



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 09:44 AM UTC

PDB ID : 5H53 / pdb_00005h53
EMDB ID : EMD-6664
Title : The structure of rabbit skeletal muscle actomyosin rigor complex at 5.2 angstrom.
Authors : Fujii, T.; Namba, K.
Deposited on : 2016-11-04
Resolution : 5.20 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

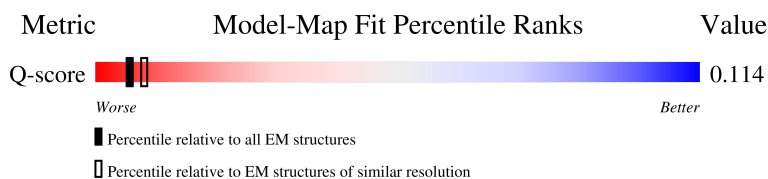
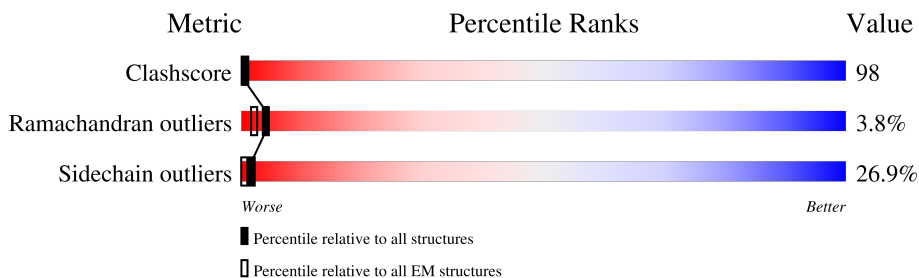
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 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	712 (4.70 - 5.70)

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	845	
2	B	146	
3	C	153	
4	D	375	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	375	14% 30% 51% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15077 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 Skeletal muscle myosin heavy chain MyHC-EO/IIL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	845	Total	C	N	O	S	0	0
			6795	4340	1155	1256	44		

- Molecule 2 is a protein called Myosin regulatory light chain 2, skeletal muscle isoform type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	146	Total	C	N	O	S	0	0
			1157	729	189	232	7		

- Molecule 3 is a protein called Myosin light chain 1/3, skeletal muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	153	Total	C	N	O	S	0	0
			1203	751	199	246	7		

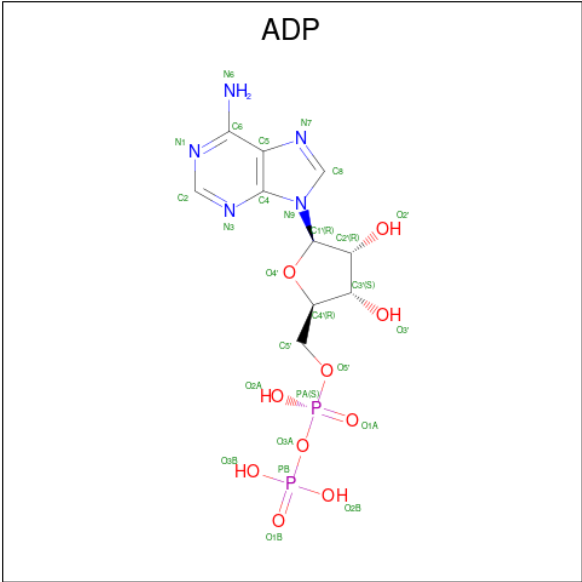
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	193	ASP	-	expression tag	UNP P02602

- Molecule 4 is a protein called Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		
4	E	375	Total	C	N	O	S	0	0
			2934	1855	493	565	21		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

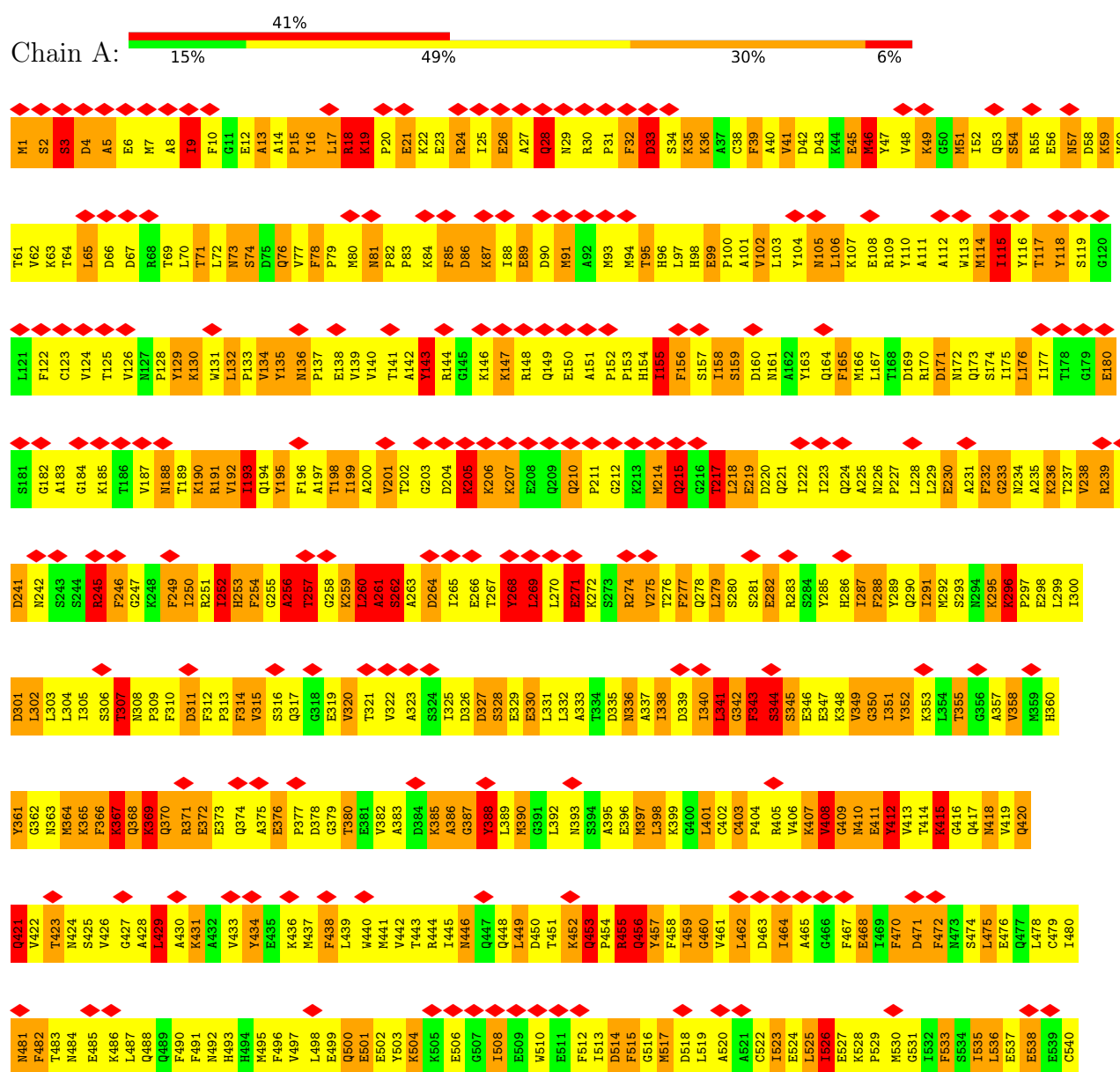


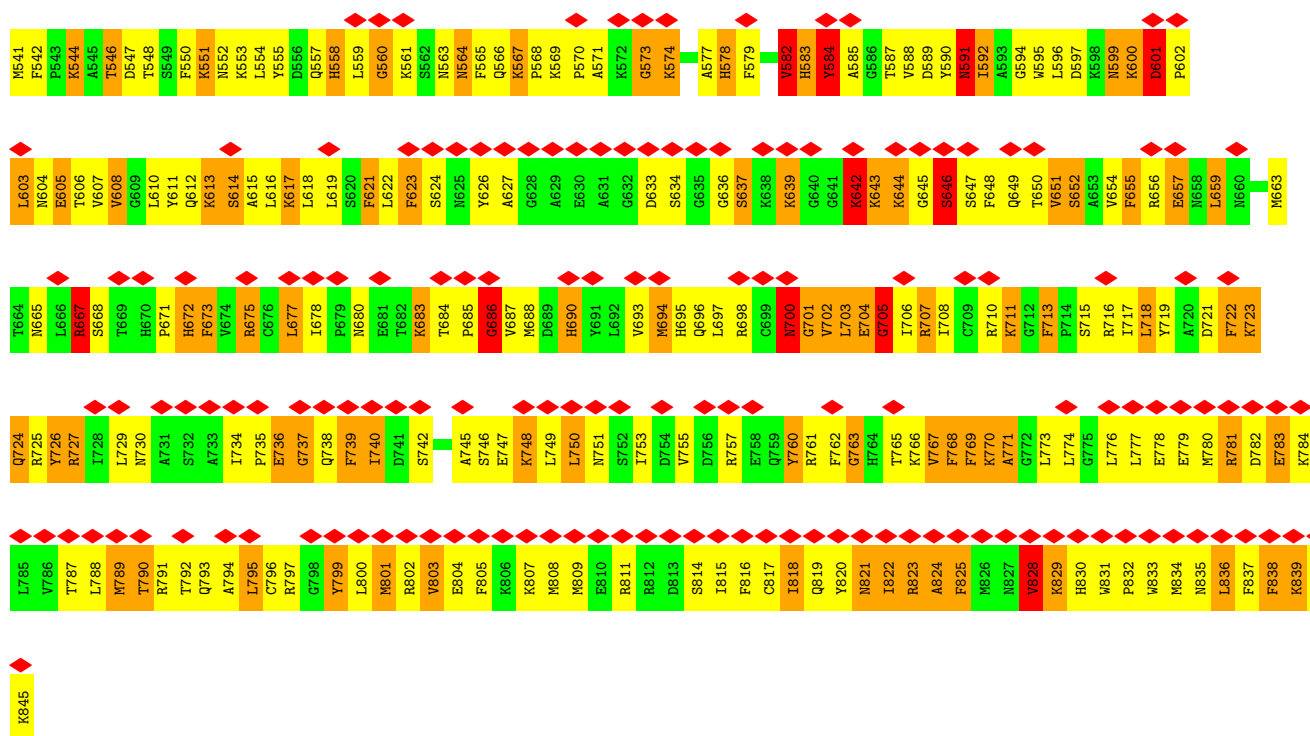
Mol	Chain	Residues	Atoms					AltConf
5	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
5	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

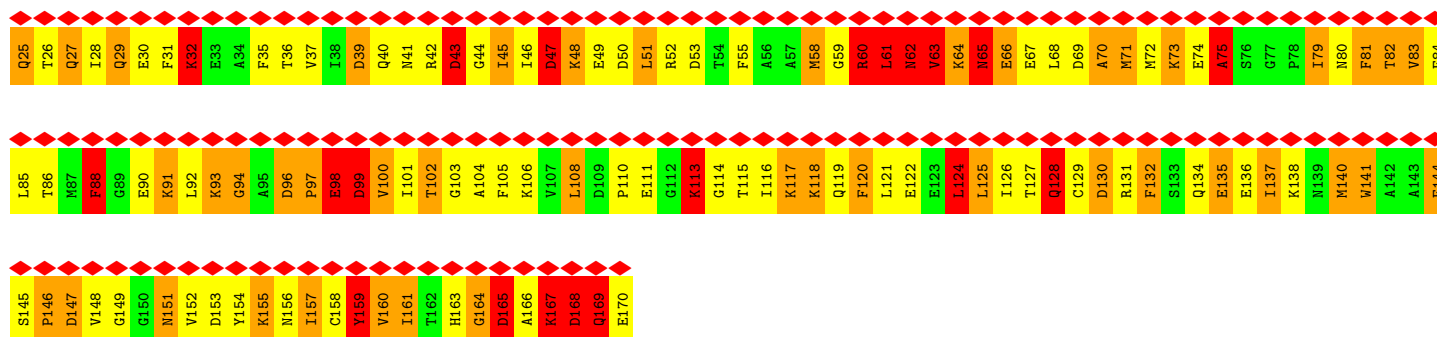
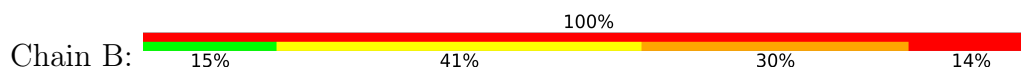
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Skeletal muscle myosin heavy chain MyHC-EO/IIL

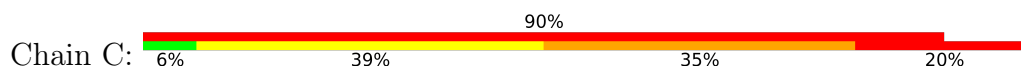




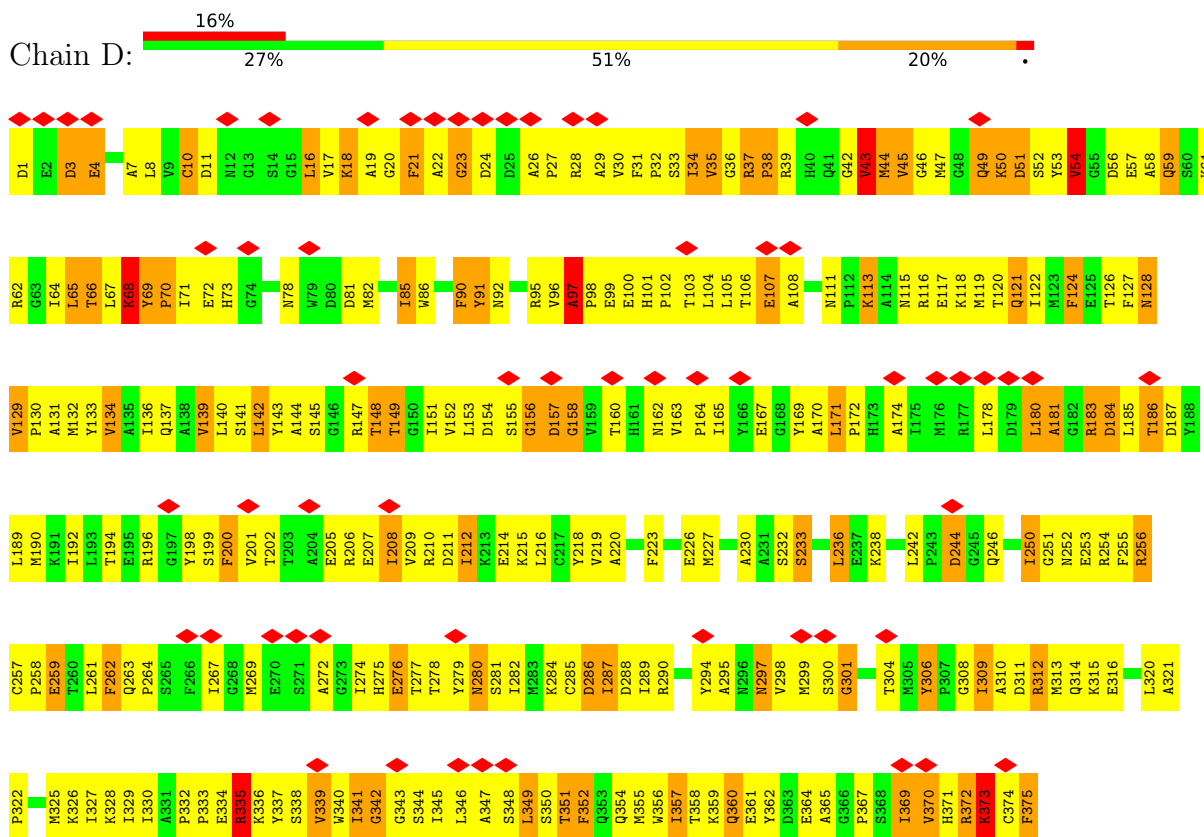
• Molecule 2: Myosin regulatory light chain 2, skeletal muscle isoform type 1



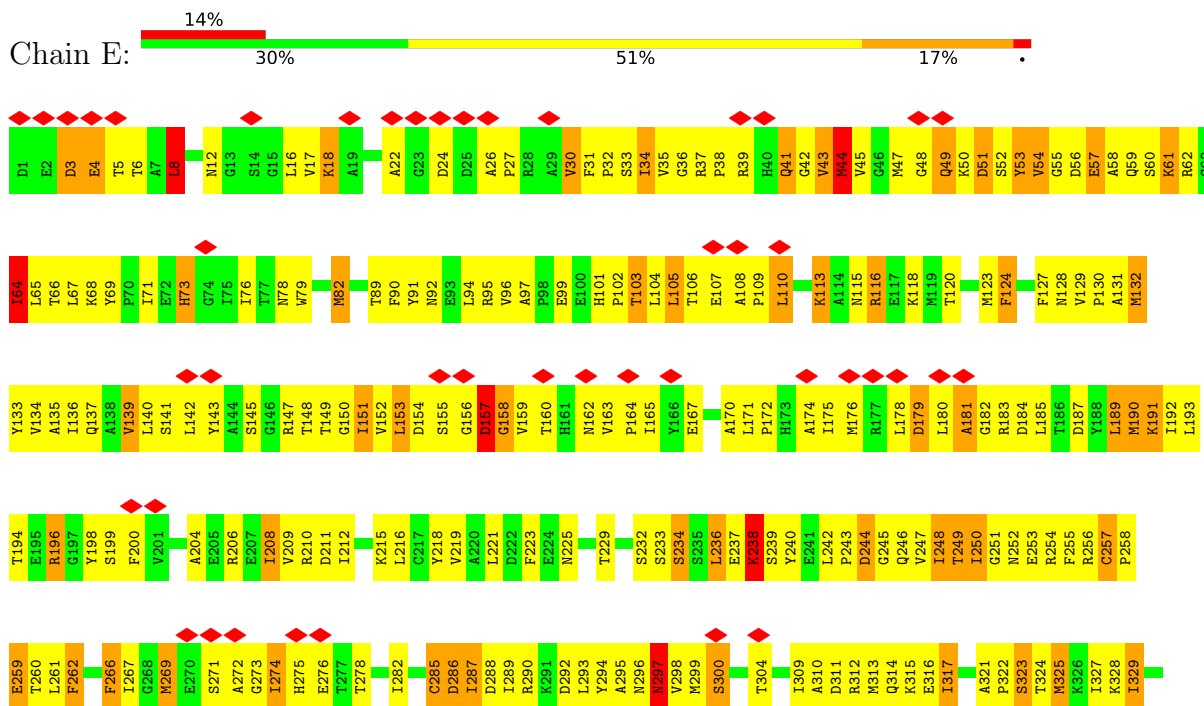
• Molecule 3: Myosin light chain 1/3, skeletal muscle isoform

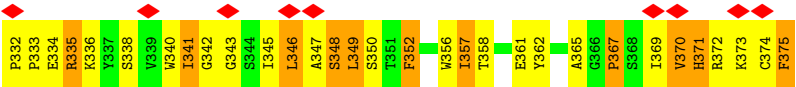


• Molecule 4: Actin, alpha skeletal muscle



• Molecule 4: Actin, alpha skeletal muscle





4 Experimental information

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=166.7°, rise=27.6 Å, axial sym=C1	Depositor
Number of segments used	31535	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL 3200FSC	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{Å}^2$)	20	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F415 (4k x 4k)	Depositor
Maximum map value	9.438	Depositor
Minimum map value	-6.853	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.746	Depositor
Recommended contour level	1.52	Depositor
Map size (Å)	337.5, 337.5, 337.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HIC, ADP

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	1.43	11/6941 (0.2%)	1.99	228/9343 (2.4%)
2	B	1.38	1/1175 (0.1%)	2.08	47/1578 (3.0%)
3	C	1.44	1/1218 (0.1%)	2.02	55/1632 (3.4%)
4	D	1.46	8/2984 (0.3%)	1.68	41/4040 (1.0%)
4	E	1.38	0/2984	1.64	39/4040 (1.0%)
All	All	1.42	21/15302 (0.1%)	1.88	410/20633 (2.0%)

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	31
2	B	0	18
3	C	0	22
4	D	0	2
4	E	0	2
All	All	0	75

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	212	ILE	C-N	16.34	1.54	1.33
4	D	214	GLU	C-N	10.28	1.47	1.33
4	D	339	VAL	C-N	9.76	1.47	1.33
4	D	70	PRO	C-N	-9.51	1.20	1.33
2	B	98	GLU	C-N	7.21	1.42	1.33
1	A	456	GLN	CA-C	7.18	1.61	1.52
4	D	306	TYR	C-N	7.07	1.42	1.33
1	A	538	GLU	CD-OE2	6.99	1.38	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	GLU	CG-CD	-6.48	1.35	1.52
4	D	351	THR	CB-CG2	6.11	1.72	1.52
1	A	256	ALA	CA-C	-5.81	1.45	1.52
1	A	254	PHE	CA-C	-5.78	1.45	1.52
4	D	54	VAL	CA-CB	-5.64	1.46	1.54
1	A	257	THR	N-CA	-5.58	1.39	1.46
3	C	121	ASN	CA-C	-5.37	1.48	1.52
4	D	335	ARG	C-N	-5.27	1.27	1.33
1	A	261	ALA	CA-C	-5.24	1.46	1.52
1	A	387	GLY	CA-C	-5.24	1.46	1.52
1	A	455	ARG	CD-NE	5.18	1.53	1.46
1	A	9	ILE	CA-CB	-5.11	1.48	1.54
1	A	268	TYR	CA-C	-5.01	1.46	1.52

All (410) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	GLU	CG-CD-OE1	-20.81	70.54	118.40
1	A	747	GLU	CG-CD-OE1	-20.61	71.00	118.40
1	A	747	GLU	CG-CD-OE2	-20.29	71.74	118.40
1	A	180	GLU	CG-CD-OE2	-20.11	72.15	118.40
1	A	81	ASN	CA-CB-CG	-16.50	96.11	112.60
2	B	99	ASP	CB-CG-OD1	-15.85	81.94	118.40
1	A	838	PHE	CA-CB-CG	-14.69	99.11	113.80
1	A	538	GLU	CG-CD-OE1	-14.28	85.56	118.40
4	E	352	PHE	CA-CB-CG	-14.14	99.66	113.80
1	A	261	ALA	N-CA-CB	12.56	128.92	110.20
1	A	261	ALA	CB-CA-C	-12.41	87.98	110.70
4	E	127	PHE	CA-CB-CG	-12.01	101.79	113.80
2	B	98	GLU	CA-C-N	11.62	136.94	120.79
2	B	98	GLU	C-N-CA	11.62	136.94	120.79
1	A	218	LEU	CA-C-N	11.22	141.90	121.70
1	A	218	LEU	C-N-CA	11.22	141.90	121.70
1	A	260	LEU	CA-C-N	-11.22	101.40	120.58
1	A	260	LEU	C-N-CA	-11.22	101.40	120.58
4	D	352	PHE	CA-CB-CG	-10.82	102.98	113.80
1	A	254	PHE	CA-CB-CG	-10.75	103.05	113.80
2	B	120	PHE	CA-CB-CG	-10.72	103.08	113.80
1	A	246	PHE	CA-CB-CG	-10.67	103.13	113.80
4	D	127	PHE	CA-CB-CG	-10.66	103.14	113.80
1	A	578	HIS	CA-CB-CG	-10.48	103.32	113.80
1	A	633	ASP	CA-CB-CG	-10.37	102.23	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	768	PHE	CA-CB-CG	-10.13	103.67	113.80
3	C	45	PHE	CA-CB-CG	-10.05	103.75	113.80
1	A	825	PHE	CA-CB-CG	-10.04	103.76	113.80
1	A	558	HIS	CA-CB-CG	-9.96	103.84	113.80
1	A	343	PHE	CA-CB-CG	-9.94	103.86	113.80
1	A	85	PHE	CA-CB-CG	-9.93	103.87	113.80
2	B	99	ASP	CB-CG-OD2	-9.86	95.72	118.40
1	A	604	ASN	CA-CB-CG	-9.84	102.76	112.60
1	A	591	ASN	CA-C-N	9.81	136.40	120.30
1	A	591	ASN	C-N-CA	9.81	136.40	120.30
1	A	655	PHE	CA-CB-CG	-9.77	104.03	113.80
1	A	218	LEU	N-CA-C	-9.70	96.17	110.23
1	A	582	VAL	CA-CB-CG1	-9.62	94.05	110.40
1	A	563	ASN	CA-CB-CG	-9.57	103.03	112.60
2	B	79	ILE	CA-C-N	9.53	138.86	121.70
2	B	79	ILE	C-N-CA	9.53	138.86	121.70
1	A	155	ILE	CB-CA-C	-9.17	99.57	112.22
1	A	129	TYR	CA-CB-CG	-9.09	97.53	113.90
1	A	39	PHE	CA-CB-CG	-9.05	104.75	113.80
4	D	351	THR	OG1-CB-CG2	9.03	127.37	109.30
2	B	167	LYS	CA-C-N	9.00	137.89	121.70
2	B	167	LYS	C-N-CA	9.00	137.89	121.70
1	A	16	TYR	CA-CB-CG	-8.95	97.78	113.90
3	C	53	PHE	CA-CB-CG	-8.90	104.90	113.80
1	A	515	PHE	CA-CB-CG	-8.83	104.97	113.80
2	B	132	PHE	CA-CB-CG	-8.82	104.98	113.80
1	A	705	GLY	CA-C-N	8.67	132.73	120.42
1	A	705	GLY	C-N-CA	8.67	132.73	120.42
1	A	601	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	143	TYR	CA-CB-CG	-8.57	98.48	113.90
4	E	375	PHE	CA-CB-CG	-8.51	105.29	113.80
4	E	262	PHE	CA-CB-CG	-8.42	105.38	113.80
4	D	262	PHE	CA-CB-CG	-8.37	105.43	113.80
2	B	168	ASP	CA-CB-CG	-8.34	104.26	112.60
2	B	160	VAL	CA-C-N	-8.34	110.71	120.88
2	B	160	VAL	C-N-CA	-8.34	110.71	120.88
1	A	726	TYR	CA-CB-CG	-8.31	98.93	113.90
1	A	747	GLU	OE1-CD-OE2	8.26	142.72	122.90
1	A	180	GLU	OE1-CD-OE2	8.24	142.67	122.90
1	A	533	PHE	CA-CB-CG	-8.20	105.60	113.80
1	A	195	TYR	CA-CB-CG	-8.19	99.16	113.90
1	A	472	PHE	CA-CB-CG	-8.16	105.64	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	TYR	CA-CB-CG	-8.13	99.27	113.90
1	A	245	ARG	CA-C-N	-8.12	109.19	122.82
1	A	245	ARG	C-N-CA	-8.12	109.19	122.82
1	A	135	TYR	CA-CB-CG	-8.09	99.33	113.90
1	A	538	GLU	CB-CG-CD	-8.07	98.89	112.60
2	B	146	PRO	CA-C-N	-8.02	106.94	121.62
2	B	146	PRO	C-N-CA	-8.02	106.94	121.62
1	A	252	ILE	CA-C-N	-7.97	108.78	123.05
1	A	252	ILE	C-N-CA	-7.97	108.78	123.05
1	A	538	GLU	OE1-CD-OE2	7.93	141.93	122.90
3	C	57	PHE	CA-CB-CG	-7.91	105.89	113.80
2	B	114	GLY	CA-C-N	7.90	135.92	121.70
2	B	114	GLY	C-N-CA	7.90	135.92	121.70
1	A	269	LEU	CA-C-N	-7.89	111.66	122.86
1	A	269	LEU	C-N-CA	-7.89	111.66	122.86
4	D	92	ASN	CA-CB-CG	-7.87	104.73	112.60
1	A	261	ALA	CA-C-O	-7.74	111.64	120.24
4	D	351	THR	N-CA-CB	7.72	121.58	110.16
1	A	387	GLY	N-CA-C	-7.71	103.47	112.73
1	A	455	ARG	CA-CB-CG	7.68	129.47	114.10
1	A	366	PHE	CA-CB-CG	-7.68	106.12	113.80
1	A	254	PHE	CA-C-O	-7.65	112.71	121.58
3	C	173	GLN	CA-C-N	7.61	131.10	120.29
3	C	173	GLN	C-N-CA	7.61	131.10	120.29
2	B	100	VAL	N-CA-C	-7.58	101.29	111.44
3	C	174	GLU	CA-C-N	-7.53	112.76	122.77
3	C	174	GLU	C-N-CA	-7.53	112.76	122.77
4	D	335	ARG	O-C-N	-7.48	113.62	122.15
3	C	183	GLU	CB-CG-CD	-7.46	99.92	112.60
1	A	491	PHE	CA-CB-CG	-7.42	106.38	113.80
4	D	335	ARG	CA-C-N	7.36	130.14	120.28
4	D	335	ARG	C-N-CA	7.36	130.14	120.28
1	A	4	ASP	CA-CB-CG	-7.35	105.25	112.60
3	C	116	GLN	CB-CG-CD	-7.34	100.12	112.60
1	A	446	ASN	CA-CB-CG	-7.34	105.26	112.60
3	C	137	PHE	N-CA-C	-7.32	103.77	114.39
3	C	67	LYS	CA-C-N	7.29	130.77	120.42
3	C	67	LYS	C-N-CA	7.29	130.77	120.42
1	A	350	GLY	CA-C-N	7.29	130.77	120.42
1	A	350	GLY	C-N-CA	7.29	130.77	120.42
1	A	28	GLN	CA-C-N	-7.23	113.10	122.79
1	A	28	GLN	C-N-CA	-7.23	113.10	122.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	124	PHE	CA-CB-CG	-7.20	106.60	113.80
1	A	314	PHE	CA-CB-CG	-7.20	106.60	113.80
1	A	657	GLU	CB-CG-CD	-7.19	100.38	112.60
3	C	90	LYS	CA-C-N	-7.16	112.55	122.93
3	C	90	LYS	C-N-CA	-7.16	112.55	122.93
4	D	252	ASN	N-CA-C	-7.14	103.57	111.36
1	A	769	PHE	CA-CB-CG	-7.10	106.70	113.80
2	B	88	PHE	CA-CB-CG	-7.08	106.72	113.80
1	A	560	GLY	N-CA-C	-7.04	106.48	115.42
4	D	351	THR	CB-CA-C	-7.03	98.89	110.85
1	A	542	PHE	CA-CB-CG	-6.97	106.83	113.80
1	A	254	PHE	CB-CA-C	-6.96	96.52	110.30
3	C	112	LEU	CA-C-N	6.96	126.21	118.97
3	C	112	LEU	C-N-CA	6.96	126.21	118.97
1	A	270	LEU	CA-C-N	-6.92	112.23	122.41
1	A	270	LEU	C-N-CA	-6.92	112.23	122.41
2	B	80	ASN	CA-CB-CG	-6.92	105.68	112.60
1	A	564	ASN	CA-CB-CG	-6.89	105.71	112.60
1	A	824	ALA	N-CA-C	-6.88	103.78	111.28
4	E	51	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	621	PHE	CA-CB-CG	-6.86	106.94	113.80
1	A	623	PHE	CA-CB-CG	-6.75	107.05	113.80
4	E	124	PHE	CA-CB-CG	-6.73	107.07	113.80
4	D	301	GLY	O-C-N	6.72	130.41	122.68
1	A	277	PHE	CA-CB-CG	-6.70	107.10	113.80
4	E	92	ASN	CA-CB-CG	-6.69	105.91	112.60
4	D	70	PRO	N-CA-C	-6.67	103.94	113.47
2	B	163	HIS	N-CA-C	-6.65	104.06	111.71
1	A	386	ALA	CB-CA-C	-6.64	100.45	110.88
1	A	739	PHE	CA-CB-CG	-6.64	107.16	113.80
1	A	722	PHE	CA-CB-CG	-6.62	107.18	113.80
3	C	193	ASP	CA-CB-CG	-6.62	105.98	112.60
1	A	288	PHE	CA-CB-CG	-6.61	107.19	113.80
3	C	181	ASN	CA-CB-CG	-6.59	106.01	112.60
3	C	45	PHE	CA-C-N	6.58	133.53	121.70
3	C	45	PHE	C-N-CA	6.58	133.53	121.70
1	A	455	ARG	CD-NE-CZ	-6.56	115.21	124.40
1	A	169	ASP	CA-CB-CG	-6.54	106.06	112.60
1	A	584	TYR	CA-C-N	6.54	134.03	121.54
1	A	584	TYR	C-N-CA	6.54	134.03	121.54
2	B	43	ASP	CA-CB-CG	-6.53	106.07	112.60
1	A	686	GLY	N-CA-C	-6.52	107.32	115.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	280	ASN	CA-CB-CG	-6.50	106.10	112.60
3	C	65	ASP	CA-CB-CG	-6.49	106.11	112.60
4	D	16	LEU	CA-C-N	-6.49	113.63	122.91
4	D	16	LEU	C-N-CA	-6.49	113.63	122.91
4	E	348	SER	CA-C-N	-6.48	114.41	122.84
4	E	348	SER	C-N-CA	-6.48	114.41	122.84
1	A	357	ALA	N-CA-C	-6.47	104.23	111.28
1	A	701	GLY	N-CA-C	-6.47	106.39	115.32
1	A	268	TYR	CA-C-N	6.46	133.87	121.54
1	A	268	TYR	C-N-CA	6.46	133.87	121.54
1	A	352	TYR	CB-CA-C	-6.45	100.75	110.88
3	C	102	ASN	CA-CB-CG	-6.45	106.15	112.60
1	A	156	PHE	N-CA-C	-6.42	104.32	111.71
1	A	268	TYR	CA-C-O	-6.40	111.57	120.21
2	B	99	ASP	CA-CB-CG	-6.36	106.24	112.60
4	E	266	PHE	CA-CB-CG	-6.35	107.45	113.80
2	B	37	VAL	CB-CA-C	-6.32	103.88	111.97
2	B	70	ALA	N-CA-C	-6.31	104.45	111.71
3	C	111	PHE	CA-CB-CG	-6.30	107.50	113.80
3	C	103	ALA	CA-C-N	-6.29	112.11	122.11
3	C	103	ALA	C-N-CA	-6.29	112.11	122.11
1	A	10	PHE	CA-CB-CG	-6.29	107.51	113.80
2	B	66	GLU	CA-C-N	6.28	128.61	120.44
2	B	66	GLU	C-N-CA	6.28	128.61	120.44
1	A	821	ASN	CA-CB-CG	-6.27	106.33	112.60
1	A	136	ASN	CA-C-N	6.25	125.94	119.56
1	A	136	ASN	C-N-CA	6.25	125.94	119.56
1	A	410	ASN	CA-CB-CG	-6.25	106.35	112.60
1	A	233	GLY	N-CA-C	-6.25	102.38	112.31
1	A	361	TYR	N-CA-C	-6.21	104.56	111.71
4	D	156	GLY	CA-C-N	6.21	129.74	120.31
4	D	156	GLY	C-N-CA	6.21	129.74	120.31
1	A	33	ASP	CA-CB-CG	-6.17	106.43	112.60
4	D	375	PHE	CA-CB-CG	-6.17	107.63	113.80
1	A	514	ASP	CA-CB-CG	-6.16	106.44	112.60
1	A	254	PHE	CA-C-N	6.15	130.51	121.05
1	A	254	PHE	C-N-CA	6.15	130.51	121.05
1	A	471	ASP	N-CA-C	-6.11	104.62	111.28
1	A	218	LEU	CB-CA-C	-6.10	99.60	109.72
1	A	470	PHE	CA-CB-CG	-6.10	107.70	113.80
3	C	116	GLN	CA-C-N	6.09	130.34	120.60
3	C	116	GLN	C-N-CA	6.09	130.34	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	268	TYR	O-C-N	6.07	130.91	123.44
1	A	403	CYS	O-C-N	6.05	124.90	121.27
1	A	232	PHE	CA-CB-CG	-6.05	107.75	113.80
4	E	154	ASP	CA-C-N	-6.05	114.24	123.07
4	E	154	ASP	C-N-CA	-6.05	114.24	123.07
4	E	292	ASP	CA-CB-CG	-6.01	106.59	112.60
2	B	81	PHE	CA-CB-CG	-6.00	107.80	113.80
4	D	259	GLU	CA-C-N	6.00	128.31	120.28
4	D	259	GLU	C-N-CA	6.00	128.31	120.28
3	C	76	VAL	N-CA-C	-5.99	104.51	110.62
3	C	64	GLY	N-CA-C	-5.99	101.95	110.63
1	A	18	ARG	N-CA-C	5.98	117.67	111.03
4	E	8	LEU	CA-C-N	-5.98	115.10	122.93
4	E	8	LEU	C-N-CA	-5.98	115.10	122.93
1	A	385	LYS	CA-C-N	5.97	128.20	120.44
1	A	385	LYS	C-N-CA	5.97	128.20	120.44
1	A	15	PRO	CA-C-N	-5.95	111.84	120.29
1	A	15	PRO	C-N-CA	-5.95	111.84	120.29
1	A	395	ALA	N-CA-C	-5.93	104.81	111.28
2	B	29	GLN	N-CA-C	-5.93	104.89	111.71
4	E	187	ASP	CA-CB-CG	-5.92	106.68	112.60
4	E	91	TYR	CA-CB-CG	-5.91	103.26	113.90
3	C	83	ASN	CA-CB-CG	-5.91	106.69	112.60
1	A	241	ASP	CA-CB-CG	-5.90	106.70	112.60
1	A	409	GLY	N-CA-C	-5.89	105.53	113.24
3	C	53	PHE	N-CA-C	-5.89	104.86	111.28
3	C	189	ILE	N-CA-CB	5.88	120.94	111.23
1	A	355	THR	N-CA-C	-5.87	104.88	111.28
1	A	398	LEU	N-CA-C	-5.86	104.80	111.07
4	D	184	ASP	CA-CB-CG	-5.85	106.75	112.60
1	A	67	ASP	CA-CB-CG	-5.84	106.76	112.60
4	D	68	LYS	CA-C-N	-5.82	113.57	122.42
4	D	68	LYS	C-N-CA	-5.82	113.57	122.42
4	E	190	MET	CG-SD-CE	-5.82	88.10	100.90
4	E	311	ASP	CA-CB-CG	-5.81	106.79	112.60
1	A	386	ALA	N-CA-C	-5.81	104.85	111.07
3	C	71	SER	CB-CA-C	-5.80	101.52	110.81
4	E	41	GLN	CA-C-N	5.80	126.42	119.98
4	E	41	GLN	C-N-CA	5.80	126.42	119.98
1	A	700	ASN	N-CA-C	-5.80	104.96	111.28
1	A	32	PHE	CA-CB-CG	-5.79	108.01	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	124	LEU	CA-C-N	-5.79	112.75	120.63
2	B	124	LEU	C-N-CA	-5.79	112.75	120.63
1	A	196	PHE	N-CA-C	-5.77	105.00	111.28
1	A	713	PHE	CB-CA-C	-5.74	104.47	110.33
1	A	751	ASN	CA-CB-CG	-5.74	106.86	112.60
1	A	105	ASN	CA-CB-CG	-5.74	106.86	112.60
4	E	179	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	311	ASP	CA-CB-CG	-5.72	106.88	112.60
1	A	490	PHE	CA-CB-CG	-5.72	108.08	113.80
1	A	673	PHE	CA-CB-CG	-5.71	108.09	113.80
1	A	269	LEU	O-C-N	-5.70	115.00	122.59
1	A	799	TYR	CA-CB-CG	-5.70	103.64	113.90
1	A	254	PHE	N-CA-C	-5.69	100.76	109.41
1	A	3	SER	CA-C-N	-5.68	114.36	122.77
1	A	3	SER	C-N-CA	-5.68	114.36	122.77
2	B	96	ASP	CA-CB-CG	-5.67	106.93	112.60
4	E	12	ASN	CA-CB-CG	-5.66	106.94	112.60
1	A	563	ASN	N-CA-C	-5.66	105.20	111.71
2	B	32	LYS	N-CA-C	-5.66	105.11	111.28
2	B	130	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	302	LEU	CA-C-N	5.65	128.42	120.28
1	A	302	LEU	C-N-CA	5.65	128.42	120.28
1	A	188	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	269	LEU	N-CA-CB	5.65	120.03	110.49
1	A	371	ARG	N-CA-C	-5.64	102.54	110.50
1	A	690	HIS	CA-CB-CG	-5.64	108.16	113.80
3	C	42	LYS	CA-C-N	5.63	131.84	121.70
3	C	42	LYS	C-N-CA	5.63	131.84	121.70
4	E	157	ASP	CA-CB-CG	-5.63	106.97	112.60
3	C	185	PHE	CB-CA-C	-5.60	102.34	110.96
3	C	58	LEU	N-CA-C	-5.60	105.08	111.07
1	A	760	TYR	CA-CB-CG	-5.58	103.86	113.90
1	A	257	THR	N-CA-C	-5.57	105.08	112.94
1	A	230	GLU	CA-C-N	-5.57	113.20	120.44
1	A	230	GLU	C-N-CA	-5.57	113.20	120.44
1	A	639	LYS	CA-C-N	5.57	130.31	120.74
1	A	639	LYS	C-N-CA	5.57	130.31	120.74
1	A	438	PHE	CA-CB-CG	-5.56	108.24	113.80
4	E	53	TYR	CA-CB-CG	-5.56	103.89	113.90
1	A	205	LYS	CA-C-N	-5.55	115.34	123.00
1	A	205	LYS	C-N-CA	-5.55	115.34	123.00
2	B	149	GLY	N-CA-C	-5.54	107.32	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	367	PRO	N-CA-C	-5.54	106.64	113.84
4	D	23	GLY	N-CA-C	-5.53	107.69	115.32
1	A	66	ASP	CA-CB-CG	-5.53	107.07	112.60
4	E	200	PHE	CB-CA-C	-5.52	103.94	111.95
1	A	672	HIS	CA-C-N	-5.52	114.24	122.74
1	A	672	HIS	C-N-CA	-5.52	114.24	122.74
1	A	58	ASP	CA-CB-CG	-5.52	107.08	112.60
2	B	151	ASN	CA-CB-CG	-5.50	107.10	112.60
1	A	388	TYR	CA-CB-CG	5.49	123.79	113.90
4	D	38	PRO	N-CA-CB	5.48	108.20	103.27
1	A	165	PHE	CA-CB-CG	-5.47	108.33	113.80
1	A	368	GLN	N-CA-C	-5.47	103.69	111.24
1	A	184	GLY	N-CA-C	-5.45	107.25	115.32
4	E	234	SER	N-CA-C	-5.45	107.64	114.56
1	A	171	ASP	CA-CB-CG	-5.44	107.16	112.60
4	E	204	ALA	N-CA-C	-5.43	105.36	111.28
1	A	114	MET	CG-SD-CE	-5.43	88.95	100.90
1	A	256	ALA	N-CA-C	-5.41	104.78	111.33
1	A	695	HIS	N-CA-C	-5.41	105.38	111.28
2	B	75	ALA	CA-C-N	-5.41	113.75	122.24
2	B	75	ALA	C-N-CA	-5.41	113.75	122.24
1	A	667	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	A	66	ASP	N-CA-C	-5.40	105.51	113.61
4	D	90	PHE	CA-CB-CG	-5.40	108.40	113.80
3	C	98	ASN	CA-CB-CG	-5.39	107.21	112.60
4	D	70	PRO	O-C-N	-5.38	116.08	122.17
4	E	341	ILE	CB-CA-C	-5.38	105.08	111.97
4	D	308	GLY	N-CA-C	-5.38	107.82	115.30
1	A	193	ILE	CB-CA-C	-5.38	105.09	111.97
3	C	75	ASP	N-CA-C	-5.37	105.46	112.23
1	A	262	SER	N-CA-CB	5.37	119.57	110.49
4	D	200	PHE	CB-CA-C	-5.37	103.76	111.70
1	A	412	TYR	N-CA-CB	5.36	119.10	111.05
2	B	159	TYR	CA-C-N	-5.36	112.32	121.97
2	B	159	TYR	C-N-CA	-5.36	112.32	121.97
1	A	65	LEU	N-CA-C	-5.35	107.30	112.97
1	A	204	ASP	N-CA-CB	5.35	119.54	110.49
4	D	128	ASN	CA-CB-CG	-5.35	107.25	112.60
4	E	259	GLU	N-CA-C	-5.34	105.56	111.71
4	D	91	TYR	CA-CB-CG	-5.34	104.29	113.90
4	D	342	GLY	CA-C-N	5.32	126.98	120.22
4	D	342	GLY	C-N-CA	5.32	126.98	120.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	ASP	CA-CB-CG	-5.32	107.28	112.60
1	A	703	LEU	N-CA-C	-5.31	105.50	111.28
3	C	70	LEU	CA-C-N	5.31	127.70	120.54
3	C	70	LEU	C-N-CA	5.31	127.70	120.54
1	A	249	PHE	CA-CB-CG	-5.30	108.50	113.80
2	B	79	ILE	O-C-N	-5.30	118.20	122.97
1	A	86	ASP	N-CA-CB	5.29	117.83	110.26
3	C	143	GLY	N-CA-C	-5.29	100.65	113.18
1	A	256	ALA	O-C-N	5.27	127.71	122.12
1	A	336	ASN	CA-CB-CG	-5.27	107.33	112.60
3	C	64	GLY	CA-C-N	-5.27	115.34	122.77
3	C	64	GLY	C-N-CA	-5.27	115.34	122.77
1	A	182	GLY	N-CA-C	-5.27	107.98	115.30
1	A	73	ASN	CA-CB-CG	-5.26	107.34	112.60
2	B	31	PHE	CA-CB-CG	-5.26	108.54	113.80
3	C	115	LEU	N-CA-C	-5.25	105.72	111.82
2	B	141	TRP	CB-CA-C	-5.25	102.64	110.88
2	B	79	ILE	N-CA-CB	-5.25	105.52	112.34
4	D	163	VAL	CB-CA-C	-5.25	106.09	111.08
4	E	24	ASP	CA-CB-CG	-5.25	107.35	112.60
1	A	552	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	597	ASP	CA-CB-CG	-5.24	107.36	112.60
1	A	271	GLU	CA-C-N	5.24	129.47	120.72
1	A	271	GLU	C-N-CA	5.24	129.47	120.72
1	A	320	VAL	CA-C-N	-5.23	113.79	122.11
1	A	320	VAL	C-N-CA	-5.23	113.79	122.11
4	D	97	ALA	CA-C-N	5.23	124.74	119.19
4	D	97	ALA	C-N-CA	5.23	124.74	119.19
4	E	225	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	393	ASN	CA-CB-CG	-5.23	107.37	112.60
3	C	167	GLU	CA-C-N	-5.22	114.42	123.25
3	C	167	GLU	C-N-CA	-5.22	114.42	123.25
1	A	828	VAL	CB-CA-C	-5.22	105.09	112.14
4	E	115	ASN	CA-CB-CG	-5.22	107.38	112.60
1	A	302	LEU	N-CA-C	-5.20	105.73	111.71
1	A	448	GLN	CA-C-N	5.19	128.20	120.31
1	A	448	GLN	C-N-CA	5.19	128.20	120.31
1	A	269	LEU	CA-C-O	5.19	127.93	120.51
1	A	482	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	402	CYS	CB-CA-C	-5.18	102.74	110.88
2	B	60	ARG	CA-C-N	5.17	130.79	121.06
2	B	60	ARG	C-N-CA	5.17	130.79	121.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	245	GLY	N-CA-C	-5.17	108.05	113.58
3	C	107	GLU	N-CA-C	-5.17	105.65	111.28
3	C	152	HIS	CB-CA-C	-5.17	100.14	110.42
1	A	592	ILE	N-CA-C	5.16	117.54	111.09
1	A	200	ALA	N-CA-C	-5.16	105.66	111.28
1	A	605	GLU	CB-CA-C	-5.15	102.79	110.88
1	A	771	ALA	CA-C-N	-5.15	117.31	123.44
1	A	771	ALA	C-N-CA	-5.15	117.31	123.44
3	C	86	ASN	CA-CB-CG	-5.15	107.45	112.60
4	E	116	ARG	N-CA-C	-5.15	105.67	111.28
4	D	157	ASP	CA-CB-CG	-5.15	107.45	112.60
1	A	601	ASP	CA-C-N	5.13	125.14	119.90
1	A	601	ASP	C-N-CA	5.13	125.14	119.90
1	A	605	GLU	CB-CG-CD	-5.13	103.88	112.60
1	A	5	ALA	CA-C-N	-5.13	114.15	122.36
1	A	5	ALA	C-N-CA	-5.13	114.15	122.36
3	C	58	LEU	CB-CA-C	-5.12	102.84	110.88
1	A	429	LEU	N-CA-C	-5.12	105.59	111.07
1	A	274	ARG	CB-CA-C	-5.12	102.30	110.79
2	B	65	ASN	N-CA-C	-5.12	99.91	110.80
1	A	118	TYR	CA-C-N	-5.11	115.42	123.13
1	A	118	TYR	C-N-CA	-5.11	115.42	123.13
1	A	89	GLU	CB-CG-CD	-5.10	103.92	112.60
1	A	571	ALA	CA-C-N	-5.10	115.80	122.99
1	A	571	ALA	C-N-CA	-5.10	115.80	122.99
1	A	155	ILE	N-CA-CB	5.10	118.23	110.58
1	A	13	ALA	N-CA-C	-5.09	105.73	111.28
1	A	215	GLN	CB-CG-CD	-5.08	103.96	112.60
3	C	191	SER	CA-C-N	5.08	131.12	121.97
3	C	191	SER	C-N-CA	5.08	131.12	121.97
1	A	481	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	823	ARG	N-CA-C	-5.07	105.75	111.28
4	E	371	HIS	CA-C-N	-5.07	115.72	122.72
4	E	371	HIS	C-N-CA	-5.07	115.72	122.72
1	A	341	LEU	N-CA-C	-5.07	106.20	112.38
1	A	342	GLY	CA-C-N	-5.07	115.96	123.05
1	A	342	GLY	C-N-CA	-5.07	115.96	123.05
1	A	747	GLU	N-CA-C	-5.06	105.66	111.07
4	E	200	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	526	ILE	CB-CA-C	-5.05	105.35	111.87
3	C	96	PRO	N-CA-C	-5.05	106.83	113.65
3	C	116	GLN	CA-CB-CG	5.04	124.18	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	455	ARG	N-CA-CB	5.04	119.28	110.81
4	D	21	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	115	ILE	CA-CB-CG2	-5.01	101.98	110.50
1	A	52	ILE	CB-CA-C	-5.01	104.12	110.98
4	D	276	GLU	CB-CG-CD	-5.01	104.08	112.60
1	A	583	HIS	N-CA-C	-5.00	102.10	109.86
1	A	291	ILE	CB-CA-C	-5.00	105.39	112.14

