD1	2.34	0.53
1:B:77:THR:HG21	1:B:80:ARG:HH21	1.73	0.53
1:B:624:LEU:CG	1:B:789:MET:HE1	2.37	0.53
1:B:714:TYR:CD1	1:B:730:PHE:HB2	2.43	0.53
1:A:377:LEU:HD23	1:A:386:TRP:CH2	2.43	0.53
1:A:623:PHE:HB3	1:A:804:TYR:HE1	1.73	0.53
1:B:426:GLY:O	1:B:453:ILE:HG23	2.08	0.53
1:B:715:GLN:HG3	1:B:837:TYR:CB	2.39	0.53
1:A:606:LYS:HB2	1:A:672:PHE:CE1	2.43	0.53
1:A:685:VAL:HG23	1:A:686:ALA:N	2.23	0.53
1:A:853:ARG:HH22	1:A:881:THR:HB	1.72	0.53
1:B:117:PRO:C	1:B:143:LYS:HD2	2.34	0.53
1:B:184:GLY:C	1:B:185:PHE:HD1	2.17	0.53
1:B:243:THR:HG21	1:B:249:ILE:HD13	1.88	0.53
1:B:336:LYS:HA	1:B:380:TYR:OH	2.08	0.53
1:B:580:PRO:C	1:B:581:LEU:HD12	2.33	0.53
1:A:119:LYS:HD2	1:A:120:GLY:HA2	1.90	0.53
1:A:606:LYS:HB2	1:A:672:PHE:CZ	2.43	0.53
1:A:705:ASN:HA	1:A:873:TRP:CE3	2.43	0.53
1:A:781:LEU:HB2	1:A:788:VAL:HG21	1.90	0.53
1:B:96:LEU:HD23	1:B:139:GLU:HG2	1.90	0.53
1:B:200:ILE:CD1	1:B:213:SER:HB2	2.33	0.53
1:B:396:PRO:HB3	1:B:443:LEU:HD13	1.89	0.53
1:B:638:GLU:H	1:B:638:GLU:CD	2.17	0.53
1:B:765:LEU:HA	1:B:773:ILE:HD12	1.90	0.53
1:A:378:LEU:HD11	1:A:419:HIS:CE1	2.44	0.53
1:A:618:THR:HA	1:A:676:LYS:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:THR:HG23	1:B:162:TYR:HB3	1.91	0.53
1:B:381:VAL:HG22	1:B:386:TRP:CE2	2.44	0.53
1:B:776:LEU:HD11	1:B:792:VAL:HG22	1.90	0.53
1:A:96:LEU:HG	1:A:139:GLU:CD	2.34	0.53
1:A:172:ALA:HB2	1:A:224:ASP:O	2.09	0.53
1:A:187:LEU:HD12	1:A:229:GLN:C	2.34	0.53
1:A:598:GLU:OE1	1:A:664:ILE:HD12	2.09	0.53
1:A:740:ALA:HB1	1:A:744:LEU:CB	2.39	0.53
1:B:144:TYR:CE2	1:B:166:ILE:HD13	2.44	0.53
1:B:244:ARG:HG3	1:B:244:ARG:HH11	1.72	0.53
1:B:429:VAL:HG22	1:B:430:ALA:N	2.22	0.53
1:B:603:ARG:NE	1:B:665:PRO:HD3	2.23	0.53
1:B:669:THR:HG22	1:B:670:SER:H	1.74	0.53
1:A:145:VAL:O	1:A:147:LEU:HD22	2.09	0.53
1:A:465:LYS:HA	1:A:466:PRO:C	2.34	0.53
1:A:650:ASN:CA	1:A:653:LYS:HG2	2.32	0.53
1:A:665:PRO:HB3	1:A:670:SER:CA	2.38	0.53
1:A:814:LYS:HD2	1:A:828:CYS:SG	2.49	0.53
1:B:88:PHE:HZ	1:B:123:PRO:HD2	1.74	0.53
1:B:466:PRO:HB2	1:B:469:TYR:HB2	1.91	0.53
1:B:666:SER:HB2	1:B:669:THR:O	2.07	0.53
1:A:103:ILE:HG21	1:A:294:PHE:HD1	1.74	0.53
1:B:715:GLN:CD	1:B:837:TYR:HB3	2.34	0.53
1:B:586:CYS:HA	1:B:592:LYS:CB	2.38	0.52
1:B:784:GLU:OE1	1:B:784:GLU:HA	2.10	0.52
1:A:207:LEU:HD13	1:A:210:THR:HG23	1.91	0.52
1:A:324:GLY:HA3	1:A:328:THR:HG21	1.92	0.52
1:A:346:ARG:CD	1:A:351:ASN:H	2.22	0.52
1:A:711:TYR:CG	1:A:840:MET:HE3	2.45	0.52
1:A:730:PHE:HE2	1:A:751:CYS:CB	2.22	0.52
1:B:114:GLU:HG3	1:B:123:PRO:HG2	1.90	0.52
1:B:138:TYR:CD2	1:B:144:TYR:HB2	2.45	0.52
1:B:363:PHE:CE1	1:B:415:PHE:HE2	2.27	0.52
1:B:604:PHE:CE2	1:B:655:ILE:HG23	2.43	0.52
1:B:606:LYS:H	1:B:606:LYS:CD	2.16	0.52
1:B:613:GLN:HB3	1:B:678:ALA:HB2	1.90	0.52
1:B:721:ASP:HB3	1:B:726:LEU:HD11	1.91	0.52
1:B:729:THR:HG22	1:B:730:PHE:H	1.73	0.52
1:A:535:ASN:HD22	1:A:536:ASP:H	1.57	0.52
1:A:839:GLU:CG	1:A:845:ARG:HH21	2.23	0.52
1:B:266:VAL:HG11	1:B:293:VAL:HG11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:LEU:HD23	1:B:694:LEU:H	1.75	0.52
1:A:92:LEU:HD21	1:A:113:THR:HB	1.91	0.52
1:A:323:VAL:HA	1:A:362:PHE:HB3	1.90	0.52
1:A:561:LEU:HD12	1:A:566:LEU:H	1.72	0.52
1:A:829:LEU:CD2	1:A:834:GLY:HA3	2.39	0.52
1:B:704:ILE:HG12	1:B:778:GLY:C	2.34	0.52
1:A:205:PRO:CB	1:A:208:TYR:HA	2.39	0.52
1:A:603:ARG:HB3	1:A:665:PRO:HG2	1.90	0.52
1:A:868:GLN:HA	1:A:868:GLN:NE2	2.25	0.52
1:B:492:THR:CG2	1:B:497:GLU:HB3	2.40	0.52
1:B:811:ASP:OD1	1:B:813:LYS:HB3	2.10	0.52
1:A:323:VAL:HG22	1:A:359:SER:HB2	1.91	0.52
1:A:738:SER:HA	1:A:745:ARG:NH2	2.25	0.52
1:B:108:ARG:CZ	1:B:108:ARG:HB2	2.40	0.52
1:B:397:HIS:CE1	1:B:595:TRP:HD1	2.27	0.52
1:B:323:VAL:HG22	1:B:362:PHE:HB3	1.90	0.52
1:B:447:TRP:O	1:B:453:ILE:HD12	2.10	0.52
1:A:207:LEU:HD22	1:A:209:VAL:HB	1.92	0.52
1:A:709:ARG:HG3	1:A:757:TYR:OH	2.10	0.52
1:A:781:LEU:HA	1:A:788:VAL:HG21	1.92	0.52
1:B:211:ARG:HB2	1:B:212:PRO:HD2	1.92	0.52
1:B:738:SER:HB3	1:B:745:ARG:HH21	1.73	0.52
1:A:200:ILE:CG2	1:A:206:LEU:HB3	2.40	0.52
1:B:207:LEU:CD2	1:B:293:VAL:HG22	2.40	0.52
1:B:381:VAL:HG12	1:B:382:LYS:N	2.21	0.52
1:B:387:PHE:HD2	1:B:429:VAL:HB	1.69	0.52
1:B:620:LEU:HD22	1:B:702:ILE:CD1	2.40	0.52
1:A:284:ASN:HD22	1:A:286:ASN:H	1.58	0.51
1:B:287:PHE:CE2	1:B:289:LEU:HB3	2.45	0.51
1:B:352:PHE:CD1	1:B:560:THR:HG21	2.45	0.51
1:B:574:PHE:CB	1:B:577:GLU:HG2	2.40	0.51
1:B:621:TYR:CD2	1:B:676:LYS:HB3	2.45	0.51
1:B:706:PRO:HD3	1:B:873:TRP:CZ2	2.44	0.51
1:B:774:LEU:HD22	1:B:795:PHE:CG	2.45	0.51
1:A:146:ASN:C	1:A:147:LEU:HD13	2.36	0.51
1:A:561:LEU:HB3	1:A:566:LEU:HB2	1.92	0.51
1:A:789:MET:HB3	1:A:804:TYR:CE2	2.46	0.51
1:A:802:ILE:HG23	1:A:804:TYR:CE2	2.45	0.51
1:B:187:LEU:HD22	1:B:188:PHE:H	1.75	0.51
1:B:466:PRO:CD	1:B:469:TYR:HB2	2.41	0.51
1:B:575:SER:O	1:B:578:LYS:HB3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:606:LYS:CE	1:B:673:TYR:H	2.11	0.51
1:B:647:ASN:ND2	1:B:679:ASN:HB3	2.25	0.51
1:B:709:ARG:NH1	1:B:754:PRO:HB2	2.25	0.51
1:A:322:PHE:CD2	1:A:363:PHE:HB2	2.45	0.51
1:A:624:LEU:CD2	1:A:630:LEU:HD13	2.41	0.51
1:A:627:HIS:HD2	1:A:630:LEU:HG	1.75	0.51
1:B:485:THR:O	1:B:514:LEU:HD13	2.10	0.51
1:A:194:GLY:HA3	1:A:244:ARG:CD	2.40	0.51
1:A:571:PHE:HD1	1:A:578:LYS:N	2.09	0.51
1:B:391:TRP:CH2	1:B:415:PHE:CB	2.94	0.51
1:B:430:ALA:HB2	1:B:436:VAL:HG13	1.91	0.51
1:B:492:THR:HB	1:B:498:TYR:CE2	2.45	0.51
1:A:409:MET:CB	1:A:451:TRP:HE1	2.24	0.51
1:A:604:PHE:CE1	1:A:693:LEU:HD11	2.37	0.51
1:A:614:LYS:CD	1:A:833:LYS:HB3	2.41	0.51
1:B:201:ASN:HD21	1:B:203:LYS:CE	2.24	0.51
1:B:782:ARG:CD	1:B:816:PHE:HE1	2.19	0.51
1:A:490:THR:HG23	1:A:527:MET:HE1	1.92	0.51
1:B:124:THR:O	1:B:124:THR:HG23	2.10	0.51
1:B:397:HIS:HE1	1:B:595:TRP:HD1	1.59	0.51
1:B:413:LYS:HA	1:B:451:TRP:CH2	2.46	0.51
1:B:597:LYS:HE3	1:B:597:LYS:N	2.24	0.51
1:B:627:HIS:CD2	1:B:802:ILE:HD11	2.46	0.51
1:A:86:LEU:HD22	1:A:133:PHE:CE2	2.46	0.51
1:A:474:ILE:HD11	1:A:571:PHE:CD2	2.44	0.51
1:A:699:VAL:HG11	1:A:764:TRP:CE3	2.45	0.51
1:A:789:MET:HG3	1:A:804:TYR:CD1	2.45	0.51
1:A:863:LEU:HD13	1:A:871:PRO:HD3	1.93	0.51
1:B:80:ARG:O	1:B:130:ARG:HB3	2.11	0.51
1:B:612:PRO:HG3	1:B:681:PHE:CD2	2.46	0.51
1:A:232:HIS:HE1	1:A:273:HIS:NE2	2.08	0.51
1:A:471:ARG:HH21	1:A:471:ARG:HG2	1.76	0.51
1:A:774:LEU:HB2	1:A:795:PHE:CG	2.45	0.51
1:B:88:PHE:CG	1:B:116:ALA:HB2	2.43	0.51
1:B:570:TYR:CE1	1:B:577:GLU:HG3	2.38	0.51
1:B:614:LYS:HG3	1:B:713:TRP:HB2	1.93	0.51
1:A:86:LEU:HB2	1:A:133:PHE:CE2	2.46	0.51
1:A:116:ALA:HB3	1:A:143:LYS:HD2	1.92	0.51
1:A:177:LEU:H	1:A:177:LEU:HD22	1.74	0.51
1:A:776:LEU:HD11	1:A:792:VAL:HG22	1.93	0.51
1:B:109:PHE:CZ	1:B:306:LEU:HB3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:619:ALA:HB2	1:B:829:LEU:CB	2.39	0.51
1:A:205:PRO:HB2	1:A:207:LEU:O	2.10	0.51
1:A:357:GLY:HA3	1:A:389:HIS:CE1	2.46	0.51
1:A:840:MET:SD	1:A:844:SER:HB3	2.51	0.51
1:B:413:LYS:CA	1:B:451:TRP:CH2	2.94	0.51
1:B:586:CYS:O	1:B:592:LYS:HD2	2.10	0.51
1:B:814:LYS:HZ2	1:B:828:CYS:HB3	1.76	0.51
1:A:89:VAL:CG2	1:A:92:LEU:HD23	2.34	0.50
1:A:147:LEU:CG	1:A:152:ARG:HD3	2.41	0.50
1:A:304:LYS:N	1:A:304:LYS:HD2	2.26	0.50
1:A:388:PRO:HD2	1:A:427:TYR:O	2.10	0.50
1:A:471:ARG:HB2	1:A:577:GLU:OE1	2.11	0.50
1:A:614:LYS:HG3	1:A:614:LYS:O	2.11	0.50
1:B:134:ALA:O	1:B:164:VAL:HG22	2.11	0.50
1:B:394:MET:HG2	1:B:395:GLN:H	1.76	0.50
1:B:733:VAL:HA	1:B:744:LEU:CD1	2.35	0.50
1:A:90:GLU:OE2	1:A:94:SER:HB2	2.11	0.50
1:A:121:ASP:HB3	1:A:151:ASN:ND2	2.25	0.50
1:A:390:MET:CB	1:A:393:HIS:H	2.17	0.50
1:A:397:HIS:CD2	1:A:594:ILE:HG22	2.45	0.50
1:A:581:LEU:N	1:A:581:LEU:HD22	2.25	0.50
1:A:604:PHE:HZ	1:A:655:ILE:HG23	1.75	0.50
1:B:103:ILE:HD13	1:B:294:PHE:HD1	1.77	0.50
1:B:324:GLY:HA3	1:B:328:THR:OG1	2.10	0.50
1:B:338:LEU:HD11	1:B:354:PHE:CE2	2.46	0.50
1:B:604:PHE:CZ	1:B:659:MET:CG	2.94	0.50
1:B:604:PHE:CE1	1:B:659:MET:HG2	2.46	0.50
1:A:474:ILE:HD11	1:A:571:PHE:CB	2.41	0.50
1:A:641:GLU:OE1	1:A:641:GLU:HA	2.11	0.50
1:A:109:PHE:CD2	1:A:306:LEU:HD13	2.46	0.50
1:A:486:CYS:HA	1:A:514:LEU:HD22	1.93	0.50
1:A:613:GLN:HG3	1:A:750:ARG:HH22	1.77	0.50
1:A:626:MET:HA	1:A:626:MET:CE	2.40	0.50
1:A:774:LEU:HD22	1:A:795:PHE:HB3	1.92	0.50
1:A:857:ILE:CG1	1:A:878:LEU:HD22	2.41	0.50
1:B:80:ARG:CB	1:B:162:TYR:CE1	2.95	0.50
1:B:299:ALA:O	1:B:304:LYS:HG3	2.11	0.50
1:B:474:ILE:O	1:B:580:PRO:HG2	2.12	0.50
1:B:492:THR:CG2	1:B:498:TYR:CE2	2.95	0.50
1:B:606:LYS:HD3	1:B:672:PHE:CD1	2.47	0.50
1:B:703:LEU:HD22	1:B:757:TYR:CG	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:HB3	1:A:290:HIS:HE1	1.75	0.50
1:B:118:GLY:N	1:B:143:LYS:HD2	2.26	0.50
1:B:479:MET:CB	1:B:567:ALA:HB1	2.40	0.50
1:A:122:MET:H	1:A:122:MET:HE3	1.77	0.50
1:A:363:PHE:CZ	1:A:364:HIS:HB2	2.46	0.50
1:A:421:ILE:HG23	1:A:422:PRO:HD2	1.94	0.50
1:A:427:TYR:HE2	1:A:455:VAL:CB	2.25	0.50
1:A:466:PRO:HD2	1:A:469:TYR:CG	2.47	0.50
1:A:598:GLU:HG2	1:A:603:ARG:HH21	1.77	0.50
1:A:740:ALA:HA	1:A:744:LEU:HD23	1.93	0.50
1:A:860:SER:CB	1:A:870:LEU:HD13	2.40	0.50
1:B:200:ILE:O	1:B:202:PRO:HD3	2.11	0.50
1:B:329:ARG:HH22	1:B:365:THR:HG22	1.73	0.50
1:B:765:LEU:HD13	1:B:866:MET:CE	2.42	0.50
1:A:125:LEU:O	1:A:132:ARG:HB2	2.12	0.50
1:B:389:HIS:CB	1:B:393:HIS:HD2	2.24	0.50
1:A:329:ARG:NH1	1:A:530:LEU:HD13	2.21	0.50
1:A:486:CYS:HB3	1:A:543:PHE:HZ	1.73	0.50
1:B:178:LEU:H	1:B:178:LEU:CD2	2.24	0.50
1:B:352:PHE:HD1	1:B:560:THR:HG21	1.77	0.50
1:B:400:HIS:O	1:B:442:GLN:HG2	2.12	0.50
1:B:789:MET:CB	1:B:804:TYR:CD2	2.94	0.50
1:A:461:TYR:HA	1:A:462:PRO:C	2.37	0.50
1:A:768:TYR:HB2	1:A:773:ILE:HD11	1.93	0.50
1:A:775:VAL:HG11	1:A:863:LEU:CD2	2.41	0.50
1:B:87:VAL:CG2	1:B:104:LEU:HD11	2.40	0.50
1:A:377:LEU:O	1:A:380:TYR:HB2	2.11	0.49
1:A:768:TYR:CD1	1:A:772:GLN:HG3	2.47	0.49
1:A:781:LEU:HD13	1:A:788:VAL:CG1	2.42	0.49
1:B:378:LEU:O	1:B:381:VAL:HB	2.12	0.49
1:B:561:LEU:HB2	1:B:566:LEU:CB	2.39	0.49
1:B:685:VAL:HG23	1:B:686:ALA:N	2.26	0.49
1:B:703:LEU:HD13	1:B:859:LEU:HD11	1.94	0.49
1:A:138:TYR:CD2	1:A:144:TYR:HB2	2.47	0.49
1:A:427:TYR:CE2	1:A:455:VAL:HG12	2.43	0.49
1:B:365:THR:HG23	1:B:366:GLY:N	2.26	0.49
1:B:378:LEU:HD11	1:B:419:HIS:CG	2.47	0.49
1:B:465:LYS:HA	1:B:466:PRO:C	2.36	0.49
1:B:612:PRO:HG3	1:B:681:PHE:HE2	1.77	0.49
1:B:634:TYR:HD2	1:B:635:PRO:HD2	1.76	0.49
1:B:820:LEU:HD11	1:B:824:GLY:HA2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:C	1:A:147:LEU:HD22	2.37	0.49
1:A:207:LEU:HD23	1:A:209:VAL:H	1.77	0.49
1:A:249:ILE:O	1:A:252:LEU:HG	2.12	0.49
1:A:730:PHE:CE2	1:A:751:CYS:HB3	2.48	0.49
1:B:384:PHE:N	1:B:384:PHE:HD2	2.09	0.49
1:B:750:ARG:O	1:B:754:PRO:HG2	2.12	0.49
1:B:782:ARG:HG3	1:B:816:PHE:HD1	1.77	0.49
1:A:283:ASN:CB	1:A:290:HIS:HE1	2.24	0.49
1:A:625:GLY:N	1:A:674:PHE:CZ	2.81	0.49
1:A:781:LEU:CB	1:A:788:VAL:HG21	2.42	0.49
1:B:103:ILE:CD1	1:B:285:LEU:HD21	2.42	0.49
1:B:174:GLU:HG2	1:B:175:ASN:H	1.77	0.49
1:B:416:ALA:CA	1:B:421:ILE:HG12	2.36	0.49
1:B:789:MET:HG3	1:B:804:TYR:CD1	2.47	0.49
1:A:84:LEU:O	1:A:133:PHE:HA	2.13	0.49
1:A:187:LEU:HD11	1:A:228:PHE:HB3	1.94	0.49
1:A:284:ASN:HD22	1:A:286:ASN:N	2.10	0.49
1:A:349:ILE:HG13	1:A:558:LEU:CB	2.42	0.49
1:A:389:HIS:HD2	1:A:431:PRO:CA	2.21	0.49
1:A:582:TRP:HB3	1:A:655:ILE:HD11	1.95	0.49
1:A:721:ASP:CA	1:A:726:LEU:HD11	2.43	0.49
1:A:727:LYS:O	1:A:728:TYR:HD1	1.94	0.49
1:B:122:MET:SD	1:B:151:ASN:HB3	2.53	0.49
1:B:386:TRP:CZ2	1:B:421:ILE:HG22	2.47	0.49
1:B:388:PRO:O	1:B:429:VAL:HG12	2.11	0.49
1:B:537:ARG:HG2	1:B:537:ARG:HH11	1.77	0.49
1:B:649:HIS:HB3	1:B:653:LYS:HZ2	1.75	0.49
1:B:860:SER:HB3	1:B:878:LEU:CD1	2.42	0.49
1:B:125:LEU:CD2	1:B:158:TYR:CG	2.96	0.49
1:B:310:LEU:HD13	1:B:557:ARG:H	1.77	0.49
1:B:471:ARG:HE	1:B:471:ARG:N	2.10	0.49
1:B:691:ALA:HB2	1:B:768:TYR:CE1	2.48	0.49
