



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 11:25 PM UTC

PDB ID : 5TBY / pdb_00005tby
EMDB ID : EMD-2240
Title : HUMAN BETA CARDIAC HEAVY MEROMYOSIN INTERACTING-HEADS MOTIF OBTAINED BY HOMOLOGY MODELING (USING SWISS-MODEL) OF HUMAN SEQUENCE FROM APHONOPELMA HOMOLOGY MODEL (PDB-3JBH), RIGIDLY FITTED TO HUMAN BETA-CARDIAC NEGATIVELY STAINED THICK FILAMENT 3D-RECONSTRUCTION (EMD-2240)
Authors : ALAMO, L.; WARE, J.S.; PINTO, A.; GILLILAN, R.E.; SEIDMAN, J.G.; SEIDMAN, C.E.; PADRON, R.
Deposited on : 2016-09-13
Resolution : 20.00 Å(reported)
Based on initial model : 3JBH

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13

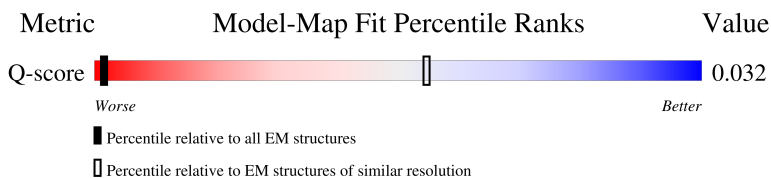
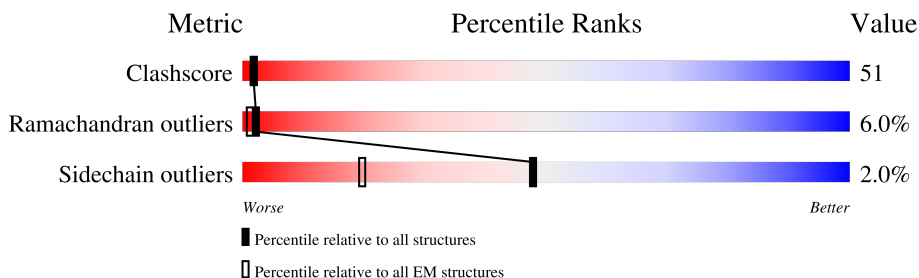
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11 (27.70 - 28.40)

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	1935	
1	B	1935	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

Mol	Chain	Length	Quality of chain
2	C	195	31% 37% 37% 2% 2% 2%
2	D	195	41% 38% 35% 2% 2% 2%
3	E	166	7% 40% 45% 8% 2% 2%
3	F	166	31% 42% 46% 7% 2% 2%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20357 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 Myosin-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	954	Total	C	N	O	S	0	0
			7704	4899	1324	1439	42		
1	B	950	Total	C	N	O	S	0	0
			7673	4877	1320	1435	41		

- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	152	Total	C	N	O	S	0	0
			1212	759	202	240	11		
2	D	152	Total	C	N	O	S	0	0
			1212	759	202	240	11		

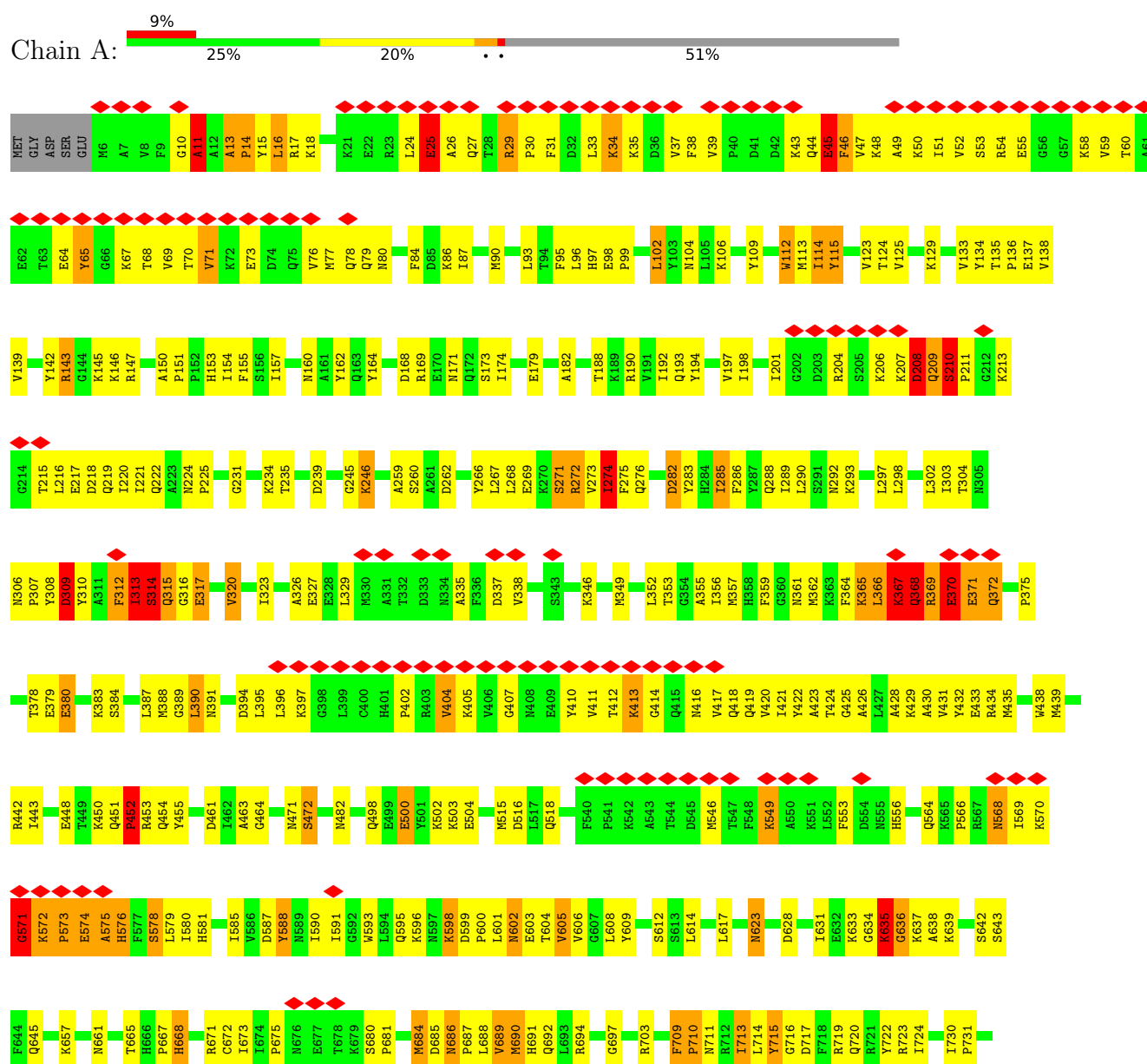
- Molecule 3 is a protein called Myosin regulatory light chain 2, ventricular/cardiac muscle isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	160	Total	C	N	O	S	0	0
			1278	808	212	252	6		
3	F	160	Total	C	N	O	S	0	0
			1278	808	212	252	6		

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.

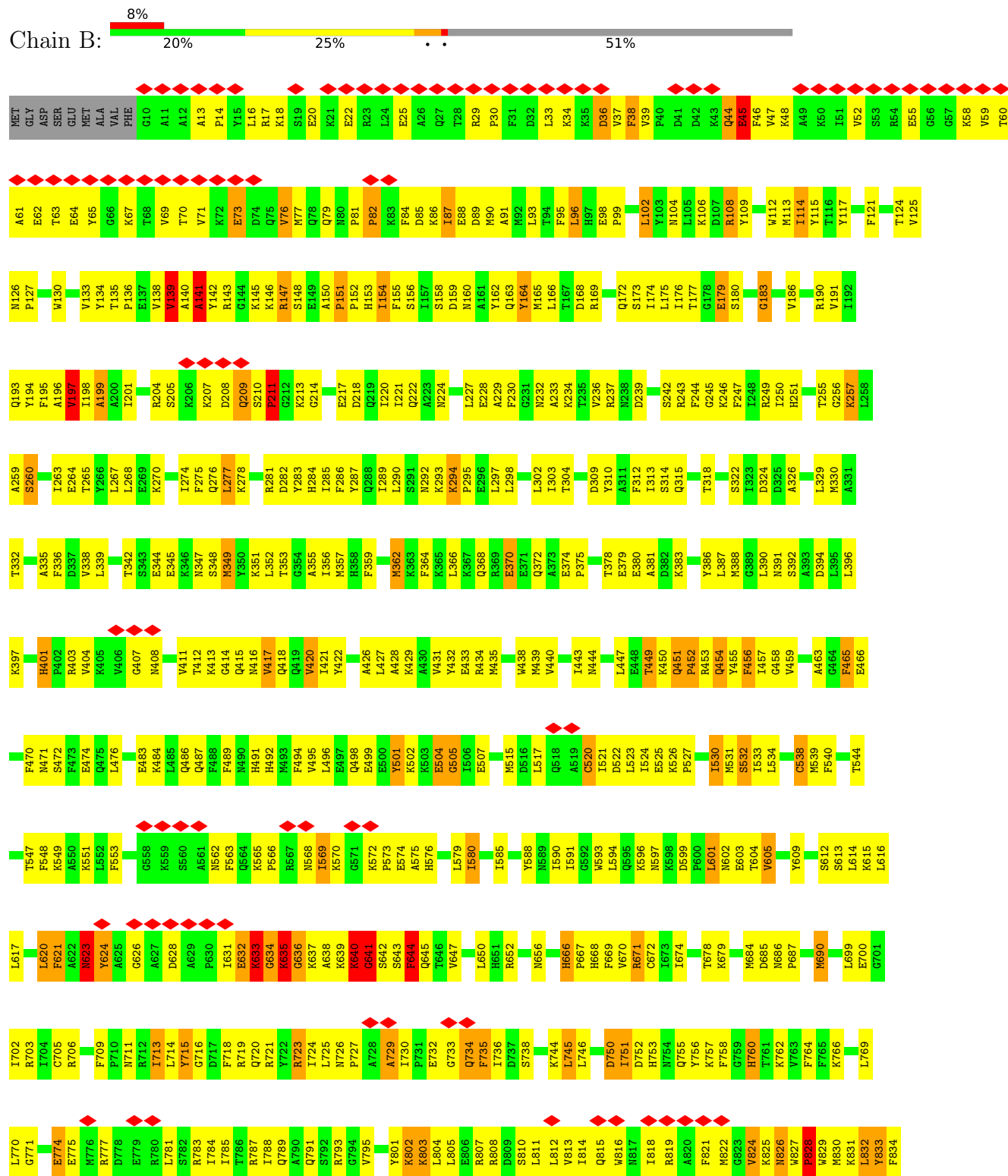
• Molecule 1: Myosin-7



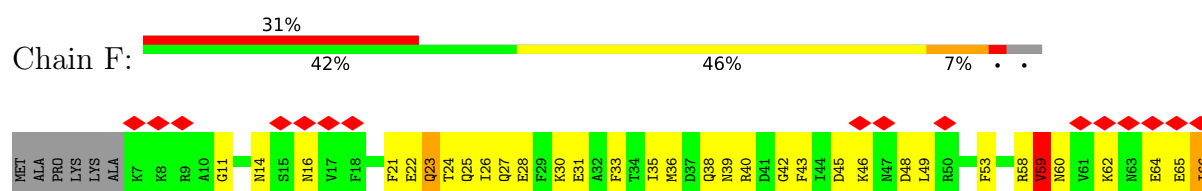


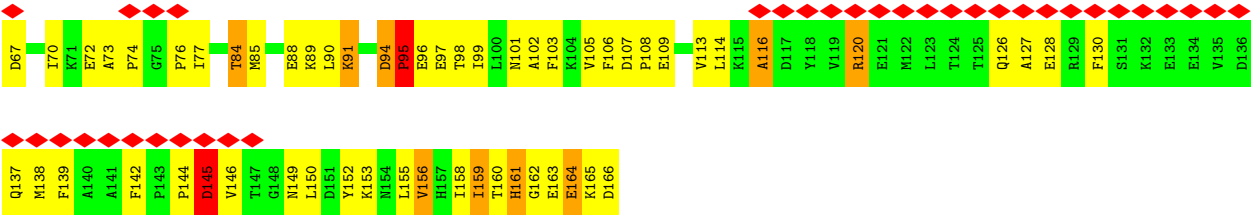
GLU	SER	GLN	VAL	ASN	LYS	LEU	ARG	ALA	LYS	SER	ARG	ASP	ILE	GLY	THR	LYS	GLY	LEU	ASN	GLU	GLU
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● Molecule 1: Myosin-7



- Molecule 2: Myosin light chain 3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	10700	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	9	Depositor
Minimum defocus (nm)	1950	Depositor
Maximum defocus (nm)	1950	Depositor
Magnification	35000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.488	Depositor
Minimum map value	-8.243	Depositor
Average map value	0.043	Depositor
Map value standard deviation	0.776	Depositor
Recommended contour level	1.5	Depositor
Map size ($\text{\AA}$)	950.4, 950.4, 950.4	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	5.94, 5.94, 5.94	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.81	2/7851 (0.0%)	1.37	94/10556 (0.9%)
1	B	0.82	5/7819 (0.1%)	1.34	53/10513 (0.5%)
2	C	0.84	0/1231	1.32	3/1651 (0.2%)
2	D	1.07	6/1231 (0.5%)	1.38	7/1651 (0.4%)
3	E	1.04	5/1301 (0.4%)	1.37	8/1747 (0.5%)
3	F	0.84	0/1301	1.33	4/1747 (0.2%)
All	All	0.85	18/20734 (0.1%)	1.35	169/27865 (0.6%)

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	20
1	B	0	19
2	C	0	2
3	E	0	3
3	F	0	4
All	All	0	48

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	129	ARG	CZ-NH1	-17.98	1.07	1.32
2	D	101	GLN	C-O	-15.26	1.02	1.24
1	B	666	HIS	CD2-NE2	-11.93	1.24	1.37
3	E	129	ARG	NE-CZ	11.07	1.45	1.33
2	D	105	ASN	C-N	-9.40	1.20	1.33
3	E	129	ARG	CZ-NH2	8.94	1.45	1.33
2	D	105	ASN	CA-C	8.08	1.63	1.52
2	D	102	GLU	N-CA	7.30	1.55	1.46
1	A	112	TRP	CD2-CE2	-6.00	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	632	GLU	C-N	-5.84	1.25	1.33
3	E	125	THR	C-O	-5.39	1.17	1.24
2	D	101	GLN	C-N	5.39	1.41	1.33
3	E	161	HIS	CD2-NE2	-5.38	1.31	1.37
1	B	760	HIS	CG-ND1	-5.29	1.32	1.38
1	A	668	HIS	CG-ND1	-5.17	1.32	1.38
2	D	106	THR	N-CA	5.17	1.52	1.46
1	B	605	VAL	C-O	-5.16	1.17	1.24
1	B	401	HIS	CG-ND1	-5.04	1.32	1.38