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	TYR	Peptide
1	A	18	ARG	Peptide
1	A	203	GLY	Peptide
1	A	217	THR	Peptide
1	A	239	ARG	Peptide
1	A	256	ALA	Peptide
1	A	261	ALA	Mainchain
1	A	268	TYR	Peptide
1	A	296	LYS	Peptide
1	A	343	PHE	Peptide
1	A	349	VAL	Peptide
1	A	367	LYS	Peptide
1	A	371	ARG	Peptide
1	A	379	GLY	Peptide
1	A	415	LYS	Peptide
1	A	421	GLN	Peptide
1	A	455	ARG	Sidechain
1	A	460	GLY	Peptide
1	A	538	GLU	Sidechain
1	A	573	GLY	Peptide
1	A	584	TYR	Peptide
1	A	594	GLY	Peptide
1	A	599	ASN	Peptide
1	A	667	ARG	Sidechain
1	A	686	GLY	Peptide
1	A	704	GLU	Peptide
1	A	707	ARG	Sidechain
1	A	736	GLU	Peptide
1	A	737	GLY	Peptide
1	A	763	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	771	ALA	Peptide
2	B	102	THR	Peptide
2	B	113	LYS	Peptide
2	B	125	LEU	Peptide
2	B	128	GLN	Peptide
2	B	144	PHE	Peptide
2	B	147	ASP	Peptide
2	B	164	GLY	Peptide
2	B	169	GLN	Peptide
2	B	43	ASP	Peptide
2	B	47	ASP	Peptide
2	B	61	LEU	Peptide
2	B	63	VAL	Peptide
2	B	65	ASN	Peptide
2	B	88	PHE	Peptide
2	B	94	GLY	Peptide
2	B	97	PRO	Peptide
2	B	99	ASP	Sidechain,Peptide
3	C	103	ALA	Peptide
3	C	116	GLN	Peptide
3	C	118	ILE	Peptide
3	C	121	ASN	Peptide
3	C	142	ASN	Peptide
3	C	143	GLY	Peptide
3	C	146	MET	Peptide
3	C	154	LEU	Peptide
3	C	168	ALA	Peptide
3	C	175	ASP	Peptide
3	C	189	ILE	Peptide
3	C	190	MET	Peptide
3	C	191	SER	Peptide
3	C	44	GLU	Peptide
3	C	45	PHE	Peptide
3	C	62	ARG	Sidechain,Peptide
3	C	66	SER	Peptide
3	C	77	LEU	Peptide
3	C	91	LYS	Peptide
3	C	93	LEU	Peptide
3	C	94	GLY	Peptide
4	D	201	VAL	Peptide
4	D	341	ILE	Peptide
4	E	297	ASN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	E	64	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6795	0	6785	1629	0
2	B	1157	0	1127	222	0
3	C	1203	0	1176	419	0
4	D	2934	0	2895	387	0
4	E	2934	0	2895	391	0
5	D	27	0	12	7	0
5	E	27	0	12	4	0
All	All	15077	0	14902	2926	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 98.