1:B:699:VAL:HG11	1:B:764:TRP:CE3	2.47	0.49
1:A:617:THR:HA	1:A:702:ILE:HD11	1.94	0.49
1:B:211:ARG:HG2	1:B:211:ARG:HH11	1.78	0.49
1:B:377:LEU:HD22	1:B:386:TRP:CH2	2.48	0.49
1:B:776:LEU:HD13	1:B:788:VAL:CG1	2.42	0.49
1:A:187:LEU:HA	1:A:230:SER:HB3	1.94	0.49
1:A:570:TYR:HE1	1:A:577:GLU:CG	2.26	0.49
1:A:681:PHE:CZ	1:A:761:ILE:HG13	2.43	0.49
1:A:715:GLN:HG3	1:A:837:TYR:CE2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:MET:CB	1:A:804:TYR:CD2	2.96	0.49
1:B:325:LYS:NZ	1:B:325:LYS:HB3	2.28	0.49
1:B:346:ARG:CA	1:B:352:PHE:HB2	2.41	0.49
1:B:394:MET:HE1	1:B:399:PHE:CZ	2.47	0.49
1:B:627:HIS:HD2	1:B:802:ILE:HG12	1.78	0.49
1:A:119:LYS:CA	1:B:128:LYS:HZ1	2.26	0.49
1:A:177:LEU:HD22	1:A:177:LEU:N	2.28	0.49
1:A:207:LEU:CG	1:A:210:THR:HG23	2.42	0.49
1:A:394:MET:HG2	1:A:395:GLN:N	2.27	0.49
1:A:433:HIS:CE1	1:A:483:ARG:HD2	2.46	0.49
1:A:703:LEU:CD2	1:A:757:TYR:HB3	2.39	0.49
1:B:715:GLN:HG3	1:B:837:TYR:CD1	2.47	0.49
1:B:749:ASN:OD1	1:B:753:VAL:HG21	2.12	0.49
1:A:315:LEU:HD21	1:A:563:PRO:HG3	1.92	0.49
1:A:621:TYR:CD2	1:A:674:PHE:CE2	3.01	0.49
1:A:694:LEU:CD2	1:A:697:ALA:HB3	2.43	0.49
1:B:248:SER:OG	1:B:260:ALA:HB2	2.13	0.49
1:B:323:VAL:HG13	1:B:362:PHE:HD2	1.67	0.49
1:B:554:THR:HB	1:B:556:LEU:HD21	1.94	0.49
1:B:714:TYR:HE2	1:B:728:TYR:O	1.95	0.49
1:A:108:ARG:NH2	1:A:468:ARG:HD3	2.27	0.48
1:A:122:MET:CE	1:A:151:ASN:HB3	2.43	0.48
1:A:285:LEU:HD13	1:A:285:LEU:C	2.38	0.48
1:A:330:MET:HB3	1:A:335:VAL:HG23	1.95	0.48
1:A:342:GLN:HE22	1:A:384:PHE:HE1	1.59	0.48
1:A:453:ILE:HD12	1:A:453:ILE:N	2.24	0.48
1:A:612:PRO:CD	1:A:681:PHE:HD1	2.19	0.48
1:A:765:LEU:CD2	1:A:862:LEU:HD11	2.42	0.48
1:B:170:PHE:CE2	1:B:189:LEU:HD22	2.47	0.48
1:B:335:VAL:HG12	1:B:380:TYR:CE2	2.48	0.48
1:A:313:TYR:CB	1:A:566:LEU:HD11	2.43	0.48
1:A:529:HIS:HB2	1:A:532:ASN:HB2	1.95	0.48
1:B:322:PHE:HA	1:B:329:ARG:HE	1.78	0.48
1:B:338:LEU:HD12	1:B:354:PHE:HE2	1.76	0.48
1:B:484:GLN:HG3	1:B:517:THR:CG2	2.43	0.48
1:B:599:LYS:HD2	1:B:659:MET:HB3	1.94	0.48
1:B:863:LEU:HD13	1:B:870:LEU:HA	1.94	0.48
1:A:181:GLN:NE2	1:A:186:PRO:HA	2.27	0.48
1:A:262:LEU:HD22	1:A:262:LEU:N	2.27	0.48
1:A:600:THR:HG21	1:A:670:SER:OG	2.12	0.48
1:A:603:ARG:HH12	1:A:664:ILE:CG2	2.17	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:THR:HB	1:A:833:LYS:NZ	2.28	0.48
1:A:711:TYR:CE1	1:A:837:TYR:CD2	3.01	0.48
1:A:857:ILE:HG12	1:A:878:LEU:HD22	1.96	0.48
1:B:172:ALA:HB2	1:B:224:ASP:O	2.12	0.48
1:B:348:HIS:CD2	1:B:547:VAL:HG11	2.48	0.48
1:B:466:PRO:HB2	1:B:469:TYR:H	1.77	0.48
1:B:554:THR:CG2	1:B:556:LEU:HD21	2.44	0.48
1:A:141:ILE:HG22	1:A:170:PHE:HD1	1.79	0.48
1:A:561:LEU:CD1	1:A:562:PRO:HD2	2.33	0.48
1:A:596:SER:H	1:A:599:LYS:HZ3	1.59	0.48
1:A:603:ARG:HB3	1:A:665:PRO:CG	2.42	0.48
1:A:607:LEU:HD13	1:A:796:LEU:HD21	1.96	0.48
1:A:802:ILE:CG2	1:A:804:TYR:CE2	2.96	0.48
1:B:88:PHE:HB3	1:B:116:ALA:HB2	1.95	0.48
1:B:606:LYS:HB2	1:B:672:PHE:CZ	2.48	0.48
1:B:621:TYR:CD2	1:B:676:LYS:CB	2.96	0.48
1:B:769:HIS:HB3	1:B:772:GLN:HB2	1.95	0.48
1:A:194:GLY:HA3	1:A:244:ARG:HD2	1.94	0.48
1:A:310:LEU:HD22	1:A:310:LEU:N	2.29	0.48
1:B:125:LEU:HD21	1:B:155:LEU:CD1	2.40	0.48
1:B:133:PHE:CD2	1:B:136:ILE:CG1	2.96	0.48
1:B:361:LYS:HE2	1:B:391:TRP:HE1	1.76	0.48
1:B:397:HIS:CD2	1:B:594:ILE:HG22	2.47	0.48
1:B:611:GLY:HA2	1:B:617:THR:CG2	2.41	0.48
1:B:684:GLU:C	1:B:687:PRO:HD2	2.39	0.48
1:A:615:THR:OG1	1:A:702:ILE:HB	2.14	0.48
1:B:606:LYS:HG3	1:B:696:LYS:HZ2	1.78	0.48
1:B:613:GLN:NE2	1:B:750:ARG:HH12	2.11	0.48
1:B:619:ALA:CB	1:B:829:LEU:HB3	2.41	0.48
1:A:115:ILE:O	1:A:117:PRO:HD3	2.13	0.48
1:A:121:ASP:HA	1:A:151:ASN:ND2	2.27	0.48
1:A:225:TRP:CZ3	1:A:290:HIS:NE2	2.82	0.48
1:A:387:PHE:HB2	1:A:428:ALA:HA	1.94	0.48
1:B:417:VAL:HG22	1:B:423:THR:HG21	1.94	0.48
1:B:599:LYS:HA	1:B:603:ARG:HH22	1.76	0.48
1:B:621:TYR:CZ	1:B:632:SER:HB2	2.48	0.48
1:B:636:SER:OG	1:B:639:THR:HB	2.14	0.48
1:A:109:PHE:CE2	1:A:306:LEU:HB3	2.49	0.48
1:A:398:LEU:HD13	1:A:398:LEU:O	2.13	0.48
1:A:495:TYR:HA	1:A:498:TYR:CE2	2.49	0.48
1:A:711:TYR:CD2	1:A:840:MET:CE	2.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:LEU:HD11	1:B:228:PHE:HD1	1.79	0.48
1:B:358:TYR:CZ	1:B:416:ALA:HB2	2.49	0.48
1:B:681:PHE:HZ	1:B:761:ILE:HG13	1.78	0.48
1:B:840:MET:HE2	1:B:845:ARG:CA	2.44	0.48
1:B:868:GLN:NE2	1:B:869:THR:H	2.12	0.48
1:A:220:LEU:HD22	1:A:220:LEU:H	1.79	0.48
1:A:494:PHE:HD2	1:A:494:PHE:HA	1.51	0.48
1:A:733:VAL:HA	1:A:744:LEU:HD11	1.95	0.48
1:A:856:ASN:O	1:A:874:LEU:HD11	2.13	0.48
1:B:356:LEU:HD13	1:B:377:LEU:HD23	1.95	0.48
1:B:363:PHE:CE1	1:B:364:HIS:HB2	2.49	0.48
1:B:710:ALA:HB1	1:B:730:PHE:HZ	1.79	0.48
1:B:740:ALA:HB1	1:B:744:LEU:CD2	2.44	0.48
1:A:127:ASP:C	1:A:128:LYS:HG2	2.38	0.48
1:A:453:ILE:HG22	1:A:455:VAL:O	2.14	0.48
1:A:617:THR:CA	1:A:702:ILE:HD12	2.44	0.48
1:B:338:LEU:CD1	1:B:354:PHE:CE2	2.96	0.48
1:B:465:LYS:HE3	1:B:465:LYS:N	2.15	0.48
1:B:471:ARG:HB3	1:B:577:GLU:CD	2.39	0.48
1:A:388:PRO:HB2	1:A:412:ASN:ND2	2.28	0.47
1:A:415:PHE:CZ	1:A:419:HIS:NE2	2.81	0.47
1:A:571:PHE:CD1	1:A:578:LYS:CA	2.96	0.47
1:B:125:LEU:CD2	1:B:158:TYR:CD1	2.96	0.47
1:B:437:TYR:HA	1:B:438:PRO:C	2.39	0.47
1:B:439:VAL:HG13	1:B:444:TYR:HE2	1.76	0.47
1:B:868:GLN:NE2	1:B:869:THR:HG22	2.20	0.47
1:A:182:LEU:HD12	1:A:183:LYS:H	1.79	0.47
1:A:388:PRO:HD2	1:A:428:ALA:HB2	1.94	0.47
1:A:409:MET:CB	1:A:450:VAL:HG11	2.43	0.47
1:B:277:GLN:NE2	1:B:300:PHE:HE1	2.11	0.47
1:B:391:TRP:HH2	1:B:415:PHE:CB	2.20	0.47
1:B:709:ARG:HH11	1:B:754:PRO:HB2	1.78	0.47
1:B:769:HIS:O	1:B:772:GLN:HB3	2.14	0.47
1:A:329:ARG:HA	1:A:329:ARG:NE	2.29	0.47
1:A:464:LEU:HD22	1:A:464:LEU:H	1.78	0.47
1:A:786:ALA:HA	1:A:804:TYR:CB	2.43	0.47
1:B:328:THR:HB	1:B:531:SER:HB3	1.95	0.47
1:B:395:GLN:HG2	1:B:432:HIS:HB3	1.96	0.47
1:B:769:HIS:CD2	1:B:771:ASN:HB3	2.46	0.47
1:B:814:LYS:HG3	1:B:818:CYS:SG	2.55	0.47
1:A:196:LYS:HA	1:A:220:LEU:HD22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:SER:OG	1:A:260:ALA:HB2	2.15	0.47
1:A:377:LEU:CD2	1:A:386:TRP:CH2	2.98	0.47
1:A:409:MET:HG2	1:A:451:TRP:HE1	1.79	0.47
1:A:471:ARG:HG2	1:A:471:ARG:NH2	2.29	0.47
1:A:711:TYR:CD2	1:A:840:MET:HE2	2.49	0.47
1:A:785:PRO:CB	1:A:808:LEU:HD13	2.43	0.47
1:B:187:LEU:HD13	1:B:188:PHE:N	2.30	0.47
1:B:378:LEU:CD2	1:B:421:ILE:HG23	2.45	0.47
1:B:384:PHE:N	1:B:384:PHE:CD2	2.83	0.47
1:B:624:LEU:HA	1:B:789:MET:HE1	1.96	0.47
1:B:768:TYR:HB2	1:B:773:ILE:CD1	2.42	0.47
1:A:173:ASN:HB2	1:A:176:SER:CB	2.45	0.47
1:A:201:ASN:HD21	1:A:203:LYS:HB2	1.80	0.47
1:A:598:GLU:HG2	1:A:603:ARG:NH2	2.28	0.47
1:A:606:LYS:CD	1:A:672:PHE:CE2	2.96	0.47
1:B:396:PRO:HB3	1:B:405:LEU:HD22	1.97	0.47
1:B:436:VAL:O	1:B:439:VAL:HA	2.13	0.47
1:A:148:ASP:OD2	1:B:128:LYS:HG3	2.15	0.47
1:A:182:LEU:CD2	1:A:185:PHE:HD2	2.26	0.47
1:A:302:THR:CG2	1:A:305:ARG:HB2	2.45	0.47
1:A:348:HIS:O	1:A:349:ILE:HD13	2.14	0.47
1:A:754:PRO:C	1:A:756:TRP:H	2.20	0.47
1:B:160:VAL:HG22	1:B:274:ASP:O	2.14	0.47
1:B:314:ILE:HD12	1:B:349:ILE:CD1	2.45	0.47
1:B:362:PHE:O	1:B:362:PHE:HD1	1.98	0.47
1:B:386:TRP:CE3	1:B:421:ILE:HD12	2.49	0.47
1:B:570:TYR:CE1	1:B:577:GLU:CG	2.97	0.47
1:A:90:GLU:HB3	1:A:140:ASN:OD1	2.15	0.47
1:A:178:LEU:O	1:A:190:HIS:HA	2.14	0.47
1:A:321:ILE:O	1:A:323:VAL:HG23	2.14	0.47
1:A:610:ILE:O	1:A:681:PHE:HB2	2.15	0.47
1:A:624:LEU:HG	1:A:789:MET:HE1	1.97	0.47
1:A:694:LEU:CB	1:A:697:ALA:HB3	2.44	0.47
1:B:313:TYR:CG	1:B:566:LEU:HD11	2.50	0.47
1:B:332:VAL:CG2	1:B:372:ALA:HB1	2.45	0.47
1:B:390:MET:HE2	1:B:408:GLN:C	2.40	0.47
1:B:396:PRO:CG	1:B:443:LEU:HD13	2.44	0.47
1:B:417:VAL:HG22	1:B:423:THR:CG2	2.44	0.47
1:B:571:PHE:CD1	1:B:577:GLU:CB	2.97	0.47
1:B:625:GLY:HA2	1:B:674:PHE:HZ	1.76	0.47
1:B:715:GLN:HE22	1:B:838:PRO:HD2	1.75	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:ASP:OD1	1:B:725:ALA:HB3	2.15	0.47
1:B:793:GLN:O	1:B:798:VAL:HG12	2.15	0.47
1:B:860:SER:HB3	1:B:878:LEU:HD11	1.96	0.47
1:B:870:LEU:H	1:B:875:ARG:HH21	1.63	0.47
1:A:460:GLU:CD	1:A:461:TYR:HE2	2.22	0.47
1:A:530:LEU:HD23	1:A:530:LEU:C	2.39	0.47
1:A:683:SER:O	1:A:687:PRO:HD3	2.15	0.47
1:A:711:TYR:CE1	1:A:837:TYR:HD2	2.32	0.47
1:A:785:PRO:CG	1:A:808:LEU:HD13	2.45	0.47
1:B:181:GLN:HE21	1:B:186:PRO:CA	2.22	0.47
1:B:223:GLU:OE1	1:B:223:GLU:HA	2.15	0.47
1:B:388:PRO:HD2	1:B:427:TYR:O	2.14	0.47
1:B:492:THR:HG22	1:B:494:PHE:O	2.15	0.47
1:B:590:ARG:O	1:B:594:ILE:HG13	2.15	0.47
1:A:381:VAL:HA	1:A:386:TRP:NE1	2.25	0.47
1:A:460:GLU:C	1:A:461:TYR:HD2	2.22	0.47
1:A:578:LYS:O	1:A:580:PRO:HD3	2.15	0.47
1:A:634:TYR:N	1:A:634:TYR:CD2	2.81	0.47
1:B:248:SER:CB	1:B:252:LEU:HD12	2.44	0.47
1:B:249:ILE:HG23	1:B:250:PRO:HD2	1.96	0.47
1:B:514:LEU:CD1	1:B:526:PHE:CE1	2.98	0.47
1:B:562:PRO:HB2	1:B:565:GLN:OE1	2.15	0.47
1:B:863:LEU:CD1	1:B:870:LEU:HA	2.45	0.47
1:A:81:THR:HB	1:A:134:ALA:HA	1.96	0.47
1:A:274:ASP:HB3	1:A:276:ILE:HD13	1.97	0.47
1:A:388:PRO:HB2	1:A:412:ASN:HD22	1.80	0.47
1:A:687:PRO:HA	1:A:764:TRP:CH2	2.49	0.47
1:B:397:HIS:HE1	1:B:595:TRP:CD1	2.33	0.47
1:B:605:PRO:HA	1:B:673:TYR:HB2	1.97	0.47
1:B:646:PHE:CD2	1:B:680:TYR:CE2	3.03	0.47
1:A:466:PRO:CB	1:A:468:ARG:HH12	2.28	0.46
1:A:488:LEU:CD1	1:A:529:HIS:HD1	2.28	0.46
1:B:82:ASP:HB3	1:B:83:PRO:HD2	1.95	0.46
1:B:225:TRP:CD2	1:B:283:ASN:HB2	2.50	0.46
1:B:378:LEU:HD22	1:B:419:HIS:HB3	1.97	0.46
1:B:416:ALA:HB1	1:B:421:ILE:HG13	1.97	0.46
1:A:486:CYS:CB	1:A:543:PHE:CZ	2.97	0.46
1:A:603:ARG:HA	1:A:673:TYR:HD2	1.74	0.46
1:A:612:PRO:HB3	1:A:754:PRO:HB3	1.97	0.46
1:A:617:THR:CG2	1:A:702:ILE:HD12	2.45	0.46
1:A:784:GLU:OE1	1:A:784:GLU:HA	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:TRP:CZ2	1:B:599:LYS:CB	2.98	0.46
1:B:687:PRO:CA	1:B:764:TRP:CZ2	2.98	0.46
1:A:207:LEU:CD2	1:A:209:VAL:H	2.28	0.46
1:A:276:ILE:O	1:A:276:ILE:HG12	2.15	0.46
1:A:329:ARG:CZ	1:A:530:LEU:HD22	2.45	0.46
1:A:461:TYR:HD2	1:A:461:TYR:N	2.13	0.46
1:A:691:ALA:CB	1:A:768:TYR:HE2	2.27	0.46
1:A:705:ASN:HA	1:A:873:TRP:CZ3	2.50	0.46
1:A:730:PHE:HE2	1:A:751:CYS:SG	2.38	0.46
1:B:207:LEU:HD11	1:B:238:VAL:HG13	1.97	0.46
1:B:484:GLN:HG3	1:B:517:THR:HG21	1.97	0.46
1:B:690:ALA:O	1:B:694:LEU:HD23	2.15	0.46
1:A:349:ILE:HA	1:A:350:PRO:HD3	1.69	0.46
1:A:495:TYR:HA	1:A:498:TYR:CD2	2.50	0.46
1:A:603:ARG:HD2	1:A:659:MET:HE3	1.96	0.46
1:A:749:ASN:O	1:A:753:VAL:HG23	2.15	0.46
1:B:349:ILE:HD12	1:B:352:PHE:CZ	2.50	0.46
1:B:413:LYS:HB2	1:B:451:TRP:CH2	2.50	0.46
1:B:461:TYR:O	1:B:470:ARG:HB3	2.15	0.46
1:B:635:PRO:CA	1:B:643:ILE:HD13	2.45	0.46
1:B:733:VAL:HG11	1:B:747:LEU:CD2	2.45	0.46
1:A:112:ARG:HB3	1:A:133:PHE:HE1	1.79	0.46
1:A:145:VAL:CB	1:A:183:LYS:HD2	2.31	0.46
1:A:402:GLN:NE2	1:A:445:GLU:HB3	2.30	0.46
1:A:536:ASP:O	1:A:537:ARG:HB2	2.15	0.46
1:A:561:LEU:HB2	1:A:566:LEU:HD13	1.92	0.46
1:A:705:ASN:CG	1:A:873:TRP:HB2	2.40	0.46
1:A:721:ASP:HA	1:A:726:LEU:HD11	1.96	0.46
1:B:201:ASN:HB2	1:B:240:LEU:HD12	1.97	0.46
1:B:386:TRP:CE2	1:B:421:ILE:CG2	2.98	0.46
1:B:465:LYS:HE3	1:B:465:LYS:O	2.15	0.46
1:B:625:GLY:CA	1:B:674:PHE:CZ	2.96	0.46
1:A:626:MET:HE3	1:A:626:MET:CA	2.41	0.46
1:B:86:LEU:HB2	1:B:133:PHE:CG	2.50	0.46
1:B:701:THR:HG21	1:B:761:ILE:HG12	1.97	0.46
1:A:125:LEU:H	1:A:125:LEU:CD2	2.26	0.46
1:B:664:ILE:HA	1:B:665:PRO:HD3	1.66	0.46
1:B:793:GLN:CB	1:B:798:VAL:HG11	2.45	0.46
1:A:378:LEU:CD2	1:A:419:HIS:CD2	2.98	0.46
1:A:461:TYR:HB3	1:A:462:PRO:HA	1.98	0.46
1:A:627:HIS:HE2	1:A:629:ASP:HB2	1.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:SER:CB	1:A:639:THR:HG23	2.46	0.46
1:A:680:TYR:HA	1:A:686:ALA:HB2	1.95	0.46
1:A:814:LYS:HG3	1:A:818:CYS:SG	2.56	0.46
1:B:200:ILE:HD11	1:B:553:TRP:CE3	2.51	0.46
1:B:281:PHE:HE1	1:B:293:VAL:HB	1.80	0.46
1:B:425:MET:HG3	1:B:427:TYR:HB2	1.98	0.46