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	641	GLY	CA-C-O	-13.94	96.31	120.57
1	B	666	HIS	CE1-NE2-CD2	13.67	122.67	109.00
3	E	129	ARG	NE-CZ-NH2	-13.00	107.50	119.20
2	D	101	GLN	CA-C-O	-12.72	104.56	119.95
1	A	366	LEU	CA-C-N	12.01	143.32	121.70
1	A	366	LEU	C-N-CA	12.01	143.32	121.70
1	B	666	HIS	CG-CD2-NE2	-11.64	95.56	107.20
1	B	36	ASP	CA-CB-CG	11.09	123.69	112.60
1	B	197	VAL	CA-C-O	-10.56	111.22	119.46
1	B	666	HIS	CB-CG-CD2	-10.32	117.78	131.20
1	B	199	ALA	N-CA-CB	-10.18	95.04	110.20
1	B	635	LYS	CA-C-N	9.74	139.23	121.70
1	B	635	LYS	C-N-CA	9.74	139.23	121.70
1	B	620	LEU	CD1-CG-CD2	-9.72	89.41	110.80
2	D	102	GLU	N-CA-CB	9.55	126.64	110.49
1	B	36	ASP	N-CA-CB	-9.49	94.85	111.08
3	E	125	THR	O-C-N	-9.48	109.98	122.59
1	B	666	HIS	ND1-CG-CD2	9.35	115.45	106.10
1	A	366	LEU	N-CA-CB	-9.32	95.76	109.83
1	A	13	ALA	CA-C-N	9.10	129.29	119.28
1	A	13	ALA	C-N-CA	9.10	129.29	119.28
1	A	309	ASP	CA-CB-CG	-8.53	104.08	112.60
1	A	365	LYS	CA-C-N	8.46	132.73	120.71
1	A	365	LYS	C-N-CA	8.46	132.73	120.71
1	B	568	ASN	N-CA-C	8.40	123.11	112.86
1	B	666	HIS	ND1-CE1-NE2	-8.16	100.24	108.40
1	A	370	GLU	CA-C-N	8.12	136.32	121.70
1	A	370	GLU	C-N-CA	8.12	136.32	121.70
1	A	756	TYR	CZ-CE2-CD2	8.00	134.00	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	102	GLU	CA-CB-CG	7.92	129.94	114.10
1	B	623	ASN	OD1-CG-ND2	-7.68	114.92	122.60
1	A	576	HIS	CA-C-O	-7.67	112.89	121.25
1	A	309	ASP	N-CA-C	7.63	127.05	110.80
1	A	452	PRO	CA-N-CD	-7.53	101.45	112.00
1	B	774	GLU	CB-CG-CD	7.43	125.23	112.60
1	A	380	GLU	N-CA-C	7.33	118.85	108.00
1	A	112	TRP	CD2-CE2-CZ2	7.28	129.68	122.40
1	B	870	ARG	CA-C-N	7.26	130.01	120.28
1	B	870	ARG	C-N-CA	7.26	130.01	120.28
1	A	690	MET	CB-CA-C	-7.17	99.33	110.81
1	A	576	HIS	O-C-N	7.17	130.49	123.04
1	A	736	ILE	CA-CB-CG2	7.16	122.67	110.50
1	A	684	MET	CG-SD-CE	7.13	116.59	100.90
1	A	314	SER	N-CA-C	7.11	125.95	110.80
1	B	102	LEU	CD1-CG-CD2	7.11	126.44	110.80
1	A	34	LYS	CA-CB-CG	7.09	128.29	114.10
1	B	632	GLU	CA-C-O	7.06	127.92	119.59
1	B	102	LEU	CB-CG-CD2	-7.03	89.62	110.70
1	A	320	VAL	CG1-CB-CG2	-6.98	95.45	110.80
1	A	312	PHE	O-C-N	6.93	129.28	121.93
1	A	327	GLU	N-CA-C	6.91	118.46	111.07
1	B	633	LYS	CA-C-O	-6.91	110.63	120.51
1	B	530	ILE	N-CA-C	-6.85	106.81	113.53
1	A	368	GLN	N-CA-C	6.73	125.13	110.80
1	B	828	PRO	CA-N-CD	-6.72	102.60	112.00
1	A	570	LYS	CA-C-N	6.71	134.55	121.41
1	A	570	LYS	C-N-CA	6.71	134.55	121.41
1	B	456	PHE	N-CA-C	6.70	119.90	109.52
3	F	145	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	312	PHE	CA-C-O	-6.60	110.18	118.43
1	A	207	LYS	CA-C-N	6.57	134.09	121.54
1	A	207	LYS	C-N-CA	6.57	134.09	121.54
3	E	139	PHE	CA-C-O	-6.53	114.14	121.00
1	A	452	PRO	N-CA-C	6.52	125.91	112.47
1	B	601	LEU	CD1-CG-CD2	-6.50	96.49	110.80
1	A	370	GLU	O-C-N	-6.47	113.98	122.59
1	A	472	SER	N-CA-CB	-6.45	105.59	111.59
1	B	504	GLU	CA-C-O	-6.43	112.84	120.10
1	B	644	PHE	CA-CB-CG	-6.42	107.38	113.80
1	A	25	GLU	CB-CA-C	-6.35	98.80	109.65
1	A	715	TYR	N-CA-C	6.33	117.98	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	SER	CA-C-N	6.33	133.09	121.70
1	A	271	SER	C-N-CA	6.33	133.09	121.70
3	E	129	ARG	CD-NE-CZ	-6.26	115.64	124.40
1	A	34	LYS	N-CA-CB	-6.25	101.38	110.70
1	B	632	GLU	O-C-N	-6.24	114.82	122.25
3	E	126	GLN	CA-C-O	-6.24	114.86	122.41
1	B	690	MET	CG-SD-CE	-6.21	87.25	100.90
1	A	734	GLN	CB-CG-CD	6.20	123.14	112.60
1	A	114	ILE	N-CA-C	6.17	116.81	110.82
1	A	390	LEU	CD1-CG-CD2	-6.17	97.24	110.80
1	A	686	ASN	CA-C-N	6.15	125.88	119.05
1	A	686	ASN	C-N-CA	6.15	125.88	119.05
1	A	598	LYS	N-CA-CB	-6.15	100.83	110.98
1	B	87	ILE	CB-CG1-CD1	-6.11	100.97	113.80
1	A	366	LEU	O-C-N	-6.09	115.38	122.87
1	A	571	GLY	CA-C-O	-6.07	110.00	120.57
1	A	45	GLU	OE1-CD-OE2	6.07	137.47	122.90
1	A	315	GLN	N-CA-C	6.03	123.64	110.80
1	B	760	HIS	CG-CD2-NE2	6.02	113.22	107.20
1	B	139	VAL	CA-CB-CG1	-5.99	100.21	110.40
1	A	29	ARG	NE-CZ-NH1	-5.99	115.51	121.50
1	A	549	LYS	CB-CG-CD	5.97	125.03	111.30
1	A	413	LYS	N-CA-C	5.95	118.19	108.55
1	B	44	GLN	O-C-N	5.92	130.85	122.20
1	B	729	ALA	N-CA-CB	-5.88	101.42	110.42
1	A	605	VAL	N-CA-C	5.87	121.55	109.34
2	C	67	CYS	CB-CA-C	5.85	123.42	116.63
1	B	349	MET	CG-SD-CE	-5.85	88.04	100.90
1	A	209	GLN	N-CA-C	5.84	119.95	112.12
1	A	207	LYS	N-CA-C	5.84	118.99	110.17
1	A	575	ALA	N-CA-CB	-5.84	100.66	110.99
1	A	14	PRO	CA-N-CD	-5.81	103.87	112.00
1	B	745	LEU	CD1-CG-CD2	-5.81	98.02	110.80
1	A	366	LEU	CA-C-O	-5.80	114.81	121.19
3	E	26	ILE	N-CA-C	5.78	115.85	110.42
1	B	635	LYS	CA-CB-CG	5.76	125.62	114.10
1	A	453	ARG	N-CA-C	5.72	118.87	109.72
1	B	148	SER	N-CA-C	-5.69	105.61	113.18
1	A	313	ILE	N-CA-C	5.66	121.12	109.34
1	A	578	SER	CA-CB-OG	5.61	122.33	111.10
2	D	180	ASN	N-CA-C	5.61	119.42	112.24
1	A	150	ALA	CA-C-N	5.61	123.75	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ALA	C-N-CA	5.61	123.75	119.66
1	B	465	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	25	GLU	CA-C-O	-5.60	114.89	121.16
1	A	372	GLN	N-CA-C	5.59	118.16	109.60
1	B	640	LYS	CG-CD-CE	5.58	124.14	111.30
1	A	568	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	828	PRO	N-CD-CG	5.54	111.51	103.20
1	A	282	ASP	CA-CB-CG	-5.53	107.07	112.60
3	F	94	ASP	O-C-N	-5.51	114.98	121.32
1	A	367	LYS	N-CA-CB	5.50	119.85	110.50
1	B	621	PHE	N-CA-C	5.49	120.64	113.88
1	A	46	PHE	CG-CD1-CE1	5.45	129.97	120.70
1	A	210	SER	N-CA-CB	5.45	119.77	110.50
2	C	119	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	A	691	HIS	CB-CG-CD2	-5.43	124.14	131.20
1	A	209	GLN	CA-C-N	5.43	131.47	121.70
1	A	209	GLN	C-N-CA	5.43	131.47	121.70
1	A	102	LEU	CD1-CG-CD2	5.40	122.67	110.80
1	A	556	HIS	N-CA-C	5.38	119.12	112.24
1	B	141	ALA	CA-C-O	-5.38	115.16	120.70
2	D	180	ASN	CA-C-N	5.35	131.33	121.70
2	D	180	ASN	C-N-CA	5.35	131.33	121.70
1	B	44	GLN	CA-C-O	-5.33	113.34	119.78
1	A	573	PRO	CA-N-CD	-5.31	104.57	112.00
1	A	709	PHE	CA-C-N	5.30	126.47	119.84
1	A	709	PHE	C-N-CA	5.30	126.47	119.84
3	F	156	VAL	CG1-CB-CG2	-5.30	99.14	110.80
1	A	367	LYS	CA-C-N	5.29	131.64	121.54
1	A	367	LYS	C-N-CA	5.29	131.64	121.54
1	A	112	TRP	CB-CG-CD1	-5.27	118.99	126.90
3	F	120	ARG	NE-CZ-NH1	5.26	126.76	121.50
1	A	135	THR	CA-C-N	5.22	126.37	119.84
1	A	135	THR	C-N-CA	5.22	126.37	119.84
2	C	194	SER	O-C-N	5.22	127.46	122.03
1	B	633	LYS	CG-CD-CE	-5.18	99.39	111.30
1	A	756	TYR	CG-CD2-CE2	-5.17	113.44	121.20
1	A	602	ASN	CA-CB-CG	5.15	117.75	112.60
1	A	208	ASP	N-CA-C	5.13	121.73	110.80
1	B	294	LYS	CA-C-N	5.12	124.92	119.28
1	B	294	LYS	C-N-CA	5.12	124.92	119.28
3	E	155	LEU	CD1-CG-CD2	-5.12	99.53	110.80
1	B	211	PRO	CA-N-CD	-5.12	104.84	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	633	LYS	CB-CA-C	5.10	120.58	110.42
1	A	604	THR	O-C-N	5.10	125.75	122.03
1	B	257	LYS	N-CA-C	5.08	116.89	110.33
1	A	404	VAL	CG1-CB-CG2	-5.07	99.64	110.80
1	B	38	PHE	CG-CD2-CE2	5.07	129.32	120.70
2	D	102	GLU	CB-CA-C	-5.07	100.33	110.42
1	A	11	ALA	N-CA-C	5.05	121.56	110.80
1	A	740	LYS	CA-C-N	-5.04	111.53	121.41
1	A	740	LYS	C-N-CA	-5.04	111.53	121.41
1	A	581	HIS	CB-CG-CD2	-5.04	124.65	131.20
1	A	689	VAL	CB-CA-C	-5.03	105.44	112.02
1	B	45	GLU	CG-CD-OE2	-5.02	106.86	118.40
1	A	710	PRO	N-CA-C	5.01	122.79	112.47
3	E	60	ASN	N-CA-CB	5.01	118.96	110.49

There are no chirality outliers.

All (48) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	TYR	Sidechain
1	A	15	TYR	Sidechain
1	A	162	TYR	Sidechain
1	A	25	GLU	Mainchain
1	A	274	ILE	Mainchain
1	A	308	TYR	Peptide
1	A	310	TYR	Peptide,Sidechain
1	A	313	ILE	Peptide
1	A	369	ARG	Peptide,Sidechain
1	A	413	LYS	Peptide
1	A	45	GLU	Mainchain
1	A	588	TYR	Sidechain
1	A	634	GLY	Peptide
1	A	635	LYS	Mainchain
1	A	722	TYR	Sidechain
1	A	756	TYR	Sidechain
1	A	821	PHE	Sidechain
1	A	870	ARG	Sidechain
1	B	108	ARG	Sidechain
1	B	141	ALA	Mainchain
1	B	164	TYR	Sidechain
1	B	197	VAL	Mainchain
1	B	209	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	B	45	GLU	Mainchain
1	B	465	PHE	Sidechain
1	B	501	TYR	Sidechain
1	B	572	LYS	Peptide
1	B	623	ASN	Peptide
1	B	633	LYS	Mainchain,Peptide
1	B	636	GLY	Mainchain
1	B	644	PHE	Sidechain
1	B	671	ARG	Sidechain
1	B	715	TYR	Sidechain
1	B	734	GLN	Mainchain,Peptide
1	B	866	SER	Peptide
2	C	101	GLN	Peptide
2	C	185	TYR	Sidechain
3	E	125	THR	Mainchain
3	E	129	ARG	Sidechain
3	E	59	VAL	Peptide
3	F	59	VAL	Peptide
3	F	84	THR	Peptide
3	F	91	LYS	Mainchain
3	F	95	PRO	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7704	0	7735	705	0
1	B	7673	0	7706	1090	0
2	C	1212	0	1182	125	0
2	D	1212	0	1184	236	0
3	E	1278	0	1241	180	0
3	F	1278	0	1239	238	0
All	All	20357	0	20287	2085	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 51.