All (2926) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ILE:HG13	2:B:83:VAL:HG13	1.20	1.19
4:E:361:GLU:HB3	4:E:369:ILE:HD13	1.25	1.19
1:A:390:MET:HB3	1:A:392:LEU:HD23	1.19	1.18
1:A:800:LEU:HG	3:C:162:LYS:HE2	1.19	1.17
4:D:142:LEU:HD21	4:D:165:ILE:HD13	1.17	1.17
1:A:833:TRP:HA	1:A:836:LEU:HD12	1.20	1.16
1:A:17:LEU:HB3	1:A:152:PRO:HG2	1.17	1.15
1:A:193:ILE:HG21	1:A:219:GLU:HB3	1.15	1.15
2:B:116:ILE:HG21	2:B:121:LEU:HD12	1.31	1.13
1:A:530:MET:HE1	4:D:351:THR:HA	1.15	1.13
3:C:191:SER:HA	3:C:192:ILE:HG22	1.17	1.12
1:A:729:LEU:HD21	1:A:781:ARG:HB3	1.30	1.12
1:A:805:PHE:HA	1:A:808:MET:HE3	1.26	1.12
2:B:108:LEU:HD22	2:B:116:ILE:HD13	1.20	1.12
1:A:390:MET:HG2	1:A:618:LEU:HD22	1.12	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HG22	1:A:126:VAL:HG23	1.13	1.11
4:D:154:ASP:HA	4:D:300:SER:HB3	1.30	1.11
1:A:207:LYS:HD2	1:A:454:PRO:HD2	1.13	1.10
1:A:32:PHE:HB3	1:A:83:PRO:HG3	1.34	1.10
1:A:360:HIS:HB3	1:A:382:VAL:HG13	1.29	1.09
3:C:68:ILE:HD12	3:C:95:ASN:HB2	1.32	1.09
4:D:212:ILE:HG23	4:D:216:LEU:HD12	1.35	1.09
4:E:76:ILE:HG21	4:E:82:MET:HG2	1.21	1.09
1:A:94:MET:HE1	1:A:101:ALA:HB1	1.16	1.09
4:D:185:LEU:HD11	4:D:261:LEU:HD21	1.18	1.08
4:D:251:GLY:HA2	4:D:254:ARG:HG3	1.32	1.08
1:A:611:TYR:HB3	1:A:622:LEU:HD13	1.09	1.08
3:C:42:LYS:HA	3:C:43:ILE:HB	1.30	1.08
1:A:173:GLN:HB2	1:A:459:ILE:HG23	1.23	1.07
1:A:295:LYS:HZ2	1:A:332:LEU:HA	1.18	1.07
1:A:296:LYS:HE2	1:A:299:LEU:HB2	1.33	1.07
1:A:351:ILE:HG12	1:A:437:MET:HE3	1.34	1.07
1:A:520:ALA:HA	1:A:523:ILE:HD11	1.31	1.07
2:B:79:ILE:HD11	2:B:84:PHE:HA	1.30	1.07
4:E:37:ARG:HG2	4:E:38:PRO:HD2	1.30	1.06
1:A:255:GLY:HA2	1:A:456:GLN:H	1.18	1.06
1:A:804:GLU:HB3	1:A:808:MET:HE2	1.38	1.06
1:A:789:MET:HE2	3:C:150:LEU:HD11	1.38	1.05
4:E:102:PRO:HB3	4:E:131:ALA:HB3	1.34	1.05
1:A:524:GLU:HG3	1:A:528:LYS:HD3	1.37	1.05
1:A:644:LYS:HD3	1:A:649:GLN:HG3	1.37	1.05
4:E:135:ALA:HB1	4:E:140:LEU:HD21	1.38	1.05
1:A:175:ILE:HD11	1:A:461:VAL:HG22	1.37	1.05
2:B:58:MET:HG3	2:B:60:ARG:H	1.15	1.04
3:C:92:VAL:HG11	3:C:100:GLU:HB2	1.06	1.04
1:A:338:ILE:HG21	1:A:348:LYS:HD2	1.36	1.04
1:A:564:ASN:HA	1:A:582:VAL:HG11	1.35	1.04
3:C:170:MET:HE3	3:C:186:VAL:HG23	1.37	1.03
1:A:1:MET:O	1:A:2:SER:O	1.76	1.03
4:E:300:SER:HA	4:E:335:ARG:HG3	1.37	1.03
1:A:569:LYS:HG2	1:A:570:PRO:HD2	1.33	1.02
1:A:46:MET:HB2	1:A:690:HIS:HB2	1.38	1.02
1:A:207:LYS:HE2	1:A:453:GLN:HB3	1.41	1.02
4:D:142:LEU:HD11	4:D:165:ILE:HD11	1.41	1.02
1:A:708:ILE:HA	1:A:711:LYS:HE2	1.40	1.01
1:A:97:LEU:HD13	1:A:706:ILE:HG23	1.41	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:299:MET:HE2	4:D:304:THR:HB	1.39	1.01
1:A:736:GLU:HA	1:A:740:ILE:HD11	1.41	1.01
4:E:61:LYS:HB3	4:E:65:LEU:HD23	1.41	1.01
4:E:120:THR:HB	4:E:367:PRO:HB3	1.40	1.00
4:D:34:ILE:HG22	4:D:68:LYS:H	1.23	1.00
4:E:151:ILE:HG23	4:E:297:ASN:HB3	1.40	1.00
4:D:299:MET:HE1	4:D:309:ILE:HG21	1.44	1.00
1:A:46:MET:HA	1:A:46:MET:HE2	1.39	1.00
3:C:54:LYS:HA	3:C:54:LYS:HE3	1.43	1.00
3:C:92:VAL:HG21	3:C:100:GLU:HG3	1.42	0.99
3:C:150:LEU:HD22	3:C:154:LEU:HD23	1.44	0.99
4:E:116:ARG:HH11	4:E:371:HIS:HA	1.25	0.99
3:C:86:ASN:HB3	3:C:91:LYS:HD3	1.43	0.98
1:A:130:LYS:HD3	1:A:132:LEU:HD11	1.45	0.98
4:D:357:ILE:HG12	4:D:370:VAL:HG23	1.45	0.97
1:A:9:ILE:HG22	1:A:20:PRO:HA	1.43	0.97
2:B:65:ASN:HB2	2:B:66:GLU:HG2	1.45	0.97
2:B:83:VAL:HA	2:B:86:THR:HG22	1.44	0.97
1:A:831:TRP:HE3	1:A:834:MET:HG2	1.28	0.96
1:A:103:LEU:HD22	1:A:690:HIS:HD2	1.28	0.96
1:A:272:LYS:HD3	1:A:431:LYS:HB3	1.45	0.96
1:A:314:PHE:CZ	1:A:362:GLY:HA2	2.01	0.96
2:B:58:MET:HE3	2:B:60:ARG:HB2	1.44	0.96
1:A:530:MET:HE1	4:D:351:THR:CA	1.95	0.96
4:D:104:LEU:HB2	4:D:356:TRP:CH2	2.01	0.96
4:D:120:THR:HB	4:D:367:PRO:HB3	1.46	0.96
4:E:34:ILE:HB	4:E:54:VAL:HG11	1.44	0.96
1:A:789:MET:HE3	3:C:130:PHE:CE1	2.01	0.96
1:A:390:MET:HB3	1:A:392:LEU:CD2	1.95	0.96
1:A:811:ARG:HG2	1:A:815:ILE:HD11	1.45	0.95
1:A:358:VAL:HG22	1:A:430:ALA:HA	1.48	0.95
1:A:296:LYS:HD2	1:A:331:LEU:HD11	1.46	0.95
1:A:225:ALA:HA	1:A:341:LEU:HD23	1.47	0.95
1:A:418:ASN:H	1:A:421:GLN:HG2	1.26	0.95
1:A:817:CYS:HA	1:A:820:TYR:CE2	2.02	0.95
4:D:272:ALA:HB1	4:D:276:GLU:HG3	1.49	0.95
4:D:35:VAL:HG12	4:D:68:LYS:HB2	1.48	0.95
4:E:198:TYR:CZ	4:E:248:ILE:HG22	2.01	0.94
2:B:120:PHE:HE2	2:B:124:LEU:HD23	1.31	0.94
1:A:799:TYR:CD1	3:C:166:VAL:HG12	2.03	0.94
1:A:128:PRO:HB2	1:A:132:LEU:HD21	1.49	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:LEU:HD21	4:D:274:ILE:HD12	1.49	0.93
4:E:140:LEU:HD13	4:E:343:GLY:CA	1.98	0.93
2:B:52:ARG:HD2	2:B:64:LYS:HG3	1.50	0.93
3:C:70:LEU:HG	3:C:91:LYS:HD2	1.47	0.93
1:A:107:LYS:CB	1:A:688:MET:HG3	1.98	0.93
1:A:247:GLY:N	1:A:269:LEU:HD11	1.84	0.93
1:A:97:LEU:HD13	1:A:706:ILE:CG2	1.97	0.93
2:B:120:PHE:CE2	2:B:124:LEU:HD23	2.02	0.93
3:C:67:LYS:HE3	3:C:101:MET:HB3	1.51	0.92
1:A:603:LEU:HG	1:A:648:PHE:CD1	2.04	0.92
4:D:39:ARG:HE	4:D:66:THR:HA	1.31	0.92
3:C:70:LEU:CG	3:C:91:LYS:HD2	2.00	0.92
4:D:37:ARG:HG2	4:D:38:PRO:HD2	1.51	0.92
4:D:297:ASN:HB2	4:D:329:ILE:HD13	1.49	0.92
4:E:34:ILE:HD12	4:E:67:LEU:HD13	1.51	0.92
3:C:42:LYS:HD2	3:C:47:LYS:CA	2.00	0.92
2:B:108:LEU:HD11	2:B:124:LEU:HD21	1.51	0.92
2:B:51:LEU:HB3	2:B:68:LEU:HD11	1.52	0.91
1:A:390:MET:CG	1:A:618:LEU:HD22	2.00	0.91
4:D:189:LEU:HD23	4:D:209:VAL:HG13	1.48	0.91
1:A:475:LEU:HD13	1:A:595:TRP:CZ3	2.05	0.91
1:A:163:TYR:CD2	1:A:199:ILE:HG21	2.06	0.91
4:E:300:SER:HA	4:E:335:ARG:CG	2.00	0.91
2:B:35:PHE:HD1	2:B:46:ILE:HD13	1.36	0.91
1:A:115:ILE:HG21	1:A:128:PRO:HD3	1.53	0.91
4:D:133:TYR:CZ	4:D:375:PHE:HB2	2.06	0.91
1:A:272:LYS:HB3	1:A:431:LYS:CG	2.00	0.90
1:A:272:LYS:HB3	1:A:431:LYS:HD2	1.54	0.90
1:A:51:MET:SD	1:A:63:LYS:HE3	2.12	0.90
1:A:825:PHE:CZ	1:A:829:LYS:HB3	2.06	0.90
1:A:377:PRO:HG2	1:A:398:LEU:HD22	1.53	0.90
2:B:58:MET:HE3	2:B:60:ARG:CB	1.99	0.90
3:C:159:GLU:HG2	3:C:162:LYS:HD3	1.53	0.90
4:D:185:LEU:HD11	4:D:261:LEU:CD2	2.00	0.90
1:A:618:LEU:HG	1:A:622:LEU:HD12	1.53	0.90
1:A:740:ILE:CG2	1:A:745:ALA:HB2	2.01	0.90
1:A:524:GLU:CG	1:A:528:LYS:HD3	2.02	0.90
1:A:236:LYS:HG2	1:A:241:ASP:HA	1.54	0.90
4:D:34:ILE:HG21	4:D:67:LEU:HB3	1.52	0.90
4:E:236:LEU:HD13	4:E:251:GLY:CA	2.02	0.90
1:A:14:ALA:HB3	1:A:15:PRO:HD3	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:HIS:CD2	1:A:592:ILE:HG12	2.06	0.90
1:A:232:PHE:CD2	1:A:287:ILE:HG12	2.07	0.89
4:D:35:VAL:HA	4:D:54:VAL:HG21	1.55	0.89
1:A:719:TYR:CE1	1:A:767:VAL:HB	2.07	0.89
4:D:287:ILE:HB	4:E:244:ASP:HB3	1.51	0.89
1:A:729:LEU:HD21	1:A:781:ARG:CB	2.03	0.89
3:C:92:VAL:HG11	3:C:100:GLU:CB	2.00	0.89
1:A:166:MET:HE1	1:A:254:PHE:CG	2.08	0.89
3:C:45:PHE:N	3:C:46:SER:HB2	1.88	0.89
3:C:123:ASP:HB3	3:C:126:THR:CG2	2.03	0.89
3:C:180:ILE:HD12	3:C:181:ASN:H	1.38	0.89
4:E:35:VAL:HG22	4:E:52:SER:HB2	1.53	0.89
1:A:102:VAL:HG21	1:A:694:MET:HE1	1.55	0.89
1:A:193:ILE:HG21	1:A:219:GLU:CB	2.02	0.89
1:A:205:LYS:CG	1:A:257:THR:HG21	2.03	0.89
2:B:65:ASN:CB	2:B:66:GLU:HG2	2.02	0.89
3:C:152:HIS:CE1	3:C:160:LYS:HA	2.07	0.89
1:A:557:GLN:HG3	1:A:558:HIS:CD2	2.08	0.89
3:C:62:ARG:HD2	3:C:63:THR:N	1.88	0.89
3:C:140:GLU:HB3	3:C:180:ILE:HD11	1.50	0.89
1:A:272:LYS:HB3	1:A:431:LYS:HG2	1.53	0.88
1:A:445:ILE:HG12	1:A:449:LEU:CD1	2.03	0.88
1:A:225:ALA:HA	1:A:341:LEU:CD2	2.03	0.88
1:A:296:LYS:CD	1:A:331:LEU:HD11	2.03	0.88
1:A:39:PHE:HB3	1:A:100:PRO:HG2	1.56	0.88
1:A:173:GLN:HB2	1:A:459:ILE:CG2	2.03	0.88
1:A:546:THR:HG23	1:A:548:THR:H	1.35	0.88
4:D:35:VAL:CA	4:D:54:VAL:HG21	2.03	0.88
3:C:62:ARG:HB3	3:C:62:ARG:HH11	1.38	0.88
4:E:357:ILE:CG1	4:E:370:VAL:HG23	2.03	0.88
1:A:406:VAL:HG12	1:A:605:GLU:HB2	1.56	0.88
1:A:39:PHE:HB2	1:A:78:PHE:HB2	1.56	0.88
2:B:79:ILE:CG1	2:B:83:VAL:HG13	2.02	0.88
1:A:115:ILE:HG22	1:A:126:VAL:CG2	2.00	0.88
1:A:749:LEU:HD11	1:A:753:ILE:HD11	1.56	0.88
4:E:113:LYS:HB3	4:E:371:HIS:CD2	2.08	0.88
1:A:730:ASN:HB3	1:A:749:LEU:HD13	1.54	0.88
4:E:123:MET:HA	4:E:123:MET:HE2	1.56	0.88
1:A:255:GLY:HA2	1:A:456:GLN:N	1.88	0.87
1:A:415:LYS:CB	4:D:333:PRO:HG2	2.04	0.87
3:C:83:ASN:HB2	3:C:84:PRO:HD3	1.56	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:LEU:HD22	3:C:154:LEU:CD2	2.04	0.87
3:C:152:HIS:HE1	3:C:160:LYS:HA	1.37	0.87
3:C:92:VAL:HG22	3:C:95:ASN:HA	1.55	0.87
1:A:578:HIS:CD2	1:A:591:ASN:HA	2.09	0.87
1:A:800:LEU:HG	3:C:162:LYS:CE	2.03	0.87
1:A:91:MET:HE2	1:A:102:VAL:HA	1.56	0.87
3:C:191:SER:HA	3:C:192:ILE:CG2	2.04	0.87
1:A:256:ALA:HA	1:A:456:GLN:HB2	1.55	0.87
1:A:296:LYS:HE2	1:A:299:LEU:CB	2.04	0.87
2:B:154:TYR:O	2:B:157:ILE:HG12	1.75	0.87
2:B:160:VAL:HG23	2:B:165:ASP:HB2	1.55	0.87
1:A:737:GLY:HA3	1:A:739:PHE:CD2	2.09	0.86
4:E:236:LEU:HD13	4:E:251:GLY:HA2	1.58	0.86
1:A:13:ALA:HB1	1:A:139:VAL:HG13	1.56	0.86
1:A:232:PHE:CG	1:A:287:ILE:HG21	2.10	0.86
1:A:404:PRO:HB3	1:A:606:THR:HB	1.57	0.86
1:A:272:LYS:HB3	1:A:431:LYS:CD	2.06	0.86
1:A:611:TYR:CD2	1:A:618:LEU:HD21	2.11	0.86
1:A:221:GLN:HE21	1:A:449:LEU:HD23	1.39	0.86
3:C:135:ARG:NH1	3:C:139:LYS:HB3	1.90	0.86
1:A:9:ILE:HD13	1:A:18:ARG:NH2	1.91	0.85
1:A:789:MET:HE3	3:C:130:PHE:CZ	2.09	0.85
4:E:190:MET:CE	4:E:206:ARG:HA	2.06	0.85
1:A:78:PHE:HD2	1:A:98:HIS:HD2	1.22	0.85
1:A:418:ASN:N	1:A:421:GLN:HG2	1.90	0.85
1:A:612:GLN:O	1:A:619:LEU:HG	1.74	0.85
1:A:421:GLN:HE21	1:A:422:VAL:HG12	1.39	0.85
4:D:357:ILE:CG1	4:D:370:VAL:HG23	2.06	0.85
1:A:207:LYS:HD3	1:A:259:LYS:HB2	1.57	0.85
1:A:375:ALA:HB3	1:A:417:GLN:HE22	1.42	0.85
3:C:41:ILE:O	3:C:43:ILE:HG13	1.76	0.85
4:D:34:ILE:HB	4:D:54:VAL:HG11	1.59	0.85
4:D:299:MET:CE	4:D:304:THR:HB	2.05	0.85
1:A:495:MET:CE	1:A:708:ILE:HG21	2.06	0.85
1:A:833:TRP:NE1	2:B:71:MET:HG2	1.91	0.85
1:A:611:TYR:CB	1:A:622:LEU:HD13	2.02	0.85
1:A:9:ILE:CG2	1:A:20:PRO:HA	2.05	0.85
1:A:290:GLN:NE2	1:A:330:GLU:HB3	1.90	0.85
1:A:9:ILE:HG21	1:A:21:GLU:H	1.41	0.85
1:A:232:PHE:CD1	1:A:287:ILE:HG21	2.11	0.85
1:A:296:LYS:CG	1:A:331:LEU:HD11	2.07	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:GLU:HB3	1:A:508:ILE:HD11	1.59	0.85
2:B:35:PHE:CD1	2:B:46:ILE:HD13	2.12	0.85
3:C:92:VAL:HG23	3:C:93:LEU:H	1.42	0.85
3:C:191:SER:CA	3:C:192:ILE:HG22	2.05	0.85
4:D:154:ASP:CA	4:D:300:SER:HB3	2.05	0.85
1:A:618:LEU:HG	1:A:622:LEU:CD1	2.05	0.84
1:A:811:ARG:HG2	1:A:815:ILE:CD1	2.05	0.84
4:D:189:LEU:HD23	4:D:209:VAL:CG1	2.06	0.84
1:A:99:GLU:HA	1:A:102:VAL:HG13	1.57	0.84
2:B:79:ILE:HD11	2:B:84:PHE:CA	2.05	0.84
1:A:335:ASP:O	1:A:338:ILE:HG22	1.78	0.84
3:C:140:GLU:HG2	3:C:180:ILE:HG12	1.59	0.84
1:A:19:LYS:H	1:A:114:MET:HE1	1.43	0.84
1:A:736:GLU:HA	1:A:740:ILE:CD1	2.08	0.84
3:C:42:LYS:HE2	3:C:113:PRO:HG3	1.56	0.84
1:A:207:LYS:HD3	1:A:259:LYS:CB	2.06	0.84
2:B:137:ILE:HD13	2:B:141:TRP:HE1	1.43	0.84
1:A:303:LEU:HD22	1:A:305:ILE:CG1	2.08	0.84
1:A:131:TRP:C	1:A:132:LEU:HD13	2.02	0.83
4:E:79:TRP:CD2	4:E:118:LYS:HG2	2.13	0.83
1:A:329:GLU:O	1:A:332:LEU:HG	1.78	0.83
1:A:833:TRP:CZ2	2:B:71:MET:HE3	2.13	0.83
3:C:90:LYS:HB2	3:C:111:PHE:HE2	1.42	0.83
4:D:35:VAL:HG12	4:D:68:LYS:CB	2.09	0.83
4:E:236:LEU:CD1	4:E:237:GLU:HG2	2.08	0.83
1:A:116:TYR:CD1	1:A:125:THR:HB	2.13	0.83
4:E:76:ILE:CG2	4:E:82:MET:HG2	2.07	0.83
1:A:495:MET:HE2	1:A:708:ILE:HG21	1.59	0.83
1:A:188:ASN:O	1:A:192:VAL:HG22	1.79	0.83
4:E:116:ARG:NH1	4:E:371:HIS:HA	1.93	0.83
4:E:133:TYR:CZ	4:E:375:PHE:HB2	2.13	0.83
1:A:223:ILE:HD12	1:A:224:GLN:N	1.94	0.83
3:C:135:ARG:HG3	3:C:138:ASP:H	1.44	0.83
4:D:104:LEU:HB2	4:D:356:TRP:HH2	1.42	0.83
1:A:111:ALA:HA	1:A:686:GLY:HA2	1.60	0.83
1:A:113:TRP:CE3	1:A:130:LYS:HE2	2.12	0.83
3:C:152:HIS:O	3:C:157:LEU:HB3	1.78	0.83
3:C:128:GLU:HB2	3:C:180:ILE:HG22	1.59	0.83
4:E:361:GLU:CB	4:E:369:ILE:HD13	2.07	0.83
1:A:253:HIS:HB2	1:A:455:ARG:CD	2.09	0.83
1:A:296:LYS:HB3	1:A:331:LEU:HD21	1.58	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PRO:O	1:A:300:ILE:HG12	1.78	0.83
4:D:285:CYS:HB3	4:D:289:ILE:HD11	1.58	0.83
1:A:16:TYR:CZ	1:A:132:LEU:HB3	2.14	0.83
1:A:295:LYS:HG3	1:A:331:LEU:HD22	1.60	0.82
1:A:611:TYR:HD2	1:A:618:LEU:HD21	1.42	0.82
1:A:801:MET:HE2	3:C:72:GLN:NE2	1.93	0.82
4:E:107:GLU:O	4:E:137:GLN:HG3	1.79	0.82
1:A:19:LYS:HD3	1:A:23:GLU:HB3	1.60	0.82
1:A:442:VAL:O	1:A:445:ILE:HG22	1.79	0.82
1:A:207:LYS:CD	1:A:259:LYS:HB2	2.09	0.82
3:C:57:PHE:HA	3:C:60:TYR:CD2	2.14	0.82
2:B:116:ILE:CG2	2:B:121:LEU:HD12	2.10	0.82
1:A:195:TYR:CZ	1:A:199:ILE:HD11	2.14	0.82
1:A:397:MET:O	1:A:401:LEU:HD23	1.80	0.82
4:E:36:GLY:O	4:E:52:SER:HA	1.79	0.82
4:E:79:TRP:CE2	4:E:118:LYS:HG2	2.14	0.82
1:A:535:ILE:HD12	1:A:557:GLN:NE2	1.95	0.82
1:A:659:LEU:HD11	1:A:663:MET:HE3	1.61	0.82
4:D:153:LEU:CD2	4:D:274:ILE:HD12	2.08	0.82
4:E:8:LEU:HD12	4:E:90:PHE:HE1	1.43	0.82
1:A:749:LEU:O	1:A:753:ILE:HG12	1.80	0.82
1:A:800:LEU:O	1:A:803:VAL:HG12	1.79	0.82
3:C:82:THR:O	3:C:85:THR:HG22	1.79	0.82
1:A:16:TYR:CD1	1:A:134:VAL:HG23	2.15	0.82
1:A:115:ILE:HG21	1:A:128:PRO:CD	2.10	0.82
3:C:42:LYS:HA	3:C:43:ILE:CB	2.09	0.82
4:D:169:TYR:CD1	4:E:42:GLY:HA3	2.14	0.82
4:D:290:ARG:NH1	4:E:244:ASP:HB2	1.94	0.82
1:A:39:PHE:CB	1:A:100:PRO:HG2	2.10	0.82
1:A:346:GLU:O	1:A:349:VAL:HG12	1.80	0.82
2:B:28:ILE:HD12	2:B:29:GLN:N	1.95	0.82
4:D:22:ALA:HB1	4:D:348:SER:HB3	1.59	0.82
4:E:106:THR:HG22	4:E:135:ALA:HB3	1.62	0.82
1:A:173:GLN:CB	1:A:459:ILE:HG23	2.08	0.82
1:A:740:ILE:HG21	1:A:745:ALA:HB2	1.62	0.82
3:C:80:LEU:HB2	3:C:121:ASN:OD1	1.80	0.82
2:B:97:PRO:O	2:B:100:VAL:HG12	1.80	0.81
1:A:73:ASN:H	1:A:76:GLN:HG2	1.43	0.81
1:A:94:MET:CE	1:A:101:ALA:HB1	2.05	0.81
1:A:144:ARG:HH22	1:A:199:ILE:HD13	1.44	0.81
1:A:445:ILE:HG23	1:A:449:LEU:HD12	1.63	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LYS:HD2	1:A:555:TYR:HE2	1.45	0.81
1:A:392:LEU:HD11	1:A:613:LYS:C	2.05	0.81
4:E:140:LEU:HD13	4:E:343:GLY:HA3	1.61	0.81
1:A:19:LYS:HD3	1:A:23:GLU:CB	2.11	0.81
1:A:49:LYS:HD3	1:A:65:LEU:HD23	1.60	0.81
1:A:530:MET:CE	4:D:351:THR:HA	2.07	0.81
1:A:817:CYS:HA	1:A:820:TYR:CZ	2.16	0.81
4:E:35:VAL:HG12	4:E:68:LYS:HB3	1.62	0.81
1:A:72:LEU:HB3	1:A:76:GLN:HG2	1.63	0.81
1:A:364:MET:CG	1:A:382:VAL:HB	2.11	0.81
1:A:366:PHE:CD2	1:A:422:VAL:HG21	2.15	0.81
1:A:468:GLU:OE2	1:A:480:ILE:HD13	1.79	0.81
1:A:175:ILE:CD1	1:A:461:VAL:HG13	2.11	0.81
1:A:428:ALA:HA	1:A:431:LYS:HE2	1.63	0.81
1:A:605:GLU:O	1:A:608:VAL:HG12	1.81	0.81
1:A:644:LYS:CD	1:A:649:GLN:HG3	2.11	0.81
3:C:137:PHE:CD2	3:C:139:LYS:HB2	2.15	0.81
1:A:19:LYS:N	1:A:114:MET:HE1	1.96	0.81
1:A:159:SER:HB3	1:A:195:TYR:CD2	2.16	0.81
1:A:424:ASN:HD21	1:A:602:PRO:HD2	1.45	0.81
1:A:787:THR:O	1:A:791:ARG:HD3	1.80	0.81
4:D:58:ALA:HB1	4:D:65:LEU:HD22	1.63	0.81
4:E:155:SER:HB3	4:E:160:THR:HG23	1.63	0.81
1:A:13:ALA:CB	1:A:139:VAL:HG22	2.11	0.81
1:A:727:ARG:NH1	1:A:745:ALA:HB1	1.96	0.81
3:C:113:PRO:O	3:C:116:GLN:HB3	1.80	0.81
1:A:232:PHE:CE1	1:A:287:ILE:HG21	2.16	0.80
3:C:90:LYS:HB2	3:C:111:PHE:CE2	2.16	0.80
4:D:209:VAL:HA	4:D:212:ILE:HD12	1.63	0.80
1:A:349:VAL:O	1:A:352:TYR:HB2	1.81	0.80
2:B:58:MET:HG3	2:B:60:ARG:N	1.96	0.80
1:A:472:PHE:CE1	1:A:591:ASN:HB3	2.16	0.80
1:A:493:HIS:HA	1:A:514:ASP:OD2	1.80	0.80
1:A:569:LYS:HD3	1:A:570:PRO:O	1.82	0.80
4:D:295:ALA:O	4:D:328:LYS:HB3	1.80	0.80
1:A:232:PHE:CD2	1:A:287:ILE:HG21	2.16	0.80
3:C:91:LYS:HE2	3:C:95:ASN:OD1	1.82	0.80
4:E:34:ILE:CB	4:E:54:VAL:HG11	2.11	0.80
1:A:805:PHE:HA	1:A:808:MET:CE	2.11	0.80
2:B:83:VAL:CA	2:B:86:THR:HG22	2.10	0.80
1:A:784:LYS:HD2	1:A:788:LEU:HD11	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:THR:HG21	2:B:154:TYR:CE2	2.17	0.80
2:B:125:LEU:HB3	2:B:132:PHE:CD1	2.17	0.80
3:C:98:ASN:HB3	3:C:99:GLU:HA	1.63	0.80
1:A:693:VAL:HA	1:A:696:GLN:HG3	1.63	0.80
3:C:72:GLN:HA	3:C:75:ASP:OD2	1.81	0.80
1:A:176:LEU:CD1	1:A:673:PHE:HA	2.12	0.80
3:C:67:LYS:CD	3:C:92:VAL:HG13	2.12	0.80
3:C:170:MET:CE	3:C:186:VAL:HG23	2.11	0.80
4:E:139:VAL:HG12	4:E:140:LEU:HD23	1.64	0.80
1:A:130:LYS:HG3	1:A:685:PRO:HG3	1.63	0.79
1:A:253:HIS:HB2	1:A:455:ARG:HD2	1.64	0.79
1:A:261:ALA:HB2	1:A:455:ARG:N	1.96	0.79
1:A:291:ILE:HG13	1:A:296:LYS:HZ2	1.46	0.79
1:A:392:LEU:HD11	1:A:613:LYS:O	1.81	0.79
2:B:43:ASP:O	2:B:45:ILE:HG23	1.79	0.79
4:E:236:LEU:HD22	4:E:251:GLY:C	2.08	0.79
4:E:300:SER:HA	4:E:335:ARG:CD	2.13	0.79
1:A:89:GLU:O	1:A:117:THR:HG23	1.83	0.79
1:A:375:ALA:HB3	1:A:417:GLN:NE2	1.96	0.79
4:E:178:LEU:HD21	4:E:180:LEU:HB3	1.65	0.79
1:A:42:ASP:HB2	1:A:48:VAL:HG23	1.65	0.79
1:A:111:ALA:CA	1:A:686:GLY:HA2	2.12	0.79
1:A:217:THR:HB	1:A:218:LEU:O	1.81	0.79
2:B:70:ALA:O	2:B:73:LYS:HG2	1.82	0.79
1:A:283:ARG:HD2	1:A:289:TYR:CE2	2.18	0.79
1:A:385:LYS:O	1:A:389:LEU:HD12	1.83	0.79
1:A:611:TYR:HB3	1:A:622:LEU:CD1	2.03	0.79
2:B:61:LEU:HD22	2:B:62:ASN:H	1.47	0.79
3:C:57:PHE:CE2	3:C:69:THR:HG21	2.16	0.79
4:D:244:ASP:OD2	4:D:246:GLN:HG3	1.82	0.79
4:D:250:ILE:HG12	4:D:251:GLY:H	1.46	0.79
1:A:256:ALA:N	1:A:456:GLN:HG3	1.98	0.79
4:E:34:ILE:HB	4:E:54:VAL:CG1	2.13	0.79
4:E:357:ILE:HG12	4:E:370:VAL:HG23	1.63	0.79
1:A:107:LYS:HB2	1:A:688:MET:HG3	1.64	0.79
1:A:568:PRO:HG2	1:A:577:ALA:HB3	1.65	0.79
1:A:644:LYS:HD3	1:A:649:GLN:CG	2.11	0.79
1:A:717:ILE:CG2	1:A:721:ASP:HB3	2.12	0.79
3:C:123:ASP:HB3	3:C:126:THR:HG22	1.64	0.79
1:A:47:TYR:CD2	1:A:100:PRO:HG3	2.18	0.79
1:A:535:ILE:HG23	1:A:553:LYS:HE2	1.63	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:ALA:HA	3:C:163:GLU:OE2	1.83	0.79
1:A:25:ILE:HD12	1:A:26:GLU:N	1.97	0.79
1:A:210:GLN:HG3	1:A:211:PRO:N	1.96	0.79
1:A:355:THR:CG2	1:A:437:MET:HE1	2.13	0.79
1:A:392:LEU:HD22	1:A:614:SER:HB3	1.65	0.79
3:C:92:VAL:N	3:C:95:ASN:HB3	1.98	0.79
3:C:127:TYR:HE2	3:C:187:LYS:HE2	1.47	0.79
4:D:321:ALA:HB1	4:D:322:PRO:HD2	1.65	0.78
4:E:237:GLU:O	4:E:249:THR:HG23	1.83	0.78
1:A:123:CYS:HG	1:A:153:PRO:HB3	1.47	0.78
1:A:287:ILE:HD12	1:A:288:PHE:N	1.98	0.78
4:D:36:GLY:O	4:D:52:SER:HA	1.82	0.78
4:D:189:LEU:HA	4:D:192:ILE:HD11	1.65	0.78
1:A:272:LYS:CD	1:A:431:LYS:HB3	2.12	0.78
1:A:436:LYS:HD3	1:A:621:PHE:HB3	1.64	0.78
1:A:737:GLY:HA3	1:A:739:PHE:HD2	1.47	0.78
3:C:71:SER:HB2	3:C:86:ASN:CG	2.08	0.78
1:A:16:TYR:CE2	1:A:132:LEU:HG	2.19	0.78
1:A:462:LEU:HD13	1:A:463:ASP:N	1.98	0.78
4:E:189:LEU:HD12	4:E:189:LEU:O	1.84	0.78
4:E:236:LEU:HD12	4:E:237:GLU:HG2	1.66	0.78
4:D:124:PHE:CE2	4:D:362:TYR:HB2	2.19	0.78
1:A:47:TYR:CB	1:A:100:PRO:HG3	2.14	0.78
1:A:176:LEU:HD11	1:A:673:PHE:CD2	2.19	0.78
1:A:247:GLY:H	1:A:269:LEU:HD11	1.45	0.78
1:A:508:ILE:HG13	1:A:768:PHE:CZ	2.19	0.78
1:A:551:LYS:HG2	1:A:555:TYR:CE2	2.18	0.78
4:D:336:LYS:HE2	5:D:401:ADP:H5'2	1.65	0.78
4:E:97:ALA:HB1	4:E:99:GLU:OE1	1.83	0.78
4:E:336:LYS:HE2	5:E:401:ADP:H5'2	1.65	0.78
1:A:476:GLU:O	1:A:480:ILE:HD12	1.83	0.78
4:E:180:LEU:HD12	4:E:181:ALA:H	1.49	0.78
1:A:79:PRO:HD2	1:A:98:HIS:NE2	1.99	0.78
1:A:795:LEU:HD23	3:C:187:LYS:HZ3	1.47	0.78
1:A:824:ALA:O	1:A:828:VAL:HG12	1.82	0.78
2:B:52:ARG:HD2	2:B:64:LYS:CG	2.14	0.78
4:D:39:ARG:HG2	4:D:66:THR:HG22	1.64	0.78
1:A:293:SER:HB3	1:A:327:ASP:HB2	1.65	0.77
3:C:62:ARG:HD2	3:C:63:THR:H	1.46	0.77
1:A:9:ILE:HG23	1:A:18:ARG:NH1	1.99	0.77
1:A:175:ILE:HD11	1:A:461:VAL:CG2	2.11	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HD2	1:A:454:PRO:CD	2.06	0.77
1:A:436:LYS:HB3	1:A:621:PHE:CD1	2.18	0.77
4:E:164:PRO:HG2	4:E:174:ALA:HB1	1.66	0.77
1:A:207:LYS:CE	1:A:259:LYS:HB2	2.13	0.77
1:A:322:VAL:O	1:A:325:ILE:HG22	1.84	0.77
1:A:831:TRP:CE3	1:A:834:MET:HG2	2.17	0.77
3:C:134:LEU:HD21	3:C:150:LEU:HG	1.67	0.77
4:D:183:ARG:HG2	4:D:184:ASP:N	1.98	0.77
1:A:613:LYS:HD3	1:A:613:LYS:N	2.00	0.77
3:C:174:GLU:O	3:C:176:SER:HA	1.85	0.77
4:D:34:ILE:CB	4:D:54:VAL:HG11	2.15	0.77
1:A:5:ALA:HB1	1:A:18:ARG:NH1	2.00	0.77
1:A:62:VAL:HG12	1:A:70:LEU:O	1.85	0.77
1:A:727:ARG:NH2	1:A:749:LEU:HB2	2.00	0.77
4:D:332:PRO:HG2	4:D:335:ARG:CZ	2.15	0.77
1:A:175:ILE:HD12	1:A:175:ILE:O	1.84	0.77
2:B:108:LEU:CD2	2:B:116:ILE:HD13	2.07	0.77
4:D:142:LEU:HD21	4:D:165:ILE:CD1	2.09	0.77
1:A:158:ILE:HA	1:A:161:ASN:HD21	1.50	0.77
3:C:142:ASN:O	3:C:177:ASN:HB3	1.85	0.77
1:A:93:MET:HE2	1:A:93:MET:HA	1.64	0.77
1:A:355:THR:O	1:A:358:VAL:HB	1.85	0.77
3:C:62:ARG:HD2	3:C:62:ARG:C	2.10	0.77
1:A:392:LEU:CD2	1:A:614:SER:HB3	2.13	0.77
1:A:795:LEU:HG	3:C:187:LYS:HD3	1.66	0.77
4:D:34:ILE:HG22	4:D:68:LYS:N	1.99	0.77
1:A:109:ARG:O	1:A:112:ALA:HB3	1.84	0.76
1:A:246:PHE:HA	1:A:269:LEU:CD1	2.15	0.76
1:A:535:ILE:HD12	1:A:557:GLN:CD	2.09	0.76
3:C:123:ASP:O	3:C:126:THR:HG23	1.85	0.76
4:D:142:LEU:CD2	4:D:165:ILE:HD13	2.10	0.76
4:D:233:SER:HB3	4:D:236:LEU:HG	1.66	0.76
4:E:365:ALA:CB	4:E:369:ILE:HD12	2.15	0.76
3:C:42:LYS:HD2	3:C:47:LYS:CB	2.16	0.76
4:E:269:MET:HG2	4:E:271:SER:OG	1.85	0.76
1:A:167:LEU:HD22	1:A:257:THR:C	2.09	0.76
1:A:312:PHE:O	1:A:315:VAL:HG23	1.86	0.76
1:A:415:LYS:CG	4:D:333:PRO:HG2	2.15	0.76
1:A:74:SER:O	1:A:77:VAL:HG22	1.83	0.76
1:A:1:MET:O	1:A:2:SER:C	2.26	0.76
1:A:40:ALA:HB1	1:A:72:LEU:CD2	2.16	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:LYS:CG	1:A:688:MET:HG3	2.16	0.76
1:A:246:PHE:CA	1:A:269:LEU:HD11	2.16	0.76
1:A:288:PHE:O	1:A:292:MET:HE2	1.84	0.76
1:A:671:PRO:HB2	1:A:673:PHE:CE1	2.21	0.76
3:C:109:GLU:O	3:C:113:PRO:HD2	1.85	0.76
3:C:128:GLU:CB	3:C:180:ILE:HG22	2.15	0.76
1:A:62:VAL:HG11	1:A:72:LEU:HD13	1.68	0.76
1:A:91:MET:HE3	1:A:105:ASN:HB3	1.68	0.76
1:A:314:PHE:CE2	1:A:362:GLY:HA2	2.20	0.76
1:A:464:ILE:HG12	1:A:465:ALA:N	1.98	0.76
3:C:92:VAL:CG2	3:C:95:ASN:HA	2.15	0.76
1:A:261:ALA:HB2	1:A:454:PRO:C	2.10	0.76
3:C:58:LEU:HD11	3:C:65:ASP:HB2	1.66	0.76
4:E:37:ARG:HG2	4:E:38:PRO:CD	2.12	0.76
4:E:149:THR:HG22	4:E:150:GLY:H	1.50	0.76
4:E:198:TYR:CE1	4:E:248:ILE:HG22	2.21	0.76
1:A:115:ILE:HG21	1:A:128:PRO:HG3	1.67	0.76
1:A:123:CYS:SG	1:A:153:PRO:HB3	2.26	0.76
1:A:694:MET:HE2	1:A:694:MET:HA	1.65	0.76
3:C:67:LYS:HA	3:C:67:LYS:HE2	1.67	0.76
1:A:360:HIS:HB3	1:A:382:VAL:CG1	2.14	0.75
1:A:838:PHE:CE1	2:B:164:GLY:HA3	2.21	0.75
4:E:299:MET:HE1	4:E:309:ILE:CG1	2.15	0.75
1:A:815:ILE:HG21	2:B:129:CYS:SG	2.26	0.75
3:C:67:LYS:O	3:C:70:LEU:HB2	1.86	0.75
4:D:287:ILE:HB	4:E:244:ASP:CB	2.16	0.75
4:E:190:MET:HE2	4:E:206:ARG:HA	1.67	0.75
1:A:253:HIS:O	1:A:260:LEU:HD22	1.87	0.75
1:A:255:GLY:CA	1:A:456:GLN:H	1.95	0.75
1:A:506:GLU:CB	1:A:508:ILE:HD11	2.16	0.75
3:C:180:ILE:O	3:C:183:GLU:HG3	1.86	0.75
4:E:140:LEU:O	4:E:342:GLY:HA3	1.86	0.75
1:A:64:THR:HG22	1:A:65:LEU:H	1.50	0.75
1:A:717:ILE:HG22	1:A:721:ASP:HB3	1.68	0.75
3:C:140:GLU:CG	3:C:180:ILE:HG12	2.17	0.75
1:A:166:MET:SD	1:A:457:TYR:HB2	2.27	0.75
1:A:424:ASN:ND2	1:A:600:LYS:HG2	2.02	0.75
1:A:825:PHE:HA	1:A:828:VAL:CG1	2.17	0.75
2:B:83:VAL:HA	2:B:86:THR:CG2	2.16	0.75
3:C:66:SER:CB	3:C:68:ILE:HG22	2.17	0.75
1:A:440:TRP:O	1:A:443:THR:HG22	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:LEU:HD11	3:C:162:LYS:HG2	1.69	0.75
1:A:833:TRP:CE2	2:B:71:MET:HG2	2.22	0.75
4:E:164:PRO:HG2	4:E:174:ALA:CB	2.16	0.75
3:C:47:LYS:HG3	3:C:109:GLU:CD	2.11	0.75
3:C:74:GLY:HA3	3:C:112:LEU:HD11	1.68	0.75
1:A:122:PHE:CE1	1:A:673:PHE:HB2	2.22	0.75
1:A:130:LYS:CD	1:A:132:LEU:HD11	2.16	0.75
1:A:421:GLN:HG3	1:A:422:VAL:N	2.02	0.75
1:A:614:SER:N	1:A:619:LEU:HD11	2.00	0.75
4:D:11:ASP:HB3	4:D:18:LYS:HG2	1.68	0.75
1:A:14:ALA:CB	1:A:18:ARG:HD2	2.17	0.74
4:D:326:LYS:C	4:D:327:ILE:HD12	2.12	0.74
4:E:33:SER:C	4:E:34:ILE:HG12	2.12	0.74
1:A:85:PHE:O	1:A:88:ILE:HB	1.87	0.74
1:A:232:PHE:CZ	1:A:287:ILE:HG21	2.23	0.74
1:A:303:LEU:HD22	1:A:305:ILE:HG13	1.66	0.74
4:D:59:GLN:O	4:D:62:ARG:HG3	1.87	0.74
4:E:47:MET:HG3	4:E:48:GLY:H	1.51	0.74
4:E:156:GLY:O	4:E:181:ALA:HB1	1.87	0.74
4:E:332:PRO:HG2	4:E:335:ARG:CZ	2.17	0.74
1:A:514:ASP:HB3	1:A:517:MET:HE3	1.68	0.74
2:B:28:ILE:HG22	2:B:85:LEU:CD2	2.17	0.74
3:C:189:ILE:HG12	3:C:190:MET:N	2.03	0.74
4:E:223:PHE:CE1	4:E:259:GLU:HG2	2.22	0.74
1:A:387:GLY:HA2	1:A:397:MET:SD	2.28	0.74
1:A:831:TRP:CE3	1:A:834:MET:HE2	2.22	0.74
3:C:137:PHE:HD2	3:C:139:LYS:HB2	1.50	0.74
1:A:142:ALA:O	1:A:146:LYS:HD2	1.88	0.74
1:A:390:MET:CB	1:A:392:LEU:HD23	2.10	0.74
1:A:436:LYS:HB3	1:A:621:PHE:HD1	1.53	0.74
1:A:789:MET:CE	3:C:150:LEU:HD11	2.16	0.74
1:A:167:LEU:HD21	1:A:258:GLY:HA3	1.69	0.74
3:C:57:PHE:HA	3:C:60:TYR:HD2	1.51	0.74
3:C:69:THR:HG22	3:C:72:GLN:HB2	1.69	0.74
4:E:39:ARG:HE	4:E:66:THR:HB	1.52	0.74
4:E:163:VAL:HG22	4:E:175:ILE:HG23	1.70	0.74
1:A:253:HIS:CB	1:A:458:PHE:HB3	2.17	0.74
1:A:583:HIS:C	1:A:585:ALA:HB3	2.13	0.74
3:C:180:ILE:HA	3:C:183:GLU:HG2	1.70	0.74
4:D:219:VAL:HG22	4:D:258:PRO:HB2	1.69	0.74
4:E:39:ARG:HE	4:E:66:THR:CB	2.01	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:HIS:CG	1:A:455:ARG:HD2	2.23	0.74
1:A:361:TYR:HA	1:A:364:MET:SD	2.28	0.74
3:C:92:VAL:H	3:C:95:ASN:HB3	1.49	0.74
4:D:158:GLY:HA2	4:D:183:ARG:HD2	1.70	0.74
4:E:365:ALA:HB3	4:E:369:ILE:HD12	1.68	0.74
1:A:159:SER:HB3	1:A:195:TYR:CG	2.22	0.73
1:A:232:PHE:CE2	1:A:287:ILE:HG21	2.24	0.73
1:A:778:GLU:O	1:A:781:ARG:HG3	1.87	0.73
2:B:70:ALA:HA	2:B:73:LYS:CE	2.18	0.73
3:C:135:ARG:CZ	3:C:137:PHE:HB3	2.17	0.73
4:E:34:ILE:CG1	4:E:54:VAL:HG11	2.18	0.73
4:E:178:LEU:HG	4:E:180:LEU:H	1.52	0.73
1:A:81:ASN:ND2	1:A:96:HIS:H	1.86	0.73
1:A:519:LEU:HD22	1:A:584:TYR:HB3	1.68	0.73
2:B:61:LEU:HD22	2:B:62:ASN:N	2.03	0.73
4:E:8:LEU:HD12	4:E:90:PHE:CE1	2.22	0.73
1:A:81:ASN:HD21	1:A:96:HIS:H	1.36	0.73
1:A:229:LEU:HD22	1:A:438:PHE:HE1	1.53	0.73
1:A:332:LEU:HD12	1:A:333:ALA:N	2.02	0.73
2:B:105:PHE:O	2:B:108:LEU:HB2	1.87	0.73
1:A:195:TYR:OH	1:A:199:ILE:HD11	1.88	0.73
1:A:205:LYS:HG2	1:A:257:THR:HG21	1.70	0.73
1:A:780:MET:O	1:A:783:GLU:HG3	1.88	0.73
3:C:142:ASN:H	3:C:177:ASN:N	1.86	0.73
4:D:287:ILE:HG12	4:D:288:ASP:N	2.02	0.73
1:A:46:MET:HA	1:A:46:MET:CE	2.17	0.73
1:A:246:PHE:HA	1:A:269:LEU:HD11	1.70	0.73
1:A:645:GLY:HA2	4:D:23:GLY:HA2	1.70	0.73
4:D:122:ILE:O	4:D:126:THR:HB	1.89	0.73
1:A:520:ALA:HA	1:A:523:ILE:CD1	2.16	0.73
1:A:644:LYS:HZ2	1:A:649:GLN:HB3	1.53	0.73
3:C:50:GLN:NE2	3:C:112:LEU:HB2	2.03	0.73
3:C:148:ALA:HA	3:C:163:GLU:CD	2.13	0.73
4:D:306:TYR:O	4:D:309:ILE:HB	1.88	0.73
1:A:47:TYR:CG	1:A:100:PRO:HG3	2.24	0.73
1:A:841:LYS:HB3	1:A:842:PRO:HD3	1.69	0.73
3:C:156:THR:O	3:C:157:LEU:HD13	1.89	0.73
4:E:206:ARG:HG2	4:E:206:ARG:HH11	1.53	0.73
1:A:197:ALA:O	1:A:201:VAL:HG22	1.88	0.73
1:A:479:CYS:O	1:A:483:THR:HG23	1.89	0.73
1:A:485:GLU:OE1	1:A:523:ILE:HG23	1.89	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:ILE:HG22	1:A:514:ASP:H	1.52	0.73
1:A:755:VAL:HG11	1:A:773:LEU:HD21	1.69	0.73
3:C:47:LYS:HG3	3:C:109:GLU:OE2	1.87	0.73
3:C:67:LYS:CE	3:C:101:MET:HB3	2.19	0.73
4:D:34:ILE:HB	4:D:54:VAL:CG1	2.19	0.73
4:E:153:LEU:HD11	4:E:274:ILE:CG2	2.19	0.73
1:A:546:THR:HG23	1:A:548:THR:N	2.03	0.73
1:A:163:TYR:CE2	1:A:199:ILE:HG21	2.23	0.72
1:A:190:LYS:O	1:A:194:GLN:HG3	1.89	0.72
1:A:220:ASP:HA	1:A:223:ILE:CG1	2.19	0.72
1:A:279:LEU:HD23	1:A:279:LEU:H	1.53	0.72
2:B:58:MET:HE1	2:B:60:ARG:HH11	1.53	0.72
1:A:245:ARG:HG3	1:A:285:TYR:CE1	2.24	0.72
1:A:295:LYS:CB	1:A:331:LEU:HB3	2.18	0.72
1:A:492:ASN:OD1	1:A:708:ILE:HD11	1.89	0.72
4:D:158:GLY:N	4:D:181:ALA:HB3	2.05	0.72
4:E:102:PRO:HB3	4:E:131:ALA:CB	2.18	0.72
1:A:166:MET:HE1	1:A:254:PHE:CD2	2.24	0.72
4:D:346:LEU:O	4:D:349:LEU:HB2	1.90	0.72
1:A:800:LEU:CG	3:C:162:LYS:HE2	2.11	0.72
4:E:189:LEU:HG	4:E:209:VAL:HG13	1.69	0.72
1:A:12:GLU:C	1:A:15:PRO:HD2	2.14	0.72
1:A:207:LYS:CD	1:A:454:PRO:HD2	2.07	0.72
4:D:156:GLY:O	4:D:181:ALA:HB1	1.89	0.72
4:D:299:MET:HE1	4:D:309:ILE:CG2	2.18	0.72
4:D:332:PRO:HG2	4:D:335:ARG:NE	2.04	0.72
1:A:46:MET:HB2	1:A:690:HIS:CB	2.19	0.72
1:A:535:ILE:HG23	1:A:553:LYS:CE	2.19	0.72
3:C:51:ASP:O	3:C:54:LYS:HB3	1.90	0.72
1:A:5:ALA:HB1	1:A:18:ARG:CZ	2.19	0.72
1:A:14:ALA:HB1	1:A:18:ARG:CD	2.20	0.72
1:A:833:TRP:HA	1:A:836:LEU:CD1	2.11	0.72
3:C:69:THR:HB	3:C:73:VAL:HG23	1.70	0.72
4:D:250:ILE:CG1	4:D:253:GLU:HB2	2.20	0.72
4:D:360:GLN:O	4:D:364:GLU:HG3	1.89	0.72
4:E:34:ILE:HD13	4:E:69:TYR:CZ	2.25	0.72
1:A:78:PHE:HB3	1:A:98:HIS:CD2	2.25	0.72
1:A:654:VAL:O	1:A:657:GLU:HB3	1.88	0.72
4:E:370:VAL:HG22	4:E:375:PHE:O	1.89	0.72
1:A:234:ASN:H	1:A:245:ARG:HG2	1.55	0.71
1:A:392:LEU:HD13	1:A:614:SER:HB2	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:736:GLU:O	1:A:740:ILE:HD12	1.90	0.71
4:E:295:ALA:O	4:E:328:LYS:HB3	1.90	0.71
1:A:14:ALA:HB1	1:A:18:ARG:HD2	1.70	0.71
1:A:417:GLN:HA	1:A:421:GLN:CD	2.14	0.71
1:A:115:ILE:HG21	1:A:128:PRO:CG	2.20	0.71
1:A:290:GLN:HE21	1:A:330:GLU:HB3	1.53	0.71
2:B:58:MET:HE1	2:B:60:ARG:NH1	2.05	0.71
1:A:298:GLU:HG3	1:A:299:LEU:N	2.04	0.71
1:A:496:PHE:CG	1:A:514:ASP:HA	2.25	0.71
1:A:584:TYR:H	1:A:584:TYR:HD1	1.36	0.71
1:A:829:LYS:HD2	1:A:830:HIS:CD2	2.25	0.71
4:E:260:THR:HG23	4:E:266:PHE:HB2	1.72	0.71
1:A:520:ALA:CA	1:A:523:ILE:HD11	2.14	0.71
4:E:143:TYR:CE2	4:E:346:LEU:HB2	2.26	0.71
1:A:230:GLU:O	1:A:234:ASN:HB2	1.91	0.71
3:C:140:GLU:CB	3:C:180:ILE:HD11	2.19	0.71
4:E:334:GLU:HA	4:E:334:GLU:OE2	1.89	0.71
1:A:39:PHE:CD1	1:A:100:PRO:HB2	2.25	0.71
1:A:253:HIS:HB3	1:A:458:PHE:HB3	1.73	0.71
1:A:283:ARG:HB2	1:A:289:TYR:OH	1.91	0.71
1:A:415:LYS:HG3	1:A:416:GLY:N	2.06	0.71
1:A:524:GLU:HG3	1:A:528:LYS:CD	2.17	0.71
1:A:32:PHE:HB3	1:A:83:PRO:CG	2.18	0.71
1:A:131:TRP:O	1:A:132:LEU:HD13	1.90	0.71
3:C:71:SER:HB2	3:C:91:LYS:HZ2	1.54	0.71
3:C:108:PHE:CZ	3:C:112:LEU:HG	2.24	0.71
3:C:159:GLU:HG2	3:C:162:LYS:CD	2.21	0.71
1:A:291:ILE:HG13	1:A:296:LYS:NZ	2.06	0.71
1:A:515:PHE:HE1	1:A:711:LYS:HG2	1.55	0.71
1:A:784:LYS:HD2	1:A:788:LEU:CD1	2.21	0.71
2:B:58:MET:CG	2:B:60:ARG:H	1.97	0.71
3:C:68:ILE:O	3:C:91:LYS:HE3	1.91	0.71
4:E:27:PRO:HG3	4:E:340:TRP:CG	2.25	0.71
4:E:34:ILE:HG13	4:E:54:VAL:HG11	1.73	0.71
1:A:267:THR:HG21	1:A:438:PHE:HE2	1.56	0.71
3:C:55:GLU:O	3:C:59:LEU:HD13	1.91	0.71
1:A:79:PRO:HD2	1:A:98:HIS:HE2	1.56	0.70
4:D:250:ILE:HG12	4:D:253:GLU:HB2	1.71	0.70
1:A:166:MET:HE3	1:A:258:GLY:HA2	1.73	0.70
1:A:291:ILE:O	1:A:296:LYS:HD3	1.91	0.70
1:A:488:GLN:HG3	1:A:584:TYR:HE2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:ILE:HG13	1:A:768:PHE:CE2	2.26	0.70
1:A:822:ILE:HG12	2:B:132:PHE:CZ	2.26	0.70
4:D:8:LEU:HD13	4:D:90:PHE:HE1	1.54	0.70
4:E:223:PHE:CD1	4:E:259:GLU:HG2	2.26	0.70
1:A:510:TRP:CE2	1:A:512:PHE:HB2	2.26	0.70
3:C:70:LEU:CB	3:C:91:LYS:HD2	2.21	0.70
4:E:362:TYR:HE1	4:E:367:PRO:HG3	1.56	0.70
1:A:78:PHE:CD2	1:A:98:HIS:HD2	2.07	0.70
1:A:176:LEU:HD11	1:A:673:PHE:HA	1.72	0.70
1:A:263:ALA:HB3	1:A:449:LEU:HD22	1.72	0.70
1:A:292:MET:CE	1:A:309:PRO:HB3	2.21	0.70
1:A:295:LYS:HG2	1:A:332:LEU:CA	2.21	0.70
3:C:45:PHE:H	3:C:46:SER:HB2	1.54	0.70
3:C:67:LYS:HD2	3:C:101:MET:CB	2.20	0.70
3:C:170:MET:HG3	3:C:182:TYR:CE1	2.27	0.70
3:C:179:CYS:O	3:C:183:GLU:HG2	1.91	0.70
4:E:134:VAL:O	4:E:375:PHE:HB3	1.90	0.70
3:C:46:SER:O	3:C:49:GLN:HG2	1.91	0.70
3:C:86:ASN:HB3	3:C:91:LYS:CD	2.21	0.70
4:D:39:ARG:NE	4:D:66:THR:HA	2.05	0.70
2:B:160:VAL:CG2	2:B:165:ASP:HB2	2.22	0.70
4:E:123:MET:HG3	4:E:132:MET:HE2	1.73	0.70
4:E:143:TYR:OH	4:E:349:LEU:HD11	1.91	0.70
1:A:345:SER:O	1:A:348:LYS:HB3	1.92	0.70
1:A:445:ILE:HG12	1:A:449:LEU:HD11	1.74	0.70
3:C:50:GLN:NE2	3:C:109:GLU:HA	2.07	0.70
3:C:57:PHE:HE2	3:C:69:THR:HG21	1.54	0.70
4:E:300:SER:CA	4:E:335:ARG:HG3	2.19	0.70
1:A:99:GLU:HA	1:A:102:VAL:CG1	2.20	0.70
1:A:103:LEU:HD22	1:A:690:HIS:CD2	2.20	0.70
1:A:475:LEU:HD22	1:A:595:TRP:CE3	2.26	0.70
1:A:569:LYS:HG2	1:A:570:PRO:CD	2.15	0.70
3:C:80:LEU:HD22	3:C:187:LYS:NZ	2.06	0.70
3:C:91:LYS:HG3	3:C:95:ASN:ND2	2.07	0.70
4:D:37:ARG:CG	4:D:38:PRO:HD2	2.21	0.70
1:A:128:PRO:CB	1:A:132:LEU:HD21	2.19	0.70
1:A:220:ASP:HA	1:A:223:ILE:HG13	1.72	0.70
3:C:180:ILE:HD12	3:C:181:ASN:N	2.06	0.70
4:D:8:LEU:HD13	4:D:90:PHE:CE1	2.26	0.70
4:D:8:LEU:O	4:D:103:THR:HG23	1.92	0.70
4:E:357:ILE:HG13	4:E:370:VAL:HG23	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:THR:HA	1:A:446:ASN:HD22	1.55	0.69
1:A:822:ILE:CD1	2:B:132:PHE:HE2	2.05	0.69
3:C:91:LYS:HB2	3:C:95:ASN:HB3	1.73	0.69
4:D:185:LEU:CD1	4:D:261:LEU:HD21	2.11	0.69
4:D:220:ALA:HB1	4:D:226:GLU:HG3	1.74	0.69
4:E:34:ILE:CG2	4:E:67:LEU:HB3	2.22	0.69
4:D:143:TYR:CD2	4:D:346:LEU:HD13	2.27	0.69
4:E:35:VAL:HG12	4:E:68:LYS:CB	2.22	0.69
4:E:132:MET:O	4:E:357:ILE:HB	1.92	0.69
1:A:176:LEU:HD11	1:A:673:PHE:CG	2.27	0.69
1:A:296:LYS:HB3	1:A:331:LEU:CD2	2.22	0.69
1:A:485:GLU:HA	1:A:584:TYR:CE1	2.27	0.69
1:A:822:ILE:HD11	2:B:132:PHE:HE2	1.57	0.69
1:A:287:ILE:HD12	1:A:288:PHE:H	1.55	0.69
1:A:405:ARG:H	1:A:606:THR:HG21	1.57	0.69
1:A:90:ASP:HA	1:A:118:TYR:O	1.93	0.69
1:A:210:GLN:HG3	1:A:211:PRO:CD	2.23	0.69
1:A:800:LEU:CD1	3:C:162:LYS:HG2	2.23	0.69
3:C:45:PHE:O	3:C:48:GLU:HG2	1.91	0.69
1:A:293:SER:OG	1:A:328:SER:HA	1.91	0.69
4:D:61:LYS:O	4:D:64:ILE:HG22	1.92	0.69
2:B:108:LEU:HD21	2:B:124:LEU:HD23	1.75	0.69
3:C:111:PHE:O	3:C:115:LEU:HB3	1.92	0.69
4:D:212:ILE:CG2	4:D:216:LEU:HD12	2.20	0.69
1:A:39:PHE:CZ	1:A:80:MET:HE3	2.28	0.69
1:A:93:MET:HE2	1:A:93:MET:CA	2.23	0.69
1:A:103:LEU:HD11	1:A:107:LYS:HD3	1.75	0.69
1:A:272:LYS:HD3	1:A:431:LYS:CB	2.20	0.69
1:A:283:ARG:HD3	1:A:322:VAL:HG23	1.74	0.69
1:A:351:ILE:CG1	1:A:437:MET:HE3	2.18	0.69
1:A:358:VAL:CG2	1:A:430:ALA:HA	2.20	0.69
1:A:541:MET:HE2	4:D:345:ILE:HG23	1.74	0.69
1:A:567:LYS:HD3	1:A:578:HIS:O	1.93	0.69
1:A:760:TYR:HE2	1:A:762:PHE:CE1	2.11	0.69
4:E:310:ALA:HB1	4:E:329:ILE:HG21	1.73	0.69
1:A:380:THR:CG2	1:A:398:LEU:HD11	2.22	0.69
1:A:380:THR:OG1	1:A:398:LEU:HD11	1.93	0.69
4:D:34:ILE:CG2	4:D:67:LEU:HB3	2.22	0.69
1:A:235:ALA:HA	1:A:286:HIS:CE1	2.28	0.69
1:A:337:ALA:O	1:A:340:ILE:HG22	1.93	0.69
1:A:344:SER:O	1:A:347:GLU:HG3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:PRO:HB2	1:A:414:THR:OG1	1.92	0.69
1:A:406:VAL:HG11	1:A:414:THR:HG21	1.74	0.69
1:A:485:GLU:HG2	1:A:584:TYR:HE1	1.58	0.69
1:A:814:SER:HB2	2:B:104:ALA:O	1.92	0.69
4:D:116:ARG:HD3	4:D:370:VAL:HG13	1.75	0.69
1:A:793:GLN:HE22	3:C:156:THR:H	1.39	0.68
3:C:80:LEU:HD22	3:C:187:LYS:HZ3	1.57	0.68
1:A:99:GLU:CA	1:A:102:VAL:HG13	2.22	0.68
1:A:603:LEU:HG	1:A:648:PHE:CG	2.27	0.68
3:C:42:LYS:NZ	3:C:47:LYS:HB2	2.07	0.68
4:E:299:MET:HE1	4:E:309:ILE:HG12	1.75	0.68
1:A:295:LYS:HB3	1:A:331:LEU:HD13	1.74	0.68
1:A:665:ASN:O	1:A:668:SER:HB2	1.93	0.68
1:A:750:LEU:O	1:A:753:ILE:HB	1.94	0.68
3:C:87:ALA:HB1	3:C:94:GLY:CA	2.24	0.68
4:E:180:LEU:HD12	4:E:181:ALA:N	2.08	0.68
1:A:478:LEU:HB2	1:A:590:TYR:CE1	2.27	0.68
2:B:52:ARG:HG2	2:B:68:LEU:CD2	2.23	0.68
4:D:39:ARG:CG	4:D:66:THR:HG22	2.24	0.68
1:A:113:TRP:CZ3	1:A:130:LYS:HE2	2.27	0.68
1:A:253:HIS:CB	1:A:455:ARG:HD2	2.23	0.68
1:A:269:LEU:O	1:A:269:LEU:HD13	1.93	0.68
1:A:383:ALA:O	1:A:386:ALA:HB3	1.93	0.68
3:C:66:SER:HB2	3:C:68:ILE:HG22	1.74	0.68
3:C:71:SER:O	3:C:75:ASP:HB3	1.93	0.68
4:D:282:ILE:HG22	4:D:290:ARG:HD3	1.75	0.68
1:A:21:GLU:HG2	1:A:22:LYS:N	2.07	0.68
1:A:528:LYS:HB2	1:A:529:PRO:HD2	1.75	0.68
2:B:28:ILE:HG22	2:B:85:LEU:HD21	1.75	0.68
4:D:158:GLY:CA	4:D:181:ALA:HB3	2.23	0.68
1:A:404:PRO:HB3	1:A:606:THR:CB	2.24	0.68
1:A:406:VAL:HB	1:A:605:GLU:CD	2.18	0.68
1:A:708:ILE:O	1:A:711:LYS:HB2	1.93	0.68
1:A:740:ILE:HG22	1:A:745:ALA:HB2	1.74	0.68
3:C:188:HIS:O	3:C:189:ILE:HG23	1.93	0.68
4:E:16:LEU:HB2	4:E:18:LYS:NZ	2.08	0.68
1:A:368:GLN:HG3	1:A:376:GLU:CB	2.23	0.68
1:A:423:THR:O	1:A:426:VAL:HG22	1.93	0.68
3:C:42:LYS:HD2	3:C:47:LYS:N	2.09	0.68
3:C:151:ARG:HD2	3:C:163:GLU:OE2	1.94	0.68
4:E:332:PRO:HG2	4:E:335:ARG:NE	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CE1	1:A:125:THR:HB	2.29	0.68
1:A:295:LYS:HB3	1:A:331:LEU:HB3	1.75	0.68
1:A:351:ILE:HG12	1:A:437:MET:CE	2.19	0.68
1:A:578:HIS:NE2	1:A:592:ILE:HG12	2.09	0.68
3:C:91:LYS:HB2	3:C:95:ASN:CG	2.18	0.68
4:D:227:MET:SD	4:D:255:PHE:HE1	2.17	0.68
4:E:113:LYS:HB3	4:E:371:HIS:NE2	2.08	0.68
3:C:167:GLU:HA	3:C:182:TYR:HE1	1.57	0.68
4:E:73:HIC:HA	4:E:183:ARG:HH12	1.59	0.68
4:E:233:SER:OG	4:E:236:LEU:HG	1.94	0.68
1:A:170:ARG:CZ	1:A:256:ALA:HB1	2.24	0.67
1:A:360:HIS:C	1:A:382:VAL:HG11	2.19	0.67
1:A:760:TYR:HE2	1:A:762:PHE:HE1	1.42	0.67
2:B:108:LEU:O	2:B:110:PRO:HD3	1.94	0.67
3:C:46:SER:H	3:C:49:GLN:H	1.40	0.67
3:C:68:ILE:HD11	3:C:95:ASN:O	1.94	0.67
4:D:212:ILE:HG23	4:D:216:LEU:CD1	2.18	0.67
1:A:701:GLY:O	1:A:704:GLU:HB3	1.93	0.67
1:A:793:GLN:NE2	3:C:156:THR:H	1.91	0.67
1:A:837:PHE:O	1:A:840:ILE:HG12	1.93	0.67
3:C:54:LYS:HE3	3:C:54:LYS:CA	2.11	0.67
3:C:167:GLU:HA	3:C:182:TYR:CE1	2.28	0.67
4:D:36:GLY:HA3	4:D:66:THR:O	1.94	0.67
1:A:515:PHE:CD1	1:A:711:LYS:HE3	2.29	0.67
1:A:88:ILE:HG22	1:A:105:ASN:OD1	1.94	0.67
1:A:418:ASN:H	1:A:421:GLN:CG	2.05	0.67
1:A:445:ILE:HG12	1:A:449:LEU:HD12	1.76	0.67
2:B:146:PRO:HG3	2:B:156:ASN:OD1	1.93	0.67
2:B:160:VAL:HG23	2:B:165:ASP:CB	2.25	0.67
3:C:62:ARG:HH11	3:C:62:ARG:CB	2.08	0.67
1:A:238:VAL:HA	1:A:281:SER:O	1.95	0.67
1:A:272:LYS:CB	1:A:431:LYS:HD2	2.24	0.67
1:A:364:MET:HG3	1:A:382:VAL:HB	1.74	0.67
1:A:9:ILE:HG21	1:A:21:GLU:N	2.10	0.67
1:A:17:LEU:HB3	1:A:152:PRO:CG	2.10	0.67
1:A:833:TRP:CH2	2:B:71:MET:HE3	2.30	0.67
2:B:125:LEU:HD22	2:B:132:PHE:CE1	2.29	0.67
4:D:58:ALA:CB	4:D:65:LEU:HD22	2.25	0.67
4:D:257:CYS:HB3	4:D:258:PRO:HD3	1.76	0.67
1:A:81:ASN:OD1	1:A:95:THR:HG22	1.95	0.67
1:A:462:LEU:HD13	1:A:463:ASP:H	1.60	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLN:NE2	1:A:449:LEU:HD23	2.09	0.67
4:D:22:ALA:CB	4:D:348:SER:HB3	2.25	0.67
3:C:170:MET:HE1	3:C:186:VAL:HA	1.75	0.67
4:D:102:PRO:HB3	4:D:131:ALA:HB3	1.75	0.67
4:D:189:LEU:HD12	4:D:192:ILE:HD11	1.76	0.67
1:A:564:ASN:CA	1:A:582:VAL:HG11	2.19	0.67
1:A:729:LEU:CD2	1:A:781:ARG:HA	2.25	0.67
3:C:127:TYR:CE2	3:C:187:LYS:HG2	2.30	0.67
4:D:133:TYR:HB2	4:D:356:TRP:CE3	2.30	0.67
1:A:226:ASN:HB2	1:A:227:PRO:HD3	1.77	0.66
1:A:253:HIS:HA	1:A:458:PHE:CB	2.25	0.66
2:B:70:ALA:HA	2:B:73:LYS:CD	2.25	0.66
3:C:86:ASN:CB	3:C:91:LYS:HD3	2.24	0.66
4:E:143:TYR:HE2	4:E:346:LEU:HB2	1.60	0.66
1:A:13:ALA:HA	1:A:139:VAL:HG22	1.77	0.66
1:A:49:LYS:HD3	1:A:65:LEU:CD2	2.25	0.66
1:A:264:ASP:C	1:A:265:ILE:HD12	2.20	0.66
3:C:91:LYS:C	3:C:95:ASN:HB3	2.20	0.66
3:C:135:ARG:HD3	3:C:139:LYS:N	2.10	0.66
1:A:56:GLU:O	1:A:59:LYS:HD3	1.95	0.66
3:C:68:ILE:CD1	3:C:95:ASN:HB2	2.20	0.66
1:A:296:LYS:HB2	1:A:299:LEU:HD12	1.76	0.66
1:A:373:GLU:OE1	1:A:373:GLU:HA	1.94	0.66
1:A:645:GLY:CA	4:D:23:GLY:HA2	2.25	0.66
1:A:719:TYR:OH	1:A:762:PHE:HA	1.96	0.66
3:C:127:TYR:CD2	3:C:187:LYS:HG2	2.30	0.66
4:D:142:LEU:HD11	4:D:165:ILE:CD1	2.20	0.66
4:D:287:ILE:CB	4:E:244:ASP:HB3	2.24	0.66
1:A:1:MET:C	1:A:2:SER:O	2.38	0.66
1:A:485:GLU:OE2	1:A:583:HIS:HB3	1.94	0.66
1:A:551:LYS:CD	1:A:555:TYR:HE2	2.08	0.66
1:A:557:GLN:O	1:A:561:LYS:HE2	1.94	0.66
3:C:135:ARG:HH11	3:C:141:GLY:H	1.42	0.66
3:C:91:LYS:HB2	3:C:95:ASN:CB	2.24	0.66
1:A:392:LEU:CD1	1:A:613:LYS:HB2	2.26	0.66
1:A:801:MET:HE3	3:C:57:PHE:HZ	1.61	0.66
2:B:124:LEU:HA	2:B:128:GLN:OE1	1.95	0.66
3:C:91:LYS:HE2	3:C:95:ASN:CG	2.19	0.66
3:C:127:TYR:O	3:C:130:PHE:HB3	1.95	0.66
4:D:357:ILE:HG12	4:D:370:VAL:CG2	2.21	0.66
1:A:5:ALA:HB1	1:A:18:ARG:NH2	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CG	1:A:100:PRO:HG2	2.30	0.66
1:A:526:ILE:HD11	1:A:583:HIS:CE1	2.30	0.66
3:C:140:GLU:HB3	3:C:180:ILE:CD1	2.25	0.66
1:A:85:PHE:CD1	1:A:94:MET:HA	2.31	0.66
1:A:110:TYR:OH	1:A:128:PRO:HA	1.96	0.66
1:A:207:LYS:HE3	1:A:259:LYS:HB2	1.78	0.66
1:A:418:ASN:OD1	1:A:421:GLN:HB3	1.96	0.66
1:A:475:LEU:HA	1:A:595:TRP:CZ3	2.30	0.66
1:A:651:VAL:O	1:A:654:VAL:HG22	1.96	0.66
1:A:836:LEU:O	1:A:840:ILE:HG23	1.96	0.66
2:B:96:ASP:HB2	2:B:97:PRO:HD2	1.77	0.66
4:D:236:LEU:HB2	4:D:251:GLY:HA3	1.76	0.66
1:A:207:LYS:HD3	1:A:259:LYS:HG3	1.78	0.66
1:A:256:ALA:CA	1:A:456:GLN:HB2	2.25	0.66
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.26	0.66
4:D:328:LYS:HD3	4:D:330:ILE:HD11	1.77	0.66
1:A:256:ALA:H	1:A:456:GLN:HG3	1.60	0.65
1:A:288:PHE:C	1:A:292:MET:HE2	2.21	0.65
3:C:135:ARG:HD3	3:C:140:GLU:H	1.61	0.65
4:D:116:ARG:HD3	4:D:370:VAL:CG1	2.27	0.65
1:A:13:ALA:HB2	1:A:139:VAL:HG22	1.78	0.65
1:A:118:TYR:CE2	1:A:153:PRO:HG3	2.31	0.65
1:A:205:LYS:CD	1:A:257:THR:HG21	2.25	0.65
3:C:58:LEU:CD1	3:C:65:ASP:HB2	2.25	0.65
1:A:380:THR:HG23	1:A:383:ALA:HB3	1.77	0.65
1:A:492:ASN:HB3	1:A:516:GLY:N	2.12	0.65
4:D:297:ASN:CB	4:D:329:ILE:HD13	2.25	0.65
4:E:32:PRO:HG3	4:E:59:GLN:NE2	2.12	0.65
1:A:12:GLU:O	1:A:15:PRO:HD2	1.96	0.65
1:A:104:TYR:CE1	1:A:108:GLU:HG3	2.30	0.65
1:A:253:HIS:HA	1:A:458:PHE:HB3	1.79	0.65
1:A:475:LEU:HD13	1:A:595:TRP:CE3	2.31	0.65
1:A:566:GLN:HG2	1:A:567:LYS:H	1.61	0.65
3:C:118:ILE:HG13	3:C:119:SER:OG	1.97	0.65
1:A:510:TRP:NE1	1:A:512:PHE:HB2	2.12	0.65
4:D:34:ILE:C	4:D:54:VAL:HG11	2.21	0.65
4:D:34:ILE:HA	4:D:68:LYS:O	1.97	0.65
1:A:5:ALA:HB1	1:A:18:ARG:HH12	1.61	0.65
1:A:173:GLN:O	1:A:459:ILE:HA	1.96	0.65
1:A:350:GLY:N	1:A:353:LYS:HG3	2.11	0.65
1:A:694:MET:CE	1:A:697:LEU:HD12	2.26	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LYS:HG2	1:A:114:MET:HE2	1.77	0.65
1:A:283:ARG:HD2	1:A:289:TYR:CD2	2.30	0.65
1:A:363:ASN:HB3	1:A:382:VAL:HG21	1.78	0.65
1:A:819:GLN:NE2	2:B:130:ASP:H	1.95	0.65
1:A:193:ILE:CG2	1:A:219:GLU:HB3	2.09	0.65
1:A:229:LEU:HD22	1:A:438:PHE:CE1	2.32	0.65
1:A:234:ASN:HD22	1:A:242:ASN:HD21	1.44	0.65
1:A:513:ILE:HG22	1:A:514:ASP:N	2.12	0.65
1:A:524:GLU:HA	1:A:527:GLU:HG2	1.79	0.65
4:D:42:GLY:O	4:D:43:VAL:HG12	1.97	0.65
4:D:101:HIS:O	4:D:129:VAL:HG12	1.96	0.65
4:D:134:VAL:O	4:D:375:PHE:HB3	1.95	0.65
4:E:153:LEU:HD11	4:E:274:ILE:HG21	1.78	0.65
1:A:27:ALA:HB1	1:A:87:LYS:HE2	1.79	0.65
1:A:261:ALA:HB3	1:A:455:ARG:NE	2.12	0.65
1:A:406:VAL:HG22	1:A:412:TYR:O	1.97	0.65
1:A:831:TRP:HE3	1:A:834:MET:CG	2.05	0.65
1:A:107:LYS:HA	1:A:688:MET:SD	2.37	0.65
1:A:451:THR:C	1:A:452:LYS:HE2	2.22	0.65
1:A:799:TYR:HA	1:A:802:ARG:HH22	1.60	0.65
1:A:801:MET:HE3	3:C:57:PHE:CZ	2.32	0.65
4:D:187:ASP:O	4:D:190:MET:HB2	1.97	0.65
4:D:341:ILE:O	4:D:344:SER:HB3	1.97	0.65
4:E:35:VAL:CG2	4:E:52:SER:HB2	2.25	0.65
1:A:39:PHE:CG	1:A:100:PRO:HB2	2.32	0.64
1:A:564:ASN:HA	1:A:582:VAL:CG1	2.19	0.64
3:C:150:LEU:O	3:C:154:LEU:HB2	1.95	0.64
3:C:170:MET:CE	3:C:186:VAL:HA	2.27	0.64
4:E:18:LYS:HD3	4:E:18:LYS:N	2.12	0.64
1:A:107:LYS:HD2	1:A:688:MET:CG	2.27	0.64
1:A:702:VAL:O	1:A:705:GLY:HA3	1.97	0.64
1:A:719:TYR:CZ	1:A:767:VAL:HB	2.32	0.64
3:C:68:ILE:HD12	3:C:95:ASN:CB	2.18	0.64
3:C:180:ILE:HA	3:C:183:GLU:CG	2.27	0.64
4:E:34:ILE:HD13	4:E:69:TYR:CE2	2.32	0.64
1:A:825:PHE:O	1:A:828:VAL:HG13	1.97	0.64
2:B:113:LYS:O	2:B:115:THR:HG23	1.97	0.64
1:A:19:LYS:CG	1:A:114:MET:HE2	2.26	0.64
1:A:238:VAL:N	1:A:282:GLU:HG3	2.12	0.64
1:A:255:GLY:HA3	1:A:259:LYS:HG2	1.79	0.64
1:A:811:ARG:CG	1:A:815:ILE:HD11	2.23	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:MET:O	3:C:165:GLU:HG2	1.98	0.64
1:A:39:PHE:HE1	1:A:49:LYS:CG	2.10	0.64
1:A:40:ALA:HB1	1:A:72:LEU:HD22	1.78	0.64
1:A:408:VAL:HG22	1:A:410:ASN:H	1.61	0.64
1:A:713:PHE:CD2	1:A:770:LYS:HD3	2.32	0.64
1:A:769:PHE:CD2	1:A:774:LEU:HD21	2.33	0.64
3:C:131:VAL:HG13	3:C:179:CYS:SG	2.37	0.64
4:D:189:LEU:CD2	4:D:209:VAL:HG13	2.26	0.64
4:D:299:MET:HE1	4:D:309:ILE:HD12	1.80	0.64
4:E:102:PRO:CB	4:E:131:ALA:HB3	2.18	0.64
1:A:644:LYS:HG3	1:A:649:GLN:HA	1.80	0.64
1:A:787:THR:O	1:A:790:THR:HG22	1.97	0.64
1:A:790:THR:CG2	1:A:791:ARG:HD2	2.28	0.64
3:C:68:ILE:HG13	3:C:95:ASN:OD1	1.97	0.64
3:C:70:LEU:HD12	3:C:86:ASN:HD22	1.63	0.64
1:A:111:ALA:HA	1:A:686:GLY:CA	2.28	0.64
1:A:198:THR:O	1:A:201:VAL:HG23	1.98	0.64
1:A:407:LYS:HA	1:A:411:GLU:HA	1.79	0.64
1:A:551:LYS:HD2	1:A:555:TYR:CE2	2.31	0.64
3:C:131:VAL:HG13	3:C:179:CYS:HB2	1.78	0.64
4:D:65:LEU:HD13	4:D:67:LEU:HD21	1.78	0.64
4:D:218:TYR:O	4:D:255:PHE:HA	1.98	0.64
4:E:149:THR:HG22	4:E:150:GLY:N	2.12	0.64
1:A:99:GLU:O	1:A:102:VAL:HG22	1.98	0.64
1:A:207:LYS:HE2	1:A:453:GLN:CB	2.23	0.64
1:A:430:ALA:O	1:A:433:VAL:HG12	1.97	0.64
3:C:66:SER:HB3	3:C:68:ILE:HG22	1.80	0.64
4:E:178:LEU:CD2	4:E:180:LEU:HB3	2.27	0.64
4:E:294:TYR:CE1	4:E:321:ALA:HB2	2.33	0.64
1:A:40:ALA:HB1	1:A:72:LEU:HD21	1.80	0.64
1:A:295:LYS:HG2	1:A:332:LEU:N	2.12	0.64
3:C:131:VAL:CG1	3:C:179:CYS:HB2	2.27	0.64
1:A:261:ALA:HB3	1:A:455:ARG:CD	2.28	0.64
3:C:42:LYS:CE	3:C:113:PRO:HG3	2.28	0.64
1:A:93:MET:HA	1:A:93:MET:CE	2.28	0.63
1:A:271:GLU:OE1	1:A:274:ARG:HG2	1.97	0.63
3:C:67:LYS:HD3	3:C:92:VAL:HG13	1.78	0.63
4:D:91:TYR:O	4:D:95:ARG:HA	1.99	0.63
1:A:20:PRO:HD2	1:A:23:GLU:OE1	1.99	0.63
1:A:65:LEU:HD12	1:A:65:LEU:O	1.98	0.63
1:A:126:VAL:O	1:A:128:PRO:HD3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:LEU:HD23	3:C:80:LEU:HD21	1.79	0.63
2:B:39:ASP:HA	2:B:50:ASP:OD2	1.98	0.63
1:A:19:LYS:CD	1:A:23:GLU:HB3	2.28	0.63
1:A:567:LYS:HG3	1:A:568:PRO:O	1.99	0.63
3:C:163:GLU:HG3	3:C:167:GLU:OE2	1.99	0.63
4:D:35:VAL:HG22	4:D:52:SER:HB2	1.80	0.63
4:E:310:ALA:HB1	4:E:329:ILE:CG2	2.28	0.63
1:A:47:TYR:HE2	1:A:78:PHE:CZ	2.17	0.63
1:A:793:GLN:NE2	3:C:157:LEU:H	1.96	0.63
1:A:837:PHE:HA	1:A:840:ILE:HG12	1.80	0.63
3:C:62:ARG:HB3	3:C:62:ARG:NH1	2.13	0.63
4:D:38:PRO:HD3	4:D:49:GLN:HE22	1.62	0.63
4:D:43:VAL:HG13	4:D:44:MET:N	2.14	0.63
4:E:104:LEU:HB2	4:E:356:TRP:CH2	2.32	0.63
2:B:61:LEU:HA	2:B:62:ASN:HB3	1.81	0.63
4:D:255:PHE:O	4:D:258:PRO:HD2	1.99	0.63
1:A:64:THR:HG22	1:A:65:LEU:N	2.14	0.63
1:A:224:GLN:HB3	1:A:340:ILE:CD1	2.28	0.63
2:B:167:LYS:HB3	2:B:168:ASP:C	2.24	0.63
3:C:87:ALA:HB1	3:C:94:GLY:HA3	1.81	0.63
4:D:104:LEU:HB2	4:D:356:TRP:CZ3	2.33	0.63
1:A:526:ILE:HD11	1:A:583:HIS:HE1	1.62	0.63
4:D:194:THR:HA	4:D:198:TYR:O	1.98	0.63
1:A:12:GLU:OE2	1:A:15:PRO:HG2	1.98	0.63
1:A:838:PHE:CD1	2:B:164:GLY:HA3	2.34	0.63
2:B:83:VAL:O	2:B:86:THR:HG22	1.99	0.63
1:A:144:ARG:HH22	1:A:199:ILE:CD1	2.10	0.63
1:A:415:LYS:HG3	1:A:416:GLY:H	1.62	0.63
1:A:475:LEU:HD22	1:A:595:TRP:HB3	1.81	0.63
1:A:588:VAL:HG11	1:A:590:TYR:CZ	2.34	0.63
1:A:797:ARG:CZ	1:A:797:ARG:HB2	2.29	0.63
2:B:147:ASP:HB3	2:B:152:VAL:HA	1.81	0.63
4:E:178:LEU:HG	4:E:180:LEU:N	2.14	0.63
1:A:47:TYR:HE2	1:A:78:PHE:CE1	2.17	0.62
1:A:349:VAL:HG22	1:A:353:LYS:HE3	1.81	0.62
2:B:102:THR:O	2:B:105:PHE:HB2	1.98	0.62
4:E:50:LYS:HG3	4:E:53:TYR:CE2	2.34	0.62
4:E:158:GLY:HA2	4:E:181:ALA:HB3	1.80	0.62
1:A:12:GLU:CD	1:A:133:PRO:HG2	2.24	0.62
1:A:583:HIS:HB2	1:A:585:ALA:CB	2.29	0.62
1:A:833:TRP:HE1	2:B:71:MET:HG2	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:58:ALA:O	4:D:65:LEU:HD21	1.97	0.62
4:D:189:LEU:HA	4:D:192:ILE:CD1	2.28	0.62
4:E:120:THR:CB	4:E:367:PRO:HB3	2.23	0.62
1:A:207:LYS:HD3	1:A:259:LYS:CG	2.28	0.62
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.80	0.62
2:B:138:LYS:HA	2:B:141:TRP:HD1	1.63	0.62
3:C:70:LEU:HB3	3:C:91:LYS:HD2	1.80	0.62
3:C:128:GLU:HA	3:C:183:GLU:CD	2.24	0.62
4:E:43:VAL:HG13	4:E:44:MET:N	2.13	0.62
4:E:61:LYS:O	4:E:64:ILE:HG22	1.99	0.62
1:A:90:ASP:OD1	1:A:119:SER:HA	1.99	0.62
1:A:115:ILE:HD13	1:A:116:TYR:CE2	2.35	0.62
4:E:155:SER:HB3	4:E:160:THR:CG2	2.30	0.62
4:E:257:CYS:HB3	4:E:258:PRO:HD3	1.81	0.62
1:A:91:MET:HE1	1:A:102:VAL:O	1.99	0.62
1:A:519:LEU:CD2	1:A:584:TYR:HB3	2.28	0.62
1:A:546:THR:HG23	1:A:547:ASP:N	2.13	0.62
3:C:128:GLU:HA	3:C:183:GLU:OE1	1.99	0.62
4:E:299:MET:HE1	4:E:309:ILE:HG13	1.80	0.62
1:A:368:GLN:HG3	1:A:376:GLU:HB3	1.82	0.62
1:A:424:ASN:ND2	1:A:602:PRO:HD2	2.14	0.62
1:A:488:GLN:HG3	1:A:584:TYR:CE2	2.35	0.62
3:C:67:LYS:HD2	3:C:101:MET:HB2	1.80	0.62
4:D:111:ASN:ND2	4:D:115:ASN:HB3	2.14	0.62
4:E:16:LEU:HB2	4:E:18:LYS:HZ2	1.64	0.62
1:A:332:LEU:HD12	1:A:332:LEU:C	2.25	0.62
4:E:39:ARG:HE	4:E:66:THR:CA	2.13	0.62
1:A:107:LYS:HD2	1:A:688:MET:HB2	1.82	0.62
1:A:210:GLN:HG3	1:A:211:PRO:HD2	1.80	0.62
1:A:722:PHE:CE1	1:A:726:TYR:HD2	2.17	0.62
1:A:81:ASN:ND2	1:A:94:MET:HB3	2.15	0.62
1:A:364:MET:HG3	1:A:382:VAL:CG2	2.29	0.62
3:C:127:TYR:CE2	3:C:187:LYS:HE2	2.32	0.62
3:C:128:GLU:HG3	3:C:180:ILE:CG2	2.29	0.62
4:E:34:ILE:C	4:E:54:VAL:HG21	2.24	0.62
1:A:795:LEU:HD23	3:C:187:LYS:NZ	2.14	0.62
3:C:67:LYS:HD2	3:C:92:VAL:HG13	1.81	0.62
4:D:99:GLU:HA	4:D:128:ASN:O	2.00	0.62
1:A:779:GLU:O	1:A:782:ASP:HB2	1.99	0.61
2:B:27:GLN:O	2:B:30:GLU:HB3	2.00	0.61
2:B:81:PHE:O	2:B:84:PHE:HB3	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:HIS:O	1:A:101:ALA:HB3	1.99	0.61
1:A:176:LEU:HD12	1:A:673:PHE:HA	1.80	0.61
1:A:799:TYR:HE1	3:C:169:LEU:HD12	1.64	0.61
2:B:93:LYS:HG2	2:B:94:GLY:N	2.14	0.61
4:D:208:ILE:HG22	4:D:209:VAL:N	2.15	0.61
4:D:321:ALA:HB1	4:D:322:PRO:CD	2.30	0.61
4:D:334:GLU:HA	4:D:334:GLU:OE2	1.99	0.61
1:A:193:ILE:HD13	1:A:219:GLU:HB3	1.82	0.61
1:A:295:LYS:CG	1:A:331:LEU:HD22	2.28	0.61
1:A:729:LEU:HD22	1:A:781:ARG:HA	1.81	0.61
4:D:39:ARG:HE	4:D:66:THR:CA	2.09	0.61
4:E:362:TYR:HE1	4:E:367:PRO:CG	2.13	0.61
1:A:42:ASP:CB	1:A:48:VAL:HG23	2.28	0.61
1:A:639:LYS:NZ	4:D:4:GLU:HB3	2.14	0.61
3:C:70:LEU:HB3	3:C:91:LYS:HE3	1.82	0.61
4:D:250:ILE:HG12	4:D:251:GLY:N	2.14	0.61
4:E:210:ARG:HG2	4:E:210:ARG:HH11	1.65	0.61
1:A:166:MET:O	1:A:170:ARG:HA	2.01	0.61
1:A:715:SER:HB3	1:A:774:LEU:HD11	1.81	0.61
1:A:789:MET:HE3	3:C:130:PHE:HE1	1.61	0.61
1:A:39:PHE:HD1	1:A:49:LYS:HA	1.66	0.61
1:A:220:ASP:O	1:A:223:ILE:HG13	2.01	0.61
1:A:607:VAL:HG12	1:A:611:TYR:CD1	2.36	0.61
1:A:59:LYS:HD3	1:A:59:LYS:O	2.01	0.61
1:A:167:LEU:HD23	1:A:167:LEU:N	2.14	0.61
1:A:348:LYS:O	1:A:351:ILE:HG22	2.00	0.61
1:A:349:VAL:C	1:A:353:LYS:HG3	2.26	0.61
4:D:37:ARG:HG2	4:D:38:PRO:CD	2.30	0.61
4:E:180:LEU:HD21	4:E:261:LEU:HD23	1.83	0.61
1:A:703:LEU:O	1:A:706:ILE:HB	2.01	0.61
3:C:42:LYS:HG3	3:C:46:SER:HB3	1.83	0.61
4:D:158:GLY:HA3	4:D:183:ARG:NE	2.16	0.61
4:E:236:LEU:HD13	4:E:251:GLY:HA3	1.82	0.61
1:A:54:SER:O	1:A:60:VAL:HG13	2.00	0.61
1:A:161:ASN:HA	1:A:164:GLN:OE1	2.01	0.61
1:A:163:TYR:CE2	1:A:199:ILE:CG2	2.83	0.61
1:A:194:GLN:O	1:A:197:ALA:HB3	2.01	0.61
1:A:519:LEU:HD13	1:A:584:TYR:HB3	1.82	0.61
1:A:578:HIS:NE2	1:A:591:ASN:HA	2.16	0.61
2:B:96:ASP:HB2	2:B:100:VAL:HG11	1.82	0.61
3:C:47:LYS:HE3	3:C:109:GLU:OE2	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:HIS:CD2	1:A:156:PHE:HD2	2.18	0.61
1:A:360:HIS:O	1:A:382:VAL:HG11	2.01	0.61
1:A:474:SER:HA	1:A:595:TRP:HZ2	1.66	0.61
3:C:70:LEU:HD12	3:C:86:ASN:ND2	2.16	0.61
3:C:166:VAL:HG23	3:C:167:GLU:N	2.16	0.61
4:D:259:GLU:HG3	4:D:263:GLN:HG3	1.81	0.61
4:D:365:ALA:HB3	4:D:369:ILE:HB	1.82	0.61
1:A:154:HIS:NE2	1:A:156:PHE:HD2	1.99	0.60
1:A:832:PRO:O	1:A:836:LEU:HG	2.00	0.60
3:C:157:LEU:O	3:C:157:LEU:HD22	2.01	0.60
4:E:189:LEU:HD13	4:E:192:ILE:HD11	1.82	0.60
1:A:13:ALA:CA	1:A:139:VAL:HG22	2.31	0.60
1:A:406:VAL:HG11	1:A:414:THR:CG2	2.31	0.60
1:A:415:LYS:HB2	4:D:333:PRO:HG2	1.82	0.60
4:D:116:ARG:HD2	4:D:371:HIS:ND1	2.16	0.60
1:A:303:LEU:HD22	1:A:305:ILE:HG12	1.81	0.60
1:A:475:LEU:HA	1:A:595:TRP:CH2	2.36	0.60
1:A:717:ILE:HG22	1:A:718:LEU:N	2.16	0.60
2:B:96:ASP:OD1	2:B:101:ILE:HG13	2.00	0.60
4:D:144:ALA:HB2	4:D:342:GLY:H	1.67	0.60
4:D:160:THR:HB	4:D:178:LEU:HB3	1.82	0.60
4:E:136:ILE:HB	4:E:139:VAL:HB	1.83	0.60
1:A:91:MET:SD	1:A:106:LEU:HD11	2.41	0.60
1:A:115:ILE:O	1:A:126:VAL:HG22	2.01	0.60
1:A:149:GLN:HG2	1:A:150:GLU:N	2.15	0.60
1:A:428:ALA:HA	1:A:431:LYS:CE	2.32	0.60
2:B:108:LEU:HD21	2:B:124:LEU:CD2	2.31	0.60
2:B:147:ASP:HB2	2:B:151:ASN:O	2.02	0.60
3:C:116:GLN:HG2	3:C:117:ALA:HA	1.82	0.60
1:A:45:GLU:O	1:A:46:MET:HB2	1.99	0.60
1:A:246:PHE:C	1:A:269:LEU:HD11	2.27	0.60
1:A:694:MET:HA	1:A:694:MET:CE	2.30	0.60
4:D:200:PHE:HA	4:D:205:GLU:OE1	2.00	0.60
1:A:24:ARG:HH22	1:A:28:GLN:HB3	1.66	0.60
1:A:224:GLN:HB3	1:A:340:ILE:HD13	1.82	0.60
3:C:58:LEU:HD12	3:C:65:ASP:OD2	2.01	0.60
4:D:3:ASP:O	4:D:4:GLU:HB2	2.01	0.60
4:D:158:GLY:CA	4:D:183:ARG:HD2	2.31	0.60
1:A:360:HIS:CB	1:A:382:VAL:HG13	2.20	0.60
1:A:525:LEU:HD11	1:A:558:HIS:CE1	2.36	0.60
1:A:535:ILE:HD12	1:A:557:GLN:HE22	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:LEU:CB	2:B:68:LEU:HD11	2.30	0.60
2:B:137:ILE:CD1	2:B:141:TRP:HE1	2.12	0.60
4:D:133:TYR:OH	4:D:375:PHE:HB2	2.02	0.60
4:D:300:SER:HA	4:D:335:ARG:HG3	1.82	0.60
1:A:295:LYS:HG2	1:A:332:LEU:HA	1.82	0.60
1:A:424:ASN:HD21	1:A:600:LYS:HG2	1.67	0.60
1:A:814:SER:O	1:A:818:ILE:HG12	2.01	0.60
3:C:68:ILE:HD13	3:C:97:SER:O	2.02	0.60
4:E:35:VAL:HG22	4:E:52:SER:CB	2.27	0.60
4:E:236:LEU:HD12	4:E:237:GLU:CG	2.32	0.60
4:E:257:CYS:CB	4:E:258:PRO:HD3	2.31	0.60
1:A:56:GLU:HG2	1:A:57:ASN:HB2	1.84	0.60
1:A:166:MET:SD	1:A:254:PHE:HB2	2.42	0.60
1:A:368:GLN:HG3	1:A:376:GLU:HB2	1.84	0.60
1:A:694:MET:HE1	1:A:697:LEU:CD1	2.32	0.60
1:A:694:MET:HE2	1:A:694:MET:CA	2.32	0.60
4:E:103:THR:HG21	4:E:105:LEU:HD21	1.83	0.60
4:E:106:THR:HG22	4:E:140:LEU:HD11	1.83	0.60
4:E:106:THR:CG2	4:E:140:LEU:HD11	2.32	0.60
4:E:180:LEU:CD2	4:E:261:LEU:HD23	2.32	0.60
1:A:254:PHE:O	1:A:455:ARG:HB2	2.01	0.60
1:A:726:TYR:O	1:A:729:LEU:HG	2.02	0.60
2:B:52:ARG:HG2	2:B:68:LEU:HD22	1.82	0.60
3:C:162:LYS:HB3	3:C:162:LYS:HZ3	1.67	0.60
3:C:183:GLU:HG3	3:C:184:ALA:N	2.16	0.60
4:D:22:ALA:HB1	4:D:348:SER:CB	2.29	0.60
1:A:729:LEU:N	1:A:729:LEU:HD23	2.16	0.59
1:A:793:GLN:OE1	3:C:156:THR:HG22	2.02	0.59
1:A:831:TRP:CD1	1:A:832:PRO:HD2	2.37	0.59
1:A:833:TRP:CA	1:A:836:LEU:HD12	2.14	0.59
4:D:171:LEU:HD13	4:D:285:CYS:SG	2.43	0.59
4:E:99:GLU:HA	4:E:128:ASN:O	2.02	0.59
1:A:22:LYS:O	1:A:25:ILE:HG13	2.02	0.59
1:A:32:PHE:CE2	1:A:82:PRO:HA	2.37	0.59
1:A:42:ASP:HB2	1:A:48:VAL:CG2	2.32	0.59
1:A:103:LEU:HD11	1:A:688:MET:HB2	1.83	0.59
1:A:175:ILE:HD12	1:A:175:ILE:C	2.26	0.59
1:A:296:LYS:HD2	1:A:331:LEU:CD1	2.29	0.59
1:A:484:ASN:HA	1:A:487:LEU:HD12	1.85	0.59
1:A:821:ASN:O	1:A:824:ALA:HB3	2.03	0.59
2:B:58:MET:N	2:B:59:GLY:HA2	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:18:LYS:HA	4:D:29:ALA:O	2.02	0.59
4:D:358:THR:OG1	4:D:361:GLU:HG3	2.03	0.59
4:E:196:ARG:NH2	4:E:251:GLY:H	2.00	0.59
4:E:299:MET:SD	4:E:304:THR:HB	2.42	0.59
1:A:45:GLU:O	1:A:690:HIS:HB2	2.01	0.59
1:A:295:LYS:NZ	1:A:332:LEU:HA	2.05	0.59
3:C:185:PHE:O	3:C:188:HIS:HB3	2.03	0.59
4:D:157:ASP:HA	5:D:401:ADP:H4'	1.83	0.59
1:A:232:PHE:O	1:A:285:TYR:HB3	2.01	0.59
1:A:252:ILE:O	1:A:458:PHE:HB2	2.01	0.59
1:A:495:MET:HE1	1:A:708:ILE:HG21	1.81	0.59
1:A:535:ILE:HD12	1:A:557:GLN:OE1	2.03	0.59
3:C:67:LYS:HE2	3:C:67:LYS:CA	2.27	0.59
3:C:131:VAL:HG11	3:C:180:ILE:N	2.18	0.59
4:D:210:ARG:HG2	4:D:210:ARG:HH11	1.67	0.59
1:A:16:TYR:HB2	1:A:134:VAL:CG2	2.32	0.59
1:A:195:TYR:O	1:A:198:THR:HG22	2.03	0.59
1:A:234:ASN:N	1:A:245:ARG:HG2	2.17	0.59
1:A:694:MET:HE1	1:A:697:LEU:HD12	1.85	0.59
3:C:142:ASN:H	3:C:177:ASN:H	1.48	0.59
4:D:18:LYS:HD3	4:D:18:LYS:N	2.17	0.59
4:E:39:ARG:HE	4:E:66:THR:HA	1.67	0.59
4:E:133:TYR:HB2	4:E:356:TRP:CE3	2.38	0.59
4:E:133:TYR:OH	4:E:375:PHE:HB2	2.02	0.59
4:E:216:LEU:HD13	4:E:250:ILE:HG21	1.84	0.59
1:A:109:ARG:HB3	1:A:114:MET:HB2	1.85	0.59
1:A:261:ALA:HB3	1:A:455:ARG:HE	1.67	0.59
1:A:351:ILE:O	1:A:355:THR:HG23	2.03	0.59
1:A:515:PHE:CE1	1:A:711:LYS:HE3	2.38	0.59
2:B:46:ILE:HG12	2:B:79:ILE:O	2.02	0.59
4:E:65:LEU:HD12	4:E:65:LEU:C	2.28	0.59
1:A:130:LYS:CE	1:A:132:LEU:HD11	2.33	0.59
1:A:296:LYS:HG3	1:A:300:ILE:HG23	1.85	0.59
1:A:361:TYR:HE1	1:A:386:ALA:CB	2.15	0.59
1:A:656:ARG:HG2	1:A:656:ARG:HH11	1.68	0.59
3:C:98:ASN:HB3	3:C:99:GLU:CA	2.33	0.59
3:C:135:ARG:O	3:C:136:VAL:HG12	2.02	0.59
4:E:287:ILE:HA	4:E:290:ARG:CD	2.33	0.59
1:A:59:LYS:HD2	1:A:59:LYS:H	1.67	0.59
1:A:207:LYS:CD	1:A:259:LYS:CB	2.76	0.59
4:D:210:ARG:HG2	4:D:210:ARG:NH1	2.18	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:357:ILE:HA	4:D:361:GLU:OE2	2.02	0.59
1:A:175:ILE:CD1	1:A:461:VAL:HG22	2.23	0.59
3:C:42:LYS:CA	3:C:43:ILE:HB	2.20	0.59
3:C:86:ASN:O	3:C:91:LYS:HG2	2.03	0.59
3:C:91:LYS:O	3:C:94:GLY:HA2	2.03	0.59
3:C:106:ILE:HD13	3:C:106:ILE:C	2.27	0.59
1:A:129:TYR:CE2	1:A:683:LYS:HB3	2.38	0.58
1:A:792:THR:HA	3:C:127:TYR:HE1	1.67	0.58
2:B:50:ASP:HA	2:B:53:ASP:OD2	2.03	0.58
3:C:142:ASN:HB3	3:C:179:CYS:SG	2.43	0.58
4:E:120:THR:HB	4:E:367:PRO:CB	2.26	0.58
4:E:250:ILE:CD1	4:E:253:GLU:HB2	2.33	0.58
1:A:236:LYS:HD3	1:A:236:LYS:C	2.28	0.58
1:A:349:VAL:HG13	1:A:350:GLY:N	2.18	0.58
1:A:727:ARG:HH11	1:A:745:ALA:HB1	1.68	0.58
1:A:814:SER:HA	2:B:104:ALA:HB1	1.85	0.58
2:B:35:PHE:CE1	2:B:46:ILE:HG23	2.38	0.58
4:D:8:LEU:HB2	4:D:103:THR:OG1	2.03	0.58
4:D:99:GLU:O	4:D:130:PRO:HG3	2.03	0.58
1:A:115:ILE:CG2	1:A:128:PRO:HG3	2.32	0.58
1:A:228:LEU:O	1:A:228:LEU:HD13	2.03	0.58
1:A:406:VAL:HB	1:A:605:GLU:OE1	2.02	0.58
1:A:816:PHE:CD2	1:A:820:TYR:HE2	2.21	0.58
3:C:42:LYS:HD2	3:C:47:LYS:HA	1.82	0.58
3:C:150:LEU:HD13	3:C:150:LEU:C	2.28	0.58
3:C:180:ILE:CA	3:C:183:GLU:HG2	2.32	0.58
4:D:153:LEU:HD21	4:D:274:ILE:CD1	2.26	0.58
4:E:34:ILE:HA	4:E:68:LYS:O	2.02	0.58
4:E:372:ARG:HG2	4:E:372:ARG:HH11	1.67	0.58
1:A:158:ILE:HA	1:A:161:ASN:ND2	2.18	0.58
1:A:175:ILE:HD12	1:A:461:VAL:HG13	1.82	0.58
1:A:220:ASP:CA	1:A:223:ILE:HG13	2.33	0.58
1:A:255:GLY:N	1:A:455:ARG:HA	2.18	0.58
1:A:421:GLN:HE21	1:A:422:VAL:CG1	2.14	0.58
3:C:42:LYS:HE2	3:C:113:PRO:CG	2.32	0.58
3:C:77:LEU:HD23	3:C:77:LEU:C	2.28	0.58
3:C:115:LEU:O	3:C:115:LEU:HD22	2.03	0.58
3:C:190:MET:O	3:C:190:MET:HE3	2.02	0.58
1:A:302:LEU:HD23	1:A:353:LYS:HE3	1.86	0.58
1:A:811:ARG:O	1:A:815:ILE:HG13	2.03	0.58
2:B:26:THR:O	2:B:27:GLN:HB2	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:TYR:O	4:D:258:PRO:HG2	2.02	0.58
4:E:180:LEU:CD1	4:E:184:ASP:HB2	2.33	0.58
1:A:81:ASN:HD21	1:A:95:THR:N	2.01	0.58
1:A:94:MET:HE1	1:A:101:ALA:CB	2.11	0.58
1:A:137:PRO:HA	1:A:140:VAL:HG23	1.85	0.58
1:A:154:HIS:HD2	1:A:156:PHE:H	1.51	0.58
1:A:289:TYR:HA	1:A:292:MET:CE	2.33	0.58
1:A:348:LYS:HA	1:A:351:ILE:HG22	1.85	0.58
1:A:377:PRO:CG	1:A:398:LEU:HD22	2.31	0.58
1:A:380:THR:CG2	1:A:383:ALA:HB3	2.33	0.58
1:A:618:LEU:HG	1:A:622:LEU:HD11	1.85	0.58
1:A:677:LEU:HD23	1:A:678:ILE:O	2.04	0.58
1:A:839:LYS:HE2	2:B:60:ARG:HH12	1.68	0.58
3:C:42:LYS:HG2	3:C:43:ILE:O	2.04	0.58
4:E:22:ALA:HB1	4:E:348:SER:HB2	1.84	0.58
4:E:47:MET:CG	4:E:48:GLY:H	2.15	0.58
4:E:238:LYS:HD3	4:E:254:ARG:NH1	2.17	0.58
1:A:256:ALA:H	1:A:259:LYS:HE2	1.69	0.58
1:A:801:MET:CE	3:C:57:PHE:HZ	2.16	0.58
3:C:135:ARG:CG	3:C:138:ASP:H	2.15	0.58
3:C:144:THR:HG23	3:C:145:VAL:N	2.18	0.58
4:D:43:VAL:HG22	4:D:44:MET:H	1.69	0.58
1:A:128:PRO:HG2	1:A:132:LEU:CD2	2.34	0.58
1:A:205:LYS:HG3	1:A:206:LYS:H	1.68	0.58
1:A:408:VAL:HG23	1:A:409:GLY:N	2.18	0.58
1:A:426:VAL:HG23	1:A:427:GLY:N	2.19	0.58
1:A:462:LEU:CD1	1:A:464:ILE:HG22	2.34	0.58
1:A:749:LEU:CD1	1:A:753:ILE:HD11	2.33	0.58
3:C:146:MET:O	3:C:149:GLU:HG3	2.04	0.58
4:E:210:ARG:HG2	4:E:210:ARG:NH1	2.18	0.58
2:B:29:GLN:O	2:B:32:LYS:HB3	2.04	0.58
4:D:148:THR:HG22	4:D:149:THR:N	2.16	0.58
1:A:170:ARG:HD2	1:A:256:ALA:O	2.02	0.58
1:A:304:LEU:O	1:A:305:ILE:HD13	2.04	0.58
1:A:610:LEU:HD13	1:A:610:LEU:C	2.28	0.58
1:A:822:ILE:C	1:A:822:ILE:HD12	2.28	0.58
4:D:26:ALA:HB1	4:D:27:PRO:HD2	1.85	0.58
4:D:236:LEU:O	4:D:251:GLY:HA3	2.04	0.58
4:E:34:ILE:HG21	4:E:67:LEU:HB3	1.86	0.58
4:E:287:ILE:HA	4:E:290:ARG:NE	2.19	0.58
1:A:12:GLU:HG3	1:A:133:PRO:HB2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:PHE:HA	1:A:269:LEU:HD13	1.85	0.57
1:A:522:CYS:SG	1:A:583:HIS:HA	2.44	0.57
1:A:839:LYS:CE	2:B:60:ARG:HH12	2.16	0.57
2:B:164:GLY:O	2:B:165:ASP:HB3	2.02	0.57
4:D:107:GLU:O	4:D:137:GLN:HG3	2.04	0.57
4:D:326:LYS:O	4:D:327:ILE:HD12	2.03	0.57
4:E:300:SER:HB3	4:E:335:ARG:NE	2.18	0.57
4:E:336:LYS:CE	5:E:401:ADP:H5'2	2.34	0.57
1:A:418:ASN:O	1:A:422:VAL:HG13	2.04	0.57
1:A:523:ILE:HD13	1:A:523:ILE:H	1.69	0.57
3:C:47:LYS:HG3	3:C:109:GLU:OE1	2.05	0.57
4:E:110:LEU:N	4:E:110:LEU:HD23	2.19	0.57
1:A:36:LYS:HD3	1:A:36:LYS:N	2.17	0.57
4:E:34:ILE:HB	4:E:54:VAL:HG21	1.87	0.57
1:A:2:SER:O	1:A:3:SER:HB2	2.04	0.57
1:A:205:LYS:HB3	1:A:257:THR:CG2	2.34	0.57
1:A:222:ILE:HD13	1:A:222:ILE:N	2.19	0.57
1:A:713:PHE:CE2	1:A:770:LYS:HG2	2.39	0.57
2:B:83:VAL:C	2:B:86:THR:HG22	2.27	0.57
4:D:336:LYS:CE	5:D:401:ADP:H5'2	2.34	0.57
4:E:34:ILE:HG22	4:E:35:VAL:N	2.19	0.57
4:E:139:VAL:HG12	4:E:140:LEU:N	2.18	0.57
1:A:396:GLU:HG2	1:A:610:LEU:HD21	1.87	0.57
3:C:54:LYS:HZ1	3:C:73:VAL:CG2	2.17	0.57
4:E:5:THR:HG23	4:E:6:THR:O	2.04	0.57
4:E:365:ALA:HB3	4:E:369:ILE:HB	1.85	0.57
1:A:250:ILE:HG23	1:A:250:ILE:O	2.04	0.57
1:A:600:LYS:C	1:A:602:PRO:HD3	2.29	0.57
1:A:610:LEU:HD13	1:A:610:LEU:O	2.05	0.57
1:A:656:ARG:HG2	1:A:656:ARG:NH1	2.19	0.57
1:A:793:GLN:OE1	3:C:155:ALA:HB3	2.03	0.57
4:D:104:LEU:HD23	4:D:104:LEU:C	2.29	0.57
4:D:287:ILE:HG12	4:D:288:ASP:OD1	2.04	0.57
4:E:244:ASP:OD2	4:E:246:GLN:HG3	2.03	0.57
4:E:321:ALA:HB1	4:E:322:PRO:HD2	1.86	0.57
1:A:39:PHE:CE1	1:A:100:PRO:HB2	2.40	0.57
1:A:110:TYR:CZ	1:A:685:PRO:HA	2.39	0.57
1:A:514:ASP:HB3	1:A:517:MET:CE	2.34	0.57
3:C:47:LYS:HG2	3:C:48:GLU:N	2.15	0.57
3:C:67:LYS:HD2	3:C:101:MET:HB3	1.87	0.57
4:E:208:ILE:HD11	4:E:243:PRO:HG2	1.85	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ILE:HD13	1:A:116:TYR:CD2	2.40	0.57
3:C:57:PHE:CD2	3:C:69:THR:HG21	2.39	0.57
3:C:140:GLU:CD	3:C:180:ILE:HG12	2.29	0.57
4:D:37:ARG:H	4:D:66:THR:HG23	1.70	0.57
4:D:37:ARG:HG3	4:D:51:ASP:OD1	2.04	0.57
4:D:64:ILE:HG23	4:D:65:LEU:N	2.20	0.57
1:A:38:CYS:HB3	1:A:78:PHE:O	2.04	0.57
1:A:172:ASN:OD1	1:A:457:TYR:HA	2.05	0.57
1:A:292:MET:SD	1:A:315:VAL:HG11	2.45	0.57
1:A:419:VAL:HG13	1:A:420:GLN:N	2.18	0.57
1:A:464:ILE:HG12	1:A:465:ALA:H	1.70	0.57
1:A:567:LYS:HG3	1:A:568:PRO:N	2.18	0.57
1:A:617:LYS:N	1:A:617:LYS:HD3	2.20	0.57
3:C:71:SER:HA	3:C:86:ASN:HD21	1.70	0.57
1:A:226:ASN:O	1:A:230:GLU:HG2	2.05	0.57
1:A:551:LYS:HG2	1:A:555:TYR:HE2	1.69	0.57
3:C:98:ASN:CB	3:C:99:GLU:HA	2.29	0.57
3:C:139:LYS:O	3:C:140:GLU:HB2	2.04	0.57
3:C:151:ARG:HG3	3:C:163:GLU:OE1	2.04	0.57
4:D:250:ILE:HD13	4:D:254:ARG:HG2	1.86	0.57
4:E:370:VAL:HG22	4:E:375:PHE:C	2.30	0.57
1:A:228:LEU:HD13	1:A:228:LEU:C	2.30	0.56
1:A:407:LYS:HG3	1:A:408:VAL:H	1.69	0.56
2:B:70:ALA:HA	2:B:73:LYS:HE3	1.84	0.56
2:B:134:GLN:O	2:B:137:ILE:HG22	2.04	0.56
4:D:352:PHE:O	4:D:355:MET:HG2	2.05	0.56
1:A:143:TYR:HE2	1:A:151:ALA:CB	2.18	0.56
1:A:291:ILE:HG23	1:A:296:LYS:HZ2	1.70	0.56
1:A:364:MET:SD	1:A:382:VAL:HB	2.44	0.56
1:A:533:PHE:O	1:A:537:GLU:HG3	2.05	0.56
1:A:790:THR:HG22	1:A:791:ARG:CD	2.34	0.56
1:A:19:LYS:HD3	1:A:23:GLU:HB2	1.84	0.56
1:A:268:TYR:C	1:A:269:LEU:HD12	2.30	0.56
1:A:290:GLN:O	1:A:331:LEU:HD12	2.05	0.56
1:A:422:VAL:HG23	1:A:423:THR:N	2.18	0.56
1:A:506:GLU:HB3	1:A:508:ILE:CD1	2.34	0.56
1:A:789:MET:HE2	3:C:150:LEU:CD1	2.25	0.56
4:E:38:PRO:HD3	4:E:49:GLN:HE22	1.69	0.56
4:E:189:LEU:HG	4:E:209:VAL:CG1	2.34	0.56
3:C:135:ARG:HH11	3:C:139:LYS:HB3	1.69	0.56
4:E:238:LYS:HD3	4:E:254:ARG:HH12	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ARG:C	1:A:456:GLN:HG2	2.15	0.56
1:A:485:GLU:HG2	1:A:584:TYR:CE1	2.39	0.56
1:A:515:PHE:CE1	1:A:711:LYS:HG2	2.39	0.56
1:A:607:VAL:O	1:A:611:TYR:HD1	1.89	0.56
1:A:811:ARG:HG2	1:A:815:ILE:CG1	2.36	0.56
2:B:124:LEU:HD12	2:B:125:LEU:N	2.21	0.56
3:C:76:VAL:HG12	3:C:77:LEU:N	2.19	0.56
3:C:128:GLU:HG3	3:C:180:ILE:HG21	1.86	0.56
4:D:31:PHE:HB2	4:D:32:PRO:HD2	1.87	0.56
4:E:194:THR:HA	4:E:198:TYR:O	2.05	0.56
4:E:54:VAL:HG12	4:E:55:GLY:N	2.19	0.56
4:E:57:GLU:O	4:E:61:LYS:HB2	2.05	0.56
4:E:287:ILE:HA	4:E:290:ARG:HD2	1.88	0.56
1:A:80:MET:HG2	1:A:81:ASN:N	2.20	0.56
1:A:233:GLY:O	1:A:234:ASN:HB2	2.04	0.56
1:A:249:PHE:HD1	1:A:462:LEU:CD2	2.18	0.56
1:A:264:ASP:HA	1:A:446:ASN:OD1	2.06	0.56
4:D:37:ARG:O	4:D:66:THR:HG23	2.06	0.56
4:E:104:LEU:HB2	4:E:356:TRP:HH2	1.69	0.56
4:E:140:LEU:HD13	4:E:343:GLY:HA2	1.83	0.56
4:E:172:PRO:HA	4:E:175:ILE:CD1	2.35	0.56
1:A:170:ARG:NH2	1:A:256:ALA:HB1	2.21	0.56
1:A:305:ILE:HD12	1:A:312:PHE:CZ	2.40	0.56
1:A:553:LYS:NZ	4:D:351:THR:HG21	2.21	0.56
2:B:28:ILE:HG22	2:B:85:LEU:HD22	1.87	0.56
2:B:124:LEU:HD12	2:B:124:LEU:C	2.30	0.56
4:D:154:ASP:CB	4:D:300:SER:HB3	2.34	0.56
4:E:34:ILE:HG22	4:E:35:VAL:H	1.71	0.56
1:A:39:PHE:CD1	1:A:49:LYS:HA	2.41	0.56
1:A:238:VAL:HG23	1:A:282:GLU:OE2	2.06	0.56
1:A:245:ARG:CG	1:A:285:TYR:HE1	2.18	0.56
1:A:255:GLY:HA3	1:A:259:LYS:CG	2.35	0.56
1:A:396:GLU:CG	1:A:610:LEU:HD21	2.36	0.56
1:A:483:THR:O	1:A:487:LEU:HG	2.06	0.56
1:A:648:PHE:HA	1:A:649:GLN:NE2	2.21	0.56
1:A:755:VAL:HG23	1:A:760:TYR:HE1	1.71	0.56
1:A:822:ILE:O	1:A:825:PHE:HB3	2.04	0.56
4:E:47:MET:HG3	4:E:48:GLY:N	2.19	0.56
4:E:153:LEU:HD11	4:E:274:ILE:HG22	1.88	0.56
4:E:372:ARG:HG2	4:E:372:ARG:NH1	2.21	0.56
1:A:406:VAL:CG1	1:A:605:GLU:HB2	2.33	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:PHE:HA	2:B:58:MET:HB3	1.87	0.56
3:C:47:LYS:HA	3:C:50:GLN:OE1	2.06	0.56
4:D:34:ILE:CA	4:D:54:VAL:HG11	2.35	0.56
4:D:151:ILE:HD12	4:D:164:PRO:HG3	1.87	0.56
4:D:164:PRO:HG2	4:D:174:ALA:CB	2.35	0.56
4:E:285:CYS:HB3	4:E:289:ILE:HD11	1.87	0.56
1:A:16:TYR:HD2	1:A:115:ILE:HG13	1.71	0.55
1:A:497:VAL:HG12	1:A:501:GLU:OE1	2.06	0.55
1:A:684:THR:O	1:A:687:VAL:HG12	2.05	0.55