1:B:505:LEU:HD21	1:B:541:TYR:HE1	1.81	0.46
1:B:716:HIS:HE1	1:B:720:HIS:NE2	2.14	0.46
1:B:776:LEU:HD13	1:B:788:VAL:HG13	1.96	0.46
1:A:488:LEU:HD12	1:A:529:HIS:HD1	1.80	0.46
1:A:645:PHE:CE2	1:A:657:TRP:CZ3	3.02	0.46
1:B:88:PHE:HB3	1:B:116:ALA:CB	2.46	0.46
1:B:604:PHE:HZ	1:B:659:MET:HG3	1.79	0.46
1:B:607:LEU:CG	1:B:796:LEU:HD21	2.45	0.46
1:B:643:ILE:H	1:B:643:ILE:HG12	1.50	0.46
1:A:349:ILE:HD11	1:A:558:LEU:HB2	1.92	0.46
1:A:438:PRO:HD3	1:A:594:ILE:CD1	2.46	0.46
1:B:116:ALA:O	1:B:143:LYS:HD2	2.16	0.46
1:B:133:PHE:CD1	1:B:133:PHE:N	2.81	0.46
1:B:185:PHE:HB3	1:B:187:LEU:H	1.80	0.46
1:B:248:SER:HB3	1:B:252:LEU:HD11	1.98	0.46
1:B:396:PRO:HG2	1:B:431:PRO:HD2	1.98	0.46
1:B:614:LYS:HG2	1:B:713:TRP:HE3	1.81	0.46
1:B:624:LEU:CA	1:B:789:MET:HE1	2.46	0.46
1:B:694:LEU:HD12	1:B:697:ALA:CB	2.20	0.46
1:B:752:LEU:HD22	1:B:851:TYR:CD1	2.49	0.46
1:B:834:GLY:H	1:B:835:ARG:NH2	2.14	0.46
1:A:582:TRP:CD1	1:A:651:TYR:HH	2.34	0.45
1:A:640:PHE:HD1	1:A:640:PHE:HA	1.44	0.45
1:A:756:TRP:HB2	1:A:760:HIS:NE2	2.31	0.45
1:A:786:ALA:HB2	1:A:804:TYR:C	2.41	0.45
1:B:313:TYR:HB2	1:B:566:LEU:HD11	1.97	0.45
1:B:322:PHE:HA	1:B:329:ARG:HH21	1.79	0.45
1:B:363:PHE:CD1	1:B:415:PHE:CE2	3.04	0.45
1:B:645:PHE:CB	1:B:650:ASN:HD22	2.25	0.45
1:B:715:GLN:C	1:B:835:ARG:HD3	2.42	0.45
1:B:764:TRP:O	1:B:773:ILE:HD11	2.16	0.45
1:A:106:SER:CB	1:A:520:LEU:HD13	2.46	0.45
1:A:610:ILE:C	1:A:681:PHE:HB2	2.41	0.45
1:B:79:SER:HB2	1:B:305:ARG:NH1	2.31	0.45
1:B:274:ASP:OD1	1:B:276:ILE:HG23	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:ILE:O	1:B:322:PHE:HB2	2.16	0.45
1:B:378:LEU:HD21	1:B:419:HIS:HB3	1.98	0.45
1:B:390:MET:C	1:B:393:HIS:H	2.23	0.45
1:A:321:ILE:HD12	1:A:530:LEU:HD12	1.98	0.45
1:A:323:VAL:CG1	1:A:362:PHE:HD2	2.20	0.45
1:A:397:HIS:CD2	1:A:594:ILE:CG2	2.99	0.45
1:A:447:TRP:O	1:A:453:ILE:HD12	2.16	0.45
1:A:840:MET:HG2	1:A:841:ASP:N	2.31	0.45
1:B:200:ILE:HD11	1:B:553:TRP:HE3	1.81	0.45
1:B:362:PHE:O	1:B:365:THR:HB	2.16	0.45
1:B:386:TRP:CE2	1:B:421:ILE:HG22	2.51	0.45
1:B:399:PHE:HD2	1:B:405:LEU:HD23	1.81	0.45
1:B:603:ARG:HE	1:B:665:PRO:CD	2.29	0.45
1:A:207:LEU:CB	1:A:210:THR:HG23	2.46	0.45
1:B:187:LEU:HD13	1:B:187:LEU:C	2.42	0.45
1:B:463:HIS:HB2	1:B:465:LYS:O	2.16	0.45
1:B:598:GLU:HG2	1:B:599:LYS:N	2.32	0.45
1:B:603:ARG:O	1:B:673:TYR:HD2	1.99	0.45
1:B:627:HIS:HD2	1:B:802:ILE:CG1	2.29	0.45
1:A:210:THR:HG21	1:A:554:THR:HA	1.97	0.45
1:A:466:PRO:HB2	1:A:468:ARG:HH12	1.81	0.45
1:A:536:ASP:CB	1:A:538:LEU:HG	2.46	0.45
1:A:600:THR:H	1:A:603:ARG:HE	1.65	0.45
1:A:624:LEU:HD23	1:A:630:LEU:CD1	2.46	0.45
1:A:664:ILE:O	1:A:664:ILE:HG13	2.16	0.45
1:A:810:PHE:O	1:A:812:PRO:HD3	2.16	0.45
1:A:814:LYS:HD2	1:A:828:CYS:CB	2.46	0.45
1:B:133:PHE:CE2	1:B:136:ILE:CD1	2.95	0.45
1:B:174:GLU:CD	1:B:174:GLU:H	2.24	0.45
1:B:313:TYR:HB3	1:B:566:LEU:CD1	2.46	0.45
1:B:598:GLU:O	1:B:600:THR:HG23	2.16	0.45
1:B:633:ASN:CA	1:B:662:PHE:HZ	2.23	0.45
1:A:117:PRO:CB	1:A:120:GLY:HA3	2.47	0.45
1:A:391:TRP:HZ3	1:A:411:LEU:O	1.98	0.45
1:B:117:PRO:CB	1:B:120:GLY:H	2.21	0.45
1:B:325:LYS:N	1:B:328:THR:HG21	2.29	0.45
1:B:495:TYR:HD1	1:B:495:TYR:HA	1.38	0.45
1:B:561:LEU:CD1	1:B:566:LEU:HD12	2.28	0.45
1:A:187:LEU:HD21	1:A:228:PHE:HB3	1.99	0.45
1:A:394:MET:SD	1:A:405:LEU:HD21	2.57	0.45
1:A:489:PHE:HD2	1:A:489:PHE:HA	1.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:SER:HB2	1:B:305:ARG:HH11	1.82	0.45
1:B:387:PHE:HB3	1:B:427:TYR:HB3	1.99	0.45
1:B:498:TYR:HA	1:B:499:PRO:HD3	1.67	0.45
1:B:508:ILE:C	1:B:512:GLY:HA3	2.41	0.45
1:B:733:VAL:CG1	1:B:747:LEU:HG	2.38	0.45
1:B:793:GLN:HE22	1:B:802:ILE:N	2.10	0.45
1:A:133:PHE:CD2	1:A:133:PHE:N	2.85	0.45
1:A:486:CYS:HA	1:A:514:LEU:CD2	2.46	0.45
1:A:617:THR:N	1:A:702:ILE:HD12	2.32	0.45
1:B:249:ILE:HA	1:B:250:PRO:HD3	1.69	0.45
1:B:283:ASN:CG	1:B:284:ASN:H	2.25	0.45
1:B:285:LEU:HD11	1:B:291:LYS:CA	2.38	0.45
1:B:345:LEU:HB3	1:B:352:PHE:CE2	2.52	0.45
1:B:582:TRP:NE1	1:B:655:ILE:CD1	2.80	0.45
1:B:703:LEU:HD11	1:B:761:ILE:HD11	1.96	0.45
1:B:774:LEU:HB2	1:B:795:PHE:CG	2.51	0.45
1:A:454:ARG:O	1:A:478:ILE:HA	2.17	0.45
1:A:703:LEU:HD13	1:A:859:LEU:HD11	1.98	0.45
1:A:839:GLU:HG2	1:A:840:MET:N	2.31	0.45
1:B:135:LEU:CD1	1:B:301:LEU:HB2	2.47	0.45
1:B:310:LEU:HD13	1:B:556:LEU:CA	2.44	0.45
1:B:730:PHE:HE2	1:B:751:CYS:SG	2.14	0.45
1:A:623:PHE:CZ	1:A:808:LEU:CD2	3.00	0.45
1:A:774:LEU:HD22	1:A:795:PHE:HB2	1.95	0.45
1:B:103:ILE:HD11	1:B:285:LEU:HD21	1.99	0.45
1:B:285:LEU:CG	1:B:291:LYS:HG2	2.46	0.45
1:A:462:PRO:CD	1:A:471:ARG:H	2.30	0.44
1:A:561:LEU:HD12	1:A:562:PRO:O	2.17	0.44
1:A:610:ILE:HD12	1:A:681:PHE:HA	1.98	0.44
1:A:717:GLN:HB3	1:A:725:ALA:CB	2.48	0.44
1:A:740:ALA:HB1	1:A:744:LEU:HG	1.99	0.44
1:B:437:TYR:CD2	1:B:438:PRO:HA	2.52	0.44
1:B:856:ASN:HB3	1:B:874:LEU:HD13	1.99	0.44
1:A:109:PHE:HD2	1:A:109:PHE:HA	1.54	0.44
1:A:112:ARG:HB3	1:A:133:PHE:CE1	2.52	0.44
1:A:117:PRO:HB2	1:A:120:GLY:HA3	2.00	0.44
1:A:425:MET:HG2	1:A:427:TYR:HB2	1.99	0.44
1:A:474:ILE:HG13	1:A:571:PHE:CE1	2.51	0.44
1:A:573:ILE:C	1:A:574:PHE:HD2	2.25	0.44
1:A:624:LEU:CD2	1:A:630:LEU:CD1	2.95	0.44
1:B:332:VAL:CG2	1:B:372:ALA:CB	2.95	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:HIS:HA	1:B:440:HIS:CE1	2.53	0.44
1:A:196:LYS:CA	1:A:220:LEU:HD23	2.46	0.44
1:A:330:MET:HG3	1:A:334:ASP:HB2	2.00	0.44
1:A:466:PRO:HB2	1:A:468:ARG:NH1	2.33	0.44
1:A:599:LYS:CD	1:A:599:LYS:H	2.30	0.44
1:A:713:TRP:NE1	1:A:750:ARG:HB3	2.33	0.44
1:A:722:ASP:HA	1:A:723:PRO:HD3	1.83	0.44
1:A:789:MET:HE2	1:A:804:TYR:CE1	2.53	0.44
1:A:856:ASN:HB3	1:A:874:LEU:CD1	2.48	0.44
1:A:868:GLN:HA	1:A:868:GLN:HE21	1.81	0.44
1:B:173:ASN:HB3	1:B:176:SER:OG	2.18	0.44
1:B:562:PRO:HA	1:B:563:PRO:HD3	1.84	0.44
1:B:753:VAL:HG12	1:B:760:HIS:NE2	2.32	0.44
1:A:429:VAL:HG22	1:A:430:ALA:N	2.32	0.44
1:B:818:CYS:SG	1:B:828:CYS:HA	2.58	0.44
1:A:206:LEU:CG	1:A:207:LEU:N	2.80	0.44
1:A:602:ASP:HB2	1:A:670:SER:HB2	2.00	0.44
1:B:381:VAL:CG1	1:B:421:ILE:HA	2.48	0.44
1:B:680:TYR:CE2	1:B:686:ALA:HB1	2.52	0.44
1:A:205:PRO:N	1:A:206:LEU:CA	2.80	0.44
1:A:578:LYS:NZ	1:A:578:LYS:HB3	2.32	0.44
1:A:704:ILE:C	1:A:873:TRP:CE2	2.95	0.44
1:B:310:LEU:HD13	1:B:557:ARG:N	2.32	0.44
1:B:627:HIS:HE1	1:B:629:ASP:HB3	1.80	0.44
1:A:145:VAL:HB	1:A:183:LYS:NZ	2.32	0.44
1:A:643:ILE:H	1:A:643:ILE:CD1	2.30	0.44
1:B:394:MET:HG2	1:B:398:LEU:HD12	1.99	0.44
1:B:461:TYR:C	1:B:461:TYR:CD2	2.92	0.44
1:B:586:CYS:HA	1:B:592:LYS:HB2	2.00	0.44
1:B:863:LEU:HD12	1:B:871:PRO:HD3	1.98	0.44
1:B:870:LEU:HD22	1:B:874:LEU:HD23	1.99	0.44
1:A:225:TRP:CH2	1:A:290:HIS:NE2	2.86	0.44
1:A:395:GLN:HG2	1:A:434:SER:OG	2.18	0.44
1:A:733:VAL:HG13	1:A:744:LEU:CD1	2.48	0.44
1:B:166:ILE:HG13	1:B:276:ILE:HD12	2.00	0.44
1:B:166:ILE:HD12	1:B:276:ILE:CD1	2.48	0.44
1:B:248:SER:CB	1:B:252:LEU:CD1	2.96	0.44
1:B:323:VAL:HG12	1:B:324:GLY:N	2.33	0.44
1:B:348:HIS:CG	1:B:547:VAL:CG1	3.01	0.44
1:B:586:CYS:SG	1:B:592:LYS:HE3	2.58	0.44
1:B:736:ALA:CB	1:B:744:LEU:HD21	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ASP:HB3	1:A:83:PRO:HD2	2.00	0.43
1:A:84:LEU:O	1:A:133:PHE:HB3	2.18	0.43
1:A:136:ILE:HG13	1:A:164:VAL:CG1	2.45	0.43
1:A:170:PHE:HD2	1:A:226:THR:HG1	1.65	0.43
1:A:386:TRP:CB	1:A:421:ILE:HG21	2.46	0.43
1:A:409:MET:HB3	1:A:450:VAL:HG11	1.99	0.43
1:A:537:ARG:CB	1:A:537:ARG:CZ	2.95	0.43
1:A:863:LEU:HD12	1:A:871:PRO:HD3	1.98	0.43
1:B:135:LEU:CD1	1:B:301:LEU:CB	2.96	0.43
1:B:330:MET:HG3	1:B:530:LEU:HD12	1.95	0.43
1:B:366:GLY:HA3	1:B:370:GLU:HB2	2.00	0.43
1:B:786:ALA:CB	1:B:804:TYR:CB	2.96	0.43
1:B:789:MET:HG3	1:B:804:TYR:CE1	2.53	0.43
1:A:397:HIS:HB2	1:A:440:HIS:CE1	2.54	0.43
1:A:399:PHE:HD1	1:A:399:PHE:HA	1.35	0.43
1:A:460:GLU:HG3	1:A:464:LEU:CD1	2.47	0.43
1:A:573:ILE:HG22	1:A:574:PHE:CE2	2.53	0.43
1:A:603:ARG:CA	1:A:673:TYR:HD2	2.32	0.43
1:A:603:ARG:CB	1:A:662:PHE:CE1	3.00	0.43
1:A:608:LEU:HD12	1:A:694:LEU:HD11	2.00	0.43
1:A:786:ALA:HB1	1:A:805:HIS:N	2.31	0.43
1:A:793:GLN:HE22	1:A:802:ILE:H	1.66	0.43
1:A:869:THR:HB	1:A:875:ARG:HH21	1.82	0.43
1:B:413:LYS:HB2	1:B:451:TRP:CZ2	2.53	0.43
1:B:530:LEU:O	1:B:533:TYR:HB2	2.18	0.43
1:B:585:PRO:HB2	1:B:595:TRP:CE3	2.53	0.43
1:B:605:PRO:CB	1:B:674:PHE:HA	2.45	0.43
1:B:640:PHE:CG	1:B:641:GLU:N	2.84	0.43
1:B:646:PHE:HD1	1:B:646:PHE:HA	1.41	0.43
1:A:211:ARG:HB2	1:A:212:PRO:HD2	2.01	0.43
1:A:575:SER:HA	1:A:578:LYS:NZ	2.34	0.43
1:A:749:ASN:CG	1:A:753:VAL:HG21	2.43	0.43
1:A:765:LEU:HD22	1:A:862:LEU:CD1	2.48	0.43
1:A:799:THR:HG23	1:A:800:ASN:H	1.83	0.43
1:B:703:LEU:HD22	1:B:757:TYR:CB	2.48	0.43
1:A:381:VAL:CA	1:A:386:TRP:HE1	2.27	0.43
1:A:614:LYS:CD	1:A:833:LYS:CB	2.97	0.43
1:A:621:TYR:CD2	1:A:676:LYS:HB2	2.53	0.43
1:B:88:PHE:CZ	1:B:123:PRO:HD2	2.52	0.43
1:B:554:THR:HB	1:B:556:LEU:CD2	2.47	0.43
1:A:709:ARG:HH11	1:A:754:PRO:HB2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:HB2	1:B:128:LYS:NZ	2.33	0.43
1:B:381:VAL:HG13	1:B:422:PRO:CD	2.46	0.43
1:B:390:MET:CG	1:B:408:GLN:CB	2.93	0.43
1:B:627:HIS:HA	1:B:628:PRO:HD3	1.79	0.43
1:A:328:THR:CG2	1:A:531:SER:CB	2.96	0.43
1:A:604:PHE:CE2	1:A:659:MET:HG2	2.53	0.43
1:B:187:LEU:HD22	1:B:188:PHE:N	2.32	0.43
1:B:196:LYS:HD3	1:B:244:ARG:HD2	2.01	0.43
1:B:201:ASN:HD21	1:B:203:LYS:HD3	1.83	0.43
1:B:276:ILE:HD11	1:B:278:ARG:NH2	2.34	0.43
1:B:287:PHE:CD1	1:B:288:TRP:N	2.87	0.43
1:B:474:ILE:HD11	1:B:571:PHE:CB	2.48	0.43
1:B:715:GLN:HG3	1:B:837:TYR:HD1	1.84	0.43
1:B:833:LYS:NZ	1:B:833:LYS:HB3	2.33	0.43
1:A:185:PHE:HB3	1:A:235:TYR:OH	2.18	0.43
1:A:381:VAL:CG2	1:A:386:TRP:NE1	2.81	0.43
1:A:610:ILE:HB	1:A:681:PHE:N	2.34	0.43
1:A:699:VAL:HG21	1:A:764:TRP:HZ3	1.77	0.43
1:A:856:ASN:C	1:A:878:LEU:HD21	2.44	0.43
1:B:330:MET:HE3	1:B:335:VAL:CA	2.48	0.43
1:B:393:HIS:CE1	1:B:432:HIS:HA	2.54	0.43
1:B:523:ILE:HD12	1:B:570:TYR:HB2	2.01	0.43
1:B:714:TYR:CZ	1:B:718:ARG:HD2	2.53	0.43
1:B:740:ALA:HB1	1:B:744:LEU:HG	2.00	0.43
1:A:185:PHE:HA	1:A:186:PRO:HD3	1.74	0.43
1:A:196:LYS:HA	1:A:220:LEU:HD23	1.98	0.43
1:A:206:LEU:HG	1:A:207:LEU:N	2.33	0.43
1:A:345:LEU:HA	1:A:348:HIS:CD2	2.47	0.43
1:A:438:PRO:HB2	1:A:595:TRP:HE1	1.84	0.43
1:A:799:THR:CG2	1:A:800:ASN:N	2.82	0.43
1:B:213:SER:CB	1:B:553:TRP:CE3	3.02	0.43
1:B:277:GLN:NE2	1:B:300:PHE:CE1	2.87	0.43
1:B:387:PHE:CE2	1:B:429:VAL:CB	3.00	0.43
1:B:717:GLN:CB	1:B:725:ALA:HB2	2.48	0.43
1:B:753:VAL:HB	1:B:754:PRO:CD	2.42	0.43
1:A:495:TYR:H	1:A:495:TYR:HD1	1.67	0.43
1:A:617:THR:HA	1:A:702:ILE:HD12	2.00	0.43
1:A:643:ILE:HG22	1:A:645:PHE:N	2.34	0.43
1:A:740:ALA:CB	1:A:744:LEU:CD2	2.95	0.43
1:B:88:PHE:HD1	1:B:116:ALA:HB2	1.71	0.43
1:B:109:PHE:CD2	1:B:306:LEU:HD23	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PHE:HB2	1:B:135:LEU:O	2.19	0.43
1:B:211:ARG:HG2	1:B:555:ASN:OD1	2.19	0.43
1:B:339:PHE:HE2	1:B:383:GLU:OE2	2.02	0.43
1:B:462:PRO:HD2	1:B:463:HIS:H	1.84	0.43
1:B:479:MET:HG2	1:B:571:PHE:CD2	2.53	0.43
1:B:814:LYS:CG	1:B:828:CYS:SG	3.07	0.43
1:B:829:LEU:HD12	1:B:829:LEU:O	2.19	0.43
1:A:201:ASN:OD1	1:A:238:VAL:HA	2.19	0.43
1:A:207:LEU:HD22	1:A:210:THR:H	1.84	0.43
1:A:214:GLU:HG3	1:A:215:VAL:H	1.84	0.43
1:A:396:PRO:HD2	1:A:435:GLY:CA	2.47	0.43
1:A:396:PRO:HA	1:A:405:LEU:HD11	2.01	0.43
1:A:613:GLN:HG3	1:A:750:ARG:NH2	2.33	0.43
1:A:734:ILE:HD12	1:A:847:PHE:CD1	2.54	0.43
1:A:740:ALA:CA	1:A:744:LEU:HD23	2.48	0.43
1:B:140:ASN:OD1	1:B:142:LEU:HB2	2.19	0.43
1:B:461:TYR:HB2	1:B:462:PRO:HA	2.00	0.43
1:B:662:PHE:HD1	1:B:662:PHE:HA	1.43	0.43
1:B:699:VAL:HG21	1:B:768:TYR:CD1	2.54	0.43
1:A:387:PHE:CD2	1:A:429:VAL:HG12	2.54	0.42
1:A:603:ARG:O	1:A:673:TYR:HD2	2.02	0.42
1:A:625:GLY:N	1:A:674:PHE:HZ	2.16	0.42
1:A:776:LEU:HD13	1:A:788:VAL:CG1	2.49	0.42
1:B:225:TRP:CZ3	1:B:283:ASN:HB2	2.51	0.42