All (2085) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:822:MET:HE1	3:E:138:MET:CE	1.27	1.64
1:B:804:LEU:CD2	2:D:63:ARG:HD3	1.21	1.56
1:A:714:LEU:HD21	1:B:396:LEU:CD1	1.15	1.55
1:B:831:LYS:HD3	3:F:163:GLU:CG	1.34	1.55
3:E:8:LYS:CD	3:F:59:VAL:HA	1.33	1.54
1:A:714:LEU:CD2	1:B:396:LEU:HD12	1.33	1.53
1:A:822:MET:CE	3:E:138:MET:CE	1.82	1.52
1:B:804:LEU:HD22	2:D:63:ARG:CD	1.03	1.49
1:A:822:MET:CE	3:E:138:MET:HE2	1.01	1.45
1:B:804:LEU:HD21	2:D:63:ARG:NH1	1.22	1.43
1:A:791:GLN:NE2	2:C:193:MET:HE1	1.18	1.42
1:B:845:ARG:CD	3:F:23:GLN:NE2	1.83	1.41
1:A:791:GLN:OE1	2:C:133:PHE:CZ	1.73	1.40
1:A:845:ARG:HH22	3:F:23:GLN:CB	1.31	1.39
1:B:791:GLN:NE2	2:D:193:MET:CE	1.86	1.38
1:A:455:TYR:CE1	1:B:403:ARG:NH1	1.73	1.37
2:D:65:PRO:HG2	3:F:126:GLN:OE1	1.19	1.36
1:A:455:TYR:HE1	1:B:403:ARG:NH1	0.86	1.35
2:D:65:PRO:CG	3:F:126:GLN:OE1	1.73	1.34
1:B:831:LYS:CD	3:F:163:GLU:CG	2.01	1.33
1:B:733:GLY:N	2:D:138:ARG:HH22	1.25	1.33
1:B:831:LYS:CD	3:F:163:GLU:HG3	1.58	1.33
1:B:791:GLN:NE2	2:D:193:MET:HE1	1.03	1.31
1:B:826:ASN:CB	3:F:59:VAL:HB	1.58	1.31
1:A:859:LEU:HD11	1:B:860:LYS:N	1.45	1.30
1:B:804:LEU:CD2	2:D:63:ARG:CD	1.88	1.30
1:B:733:GLY:N	2:D:138:ARG:NH2	1.79	1.29
1:B:826:ASN:HB3	3:F:59:VAL:CB	1.63	1.29
2:D:65:PRO:HG2	3:F:126:GLN:CD	1.57	1.27
1:B:804:LEU:CD2	2:D:63:ARG:HH11	1.47	1.25
1:B:821:PHE:CE2	3:F:138:MET:HG2	1.69	1.25
1:B:733:GLY:H	2:D:138:ARG:NH2	1.34	1.25
1:A:791:GLN:NE2	2:C:193:MET:CE	2.02	1.23
1:B:719:ARG:NH1	2:D:139:VAL:O	1.70	1.23
1:A:849:MET:HE1	1:B:852:MET:CE	1.67	1.23
1:A:845:ARG:NH2	3:F:23:GLN:CB	1.87	1.22
3:E:8:LYS:HD3	3:F:59:VAL:CA	1.68	1.21
1:A:791:GLN:OE1	2:C:133:PHE:CE2	1.95	1.20
1:B:635:LYS:HG3	1:B:636:GLY:HA3	1.21	1.20
3:E:8:LYS:HB3	3:F:58:ARG:O	1.38	1.20
1:B:733:GLY:CA	2:D:138:ARG:HH22	1.54	1.19
1:A:856:PHE:CE1	1:B:855:GLU:HB3	1.78	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:LYS:HD2	3:F:163:GLU:CD	1.67	1.19
3:E:100:LEU:HA	3:E:155:LEU:HD23	1.21	1.19
1:A:835:LYS:HE3	3:E:165:LYS:NZ	1.58	1.16
1:B:256:GLY:N	2:D:154:ARG:HH22	1.42	1.16
3:E:27:GLN:NE2	3:F:24:THR:HG22	1.61	1.16
1:B:869:ARG:CD	2:D:177:GLU:OE2	1.93	1.16
3:E:80:THR:HG23	3:F:40:ARG:CD	1.75	1.16
3:E:80:THR:HG23	3:F:40:ARG:HD2	1.28	1.15
1:B:822:MET:HE1	3:F:137:GLN:HG3	1.25	1.15
1:B:869:ARG:HD2	2:D:177:GLU:OE2	0.98	1.15
1:A:845:ARG:NH2	3:F:23:GLN:HB2	1.21	1.14
1:A:849:MET:HE1	1:B:852:MET:SD	1.87	1.13
1:B:827:TRP:N	3:F:58:ARG:CZ	2.11	1.13
2:D:66:LYS:HD3	3:F:126:GLN:HG2	1.21	1.13
2:D:66:LYS:HE3	3:F:126:GLN:HG3	1.27	1.12
3:E:8:LYS:CB	3:F:58:ARG:O	1.96	1.12
3:E:8:LYS:HD2	3:F:58:ARG:O	1.48	1.12
1:A:805:LEU:HD11	2:C:60:LEU:HD22	1.17	1.11
1:B:733:GLY:C	2:D:138:ARG:NH2	2.09	1.11
3:E:8:LYS:CD	3:F:59:VAL:CA	2.22	1.11
1:A:60:THR:HG22	1:A:70:THR:HG22	1.31	1.11
1:A:922:MET:HE1	1:B:919:VAL:HG13	1.29	1.11
2:C:98:LYS:HE3	2:C:100:ARG:HB3	1.30	1.10
1:A:735:PHE:HA	1:A:736:ILE:HG22	1.23	1.10
2:D:66:LYS:CD	3:F:126:GLN:HG2	1.81	1.10
1:B:733:GLY:HA2	2:D:134:VAL:HG13	1.10	1.10
1:A:835:LYS:HE3	3:E:165:LYS:HZ1	1.03	1.09
3:E:8:LYS:CG	3:F:58:ARG:O	2.00	1.09
1:A:860:LYS:N	1:B:859:LEU:HD11	1.68	1.09
1:A:87:ILE:HD12	1:A:93:LEU:HD11	1.30	1.09
1:A:367:LYS:HE2	1:A:370:GLU:HB2	1.35	1.09
1:B:804:LEU:HD22	2:D:63:ARG:HD2	1.33	1.09
1:A:805:LEU:CD1	2:C:60:LEU:HD22	1.83	1.08
2:D:66:LYS:HD2	3:F:127:ALA:CB	1.82	1.08
1:B:292:ASN:HD21	1:B:330:MET:HG3	0.97	1.08
1:B:827:TRP:N	3:F:58:ARG:NH1	1.98	1.08
1:B:845:ARG:HD2	3:F:23:GLN:NE2	1.49	1.08
1:A:375:PRO:HG2	1:A:380:GLU:HA	1.35	1.08
1:A:169:ARG:HB3	1:B:403:ARG:HH21	0.94	1.08
1:A:788:ILE:CD1	2:C:133:PHE:CE2	2.32	1.08
1:B:791:GLN:CD	2:D:193:MET:HE1	1.77	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:ASN:HA	1:B:637:LYS:HE2	1.35	1.07
1:B:734:GLN:N	2:D:138:ARG:NH2	2.03	1.07
1:B:783:ARG:HH12	2:D:126:ASP:CB	1.66	1.07
3:F:153:LYS:HA	3:F:156:VAL:HG12	1.33	1.07
1:B:869:ARG:HD2	2:D:177:GLU:CD	1.79	1.07
1:A:33:LEU:HD23	1:A:50:LYS:HE2	1.36	1.06
1:A:853:LYS:NZ	1:B:841:LYS:NZ	2.04	1.06
1:A:808:ARG:CZ	2:C:63:ARG:HA	1.85	1.06
1:B:733:GLY:C	2:D:138:ARG:HH22	1.62	1.06
3:E:8:LYS:CD	3:F:58:ARG:O	2.03	1.06
1:A:784:ILE:HD13	2:C:140:PHE:HE2	1.17	1.05
1:B:831:LYS:CD	3:F:163:GLU:CD	2.28	1.05
1:B:807:ARG:HD2	2:D:63:ARG:HB2	1.06	1.05
1:B:733:GLY:C	2:D:138:ARG:NH1	2.15	1.05
1:B:388:MET:HA	1:B:617:LEU:HD23	1.38	1.04
1:B:831:LYS:HD3	3:F:163:GLU:HG2	1.37	1.04
1:A:849:MET:HE1	1:B:852:MET:HE1	1.34	1.04
1:B:723:ARG:HH21	1:B:785:ILE:HA	1.22	1.04
1:A:822:MET:HE1	3:E:138:MET:HE3	1.08	1.04
1:B:635:LYS:NZ	1:B:647:VAL:HA	1.72	1.04
1:B:834:PHE:CD1	3:F:163:GLU:O	2.11	1.04
3:E:8:LYS:CG	3:F:59:VAL:HA	1.87	1.04
1:A:735:PHE:CD1	1:A:741:GLY:HA3	1.91	1.04
1:A:808:ARG:NH2	2:C:63:ARG:HA	1.71	1.04
1:A:873:LEU:HD12	1:B:870:ARG:HD2	1.35	1.04
1:B:733:GLY:CA	2:D:138:ARG:HH12	1.69	1.04
3:E:80:THR:CG2	3:F:40:ARG:HD2	1.88	1.03
1:B:631:ILE:HB	1:B:641:GLY:HA2	1.34	1.03
1:B:783:ARG:NH1	2:D:126:ASP:HB3	1.74	1.03
2:D:66:LYS:HD2	3:F:127:ALA:HB2	1.04	1.02
1:A:430:ALA:HB2	1:A:601:LEU:HD21	1.42	1.02
1:B:733:GLY:CA	2:D:134:VAL:HG13	1.88	1.02
1:A:849:MET:CE	1:B:852:MET:HE1	1.90	1.01
1:A:169:ARG:HB3	1:B:403:ARG:NH2	1.74	1.01
1:B:36:ASP:HB3	1:B:48:LYS:NZ	1.76	1.01
1:B:827:TRP:CD1	1:B:828:PRO:HD2	1.95	1.01
1:B:845:ARG:HD3	3:F:23:GLN:HE22	0.89	1.01
1:A:147:ARG:HB2	1:A:160:ASN:HD22	1.24	1.01
1:A:572:LYS:HB2	1:A:573:PRO:HD3	1.36	1.01
1:A:856:PHE:HE1	1:B:855:GLU:HB3	0.88	1.00
1:A:881:LEU:HD12	2:D:180:ASN:HD21	1.20	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:LYS:O	1:B:640:LYS:HD3	1.60	1.00
1:B:831:LYS:HG3	3:F:163:GLU:OE2	1.61	1.00
1:B:160:ASN:HD21	1:B:711:ASN:HA	1.22	1.00
1:B:804:LEU:HD11	2:D:75:GLN:NE2	1.77	1.00
1:B:45:GLU:HG3	1:B:690:MET:SD	2.01	1.00
1:B:733:GLY:C	2:D:138:ARG:HH12	1.70	0.99
1:A:873:LEU:CD1	1:B:870:ARG:HD2	1.92	0.99
1:A:815:GLN:OE1	3:E:127:ALA:HB3	1.61	0.99
1:B:733:GLY:HA2	2:D:138:ARG:HH12	1.27	0.98
1:B:160:ASN:ND2	1:B:711:ASN:HA	1.77	0.98
1:B:733:GLY:C	2:D:138:ARG:CZ	2.36	0.98
1:A:45:GLU:HG3	1:A:46:PHE:CD1	1.99	0.98
1:B:190:ARG:HA	1:B:193:GLN:HG2	1.46	0.98
1:B:603:GLU:HG3	1:B:604:THR:H	1.28	0.98
1:A:908:LEU:HD11	1:B:908:LEU:C	1.88	0.97
1:B:821:PHE:CD2	3:F:138:MET:HG2	1.99	0.97
1:B:827:TRP:H	3:F:58:ARG:NH1	1.57	0.97
1:B:791:GLN:HE22	2:D:193:MET:CE	1.65	0.97
1:A:112:TRP:HE1	1:A:129:LYS:NZ	1.61	0.97
1:B:84:PHE:HZ	1:B:90:MET:HA	1.29	0.97
1:B:804:LEU:HD21	2:D:63:ARG:CZ	1.95	0.97
1:B:613:SER:HB2	2:C:144:GLY:O	1.65	0.97
1:A:798:ARG:HD2	2:C:82:ALA:HA	1.47	0.96
1:B:733:GLY:O	2:D:138:ARG:NH1	1.97	0.96
1:A:806:GLU:HB3	3:E:105:VAL:HG21	1.46	0.96
1:B:639:LYS:HG2	1:B:640:LYS:HG3	1.42	0.96
1:B:65:TYR:HE1	1:B:67:LYS:HB3	1.29	0.96
1:B:292:ASN:ND2	1:B:330:MET:HG3	1.80	0.96
1:A:859:LEU:HD11	1:B:860:LYS:CA	1.95	0.96
1:B:845:ARG:HD3	3:F:23:GLN:NE2	1.47	0.96
1:B:109:TYR:HB2	1:B:125:VAL:HG11	1.47	0.95
1:B:783:ARG:HH12	2:D:126:ASP:CG	1.73	0.95
1:B:783:ARG:HH12	2:D:126:ASP:HB3	1.25	0.95
1:A:714:LEU:CD2	1:B:396:LEU:CD1	2.09	0.95
1:A:791:GLN:HE22	2:C:193:MET:CE	1.71	0.95
1:B:17:ARG:HD3	1:B:20:GLU:HB3	1.48	0.95
1:B:65:TYR:CE1	1:B:67:LYS:HB3	2.00	0.95
1:A:827:TRP:CE3	1:A:828:PRO:HD2	2.01	0.95
1:B:803:LYS:NZ	3:F:107:ASP:O	2.00	0.95
1:A:293:LYS:HD3	1:A:298:LEU:HA	1.48	0.95
1:A:147:ARG:HB2	1:A:160:ASN:ND2	1.81	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:ILE:HG22	1:B:714:LEU:H	1.32	0.94
1:A:169:ARG:CB	1:B:403:ARG:HH21	1.79	0.94
1:A:805:LEU:HD11	2:C:60:LEU:CD2	1.97	0.94
1:A:713:ILE:HG22	1:A:714:LEU:H	1.32	0.94
1:B:198:ILE:HD13	1:B:204:ARG:NH2	1.82	0.94
1:B:723:ARG:NH2	1:B:785:ILE:HA	1.83	0.94
1:B:810:SER:OG	3:F:102:ALA:HA	1.68	0.94
1:A:784:ILE:HD13	2:C:140:PHE:CE2	2.02	0.94
1:A:735:PHE:HA	1:A:736:ILE:CG2	1.98	0.93
1:A:791:GLN:HE21	2:C:193:MET:HE1	1.25	0.93