1:A:722:PHE:CZ	1:A:777:LEU:HD11	2.40	0.55
4:D:116:ARG:HH12	4:D:375:PHE:HA	1.72	0.55
4:E:78:ASN:O	4:E:82:MET:HB2	2.06	0.55
4:E:99:GLU:O	4:E:130:PRO:HG3	2.06	0.55
1:A:47:TYR:CE2	1:A:78:PHE:CE1	2.94	0.55
1:A:110:TYR:OH	1:A:685:PRO:HA	2.06	0.55
1:A:269:LEU:HD12	1:A:269:LEU:N	2.21	0.55
1:A:584:TYR:CD1	1:A:584:TYR:N	2.74	0.55
1:A:735:PRO:HB2	1:A:739:PHE:CD2	2.42	0.55
1:A:795:LEU:HD23	3:C:80:LEU:CD2	2.36	0.55
2:B:46:ILE:HG13	2:B:46:ILE:O	2.06	0.55
2:B:65:ASN:HB3	2:B:66:GLU:HG2	1.85	0.55
1:A:170:ARG:NE	1:A:256:ALA:HB1	2.21	0.55
1:A:237:THR:C	1:A:282:GLU:HG3	2.30	0.55
2:B:68:LEU:O	2:B:71:MET:HB2	2.06	0.55
2:B:79:ILE:O	2:B:79:ILE:HG23	2.06	0.55
3:C:183:GLU:HG3	3:C:184:ALA:H	1.71	0.55
4:D:220:ALA:CB	4:D:226:GLU:HG3	2.35	0.55
1:A:17:LEU:CD1	1:A:152:PRO:HB2	2.36	0.55
1:A:163:TYR:CZ	1:A:167:LEU:HD11	2.41	0.55
1:A:260:LEU:O	1:A:260:LEU:HD13	2.06	0.55
1:A:536:LEU:HA	1:A:550:PHE:CE1	2.41	0.55
1:A:439:LEU:O	1:A:439:LEU:HD13	2.07	0.55
1:A:475:LEU:HD22	1:A:595:TRP:CD2	2.41	0.55
1:A:607:VAL:HG12	1:A:611:TYR:CE1	2.41	0.55
3:C:104:LYS:NZ	3:C:104:LYS:HB3	2.22	0.55
4:E:35:VAL:N	4:E:54:VAL:HG21	2.21	0.55
4:E:35:VAL:CA	4:E:54:VAL:HG21	2.36	0.55
4:E:309:ILE:HG23	4:E:310:ALA:N	2.21	0.55
1:A:128:PRO:HG2	1:A:132:LEU:HD23	1.87	0.55
1:A:245:ARG:HH22	1:A:274:ARG:HE	1.55	0.55
1:A:291:ILE:HG23	1:A:296:LYS:NZ	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:O	1:A:615:ALA:HB2	2.07	0.55
1:A:420:GLN:H	1:A:420:GLN:CD	2.14	0.55
1:A:565:PHE:CE2	1:A:579:PHE:CD2	2.95	0.55
1:A:583:HIS:HB2	1:A:585:ALA:HB3	1.88	0.55
2:B:39:ASP:HA	2:B:46:ILE:HG22	1.88	0.55
3:C:113:PRO:C	3:C:116:GLN:HB3	2.31	0.55
1:A:104:TYR:CZ	1:A:108:GLU:HG3	2.41	0.55
1:A:107:LYS:HD2	1:A:688:MET:CB	2.36	0.55
4:D:34:ILE:HG21	4:D:67:LEU:CB	2.32	0.55
4:E:300:SER:HA	4:E:335:ARG:NE	2.21	0.55
1:A:143:TYR:HE2	1:A:151:ALA:HB3	1.72	0.55
1:A:392:LEU:HD22	1:A:614:SER:CB	2.35	0.55
1:A:426:VAL:O	1:A:429:LEU:HB3	2.07	0.55
1:A:474:SER:HA	1:A:595:TRP:CZ2	2.41	0.55
1:A:816:PHE:CD2	1:A:820:TYR:CE2	2.95	0.55
1:A:818:ILE:O	1:A:822:ILE:HG23	2.07	0.55
4:E:275:HIS:HA	4:E:313:MET:HE1	1.89	0.55
4:E:358:THR:OG1	4:E:361:GLU:HG3	2.07	0.55
1:A:167:LEU:HD13	1:A:257:THR:O	2.07	0.55
1:A:167:LEU:CD2	1:A:258:GLY:HA3	2.35	0.55
1:A:644:LYS:CG	1:A:649:GLN:HA	2.36	0.55
3:C:68:ILE:HD13	3:C:97:SER:C	2.31	0.55
4:D:124:PHE:CD2	4:D:362:TYR:CG	2.95	0.55
4:E:8:LEU:HB2	4:E:103:THR:OG1	2.07	0.55
4:E:106:THR:HG21	4:E:140:LEU:CD1	2.37	0.55
1:A:32:PHE:CD2	1:A:83:PRO:HD3	2.41	0.55
4:E:208:ILE:O	4:E:212:ILE:HD12	2.07	0.55
1:A:249:PHE:CD1	1:A:462:LEU:HD23	2.42	0.54
1:A:283:ARG:HH22	1:A:325:ILE:CD1	2.20	0.54
4:E:36:GLY:HA2	4:E:66:THR:HG23	1.87	0.54
4:E:316:GLU:OE1	4:E:316:GLU:HA	2.07	0.54
1:A:220:ASP:C	1:A:223:ILE:HG13	2.32	0.54
1:A:338:ILE:O	1:A:341:LEU:HD12	2.07	0.54
1:A:835:ASN:O	1:A:839:LYS:HD3	2.08	0.54
2:B:82:THR:O	2:B:85:LEU:HB2	2.07	0.54
2:B:115:THR:HG21	2:B:154:TYR:CZ	2.42	0.54
4:E:158:GLY:CA	4:E:181:ALA:HB3	2.38	0.54
1:A:221:GLN:NE2	1:A:449:LEU:HA	2.22	0.54
1:A:780:MET:HA	1:A:783:GLU:CG	2.37	0.54
2:B:108:LEU:HD11	2:B:124:LEU:CD2	2.33	0.54
3:C:136:VAL:O	3:C:136:VAL:HG13	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:158:GLY:HA2	4:D:181:ALA:HB3	1.89	0.54
4:E:3:ASP:O	4:E:4:GLU:HG3	2.07	0.54
4:E:45:VAL:HG13	4:E:45:VAL:O	2.08	0.54
1:A:136:ASN:HB2	1:A:139:VAL:HG23	1.89	0.54
1:A:283:ARG:HB2	1:A:289:TYR:CZ	2.42	0.54
1:A:338:ILE:CG2	1:A:348:LYS:HD2	2.24	0.54
1:A:418:ASN:HB2	1:A:420:GLN:NE2	2.23	0.54
3:C:118:ILE:HG23	3:C:118:ILE:O	2.07	0.54
3:C:131:VAL:HG13	3:C:179:CYS:CB	2.38	0.54
4:D:121:GLN:HA	4:D:362:TYR:OH	2.07	0.54
4:E:148:THR:HG23	4:E:149:THR:N	2.22	0.54
4:E:182:GLY:HA2	4:E:185:LEU:HG	1.90	0.54
4:E:193:LEU:HD22	4:E:198:TYR:HD2	1.73	0.54
1:A:253:HIS:CA	1:A:458:PHE:HB3	2.36	0.54
1:A:296:LYS:HG2	1:A:331:LEU:HD11	1.86	0.54
2:B:159:TYR:O	2:B:159:TYR:HD2	1.91	0.54
4:D:154:ASP:HA	4:D:300:SER:CB	2.22	0.54
4:D:261:LEU:N	4:D:261:LEU:HD23	2.22	0.54
4:E:37:ARG:H	4:E:66:THR:HG22	1.70	0.54
4:E:282:ILE:HA	4:E:285:CYS:SG	2.47	0.54
1:A:176:LEU:CD1	1:A:675:ARG:HH21	2.21	0.54
1:A:205:LYS:CB	1:A:257:THR:HG21	2.36	0.54
1:A:255:GLY:HA3	1:A:259:LYS:CE	2.38	0.54
1:A:645:GLY:N	4:D:23:GLY:HA2	2.21	0.54
1:A:722:PHE:HZ	1:A:777:LEU:HD11	1.73	0.54
4:D:255:PHE:C	4:D:258:PRO:HD2	2.33	0.54
4:E:157:ASP:OD1	5:E:401:ADP:H3'	2.08	0.54
4:E:172:PRO:HA	4:E:175:ILE:HD12	1.90	0.54
4:E:286:ASP:O	4:E:290:ARG:HG3	2.07	0.54
1:A:308:ASN:OD1	1:A:310:PHE:HB3	2.08	0.54
1:A:365:LYS:HB2	1:A:378:ASP:HB3	1.89	0.54
1:A:639:LYS:HZ2	4:D:4:GLU:HB3	1.72	0.54
1:A:715:SER:CB	1:A:774:LEU:HD11	2.37	0.54
4:E:34:ILE:HG13	4:E:54:VAL:CG1	2.37	0.54
4:E:107:GLU:OE1	4:E:116:ARG:HG3	2.07	0.54
1:A:91:MET:HE3	1:A:105:ASN:CB	2.36	0.54
1:A:93:MET:HE2	1:A:93:MET:N	2.22	0.54
1:A:407:LYS:O	1:A:408:VAL:HG12	2.07	0.54
1:A:500:GLN:O	1:A:504:LYS:HG2	2.08	0.54
3:C:80:LEU:CD2	3:C:187:LYS:HZ3	2.21	0.54
3:C:135:ARG:HE	3:C:135:ARG:C	2.16	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:GLN:HB2	4:D:362:TYR:OH	2.07	0.54
4:D:311:ASP:O	4:D:314:GLN:HB3	2.08	0.54
4:E:101:HIS:O	4:E:130:PRO:HD2	2.08	0.54
1:A:16:TYR:OH	1:A:132:LEU:HD12	2.08	0.54
1:A:287:ILE:HA	1:A:290:GLN:HG3	1.88	0.54
1:A:408:VAL:HG23	1:A:409:GLY:H	1.73	0.54
1:A:645:GLY:O	1:A:646:SER:HB2	2.08	0.54
3:C:106:ILE:HA	3:C:109:GLU:CG	2.38	0.54
4:E:49:GLN:C	4:E:50:LYS:HD3	2.33	0.54
4:E:190:MET:HE3	4:E:206:ARG:HG3	1.88	0.54
4:E:250:ILE:O	4:E:250:ILE:HG23	2.08	0.54
4:E:365:ALA:HB2	4:E:369:ILE:HD12	1.88	0.54
1:A:155:ILE:CD1	1:A:191:ARG:HB3	2.38	0.54
1:A:236:LYS:HA	1:A:241:ASP:O	2.07	0.54
1:A:364:MET:HG3	1:A:382:VAL:CB	2.37	0.54
2:B:52:ARG:NH1	2:B:64:LYS:HG2	2.22	0.54
4:D:211:ASP:OD1	4:D:215:LYS:HD2	2.08	0.54
4:E:34:ILE:HG23	4:E:67:LEU:HB3	1.90	0.54
1:A:433:VAL:HG13	1:A:434:TYR:N	2.22	0.53
1:A:554:LEU:O	1:A:557:GLN:HG2	2.08	0.53
1:A:723:LYS:NZ	1:A:723:LYS:HB3	2.23	0.53
1:A:524:GLU:OE2	1:A:528:LYS:HB3	2.08	0.53
1:A:205:LYS:CB	1:A:257:THR:CG2	2.86	0.53
1:A:526:ILE:HG22	1:A:533:PHE:CD1	2.43	0.53
1:A:535:ILE:HD13	1:A:553:LYS:HE2	1.90	0.53
1:A:600:LYS:HB3	1:A:600:LYS:NZ	2.22	0.53
3:C:54:LYS:HZ1	3:C:73:VAL:HG21	1.72	0.53
3:C:192:ILE:O	3:C:193:ASP:HB2	2.08	0.53
4:D:106:THR:HG22	4:D:140:LEU:HD11	1.90	0.53
1:A:332:LEU:HD12	1:A:333:ALA:CA	2.37	0.53
4:D:136:ILE:HB	4:D:139:VAL:HB	1.91	0.53
1:A:103:LEU:CD1	1:A:107:LYS:HB2	2.39	0.53
1:A:249:PHE:CE2	1:A:251:ARG:HG2	2.44	0.53
1:A:380:THR:HG23	1:A:398:LEU:HD11	1.89	0.53
1:A:482:PHE:HZ	1:A:527:GLU:HB3	1.72	0.53
2:B:74:GLU:HG3	2:B:74:GLU:O	2.09	0.53
3:C:135:ARG:HD3	3:C:139:LYS:H	1.72	0.53
4:D:180:LEU:HD12	4:D:181:ALA:N	2.23	0.53
1:A:347:GLU:O	1:A:350:GLY:HA3	2.08	0.53
1:A:677:LEU:HG	1:A:696:GLN:OE1	2.09	0.53
1:A:801:MET:HG2	3:C:72:GLN:HB3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:PHE:CD1	4:D:209:VAL:HG23	2.44	0.53
1:A:81:ASN:CG	1:A:96:HIS:H	2.16	0.53
1:A:578:HIS:CD2	1:A:578:HIS:H	2.25	0.53
1:A:644:LYS:CG	1:A:649:GLN:HG3	2.39	0.53
4:D:157:ASP:HB2	5:D:401:ADP:PB	2.49	0.53
1:A:255:GLY:HA3	1:A:259:LYS:CD	2.38	0.53
1:A:319:GLU:CD	1:A:320:VAL:H	2.17	0.53
1:A:405:ARG:H	1:A:606:THR:CG2	2.21	0.53
1:A:790:THR:HG22	1:A:791:ARG:HH11	1.73	0.53
3:C:134:LEU:CD2	3:C:150:LEU:HG	2.36	0.53
3:C:163:GLU:O	3:C:166:VAL:HG22	2.09	0.53
4:D:16:LEU:HD23	4:D:32:PRO:HA	1.89	0.53
1:A:176:LEU:HD13	1:A:675:ARG:NH2	2.24	0.53
1:A:272:LYS:O	1:A:275:VAL:HB	2.09	0.53
1:A:544:LYS:HD2	4:D:148:THR:OG1	2.08	0.53
2:B:81:PHE:HA	2:B:84:PHE:HB3	1.90	0.53
2:B:126:ILE:HG23	2:B:127:THR:N	2.24	0.53
3:C:71:SER:HB2	3:C:86:ASN:ND2	2.24	0.53
4:D:186:THR:HG21	4:D:206:ARG:CZ	2.39	0.53
1:A:79:PRO:HB2	1:A:96:HIS:CD2	2.44	0.53
1:A:559:LEU:HD12	1:A:560:GLY:N	2.24	0.53
2:B:96:ASP:HB2	2:B:97:PRO:CD	2.39	0.53
2:B:97:PRO:HD2	2:B:100:VAL:HG11	1.90	0.53
2:B:108:LEU:HD21	2:B:120:PHE:HE2	1.74	0.53
3:C:162:LYS:HA	3:C:165:GLU:CD	2.34	0.53
4:D:143:TYR:CE2	4:D:346:LEU:HD13	2.43	0.53
4:D:169:TYR:CE1	4:E:42:GLY:HA3	2.44	0.53
4:E:123:MET:HG3	4:E:132:MET:CE	2.36	0.53
1:A:220:ASP:O	1:A:224:GLN:HG3	2.09	0.52
1:A:238:VAL:HG12	1:A:239:ARG:N	2.24	0.52
1:A:312:PHE:O	1:A:316:SER:HB2	2.09	0.52
1:A:338:ILE:O	1:A:338:ILE:HD13	2.09	0.52
1:A:340:ILE:HG23	1:A:341:LEU:N	2.23	0.52
1:A:642:LYS:CG	1:A:643:LYS:H	2.21	0.52
3:C:106:ILE:HA	3:C:109:GLU:HG2	1.90	0.52
4:E:39:ARG:NE	4:E:66:THR:HA	2.24	0.52
4:E:42:GLY:O	4:E:43:VAL:HG12	2.08	0.52
4:E:66:THR:C	4:E:67:LEU:HD23	2.33	0.52
4:E:105:LEU:O	4:E:134:VAL:HA	2.09	0.52
1:A:254:PHE:HB2	1:A:457:TYR:O	2.10	0.52
1:A:765:THR:OG1	1:A:766:LYS:HG2	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ILE:O	2:B:45:ILE:HG12	2.08	0.52
3:C:42:LYS:HZ1	3:C:47:LYS:HB2	1.73	0.52
3:C:140:GLU:O	3:C:178:GLY:HA2	2.08	0.52
4:E:58:ALA:O	4:E:65:LEU:HD21	2.09	0.52
4:E:190:MET:CE	4:E:206:ARG:HG3	2.40	0.52
1:A:88:ILE:HD11	1:A:93:MET:HB3	1.92	0.52
1:A:175:ILE:O	1:A:461:VAL:HA	2.08	0.52
1:A:544:LYS:HD2	4:D:148:THR:CB	2.38	0.52
2:B:160:VAL:CA	2:B:165:ASP:HB2	2.40	0.52
3:C:68:ILE:HG23	3:C:69:THR:N	2.25	0.52
3:C:157:LEU:HD22	3:C:157:LEU:C	2.34	0.52
4:D:290:ARG:HH11	4:E:244:ASP:HB2	1.69	0.52
4:E:79:TRP:CZ2	4:E:118:LYS:HB3	2.44	0.52
1:A:39:PHE:HZ	1:A:80:MET:HE3	1.71	0.52
1:A:205:LYS:HD3	1:A:257:THR:OG1	2.10	0.52
1:A:363:ASN:HB3	1:A:382:VAL:CG2	2.40	0.52
2:B:108:LEU:HD21	2:B:120:PHE:CE2	2.44	0.52
2:B:159:TYR:O	2:B:165:ASP:HA	2.08	0.52
4:D:335:ARG:NH2	4:D:338:SER:HB2	2.24	0.52
4:E:31:PHE:HB2	4:E:32:PRO:HD2	1.91	0.52
1:A:519:LEU:CD1	1:A:584:TYR:HB3	2.38	0.52
1:A:659:LEU:HD12	1:A:663:MET:HG2	1.92	0.52
1:A:805:PHE:CE1	3:C:53:PHE:CD1	2.98	0.52
3:C:67:LYS:CD	3:C:101:MET:HB3	2.40	0.52
4:D:53:TYR:O	4:D:54:VAL:HB	2.09	0.52
4:E:124:PHE:CE2	4:E:362:TYR:HB2	2.44	0.52
1:A:14:ALA:HB2	1:A:18:ARG:HD2	1.88	0.52
1:A:122:PHE:HE1	1:A:673:PHE:HB2	1.70	0.52
1:A:255:GLY:HA2	1:A:456:GLN:CG	2.39	0.52
1:A:283:ARG:HH22	1:A:325:ILE:HD13	1.74	0.52
1:A:287:ILE:O	1:A:291:ILE:HD13	2.08	0.52
1:A:292:MET:HE3	1:A:309:PRO:HG3	1.91	0.52
1:A:729:LEU:HD21	1:A:781:ARG:CA	2.40	0.52
2:B:135:GLU:O	2:B:138:LYS:HB3	2.10	0.52
2:B:167:LYS:HB3	2:B:168:ASP:CA	2.38	0.52
4:E:206:ARG:HG2	4:E:206:ARG:NH1	2.23	0.52
1:A:5:ALA:HB1	1:A:18:ARG:HH22	1.74	0.52
1:A:617:LYS:O	1:A:621:PHE:HD2	1.92	0.52
1:A:760:TYR:CE2	1:A:762:PHE:CE1	2.96	0.52
1:A:773:LEU:C	1:A:773:LEU:HD13	2.35	0.52
1:A:818:ILE:HG21	2:B:125:LEU:HD21	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:TRP:CZ2	2:B:71:MET:HG2	2.44	0.52
3:C:156:THR:C	3:C:157:LEU:HD13	2.34	0.52
4:D:61:LYS:HG2	4:D:64:ILE:HG21	1.92	0.52
4:D:120:THR:CB	4:D:367:PRO:HB3	2.31	0.52
4:E:336:LYS:HE2	5:E:401:ADP:C5'	2.38	0.52
1:A:73:ASN:O	1:A:77:VAL:HG13	2.10	0.52
1:A:107:LYS:CA	1:A:688:MET:HG3	2.39	0.52
1:A:250:ILE:C	1:A:250:ILE:HD13	2.35	0.52
2:B:48:LYS:NZ	2:B:69:ASP:HB3	2.25	0.52
2:B:137:ILE:HG23	2:B:138:LYS:N	2.24	0.52
4:D:180:LEU:HD21	4:D:261:LEU:HD22	1.92	0.52
4:E:58:ALA:HB1	4:E:65:LEU:CD2	2.40	0.52
1:A:228:LEU:HB2	1:A:337:ALA:HB1	1.90	0.52
1:A:361:TYR:CE1	1:A:386:ALA:CB	2.93	0.52
1:A:405:ARG:HG2	1:A:413:VAL:HG23	1.92	0.52
1:A:417:GLN:HG2	1:A:421:GLN:NE2	2.24	0.52
3:C:54:LYS:NZ	3:C:73:VAL:HG21	2.25	0.52
3:C:92:VAL:H	3:C:95:ASN:CB	2.19	0.52
1:A:85:PHE:HD1	1:A:94:MET:HA	1.75	0.52
1:A:107:LYS:CD	1:A:688:MET:HG3	2.40	0.52
1:A:643:LYS:O	1:A:644:LYS:HG2	2.10	0.52
3:C:41:ILE:HG12	3:C:42:LYS:N	2.25	0.52
4:D:35:VAL:C	4:D:54:VAL:HG21	2.35	0.52
4:D:169:TYR:CE1	4:E:42:GLY:CA	2.93	0.52
4:D:287:ILE:CG2	4:E:244:ASP:HB3	2.40	0.52
4:E:59:GLN:O	4:E:62:ARG:HG3	2.09	0.52
4:E:250:ILE:HD11	4:E:253:GLU:HB2	1.91	0.52
4:E:299:MET:SD	4:E:309:ILE:HG12	2.49	0.52
1:A:795:LEU:HD11	3:C:186:VAL:O	2.10	0.51
1:A:825:PHE:HA	1:A:828:VAL:HG13	1.92	0.51
3:C:44:GLU:O	3:C:48:GLU:HB3	2.10	0.51
4:D:10:CYS:HB2	4:D:19:ALA:HB2	1.92	0.51
4:D:17:VAL:O	4:D:30:VAL:HA	2.10	0.51
4:E:18:LYS:HG3	4:E:30:VAL:HG13	1.92	0.51
4:E:153:LEU:CD1	4:E:274:ILE:HG22	2.40	0.51
1:A:137:PRO:HA	1:A:140:VAL:CG2	2.40	0.51
1:A:230:GLU:HB2	1:A:234:ASN:ND2	2.25	0.51
1:A:291:ILE:CG1	1:A:296:LYS:HZ2	2.19	0.51
1:A:530:MET:CE	4:D:351:THR:HG22	2.41	0.51
1:A:644:LYS:NZ	1:A:649:GLN:HB3	2.24	0.51
2:B:144:PHE:HA	2:B:145:SER:OG	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:PRO:HG2	4:D:174:ALA:HB1	1.92	0.51
4:E:178:LEU:HD13	4:E:271:SER:CB	2.40	0.51
1:A:249:PHE:HD1	1:A:462:LEU:HD22	1.74	0.51
1:A:388:TYR:C	1:A:388:TYR:CD2	2.88	0.51
1:A:822:ILE:HG12	2:B:132:PHE:CE2	2.45	0.51
1:A:828:VAL:HG22	1:A:829:LYS:N	2.24	0.51
1:A:837:PHE:CA	1:A:840:ILE:HG12	2.40	0.51
3:C:51:ASP:CG	3:C:105:LYS:HE3	2.36	0.51
1:A:564:ASN:O	1:A:582:VAL:HG12	2.09	0.51
3:C:83:ASN:CB	3:C:84:PRO:HD3	2.36	0.51
4:D:103:THR:HG22	4:D:105:LEU:HD23	1.92	0.51
4:D:236:LEU:HB2	4:D:251:GLY:CA	2.40	0.51
1:A:84:LYS:HD3	1:A:778:GLU:OE2	2.11	0.51
1:A:295:LYS:C	1:A:297:PRO:HD3	2.36	0.51
1:A:531:GLY:O	1:A:535:ILE:HG13	2.10	0.51
1:A:582:VAL:HG13	1:A:582:VAL:O	2.10	0.51
3:C:54:LYS:NZ	3:C:73:VAL:HG11	2.25	0.51
4:D:141:SER:HA	4:D:338:SER:O	2.11	0.51
4:D:336:LYS:HE2	5:D:401:ADP:C5'	2.38	0.51
4:E:34:ILE:HG22	4:E:68:LYS:H	1.76	0.51
1:A:12:GLU:CG	1:A:133:PRO:HB2	2.41	0.51
1:A:47:TYR:HB3	1:A:100:PRO:HG3	1.90	0.51
1:A:88:ILE:HD13	1:A:93:MET:HB2	1.93	0.51
1:A:103:LEU:CD2	1:A:690:HIS:HD2	2.12	0.51
1:A:129:TYR:CZ	1:A:683:LYS:HB3	2.46	0.51
1:A:508:ILE:CD1	1:A:768:PHE:CE1	2.94	0.51
1:A:559:LEU:C	1:A:561:LYS:H	2.18	0.51
1:A:613:LYS:C	1:A:619:LEU:HD11	2.34	0.51
2:B:81:PHE:C	2:B:84:PHE:HB3	2.36	0.51
3:C:149:GLU:O	3:C:153:VAL:HG23	2.11	0.51
1:A:27:ALA:HB1	1:A:87:LYS:HG2	1.93	0.51
1:A:71:THR:HG23	1:A:71:THR:O	2.10	0.51
1:A:73:ASN:HB3	1:A:76:GLN:HB3	1.92	0.51
1:A:333:ALA:O	1:A:336:ASN:HB3	2.10	0.51
1:A:677:LEU:HD21	1:A:696:GLN:NE2	2.26	0.51
1:A:698:ARG:HG2	1:A:703:LEU:CD1	2.41	0.51
1:A:790:THR:HA	1:A:793:GLN:OE1	2.11	0.51
1:A:34:SER:HB2	1:A:779:GLU:OE1	2.10	0.51
1:A:249:PHE:CD2	1:A:251:ARG:HG2	2.46	0.51
1:A:260:LEU:HD13	1:A:261:ALA:C	2.36	0.51
1:A:600:LYS:CG	1:A:602:PRO:HD3	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:LYS:HD3	1:A:617:LYS:H	1.74	0.51
1:A:773:LEU:HD13	1:A:773:LEU:O	2.11	0.51
1:A:795:LEU:HD12	3:C:186:VAL:HG13	1.93	0.51
2:B:160:VAL:HA	2:B:165:ASP:HB2	1.93	0.51
4:D:69:TYR:HB2	4:D:72:GLU:HA	1.92	0.51
4:D:157:ASP:OD1	5:D:401:ADP:H3'	2.11	0.51
1:A:9:ILE:HA	1:A:18:ARG:CZ	2.41	0.51
1:A:332:LEU:HD12	1:A:333:ALA:HA	1.93	0.51
1:A:392:LEU:HD21	1:A:614:SER:HB3	1.93	0.51
1:A:484:ASN:O	1:A:487:LEU:HB2	2.11	0.51
1:A:537:GLU:HG2	1:A:652:SER:OG	2.11	0.51
1:A:613:LYS:HD3	1:A:613:LYS:H	1.76	0.51
4:D:103:THR:O	4:D:132:MET:HA	2.11	0.51
1:A:143:TYR:CE2	1:A:151:ALA:CB	2.94	0.51
1:A:268:TYR:N	1:A:268:TYR:CD1	2.79	0.51
1:A:445:ILE:HG23	1:A:449:LEU:CD1	2.38	0.51
2:B:100:VAL:O	2:B:103:GLY:HA3	2.10	0.51
2:B:147:ASP:OD1	2:B:152:VAL:HG22	2.11	0.51
2:B:161:ILE:O	2:B:164:GLY:HA2	2.10	0.51
3:C:170:MET:SD	3:C:186:VAL:HA	2.50	0.51
4:D:7:ALA:HB1	4:D:356:TRP:CH2	2.47	0.51
4:E:58:ALA:HA	4:E:65:LEU:CD2	2.40	0.51
1:A:283:ARG:NH2	1:A:325:ILE:HD13	2.27	0.50
1:A:837:PHE:C	1:A:840:ILE:HG12	2.36	0.50
2:B:71:MET:O	2:B:74:GLU:HG2	2.11	0.50
2:B:167:LYS:HB3	2:B:168:ASP:O	2.12	0.50
3:C:70:LEU:C	3:C:70:LEU:HD13	2.36	0.50
3:C:122:LYS:O	3:C:187:LYS:HE3	2.11	0.50
4:D:287:ILE:HG22	4:D:290:ARG:NH1	2.25	0.50
1:A:16:TYR:HH	1:A:113:TRP:HE3	1.59	0.50
1:A:128:PRO:HB3	1:A:130:LYS:NZ	2.26	0.50
1:A:176:LEU:O	1:A:177:ILE:HD13	2.11	0.50
1:A:614:SER:C	1:A:619:LEU:HD11	2.36	0.50
1:A:790:THR:HG22	1:A:791:ARG:HD2	1.92	0.50
1:A:822:ILE:HD11	2:B:132:PHE:CE2	2.43	0.50
3:C:69:THR:HB	3:C:73:VAL:CG2	2.39	0.50
4:D:262:PHE:C	4:D:264:PRO:HD3	2.36	0.50
4:E:162:ASN:ND2	4:E:278:THR:HA	2.26	0.50
1:A:115:ILE:CD1	1:A:116:TYR:CD2	2.95	0.50
1:A:564:ASN:CA	1:A:582:VAL:CG1	2.87	0.50
1:A:603:LEU:HB2	1:A:648:PHE:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:ILE:HG12	2:B:132:PHE:HZ	1.71	0.50
1:A:254:PHE:HB3	1:A:259:LYS:O	2.12	0.50
1:A:415:LYS:CD	4:D:333:PRO:HG2	2.41	0.50
1:A:791:ARG:O	1:A:794:ALA:HB3	2.11	0.50
2:B:55:PHE:CD2	2:B:62:ASN:HB2	2.47	0.50
3:C:105:LYS:HD3	3:C:106:ILE:HA	1.93	0.50
4:D:8:LEU:H	4:D:103:THR:HA	1.76	0.50
4:E:285:CYS:CB	4:E:289:ILE:HD11	2.41	0.50
1:A:17:LEU:HG	1:A:143:TYR:OH	2.10	0.50
1:A:91:MET:CE	1:A:105:ASN:HB3	2.40	0.50
1:A:118:TYR:CD2	1:A:153:PRO:HG3	2.47	0.50
1:A:296:LYS:CB	1:A:331:LEU:HD11	2.42	0.50
1:A:551:LYS:CG	1:A:555:TYR:HE2	2.23	0.50
2:B:42:ARG:NH1	2:B:42:ARG:HG2	2.27	0.50
3:C:108:PHE:CE1	3:C:112:LEU:CD2	2.95	0.50
3:C:112:LEU:O	3:C:116:GLN:HB2	2.12	0.50
4:E:58:ALA:HB1	4:E:65:LEU:HD22	1.92	0.50
4:E:211:ASP:OD2	4:E:215:LYS:HE3	2.11	0.50
1:A:603:LEU:HD23	1:A:648:PHE:CD2	2.47	0.50
1:A:776:LEU:O	1:A:780:MET:HG3	2.12	0.50
3:C:87:ALA:CB	3:C:94:GLY:HA3	2.41	0.50
4:D:58:ALA:HA	4:D:65:LEU:CD2	2.42	0.50
4:D:70:PRO:HG2	4:D:85:ILE:CD1	2.42	0.50
1:A:88:ILE:HD11	1:A:93:MET:CB	2.42	0.50
1:A:159:SER:CB	1:A:195:TYR:CG	2.93	0.50
1:A:603:LEU:CD2	1:A:648:PHE:CD2	2.95	0.50
1:A:755:VAL:CG1	1:A:773:LEU:HD21	2.41	0.50
1:A:815:ILE:HD13	2:B:129:CYS:SG	2.52	0.50
2:B:27:GLN:C	2:B:30:GLU:HB3	2.37	0.50
4:E:240:TYR:O	4:E:247:VAL:HG13	2.12	0.50
4:E:244:ASP:CG	4:E:246:GLN:H	2.19	0.50
4:E:294:TYR:CD1	4:E:327:ILE:CD1	2.95	0.50
1:A:154:HIS:HE2	1:A:156:PHE:HD2	1.60	0.50
1:A:167:LEU:HD21	1:A:258:GLY:CA	2.39	0.50
1:A:232:PHE:HB3	1:A:434:TYR:OH	2.12	0.50
1:A:557:GLN:HG2	1:A:558:HIS:H	1.77	0.50
1:A:601:ASP:N	1:A:602:PRO:HD3	2.27	0.50
1:A:659:LEU:HD11	1:A:663:MET:CE	2.37	0.50
1:A:724:GLN:HG3	1:A:725:ARG:N	2.25	0.50
2:B:41:ASN:HB3	2:B:45:ILE:O	2.12	0.50
2:B:137:ILE:HD13	2:B:141:TRP:NE1	2.22	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:144:THR:HG23	3:C:145:VAL:H	1.75	0.50
4:D:10:CYS:HA	4:D:19:ALA:HA	1.94	0.50
4:D:279:TYR:HB2	4:D:320:LEU:HD13	1.93	0.50
4:D:335:ARG:HH21	4:D:338:SER:CB	2.25	0.50
4:E:17:VAL:C	4:E:18:LYS:HD3	2.37	0.50
4:E:45:VAL:O	4:E:45:VAL:HG22	2.11	0.50
1:A:17:LEU:HD13	1:A:152:PRO:HB2	1.94	0.50
1:A:292:MET:SD	1:A:309:PRO:HA	2.52	0.50
1:A:646:SER:O	1:A:647:SER:HB2	2.12	0.50
1:A:844:LEU:HD22	1:A:844:LEU:N	2.27	0.50
4:E:299:MET:CE	4:E:309:ILE:HG12	2.40	0.50
1:A:292:MET:HE1	1:A:309:PRO:HB3	1.93	0.49
1:A:343:PHE:CE2	1:A:441:MET:SD	3.05	0.49
1:A:520:ALA:O	1:A:523:ILE:HG12	2.12	0.49
1:A:838:PHE:CE1	2:B:164:GLY:CA	2.95	0.49
1:A:839:LYS:HE2	2:B:60:ARG:NH1	2.26	0.49
4:D:107:GLU:HG3	4:D:111:ASN:HB2	1.94	0.49
4:E:89:THR:HG22	4:E:94:LEU:HD12	1.93	0.49
1:A:205:LYS:HD3	1:A:257:THR:CG2	2.43	0.49
1:A:296:LYS:N	1:A:297:PRO:HD3	2.27	0.49
1:A:512:PHE:HZ	1:A:711:LYS:O	1.94	0.49
1:A:544:LYS:HD2	4:D:148:THR:HB	1.93	0.49
1:A:755:VAL:CG2	1:A:760:TYR:CE1	2.95	0.49
2:B:70:ALA:HA	2:B:73:LYS:HD3	1.93	0.49
4:D:7:ALA:HB3	4:D:347:ALA:HB1	1.94	0.49
4:D:26:ALA:HB1	4:D:27:PRO:CD	2.42	0.49
4:D:140:LEU:HD13	4:D:343:GLY:N	2.27	0.49
1:A:207:LYS:CE	1:A:453:GLN:HB3	2.29	0.49
4:E:211:ASP:CG	4:E:215:LYS:HE3	2.38	0.49
1:A:185:LYS:O	1:A:189:THR:HG23	2.12	0.49
1:A:361:TYR:HE1	1:A:386:ALA:HB1	1.78	0.49
1:A:761:ARG:HG2	1:A:761:ARG:HH11	1.76	0.49
2:B:152:VAL:HG12	2:B:153:ASP:N	2.26	0.49
3:C:58:LEU:HG	3:C:64:GLY:C	2.38	0.49
4:D:148:THR:HG22	4:D:149:THR:CB	2.43	0.49
4:E:38:PRO:CD	4:E:49:GLN:HE22	2.26	0.49
1:A:39:PHE:CE2	1:A:80:MET:HE3	2.47	0.49
1:A:348:LYS:HG2	1:A:352:TYR:CE2	2.48	0.49
1:A:349:VAL:O	1:A:353:LYS:HG3	2.11	0.49
1:A:392:LEU:HD12	1:A:613:LYS:HB2	1.94	0.49
1:A:519:LEU:HD13	1:A:584:TYR:CG	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:730:ASN:HB3	1:A:749:LEU:CD1	2.36	0.49
1:A:792:THR:HA	3:C:127:TYR:CE1	2.47	0.49
3:C:127:TYR:HE2	3:C:187:LYS:CE	2.21	0.49
4:E:123:MET:HA	4:E:123:MET:CE	2.37	0.49
4:E:192:ILE:HG22	4:E:256:ARG:CZ	2.42	0.49
4:E:193:LEU:HD22	4:E:198:TYR:CD2	2.48	0.49
1:A:176:LEU:HD11	1:A:673:PHE:CA	2.41	0.49
1:A:234:ASN:ND2	1:A:242:ASN:HD21	2.10	0.49
1:A:361:TYR:CE1	1:A:386:ALA:HB1	2.48	0.49
2:B:122:GLU:HG3	2:B:137:ILE:HD12	1.93	0.49
3:C:188:HIS:NE2	3:C:192:ILE:HA	2.27	0.49
1:A:30:ARG:HB2	1:A:31:PRO:HD2	1.95	0.49
1:A:155:ILE:HD12	1:A:191:ARG:HB3	1.95	0.49
1:A:287:ILE:CD1	1:A:288:PHE:CD2	2.96	0.49
1:A:607:VAL:CG1	1:A:611:TYR:CE1	2.95	0.49
1:A:612:GLN:HB3	1:A:623:PHE:CZ	2.48	0.49
1:A:760:TYR:HA	1:A:768:PHE:O	2.12	0.49
1:A:799:TYR:CE2	3:C:170:MET:CE	2.95	0.49
1:A:825:PHE:CE1	1:A:829:LYS:HB3	2.47	0.49
4:D:69:TYR:N	4:D:69:TYR:CD1	2.81	0.49
4:E:190:MET:HE1	4:E:206:ARG:CG	2.43	0.49
1:A:348:LYS:HG2	1:A:352:TYR:HE2	1.76	0.49
1:A:375:ALA:CB	1:A:417:GLN:HE22	2.19	0.49
1:A:508:ILE:CG1	1:A:768:PHE:CZ	2.94	0.49
1:A:801:MET:CE	3:C:57:PHE:CZ	2.95	0.49
2:B:154:TYR:CD1	2:B:155:LYS:N	2.81	0.49
3:C:45:PHE:CA	3:C:46:SER:HB2	2.42	0.49
3:C:142:ASN:N	3:C:176:SER:HB3	2.27	0.49
3:C:189:ILE:HG12	3:C:190:MET:H	1.75	0.49
4:D:143:TYR:CE2	4:D:346:LEU:CD1	2.96	0.49
4:E:34:ILE:HB	4:E:54:VAL:CG2	2.43	0.49
4:E:106:THR:HG21	4:E:140:LEU:HD12	1.93	0.49
4:E:179:ASP:HB3	4:E:269:MET:HE1	1.93	0.49
1:A:151:ALA:HB1	1:A:152:PRO:HD2	1.94	0.49
1:A:300:ILE:O	1:A:303:LEU:HB3	2.13	0.49
1:A:441:MET:O	1:A:444:ARG:HB2	2.13	0.49
1:A:722:PHE:CE1	1:A:777:LEU:CD1	2.96	0.49
3:C:56:ALA:O	3:C:59:LEU:HB2	2.13	0.49
4:E:26:ALA:HB1	4:E:27:PRO:HD2	1.94	0.49
4:E:94:LEU:HB3	4:E:96:VAL:HG13	1.95	0.49
4:E:143:TYR:HD1	4:E:143:TYR:O	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:ND2	1:A:94:MET:HE2	2.27	0.49
1:A:279:LEU:H	1:A:279:LEU:CD2	2.24	0.49
1:A:295:LYS:HB3	1:A:331:LEU:CB	2.41	0.49
4:D:132:MET:HE2	4:D:132:MET:HB2	1.72	0.49
4:D:151:ILE:HA	4:D:164:PRO:HA	1.95	0.49
4:D:194:THR:HG23	4:D:198:TYR:O	2.13	0.49
4:D:294:TYR:CD2	4:D:325:MET:HG2	2.48	0.49
1:A:287:ILE:HD12	1:A:288:PHE:CD2	2.47	0.48
1:A:312:PHE:CD1	1:A:312:PHE:N	2.81	0.48
1:A:557:GLN:O	1:A:561:LYS:HG3	2.13	0.48
1:A:697:LEU:HB3	1:A:703:LEU:HG	1.94	0.48
3:C:54:LYS:HZ1	3:C:73:VAL:CG1	2.25	0.48
4:D:339:VAL:O	4:D:342:GLY:HA3	2.13	0.48
1:A:16:TYR:CD1	1:A:16:TYR:N	2.79	0.48
1:A:30:ARG:HB2	1:A:31:PRO:CD	2.42	0.48
1:A:319:GLU:HG3	1:A:321:THR:H	1.78	0.48
1:A:722:PHE:CZ	1:A:777:LEU:CD1	2.96	0.48
3:C:71:SER:HB2	3:C:86:ASN:OD1	2.13	0.48
3:C:144:THR:HG23	3:C:145:VAL:HG13	1.95	0.48
4:E:219:VAL:HG22	4:E:258:PRO:HB2	1.95	0.48
1:A:33:ASP:CG	1:A:35:LYS:H	2.21	0.48
1:A:129:TYR:CD2	1:A:683:LYS:HB3	2.48	0.48
1:A:130:LYS:HE2	1:A:132:LEU:HD11	1.94	0.48
1:A:205:LYS:HG3	1:A:206:LYS:N	2.28	0.48
1:A:275:VAL:HG12	1:A:276:THR:N	2.27	0.48
1:A:372:GLU:H	1:A:372:GLU:HG2	1.43	0.48
1:A:485:GLU:HB3	1:A:523:ILE:CG2	2.43	0.48
2:B:108:LEU:CD2	2:B:120:PHE:CE2	2.95	0.48
2:B:147:ASP:CB	2:B:152:VAL:HA	2.44	0.48
4:D:189:LEU:O	4:D:192:ILE:HG12	2.12	0.48
4:E:238:LYS:O	4:E:250:ILE:HG22	2.13	0.48
1:A:39:PHE:CE1	1:A:49:LYS:CG	2.95	0.48
1:A:98:HIS:O	1:A:102:VAL:HG13	2.14	0.48
1:A:176:LEU:HD13	1:A:675:ARG:HH21	1.76	0.48
1:A:205:LYS:HZ2	1:A:257:THR:HG21	1.79	0.48
1:A:268:TYR:O	1:A:269:LEU:HD12	2.13	0.48
1:A:348:LYS:C	1:A:351:ILE:HG22	2.38	0.48
1:A:348:LYS:CA	1:A:351:ILE:HG22	2.43	0.48
1:A:519:LEU:HD13	1:A:584:TYR:CB	2.43	0.48
1:A:557:GLN:HG2	1:A:558:HIS:N	2.28	0.48
1:A:722:PHE:CE1	1:A:726:TYR:CD2	2.98	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:PHE:CA	2:B:84:PHE:HB3	2.43	0.48
2:B:120:PHE:CZ	2:B:124:LEU:HB3	2.48	0.48
3:C:122:LYS:HB3	3:C:127:TYR:CZ	2.48	0.48
4:D:362:TYR:CE1	4:D:367:PRO:HG3	2.47	0.48
1:A:16:TYR:CG	1:A:134:VAL:HG23	2.48	0.48
1:A:166:MET:CG	1:A:457:TYR:HB2	2.43	0.48
1:A:219:GLU:H	1:A:219:GLU:CD	2.13	0.48
1:A:228:LEU:HD23	1:A:337:ALA:HB3	1.94	0.48
1:A:240:ASN:HD22	1:A:241:ASP:N	2.11	0.48
1:A:249:PHE:CD1	1:A:462:LEU:CD2	2.96	0.48
1:A:463:ASP:C	1:A:464:ILE:HG22	2.38	0.48
1:A:639:LYS:HZ2	1:A:639:LYS:HB3	1.78	0.48
2:B:160:VAL:HA	2:B:165:ASP:HA	1.95	0.48
3:C:90:LYS:HG3	3:C:90:LYS:O	2.13	0.48
3:C:142:ASN:C	3:C:177:ASN:H	2.21	0.48
3:C:143:GLY:N	3:C:176:SER:HB3	2.28	0.48
4:D:7:ALA:HA	4:D:102:PRO:O	2.13	0.48
4:E:32:PRO:HG2	4:E:55:GLY:O	2.14	0.48
4:E:58:ALA:CA	4:E:65:LEU:CD2	2.91	0.48
1:A:14:ALA:HB1	1:A:18:ARG:HB2	1.94	0.48
1:A:170:ARG:HB3	1:A:457:TYR:OH	2.14	0.48
1:A:713:PHE:HE2	1:A:770:LYS:HG2	1.79	0.48
4:E:16:LEU:HD23	4:E:32:PRO:HA	1.95	0.48
4:E:223:PHE:CD1	4:E:259:GLU:CG	2.96	0.48
4:E:229:THR:HG22	4:E:233:SER:HB3	1.95	0.48
1:A:286:HIS:O	1:A:290:GLN:HG3	2.13	0.48
1:A:582:VAL:HA	1:A:587:THR:HA	1.95	0.48
2:B:85:LEU:O	2:B:88:PHE:HB2	2.14	0.48
3:C:127:TYR:CE2	3:C:187:LYS:CG	2.96	0.48
4:D:20:GLY:HA3	4:D:340:TRP:HZ2	1.78	0.48
4:D:153:LEU:HD11	4:D:160:THR:CG2	2.43	0.48
4:E:103:THR:CG2	4:E:105:LEU:HD21	2.42	0.48
1:A:176:LEU:HD11	1:A:673:PHE:CB	2.44	0.48
1:A:367:LYS:HD3	1:A:378:ASP:OD2	2.13	0.48
1:A:704:GLU:O	1:A:707:ARG:HB3	2.12	0.48
3:C:51:ASP:OD2	3:C:105:LYS:HE3	2.13	0.48
3:C:92:VAL:HG23	3:C:93:LEU:N	2.19	0.48
4:D:106:THR:HG22	4:D:140:LEU:CD1	2.43	0.48
4:E:73:HIC:HD2	4:E:183:ARG:NH1	2.29	0.48
1:A:789:MET:HB3	3:C:155:ALA:HB2	1.95	0.48
1:A:799:TYR:CE1	3:C:169:LEU:HD12	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:GLU:CB	1:A:808:MET:HE2	2.26	0.48
3:C:71:SER:CB	3:C:91:LYS:HZ2	2.24	0.48
3:C:146:MET:N	3:C:147:GLY:HA3	2.28	0.48
3:C:162:LYS:HB3	3:C:162:LYS:NZ	2.28	0.48
4:D:115:ASN:O	4:D:119:MET:HG3	2.13	0.48
4:E:262:PHE:O	4:E:273:GLY:HA3	2.14	0.48
1:A:159:SER:CB	1:A:195:TYR:CD2	2.93	0.48
1:A:472:PHE:CE1	1:A:591:ASN:CB	2.93	0.48
1:A:729:LEU:HD21	1:A:781:ARG:HA	1.93	0.48
1:A:790:THR:HG22	1:A:791:ARG:HD3	1.96	0.48
4:D:58:ALA:HB1	4:D:65:LEU:CD2	2.40	0.48
4:D:157:ASP:OD1	5:D:401:ADP:C3'	2.62	0.48
4:D:335:ARG:HD3	4:D:335:ARG:HA	1.51	0.48
4:E:314:GLN:NE2	4:E:327:ILE:HB	2.28	0.48
1:A:7:MET:HB2	1:A:8:ALA:H	1.21	0.47
1:A:476:GLU:H	1:A:476:GLU:CD	2.21	0.47
1:A:515:PHE:CD1	1:A:711:LYS:CE	2.97	0.47
1:A:544:LYS:CD	4:D:148:THR:HB	2.44	0.47
1:A:600:LYS:HG2	1:A:602:PRO:CD	2.43	0.47
4:D:85:ILE:HG22	4:D:86:TRP:N	2.27	0.47
4:D:357:ILE:HD13	4:D:357:ILE:N	2.28	0.47
4:E:58:ALA:CB	4:E:65:LEU:HD22	2.44	0.47
4:E:198:TYR:CE2	4:E:248:ILE:HG22	2.46	0.47
4:E:240:TYR:HB3	4:E:248:ILE:HG13	1.96	0.47
1:A:805:PHE:CE2	1:A:809:MET:SD	3.07	0.47
4:D:236:LEU:HB2	4:D:251:GLY:C	2.39	0.47
4:E:294:TYR:CE1	4:E:321:ALA:CB	2.97	0.47
4:E:347:ALA:HA	4:E:356:TRP:CZ2	2.49	0.47
1:A:253:HIS:HB2	1:A:455:ARG:CG	2.44	0.47
1:A:418:ASN:CG	1:A:420:GLN:HE22	2.22	0.47
1:A:790:THR:CG2	1:A:791:ARG:HH11	2.26	0.47
1:A:805:PHE:O	1:A:809:MET:HG3	2.14	0.47
1:A:39:PHE:HE1	1:A:49:LYS:HG2	1.78	0.47
1:A:328:SER:O	1:A:331:LEU:HB3	2.15	0.47
1:A:439:LEU:HD13	1:A:439:LEU:C	2.39	0.47
1:A:808:MET:HB3	3:C:60:TYR:OH	2.14	0.47
1:A:837:PHE:CE2	1:A:838:PHE:CE1	3.02	0.47
3:C:42:LYS:HD2	3:C:47:LYS:HB3	1.96	0.47
3:C:122:LYS:C	3:C:187:LYS:HE2	2.39	0.47
4:D:35:VAL:HG12	4:D:68:LYS:HB3	1.93	0.47
4:D:66:THR:O	4:D:67:LEU:HD23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:373:LYS:HA	4:D:373:LYS:HD2	1.67	0.47
4:E:285:CYS:SG	4:E:293:LEU:HD11	2.53	0.47
4:E:362:TYR:CE1	4:E:367:PRO:HG3	2.44	0.47
1:A:9:ILE:HD13	1:A:18:ARG:HH22	1.74	0.47
1:A:9:ILE:HA	1:A:18:ARG:NE	2.30	0.47
1:A:135:TYR:N	1:A:135:TYR:CD1	2.82	0.47
1:A:295:LYS:HB3	1:A:331:LEU:CD1	2.42	0.47
1:A:361:TYR:HE1	1:A:386:ALA:HB2	1.79	0.47
1:A:445:ILE:CG2	1:A:449:LEU:HD12	2.38	0.47
1:A:526:ILE:CG2	1:A:533:PHE:CD1	2.98	0.47
1:A:783:GLU:O	1:A:787:THR:HG23	2.14	0.47
2:B:25:GLN:HE21	2:B:29:GLN:CD	2.22	0.47
3:C:105:LYS:O	3:C:108:PHE:HB3	2.15	0.47
4:D:158:GLY:HA3	4:D:183:ARG:CD	2.45	0.47
4:D:194:THR:HG23	4:D:199:SER:HA	1.96	0.47
4:E:236:LEU:HD22	4:E:252:ASN:HA	1.96	0.47
1:A:103:LEU:HD12	1:A:107:LYS:HB2	1.96	0.47
1:A:312:PHE:HB2	1:A:315:VAL:CG2	2.45	0.47
1:A:396:GLU:HG2	1:A:610:LEU:CD2	2.44	0.47
1:A:474:SER:HG	1:A:595:TRP:NE1	2.12	0.47
1:A:726:TYR:HD1	1:A:726:TYR:HA	1.35	0.47
1:A:825:PHE:CE1	2:B:161:ILE:CG2	2.97	0.47
2:B:47:ASP:O	2:B:50:ASP:HB2	2.14	0.47
4:D:121:GLN:HA	4:D:362:TYR:CZ	2.49	0.47
4:E:335:ARG:HD3	4:E:335:ARG:HA	1.65	0.47
1:A:27:ALA:CB	1:A:87:LYS:HG2	2.45	0.47
1:A:103:LEU:HD11	1:A:688:MET:CB	2.44	0.47
1:A:107:LYS:HA	1:A:688:MET:HG3	1.97	0.47
1:A:110:TYR:CE1	1:A:128:PRO:HA	2.49	0.47
1:A:128:PRO:HB3	1:A:130:LYS:HZ2	1.80	0.47
1:A:167:LEU:HD22	1:A:258:GLY:N	2.30	0.47
1:A:210:GLN:CG	1:A:211:PRO:HD2	2.45	0.47
1:A:226:ASN:CB	1:A:227:PRO:HD3	2.42	0.47
1:A:234:ASN:H	1:A:245:ARG:CG	2.27	0.47
1:A:259:LYS:H	1:A:259:LYS:HD3	1.79	0.47
1:A:350:GLY:H	1:A:353:LYS:HG3	1.78	0.47
1:A:566:GLN:HG2	1:A:567:LYS:N	2.29	0.47
1:A:603:LEU:HG	1:A:648:PHE:CE1	2.46	0.47
1:A:603:LEU:CG	1:A:648:PHE:CG	2.97	0.47
1:A:678:ILE:O	1:A:678:ILE:HG23	2.15	0.47
1:A:763:GLY:HA3	1:A:766:LYS:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:MET:SD	3:C:57:PHE:CE1	3.08	0.47
2:B:63:VAL:CG1	2:B:67:GLU:HB2	2.45	0.47
3:C:70:LEU:HB3	3:C:91:LYS:CD	2.44	0.47
3:C:85:THR:O	3:C:89:VAL:HB	2.15	0.47
3:C:89:VAL:O	3:C:90:LYS:HB2	2.14	0.47
3:C:90:LYS:CD	3:C:111:PHE:HZ	2.28	0.47
3:C:115:LEU:HD13	3:C:115:LEU:C	2.39	0.47
3:C:135:ARG:CD	3:C:140:GLU:H	2.27	0.47
4:D:35:VAL:HA	4:D:54:VAL:CG2	2.35	0.47
4:E:65:LEU:HD13	4:E:67:LEU:HD23	1.95	0.47
1:A:17:LEU:HD12	1:A:152:PRO:CB	2.45	0.47
1:A:88:ILE:CD1	1:A:93:MET:HB2	2.44	0.47
1:A:189:THR:HA	1:A:192:VAL:CG2	2.45	0.47
1:A:361:TYR:O	1:A:364:MET:HE1	2.14	0.47
1:A:412:TYR:HE2	4:D:337:TYR:CD2	2.33	0.47
3:C:70:LEU:O	3:C:73:VAL:HB	2.15	0.47
4:E:159:VAL:HG22	4:E:160:THR:N	2.30	0.47
1:A:166:MET:HE1	1:A:254:PHE:CB	2.45	0.47
1:A:167:LEU:CD2	1:A:258:GLY:CA	2.93	0.47
1:A:246:PHE:CA	1:A:269:LEU:CD1	2.82	0.47
1:A:485:GLU:HA	1:A:584:TYR:CZ	2.49	0.47
1:A:673:PHE:CD1	1:A:673:PHE:N	2.82	0.47
2:B:69:ASP:O	2:B:72:MET:HB2	2.14	0.47
2:B:81:PHE:HA	2:B:84:PHE:CB	2.45	0.47
4:D:133:TYR:CE2	4:D:375:PHE:HB2	2.46	0.47
4:E:218:TYR:O	4:E:255:PHE:HA	2.14	0.47
1:A:24:ARG:HH11	1:A:27:ALA:HB3	1.80	0.47
1:A:39:PHE:CZ	1:A:80:MET:CE	2.96	0.47
1:A:117:THR:HB	1:A:124:VAL:CG2	2.45	0.47
1:A:139:VAL:HG12	1:A:143:TYR:CE1	2.50	0.47
1:A:230:GLU:HB2	1:A:234:ASN:CG	2.40	0.47
1:A:236:LYS:HD3	1:A:237:THR:O	2.14	0.47
1:A:245:ARG:CD	1:A:285:TYR:HE1	2.28	0.47
1:A:408:VAL:HG22	1:A:410:ASN:O	2.13	0.47
1:A:415:LYS:HE3	4:D:333:PRO:CG	2.45	0.47
1:A:458:PHE:C	1:A:458:PHE:CD1	2.93	0.47
1:A:644:LYS:C	1:A:646:SER:H	2.23	0.47
1:A:651:VAL:O	1:A:655:PHE:HD1	1.98	0.47
1:A:755:VAL:CG2	1:A:760:TYR:HE1	2.27	0.47
3:C:69:THR:CB	3:C:73:VAL:HG23	2.41	0.47
3:C:87:ALA:CB	3:C:94:GLY:CA	2.93	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:LYS:HB3	3:C:127:TYR:CE2	2.50	0.47
3:C:167:GLU:O	3:C:170:MET:HB2	2.15	0.47
4:D:230:ALA:HA	4:D:233:SER:HB2	1.96	0.47
4:E:54:VAL:HA	4:E:58:ALA:HB2	1.97	0.47
1:A:80:MET:HG2	1:A:81:ASN:H	1.80	0.46
1:A:254:PHE:HD1	1:A:458:PHE:HA	1.79	0.46
1:A:525:LEU:HD11	1:A:558:HIS:ND1	2.29	0.46
1:A:558:HIS:O	1:A:561:LYS:HB2	2.15	0.46
1:A:583:HIS:CB	1:A:585:ALA:HB3	2.45	0.46
1:A:831:TRP:CE3	1:A:834:MET:CE	2.97	0.46
4:E:294:TYR:HD1	4:E:327:ILE:HD12	1.80	0.46
1:A:14:ALA:HB3	1:A:15:PRO:CD	2.37	0.46
1:A:80:MET:CG	1:A:81:ASN:N	2.78	0.46
1:A:118:TYR:OH	1:A:148:ARG:HD3	2.16	0.46
1:A:193:ILE:HG22	1:A:194:GLN:N	2.26	0.46
1:A:392:LEU:HD11	1:A:613:LYS:HB2	1.95	0.46
1:A:417:GLN:HG2	1:A:422:VAL:CG1	2.45	0.46
1:A:451:THR:OG1	1:A:452:LYS:N	2.45	0.46
1:A:708:ILE:HA	1:A:711:LYS:CE	2.29	0.46
3:C:73:VAL:HG12	3:C:108:PHE:CZ	2.50	0.46
3:C:182:TYR:CD2	3:C:182:TYR:C	2.94	0.46
4:D:104:LEU:HD23	4:D:105:LEU:N	2.30	0.46
1:A:408:VAL:CG2	1:A:410:ASN:H	2.27	0.46
1:A:498:LEU:O	1:A:501:GLU:HB2	2.15	0.46
1:A:578:HIS:HD2	1:A:591:ASN:HA	1.71	0.46
3:C:183:GLU:HA	3:C:186:VAL:HG12	1.97	0.46
4:E:294:TYR:HE1	4:E:321:ALA:HB2	1.76	0.46
1:A:130:LYS:HD3	1:A:132:LEU:CD1	2.32	0.46
1:A:388:TYR:C	1:A:388:TYR:HD2	2.24	0.46
1:A:408:VAL:CG2	1:A:409:GLY:N	2.78	0.46
2:B:108:LEU:CD2	2:B:120:PHE:HE2	2.28	0.46
4:D:134:VAL:HG12	4:D:375:PHE:OXT	2.15	0.46
1:A:9:ILE:HA	1:A:18:ARG:HD3	1.97	0.46
1:A:220:ASP:HA	1:A:223:ILE:HG12	1.97	0.46
2:B:82:THR:HG23	2:B:83:VAL:H	1.80	0.46
4:E:370:VAL:CG1	4:E:371:HIS:N	2.78	0.46
1:A:122:PHE:HE1	1:A:673:PHE:CB	2.27	0.46
1:A:129:TYR:OH	1:A:678:ILE:HG13	2.14	0.46
1:A:264:ASP:O	1:A:265:ILE:HD12	2.16	0.46
1:A:309:PRO:HB2	1:A:320:VAL:HG13	1.97	0.46
1:A:537:GLU:HA	1:A:540:CYS:SG	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:LYS:HG3	1:A:643:LYS:H	1.79	0.46
1:A:723:LYS:HB3	1:A:723:LYS:HZ3	1.81	0.46
4:E:65:LEU:HD13	4:E:67:LEU:CD2	2.45	0.46
4:E:321:ALA:HB1	4:E:322:PRO:CD	2.45	0.46
1:A:51:MET:O	1:A:62:VAL:HG23	2.16	0.46
1:A:81:ASN:HD22	1:A:94:MET:CE	2.29	0.46
1:A:260:LEU:HD13	1:A:260:LEU:C	2.40	0.46
1:A:475:LEU:HD22	1:A:595:TRP:CG	2.50	0.46
1:A:488:GLN:CB	1:A:584:TYR:CE2	2.98	0.46
1:A:680:ASN:OD1	1:A:687:VAL:HG11	2.16	0.46
1:A:819:GLN:OE1	2:B:130:ASP:HB2	2.16	0.46
3:C:130:PHE:C	3:C:130:PHE:CD1	2.92	0.46
4:D:90:PHE:CD2	4:D:98:PRO:HG3	2.51	0.46
4:D:180:LEU:HD12	4:D:181:ALA:H	1.80	0.46
4:E:116:ARG:HD3	4:E:370:VAL:HG13	1.98	0.46
1:A:47:TYR:CD1	1:A:99:GLU:CD	2.92	0.46
1:A:94:MET:HE2	1:A:96:HIS:O	2.15	0.46
1:A:99:GLU:HG2	1:A:100:PRO:N	2.31	0.46
1:A:255:GLY:CA	1:A:259:LYS:HG2	2.45	0.46
1:A:412:TYR:N	1:A:412:TYR:HD1	2.14	0.46
1:A:588:VAL:HG12	1:A:590:TYR:CE2	2.50	0.46
1:A:793:GLN:HE22	3:C:155:ALA:N	2.14	0.46
1:A:802:ARG:O	1:A:805:PHE:HB3	2.15	0.46
1:A:805:PHE:O	1:A:808:MET:HB2	2.16	0.46
2:B:39:ASP:C	2:B:41:ASN:H	2.23	0.46
4:D:34:ILE:O	4:D:54:VAL:HG11	2.16	0.46
4:D:351:THR:OG1	4:D:352:PHE:CD1	2.68	0.46
1:A:408:VAL:CG1	1:A:412:TYR:CE1	2.99	0.46
2:B:124:LEU:C	2:B:124:LEU:CD1	2.89	0.46
3:C:57:PHE:CD1	3:C:60:TYR:HE2	2.34	0.46
3:C:106:ILE:HG23	3:C:107:GLU:N	2.30	0.46
4:D:45:VAL:O	4:D:45:VAL:HG13	2.16	0.46
4:E:189:LEU:HD12	4:E:189:LEU:C	2.40	0.46
4:E:335:ARG:O	4:E:338:SER:HB3	2.16	0.46
1:A:22:LYS:HA	1:A:25:ILE:HG13	1.97	0.46
1:A:24:ARG:HA	1:A:24:ARG:HD2	1.72	0.46
1:A:60:VAL:HG12	1:A:61:THR:N	2.31	0.46
1:A:95:THR:CG2	1:A:96:HIS:ND1	2.79	0.46
1:A:261:ALA:HB1	1:A:453:GLN:O	2.16	0.46
1:A:755:VAL:HG21	1:A:760:TYR:CE1	2.51	0.46
1:A:761:ARG:HG2	1:A:761:ARG:NH1	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:VAL:HA	4:D:330:ILE:O	2.15	0.46
4:D:362:TYR:HE1	4:D:367:PRO:HG3	1.79	0.46
4:E:294:TYR:CD2	4:E:325:MET:SD	3.10	0.46
1:A:210:GLN:CG	1:A:212:GLY:N	2.79	0.45
1:A:535:ILE:CG2	1:A:553:LYS:HE2	2.39	0.45
4:D:278:THR:O	4:D:282:ILE:HG13	2.15	0.45
4:E:181:ALA:O	4:E:185:LEU:HG	2.16	0.45
1:A:9:ILE:HA	1:A:18:ARG:CD	2.46	0.45
1:A:48:VAL:HG12	1:A:49:LYS:O	2.16	0.45
1:A:88:ILE:CD1	1:A:93:MET:CB	2.95	0.45
1:A:107:LYS:CD	1:A:688:MET:CG	2.94	0.45
1:A:173:GLN:C	1:A:459:ILE:HG23	2.41	0.45
1:A:254:PHE:C	1:A:455:ARG:HA	2.40	0.45
1:A:644:LYS:HG2	1:A:649:GLN:HG3	1.98	0.45
1:A:825:PHE:CE1	2:B:161:ILE:HG21	2.51	0.45
2:B:122:GLU:HG3	2:B:137:ILE:CD1	2.46	0.45
3:C:162:LYS:O	3:C:165:GLU:HG2	2.16	0.45
4:D:164:PRO:HG3	4:D:281:SER:OG	2.16	0.45
4:E:34:ILE:CD1	4:E:69:TYR:CZ	2.98	0.45
4:E:140:LEU:HB3	4:E:343:GLY:N	2.32	0.45
1:A:16:TYR:CG	1:A:134:VAL:CG2	2.99	0.45
1:A:130:LYS:HG3	1:A:685:PRO:CG	2.42	0.45
1:A:292:MET:HB2	1:A:309:PRO:HG3	1.98	0.45
1:A:396:GLU:CG	1:A:610:LEU:CD2	2.94	0.45
1:A:452:LYS:N	1:A:452:LYS:CD	2.79	0.45
1:A:574:LYS:HB2	1:A:574:LYS:HE3	1.56	0.45
2:B:58:MET:HG3	2:B:59:GLY:N	2.30	0.45
3:C:157:LEU:HB2	3:C:158:GLY:O	2.16	0.45
4:D:107:GLU:HG3	4:D:111:ASN:CB	2.46	0.45
1:A:36:LYS:HB3	1:A:51:MET:HB3	1.98	0.45
1:A:113:TRP:CE3	1:A:130:LYS:CE	2.95	0.45
1:A:160:ASP:HA	1:A:195:TYR:OH	2.17	0.45
1:A:595:TRP:N	1:A:595:TRP:CD1	2.85	0.45
1:A:760:TYR:CD1	1:A:760:TYR:N	2.84	0.45
2:B:125:LEU:HB3	2:B:132:PHE:HD1	1.74	0.45
2:B:147:ASP:HA	2:B:148:VAL:HG23	1.98	0.45
2:B:159:TYR:C	2:B:159:TYR:CD2	2.94	0.45
4:D:153:LEU:HD13	4:D:162:ASN:ND2	2.31	0.45
4:E:123:MET:HE2	4:E:123:MET:CA	2.38	0.45
4:E:346:LEU:HA	4:E:349:LEU:HG	1.99	0.45
1:A:16:TYR:HE2	1:A:132:LEU:HG	1.78	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:HB3	1:A:153:PRO:HG2	1.98	0.45
1:A:279:LEU:HD23	1:A:279:LEU:N	2.26	0.45
1:A:615:ALA:O	1:A:619:LEU:HD13	2.16	0.45
1:A:671:PRO:HB2	1:A:673:PHE:HE1	1.73	0.45
1:A:716:ARG:O	1:A:717:ILE:HG13	2.17	0.45
3:C:67:LYS:CD	3:C:92:VAL:CG1	2.92	0.45
3:C:73:VAL:CG1	3:C:108:PHE:CZ	2.99	0.45
3:C:83:ASN:HB2	3:C:84:PRO:CD	2.38	0.45
3:C:105:LYS:CD	3:C:106:ILE:N	2.79	0.45
4:D:58:ALA:CA	4:D:65:LEU:CD2	2.94	0.45
4:D:314:GLN:OE1	4:D:314:GLN:HA	2.15	0.45
1:A:295:LYS:HB2	1:A:328:SER:O	2.16	0.45
1:A:510:TRP:CZ2	1:A:512:PHE:HB2	2.51	0.45
1:A:717:ILE:HG22	1:A:718:LEU:O	2.16	0.45
1:A:805:PHE:CE1	3:C:53:PHE:HD1	2.34	0.45
1:A:825:PHE:CD1	2:B:161:ILE:HG21	2.51	0.45
4:E:191:LYS:HD2	4:E:191:LYS:HA	1.57	0.45
1:A:19:LYS:CG	1:A:114:MET:CE	2.93	0.45
1:A:53:GLN:NE2	1:A:53:GLN:HA	2.31	0.45
1:A:62:VAL:HG22	1:A:63:LYS:N	2.32	0.45
1:A:81:ASN:OD1	1:A:96:HIS:HB2	2.17	0.45
1:A:110:TYR:CE2	1:A:686:GLY:N	2.84	0.45
1:A:205:LYS:HD3	1:A:257:THR:HG21	1.97	0.45
1:A:221:GLN:HG2	1:A:449:LEU:CD2	2.46	0.45
1:A:526:ILE:CD1	1:A:583:HIS:HE1	2.28	0.45
1:A:583:HIS:CB	1:A:585:ALA:CB	2.94	0.45
1:A:688:MET:HB3	1:A:688:MET:HE3	1.62	0.45
1:A:738:GLN:HG2	1:A:738:GLN:O	2.16	0.45
1:A:836:LEU:HA	1:A:839:LYS:CG	2.47	0.45
4:E:236:LEU:HD22	4:E:251:GLY:O	2.17	0.45
4:E:236:LEU:HD22	4:E:252:ASN:N	2.32	0.45
4:E:244:ASP:CG	4:E:246:GLN:HE21	2.24	0.45
1:A:39:PHE:HZ	1:A:80:MET:CE	2.30	0.45
1:A:314:PHE:CE2	1:A:362:GLY:CA	2.97	0.45
1:A:392:LEU:HD22	1:A:392:LEU:N	2.30	0.45
1:A:462:LEU:CD1	1:A:464:ILE:CG2	2.94	0.45
1:A:499:GLU:O	1:A:503:TYR:HD1	2.00	0.45
1:A:528:LYS:HB2	1:A:529:PRO:CD	2.46	0.45
1:A:727:ARG:HH12	1:A:745:ALA:HB1	1.77	0.45
1:A:757:ARG:NH1	1:A:757:ARG:HG2	2.31	0.45
2:B:146:PRO:HD3	2:B:157:ILE:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:SER:N	3:C:49:GLN:H	2.12	0.45
3:C:67:LYS:HD2	3:C:92:VAL:CG1	2.47	0.45
3:C:122:LYS:HD2	3:C:122:LYS:HA	1.86	0.45
3:C:190:MET:HE3	3:C:190:MET:C	2.41	0.45
4:D:370:VAL:HG12	4:D:371:HIS:N	2.32	0.45
4:E:16:LEU:HB2	4:E:18:LYS:HZ3	1.82	0.45
4:E:106:THR:HA	4:E:135:ALA:H	1.82	0.45
4:E:129:VAL:O	4:E:129:VAL:HG23	2.14	0.45
4:E:287:ILE:HG12	4:E:288:ASP:OD1	2.16	0.45
4:E:329:ILE:O	4:E:329:ILE:HG22	2.16	0.45
1:A:13:ALA:HA	1:A:139:VAL:CG2	2.45	0.45
1:A:27:ALA:CB	1:A:87:LYS:HE2	2.47	0.45
1:A:136:ASN:HA	1:A:137:PRO:HD3	1.69	0.45
1:A:277:PHE:CG	1:A:278:GLN:N	2.84	0.45
1:A:517:MET:HE3	1:A:517:MET:HB2	1.67	0.45
1:A:557:GLN:CG	1:A:558:HIS:N	2.80	0.45
1:A:795:LEU:HA	3:C:80:LEU:HD21	1.99	0.45
3:C:135:ARG:HD3	3:C:140:GLU:N	2.28	0.45
3:C:188:HIS:C	3:C:189:ILE:HG23	2.42	0.45
4:E:221:LEU:HD12	4:E:221:LEU:HA	1.85	0.45
1:A:17:LEU:HD22	1:A:17:LEU:N	2.31	0.45
1:A:254:PHE:N	1:A:254:PHE:CD1	2.84	0.45
1:A:296:LYS:HB3	1:A:331:LEU:HD11	1.99	0.45
1:A:472:PHE:HZ	1:A:591:ASN:OD1	2.00	0.45
1:A:482:PHE:CE1	1:A:526:ILE:HB	2.52	0.45
1:A:648:PHE:CG	1:A:649:GLN:N	2.83	0.45
4:D:36:GLY:N	4:D:54:VAL:CG2	2.80	0.45
4:E:39:ARG:NE	4:E:66:THR:HB	2.28	0.45
4:E:143:TYR:C	4:E:143:TYR:CD1	2.95	0.45
1:A:85:PHE:HE1	1:A:93:MET:O	2.00	0.44
1:A:155:ILE:HD12	1:A:191:ARG:CG	2.47	0.44
1:A:210:GLN:HG3	1:A:212:GLY:N	2.32	0.44
1:A:237:THR:HG22	1:A:274:ARG:NH2	2.32	0.44
1:A:245:ARG:CG	1:A:285:TYR:CE1	2.94	0.44
1:A:260:LEU:O	1:A:453:GLN:CB	2.65	0.44
1:A:322:VAL:HG12	1:A:323:ALA:N	2.31	0.44
1:A:358:VAL:HG22	1:A:430:ALA:CA	2.33	0.44
1:A:508:ILE:HD13	1:A:508:ILE:N	2.32	0.44
1:A:748:LYS:HE3	1:A:748:LYS:HB2	1.68	0.44
3:C:70:LEU:HB3	3:C:91:LYS:CE	2.45	0.44
3:C:134:LEU:H	3:C:134:LEU:HD12	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:192:ILE:HG22	4:D:256:ARG:NH1	2.32	0.44
4:D:341:ILE:HG22	4:D:345:ILE:HD11	1.99	0.44
4:E:35:VAL:CA	4:E:54:VAL:CG2	2.95	0.44
1:A:245:ARG:HA	1:A:245:ARG:HE	1.82	0.44
1:A:295:LYS:HB3	1:A:331:LEU:CG	2.47	0.44
1:A:493:HIS:HA	1:A:514:ASP:CG	2.41	0.44
1:A:648:PHE:CD1	1:A:649:GLN:NE2	2.85	0.44
3:C:54:LYS:HZ1	3:C:73:VAL:HG11	1.82	0.44
4:D:24:ASP:HB2	4:D:340:TRP:HH2	1.81	0.44
4:D:38:PRO:CD	4:D:49:GLN:HE22	2.28	0.44
4:E:34:ILE:HG21	4:E:67:LEU:CB	2.46	0.44
4:E:162:ASN:HD22	4:E:278:THR:HA	1.82	0.44
1:A:16:TYR:CZ	1:A:132:LEU:HG	2.51	0.44
1:A:41:VAL:HG23	1:A:78:PHE:CE1	2.53	0.44
1:A:167:LEU:O	1:A:170:ARG:HG2	2.17	0.44
1:A:301:ASP:O	1:A:304:LEU:HD23	2.18	0.44
1:A:698:ARG:CG	1:A:703:LEU:CD1	2.95	0.44
1:A:730:ASN:CB	1:A:749:LEU:HD13	2.36	0.44
1:A:805:PHE:CE1	3:C:53:PHE:CE1	3.06	0.44
2:B:51:LEU:CD1	2:B:71:MET:CE	2.95	0.44
2:B:52:ARG:CZ	2:B:64:LYS:HG2	2.47	0.44
4:D:169:TYR:CE1	4:E:42:GLY:HA2	2.52	0.44
4:D:332:PRO:HA	4:D:333:PRO:HD3	1.71	0.44
1:A:47:TYR:CD1	1:A:47:TYR:N	2.85	0.44
1:A:107:LYS:HA	1:A:688:MET:CG	2.46	0.44
1:A:187:VAL:O	1:A:190:LYS:HB2	2.18	0.44
1:A:245:ARG:NH1	1:A:274:ARG:HD2	2.33	0.44
1:A:283:ARG:NE	1:A:322:VAL:HG21	2.32	0.44
1:A:412:TYR:N	1:A:412:TYR:CD1	2.85	0.44
1:A:526:ILE:HG22	1:A:533:PHE:HD1	1.82	0.44
1:A:799:TYR:CE2	3:C:170:MET:HE2	2.52	0.44
3:C:140:GLU:OE1	3:C:180:ILE:HG12	2.18	0.44
4:D:158:GLY:CA	4:D:183:ARG:CD	2.95	0.44
4:D:180:LEU:HD21	4:D:261:LEU:HA	1.99	0.44
4:D:335:ARG:HH21	4:D:338:SER:HB2	1.81	0.44
4:E:65:LEU:CD1	4:E:67:LEU:CD2	2.95	0.44
1:A:81:ASN:HB2	1:A:94:MET:HE3	1.99	0.44
1:A:235:ALA:HA	1:A:286:HIS:ND1	2.32	0.44
1:A:253:HIS:CD2	1:A:253:HIS:N	2.86	0.44
1:A:260:LEU:O	1:A:453:GLN:HB3	2.17	0.44
1:A:541:MET:CE	4:D:345:ILE:HG23	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:716:ARG:C	1:A:717:ILE:HD12	2.42	0.44
1:A:802:ARG:CZ	1:A:802:ARG:HB2	2.47	0.44
2:B:97:PRO:HD2	2:B:100:VAL:CG1	2.48	0.44
3:C:131:VAL:HG21	3:C:179:CYS:O	2.17	0.44
3:C:180:ILE:CD1	3:C:181:ASN:N	2.79	0.44
4:D:223:PHE:CD1	4:D:259:GLU:HG2	2.53	0.44
4:D:223:PHE:HB2	4:D:259:GLU:OE2	2.17	0.44
4:D:251:GLY:CA	4:D:254:ARG:HG3	2.24	0.44
4:E:108:ALA:HB1	4:E:109:PRO:HD2	1.98	0.44
4:E:325:MET:HB2	4:E:325:MET:HE2	1.60	0.44
1:A:205:LYS:CG	1:A:206:LYS:N	2.80	0.44
1:A:445:ILE:HG23	1:A:446:ASN:N	2.33	0.44
1:A:802:ARG:NH2	1:A:802:ARG:HB3	2.33	0.44
2:B:51:LEU:HD12	2:B:68:LEU:CD1	2.48	0.44
2:B:166:ALA:O	2:B:167:LYS:HD3	2.18	0.44
3:C:163:GLU:HG3	3:C:163:GLU:O	2.15	0.44
4:D:27:PRO:HG3	4:D:340:TRP:CG	2.52	0.44
4:D:70:PRO:HG3	4:D:81:ASP:HB3	1.99	0.44
4:D:280:ASN:O	4:D:284:LYS:HG3	2.16	0.44
4:E:36:GLY:HA3	4:E:66:THR:O	2.18	0.44
4:E:53:TYR:HD1	4:E:53:TYR:HA	1.42	0.44
1:A:16:TYR:CD1	1:A:134:VAL:CG2	2.96	0.44
1:A:91:MET:HE1	1:A:106:LEU:HD12	1.99	0.44
1:A:245:ARG:HA	1:A:245:ARG:NE	2.33	0.44
1:A:496:PHE:CD1	1:A:514:ASP:HA	2.53	0.44
1:A:642:LYS:HG3	1:A:643:LYS:N	2.32	0.44
1:A:735:PRO:O	1:A:739:PHE:HB2	2.17	0.44
2:B:154:TYR:HD1	2:B:155:LYS:N	2.15	0.44
4:D:39:ARG:HD2	4:D:65:LEU:O	2.18	0.44
4:E:8:LEU:HD11	4:E:96:VAL:HG21	2.00	0.44
4:E:261:LEU:HB3	4:E:274:ILE:HD11	2.00	0.44
1:A:70:LEU:N	1:A:70:LEU:HD12	2.33	0.44
1:A:246:PHE:N	1:A:246:PHE:CD1	2.85	0.44
1:A:254:PHE:O	1:A:456:GLN:C	2.60	0.44
1:A:283:ARG:CD	1:A:322:VAL:HG23	2.45	0.44
1:A:368:GLN:CG	1:A:376:GLU:HB3	2.48	0.44
1:A:693:VAL:O	1:A:696:GLN:HB2	2.18	0.44
1:A:760:TYR:CD2	1:A:760:TYR:C	2.95	0.44
1:A:778:GLU:OE1	1:A:778:GLU:HA	2.18	0.44
1:A:790:THR:HG23	1:A:791:ARG:HD2	1.98	0.44
4:E:282:ILE:HG12	4:E:293:LEU:HD13	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:CZ	1:A:132:LEU:CB	2.94	0.44
1:A:32:PHE:HD2	1:A:83:PRO:HD3	1.83	0.44
1:A:175:ILE:HD11	1:A:461:VAL:HG13	1.97	0.44
1:A:380:THR:O	1:A:380:THR:HG22	2.17	0.44
1:A:406:VAL:HB	1:A:605:GLU:OE2	2.17	0.44
1:A:519:LEU:HD22	1:A:584:TYR:CB	2.43	0.44
1:A:536:LEU:CD1	1:A:596:LEU:CD2	2.95	0.44
1:A:603:LEU:HD22	1:A:603:LEU:HA	1.76	0.44
1:A:700:ASN:HB3	1:A:702:VAL:HG23	1.99	0.44
1:A:822:ILE:HG13	1:A:823:ARG:N	2.32	0.44
1:A:825:PHE:CD1	1:A:828:VAL:HG13	2.53	0.44
2:B:88:PHE:HD2	2:B:91:LYS:HE2	1.82	0.44
1:A:22:LYS:HA	1:A:25:ILE:CG1	2.48	0.43
1:A:99:GLU:OE1	1:A:694:MET:HG3	2.17	0.43
1:A:415:LYS:HB2	1:A:415:LYS:HE2	1.40	0.43
1:A:418:ASN:CB	1:A:420:GLN:HE22	2.31	0.43
1:A:642:LYS:CG	1:A:643:LYS:N	2.80	0.43
1:A:693:VAL:CA	1:A:696:GLN:HG3	2.42	0.43
2:B:115:THR:CG2	2:B:154:TYR:CE2	2.96	0.43
2:B:137:ILE:CD1	2:B:141:TRP:NE1	2.79	0.43
4:D:50:LYS:HG3	4:D:53:TYR:CE2	2.53	0.43
4:D:53:TYR:HD1	4:D:53:TYR:HA	1.57	0.43
4:D:299:MET:CE	4:D:309:ILE:HG21	2.31	0.43
4:E:347:ALA:O	4:E:356:TRP:HZ2	2.01	0.43
1:A:117:THR:CG2	1:A:118:TYR:N	2.81	0.43
1:A:210:GLN:HE21	1:A:211:PRO:HD2	1.83	0.43
1:A:262:SER:CB	1:A:455:ARG:HH21	2.31	0.43
1:A:283:ARG:HD3	1:A:322:VAL:CG2	2.46	0.43
1:A:595:TRP:CD1	1:A:595:TRP:H	2.36	0.43
1:A:792:THR:HG1	3:C:127:TYR:HE1	1.64	0.43
4:E:190:MET:HE1	4:E:206:ARG:CB	2.47	0.43
4:E:236:LEU:HD12	4:E:237:GLU:N	2.34	0.43
4:E:342:GLY:HA2	4:E:345:ILE:HD12	2.01	0.43
1:A:17:LEU:N	1:A:17:LEU:CD2	2.80	0.43
1:A:99:GLU:CD	1:A:694:MET:CG	2.91	0.43
1:A:155:ILE:CD1	1:A:191:ARG:CB	2.96	0.43
1:A:198:THR:CG2	1:A:199:ILE:N	2.81	0.43
1:A:255:GLY:CA	1:A:455:ARG:HA	2.48	0.43
1:A:289:TYR:HA	1:A:292:MET:HE3	2.01	0.43
1:A:380:THR:CB	1:A:398:LEU:HD11	2.49	0.43
1:A:452:LYS:H	1:A:452:LYS:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:VAL:CG1	1:A:589:ASP:N	2.80	0.43
1:A:592:ILE:O	1:A:595:TRP:CD1	2.71	0.43
1:A:672:HIS:C	1:A:673:PHE:CD1	2.97	0.43
1:A:719:TYR:CE2	1:A:766:LYS:C	2.97	0.43
1:A:796:CYS:O	1:A:799:TYR:HB3	2.19	0.43
1:A:822:ILE:CD1	2:B:132:PHE:CE2	2.94	0.43
2:B:98:GLU:HB3	2:B:99:ASP:H	1.50	0.43
4:D:107:GLU:HG2	4:D:108:ALA:N	2.28	0.43
4:D:299:MET:CE	4:D:309:ILE:HD12	2.46	0.43
4:E:8:LEU:CD1	4:E:90:PHE:CE1	2.97	0.43
1:A:16:TYR:HB3	1:A:115:ILE:HD11	2.00	0.43
1:A:19:LYS:CA	1:A:114:MET:HE1	2.48	0.43
1:A:139:VAL:O	1:A:142:ALA:HB3	2.18	0.43
2:B:55:PHE:CG	2:B:62:ASN:HB2	2.54	0.43
4:D:78:ASN:O	4:D:82:MET:HB2	2.18	0.43
4:D:335:ARG:HD2	4:D:338:SER:HB3	1.99	0.43
4:E:158:GLY:CA	4:E:181:ALA:CB	2.96	0.43
4:E:164:PRO:CG	4:E:174:ALA:HB1	2.44	0.43
1:A:214:MET:O	1:A:215:GLN:HG3	2.18	0.43
1:A:348:LYS:HA	1:A:351:ILE:CG2	2.47	0.43
1:A:370:GLN:HG2	1:A:373:GLU:O	2.18	0.43
1:A:406:VAL:CG1	1:A:414:THR:CG2	2.95	0.43
1:A:415:LYS:C	1:A:417:GLN:H	2.26	0.43
1:A:452:LYS:HE2	1:A:452:LYS:N	2.34	0.43
1:A:551:LYS:CG	1:A:555:TYR:CE2	2.94	0.43
1:A:724:GLN:CG	1:A:725:ARG:N	2.81	0.43
1:A:795:LEU:CA	3:C:80:LEU:HD21	2.49	0.43
2:B:159:TYR:HD2	2:B:159:TYR:C	2.26	0.43
3:C:122:LYS:C	3:C:187:LYS:CE	2.92	0.43
3:C:140:GLU:CB	3:C:180:ILE:CD1	2.93	0.43
4:D:44:MET:HG3	4:D:46:GLY:O	2.18	0.43
4:D:189:LEU:HD23	4:D:209:VAL:HG12	1.98	0.43
4:E:103:THR:CG2	4:E:105:LEU:CD2	2.96	0.43
4:E:369:ILE:CG2	4:E:370:VAL:N	2.81	0.43
1:A:102:VAL:CG2	1:A:694:MET:HE1	2.36	0.43
1:A:128:PRO:CG	1:A:132:LEU:HD21	2.48	0.43
1:A:325:ILE:CG1	1:A:326:ASP:N	2.81	0.43
1:A:820:TYR:HE1	1:A:821:ASN:HD21	1.67	0.43
2:B:58:MET:HE3	2:B:60:ARG:HB3	1.90	0.43
3:C:67:LYS:H	3:C:103:ALA:H	1.67	0.43
4:D:31:PHE:HB2	4:D:32:PRO:CD	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:165:ILE:HG23	4:D:169:TYR:C	2.43	0.43
1:A:31:PRO:O	1:A:32:PHE:HB2	2.19	0.43
1:A:293:SER:HG	1:A:328:SER:HA	1.83	0.43
1:A:407:LYS:CG	1:A:408:VAL:H	2.32	0.43
1:A:524:GLU:HA	1:A:527:GLU:CG	2.47	0.43
1:A:592:ILE:O	1:A:592:ILE:HG22	2.19	0.43
1:A:726:TYR:N	1:A:726:TYR:CD1	2.82	0.43
1:A:793:GLN:HE22	3:C:156:THR:N	2.11	0.43
1:A:795:LEU:CD1	3:C:186:VAL:HG22	2.49	0.43
1:A:835:ASN:O	1:A:839:LYS:HG2	2.18	0.43
3:C:112:LEU:HD22	3:C:112:LEU:HA	1.53	0.43
4:D:272:ALA:HB3	4:D:277:THR:HG23	2.00	0.43
4:E:158:GLY:N	4:E:181:ALA:CB	2.81	0.43
1:A:81:ASN:HA	1:A:82:PRO:HD3	1.66	0.43
1:A:103:LEU:CD1	1:A:688:MET:CB	2.97	0.43
1:A:176:LEU:CD1	1:A:673:PHE:CD2	2.96	0.43
1:A:207:LYS:HZ3	1:A:453:GLN:CG	2.31	0.43
1:A:408:VAL:HG11	1:A:412:TYR:CE1	2.54	0.43
1:A:790:THR:CG2	1:A:791:ARG:N	2.81	0.43
1:A:831:TRP:CE3	1:A:834:MET:SD	3.12	0.43
2:B:126:ILE:CG2	2:B:127:THR:N	2.82	0.43
4:D:242:LEU:HG	4:D:246:GLN:O	2.18	0.43
4:E:94:LEU:HD23	4:E:94:LEU:HA	1.96	0.43
4:E:272:ALA:HB1	4:E:276:GLU:HB2	2.01	0.43
4:E:356:TRP:C	4:E:357:ILE:HD13	2.44	0.43
1:A:99:GLU:O	1:A:102:VAL:N	2.51	0.43
1:A:154:HIS:O	1:A:157:SER:HB2	2.19	0.43
1:A:163:TYR:CE2	1:A:167:LEU:HD11	2.54	0.43
1:A:338:ILE:CG2	1:A:339:ASP:N	2.82	0.43
1:A:358:VAL:HG23	1:A:433:VAL:HG11	2.01	0.43
1:A:406:VAL:O	1:A:411:GLU:HB3	2.19	0.43
1:A:467:PHE:CZ	1:A:481:ASN:CG	2.97	0.43
1:A:529:PRO:HG3	4:D:4:GLU:OE2	2.19	0.43
1:A:550:PHE:CE2	1:A:554:LEU:HD11	2.53	0.43
1:A:636:GLY:HA2	1:A:637:SER:HA	1.74	0.43
1:A:698:ARG:HG2	1:A:703:LEU:HD13	2.01	0.43
1:A:800:LEU:CG	3:C:162:LYS:HG2	2.49	0.43
1:A:825:PHE:CA	1:A:828:VAL:CG1	2.94	0.43
2:B:51:LEU:HD12	2:B:68:LEU:HD11	2.00	0.43
2:B:124:LEU:O	2:B:128:GLN:HB3	2.19	0.43
3:C:108:PHE:CZ	3:C:112:LEU:CG	2.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:ILE:HA	3:C:119:SER:OG	2.18	0.43
4:D:143:TYR:O	4:D:143:TYR:HD1	2.02	0.43
4:D:153:LEU:HD13	4:D:162:ASN:HD22	1.84	0.43
1:A:30:ARG:HH21	1:A:30:ARG:HD2	1.72	0.43
1:A:39:PHE:HA	1:A:49:LYS:HA	2.00	0.43
1:A:147:LYS:HG2	1:A:149:GLN:OE1	2.19	0.43
1:A:217:THR:HB	1:A:218:LEU:C	2.42	0.43
1:A:221:GLN:CD	1:A:449:LEU:HA	2.44	0.43
1:A:222:ILE:CD1	1:A:449:LEU:HD21	2.49	0.43
1:A:239:ARG:NH2	1:A:470:PHE:HA	2.34	0.43
1:A:415:LYS:CE	4:D:333:PRO:HG2	2.48	0.43
1:A:433:VAL:CG1	1:A:434:TYR:N	2.82	0.43
1:A:588:VAL:CG1	1:A:590:TYR:CE2	3.01	0.43
2:B:55:PHE:CA	2:B:58:MET:HB3	2.48	0.43
3:C:108:PHE:CE1	3:C:112:LEU:HD23	2.53	0.43
3:C:134:LEU:HD21	3:C:150:LEU:CG	2.44	0.43
3:C:134:LEU:O	3:C:136:VAL:HB	2.19	0.43
3:C:135:ARG:HG2	3:C:138:ASP:HA	2.00	0.43
4:D:65:LEU:H	4:D:65:LEU:HG	1.54	0.43
4:D:262:PHE:CB	4:D:312:ARG:HH21	2.31	0.43
4:E:183:ARG:CG	4:E:184:ASP:N	2.82	0.43
1:A:16:TYR:CB	1:A:134:VAL:CG2	2.97	0.42
1:A:239:ARG:HG3	1:A:470:PHE:CE2	2.54	0.42
1:A:462:LEU:HD11	1:A:464:ILE:HG22	2.00	0.42
1:A:736:GLU:HG2	1:A:737:GLY:H	1.84	0.42
2:B:81:PHE:C	2:B:81:PHE:CD1	2.93	0.42
2:B:170:GLU:OE2	2:B:170:GLU:HA	2.18	0.42
3:C:57:PHE:CD1	3:C:60:TYR:CE2	3.07	0.42
4:D:309:ILE:CG2	4:D:310:ALA:N	2.82	0.42
4:E:287:ILE:CG1	4:E:288:ASP:N	2.82	0.42
4:E:309:ILE:CG2	4:E:310:ALA:N	2.81	0.42
1:A:19:LYS:NZ	1:A:112:ALA:HB1	2.34	0.42
1:A:76:GLN:O	1:A:78:PHE:CE1	2.72	0.42
1:A:279:LEU:CD2	1:A:279:LEU:N	2.82	0.42
1:A:339:ASP:O	1:A:342:GLY:HA2	2.19	0.42
1:A:401:LEU:N	1:A:401:LEU:CD2	2.82	0.42
1:A:413:VAL:O	1:A:413:VAL:HG13	2.17	0.42
1:A:452:LYS:N	1:A:452:LYS:HD2	2.34	0.42
1:A:614:SER:C	1:A:619:LEU:CD1	2.92	0.42
1:A:820:TYR:CE1	1:A:821:ASN:ND2	2.88	0.42
1:A:836:LEU:O	1:A:839:LYS:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:LYS:HE3	2:B:141:TRP:CZ3	2.54	0.42
3:C:131:VAL:HG12	3:C:132:GLU:N	2.33	0.42
3:C:157:LEU:C	3:C:157:LEU:CD2	2.92	0.42
3:C:162:LYS:C	3:C:165:GLU:HG2	2.44	0.42
4:D:152:VAL:O	4:D:162:ASN:HA	2.19	0.42
4:D:223:PHE:CD1	4:D:259:GLU:CD	2.97	0.42
1:A:22:LYS:C	1:A:25:ILE:HG13	2.44	0.42
1:A:488:GLN:CG	1:A:584:TYR:HE2	2.28	0.42
2:B:160:VAL:O	2:B:165:ASP:HA	2.20	0.42
3:C:105:LYS:CD	3:C:105:LYS:C	2.92	0.42
4:E:349:LEU:HB3	4:E:352:PHE:HB2	2.01	0.42
1:A:39:PHE:CG	1:A:100:PRO:CG	3.02	0.42
1:A:87:LYS:N	1:A:87:LYS:HD3	2.35	0.42
1:A:295:LYS:HB2	1:A:331:LEU:HB3	1.98	0.42
1:A:369:LYS:HB3	1:A:369:LYS:HE2	1.92	0.42
2:B:42:ARG:HA	2:B:43:ASP:HA	1.77	0.42
2:B:144:PHE:O	2:B:144:PHE:CG	2.72	0.42
2:B:160:VAL:HA	2:B:165:ASP:CB	2.50	0.42
3:C:135:ARG:HH11	3:C:141:GLY:N	2.11	0.42
3:C:170:MET:SD	3:C:185:PHE:HB3	2.59	0.42
4:D:297:ASN:N	4:D:297:ASN:HD22	2.18	0.42
4:D:369:ILE:CG2	4:D:370:VAL:N	2.82	0.42
4:E:153:LEU:CD2	4:E:299:MET:HE2	2.50	0.42
1:A:188:ASN:HD22	1:A:188:ASN:N	2.17	0.42
1:A:305:ILE:CG2	1:A:306:SER:N	2.82	0.42
1:A:312:PHE:HA	1:A:313:PRO:HD3	1.89	0.42
1:A:380:THR:CG2	1:A:398:LEU:CD1	2.97	0.42
1:A:415:LYS:HE3	4:D:333:PRO:HG3	2.01	0.42
1:A:475:LEU:N	1:A:595:TRP:CZ2	2.87	0.42
1:A:734:ILE:HA	1:A:735:PRO:HD3	1.70	0.42
1:A:820:TYR:O	1:A:823:ARG:HB3	2.19	0.42
2:B:152:VAL:CG1	2:B:153:ASP:N	2.82	0.42
3:C:159:GLU:CG	3:C:162:LYS:HG3	2.50	0.42
3:C:170:MET:SD	3:C:186:VAL:CA	3.08	0.42
4:D:279:TYR:HB2	4:D:320:LEU:CD1	2.48	0.42
4:E:152:VAL:CG1	4:E:153:LEU:N	2.83	0.42
4:E:170:ALA:O	4:E:172:PRO:HD3	2.19	0.42
4:E:300:SER:O	4:E:304:THR:CG2	2.67	0.42
4:E:300:SER:O	4:E:304:THR:HG23	2.18	0.42
1:A:6:GLU:O	1:A:7:MET:HB2	2.20	0.42
1:A:175:ILE:CD1	1:A:175:ILE:C	2.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:VAL:H	1:A:282:GLU:CD	2.27	0.42
1:A:406:VAL:HG12	1:A:605:GLU:CB	2.38	0.42
1:A:478:LEU:O	1:A:478:LEU:HD12	2.18	0.42
1:A:506:GLU:CB	1:A:508:ILE:CD1	2.94	0.42
1:A:541:MET:HE2	4:D:345:ILE:CG2	2.46	0.42
1:A:573:GLY:N	1:A:574:LYS:HA	2.33	0.42
1:A:671:PRO:HB2	1:A:673:PHE:CZ	2.53	0.42
1:A:717:ILE:CG2	1:A:718:LEU:N	2.82	0.42
2:B:74:GLU:O	2:B:75:ALA:HB2	2.19	0.42
2:B:137:ILE:CG2	2:B:138:LYS:N	2.82	0.42
3:C:42:LYS:HZ3	3:C:113:PRO:CG	2.33	0.42
3:C:95:ASN:N	3:C:96:PRO:HD3	2.34	0.42
3:C:108:PHE:CZ	3:C:112:LEU:CD2	3.02	0.42
3:C:190:MET:HE2	3:C:190:MET:HB3	1.62	0.42
4:D:21:PHE:CZ	4:D:96:VAL:HG11	2.55	0.42
4:D:64:ILE:CG2	4:D:65:LEU:N	2.82	0.42
4:D:65:LEU:HD13	4:D:67:LEU:CD2	2.48	0.42
4:D:286:ASP:O	4:D:290:ARG:HG3	2.20	0.42
4:E:132:MET:HE2	4:E:132:MET:HB2	1.69	0.42
4:E:242:LEU:HB2	4:E:244:ASP:OD1	2.20	0.42
4:E:332:PRO:HD2	4:E:335:ARG:HG2	2.01	0.42
1:A:17:LEU:HD12	1:A:152:PRO:C	2.45	0.42
1:A:47:TYR:CE1	1:A:99:GLU:CD	2.98	0.42
1:A:80:MET:CG	1:A:81:ASN:H	2.33	0.42
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.76	0.42
1:A:151:ALA:HB1	1:A:152:PRO:CD	2.49	0.42
1:A:172:ASN:HB3	1:A:458:PHE:O	2.19	0.42
1:A:195:TYR:CD2	1:A:195:TYR:C	2.96	0.42
1:A:210:GLN:HG3	1:A:212:GLY:H	1.85	0.42
1:A:287:ILE:H	1:A:287:ILE:HG13	1.51	0.42
1:A:319:GLU:OE2	1:A:319:GLU:HA	2.19	0.42
1:A:407:LYS:CG	1:A:408:VAL:N	2.82	0.42
1:A:475:LEU:CD2	1:A:595:TRP:HB3	2.48	0.42
1:A:608:VAL:O	1:A:612:GLN:HG3	2.20	0.42
1:A:697:LEU:O	1:A:700:ASN:HB2	2.19	0.42
1:A:787:THR:HB	1:A:791:ARG:NH1	2.35	0.42
1:A:788:LEU:CD1	1:A:788:LEU:N	2.83	0.42
1:A:811:ARG:NH1	2:B:120:PHE:CZ	2.87	0.42
3:C:178:GLY:C	3:C:180:ILE:HD12	2.45	0.42
4:E:134:VAL:HB	4:E:375:PHE:OXT	2.20	0.42
4:E:236:LEU:O	4:E:251:GLY:HA2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:357:ILE:HD13	4:E:357:ILE:N	2.35	0.42
1:A:144:ARG:NH2	1:A:198:THR:HG23	2.34	0.42
1:A:170:ARG:O	1:A:457:TYR:CZ	2.73	0.42
1:A:177:ILE:HD13	1:A:177:ILE:HA	1.86	0.42
1:A:188:ASN:HD22	1:A:188:ASN:H	1.67	0.42
1:A:219:GLU:CD	1:A:219:GLU:N	2.77	0.42
1:A:249:PHE:CD2	1:A:251:ARG:CG	3.02	0.42
1:A:755:VAL:HG23	1:A:760:TYR:CE1	2.52	0.42
1:A:801:MET:O	1:A:804:GLU:HB2	2.19	0.42
1:A:811:ARG:HG2	1:A:815:ILE:HG13	2.01	0.42
3:C:85:THR:CG2	3:C:86:ASN:N	2.82	0.42
3:C:183:GLU:O	3:C:187:LYS:HB2	2.19	0.42
3:C:187:LYS:HD2	3:C:187:LYS:HA	1.48	0.42
4:D:99:GLU:HG2	4:D:100:GLU:HG2	2.02	0.42
4:D:155:SER:O	4:D:301:GLY:HA3	2.20	0.42
4:D:275:HIS:CG	4:D:276:GLU:N	2.87	0.42
4:D:316:GLU:HA	4:D:316:GLU:OE1	2.19	0.42
4:D:357:ILE:HA	4:D:357:ILE:HD12	1.85	0.42
4:D:357:ILE:CG2	4:D:358:THR:N	2.83	0.42
4:D:357:ILE:HG13	4:D:370:VAL:HG23	1.96	0.42
1:A:232:PHE:CG	1:A:287:ILE:CG2	2.94	0.42
1:A:349:VAL:CG1	1:A:350:GLY:N	2.82	0.42
1:A:600:LYS:HG2	1:A:602:PRO:HD3	2.01	0.42
1:A:805:PHE:CA	1:A:808:MET:HE3	2.19	0.42
2:B:61:LEU:CD2	2:B:62:ASN:N	2.80	0.42
2:B:157:ILE:O	2:B:160:VAL:HG13	2.19	0.42
4:D:202:THR:OG1	4:D:205:GLU:HG3	2.18	0.42
4:D:335:ARG:O	4:D:338:SER:HB3	2.20	0.42
4:E:150:GLY:HA3	4:E:296:ASN:HB2	2.01	0.42
4:E:193:LEU:HD23	4:E:193:LEU:HA	1.71	0.42
4:E:236:LEU:CD1	4:E:236:LEU:C	2.93	0.42
1:A:19:LYS:HG3	1:A:114:MET:HE2	2.01	0.42
1:A:41:VAL:HB	1:A:76:GLN:NE2	2.35	0.42
1:A:113:TRP:CZ3	1:A:132:LEU:HD12	2.54	0.42
1:A:155:ILE:HG21	1:A:192:VAL:HG13	2.01	0.42
1:A:261:ALA:H	1:A:455:ARG:HB3	1.85	0.42
1:A:289:TYR:CD1	1:A:320:VAL:O	2.73	0.42
1:A:301:ASP:C	1:A:304:LEU:H	2.27	0.42
1:A:419:VAL:CG1	1:A:420:GLN:N	2.83	0.42
1:A:737:GLY:C	1:A:739:PHE:H	2.27	0.42
1:A:796:CYS:O	1:A:800:LEU:HD23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:ALA:C	2:B:167:LYS:HD3	2.45	0.42
3:C:57:PHE:HA	3:C:60:TYR:CE2	2.52	0.42
3:C:88:GLU:CG	3:C:89:VAL:N	2.83	0.42
3:C:92:VAL:HG22	3:C:95:ASN:CA	2.37	0.42
4:D:113:LYS:HB3	4:D:371:HIS:CD2	2.55	0.42
4:D:299:MET:HE2	4:D:299:MET:HB3	1.82	0.42
4:D:371:HIS:CD2	4:D:372:ARG:HH11	2.38	0.42
4:E:67:LEU:HD23	4:E:67:LEU:N	2.35	0.42
4:E:190:MET:CE	4:E:206:ARG:CG	2.98	0.42
1:A:2:SER:O	1:A:3:SER:CB	2.68	0.41
1:A:76:GLN:O	1:A:76:GLN:HG3	2.20	0.41
1:A:111:ALA:N	1:A:686:GLY:HA2	2.35	0.41
2:B:157:ILE:CG1	2:B:158:CYS:N	2.82	0.41
2:B:160:VAL:HG13	2:B:161:ILE:N	2.35	0.41
3:C:104:LYS:HB3	3:C:104:LYS:HZ1	1.82	0.41
3:C:120:ASN:HD22	3:C:120:ASN:HA	1.41	0.41
3:C:170:MET:SD	3:C:186:VAL:HB	2.60	0.41
1:A:103:LEU:HD11	1:A:107:LYS:CD	2.45	0.41
1:A:170:ARG:HB3	1:A:457:TYR:CZ	2.55	0.41
1:A:406:VAL:CG1	1:A:414:THR:HG23	2.49	0.41
1:A:486:LYS:HB3	1:A:486:LYS:HE3	1.93	0.41
1:A:554:LEU:HA	1:A:557:GLN:CD	2.45	0.41
1:A:802:ARG:CZ	1:A:802:ARG:CB	2.99	0.41
1:A:844:LEU:N	1:A:844:LEU:CD2	2.84	0.41
2:B:60:ARG:HB2	2:B:60:ARG:HE	1.48	0.41
3:C:68:ILE:CG2	3:C:69:THR:N	2.83	0.41
3:C:123:ASP:O	3:C:127:TYR:CD2	2.73	0.41
4:D:117:GLU:HG2	4:D:367:PRO:HB2	2.02	0.41
4:D:140:LEU:HD22	4:D:343:GLY:HA2	2.02	0.41
4:D:227:MET:O	4:D:230:ALA:HB3	2.19	0.41
1:A:295:LYS:O	1:A:295:LYS:HD2	2.19	0.41
1:A:418:ASN:HB2	1:A:420:GLN:CD	2.45	0.41
1:A:429:LEU:CD2	1:A:429:LEU:C	2.93	0.41
1:A:482:PHE:CZ	1:A:527:GLU:HB3	2.54	0.41
2:B:147:ASP:C	2:B:148:VAL:HG23	2.45	0.41
3:C:137:PHE:C	3:C:139:LYS:N	2.78	0.41
3:C:192:ILE:O	3:C:192:ILE:HG23	2.20	0.41
4:D:97:ALA:HA	4:D:98:PRO:HD3	1.67	0.41
4:D:207:GLU:OE2	4:D:207:GLU:HA	2.20	0.41
4:E:143:TYR:CD2	4:E:346:LEU:HB2	2.54	0.41
4:E:317:ILE:HD13	4:E:317:ILE:HA	1.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:CD	1:A:694:MET:HG3	2.45	0.41
1:A:125:THR:O	1:A:125:THR:HG23	2.19	0.41
1:A:245:ARG:NH2	1:A:274:ARG:HE	2.17	0.41
1:A:364:MET:SD	1:A:382:VAL:HG11	2.60	0.41
1:A:462:LEU:HD11	1:A:464:ILE:CG2	2.50	0.41
1:A:475:LEU:HD22	1:A:595:TRP:CB	2.48	0.41
3:C:106:ILE:HD13	3:C:106:ILE:O	2.20	0.41
4:D:183:ARG:HG2	4:D:184:ASP:H	1.77	0.41
1:A:89:GLU:HA	1:A:109:ARG:NH1	2.35	0.41
1:A:171:ASP:HA	1:A:457:TYR:CD1	2.55	0.41
1:A:291:ILE:CG2	1:A:296:LYS:HZ2	2.32	0.41
1:A:306:SER:O	1:A:307:THR:HG23	2.21	0.41
1:A:340:ILE:CG2	1:A:341:LEU:N	2.83	0.41
1:A:367:LYS:HG2	1:A:378:ASP:HB2	2.01	0.41
1:A:645:GLY:HA2	4:D:23:GLY:CA	2.43	0.41
1:A:819:GLN:HE22	2:B:130:ASP:H	1.66	0.41
1:A:839:LYS:O	1:A:842:PRO:HD2	2.19	0.41
2:B:55:PHE:O	2:B:58:MET:HB3	2.19	0.41
2:B:88:PHE:CD2	2:B:91:LYS:HE2	2.56	0.41
3:C:43:ILE:HG22	3:C:45:PHE:H	1.84	0.41
3:C:98:ASN:CB	3:C:99:GLU:CA	2.92	0.41
3:C:131:VAL:CG1	3:C:179:CYS:CB	2.96	0.41
3:C:137:PHE:C	3:C:139:LYS:H	2.27	0.41
3:C:180:ILE:CA	3:C:183:GLU:CG	2.95	0.41
4:D:200:PHE:CD1	4:D:209:VAL:CG2	3.03	0.41
4:D:349:LEU:HD23	4:D:349:LEU:HA	1.80	0.41
4:E:106:THR:CG2	4:E:140:LEU:CD1	2.96	0.41
4:E:294:TYR:HD1	4:E:327:ILE:CD1	2.32	0.41
1:A:78:PHE:HD2	1:A:98:HIS:CD2	2.15	0.41
1:A:199:ILE:HA	1:A:202:THR:OG1	2.20	0.41
1:A:235:ALA:HB3	1:A:245:ARG:HH11	1.86	0.41
1:A:429:LEU:O	1:A:429:LEU:HD23	2.21	0.41
1:A:513:ILE:CG2	1:A:514:ASP:N	2.82	0.41
1:A:524:GLU:CA	1:A:527:GLU:HG2	2.48	0.41
1:A:599:ASN:OD1	1:A:650:THR:HB	2.21	0.41
1:A:800:LEU:HD21	3:C:162:LYS:HB3	2.02	0.41
1:A:836:LEU:HA	1:A:839:LYS:HG3	2.02	0.41
2:B:116:ILE:HG22	2:B:117:LYS:O	2.20	0.41
3:C:70:LEU:CD1	3:C:71:SER:N	2.84	0.41
4:E:37:ARG:H	4:E:66:THR:CG2	2.34	0.41
1:A:205:LYS:HZ1	1:A:257:THR:HB	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:CD	1:A:322:VAL:CG2	2.98	0.41
1:A:364:MET:SD	1:A:382:VAL:CB	3.08	0.41
1:A:404:PRO:CB	1:A:606:THR:HB	2.41	0.41
1:A:504:LYS:HA	1:A:504:LYS:HD2	1.90	0.41
1:A:578:HIS:NE2	1:A:591:ASN:CA	2.81	0.41
1:A:618:LEU:CG	1:A:622:LEU:HD11	2.49	0.41
1:A:687:VAL:C	1:A:688:MET:HG2	2.44	0.41
4:D:69:TYR:HB2	4:D:72:GLU:CA	2.50	0.41
4:D:82:MET:HE2	4:D:86:TRP:CE2	2.56	0.41
4:E:120:THR:HG23	4:E:132:MET:SD	2.60	0.41
1:A:231:ALA:O	1:A:286:HIS:HB2	2.21	0.41
1:A:236:LYS:CG	1:A:241:ASP:HA	2.36	0.41
1:A:519:LEU:CD1	1:A:584:TYR:CB	2.98	0.41
2:B:51:LEU:CD1	2:B:68:LEU:HD11	2.50	0.41
3:C:137:PHE:CD2	3:C:137:PHE:O	2.74	0.41
4:D:33:SER:O	4:D:69:TYR:CD2	2.74	0.41
4:D:50:LYS:CG	4:D:53:TYR:CE2	3.03	0.41
4:D:107:GLU:HG2	4:D:108:ALA:O	2.20	0.41
4:D:285:CYS:CB	4:D:289:ILE:HD11	2.41	0.41
4:D:313:MET:CA	4:D:313:MET:HE3	2.51	0.41
4:D:372:ARG:O	4:D:373:LYS:HB2	2.20	0.41
4:E:47:MET:CG	4:E:48:GLY:N	2.82	0.41
4:E:143:TYR:CZ	4:E:345:ILE:HG21	2.56	0.41
4:E:148:THR:CG2	4:E:149:THR:N	2.82	0.41
4:E:282:ILE:HG12	4:E:293:LEU:CD1	2.50	0.41
1:A:147:LYS:HB3	1:A:150:GLU:HG3	2.03	0.41
1:A:170:ARG:C	1:A:457:TYR:CZ	2.99	0.41
1:A:174:SER:HA	1:A:460:GLY:H	1.86	0.41
1:A:261:ALA:CB	1:A:455:ARG:HB3	2.51	0.41
1:A:262:SER:HB3	1:A:451:THR:H	1.86	0.41
1:A:311:ASP:HB2	1:A:312:PHE:CE1	2.56	0.41
1:A:343:PHE:CD1	1:A:444:ARG:NH2	2.89	0.41
1:A:355:THR:HG23	1:A:437:MET:HE1	2.00	0.41
1:A:368:GLN:CG	1:A:376:GLU:CB	2.95	0.41
1:A:485:GLU:HB3	1:A:523:ILE:HG21	2.03	0.41
1:A:506:GLU:HB2	1:A:508:ILE:HD11	1.98	0.41
1:A:537:GLU:O	1:A:540:CYS:HB2	2.20	0.41
1:A:544:LYS:HE2	1:A:544:LYS:HB2	1.87	0.41
1:A:762:PHE:CD1	1:A:762:PHE:N	2.89	0.41
1:A:784:LYS:O	1:A:788:LEU:HD13	2.21	0.41
1:A:795:LEU:CD2	3:C:80:LEU:HD21	2.48	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:PHE:CD1	3:C:53:PHE:HE1	2.38	0.41
1:A:822:ILE:CG1	1:A:823:ARG:N	2.83	0.41
2:B:42:ARG:HH11	2:B:42:ARG:CG	2.34	0.41
2:B:55:PHE:O	2:B:59:GLY:HA2	2.21	0.41
2:B:159:TYR:CE2	2:B:165:ASP:O	2.74	0.41
2:B:169:GLN:O	2:B:169:GLN:HG2	2.20	0.41
3:C:43:ILE:CG2	3:C:44:GLU:N	2.83	0.41
3:C:70:LEU:HB3	3:C:71:SER:H	1.62	0.41
3:C:114:MET:HB2	3:C:114:MET:HE2	1.78	0.41
3:C:145:VAL:CG2	3:C:146:MET:N	2.82	0.41
4:D:143:TYR:HD2	4:D:346:LEU:HD13	1.80	0.41
4:D:170:ALA:O	4:D:172:PRO:HD3	2.21	0.41
4:D:219:VAL:HG12	4:D:220:ALA:N	2.36	0.41
4:D:251:GLY:HA2	4:D:254:ARG:CG	2.23	0.41
4:E:171:LEU:HA	4:E:172:PRO:HD3	1.85	0.41
4:E:189:LEU:HA	4:E:192:ILE:HG12	2.03	0.41
4:E:275:HIS:CA	4:E:313:MET:HE1	2.49	0.41
4:E:299:MET:O	4:E:332:PRO:HD2	2.21	0.41
4:E:365:ALA:HB3	4:E:369:ILE:CD1	2.46	0.41
1:A:25:ILE:HD12	1:A:26:GLU:H	1.78	0.41
1:A:91:MET:CE	1:A:102:VAL:HA	2.40	0.41
1:A:137:PRO:O	1:A:141:THR:HG23	2.21	0.41
1:A:205:LYS:HB3	1:A:257:THR:HG23	2.02	0.41
1:A:265:ILE:N	1:A:265:ILE:CD1	2.85	0.41
1:A:338:ILE:HA	1:A:341:LEU:CD1	2.50	0.41
3:C:90:LYS:CB	3:C:111:PHE:CE2	2.95	0.41
3:C:148:ALA:HB1	3:C:163:GLU:HG2	2.01	0.41
4:D:210:ARG:HH11	4:D:210:ARG:CG	2.34	0.41
4:D:236:LEU:CB	4:D:251:GLY:C	2.94	0.41
4:E:149:THR:CG2	4:E:150:GLY:N	2.82	0.41
4:E:150:GLY:CA	4:E:296:ASN:HB2	2.50	0.41
1:A:32:PHE:CD2	1:A:83:PRO:CD	3.03	0.40
1:A:104:TYR:CE1	1:A:108:GLU:CG	3.03	0.40
1:A:161:ASN:O	1:A:165:PHE:CD2	2.74	0.40
1:A:277:PHE:CZ	1:A:278:GLN:O	2.75	0.40
1:A:474:SER:CA	1:A:595:TRP:CZ2	3.04	0.40
2:B:140:MET:SD	2:B:145:SER:HB3	2.61	0.40
3:C:166:VAL:CG2	3:C:167:GLU:N	2.84	0.40
4:D:37:ARG:HH11	4:D:37:ARG:HD3	1.75	0.40
4:D:143:TYR:C	4:D:143:TYR:CD1	2.95	0.40
4:D:288:ASP:HA	4:E:243:PRO:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:VAL:CG2	1:A:103:LEU:N	2.84	0.40
1:A:183:ALA:HB3	1:A:185:LYS:H	1.87	0.40
1:A:306:SER:C	1:A:307:THR:CG2	2.94	0.40
1:A:351:ILE:HG23	1:A:352:TYR:N	2.35	0.40
3:C:54:LYS:HE2	3:C:65:ASP:OD2	2.20	0.40
4:E:165:ILE:N	4:E:165:ILE:HD12	2.36	0.40
4:E:297:ASN:OD1	4:E:329:ILE:HD11	2.21	0.40
4:E:332:PRO:HA	4:E:333:PRO:HD3	1.81	0.40
1:A:115:ILE:CD1	1:A:116:TYR:CE2	3.04	0.40
1:A:234:ASN:N	1:A:245:ARG:CG	2.83	0.40
1:A:234:ASN:O	1:A:235:ALA:HB2	2.21	0.40
1:A:351:ILE:CD1	1:A:437:MET:CE	2.99	0.40
1:A:626:TYR:CG	1:A:627:ALA:N	2.89	0.40
2:B:147:ASP:C	2:B:148:VAL:CG2	2.94	0.40
3:C:53:PHE:CE2	3:C:73:VAL:O	2.75	0.40
3:C:70:LEU:C	3:C:70:LEU:CD1	2.95	0.40
3:C:128:GLU:CG	3:C:180:ILE:CG2	2.99	0.40
4:D:140:LEU:HD23	4:D:140:LEU:HA	1.85	0.40
4:D:233:SER:HB3	4:D:236:LEU:CG	2.45	0.40
1:A:16:TYR:HB2	1:A:134:VAL:HG22	2.02	0.40
1:A:72:LEU:HB3	1:A:76:GLN:CG	2.43	0.40
1:A:159:SER:HB3	1:A:195:TYR:CE2	2.55	0.40
1:A:245:ARG:HG2	1:A:245:ARG:H	1.56	0.40
1:A:292:MET:SD	1:A:309:PRO:HB3	2.62	0.40
1:A:364:MET:HE2	1:A:364:MET:HB2	1.64	0.40
1:A:398:LEU:HD23	1:A:398:LEU:HA	1.87	0.40
1:A:445:ILE:CG2	1:A:446:ASN:N	2.83	0.40
3:C:53:PHE:CD2	3:C:53:PHE:C	2.93	0.40
4:D:104:LEU:C	4:D:104:LEU:CD2	2.95	0.40
4:E:8:LEU:HD23	4:E:8:LEU:HA	1.92	0.40
4:E:148:THR:O	4:E:165:ILE:HG22	2.21	0.40
1:A:38:CYS:HB3	1:A:39:PHE:H	1.54	0.40
1:A:116:TYR:CE1	1:A:125:THR:CB	3.02	0.40
1:A:192:VAL:O	1:A:195:TYR:HB3	2.22	0.40
1:A:360:HIS:C	1:A:382:VAL:CG1	2.93	0.40
1:A:446:ASN:HA	1:A:449:LEU:HB2	2.03	0.40
1:A:789:MET:HG3	3:C:130:PHE:CZ	2.57	0.40
4:D:36:GLY:H	4:D:52:SER:HB2	1.86	0.40
4:E:49:GLN:O	4:E:50:LYS:HD3	2.21	0.40
4:E:142:LEU:HD21	4:E:165:ILE:HG12	2.03	0.40
4:E:143:TYR:CE2	4:E:346:LEU:CB	3.02	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	843/845 (100%)	776 (92%)	42 (5%)	25 (3%)	3	22
2	B	144/146 (99%)	116 (81%)	17 (12%)	11 (8%)	1	9
3	C	151/153 (99%)	121 (80%)	15 (10%)	15 (10%)	0	7
4	D	372/375 (99%)	338 (91%)	24 (6%)	10 (3%)	4	24
4	E	372/375 (99%)	343 (92%)	18 (5%)	11 (3%)	3	22
All	All	1882/1894 (99%)	1694 (90%)	116 (6%)	72 (4%)	4	18