1:B:581:LEU:N	1:B:581:LEU:CD1	2.82	0.42
1:B:821:LEU:HD11	1:B:827:LYS:HB2	2.01	0.42
1:A:356:LEU:HD13	1:A:377:LEU:CD2	2.49	0.42
1:A:381:VAL:CG1	1:A:382:LYS:N	2.82	0.42
1:A:474:ILE:CD1	1:A:571:PHE:CG	2.96	0.42
1:A:646:PHE:HB2	1:A:680:TYR:HE1	1.82	0.42
1:A:754:PRO:O	1:A:757:TYR:CE1	2.72	0.42
1:A:818:CYS:SG	1:A:828:CYS:CB	3.07	0.42
1:A:831:LYS:CE	1:A:832:SER:HA	2.48	0.42
1:B:96:LEU:HD21	1:B:169:PHE:HB2	2.01	0.42
1:B:388:PRO:HB2	1:B:412:ASN:HD22	1.83	0.42
1:B:388:PRO:CG	1:B:451:TRP:CZ2	3.01	0.42
1:B:604:PHE:CZ	1:B:655:ILE:HG23	2.54	0.42
1:B:871:PRO:HD2	1:B:874:LEU:HD23	2.01	0.42
1:A:320:ASP:O	1:A:323:VAL:HB	2.19	0.42
1:A:361:LYS:N	1:A:391:TRP:NE1	2.67	0.42
1:A:604:PHE:CZ	1:A:655:ILE:HG23	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:ILE:CG2	1:A:709:ARG:HB2	2.49	0.42
1:A:761:ILE:CG2	1:A:862:LEU:HD21	2.49	0.42
1:A:781:LEU:HA	1:A:788:VAL:CG2	2.50	0.42
1:A:831:LYS:CD	1:A:832:SER:N	2.83	0.42
1:B:167:ILE:HD11	1:B:297:ALA:C	2.45	0.42
1:B:320:ASP:O	1:B:323:VAL:HB	2.19	0.42
1:B:386:TRP:CZ2	1:B:421:ILE:CG2	3.02	0.42
1:B:604:PHE:HA	1:B:605:PRO:HD3	1.84	0.42
1:A:377:LEU:O	1:A:386:TRP:HZ2	2.02	0.42
1:B:173:ASN:HB3	1:B:176:SER:CB	2.49	0.42
1:B:322:PHE:HE2	1:B:415:PHE:CE1	2.38	0.42
1:B:810:PHE:O	1:B:812:PRO:HD3	2.18	0.42
1:A:108:ARG:HH22	1:A:468:ARG:CD	2.31	0.42
1:A:144:TYR:CE2	1:A:166:ILE:HD13	2.54	0.42
1:A:146:ASN:C	1:A:147:LEU:HD22	2.44	0.42
1:A:205:PRO:HB2	1:A:206:LEU:C	2.44	0.42
1:A:210:THR:HA	1:A:555:ASN:CB	2.49	0.42
1:A:312:ARG:HD3	1:A:522:PRO:HA	2.02	0.42
1:A:816:PHE:CD2	1:A:834:GLY:CA	2.98	0.42
1:B:740:ALA:CB	1:B:744:LEU:CD2	2.95	0.42
1:B:785:PRO:HB2	1:B:808:LEU:HD13	2.01	0.42
1:A:205:PRO:HB3	1:A:208:TYR:HA	2.01	0.42
1:A:469:TYR:HD1	1:A:469:TYR:HA	1.50	0.42
1:A:603:ARG:CD	1:A:659:MET:CE	2.94	0.42
1:A:717:GLN:O	1:A:720:HIS:HB2	2.20	0.42
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.83	0.42
1:B:489:PHE:HD2	1:B:489:PHE:HA	1.57	0.42
1:B:578:LYS:C	1:B:580:PRO:HD3	2.45	0.42
1:B:586:CYS:O	1:B:592:LYS:HB2	2.19	0.42
1:B:609:ILE:HD11	1:B:624:LEU:CD1	2.49	0.42
1:B:612:PRO:HG2	1:B:757:TYR:HE1	1.73	0.42
1:B:619:ALA:HB2	1:B:829:LEU:CD2	2.50	0.42
1:A:119:LYS:HB2	1:B:128:LYS:NZ	2.34	0.42
1:A:206:LEU:CD1	1:A:293:VAL:HG22	2.49	0.42
1:A:498:TYR:HA	1:A:499:PRO:HD3	1.73	0.42
1:A:571:PHE:CD1	1:A:577:GLU:HB2	2.55	0.42
1:A:728:TYR:HD1	1:A:728:TYR:HA	1.66	0.42
1:A:764:TRP:HB3	1:A:773:ILE:CD1	2.50	0.42
1:A:789:MET:CE	1:A:804:TYR:CZ	3.01	0.42
1:B:118:GLY:N	1:B:143:LYS:CD	2.82	0.42
1:B:308:LEU:HA	1:B:309:PRO:HD3	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:MET:SD	1:B:567:ALA:C	3.03	0.42
1:B:597:LYS:HG2	1:B:598:GLU:N	2.34	0.42
1:B:606:LYS:O	1:B:697:ALA:HB1	2.20	0.42
1:B:662:PHE:HA	1:B:663:PRO:HD3	1.72	0.42
1:A:122:MET:HE1	1:A:151:ASN:HB3	2.02	0.42
1:A:486:CYS:CA	1:A:514:LEU:HD22	2.49	0.42
1:A:518:VAL:HG22	1:A:526:PHE:CZ	2.53	0.42
1:A:831:LYS:CE	1:A:832:SER:CA	2.98	0.42
1:B:83:PRO:HG3	1:B:305:ARG:HE	1.84	0.42
1:B:471:ARG:HB2	1:B:577:GLU:OE1	2.19	0.42
1:B:582:TRP:HE1	1:B:655:ILE:HG13	1.84	0.42
1:B:724:VAL:CG2	1:B:743:LYS:HD3	2.49	0.42
1:B:762:GLU:HG2	1:B:862:LEU:HD22	2.02	0.42
1:B:772:GLN:O	1:B:795:PHE:CZ	2.73	0.42
1:A:131:GLY:HA3	1:A:158:TYR:OH	2.19	0.42
1:A:132:ARG:HH11	1:A:132:ARG:HD2	1.73	0.42
1:A:505:LEU:HD23	1:A:538:LEU:HD22	2.00	0.42
1:B:206:LEU:C	1:B:206:LEU:HD13	2.45	0.42
1:B:473:PHE:C	1:B:571:PHE:CZ	2.97	0.42
1:B:576:GLU:HG2	1:B:577:GLU:N	2.34	0.42
1:B:585:PRO:HG2	1:B:595:TRP:CE3	2.55	0.42
1:A:196:LYS:CA	1:A:220:LEU:CD2	2.97	0.42
1:A:209:VAL:HG12	1:A:555:ASN:CB	2.38	0.42
1:A:304:LYS:N	1:A:304:LYS:CD	2.83	0.42
1:A:602:ASP:CB	1:A:670:SER:HB3	2.41	0.42
1:A:785:PRO:CD	1:A:817:TRP:CG	3.03	0.42
1:B:81:THR:HG22	1:B:131:GLY:CA	2.28	0.42
1:B:330:MET:HB3	1:B:334:ASP:HB2	2.02	0.42
1:B:389:HIS:HB3	1:B:393:HIS:CD2	2.48	0.42
1:B:586:CYS:HB3	1:B:592:LYS:HD2	2.02	0.42
1:B:598:GLU:CG	1:B:599:LYS:N	2.83	0.42
1:B:821:LEU:N	1:B:821:LEU:CD1	2.83	0.42
1:A:302:THR:CG2	1:A:305:ARG:H	2.19	0.41
1:A:409:MET:CG	1:A:451:TRP:HE1	2.33	0.41
1:A:730:PHE:CE2	1:A:751:CYS:SG	3.13	0.41
1:A:762:GLU:HG2	1:A:862:LEU:HD13	2.02	0.41
1:B:438:PRO:HG3	1:B:591:HIS:O	2.20	0.41
1:B:606:LYS:HD3	1:B:672:PHE:HA	2.03	0.41
1:B:705:ASN:CA	1:B:873:TRP:CE2	3.03	0.41
1:B:784:GLU:HA	1:B:785:PRO:HD2	1.87	0.41
1:A:363:PHE:CD2	1:A:364:HIS:N	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:ARG:CD	1:A:659:MET:HE2	2.49	0.41
1:B:96:LEU:HG	1:B:139:GLU:CG	2.40	0.41
1:B:288:TRP:CZ2	1:B:549:PHE:HZ	2.38	0.41
1:B:346:ARG:CG	1:B:352:PHE:HB2	2.48	0.41
1:B:366:GLY:HA3	1:B:370:GLU:CB	2.50	0.41
1:B:367:THR:CG2	1:B:368:ASN:H	2.23	0.41
1:B:606:LYS:O	1:B:697:ALA:HA	2.20	0.41
1:B:762:GLU:OE1	1:B:862:LEU:HD13	2.20	0.41
1:B:786:ALA:CB	1:B:804:TYR:HB2	2.50	0.41
1:B:789:MET:HE2	1:B:804:TYR:CZ	2.55	0.41
1:A:397:HIS:CA	1:A:440:HIS:CE1	3.04	0.41
1:A:602:ASP:O	1:A:673:TYR:CD2	2.73	0.41
1:B:310:LEU:HD21	1:B:555:ASN:O	2.20	0.41
1:B:322:PHE:CD2	1:B:363:PHE:HB2	2.55	0.41
1:B:388:PRO:HG3	1:B:451:TRP:CD2	2.54	0.41
1:B:388:PRO:HG3	1:B:451:TRP:CH2	2.55	0.41
1:B:625:GLY:HA2	1:B:674:PHE:CE1	2.54	0.41
1:B:645:PHE:HB2	1:B:650:ASN:ND2	2.26	0.41
1:B:733:VAL:HG21	1:B:747:LEU:HD21	2.00	0.41
1:B:772:GLN:O	1:B:795:PHE:HZ	2.02	0.41
1:B:860:SER:CB	1:B:878:LEU:CD1	2.98	0.41
1:A:138:TYR:CE1	1:A:144:TYR:HA	2.55	0.41
1:A:172:ALA:CB	1:A:224:ASP:HB3	2.50	0.41
1:A:466:PRO:HD2	1:A:469:TYR:HB2	2.01	0.41
1:A:621:TYR:CD2	1:A:674:PHE:HE2	2.38	0.41
1:A:839:GLU:HG3	1:A:845:ARG:HH21	1.85	0.41
1:B:399:PHE:HD1	1:B:399:PHE:HA	1.56	0.41
1:B:466:PRO:HG2	1:B:469:TYR:HB2	1.99	0.41
1:B:595:TRP:CZ2	1:B:599:LYS:HB3	2.55	0.41
1:B:604:PHE:HA	1:B:604:PHE:HD1	1.52	0.41
1:B:627:HIS:HD2	1:B:802:ILE:CD1	2.34	0.41
1:B:704:ILE:CG2	1:B:705:ASN:N	2.83	0.41
1:B:717:GLN:HB3	1:B:725:ALA:CB	2.48	0.41
1:B:835:ARG:H	1:B:835:ARG:NE	2.18	0.41
1:A:302:THR:CG2	1:A:305:ARG:N	2.82	0.41
1:A:419:HIS:HB2	1:A:421:ILE:HG13	2.02	0.41
1:A:509:ILE:HD13	1:A:542:THR:HA	2.02	0.41
1:A:700:LEU:HD11	1:A:792:VAL:HG22	2.03	0.41
1:A:758:ALA:HB2	1:A:859:LEU:HA	2.00	0.41
1:A:831:LYS:HD2	1:A:832:SER:N	2.35	0.41
1:B:184:GLY:O	1:B:185:PHE:HD1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:LEU:O	1:B:348:HIS:HB2	2.21	0.41
1:B:484:GLN:CG	1:B:517:THR:HG21	2.50	0.41
1:B:729:THR:CG2	1:B:730:PHE:N	2.83	0.41
1:B:833:LYS:HA	1:B:835:ARG:HH21	1.83	0.41
1:A:81:THR:CB	1:A:134:ALA:HA	2.51	0.41
1:A:322:PHE:CE1	1:A:374:ASP:HA	2.55	0.41
1:A:391:TRP:CE3	1:A:412:ASN:CA	3.02	0.41
1:A:627:HIS:HA	1:A:628:PRO:HD3	1.78	0.41
1:B:204:SER:CB	1:B:238:VAL:HG22	2.50	0.41
1:B:599:LYS:NZ	1:B:660:GLU:HA	2.35	0.41
1:B:657:TRP:CH2	1:B:661:PHE:CE2	3.07	0.41
1:A:107:SER:HB3	1:A:109:PHE:CE1	2.56	0.41
1:A:108:ARG:HH22	1:A:468:ARG:HD3	1.85	0.41
1:A:684:GLU:C	1:A:687:PRO:HD2	2.44	0.41
1:B:167:ILE:CG1	1:B:301:LEU:HD12	2.51	0.41
1:B:225:TRP:CH2	1:B:287:PHE:CD2	2.99	0.41
1:B:322:PHE:CA	1:B:329:ARG:HH21	2.33	0.41
1:B:365:THR:CG2	1:B:366:GLY:N	2.83	0.41
1:B:617:THR:C	1:B:676:LYS:HD2	2.46	0.41
1:B:621:TYR:HD2	1:B:676:LYS:HB2	1.85	0.41
1:B:866:MET:CG	1:B:868:GLN:CB	2.95	0.41
1:A:225:TRP:CZ2	1:A:287:PHE:HD2	2.39	0.41
1:A:495:TYR:CG	1:A:496:ASN:N	2.88	0.41
1:A:507:LYS:O	1:A:512:GLY:HA3	2.20	0.41
1:A:754:PRO:O	1:A:757:TYR:CD1	2.74	0.41
1:A:786:ALA:CB	1:A:805:HIS:N	2.83	0.41
1:A:816:PHE:CE2	1:A:834:GLY:CA	2.97	0.41
1:A:829:LEU:HD22	1:A:829:LEU:C	2.45	0.41
1:B:182:LEU:HD23	1:B:185:PHE:CD2	2.56	0.41
1:B:396:PRO:O	1:B:405:LEU:HD11	2.20	0.41
1:B:399:PHE:CE2	1:B:404:VAL:CG1	3.03	0.41
1:B:621:TYR:OH	1:B:632:SER:HB2	2.20	0.41
1:B:626:MET:SD	1:B:804:TYR:CE1	3.14	0.41
1:B:781:LEU:HD13	1:B:788:VAL:HG11	2.01	0.41
1:B:781:LEU:HA	1:B:788:VAL:HG21	2.02	0.41
1:A:274:ASP:CB	1:A:278:ARG:HH12	2.34	0.41
1:A:391:TRP:CZ3	1:A:412:ASN:CA	2.95	0.41
1:A:437:TYR:CA	1:A:438:PRO:C	2.93	0.41
1:A:571:PHE:CD1	1:A:578:LYS:N	2.88	0.41
1:A:694:LEU:HB3	1:A:697:ALA:N	2.27	0.41
1:A:709:ARG:NH1	1:A:754:PRO:HB2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:GLN:HE21	1:A:868:GLN:CA	2.34	0.41
1:B:170:PHE:HD1	1:B:170:PHE:HA	1.61	0.41
1:B:310:LEU:CD1	1:B:556:LEU:HA	2.45	0.41
1:B:313:TYR:CE1	1:B:561:LEU:CG	3.03	0.41
1:B:349:ILE:CG1	1:B:558:LEU:HB3	2.51	0.41
1:B:413:LYS:CB	1:B:451:TRP:CH2	3.04	0.41
1:B:454:ARG:HA	1:B:454:ARG:HH11	1.86	0.41
1:B:510:ASN:OD1	1:B:549:PHE:CZ	2.74	0.41
1:B:615:THR:CG2	1:B:702:ILE:CB	2.95	0.41
1:B:633:ASN:H	1:B:633:ASN:HD22	1.68	0.41
1:B:645:PHE:HB2	1:B:650:ASN:CB	2.51	0.41
1:B:646:PHE:HE2	1:B:690:ALA:N	2.19	0.41
1:B:718:ARG:HG2	1:B:725:ALA:O	2.20	0.41
1:B:758:ALA:HB2	1:B:859:LEU:CA	2.51	0.41
1:B:771:ASN:O	1:B:795:PHE:HE2	2.03	0.41
1:B:868:GLN:HE21	1:B:869:THR:H	1.68	0.41
1:A:363:PHE:CG	1:A:364:HIS:N	2.83	0.41
1:A:591:HIS:HA	1:A:594:ILE:HD12	2.03	0.41
1:A:733:VAL:HG13	1:A:744:LEU:HD12	2.02	0.41
1:B:313:TYR:CG	1:B:566:LEU:CD1	3.04	0.41
1:B:339:PHE:CB	1:B:380:TYR:CZ	3.02	0.41
1:B:349:ILE:HG12	1:B:558:LEU:HB3	2.01	0.41
1:B:428:ALA:HB3	1:B:453:ILE:HG12	2.03	0.41
1:B:494:PHE:O	1:B:498:TYR:CD2	2.74	0.41
1:B:586:CYS:HB3	1:B:592:LYS:CE	2.51	0.41
1:B:837:TYR:C	1:B:837:TYR:CD2	2.99	0.41
1:A:234:THR:HG22	1:A:273:HIS:ND1	2.36	0.40
1:A:321:ILE:HG22	1:A:322:PHE:CD1	2.56	0.40
1:A:462:PRO:HG2	1:A:471:ARG:HG2	2.02	0.40
1:A:514:LEU:HD11	1:A:526:PHE:CE1	2.56	0.40
1:A:610:ILE:CD1	1:A:681:PHE:CD2	3.01	0.40
1:A:765:LEU:CD2	1:A:862:LEU:CD1	2.99	0.40
1:A:776:LEU:HD13	1:A:788:VAL:HG13	2.02	0.40
1:A:802:ILE:HG23	1:A:802:ILE:O	2.20	0.40
1:A:837:TYR:CD1	1:A:837:TYR:N	2.89	0.40
1:B:736:ALA:HB2	1:B:744:LEU:HD21	2.03	0.40
1:A:96:LEU:CD2	1:A:139:GLU:HG3	2.52	0.40
1:A:119:LYS:HA	1:B:128:LYS:HZ1	1.85	0.40
1:A:147:LEU:HG	1:A:152:ARG:HD3	2.04	0.40
1:A:183:LYS:O	1:A:183:LYS:HG3	2.20	0.40
1:A:207:LEU:HD13	1:A:210:THR:HG21	1.99	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:TYR:CD2	1:A:384:PHE:CE2	3.10	0.40
1:A:392:SER:O	1:A:393:HIS:HB2	2.21	0.40
1:A:425:MET:HG2	1:A:427:TYR:CB	2.51	0.40
1:A:762:GLU:HG2	1:A:862:LEU:HD22	2.04	0.40
1:B:103:ILE:CD1	1:B:294:PHE:CD1	3.04	0.40
1:B:114:GLU:HG3	1:B:123:PRO:HG3	2.03	0.40
1:B:147:LEU:HB3	1:B:152:ARG:HB2	2.04	0.40
1:B:214:GLU:O	1:B:553:TRP:CH2	2.74	0.40
1:B:220:LEU:HA	1:B:221:PRO:HD3	1.74	0.40
1:B:768:TYR:HB3	1:B:773:ILE:HG13	2.01	0.40
1:A:182:LEU:HD23	1:A:185:PHE:CD2	2.46	0.40
1:A:225:TRP:CE3	1:A:283:ASN:HB2	2.56	0.40
1:A:388:PRO:CD	1:A:428:ALA:HB2	2.51	0.40
1:A:409:MET:HB3	1:A:451:TRP:CD1	2.56	0.40
1:A:618:THR:HB	1:A:833:LYS:CE	2.51	0.40
1:B:211:ARG:HB3	1:B:555:ASN:OD1	2.21	0.40
1:B:313:TYR:CB	1:B:566:LEU:CD1	2.95	0.40
1:B:613:GLN:NE2	1:B:613:GLN:H	2.19	0.40
1:B:635:PRO:HA	1:B:643:ILE:HD13	2.02	0.40
1:A:322:PHE:CD1	1:A:322:PHE:N	2.85	0.40
1:A:390:MET:HB2	1:A:393:HIS:CA	2.51	0.40
1:A:394:MET:SD	1:A:405:LEU:CD2	3.10	0.40
1:A:602:ASP:OD2	1:A:606:LYS:HE3	2.22	0.40
1:B:198:CYS:HB2	1:B:220:LEU:HD11	2.02	0.40
1:B:234:THR:O	1:B:269:ASP:HA	2.21	0.40
1:B:325:LYS:N	1:B:328:THR:CG2	2.85	0.40
1:B:393:HIS:CE1	1:B:432:HIS:H	2.38	0.40
1:A:97:GLY:HA2	1:A:139:GLU:OE1	2.21	0.40
1:A:397:HIS:HA	1:A:440:HIS:CE1	2.56	0.40
1:A:488:LEU:O	1:A:489:PHE:HD2	2.05	0.40
1:A:680:TYR:CA	1:A:686:ALA:CB	2.94	0.40
1:B:103:ILE:HD13	1:B:294:PHE:CD1	2.55	0.40
1:B:292:LEU:CD1	1:B:519:LEU:HD13	2.52	0.40
1:B:642:GLU:C	1:B:644:GLN:HG3	2.46	0.40
1:B:680:TYR:HA	1:B:686:ALA:CB	2.51	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	801/858 (93%)	794 (99%)	5 (1%)	2 (0%)	43	77
1	B	804/858 (94%)	791 (98%)	11 (1%)	2 (0%)	43	77
All	All	1605/1716 (94%)	1585 (99%)	16 (1%)	4 (0%)	44	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	535	ASN
1	B	535	ASN
1	A	640	PHE
1	B	756	TRP