1:A:860:LYS:CA	1:B:859:LEU:HD11	1.98	0.93
1:A:800:GLU:OE2	3:E:108:PRO:HG3	1.69	0.93
1:B:873:LEU:HD23	1:B:876:LYS:HD3	1.47	0.92
1:A:112:TRP:HE1	1:A:129:LYS:HZ3	1.07	0.92
1:B:635:LYS:CG	1:B:636:GLY:HA3	1.99	0.92
1:B:290:LEU:HG	1:B:303:ILE:HD11	1.50	0.92
1:B:827:TRP:CG	1:B:828:PRO:HD2	2.03	0.92
2:D:66:LYS:CE	3:F:126:GLN:HG3	2.00	0.92
1:A:922:MET:CE	1:B:919:VAL:HG13	2.00	0.92
1:B:388:MET:HA	1:B:617:LEU:CD2	1.99	0.92
1:A:17:ARG:HD3	1:A:151:PRO:HG3	1.49	0.91
1:A:853:LYS:NZ	1:B:841:LYS:HZ3	1.67	0.91
1:A:922:MET:HE1	1:B:919:VAL:CG1	2.00	0.91
1:B:845:ARG:CD	3:F:23:GLN:HE22	1.60	0.91
1:B:723:ARG:HA	1:B:745:LEU:HD21	1.48	0.91
1:B:84:PHE:CE1	1:B:87:ILE:HD11	2.06	0.91
1:A:289:ILE:O	1:A:293:LYS:HB2	1.69	0.91
1:A:849:MET:CE	1:B:852:MET:CE	2.46	0.91
1:A:735:PHE:CD2	1:B:379:GLU:OE2	2.24	0.90
1:B:827:TRP:HB2	3:F:58:ARG:NH2	1.85	0.90
1:A:434:ARG:HH12	1:A:623:ASN:HD22	1.17	0.90
1:B:335:ALA:HA	1:B:338:VAL:HG22	1.54	0.90
1:B:270:LYS:HD3	1:B:433:GLU:HB2	1.51	0.90
1:B:831:LYS:HD3	3:F:163:GLU:HG3	0.90	0.90
3:E:21:PHE:CD2	3:E:26:ILE:HG21	2.07	0.90
1:B:733:GLY:CA	2:D:138:ARG:NH2	2.24	0.90
1:A:274:ILE:HD12	1:A:422:TYR:HA	1.52	0.89
1:A:735:PHE:CD2	1:A:738:SER:HA	2.07	0.89
1:B:135:THR:O	1:B:138:VAL:HG12	1.72	0.89
1:A:873:LEU:HD12	1:B:870:ARG:CD	2.01	0.89
1:B:18:LYS:CD	1:B:108:ARG:HD2	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:755:GLN:HB2	1:B:769:LEU:HD13	1.50	0.89
1:B:549:LYS:HG2	1:B:553:PHE:CE2	2.06	0.89
1:B:635:LYS:HZ2	1:B:647:VAL:HA	1.37	0.89
1:A:289:ILE:HD11	1:A:357:MET:HE2	1.54	0.89
1:A:791:GLN:HE22	2:C:193:MET:HE1	1.06	0.89
1:B:807:ARG:HD2	2:D:63:ARG:CB	1.99	0.89
1:A:822:MET:HE3	3:E:138:MET:CE	1.73	0.89
1:A:33:LEU:HB3	1:A:50:LYS:NZ	1.86	0.89
1:A:633:LYS:HA	1:A:636:GLY:HA2	1.52	0.89
1:A:684:MET:HE3	1:A:689:VAL:HG22	1.52	0.89
1:A:859:LEU:HD11	1:B:859:LEU:C	1.97	0.88
1:B:733:GLY:HA2	2:D:134:VAL:CG1	2.00	0.88
2:C:114:PHE:CE1	2:C:118:LEU:HD11	2.08	0.88
3:F:73:ALA:HB2	3:F:85:MET:HE3	1.52	0.88
1:A:791:GLN:OE1	2:C:133:PHE:HZ	1.54	0.88
1:B:831:LYS:CG	3:F:163:GLU:HG3	2.04	0.88
1:A:734:GLN:HG2	1:A:735:PHE:CD1	2.07	0.88
1:A:845:ARG:NH2	3:F:23:GLN:HB3	1.89	0.88
1:B:783:ARG:NH2	2:D:126:ASP:OD2	2.07	0.88
2:D:65:PRO:HG3	3:F:126:GLN:OE1	1.71	0.88
2:D:66:LYS:CD	3:F:126:GLN:CG	2.52	0.88
3:E:164:GLU:HG2	3:E:165:LYS:HA	1.54	0.88
1:A:168:ASP:OD1	1:B:397:LYS:HE3	1.74	0.88
1:A:834:PHE:CE2	3:E:163:GLU:HA	2.09	0.88
2:D:66:LYS:CD	3:F:127:ALA:HB2	1.99	0.88
1:A:853:LYS:HZ3	1:B:841:LYS:NZ	1.71	0.88
1:B:804:LEU:CG	2:D:63:ARG:HD3	2.04	0.88
1:B:804:LEU:CD2	2:D:63:ARG:HD2	1.95	0.87
1:A:428:ALA:HA	1:A:431:VAL:HG12	1.56	0.87
1:B:729:ALA:HB1	1:B:744:LYS:HE2	1.56	0.87
2:D:65:PRO:CG	3:F:126:GLN:CD	2.34	0.87
1:B:733:GLY:CA	2:D:138:ARG:NH1	2.35	0.87
1:A:45:GLU:HG2	1:A:102:LEU:CD2	2.04	0.87
1:A:168:ASP:OD1	1:B:397:LYS:CE	2.22	0.87
1:A:564:GLN:HG3	1:A:578:SER:HB2	1.57	0.87
1:B:791:GLN:HE21	2:D:193:MET:HE1	1.35	0.87
1:B:831:LYS:CG	3:F:163:GLU:OE2	2.23	0.87
1:B:821:PHE:CD2	3:F:138:MET:CG	2.58	0.87
1:A:853:LYS:NZ	1:B:841:LYS:HZ1	1.71	0.87
1:B:84:PHE:CZ	1:B:90:MET:HA	2.09	0.87
1:B:723:ARG:CZ	1:B:785:ILE:HG12	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:LEU:CD1	2:D:180:ASN:ND2	2.38	0.86
1:B:549:LYS:HE2	1:B:553:PHE:CE2	2.10	0.86
1:A:734:GLN:HG2	1:A:735:PHE:HD1	1.39	0.86
1:A:735:PHE:HE2	1:B:379:GLU:OE1	1.57	0.86
1:B:734:GLN:N	2:D:138:ARG:HH22	1.68	0.86
1:B:298:LEU:HG	1:B:303:ILE:CG2	2.05	0.86
1:A:455:TYR:HE1	1:B:403:ARG:HH11	1.21	0.86
1:B:635:LYS:HG3	1:B:636:GLY:CA	2.06	0.86
3:E:80:THR:HA	3:F:40:ARG:HD3	1.58	0.86
1:A:810:SER:HB2	3:E:105:VAL:CG1	2.06	0.85
1:B:260:SER:HB2	1:B:447:LEU:O	1.76	0.85
1:B:268:LEU:HD21	1:B:432:TYR:CE2	2.11	0.85
1:A:631:ILE:HD11	1:A:639:LYS:HB3	1.54	0.85
1:B:781:LEU:HD13	1:B:785:ILE:HD12	1.59	0.85
2:C:114:PHE:CZ	2:C:118:LEU:HD11	2.11	0.85
1:A:18:LYS:HD2	1:A:113:MET:HE1	1.57	0.85
1:A:375:PRO:CG	1:A:380:GLU:HA	2.07	0.85
1:B:292:ASN:HD21	1:B:330:MET:CG	1.88	0.85
1:B:829:TRP:CG	3:F:89:LYS:HE2	2.11	0.85
2:D:66:LYS:HD3	3:F:126:GLN:CG	2.04	0.85
3:E:80:THR:HG23	3:F:40:ARG:NE	1.91	0.85
1:A:881:LEU:CD1	2:D:180:ASN:HD21	1.89	0.85
1:B:45:GLU:CD	1:B:102:LEU:HD21	2.02	0.85
1:A:67:LYS:HG2	1:A:68:THR:H	1.42	0.84
3:F:35:ILE:HG13	3:F:36:MET:HG3	1.59	0.84
1:B:832:LEU:HD23	3:F:164:GLU:HG2	1.58	0.84
1:A:853:LYS:HZ1	1:B:841:LYS:NZ	1.67	0.84
1:B:180:SER:HB2	1:B:466:GLU:HA	1.58	0.84
1:B:38:PHE:CE1	1:B:79:GLN:HA	2.13	0.84
1:B:735:PHE:HB3	2:D:138:ARG:NE	1.90	0.84
1:B:807:ARG:CD	2:D:63:ARG:HB2	2.00	0.84
1:A:112:TRP:NE1	1:A:129:LYS:NZ	2.26	0.84
1:A:134:TYR:CD1	1:A:190:ARG:HD3	2.12	0.84
1:A:404:VAL:HG12	1:A:411:VAL:O	1.78	0.84
1:A:815:GLN:OE1	3:E:127:ALA:CB	2.25	0.84
1:A:878:VAL:HG12	1:B:453:ARG:HB2	1.57	0.84
1:B:827:TRP:CB	3:F:58:ARG:HH12	1.90	0.84
2:D:65:PRO:CG	3:F:126:GLN:NE2	2.41	0.84
1:A:936:LEU:HD11	1:B:933:ASN:OD1	1.78	0.84
1:A:58:LYS:CE	1:A:70:THR:HB	2.08	0.83
1:A:293:LYS:HD3	1:A:298:LEU:CA	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ALA:HA	1:B:429:LYS:HE2	1.60	0.83
2:D:65:PRO:HG2	3:F:126:GLN:NE2	1.92	0.83
1:B:255:THR:HB	2:D:154:ARG:NH1	1.93	0.83
1:B:821:PHE:CE2	3:F:138:MET:CG	2.60	0.83
1:A:856:PHE:HE1	1:B:855:GLU:CB	1.83	0.83
1:B:162:TYR:CZ	1:B:199:ALA:HB1	2.14	0.83
1:B:179:GLU:HB3	1:B:674:ILE:HD12	1.61	0.83
1:A:746:LEU:HD22	1:A:751:ILE:HD11	1.57	0.83
1:B:18:LYS:NZ	1:B:88:GLU:HA	1.93	0.83
1:A:434:ARG:HH12	1:A:623:ASN:ND2	1.75	0.83
3:E:67:ASP:O	3:E:70:ILE:HG12	1.79	0.83
1:B:635:LYS:HB3	1:B:640:LYS:O	1.79	0.83
1:A:810:SER:OG	3:E:102:ALA:O	1.97	0.83
1:B:46:PHE:CD2	1:B:99:PRO:HB3	2.14	0.82
1:B:531:MET:SD	1:B:532:SER:HB3	2.19	0.82
1:A:714:LEU:HD21	1:B:396:LEU:CG	2.07	0.82
1:A:835:LYS:CE	3:E:165:LYS:NZ	2.39	0.82
1:A:881:LEU:HD12	2:D:180:ASN:ND2	1.94	0.82
3:E:99:ILE:HD12	3:E:159:ILE:HD13	1.59	0.82
1:A:806:GLU:HB3	3:E:105:VAL:CG2	2.09	0.82
1:B:633:LYS:H	1:B:641:GLY:HA3	1.43	0.82
3:F:66:ILE:HG13	3:F:67:ASP:H	1.42	0.82
3:E:80:THR:CB	3:F:40:ARG:HD2	2.08	0.82
1:B:872:GLU:O	1:B:875:GLU:HG2	1.80	0.82
1:B:815:GLN:HA	1:B:818:ILE:HG12	1.62	0.82
1:A:755:GLN:HG2	1:A:769:LEU:HD12	1.60	0.82
3:E:56:LEU:C	3:E:165:LYS:HE2	2.05	0.82
1:A:58:LYS:HE2	1:A:70:THR:HB	1.59	0.82
1:A:45:GLU:CD	1:A:690:MET:HB2	2.05	0.81
1:B:47:VAL:HG22	1:B:48:LYS:H	1.45	0.81
3:E:59:VAL:HA	3:E:60:ASN:HB2	1.60	0.81
1:B:160:ASN:HA	1:B:163:GLN:CD	2.05	0.81
1:B:256:GLY:N	2:D:154:ARG:NH2	2.27	0.81
1:B:352:LEU:HD11	1:B:620:LEU:HD12	1.60	0.81
1:A:730:ILE:HB	1:A:734:GLN:HG3	1.63	0.81
1:A:77:MET:SD	1:A:99:PRO:HD3	2.21	0.81
1:A:832:LEU:HA	3:E:164:GLU:HG3	1.62	0.81
1:A:675:PRO:HA	1:A:684:MET:SD	2.21	0.81
2:D:73:TYR:CE1	2:D:106:THR:HB	2.15	0.81
2:C:54:PHE:CZ	2:C:118:LEU:HD23	2.16	0.81
1:B:418:GLN:HA	1:B:421:ILE:HG12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLN:HG2	1:A:95:PHE:CE1	2.16	0.80
1:A:922:MET:CE	1:B:923:ASN:OD1	2.30	0.80
1:B:351:LYS:HD3	1:B:614:LEU:HD23	1.62	0.80
3:E:8:LYS:HD3	3:F:59:VAL:HA	0.81	0.80
3:E:8:LYS:HG2	3:F:59:VAL:CA	2.11	0.80
1:B:726:ASN:HD22	1:B:744:LYS:HB3	1.45	0.80
1:A:353:THR:O	1:A:356:ILE:HG12	1.81	0.80
1:A:735:PHE:CE2	1:B:379:GLU:OE1	2.34	0.80
1:B:635:LYS:HZ1	1:B:650:LEU:HB2	1.46	0.80
2:D:147:THR:HG22	2:D:184:ASN:HD21	1.44	0.80
3:E:27:GLN:HE22	3:F:24:THR:HG22	1.46	0.80
1:A:810:SER:HB2	3:E:105:VAL:HG11	1.63	0.80
1:A:25:GLU:C	1:A:29:ARG:HH12	1.89	0.80
1:B:146:LYS:HD2	1:B:774:GLU:HG2	1.63	0.80
3:E:78:ASN:H	3:E:81:VAL:HG12	1.47	0.80
1:B:151:PRO:HB2	1:B:152:PRO:HD2	1.61	0.80
1:B:609:TYR:O	1:B:612:SER:HB2	1.82	0.80
1:B:534:LEU:HA	1:B:538:CYS:SG	2.22	0.80
1:B:939:LYS:NZ	1:B:943:LEU:HD21	1.97	0.80
1:B:804:LEU:CD2	2:D:63:ARG:NH1	2.19	0.79
1:A:194:TYR:O	1:A:197:VAL:HG12	1.82	0.79
1:A:834:PHE:HE2	3:E:163:GLU:HA	1.47	0.79
1:A:45:GLU:OE1	1:A:690:MET:HB2	1.82	0.79