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	SER
1	A	46	MET
1	A	215	GLN
1	A	269	LEU
1	A	307	THR
1	A	367	LYS
1	A	369	LYS
1	A	380	THR
1	A	453	GLN
1	A	614	SER
2	B	39	ASP
2	B	62	ASN
2	B	75	ALA
2	B	111	GLU
2	B	167	LYS
3	C	46	SER
3	C	62	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	67	LYS
3	C	94	GLY
3	C	116	GLN
3	C	136	VAL
3	C	157	LEU
4	D	43	VAL
4	D	97	ALA
4	D	373	LYS
4	E	3	ASP
4	E	4	GLU
4	E	43	VAL
4	E	44	MET
1	A	262	SER
1	A	408	VAL
1	A	642	LYS
1	A	705	GLY
2	B	44	GLY
2	B	65	ASN
2	B	165	ASP
3	C	43	ILE
3	C	90	LYS
3	C	189	ILE
4	D	3	ASP
4	D	238	LYS
1	A	19	LYS
1	A	205	LYS
1	A	280	SER
1	A	344	SER
1	A	425	SER
1	A	646	SER
2	B	98	GLU
3	C	70	LEU
3	C	192	ILE
4	D	4	GLU
4	D	44	MET
4	D	158	GLY
4	D	181	ALA
4	E	41	GLN
4	E	54	VAL
1	A	624	SER
2	B	27	GLN
2	B	169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	97	SER
3	C	154	LEU
4	E	181	ALA
4	E	323	SER
4	E	374	CYS
1	A	296	LYS
1	A	457	TYR
1	A	601	ASP
3	C	152	HIS
4	E	238	LYS
4	D	54	VAL
4	E	158	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	738/738 (100%)	536 (73%)	202 (27%)	0	3
2	B	125/125 (100%)	82 (66%)	43 (34%)	0	2
3	C	131/131 (100%)	73 (56%)	58 (44%)	0	0
4	D	317/317 (100%)	250 (79%)	67 (21%)	1	7
4	E	317/317 (100%)	249 (78%)	68 (22%)	1	7
All	All	1628/1628 (100%)	1190 (73%)	438 (27%)	2	3