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	705/750 (94%)	664 (94%)	41 (6%)	18	40
1	B	708/750 (94%)	653 (92%)	55 (8%)	11	32
All	All	1413/1500 (94%)	1317 (93%)	96 (7%)	16	37

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	LEU
1	A	93	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	113	THR
1	A	119	LYS
1	A	122	MET
1	A	125	LEU
1	A	132	ARG
1	A	147	LEU
1	A	177	LEU
1	A	211	ARG
1	A	220	LEU
1	A	276	ILE
1	A	308	LEU
1	A	329	ARG
1	A	333	GLU
1	A	352	PHE
1	A	363	PHE
1	A	377	LEU
1	A	391	TRP
1	A	399	PHE
1	A	419	HIS
1	A	453	ILE
1	A	465	LYS
1	A	468	ARG
1	A	469	TYR
1	A	494	PHE
1	A	502	SER
1	A	535	ASN
1	A	561	LEU
1	A	578	LYS
1	A	597	LYS
1	A	604	PHE
1	A	622	LEU
1	A	640	PHE
1	A	675	GLU
1	A	720	HIS
1	A	825	LYS
1	A	829	LEU
1	A	831	LYS
1	A	836	LYS
1	A	850	ASP
1	B	84	LEU
1	B	109	PHE
1	B	113	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	121	ASP
1	B	122	MET
1	B	125	LEU
1	B	128	LYS
1	B	133	PHE
1	B	207	LEU
1	B	219	VAL
1	B	234	THR
1	B	310	LEU
1	B	325	LYS
1	B	331	LYS
1	B	352	PHE
1	B	361	LYS
1	B	362	PHE
1	B	377	LEU
1	B	381	VAL
1	B	390	MET
1	B	399	PHE
1	B	419	HIS
1	B	427	TYR
1	B	436	VAL
1	B	453	ILE
1	B	461	TYR
1	B	465	LYS
1	B	471	ARG
1	B	489	PHE
1	B	495	TYR
1	B	502	SER
1	B	535	ASN
1	B	556	LEU
1	B	577	GLU
1	B	597	LYS
1	B	606	LYS
1	B	613	GLN
1	B	614	LYS
1	B	615	THR
1	B	622	LEU
1	B	633	ASN
1	B	643	ILE
1	B	646	PHE
1	B	651	TYR
1	B	661	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	662	PHE
1	B	669	THR
1	B	675	GLU
1	B	681	PHE
1	B	694	LEU
1	B	771	ASN
1	B	833	LYS
1	B	835	ARG
1	B	837	TYR
1	B	850	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	181	GLN
1	A	232	HIS
1	A	277	GLN
1	A	284	ASN
1	A	342	GLN
1	A	348	HIS
1	A	355	ASN
1	A	389	HIS
1	A	397	HIS
1	A	402	GLN
1	A	412	ASN
1	A	433	HIS
1	A	475	HIS
1	A	521	ASN
1	A	532	ASN
1	A	535	ASN
1	A	551	HIS
1	A	559	GLN
1	A	572	GLN
1	A	583	GLN
1	A	633	ASN
1	A	652	HIS
1	A	717	GLN
1	A	720	HIS
1	A	769	HIS
1	A	805	HIS
1	A	819	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	868	GLN
1	B	98	GLN
1	B	175	ASN
1	B	181	GLN
1	B	201	ASN
1	B	263	HIS
1	B	283	ASN
1	B	284	ASN
1	B	286	ASN
1	B	290	HIS
1	B	348	HIS
1	B	355	ASN
1	B	364	HIS
1	B	389	HIS
1	B	395	GLN
1	B	397	HIS
1	B	400	HIS
1	B	412	ASN
1	B	433	HIS
1	B	476	ASN
1	B	510	ASN
1	B	535	ASN
1	B	613	GLN
1	B	647	ASN
1	B	650	ASN
1	B	715	GLN
1	B	716	HIS
1	B	720	HIS
1	B	769	HIS
1	B	772	GLN
1	B	819	GLN
1	B	855	HIS
1	B	868	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](#)