1:B:260:SER:OG	1:B:449:THR:HB	1.83	0.79
1:B:520:CYS:SG	1:B:579:LEU:HD11	2.22	0.79
1:B:810:SER:OG	3:F:102:ALA:CA	2.31	0.79
3:E:56:LEU:HB3	3:E:165:LYS:HD3	1.64	0.79
1:A:574:GLU:OE2	1:A:591:ILE:HG21	1.83	0.79
3:E:142:PHE:O	3:E:144:PRO:HD3	1.83	0.79
1:B:18:LYS:HD3	1:B:108:ARG:HD2	1.65	0.79
1:B:84:PHE:CD2	1:B:93:LEU:HD13	2.17	0.79
1:B:208:ASP:O	1:B:210:SER:HA	1.82	0.79
3:F:139:PHE:HA	3:F:142:PHE:CD2	2.18	0.79
1:B:822:MET:CE	3:F:137:GLN:HG3	2.10	0.78
1:B:190:ARG:HA	1:B:193:GLN:CG	2.14	0.78
1:A:359:PHE:CE1	1:A:384:SER:HB2	2.18	0.78
1:B:17:ARG:HD3	1:B:20:GLU:CB	2.13	0.78
1:B:910:LYS:O	1:B:913:ILE:HG12	1.84	0.78
2:D:134:VAL:HG13	2:D:138:ARG:HH12	1.48	0.78
1:B:162:TYR:CZ	1:B:166:LEU:HD11	2.18	0.78
1:A:804:LEU:HA	1:A:807:ARG:HE	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:OE2	1:B:690:MET:HA	1.83	0.78
1:B:831:LYS:HD2	3:F:163:GLU:OE2	1.82	0.78
1:B:164:TYR:HE1	1:B:762:LYS:HG2	1.46	0.78
1:A:10:GLY:O	1:A:14:PRO:HD3	1.84	0.78
1:A:791:GLN:CD	2:C:133:PHE:CZ	2.60	0.78
3:F:103:PHE:CD1	3:F:114:LEU:HD22	2.19	0.78
1:A:97:HIS:C	1:A:99:PRO:HD2	2.09	0.78
1:A:803:LYS:NZ	3:E:109:GLU:OE1	2.13	0.78
1:B:88:GLU:HG3	1:B:89:ASP:H	1.48	0.78
1:A:690:MET:HG2	1:A:694:ARG:NH1	1.99	0.78
2:C:46:PHE:HD1	2:C:119:GLN:HE21	1.30	0.78
1:A:370:GLU:HB3	1:A:371:GLU:HB2	1.66	0.77
1:B:294:LYS:HE3	1:B:295:PRO:HD2	1.66	0.77
1:A:38:PHE:CE1	1:A:79:GLN:HA	2.20	0.77
1:A:298:LEU:HG	1:A:303:ILE:CG1	2.13	0.77
1:B:730:ILE:HD12	1:B:745:LEU:HD13	1.65	0.77
1:B:353:THR:O	1:B:356:ILE:HG12	1.85	0.77
1:A:822:MET:HE3	3:E:138:MET:HE2	0.78	0.77
1:B:139:VAL:HG11	1:B:197:VAL:HG13	1.67	0.77
1:B:635:LYS:NZ	1:B:650:LEU:HB2	1.99	0.77
1:B:915:LEU:HD23	1:B:918:LYS:HD3	1.64	0.77
1:B:84:PHE:CE2	1:B:104:ASN:ND2	2.53	0.77
3:F:152:TYR:CE2	3:F:153:LYS:HG3	2.20	0.77
1:A:859:LEU:CD1	1:B:860:LYS:N	2.39	0.76
1:A:910:LYS:O	1:A:913:ILE:HG12	1.84	0.76
2:D:87:PRO:HA	2:D:91:GLU:OE1	1.85	0.76
2:D:135:GLU:HG2	2:D:138:ARG:HH22	1.47	0.76
1:A:808:ARG:NH2	2:C:62:ASP:O	2.18	0.76
1:B:387:LEU:O	1:B:617:LEU:HD21	1.84	0.76
1:B:834:PHE:CG	3:F:163:GLU:O	2.38	0.76
3:E:21:PHE:HD2	3:E:26:ILE:HG21	1.51	0.76
1:A:352:LEU:HD22	1:A:435:MET:HE2	1.67	0.76
1:B:733:GLY:HA2	2:D:138:ARG:NH1	1.98	0.76
1:B:827:TRP:HB3	3:F:58:ARG:HH12	1.49	0.76
3:E:8:LYS:CG	3:F:59:VAL:CA	2.56	0.76
1:A:372:GLN:HA	1:A:420:VAL:HG21	1.67	0.76
1:A:389:GLY:C	1:A:390:LEU:HD12	2.11	0.76
1:A:800:GLU:OE2	3:E:108:PRO:CG	2.34	0.76
2:D:114:PHE:CE2	2:D:118:LEU:HD11	2.20	0.76
1:B:746:LEU:HB3	1:B:751:ILE:CD1	2.16	0.76
3:E:8:LYS:HD2	3:F:58:ARG:C	2.09	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HB3	1:A:50:LYS:HZ3	1.50	0.75
1:A:45:GLU:HG2	1:A:102:LEU:HD22	1.66	0.75
1:A:549:LYS:HD3	1:A:575:ALA:HB1	1.67	0.75
1:B:22:GLU:OE1	1:B:87:ILE:HG22	1.85	0.75
1:B:36:ASP:HB3	1:B:48:LYS:HZ2	1.50	0.75
1:B:549:LYS:HE2	1:B:553:PHE:CZ	2.20	0.75
1:B:723:ARG:HA	1:B:745:LEU:CD2	2.16	0.75
1:B:826:ASN:HB3	3:F:59:VAL:HB	0.80	0.75
1:B:831:LYS:CD	3:F:163:GLU:OE2	2.33	0.75
1:A:109:TYR:CD1	1:A:125:VAL:HG13	2.21	0.75
2:D:65:PRO:CG	3:F:126:GLN:HE22	1.98	0.75
3:F:94:ASP:O	3:F:99:ILE:HG12	1.85	0.75
2:C:94:ARG:HH22	2:C:124:ASN:ND2	1.84	0.75
1:B:36:ASP:HB3	1:B:48:LYS:CE	2.16	0.75
1:B:821:PHE:O	1:B:824:VAL:HG12	1.86	0.75
1:B:783:ARG:NH1	2:D:126:ASP:CB	2.40	0.75
1:B:63:THR:HG21	1:B:65:TYR:CE2	2.21	0.75
1:B:303:ILE:HD12	1:B:310:TYR:OH	1.87	0.75
1:B:836:ILE:HG21	3:F:28:GLU:OE1	1.87	0.75
1:A:48:LYS:CE	1:A:79:GLN:HE21	1.98	0.75
1:A:404:VAL:HG13	1:A:411:VAL:HB	1.69	0.75
1:B:427:LEU:HA	1:B:601:LEU:HD11	1.66	0.75
1:B:614:LEU:HB2	1:B:617:LEU:HD22	1.67	0.75
1:B:623:ASN:HA	1:B:637:LYS:CE	2.14	0.75
1:B:746:LEU:HB3	1:B:751:ILE:HD11	1.68	0.75
3:E:32:ALA:O	3:E:35:ILE:HG12	1.86	0.75
1:B:46:PHE:HD2	1:B:99:PRO:HB3	1.52	0.74
1:B:544:THR:HA	1:B:594:LEU:HD11	1.68	0.74
1:B:623:ASN:HB2	1:B:637:LYS:HZ3	1.52	0.74
3:E:23:GLN:HG3	3:E:24:THR:HG23	1.68	0.74
3:E:61:VAL:HG23	3:E:66:ILE:HG23	1.68	0.74
1:B:256:GLY:CA	2:D:154:ARG:HH22	1.99	0.74
1:B:569:ILE:HD13	1:B:574:GLU:OE1	1.87	0.74
1:A:38:PHE:CD2	1:A:99:PRO:HB2	2.21	0.74
3:E:22:GLU:HG2	3:E:25:GLN:HE21	1.52	0.74
3:F:67:ASP:HA	3:F:70:ILE:HG22	1.69	0.74
1:B:390:LEU:HD12	1:B:609:TYR:HA	1.70	0.74
1:B:633:LYS:H	1:B:641:GLY:CA	1.99	0.74
2:D:66:LYS:CE	3:F:126:GLN:CG	2.66	0.74
1:B:293:LYS:HZ1	1:B:303:ILE:HB	1.50	0.74
1:B:601:LEU:HD23	1:B:602:ASN:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLY:CA	2:D:138:ARG:CZ	2.66	0.74
1:B:832:LEU:HD23	3:F:164:GLU:CG	2.17	0.74
1:A:955:ASP:O	1:A:958:GLU:HG2	1.87	0.74
2:D:66:LYS:HD3	3:F:126:GLN:C	2.12	0.74
1:A:428:ALA:HA	1:A:431:VAL:CG1	2.17	0.74
1:B:549:LYS:NZ	1:B:566:PRO:HG3	2.03	0.74
1:B:366:LEU:HD21	1:B:368:GLN:HB3	1.70	0.73
2:C:101:GLN:HB2	2:C:102:GLU:HB2	1.70	0.73
2:D:45:GLU:HA	2:D:119:GLN:NE2	2.03	0.73
2:D:109:MET:HE3	2:D:113:THR:HB	1.69	0.73
3:F:138:MET:HB3	3:F:142:PHE:CE1	2.22	0.73
1:A:804:LEU:HA	1:A:807:ARG:NE	2.03	0.73
2:C:67:CYS:CB	2:C:68:GLU:HA	2.16	0.73
2:D:147:THR:HG22	2:D:184:ASN:ND2	2.04	0.73
1:A:143:ARG:HG3	1:A:198:ILE:HG22	1.70	0.73
1:A:735:PHE:HB2	1:A:737:ASP:O	1.86	0.73
1:B:352:LEU:HD12	1:B:617:LEU:HA	1.70	0.73
1:B:633:LYS:HB2	1:B:642:SER:H	1.54	0.73
1:B:139:VAL:HG11	1:B:197:VAL:CG1	2.18	0.73
1:B:336:PHE:CE1	1:B:349:MET:HE1	2.24	0.73
1:B:785:ILE:O	1:B:788:ILE:HG12	1.87	0.73
1:A:822:MET:CE	3:E:138:MET:HB3	2.17	0.73
1:B:434:ARG:NH1	1:B:621:PHE:HA	2.03	0.73
1:B:549:LYS:HZ1	1:B:566:PRO:HG3	1.54	0.73
3:E:27:GLN:NE2	3:F:24:THR:CG2	2.47	0.73
1:B:605:VAL:O	1:B:609:TYR:CD1	2.40	0.73
1:B:818:ILE:HD12	3:F:130:PHE:CE2	2.24	0.73
1:A:756:TYR:HE2	1:A:758:PHE:CZ	2.07	0.73
1:A:84:PHE:CD2	1:A:93:LEU:HG	2.24	0.72
1:B:520:CYS:SG	1:B:579:LEU:HD21	2.28	0.72
2:D:98:LYS:HD2	2:D:99:PRO:HD2	1.71	0.72
3:E:24:THR:HB	3:E:161:HIS:NE2	2.03	0.72
1:A:168:ASP:OD1	1:B:397:LYS:CD	2.36	0.72
1:A:735:PHE:HD1	1:A:741:GLY:HA3	1.54	0.72
1:A:798:ARG:CD	2:C:82:ALA:HA	2.18	0.72
1:B:635:LYS:HD2	1:B:645:GLN:O	1.90	0.72
1:B:924:GLU:O	1:B:927:GLU:HG2	1.89	0.72
1:A:853:LYS:HZ1	1:B:841:LYS:HZ1	1.32	0.72
2:C:114:PHE:CE2	2:C:118:LEU:HD21	2.24	0.72
1:A:217:GLU:O	1:A:220:ILE:HG12	1.89	0.72
1:B:605:VAL:HG22	1:B:609:TYR:CE1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:98:LYS:HD3	2:C:106:THR:HG21	1.70	0.72
1:A:222:GLN:HG3	1:A:338:VAL:HG21	1.70	0.72
1:B:723:ARG:HG3	1:B:724:ILE:H	1.52	0.72
1:A:298:LEU:HG	1:A:303:ILE:HG13	1.72	0.72
1:A:553:PHE:CE1	1:A:566:PRO:HD3	2.24	0.72
1:A:735:PHE:HD2	1:A:738:SER:HA	1.53	0.72
1:A:804:LEU:HD22	1:A:807:ARG:HH21	1.55	0.72
1:A:45:GLU:HG3	1:A:46:PHE:HD1	1.49	0.72
1:A:375:PRO:HG2	1:A:380:GLU:CA	2.18	0.72
1:A:798:ARG:CZ	2:C:82:ALA:O	2.37	0.72
1:A:820:ALA:O	1:A:824:VAL:HG12	1.90	0.72
1:B:827:TRP:CB	3:F:58:ARG:NH1	2.52	0.72
3:F:73:ALA:HB2	3:F:85:MET:CE	2.20	0.72
1:B:73:GLU:O	1:B:76:VAL:HG12	1.90	0.72
1:B:96:LEU:HD23	1:B:703:ARG:HG2	1.72	0.72
1:B:277:LEU:HD23	1:B:278:LYS:N	2.05	0.72
1:B:633:LYS:HA	1:B:641:GLY:CA	2.18	0.72
1:B:733:GLY:HA2	2:D:135:GLU:N	2.05	0.72
2:D:65:PRO:CD	3:F:126:GLN:HE22	2.03	0.72
2:D:95:VAL:HB	2:D:117:MET:SD	2.29	0.72
3:F:113:VAL:HG21	3:F:150:LEU:HD12	1.71	0.72
1:B:275:PHE:CE1	1:B:314:SER:HB2	2.24	0.71
1:B:401:HIS:CD2	1:B:414:GLY:HA2	2.25	0.71
1:B:428:ALA:O	1:B:431:VAL:HG12	1.91	0.71
1:B:791:GLN:O	1:B:795:VAL:HG23	1.90	0.71
1:B:218:ASP:O	1:B:221:ILE:HG12	1.90	0.71
2:C:67:CYS:HB3	2:C:68:GLU:HA	1.71	0.71
1:B:721:ARG:HD2	2:D:159:THR:OG1	1.91	0.71
1:B:830:MET:HB3	3:F:166:ASP:O	1.90	0.71
2:C:48:PRO:O	2:C:51:ILE:HG12	1.90	0.71
3:E:53:PHE:HB3	3:E:60:ASN:OD1	1.90	0.71
3:E:106:PHE:CZ	3:E:114:LEU:HD11	2.26	0.71
1:A:684:MET:HE3	1:A:689:VAL:CG2	2.20	0.71
1:A:822:MET:HE2	3:E:138:MET:HB3	1.72	0.71
1:B:286:PHE:O	1:B:289:ILE:HG12	1.91	0.71
3:F:153:LYS:HA	3:F:156:VAL:CG1	2.17	0.71