All (438) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ASP
1	A	9	ILE
1	A	17	LEU
1	A	18	ARG
1	A	19	LYS
1	A	21	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	24	ARG
1	A	26	GLU
1	A	28	GLN
1	A	29	ASN
1	A	33	ASP
1	A	35	LYS
1	A	36	LYS
1	A	41	VAL
1	A	43	ASP
1	A	45	GLU
1	A	46	MET
1	A	49	LYS
1	A	51	MET
1	A	54	SER
1	A	55	ARG
1	A	57	ASN
1	A	59	LYS
1	A	69	THR
1	A	71	THR
1	A	74	SER
1	A	76	GLN
1	A	86	ASP
1	A	87	LYS
1	A	91	MET
1	A	95	THR
1	A	99	GLU
1	A	102	VAL
1	A	106	LEU
1	A	115	ILE
1	A	117	THR
1	A	130	LYS
1	A	132	LEU
1	A	134	VAL
1	A	138	GLU
1	A	147	LYS
1	A	155	ILE
1	A	158	ILE
1	A	159	SER
1	A	176	LEU
1	A	180	GLU
1	A	190	LYS
1	A	191	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	192	VAL
1	A	193	ILE
1	A	198	THR
1	A	199	ILE
1	A	201	VAL
1	A	206	LYS
1	A	207	LYS
1	A	210	GLN
1	A	214	MET
1	A	217	THR
1	A	219	GLU
1	A	236	LYS
1	A	238	VAL
1	A	245	ARG
1	A	250	ILE
1	A	252	ILE
1	A	253	HIS
1	A	257	THR
1	A	259	LYS
1	A	260	LEU
1	A	262	SER
1	A	264	ASP
1	A	266	GLU
1	A	268	TYR
1	A	269	LEU
1	A	271	GLU
1	A	275	VAL
1	A	279	LEU
1	A	282	GLU
1	A	287	ILE
1	A	295	LYS
1	A	301	ASP
1	A	307	THR
1	A	315	VAL
1	A	317	GLN
1	A	327	ASP
1	A	328	SER
1	A	330	GLU
1	A	338	ILE
1	A	340	ILE
1	A	341	LEU
1	A	344	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	345	SER
1	A	351	ILE
1	A	358	VAL
1	A	364	MET
1	A	365	LYS
1	A	367	LYS
1	A	369	LYS
1	A	370	GLN
1	A	372	GLU
1	A	374	GLN
1	A	376	GLU
1	A	388	TYR
1	A	390	MET
1	A	397	MET
1	A	399	LYS
1	A	401	LEU
1	A	403	CYS
1	A	407	LYS
1	A	408	VAL
1	A	411	GLU
1	A	412	TYR
1	A	415	LYS
1	A	418	ASN
1	A	420	GLN
1	A	421	GLN
1	A	423	THR
1	A	429	LEU
1	A	431	LYS
1	A	449	LEU
1	A	452	LYS
1	A	453	GLN
1	A	455	ARG
1	A	456	GLN
1	A	459	ILE
1	A	462	LEU
1	A	464	ILE
1	A	468	GLU
1	A	471	ASP
1	A	475	LEU
1	A	500	GLN
1	A	501	GLU
1	A	502	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	504	LYS
1	A	508	ILE
1	A	517	MET
1	A	518	ASP
1	A	523	ILE
1	A	525	LEU
1	A	526	ILE
1	A	535	ILE
1	A	536	LEU
1	A	544	LYS
1	A	546	THR
1	A	551	LYS
1	A	567	LYS
1	A	574	LYS
1	A	582	VAL
1	A	584	TYR
1	A	591	ASN
1	A	600	LYS
1	A	601	ASP
1	A	603	LEU
1	A	608	VAL
1	A	613	LYS
1	A	616	LEU
1	A	617	LYS
1	A	634	SER
1	A	637	SER
1	A	642	LYS
1	A	643	LYS
1	A	644	LYS
1	A	646	SER
1	A	651	VAL
1	A	652	SER
1	A	659	LEU
1	A	667	ARG
1	A	675	ARG
1	A	677	LEU
1	A	683	LYS
1	A	694	MET
1	A	700	ASN
1	A	702	VAL
1	A	710	ARG
1	A	711	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	718	LEU
1	A	723	LYS
1	A	724	GLN
1	A	727	ARG
1	A	740	ILE
1	A	742	SER
1	A	746	SER
1	A	748	LYS
1	A	750	LEU
1	A	767	VAL
1	A	770	LYS
1	A	781	ARG
1	A	783	GLU
1	A	789	MET
1	A	790	THR
1	A	795	LEU
1	A	801	MET
1	A	803	VAL
1	A	807	LYS
1	A	818	ILE
1	A	822	ILE
1	A	828	VAL
1	A	829	LYS
1	A	836	LEU
1	A	839	LYS
1	A	841	LYS
1	A	845	LYS
2	B	25	GLN
2	B	32	LYS
2	B	36	THR
2	B	40	GLN
2	B	45	ILE
2	B	47	ASP
2	B	48	LYS
2	B	49	GLU
2	B	51	LEU
2	B	58	MET
2	B	60	ARG
2	B	61	LEU
2	B	62	ASN
2	B	63	VAL
2	B	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	71	MET
2	B	73	LYS
2	B	82	THR
2	B	83	VAL
2	B	90	GLU
2	B	91	LYS
2	B	92	LEU
2	B	93	LYS
2	B	106	LYS
2	B	108	LEU
2	B	113	LYS
2	B	117	LYS
2	B	118	LYS
2	B	119	GLN
2	B	124	LEU
2	B	128	GLN
2	B	131	ARG
2	B	135	GLU
2	B	136	GLU
2	B	137	ILE
2	B	140	MET
2	B	155	LYS
2	B	157	ILE
2	B	159	TYR
2	B	161	ILE
2	B	165	ASP
2	B	167	LYS
2	B	168	ASP
3	C	41	ILE
3	C	45	PHE
3	C	46	SER
3	C	47	LYS
3	C	48	GLU
3	C	50	GLN
3	C	52	GLU
3	C	54	LYS
3	C	57	PHE
3	C	58	LEU
3	C	62	ARG
3	C	67	LYS
3	C	68	ILE
3	C	73	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	75	ASP
3	C	76	VAL
3	C	77	LEU
3	C	78	ARG
3	C	80	LEU
3	C	90	LYS
3	C	91	LYS
3	C	92	VAL
3	C	95	ASN
3	C	104	LYS
3	C	105	LYS
3	C	106	ILE
3	C	112	LEU
3	C	115	LEU
3	C	120	ASN
3	C	122	LYS
3	C	124	GLN
3	C	126	THR
3	C	128	GLU
3	C	130	PHE
3	C	131	VAL
3	C	132	GLU
3	C	136	VAL
3	C	138	ASP
3	C	139	LYS
3	C	142	ASN
3	C	144	THR
3	C	145	VAL
3	C	149	GLU
3	C	153	VAL
3	C	156	THR
3	C	157	LEU
3	C	160	LYS
3	C	163	GLU
3	C	164	GLU
3	C	167	GLU
3	C	174	GLU
3	C	179	CYS
3	C	180	ILE
3	C	183	GLU
3	C	187	LYS
3	C	189	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	190	MET
3	C	192	ILE
4	D	1	ASP
4	D	10	CYS
4	D	18	LYS
4	D	28	ARG
4	D	34	ILE
4	D	35	VAL
4	D	37	ARG
4	D	43	VAL
4	D	45	VAL
4	D	47	MET
4	D	49	GLN
4	D	50	LYS
4	D	51	ASP
4	D	56	ASP
4	D	57	GLU
4	D	59	GLN
4	D	65	LEU
4	D	66	THR
4	D	68	LYS
4	D	69	TYR
4	D	71	ILE
4	D	85	ILE
4	D	107	GLU
4	D	113	LYS
4	D	118	LYS
4	D	121	GLN
4	D	129	VAL
4	D	134	VAL
4	D	139	VAL
4	D	142	LEU
4	D	145	SER
4	D	147	ARG
4	D	148	THR
4	D	149	THR
4	D	167	GLU
4	D	171	LEU
4	D	180	LEU
4	D	183	ARG
4	D	186	THR
4	D	196	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	208	ILE
4	D	232	SER
4	D	233	SER
4	D	236	LEU
4	D	244	ASP
4	D	250	ILE
4	D	256	ARG
4	D	267	ILE
4	D	269	MET
4	D	286	ASP
4	D	287	ILE
4	D	297	ASN
4	D	309	ILE
4	D	312	ARG
4	D	315	LYS
4	D	335	ARG
4	D	349	LEU
4	D	350	SER
4	D	354	GLN
4	D	357	ILE
4	D	359	LYS
4	D	360	GLN
4	D	369	ILE
4	D	370	VAL
4	D	372	ARG
4	D	373	LYS
4	D	374	CYS
4	E	8	LEU
4	E	18	LYS
4	E	30	VAL
4	E	34	ILE
4	E	44	MET
4	E	49	GLN
4	E	51	ASP
4	E	56	ASP
4	E	57	GLU
4	E	60	SER
4	E	61	LYS
4	E	64	ILE
4	E	71	ILE
4	E	82	MET
4	E	95	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	103	THR
4	E	105	LEU
4	E	110	LEU
4	E	113	LYS
4	E	132	MET
4	E	139	VAL
4	E	141	SER
4	E	145	SER
4	E	147	ARG
4	E	151	ILE
4	E	153	LEU
4	E	157	ASP
4	E	167	GLU
4	E	176	MET
4	E	189	LEU
4	E	191	LYS
4	E	196	ARG
4	E	199	SER
4	E	208	ILE
4	E	232	SER
4	E	234	SER
4	E	236	LEU
4	E	238	LYS
4	E	239	SER
4	E	244	ASP
4	E	248	ILE
4	E	249	THR
4	E	250	ILE
4	E	257	CYS
4	E	267	ILE
4	E	269	MET
4	E	274	ILE
4	E	285	CYS
4	E	286	ASP
4	E	287	ILE
4	E	297	ASN
4	E	298	VAL
4	E	300	SER
4	E	312	ARG
4	E	315	LYS
4	E	317	ILE
4	E	323	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	324	THR
4	E	325	MET
4	E	329	ILE
4	E	335	ARG
4	E	341	ILE
4	E	346	LEU
4	E	349	LEU
4	E	350	SER
4	E	357	ILE
4	E	370	VAL
4	E	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	53	GLN
1	A	76	GLN
1	A	105	ASN
1	A	161	ASN
1	A	188	ASN
1	A	210	GLN
1	A	221	GLN
1	A	234	ASN
1	A	240	ASN
1	A	360	HIS
1	A	363	ASN
1	A	393	ASN
1	A	420	GLN
1	A	421	GLN
1	A	424	ASN
1	A	453	GLN
1	A	456	GLN
1	A	488	GLN
1	A	558	HIS
1	A	583	HIS
1	A	649	GLN
1	A	665	ASN
1	A	670	HIS
1	A	672	HIS
1	A	690	HIS
1	A	793	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	819	GLN
1	A	821	ASN
1	A	827	ASN
1	A	835	ASN
2	B	25	GLN
2	B	27	GLN
2	B	29	GLN
2	B	62	ASN
2	B	65	ASN
2	B	119	GLN
2	B	139	ASN
3	C	72	GLN
3	C	86	ASN
3	C	98	ASN
3	C	116	GLN
3	C	120	ASN
3	C	142	ASN
3	C	152	HIS
3	C	177	ASN
4	D	41	GLN
4	D	49	GLN
4	D	87	HIS
4	D	92	ASN
4	D	162	ASN
4	D	297	ASN
4	D	353	GLN
4	D	360	GLN
4	E	59	GLN
4	E	92	ASN
4	E	162	ASN
4	E	246	GLN
4	E	353	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HIC	E	73	4	10,11,12	0.69	0	9,14,16	3.35	4 (44%)
4	HIC	D	73	4	10,11,12	0.68	0	9,14,16	3.34	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HIC	E	73	4	-	1/5/6/8	0/1/1/1
4	HIC	D	73	4	-	1/5/6/8	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	73	HIC	NE2-CE1-ND1	-8.89	109.26	112.66
4	E	73	HIC	NE2-CE1-ND1	-8.79	109.30	112.66
4	E	73	HIC	CE1-ND1-CG	2.72	110.15	105.80
4	D	73	HIC	CE1-ND1-CG	2.69	110.11	105.80
4	E	73	HIC	CD2-NE2-CE1	-2.66	105.66	106.71
4	D	73	HIC	CD2-NE2-CE1	-2.35	105.78	106.71
4	E	73	HIC	CD2-CG-ND1	-2.17	104.71	109.43
4	D	73	HIC	CD2-CG-ND1	-2.13	104.79	109.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	73	HIC	O-C-CA-CB
4	E	73	HIC	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	73	HIC	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ADP	D	401	-	28,29,29	1.13	2 (7%)	43,45,45	1.26	7 (16%)
5	ADP	E	401	-	28,29,29	1.14	2 (7%)	43,45,45	1.26	7 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	D	401	-	-	0/16/32/32	0/3/3/3
5	ADP	E	401	-	-	0/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	401	ADP	C2-N1	3.15	1.39	1.33
5	E	401	ADP	C5-N7	-3.10	1.33	1.39
5	D	401	ADP	C5-N7	-3.07	1.33	1.39
5	D	401	ADP	C2-N1	3.05	1.39	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	401	ADP	C5-C4-N3	2.59	130.28	126.72
5	D	401	ADP	C5-C4-N3	2.55	130.22	126.72
5	E	401	ADP	C4-C5-N7	2.54	113.48	110.58
5	D	401	ADP	C4-C5-N7	2.50	113.44	110.58
5	D	401	ADP	C4-N9-C8	-2.39	103.23	105.74
5	D	401	ADP	C2-N1-C6	2.39	122.65	118.73
5	E	401	ADP	C2-N1-C6	2.36	122.61	118.73
5	E	401	ADP	C4-N9-C8	-2.34	103.28	105.74
5	D	401	ADP	N3-C2-N1	-2.24	125.19	128.58
5	E	401	ADP	N3-C2-N1	-2.21	125.24	128.58
5	D	401	ADP	O3B-PB-O2B	2.20	116.04	107.80
5	E	401	ADP	O3B-PB-O2B	2.18	115.98	107.80
5	E	401	ADP	O2A-PA-O3A	2.16	113.11	107.27
5	D	401	ADP	O2A-PA-O3A	2.13	113.04	107.27