There are no chain breaks in this entry.

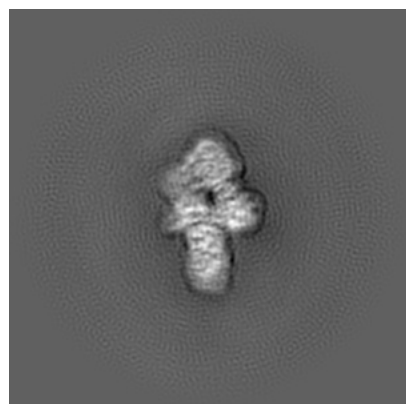
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17349. These allow visual inspection of the internal detail of the map and identification of artifacts.

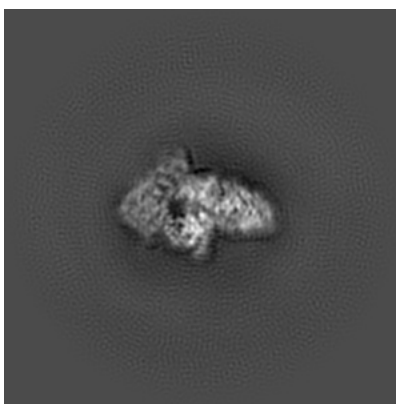
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

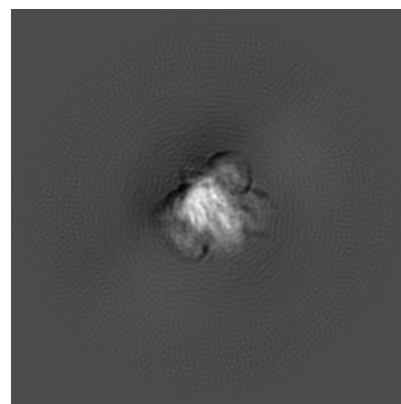
6.1.1 Primary map



X

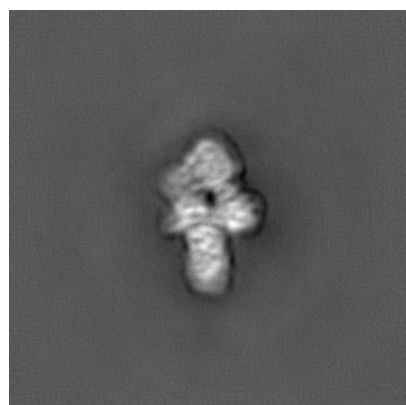


Y

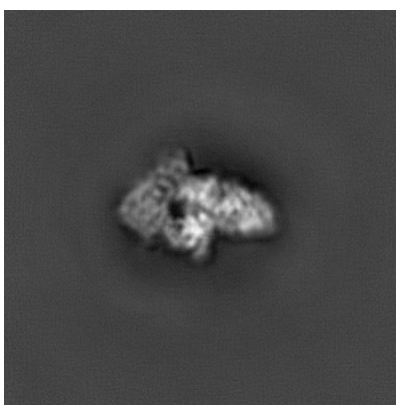


Z

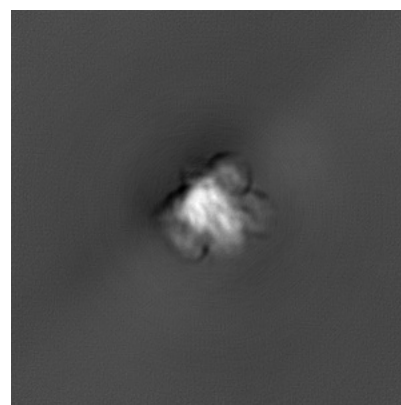
6.1.2 Raw map



X



Y

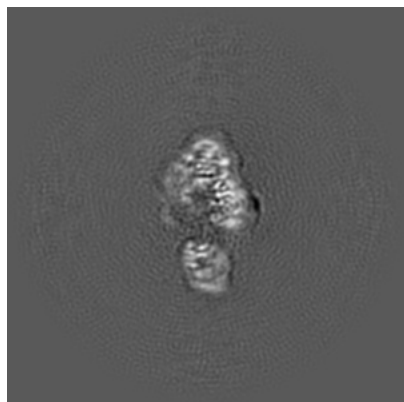


Z

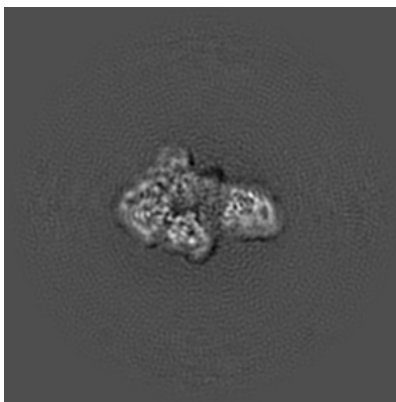
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