1:B:45:GLU:CG	1:B:102:LEU:HD21	2.19	0.71
1:B:826:ASN:HB3	3:F:59:VAL:CG1	2.19	0.71
2:D:66:LYS:HE3	3:F:126:GLN:CG	2.14	0.71
1:A:637:LYS:HG3	1:A:638:ALA:H	1.53	0.71
1:B:639:LYS:CG	1:B:640:LYS:HG3	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:135:GLU:HA	2:D:138:ARG:CZ	2.21	0.71
1:B:109:TYR:CD2	1:B:684:MET:HE2	2.25	0.71
2:C:87:PRO:HA	2:C:91:GLU:OE1	1.91	0.71
1:A:18:LYS:HE2	1:A:86:LYS:HD3	1.72	0.71
1:A:751:ILE:HD12	1:A:756:TYR:CE1	2.26	0.71
1:B:427:LEU:HD21	1:B:609:TYR:OH	1.91	0.71
1:A:136:PRO:HD2	1:A:209:GLN:O	1.90	0.70
1:B:848:GLU:O	1:B:852:MET:HG3	1.92	0.70
1:B:709:PHE:CZ	1:B:757:LYS:HG3	2.26	0.70
1:A:855:GLU:HB3	1:B:856:PHE:HE1	1.55	0.70
1:B:723:ARG:NH2	1:B:785:ILE:HG12	2.06	0.70
1:B:810:SER:OG	3:F:102:ALA:CB	2.39	0.70
1:B:633:LYS:HA	1:B:641:GLY:C	2.17	0.70
1:B:633:LYS:N	1:B:641:GLY:HA3	2.06	0.70
1:B:867:GLU:HA	1:B:871:LYS:HG2	1.72	0.70
1:B:623:ASN:OD1	1:B:624:TYR:HA	1.92	0.70
1:A:872:GLU:O	1:A:875:GLU:HG2	1.92	0.69
1:B:142:TYR:O	1:B:198:ILE:HD12	1.91	0.69
1:B:730:ILE:HD12	1:B:745:LEU:CD1	2.21	0.69
1:A:572:LYS:HB2	1:A:573:PRO:CD	2.21	0.69
1:B:275:PHE:CD1	1:B:314:SER:HB3	2.25	0.69
2:D:131:GLU:HA	2:D:134:VAL:HG12	1.72	0.69
1:B:631:ILE:HB	1:B:641:GLY:CA	2.18	0.69
1:B:635:LYS:HG2	1:B:639:LYS:C	2.17	0.69
1:B:635:LYS:HG2	1:B:639:LYS:O	1.91	0.69
1:A:335:ALA:O	1:A:338:VAL:HG22	1.93	0.69
1:A:790:ALA:HB2	2:C:88:THR:HG22	1.74	0.69
1:A:290:LEU:HD23	1:A:303:ILE:HD13	1.74	0.69
1:B:869:ARG:HG3	1:B:870:ARG:H	1.58	0.69
1:B:190:ARG:CA	1:B:193:GLN:HG2	2.20	0.69
1:B:633:LYS:H	1:B:641:GLY:N	1.91	0.69
3:E:76:PRO:O	3:E:81:VAL:HG11	1.93	0.69
3:F:156:VAL:HG23	3:F:159:ILE:HD11	1.74	0.69
1:B:652:ARG:HA	1:B:652:ARG:HE	1.58	0.69
2:D:66:LYS:CG	3:F:126:GLN:HG2	2.23	0.69
2:D:135:GLU:HA	2:D:138:ARG:NH2	2.07	0.69
1:A:112:TRP:NE1	1:A:129:LYS:HZ2	1.89	0.68
1:A:793:ARG:HH21	2:C:162:GLU:HB3	1.57	0.68
1:B:401:HIS:HD2	1:B:414:GLY:HA2	1.58	0.68
2:D:45:GLU:HA	2:D:119:GLN:HE21	1.58	0.68
2:D:65:PRO:HD2	3:F:126:GLN:HE22	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:13:ALA:HA	3:F:165:LYS:O	1.92	0.68
1:A:46:PHE:CD2	1:A:99:PRO:HB3	2.29	0.68
1:B:52:VAL:HG12	1:B:60:THR:O	1.94	0.68
2:C:44:ILE:HD11	2:C:123:LYS:HG2	1.74	0.68
1:A:11:ALA:C	1:A:14:PRO:HD2	2.17	0.68
1:A:735:PHE:CG	1:A:741:GLY:HA3	2.29	0.68
3:F:139:PHE:HA	3:F:142:PHE:CE2	2.28	0.68
1:A:714:LEU:HD21	1:B:396:LEU:HD13	1.60	0.68
1:B:826:ASN:OD1	3:E:8:LYS:NZ	2.18	0.68
1:A:84:PHE:CE2	1:A:93:LEU:HA	2.27	0.68
1:A:761:THR:HG21	1:B:374:GLU:HB3	1.75	0.68
1:B:335:ALA:CA	1:B:338:VAL:HG22	2.22	0.68
1:B:716:GLY:HA2	1:B:719:ARG:NH2	2.08	0.68
3:E:8:LYS:CG	3:F:58:ARG:C	2.67	0.68
3:F:67:ASP:HA	3:F:70:ILE:CG2	2.24	0.68
1:B:198:ILE:HD13	1:B:204:ARG:HH21	1.55	0.68
1:A:289:ILE:O	1:A:293:LYS:HE3	1.94	0.68
1:A:804:LEU:HD23	1:A:807:ARG:HE	1.57	0.68
3:E:8:LYS:HD3	3:F:59:VAL:CB	2.24	0.68
1:A:18:LYS:HE2	1:A:86:LYS:HE2	1.75	0.68
1:A:259:ALA:HB1	1:A:450:LYS:HG3	1.75	0.68
1:B:814:ILE:O	1:B:818:ILE:HG23	1.94	0.68
2:C:130:TYR:OH	2:C:186:GLU:HG3	1.94	0.68
3:F:108:PRO:HG2	3:F:109:GLU:OE1	1.94	0.68
1:A:224:ASN:HB3	1:A:225:PRO:HD3	1.76	0.67
1:A:756:TYR:HB3	1:A:769:LEU:HD13	1.74	0.67
1:A:845:ARG:HH22	3:F:23:GLN:HB2	0.59	0.67
1:B:432:TYR:HA	1:B:435:MET:HG2	1.75	0.67
1:B:787:ARG:HH12	2:D:127:THR:HA	1.59	0.67
1:A:286:PHE:O	1:A:289:ILE:HG12	1.94	0.67
1:A:454:GLN:HB3	1:A:455:TYR:HA	1.76	0.67
1:B:791:GLN:CD	2:D:193:MET:CE	2.50	0.67
1:A:922:MET:HE2	1:B:923:ASN:OD1	1.94	0.67
1:B:286:PHE:CZ	1:B:356:ILE:HG13	2.30	0.67
1:B:335:ALA:HA	1:B:338:VAL:CG2	2.23	0.67
1:B:815:GLN:HE22	2:D:66:LYS:HA	1.60	0.67
1:A:260:SER:OG	1:A:448:GLU:HA	1.95	0.67
1:A:11:ALA:O	1:A:14:PRO:HD2	1.94	0.67
1:B:735:PHE:CB	2:D:138:ARG:NE	2.58	0.67
1:A:564:GLN:NE2	1:A:578:SER:HB3	2.10	0.67
1:B:633:LYS:CB	1:B:642:SER:H	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:832:LEU:HA	3:F:164:GLU:HG3	1.77	0.67
1:B:89:ASP:HA	1:B:117:TYR:HB2	1.77	0.67
2:C:131:GLU:HA	2:C:134:VAL:HG12	1.77	0.67
2:C:172:LEU:HD21	2:C:188:PHE:CE1	2.30	0.67
1:B:18:LYS:HD2	1:B:108:ARG:HD2	1.75	0.67
1:B:44:GLN:O	1:B:45:GLU:HB2	1.95	0.67
1:B:834:PHE:CE1	3:F:163:GLU:O	2.48	0.67
2:D:66:LYS:CD	3:F:127:ALA:CB	2.64	0.67
1:B:849:MET:HA	1:B:852:MET:HG3	1.76	0.66
2:C:109:MET:HE3	2:C:113:THR:HB	1.76	0.66
2:C:172:LEU:HD21	2:C:188:PHE:CZ	2.30	0.66
1:A:289:ILE:HD11	1:A:357:MET:CE	2.24	0.66
1:A:834:PHE:HE2	3:E:163:GLU:CA	2.07	0.66
1:A:908:LEU:HD11	1:B:908:LEU:O	1.95	0.66
1:B:888:GLN:HA	1:B:891:VAL:HG12	1.77	0.66
2:C:47:THR:HB	2:C:48:PRO:HD2	1.76	0.66
1:A:713:ILE:CG2	1:A:714:LEU:H	2.07	0.66
1:B:38:PHE:HE1	1:B:79:GLN:HA	1.60	0.66
2:D:111:PHE:CE2	2:D:115:LEU:HD11	2.30	0.66
1:B:603:GLU:HG3	1:B:604:THR:N	2.06	0.66
1:A:827:TRP:CD2	1:A:828:PRO:HD2	2.30	0.66
1:B:867:GLU:CA	1:B:871:LYS:HG2	2.25	0.66
3:F:160:THR:HG22	3:F:161:HIS:H	1.61	0.66
1:A:908:LEU:HD13	1:B:908:LEU:HB3	1.76	0.66
1:B:77:MET:SD	1:B:99:PRO:HD3	2.35	0.66
1:B:213:LYS:HB3	1:B:214:GLY:HA2	1.78	0.66
1:A:756:TYR:CE2	1:A:758:PHE:CE2	2.84	0.66
1:B:292:ASN:HB3	1:B:329:LEU:HD23	1.78	0.66
2:C:54:PHE:CE2	2:C:118:LEU:HD23	2.30	0.66
2:D:64:THR:HB	2:D:67:CYS:HA	1.78	0.66
1:A:45:GLU:HG2	1:A:102:LEU:HD21	1.77	0.65
1:A:370:GLU:HB2	1:A:372:GLN:H	1.62	0.65
1:B:164:TYR:OH	1:B:762:LYS:HD2	1.95	0.65
1:B:614:LEU:HB3	1:B:617:LEU:HD13	1.77	0.65
1:A:17:ARG:HD3	1:A:151:PRO:CG	2.25	0.65
1:A:346:LYS:HA	1:A:349:MET:HE3	1.77	0.65
1:B:88:GLU:HG3	1:B:89:ASP:N	2.10	0.65
1:B:256:GLY:H	2:D:154:ARG:HH22	1.38	0.65
1:B:726:ASN:HD22	1:B:744:LYS:CB	2.09	0.65
1:B:726:ASN:ND2	1:B:745:LEU:HD12	2.12	0.65
1:B:45:GLU:HG2	1:B:102:LEU:HD21	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ARG:HA	1:B:193:GLN:CD	2.22	0.65
3:E:8:LYS:HE2	3:F:60:ASN:HD21	1.62	0.65
1:A:33:LEU:HB3	1:A:50:LYS:HZ1	1.60	0.65
1:B:713:ILE:HG22	1:B:714:LEU:N	2.08	0.65
1:B:18:LYS:HZ1	1:B:88:GLU:HA	1.62	0.65
1:B:164:TYR:CE1	1:B:762:LYS:HG2	2.30	0.65
1:B:417:VAL:HG13	1:B:418:GLN:H	1.61	0.65
1:B:729:ALA:CB	1:B:744:LYS:HE2	2.26	0.65
1:B:808:ARG:HB2	2:D:62:ASP:O	1.96	0.65
1:A:25:GLU:C	1:A:29:ARG:NH1	2.55	0.65
1:A:312:PHE:O	1:A:313:ILE:HG12	1.96	0.65
1:A:810:SER:CB	3:E:105:VAL:CG1	2.74	0.65
1:B:143:ARG:NH2	2:D:166:GLU:OE2	2.29	0.65
1:B:162:TYR:OH	1:B:199:ALA:HB1	1.95	0.65
1:B:829:TRP:CD2	3:F:89:LYS:HE2	2.31	0.65
1:A:736:ILE:HG23	1:A:737:ASP:H	1.62	0.65
1:B:549:LYS:HE2	1:B:553:PHE:HE2	1.57	0.65
1:B:634:GLY:O	1:B:635:LYS:HB2	1.94	0.65
1:B:635:LYS:HZ1	1:B:650:LEU:CB	2.09	0.65
1:B:803:LYS:NZ	3:F:107:ASP:C	2.55	0.65
2:C:54:PHE:CD1	2:C:83:LEU:HD13	2.31	0.65
1:A:313:ILE:HG13	1:A:314:SER:N	2.12	0.65
1:A:860:LYS:HA	1:B:859:LEU:HD11	1.79	0.65
1:B:38:PHE:HD2	1:B:99:PRO:HB2	1.62	0.65
1:B:146:LYS:HD2	1:B:774:GLU:CG	2.26	0.65
3:E:20:MET:HG3	3:E:90:LEU:HD13	1.79	0.65
1:B:849:MET:HA	1:B:852:MET:SD	2.36	0.64
2:C:111:PHE:CE2	2:C:112:GLU:HG3	2.31	0.64
2:D:47:THR:HB	2:D:48:PRO:HD2	1.77	0.64
1:A:716:GLY:C	1:B:392:SER:OG	2.40	0.64
1:B:623:ASN:CB	1:B:637:LYS:HZ3	2.08	0.64
1:B:632:GLU:O	1:B:632:GLU:CD	2.40	0.64
1:B:834:PHE:CE1	3:F:163:GLU:C	2.75	0.64
1:B:158:SER:HB3	1:B:195:PHE:HE1	1.62	0.64
1:B:210:SER:N	1:B:211:PRO:HD2	2.12	0.64
1:B:709:PHE:CE2	1:B:757:LYS:HG3	2.33	0.64
1:B:733:GLY:H	2:D:138:ARG:CZ	2.08	0.64
1:A:24:LEU:C	1:A:29:ARG:HH22	2.05	0.64
1:A:84:PHE:HD2	1:A:93:LEU:HG	1.61	0.64
1:A:209:GLN:HB2	1:A:210:SER:HB2	1.78	0.64
1:B:540:PHE:CZ	1:B:913:ILE:HG21	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ASN:HD21	1:B:730:ILE:HD12	1.63	0.64
1:B:849:MET:SD	1:B:852:MET:SD	2.96	0.64
3:E:100:LEU:CA	3:E:155:LEU:HD23	2.13	0.64
1:A:685:ASP:OD1	1:A:687:PRO:HD2	1.97	0.64
1:B:734:GLN:O	1:B:735:PHE:CD1	2.51	0.64
2:D:61:PHE:CE2	2:D:79:VAL:HB	2.32	0.64
1:B:390:LEU:CD1	1:B:609:TYR:CD1	2.80	0.64
2:D:46:PHE:CE2	2:D:54:PHE:CE2	2.85	0.64