There are no chirality outliers.

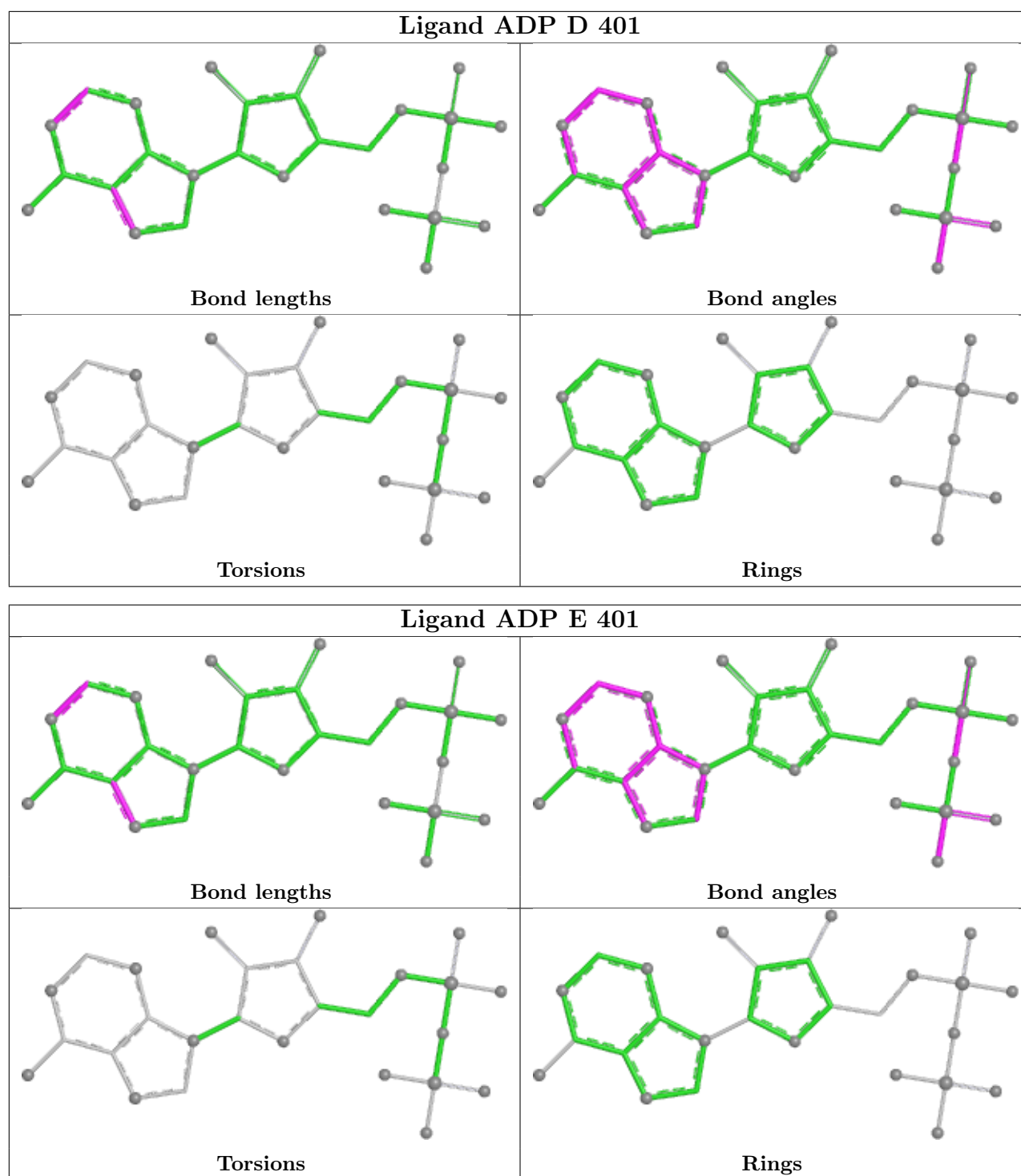
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	ADP	7	0
5	E	401	ADP	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