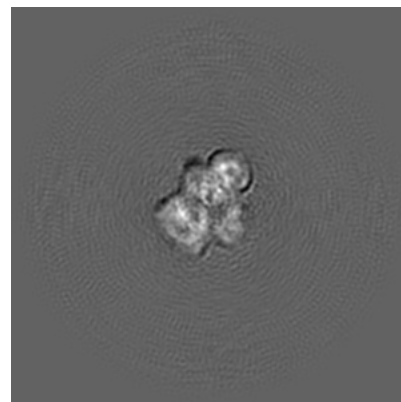
6.2.1 Primary map



X Index: 160

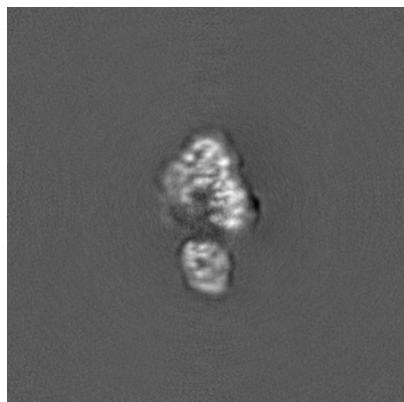


Y Index: 160

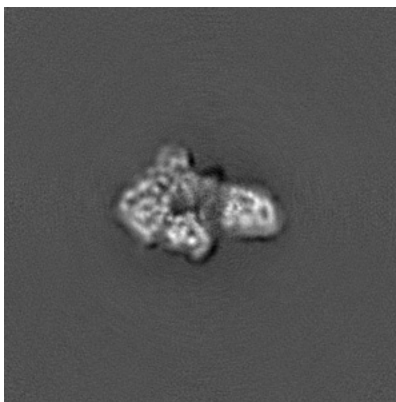


Z Index: 160

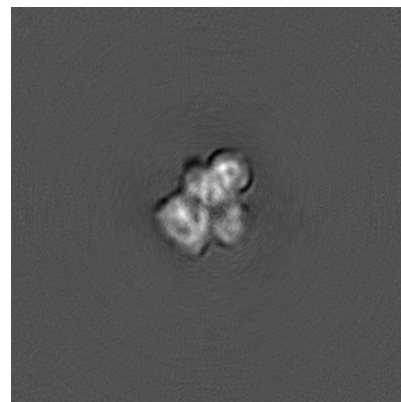
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

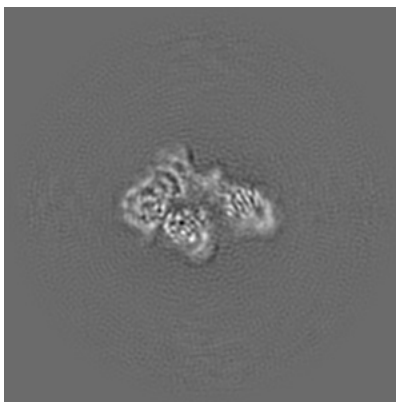
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

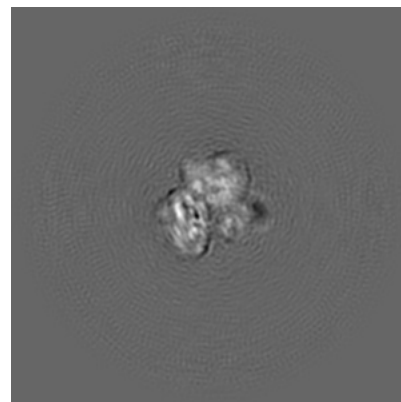
6.3.1 Primary map



X Index: 153

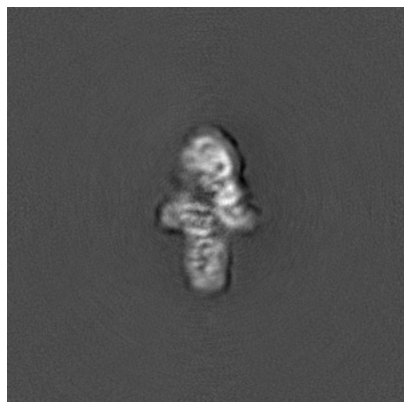


Y Index: 155

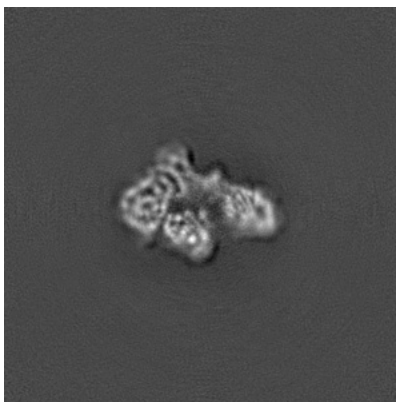


Z Index: 150

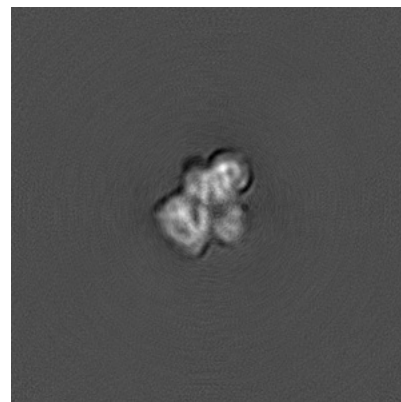
6.3.2 Raw map



X Index: 151



Y Index: 156

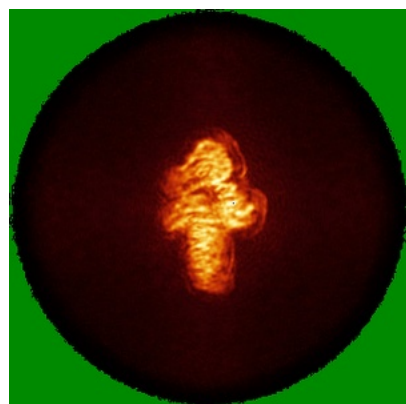


Z Index: 159

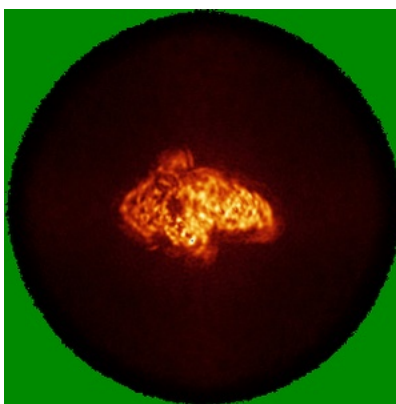
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

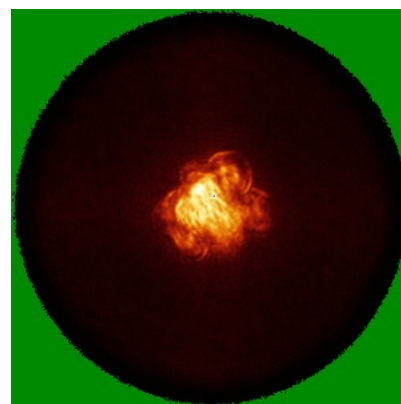
6.4.1 Primary map



X

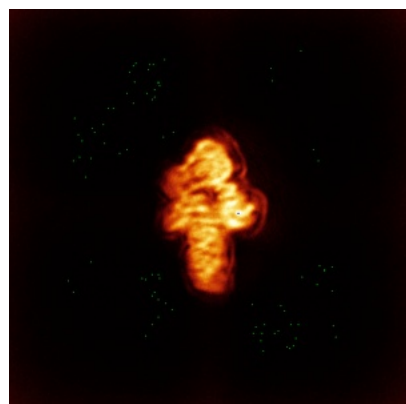


Y

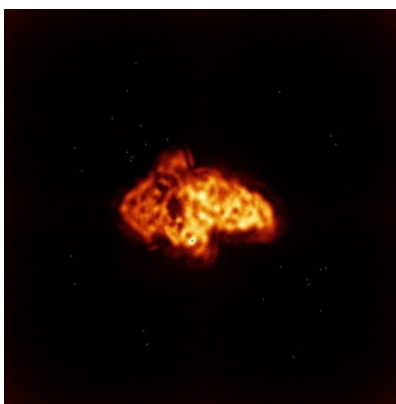


Z

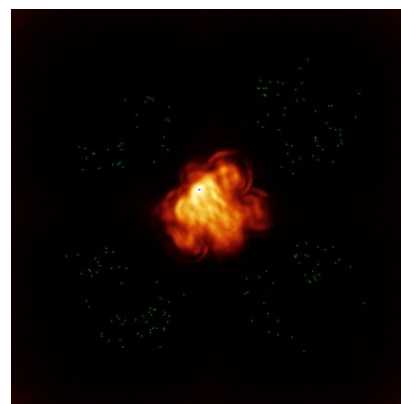
6.4.2 Raw map



X



Y



Z

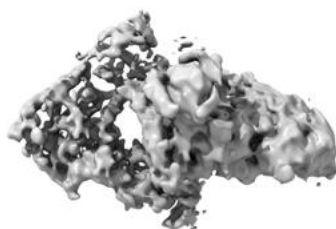
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

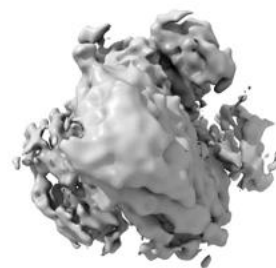
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.262. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

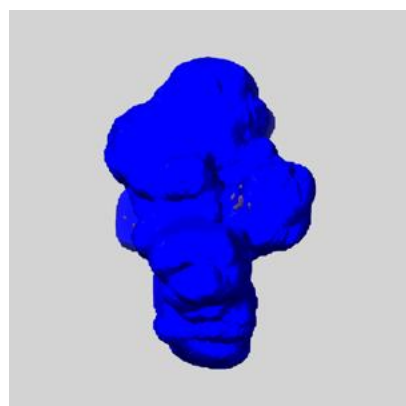
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

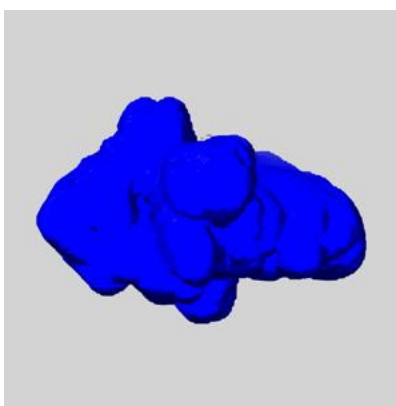
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

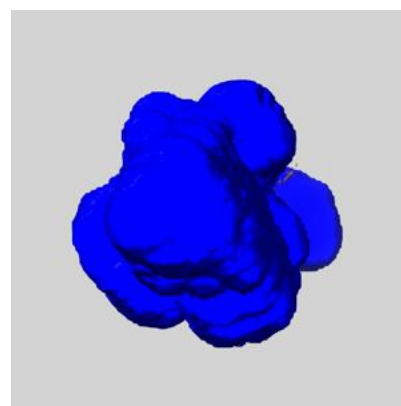
6.6.1 emd_17349_msk_1.map [i](#)



X



Y

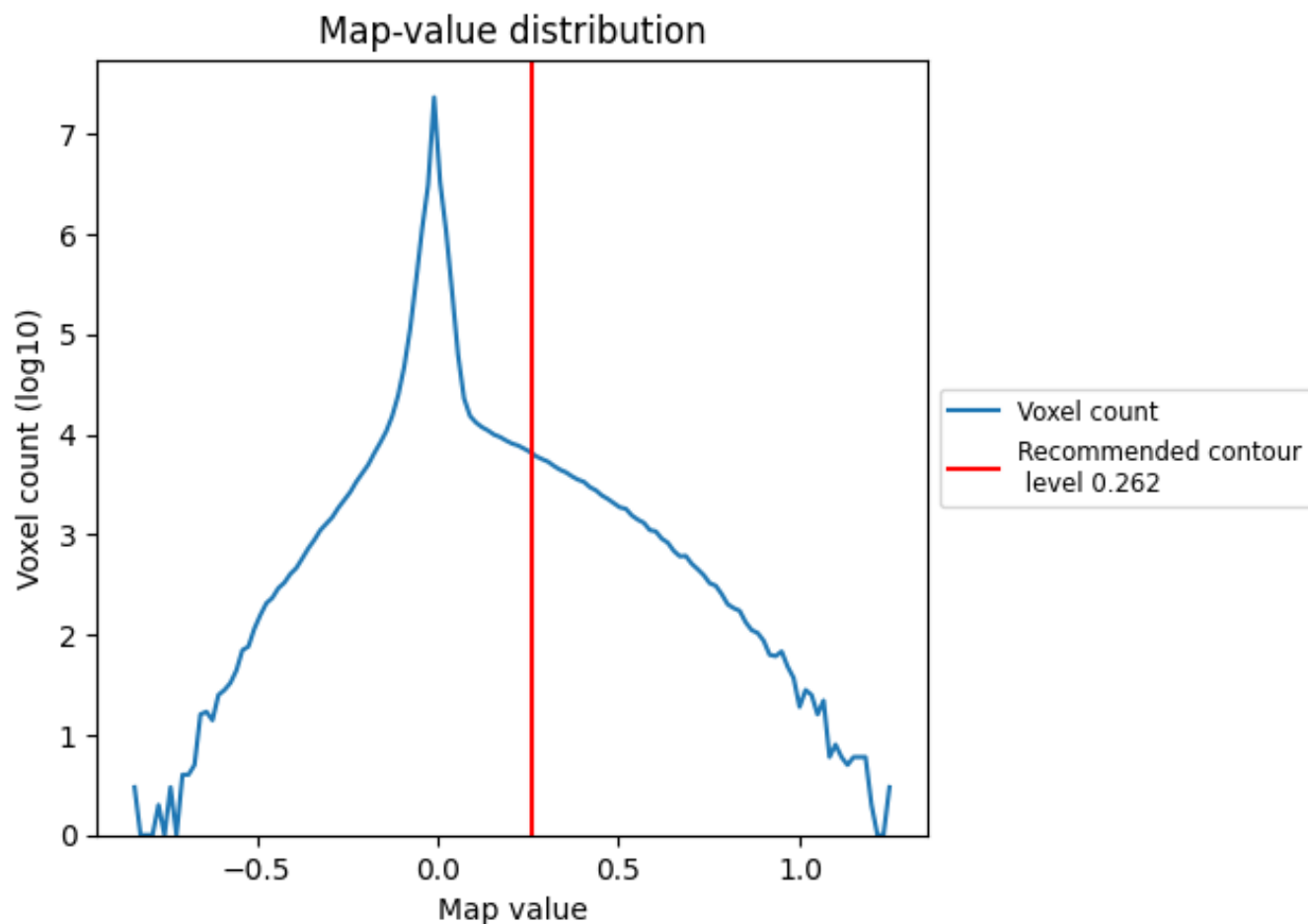


Z

7 Map analysis [i](#)

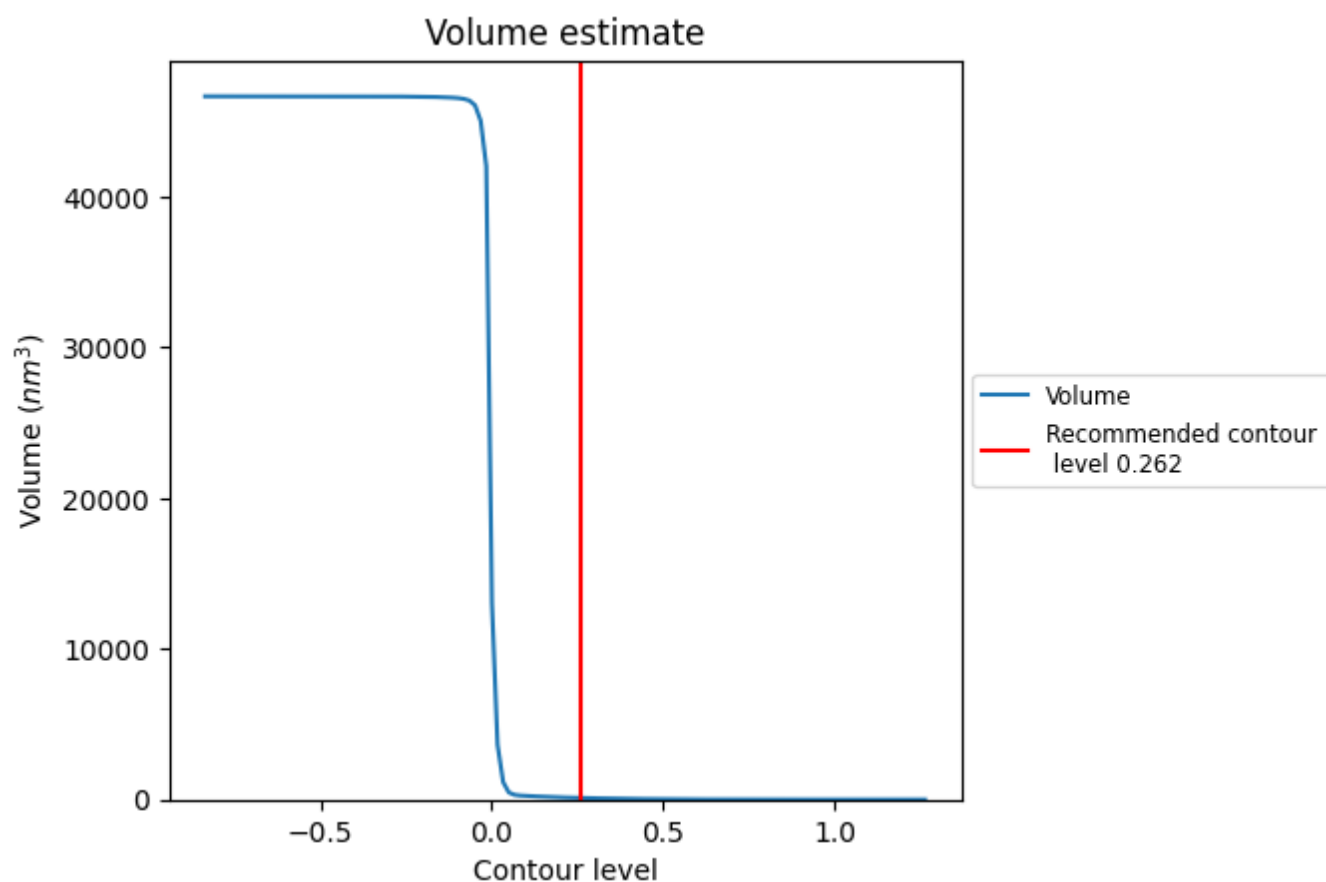
This section contains the results of statistical analysis of the map.