3:E:33:PHE:HA	3:E:36:MET:HG2	1.79	0.64
1:A:174:ILE:CD1	1:A:668:HIS:HB2	2.27	0.64
1:A:564:GLN:HG3	1:A:578:SER:CB	2.27	0.64
1:B:804:LEU:CD2	2:D:63:ARG:NE	2.60	0.64
1:B:155:PHE:HE1	1:B:193:GLN:HG3	1.63	0.64
1:A:849:MET:SD	1:B:852:MET:HE1	2.38	0.64
1:B:835:LYS:HB3	3:E:16:ASN:HB3	1.79	0.64
1:A:375:PRO:HG2	1:A:380:GLU:HG2	1.80	0.63
1:B:432:TYR:HA	1:B:435:MET:HE3	1.80	0.63
1:B:525:GLU:OE1	1:B:656:ASN:HB2	1.97	0.63
1:B:666:HIS:NE2	1:B:762:LYS:NZ	2.45	0.63
1:B:734:GLN:C	1:B:735:PHE:CD1	2.76	0.63
1:A:137:GLU:HG3	1:A:208:ASP:O	1.99	0.63
1:B:59:VAL:HG13	1:B:71:VAL:HB	1.80	0.63
1:B:364:PHE:CE2	1:B:375:PRO:HD3	2.34	0.63
1:B:16:LEU:O	1:B:113:MET:HE1	1.99	0.63
1:B:735:PHE:N	2:D:138:ARG:HH21	1.96	0.63
1:B:834:PHE:CD2	1:B:835:LYS:N	2.66	0.63
2:D:54:PHE:CD1	2:D:118:LEU:HD13	2.32	0.63
2:D:73:TYR:HE1	2:D:106:THR:H	1.46	0.63
1:A:18:LYS:HE2	1:A:86:LYS:CE	2.29	0.63
1:A:87:ILE:HG12	1:A:104:ASN:ND2	2.14	0.63
1:A:690:MET:HG2	1:A:694:ARG:HH12	1.61	0.63
1:A:849:MET:SD	1:B:852:MET:CE	2.87	0.63
1:A:856:PHE:CE1	1:B:855:GLU:CB	2.68	0.63
1:B:751:ILE:HG13	1:B:751:ILE:O	1.99	0.63
1:B:85:ASP:OD1	1:B:86:LYS:HG3	1.97	0.63
1:B:526:LYS:O	1:B:530:ILE:HG13	1.98	0.63
1:B:59:VAL:CG1	1:B:71:VAL:HB	2.28	0.63
1:B:310:TYR:O	1:B:313:ILE:HG22	1.98	0.63
1:B:336:PHE:CE1	1:B:349:MET:SD	2.92	0.63
2:D:134:VAL:HG22	2:D:138:ARG:HH11	1.63	0.63
1:A:790:ALA:CB	2:C:88:THR:HG22	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:GLN:HE22	2:D:66:LYS:CB	2.12	0.63
1:A:31:PHE:CE2	1:A:34:LYS:HB2	2.34	0.63
1:A:688:LEU:O	1:A:692:GLN:HG3	1.98	0.63
2:C:73:TYR:CE2	2:C:106:THR:HB	2.33	0.63
3:E:80:THR:HA	3:F:40:ARG:CD	2.28	0.63
1:B:671:ARG:HB3	1:B:671:ARG:HH11	1.64	0.63
1:B:804:LEU:CD1	2:D:75:GLN:NE2	2.56	0.63
1:B:133:VAL:O	1:B:138:VAL:HG11	1.98	0.62
1:B:700:GLU:HG3	1:B:703:ARG:NH2	2.14	0.62
1:B:826:ASN:CB	3:F:59:VAL:CB	2.45	0.62
1:B:48:LYS:NZ	1:B:79:GLN:HB2	2.13	0.62
2:D:85:GLN:O	2:D:87:PRO:HD3	1.99	0.62
1:A:404:VAL:CG1	1:A:411:VAL:HB	2.29	0.62
1:A:574:GLU:OE2	1:A:591:ILE:HD13	1.99	0.62
1:B:217:GLU:O	1:B:221:ILE:HG23	1.99	0.62
1:A:142:TYR:O	1:A:145:LYS:HG2	1.99	0.62
1:A:367:LYS:HD2	1:A:372:GLN:N	2.15	0.62
1:A:788:ILE:HD13	1:A:791:GLN:OE1	1.98	0.62
1:B:298:LEU:HG	1:B:303:ILE:HG22	1.80	0.62
3:E:56:LEU:O	3:E:165:LYS:HE2	1.99	0.62
3:F:91:LYS:O	3:F:95:PRO:HD2	1.98	0.62
1:A:209:GLN:HB2	1:A:210:SER:CB	2.30	0.62
1:A:245:GLY:HA3	1:A:266:TYR:HB3	1.81	0.62
1:A:791:GLN:CD	2:C:133:PHE:HZ	2.04	0.62
1:B:174:ILE:HB	1:B:459:VAL:HG22	1.80	0.62
1:B:815:GLN:HA	1:B:818:ILE:CG1	2.29	0.62
1:A:123:VAL:HA	1:A:671:ARG:O	2.00	0.62
1:B:734:GLN:H	2:D:138:ARG:NH2	1.97	0.62
1:B:815:GLN:HE22	2:D:66:LYS:CA	2.12	0.62
1:A:31:PHE:CD2	1:A:34:LYS:HE3	2.34	0.62
1:A:402:PRO:O	1:A:412:THR:HA	1.99	0.62
1:A:746:LEU:O	1:A:751:ILE:HG12	2.00	0.62
1:A:31:PHE:CE2	1:A:34:LYS:CB	2.83	0.62
1:A:806:GLU:CB	3:E:105:VAL:CG2	2.77	0.62
1:B:193:GLN:O	1:B:197:VAL:HG12	2.00	0.62
1:B:293:LYS:HZ1	1:B:303:ILE:CB	2.12	0.62
1:B:484:LYS:HD3	1:B:523:LEU:HA	1.82	0.62
1:B:808:ARG:NH1	2:D:67:CYS:SG	2.72	0.62
1:A:39:VAL:CG1	1:A:49:ALA:HB2	2.30	0.62
1:A:834:PHE:HE2	3:E:163:GLU:N	1.89	0.62
1:B:533:ILE:HG12	1:B:551:LYS:HB2	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:TRP:CD2	1:B:828:PRO:HD2	2.34	0.61
1:B:925:ARG:HA	1:B:928:ASP:OD2	2.00	0.61
1:B:222:GLN:HG3	1:B:338:VAL:HG21	1.81	0.61
1:B:735:PHE:N	2:D:138:ARG:NH2	2.48	0.61
1:B:815:GLN:NE2	2:D:66:LYS:HA	2.14	0.61
1:A:815:GLN:CD	3:E:127:ALA:HB3	2.23	0.61
1:B:146:LYS:HE3	2:D:160:LEU:HD21	1.81	0.61
1:A:84:PHE:HE2	1:A:93:LEU:HA	1.65	0.61
1:A:579:LEU:HD23	1:A:580:ILE:N	2.16	0.61
1:A:612:SER:HB3	1:A:617:LEU:HD22	1.82	0.61
1:A:675:PRO:CA	1:A:684:MET:SD	2.88	0.61
1:A:731:PRO:HD2	1:A:734:GLN:HB3	1.83	0.61
1:A:168:ASP:OD1	1:B:397:LYS:HD3	1.99	0.61
1:A:262:ASP:HB2	1:A:448:GLU:OE2	2.00	0.61
1:A:79:GLN:HG2	1:A:80:ASN:O	2.01	0.61
1:A:428:ALA:CA	1:A:431:VAL:HG12	2.27	0.61
1:B:48:LYS:HZ3	1:B:79:GLN:HB2	1.66	0.61
1:B:63:THR:HG22	1:B:64:GLU:N	2.15	0.61
1:B:752:ASP:HB2	1:B:769:LEU:CD1	2.31	0.61
1:B:830:MET:HG3	1:B:831:LYS:HG2	1.82	0.61
1:B:929:GLU:HA	1:B:932:MET:HB3	1.83	0.61
3:E:8:LYS:CD	3:F:58:ARG:C	2.71	0.61
3:E:125:THR:O	3:E:129:ARG:CZ	2.49	0.61
1:A:835:LYS:HE3	3:E:165:LYS:HZ2	1.59	0.61
1:B:440:VAL:HA	1:B:443:ILE:HG12	1.83	0.61
2:C:148:VAL:HG13	2:C:183:ILE:HG13	1.81	0.61
1:B:491:HIS:O	1:B:495:VAL:HB	2.00	0.61
3:F:120:ARG:HH22	3:F:139:PHE:HE1	1.47	0.61
1:A:53:SER:O	1:A:59:VAL:HG23	2.01	0.60
1:A:859:LEU:C	1:B:859:LEU:HD11	2.26	0.60
1:B:335:ALA:C	1:B:338:VAL:HG22	2.26	0.60
2:C:175:GLY:HA2	2:C:177:GLU:H	1.65	0.60
3:F:21:PHE:C	3:F:22:GLU:HG2	2.26	0.60
1:A:271:SER:N	1:A:272:ARG:HB2	2.15	0.60
1:B:109:TYR:CE2	1:B:684:MET:HE2	2.36	0.60
1:B:293:LYS:HE3	1:B:298:LEU:HA	1.83	0.60
1:B:347:ASN:OD1	1:B:351:LYS:HE3	2.01	0.60
1:B:65:TYR:CE1	1:B:67:LYS:HE2	2.35	0.60
1:B:168:ASP:OD2	1:B:762:LYS:HG3	2.02	0.60
1:B:870:ARG:HB3	1:B:871:LYS:HE2	1.81	0.60
3:E:8:LYS:HG2	3:F:58:ARG:C	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:142:PHE:CD2	3:E:144:PRO:HB3	2.37	0.60
1:A:417:VAL:HG23	1:A:418:GLN:H	1.66	0.60
1:B:418:GLN:HA	1:B:421:ILE:CG1	2.31	0.60
1:A:18:LYS:HG3	1:A:113:MET:SD	2.42	0.60
1:A:46:PHE:CE1	1:A:690:MET:SD	2.94	0.60
1:A:836:ILE:HG12	3:E:164:GLU:OE2	2.01	0.60
1:A:855:GLU:CB	1:B:856:PHE:HE1	2.13	0.60
1:B:48:LYS:HD3	1:B:79:GLN:OE1	2.01	0.60
1:B:292:ASN:HB3	1:B:329:LEU:CD2	2.31	0.60
1:B:724:ILE:O	1:B:727:PRO:HD3	2.01	0.60
2:D:100:ARG:HG2	2:D:106:THR:OG1	2.01	0.60
3:F:88:GLU:HA	3:F:91:LYS:HB3	1.82	0.60
1:A:810:SER:OG	3:E:102:ALA:HA	2.01	0.60
1:B:762:LYS:HE2	1:B:764:PHE:CZ	2.36	0.60
1:B:896:ASP:HA	1:B:899:ALA:HB3	1.81	0.60
2:C:93:LEU:HD21	2:C:101:GLN:HG3	1.84	0.60
1:A:859:LEU:CD1	1:B:859:LEU:C	2.73	0.60
1:B:735:PHE:CB	2:D:138:ARG:HE	2.14	0.60
3:E:80:THR:OG1	3:F:40:ARG:HD2	2.00	0.60
1:B:45:GLU:OE2	1:B:690:MET:HG3	2.02	0.60
1:B:84:PHE:HD2	1:B:93:LEU:HD13	1.66	0.60
1:B:255:THR:C	2:D:154:ARG:HH12	2.10	0.60
2:D:131:GLU:O	2:D:134:VAL:HG12	2.02	0.60
1:A:608:LEU:O	1:A:608:LEU:HD23	2.02	0.60
1:A:675:PRO:HA	1:A:684:MET:HE1	1.84	0.60
1:B:277:LEU:HD23	1:B:278:LYS:H	1.64	0.60
1:A:735:PHE:HD2	1:B:379:GLU:OE2	1.81	0.59
1:A:756:TYR:HE2	1:A:758:PHE:CE2	2.19	0.59
1:A:805:LEU:CD1	2:C:60:LEU:HD13	2.32	0.59
1:B:289:ILE:HG13	1:B:290:LEU:HD12	1.84	0.59
1:B:534:LEU:CA	1:B:538:CYS:SG	2.90	0.59
1:B:709:PHE:CZ	1:B:757:LYS:CG	2.85	0.59
1:B:781:LEU:HD13	1:B:785:ILE:CD1	2.30	0.59
1:A:772:LEU:O	1:A:776:MET:HG3	2.02	0.59
1:A:87:ILE:HG12	1:A:104:ASN:CG	2.27	0.59
1:A:306:ASN:HB3	1:A:309:ASP:CG	2.26	0.59
1:A:362:MET:HE3	1:A:421:ILE:HG22	1.83	0.59
1:B:155:PHE:CZ	1:B:193:GLN:NE2	2.65	0.59
1:B:201:ILE:HG23	1:B:257:LYS:HD3	1.83	0.59
1:B:585:ILE:HG13	1:B:585:ILE:O	2.01	0.59
1:B:827:TRP:HB2	3:F:58:ARG:CZ	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:C	1:A:426:ALA:HB3	2.27	0.59
1:A:451:GLN:HB2	1:A:452:PRO:HD2	1.84	0.59
1:A:775:GLU:O	1:A:779:GLU:HG3	2.02	0.59
1:A:784:ILE:CD1	2:C:140:PHE:CE2	2.82	0.59
1:B:431:VAL:HG22	1:B:435:MET:HE2	1.84	0.59
1:B:827:TRP:H	3:F:58:ARG:HG2	1.68	0.59
3:F:150:LEU:HG	3:F:152:TYR:CE1	2.37	0.59
1:A:714:LEU:CG	1:B:396:LEU:CD1	2.75	0.59
1:B:234:LYS:HG3	1:B:239:ASP:HA	1.84	0.59
1:B:835:LYS:O	1:B:835:LYS:HD2	2.02	0.59
1:A:78:GLN:HG2	1:A:95:PHE:CD1	2.37	0.59
1:A:293:LYS:HD2	1:A:303:ILE:HD11	1.85	0.59
1:B:565:LYS:HB2	1:B:566:PRO:HD2	1.85	0.59
1:B:918:LYS:O	1:B:922:MET:HG3	2.03	0.59
1:A:69:VAL:HG22	1:A:71:VAL:HG13	1.84	0.59
1:A:735:PHE:CA	1:A:736:ILE:HG22	2.15	0.59
1:A:778:ASP:HA	1:A:781:LEU:HB2	1.85	0.59
1:B:17:ARG:HG2	1:B:18:LYS:N	2.18	0.59
1:B:623:ASN:CA	1:B:637:LYS:HE2	2.21	0.59
1:B:632:GLU:O	1:B:633:LYS:HG2	2.03	0.59
1:A:362:MET:HG3	1:A:421:ILE:HG22	1.83	0.59
1:B:13:ALA:HB1	1:B:14:PRO:HD2	1.85	0.59