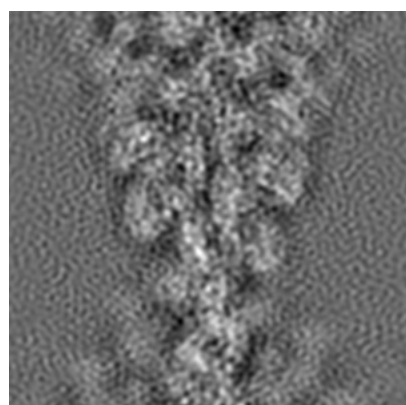
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6664. These allow visual inspection of the internal detail of the map and identification of artifacts.

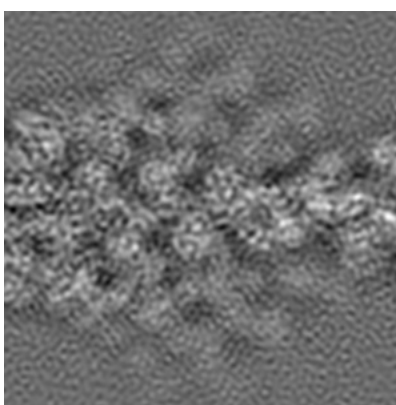
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

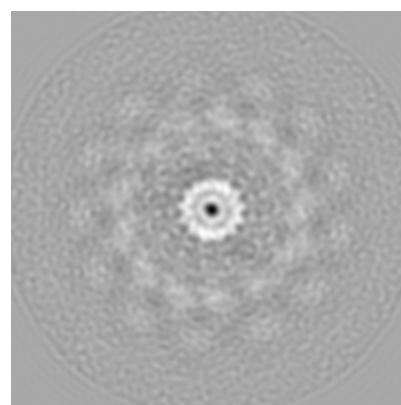
6.1.1 Primary map



X



Y



Z

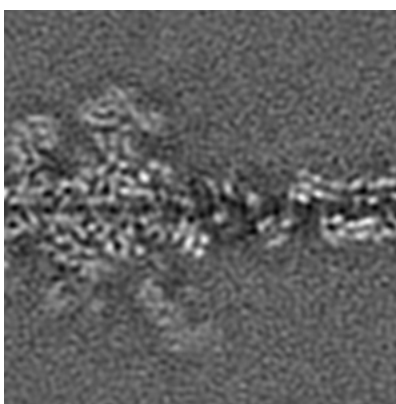
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

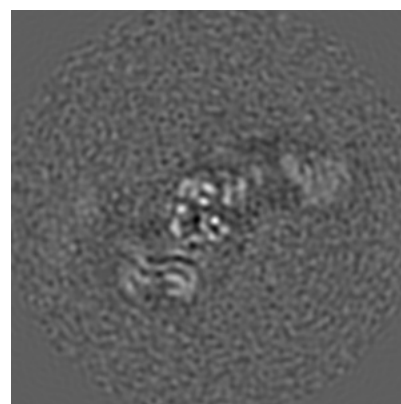
6.2.1 Primary map



X Index: 125



Y Index: 125



Z Index: 125

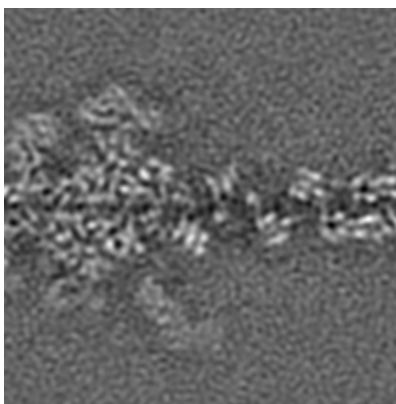
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

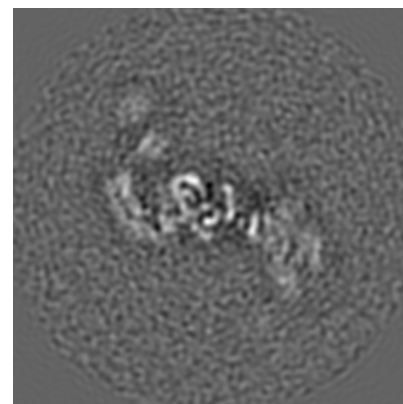
6.3.1 Primary map



X Index: 125



Y Index: 126

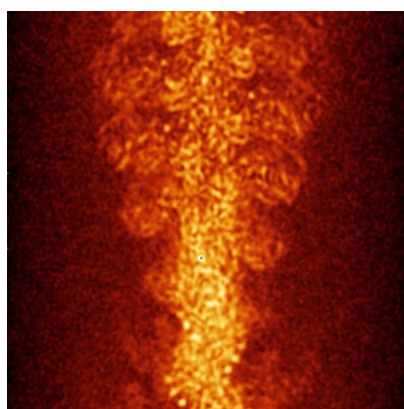


Z Index: 33

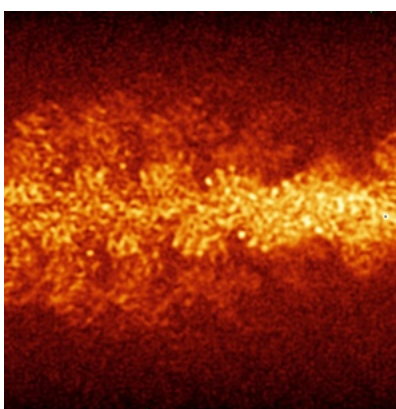
The images above show the largest variance slices of the map in three orthogonal directions.

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

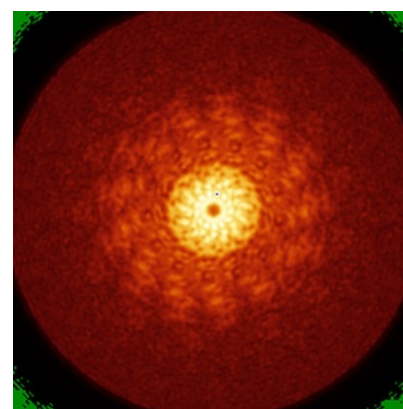
6.4.1 Primary map



X



Y

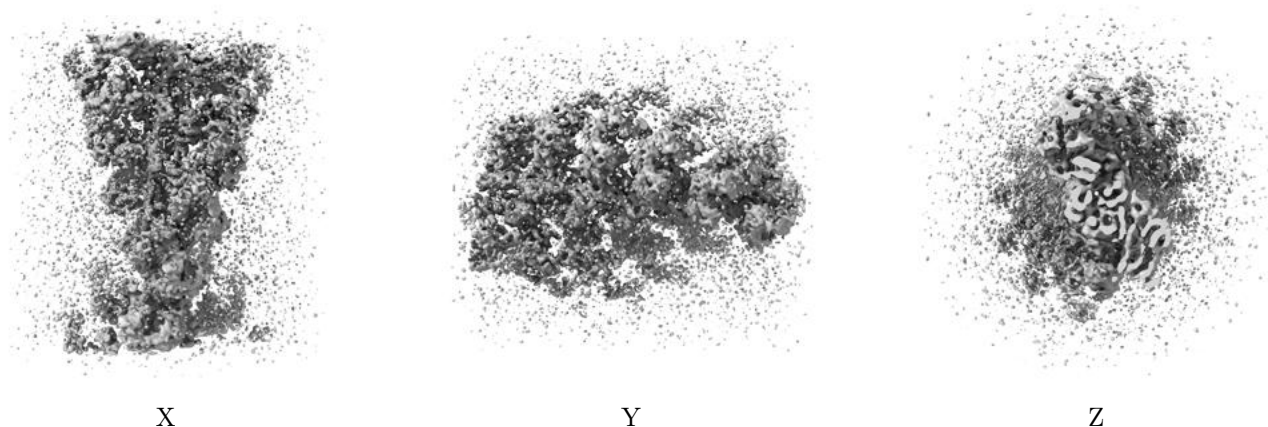


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.52. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

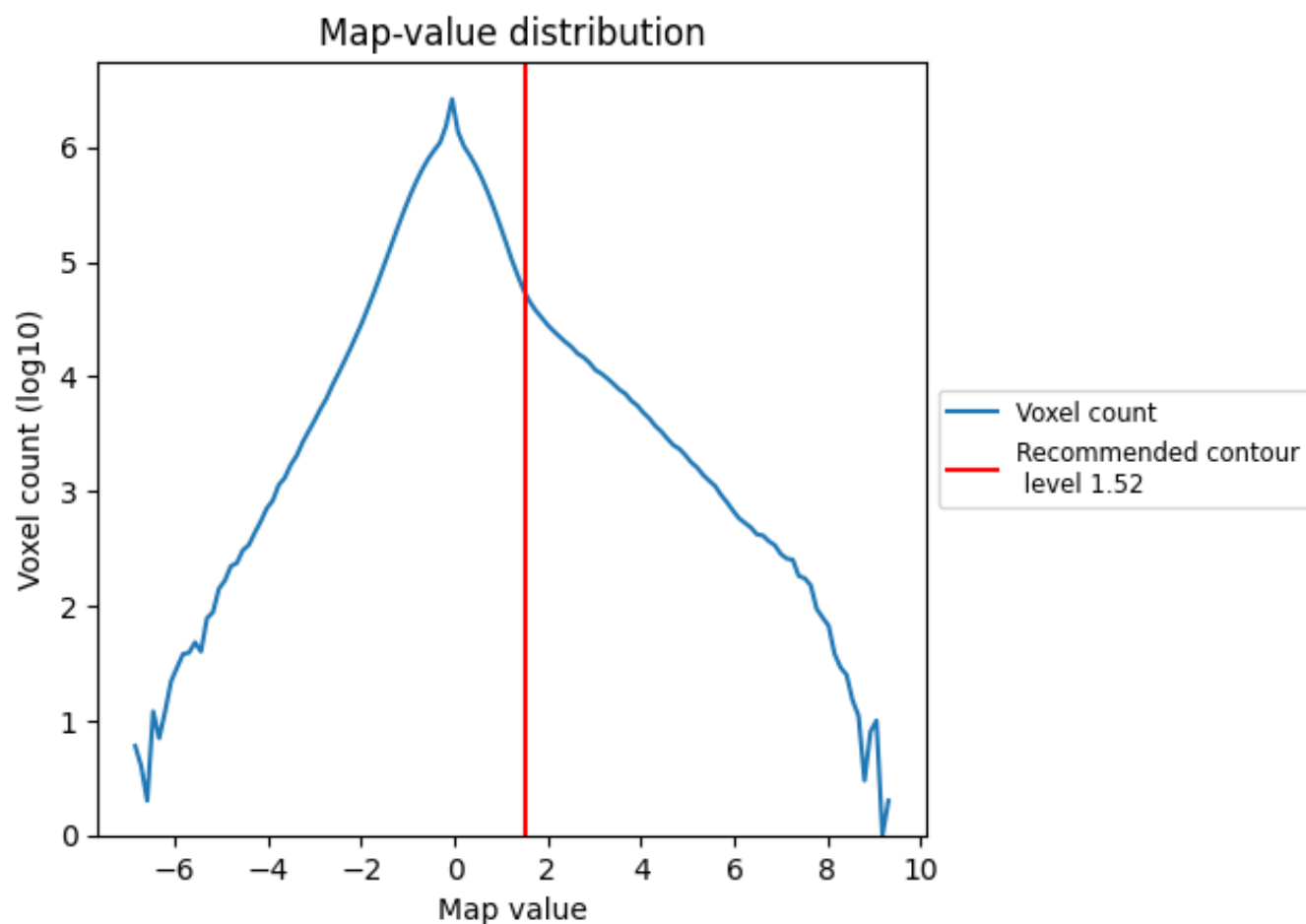
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

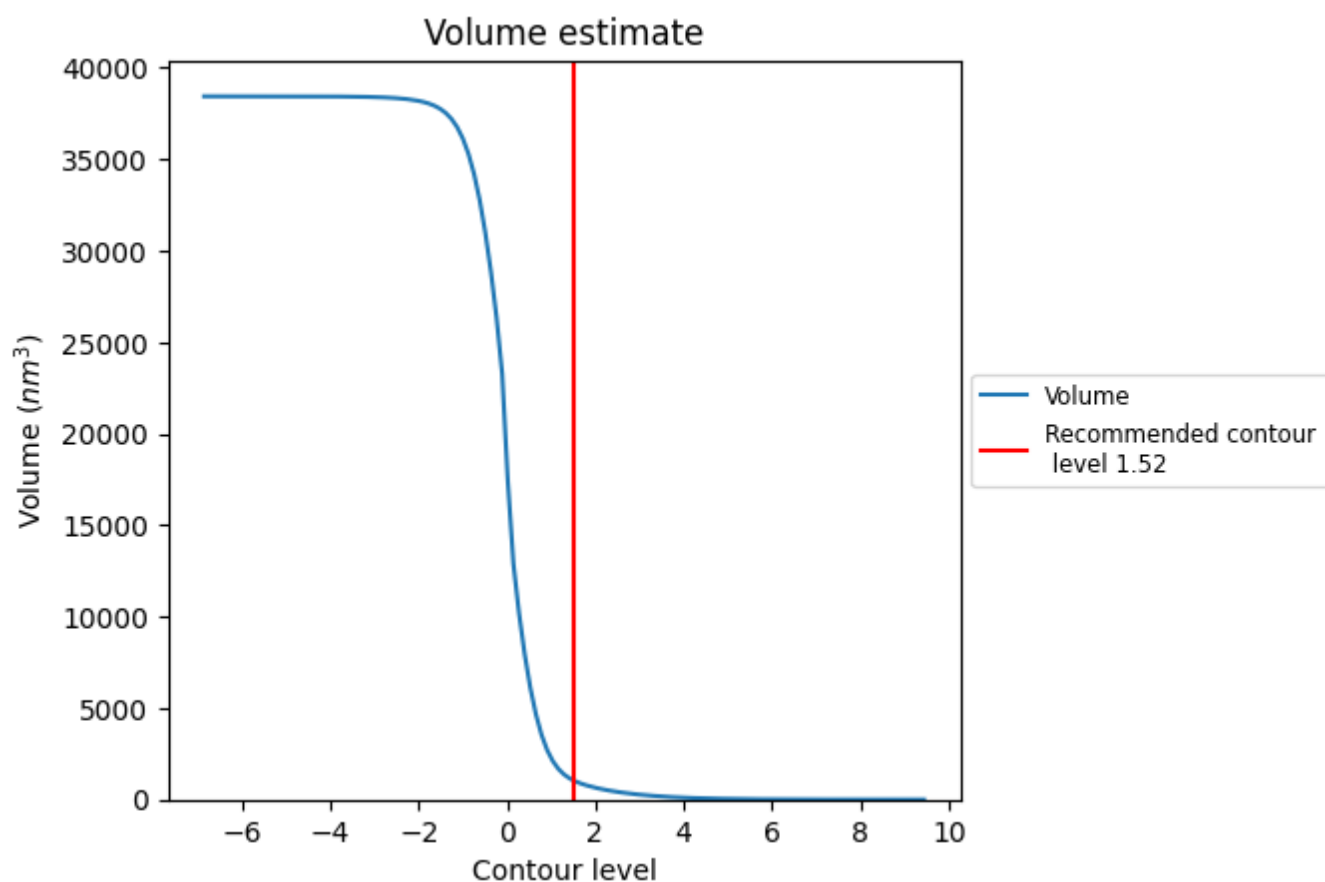
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

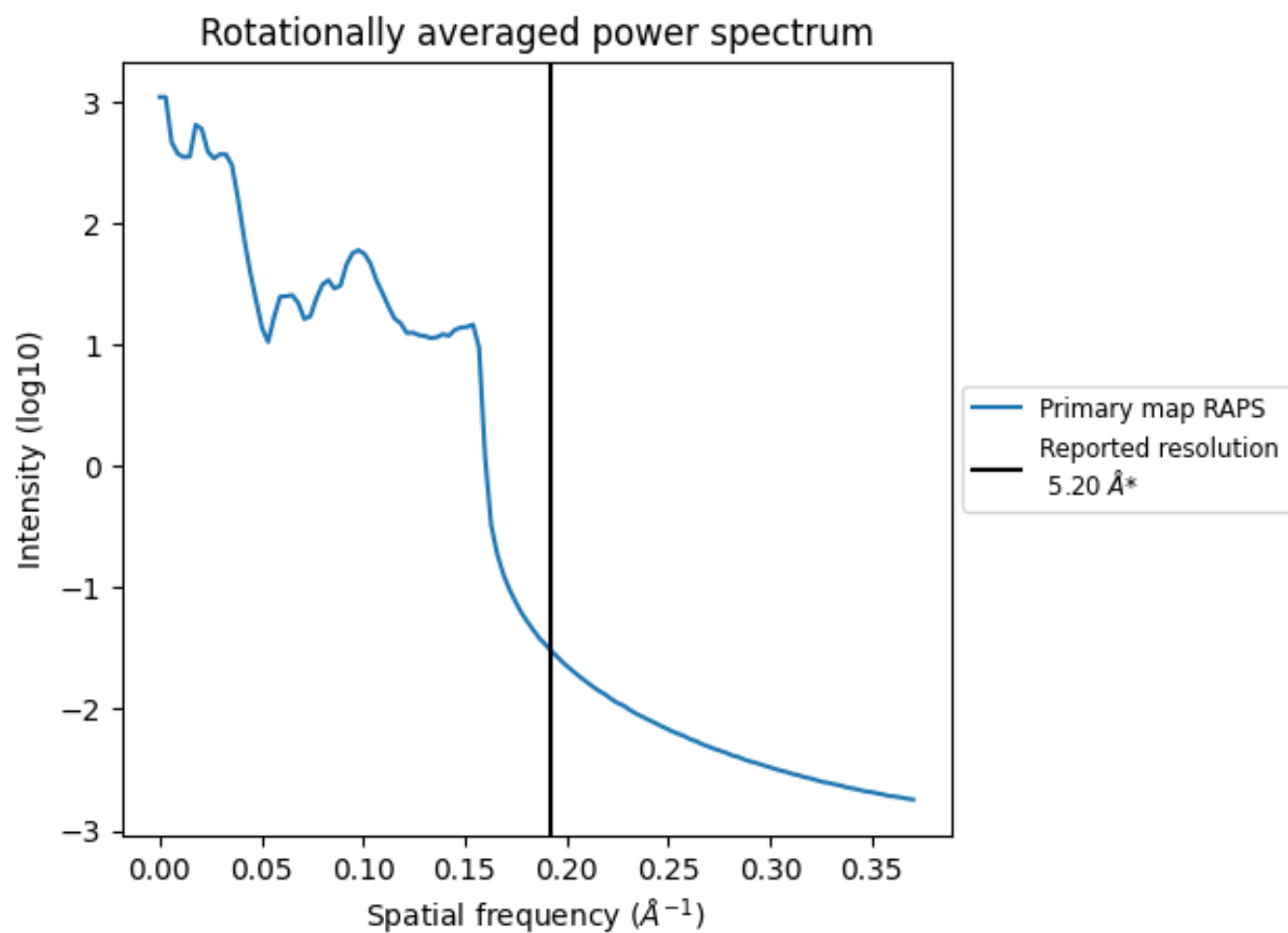
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1033 nm³; this corresponds to an approximate mass of 933 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 0.192 Å⁻¹

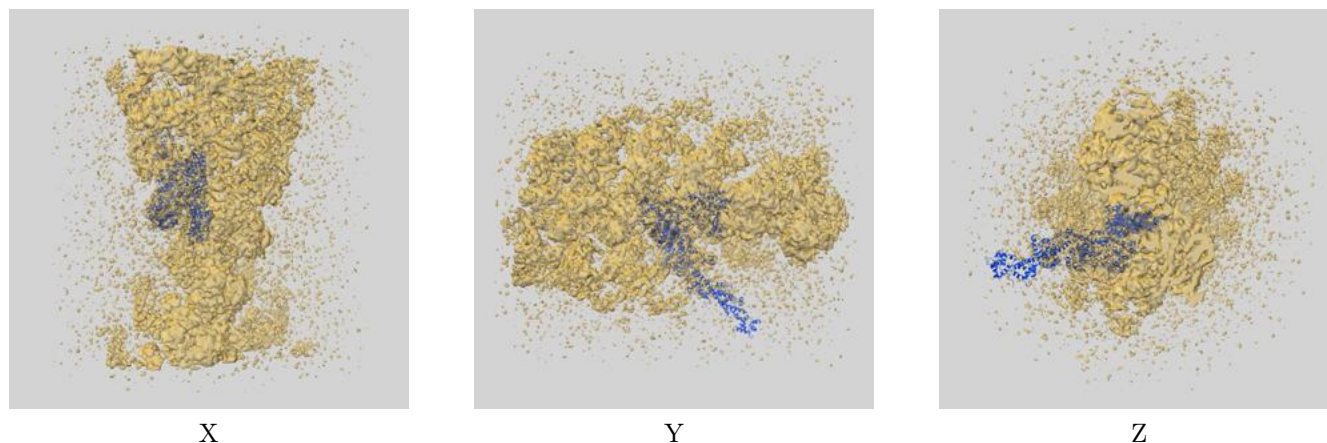
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

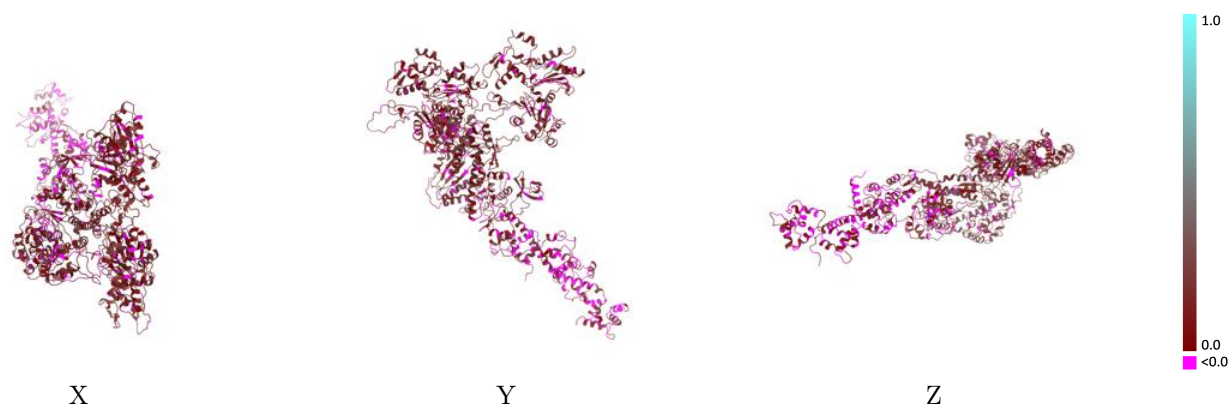
This section contains information regarding the fit between EMDB map EMD-6664 and PDB model 5H53. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



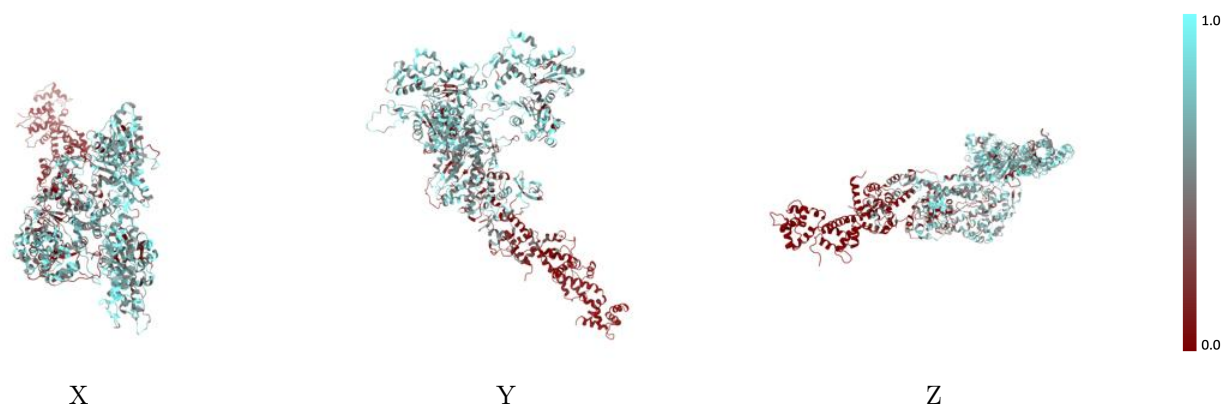
The images above show the 3D surface view of the map at the recommended contour level 1.52 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



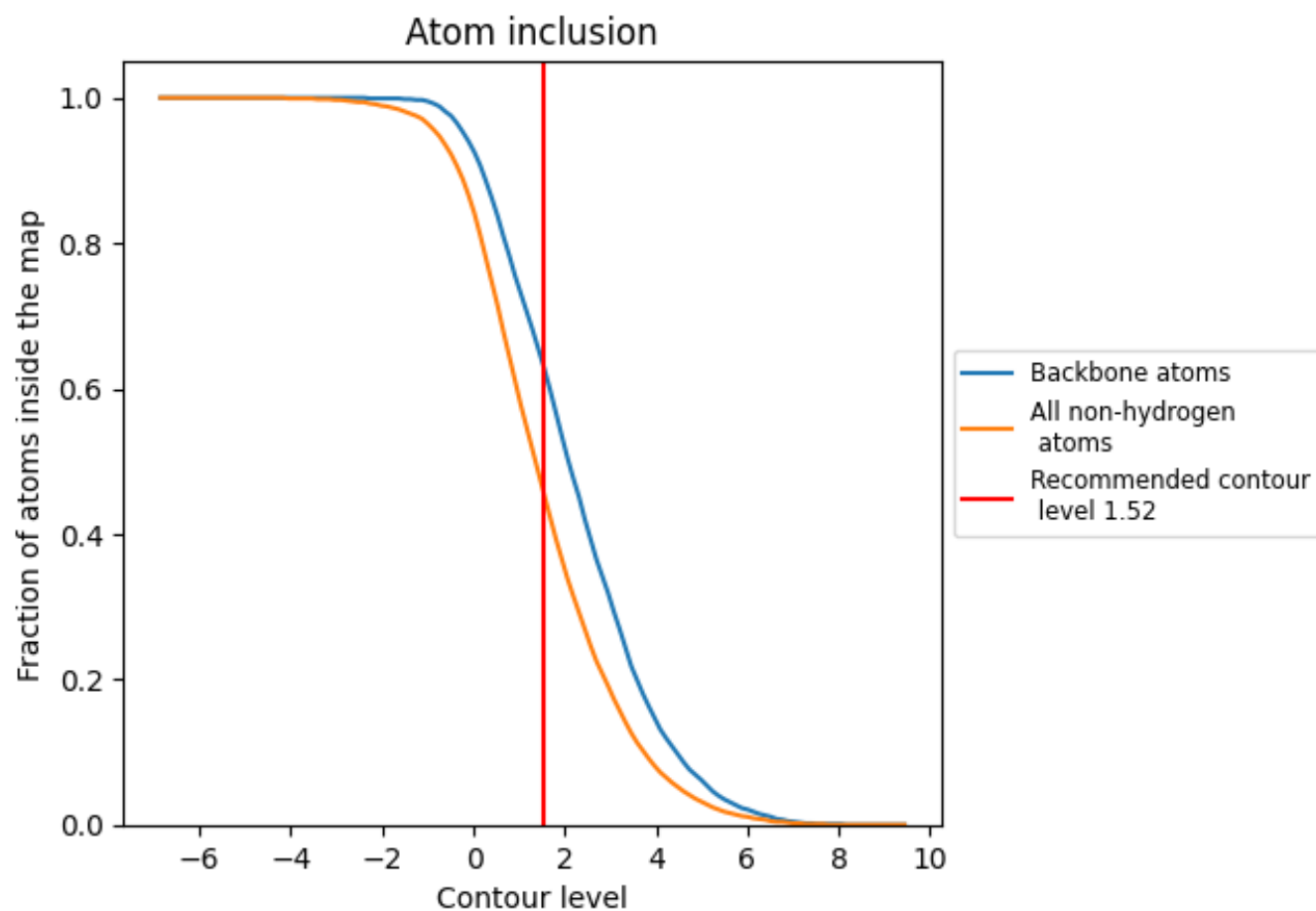
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.52).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 46% 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 (1.52) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4590	0.1140
A	0.4600	0.1190
B	0.0000	0.0200
C	0.1040	0.0340
D	0.6210	0.1430
E	0.6220	0.1450