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.

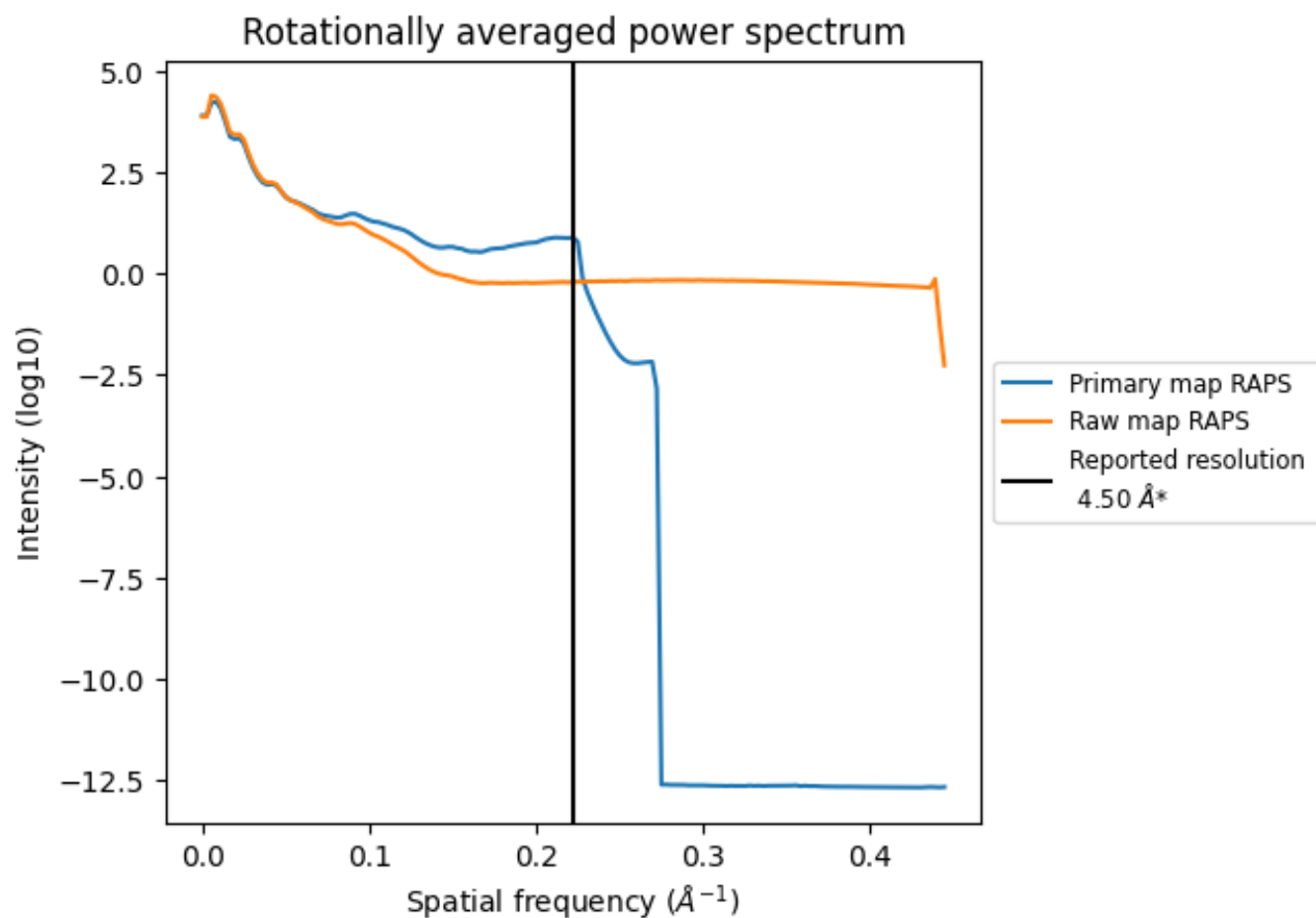
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 107 nm³; this corresponds to an approximate mass of 96 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 ⓘ

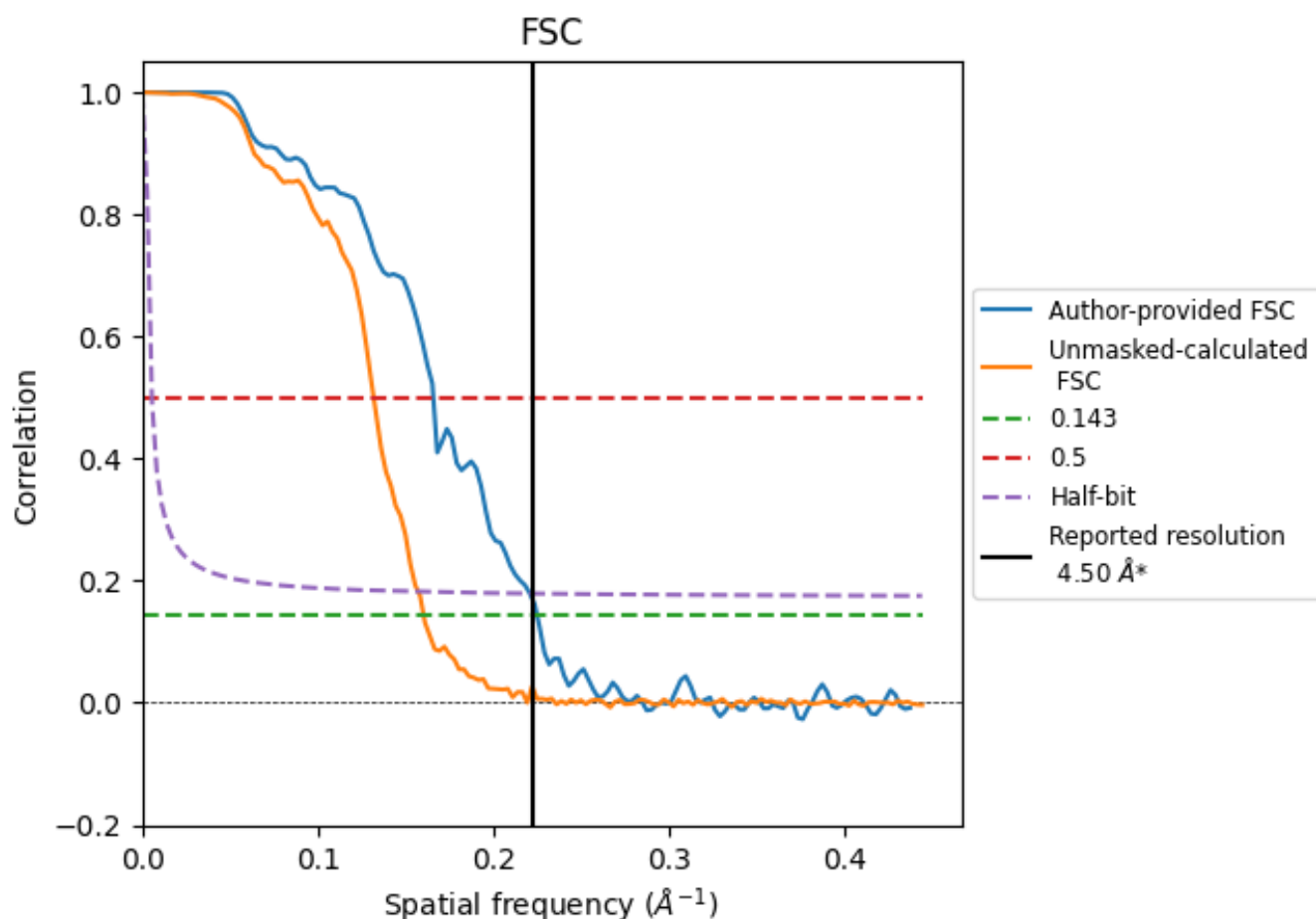


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.222 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.44	6.03	4.53
Unmasked-calculated*	6.23	7.58	6.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.23 differs from the reported value 4.5 by more than 10 %

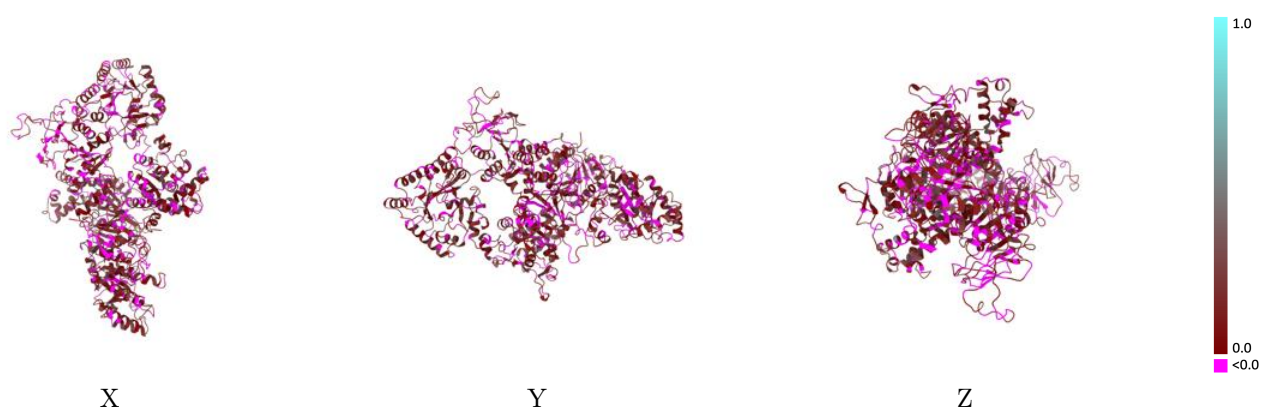
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-17349 and PDB model 9F6Z. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)

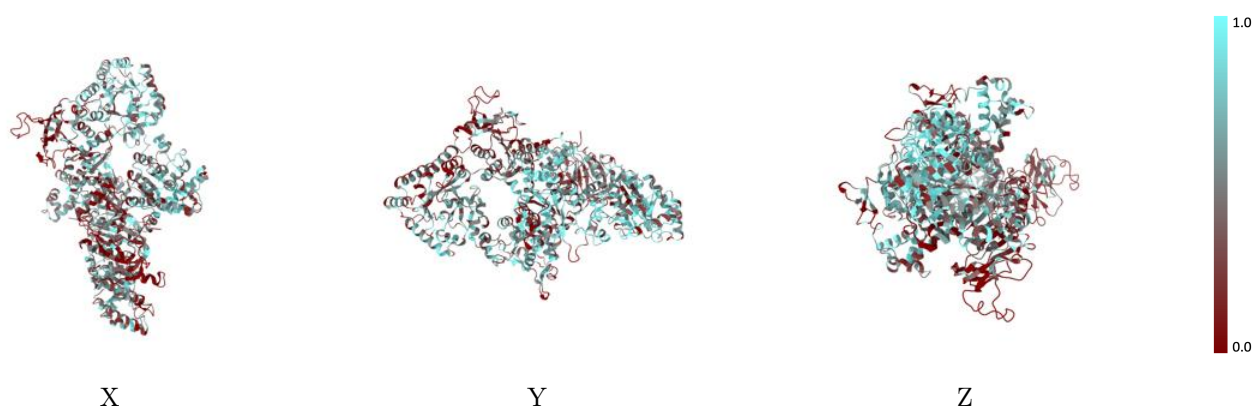
This section was not generated.

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



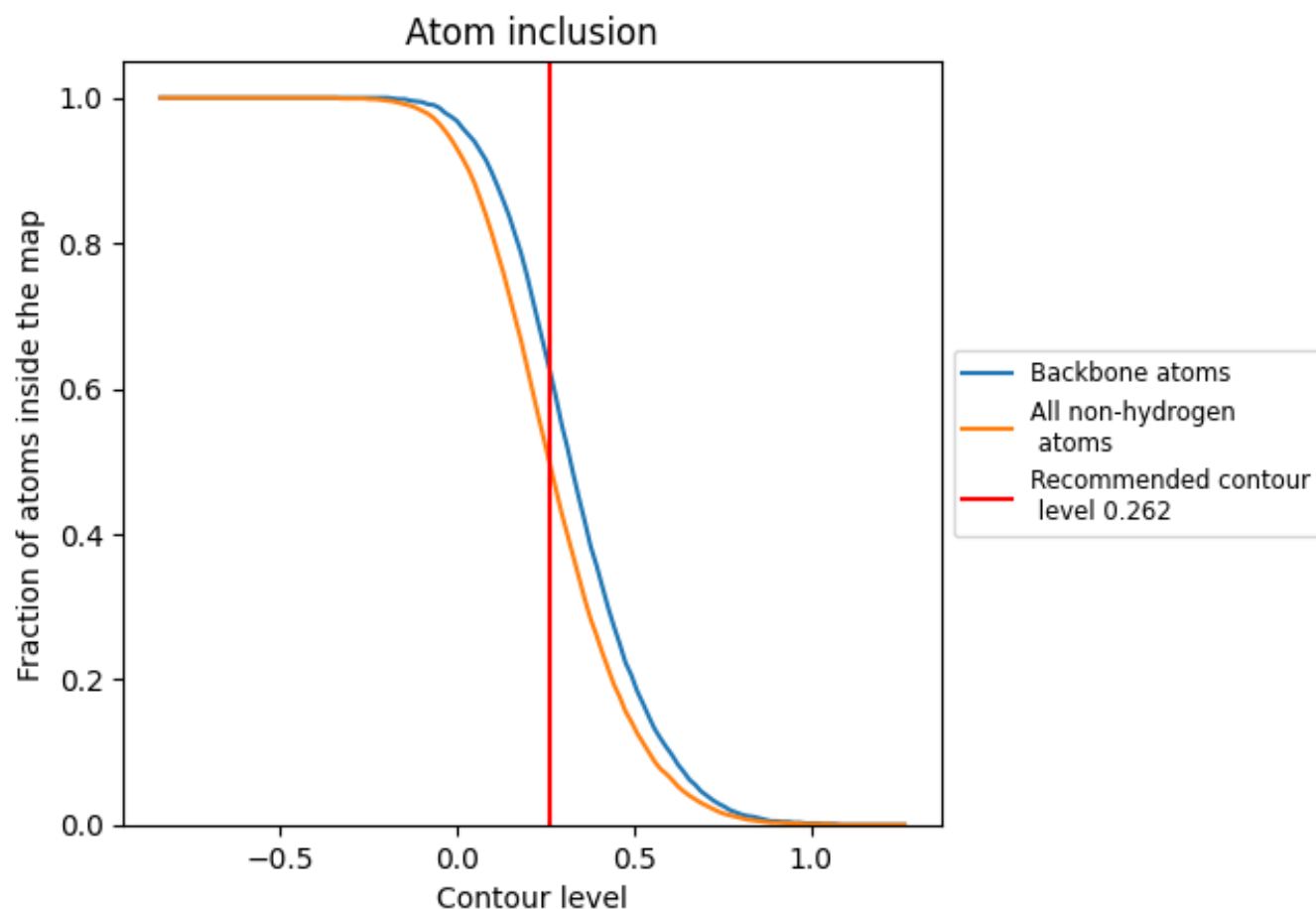
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.262).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 50% 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 (0.262) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4980	0.0970
A	0.4500	0.1170
B	0.5470	0.0760