2:C:193:MET:HA	2:C:193:MET:HE2	1.84	0.59
3:F:145:ASP:HB3	3:F:150:LEU:CD1	2.32	0.59
1:A:290:LEU:HD23	1:A:303:ILE:CD1	2.33	0.59
1:B:449:THR:OG1	1:B:452:PRO:HG2	2.03	0.59
1:B:815:GLN:O	1:B:818:ILE:HG12	2.03	0.59
1:B:866:SER:HA	1:B:869:ARG:HH12	1.68	0.59
1:A:355:ALA:O	1:A:359:PHE:CD1	2.56	0.58
1:B:624:TYR:CE2	1:B:626:GLY:HA2	2.38	0.58
1:B:735:PHE:H	2:D:138:ARG:HH21	1.51	0.58
1:B:109:TYR:CD1	1:B:125:VAL:HG13	2.38	0.58
1:B:221:ILE:HG13	1:B:222:GLN:N	2.18	0.58
1:B:730:ILE:HG23	1:B:736:ILE:HD13	1.85	0.58
1:B:868:ALA:O	1:B:872:GLU:HG3	2.03	0.58
1:A:275:PHE:CD1	1:A:421:ILE:HD12	2.38	0.58
1:A:471:ASN:HB2	1:A:587:ASP:O	2.03	0.58
3:E:17:VAL:HG23	3:E:18:PHE:H	1.68	0.58
3:E:27:GLN:HE22	3:F:24:THR:CG2	2.13	0.58
3:F:145:ASP:H	3:F:150:LEU:HD13	1.67	0.58
1:B:347:ASN:O	1:B:351:LYS:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:CA	1:B:421:ILE:HG12	2.33	0.58
1:B:435:MET:HA	1:B:620:LEU:HD22	1.85	0.58
1:B:863:LEU:O	1:B:867:GLU:HG2	2.04	0.58
1:A:18:LYS:HE2	1:A:86:LYS:CD	2.33	0.58
1:A:190:ARG:O	1:A:193:GLN:HG2	2.02	0.58
1:B:115:TYR:HA	1:B:124:THR:HG22	1.85	0.58
1:B:160:ASN:HA	1:B:163:GLN:CG	2.34	0.58
1:B:160:ASN:HD21	1:B:711:ASN:CA	2.07	0.58
1:B:298:LEU:HG	1:B:303:ILE:HG23	1.85	0.58
1:B:539:MET:HE1	1:B:910:LYS:HD3	1.86	0.58
1:B:788:ILE:HG13	1:B:789:GLN:N	2.18	0.58
3:E:8:LYS:HG2	3:F:59:VAL:C	2.28	0.58
3:F:39:ASN:HB2	3:F:43:PHE:HB2	1.85	0.58
1:A:146:LYS:HZ1	1:A:775:GLU:HA	1.69	0.58
1:A:804:LEU:CD2	1:A:807:ARG:HE	2.17	0.58
1:A:834:PHE:CE2	3:E:163:GLU:CA	2.81	0.58
1:B:109:TYR:CB	1:B:125:VAL:HG11	2.28	0.58
1:B:944:GLU:HA	1:B:947:CYS:SG	2.43	0.58
1:B:352:LEU:CD1	1:B:617:LEU:HA	2.33	0.58
3:E:115:LYS:HD3	3:E:118:TYR:CE1	2.39	0.58
1:B:165:MET:SD	1:B:457:ILE:HD11	2.43	0.58
1:B:194:TYR:HD2	1:B:195:PHE:CD1	2.21	0.58
3:E:21:PHE:HB2	3:F:31:GLU:HG2	1.86	0.58
1:A:950:LEU:HD11	1:B:951:LYS:CE	2.33	0.57
1:B:802:LYS:HA	1:B:805:LEU:HD12	1.86	0.57
1:B:898:LEU:O	1:B:902:GLU:HG2	2.03	0.57
1:B:901:ALA:HA	1:B:904:ARG:HB2	1.86	0.57
1:B:955:ASP:O	1:B:958:GLU:HG2	2.03	0.57
3:E:80:THR:CG2	3:F:40:ARG:CD	2.58	0.57
1:A:389:GLY:O	1:A:390:LEU:HD12	2.03	0.57
1:B:84:PHE:HE1	1:B:87:ILE:HD11	1.62	0.57
1:B:549:LYS:HG2	1:B:553:PHE:CZ	2.39	0.57
3:E:164:GLU:CG	3:E:165:LYS:HA	2.29	0.57
1:A:48:LYS:HE3	1:A:79:GLN:HE21	1.68	0.57
1:B:294:LYS:HB3	1:B:295:PRO:HD2	1.86	0.57
1:A:860:LYS:N	1:B:859:LEU:CD1	2.58	0.57
1:B:522:ASP:HB3	1:B:527:PRO:HB2	1.86	0.57
3:F:142:PHE:C	3:F:144:PRO:HD3	2.30	0.57
1:A:735:PHE:CE2	1:B:379:GLU:CD	2.83	0.57
1:A:898:LEU:HD11	1:B:897:ASN:OD1	2.04	0.57
1:B:788:ILE:HG22	2:D:133:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:108:PRO:HG2	3:E:109:GLU:OE1	2.04	0.57
1:A:39:VAL:HG12	1:A:49:ALA:HB2	1.86	0.57
1:B:198:ILE:HA	1:B:204:ARG:HH21	1.69	0.57
1:B:421:ILE:HG13	1:B:422:TYR:N	2.19	0.57
2:D:114:PHE:CZ	2:D:118:LEU:HD11	2.39	0.57
1:A:18:LYS:HD2	1:A:113:MET:CE	2.33	0.57
1:A:810:SER:CB	3:E:105:VAL:HG13	2.35	0.57
1:A:831:LYS:O	3:E:164:GLU:HA	2.05	0.57
3:E:142:PHE:CE2	3:E:144:PRO:HB3	2.39	0.57
1:A:46:PHE:HE1	1:A:690:MET:SD	2.27	0.57
1:A:90:MET:HA	1:A:93:LEU:HD13	1.85	0.57
1:A:710:PRO:HD2	1:A:766:LYS:HA	1.87	0.57
1:B:275:PHE:CD1	1:B:314:SER:CB	2.87	0.57
1:B:635:LYS:CB	1:B:640:LYS:H	2.18	0.57
1:B:810:SER:OG	3:F:102:ALA:HB2	2.04	0.57
1:A:735:PHE:O	1:B:379:GLU:OE2	2.23	0.57
3:F:102:ALA:O	3:F:105:VAL:HG12	2.04	0.57
1:B:336:PHE:CZ	1:B:349:MET:HE1	2.39	0.57
1:B:633:LYS:N	1:B:641:GLY:CA	2.67	0.57
1:B:815:GLN:HA	1:B:818:ILE:CD1	2.34	0.57
1:B:826:ASN:CB	3:F:58:ARG:HG3	2.16	0.56
3:E:77:ILE:HA	3:E:81:VAL:CG1	2.34	0.56
3:E:116:ALA:HA	3:E:119:VAL:HG12	1.86	0.56
1:A:29:ARG:HB2	1:A:30:PRO:HD3	1.86	0.56
1:A:367:LYS:HD2	1:A:372:GLN:O	2.05	0.56
1:A:390:LEU:CD2	1:A:609:TYR:CE2	2.88	0.56
1:A:549:LYS:HG2	1:A:553:PHE:HE2	1.70	0.56
1:B:36:ASP:HB3	1:B:48:LYS:HE3	1.86	0.56
1:B:562:ASN:OD1	1:B:580:ILE:HG21	2.05	0.56
2:D:73:TYR:HB2	2:D:96:LEU:CD1	2.35	0.56
1:A:213:LYS:HE2	1:A:221:ILE:HD11	1.86	0.56
1:A:286:PHE:CE1	1:A:356:ILE:HG13	2.39	0.56
1:A:438:TRP:O	1:A:442:ARG:HG2	2.05	0.56
1:A:791:GLN:CD	2:C:133:PHE:CE2	2.80	0.56
1:B:496:LEU:HA	1:B:499:GLU:HB2	1.87	0.56
1:B:733:GLY:CA	2:D:135:GLU:N	2.67	0.56
1:B:810:SER:HG	3:F:102:ALA:HB2	1.70	0.56
1:B:827:TRP:CA	3:F:58:ARG:NH1	2.68	0.56
3:E:8:LYS:HD3	3:F:60:ASN:ND2	2.20	0.56
1:A:352:LEU:HD21	1:A:431:VAL:CG2	2.36	0.56
1:A:390:LEU:HD23	1:A:608:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:765:PHE:CD1	1:A:769:LEU:HD22	2.41	0.56
1:B:277:LEU:HD23	1:B:278:LYS:CB	2.34	0.56
1:B:726:ASN:CG	1:B:745:LEU:HD12	2.30	0.56
1:B:835:LYS:O	1:B:838:PRO:HD2	2.04	0.56
1:B:18:LYS:HG3	1:B:113:MET:HE3	1.88	0.56
1:B:259:ALA:O	1:B:260:SER:HB3	2.06	0.56
1:B:391:ASN:HB3	1:B:394:ASP:HB2	1.87	0.56
1:B:569:ILE:HG22	1:B:569:ILE:O	2.06	0.56
1:B:549:LYS:CE	1:B:553:PHE:CZ	2.89	0.56
1:B:713:ILE:O	1:B:762:LYS:HA	2.06	0.56
2:D:78:ASP:HA	2:D:81:ARG:HD2	1.87	0.56
3:E:8:LYS:CD	3:F:60:ASN:ND2	2.69	0.56
1:A:426:ALA:O	1:A:429:LYS:HB3	2.06	0.56
1:A:595:GLN:HG2	1:A:600:PRO:HB3	1.88	0.56
1:B:719:ARG:HB3	2:D:139:VAL:HG12	1.86	0.56
1:B:815:GLN:NE2	2:D:66:LYS:CA	2.69	0.56
3:E:33:PHE:O	3:E:36:MET:HG2	2.05	0.56
3:E:59:VAL:HA	3:E:60:ASN:CB	2.35	0.56
1:A:46:PHE:HE2	1:A:77:MET:SD	2.29	0.56
1:A:675:PRO:HA	1:A:684:MET:CE	2.36	0.56
1:A:711:ASN:HB2	1:A:765:PHE:HB2	1.86	0.56
1:A:784:ILE:HG21	2:C:140:PHE:CE2	2.40	0.56
1:A:160:ASN:O	1:A:164:TYR:CD1	2.58	0.56
1:B:351:LYS:HD3	1:B:614:LEU:CD2	2.34	0.56
1:B:84:PHE:CD2	1:B:104:ASN:ND2	2.74	0.56
1:B:569:ILE:CG2	1:B:574:GLU:H	2.19	0.56
1:B:787:ARG:O	1:B:791:GLN:HG3	2.06	0.56
1:B:789:GLN:O	1:B:793:ARG:HG2	2.06	0.56
2:D:115:LEU:HB2	2:D:116:PRO:HD3	1.87	0.56
3:F:94:ASP:HB3	3:F:98:THR:OG1	2.06	0.56
1:A:134:TYR:CE1	1:A:190:ARG:HD3	2.40	0.55
1:B:418:GLN:HA	1:B:421:ILE:CD1	2.35	0.55
1:B:451:GLN:N	1:B:452:PRO:HD3	2.21	0.55
1:B:813:VAL:HA	1:B:816:TRP:HD1	1.71	0.55
2:D:61:PHE:HE2	2:D:79:VAL:HB	1.70	0.55
2:D:155:HIS:NE2	2:D:159:THR:HG21	2.20	0.55
1:B:45:GLU:HG2	1:B:46:PHE:CD1	2.41	0.55
1:B:293:LYS:CG	1:B:297:LEU:HB2	2.36	0.55
1:B:304:THR:HG21	1:B:309:ASP:OD2	2.05	0.55
1:B:234:LYS:HB3	1:B:281:ARG:HB2	1.89	0.55
1:B:275:PHE:CE1	1:B:314:SER:CB	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:TYR:HB2	2:D:96:LEU:HD13	1.88	0.55
1:A:98:GLU:N	1:A:99:PRO:HD2	2.22	0.55
1:A:887:LEU:O	1:A:891:VAL:HG23	2.06	0.55
1:B:55:GLU:O	1:B:55:GLU:CD	2.49	0.55
1:B:815:GLN:CA	1:B:818:ILE:HG12	2.34	0.55
1:B:822:MET:HE1	3:F:137:GLN:CG	2.18	0.55
3:F:138:MET:HB3	3:F:142:PHE:CZ	2.40	0.55
1:B:434:ARG:HH12	1:B:621:PHE:HA	1.67	0.55
1:B:633:LYS:HA	1:B:642:SER:N	2.21	0.55
1:B:733:GLY:CA	2:D:134:VAL:CG1	2.74	0.55
1:A:320:VAL:HG12	1:A:323:ILE:HG22	1.89	0.55
1:A:367:LYS:HD2	1:A:372:GLN:C	2.32	0.55
1:A:434:ARG:NH1	1:A:623:ASN:HD22	1.96	0.55
1:A:827:TRP:O	3:E:166:ASP:OD2	2.24	0.55
1:B:33:LEU:HA	1:B:34:LYS:HB2	1.89	0.55
1:B:791:GLN:NE2	2:D:193:MET:SD	2.77	0.55
3:E:65:GLU:O	3:E:68:GLU:HG2	2.06	0.55
3:F:49:LEU:HD11	3:F:70:ILE:HD13	1.88	0.55
1:A:124:THR:O	1:A:672:CYS:HA	2.07	0.55
1:A:765:PHE:HD1	1:A:769:LEU:HD22	1.71	0.55
1:B:38:PHE:CD2	1:B:99:PRO:HG2	2.42	0.55
1:B:236:VAL:HG22	1:B:278:LYS:O	2.07	0.55
1:B:635:LYS:HZ2	1:B:647:VAL:CA	2.16	0.55
1:B:849:MET:HA	1:B:852:MET:CG	2.36	0.55
3:E:58:ARG:HG3	3:E:58:ARG:O	2.07	0.55
1:A:18:LYS:CD	1:A:86:LYS:HD3	2.37	0.55
1:A:292:ASN:ND2	1:A:326:ALA:HA	2.22	0.55
1:B:16:LEU:HD23	1:B:133:VAL:HG23	1.89	0.55
1:B:534:LEU:C	1:B:538:CYS:SG	2.90	0.55
1:B:732:GLU:HG2	2:D:132:ASP:O	2.07	0.55
1:B:826:ASN:CG	3:F:59:VAL:HB	2.29	0.55
1:B:827:TRP:N	3:F:58:ARG:HG2	2.21	0.55
1:A:746:LEU:CD2	1:A:751:ILE:HD11	2.33	0.55
1:A:808:ARG:CZ	2:C:63:ARG:CA	2.75	0.55
1:A:900:ASP:HB3	1:B:526:LYS:HD3	1.88	0.55
1:B:98:GLU:CD	1:B:699:LEU:HD22	2.32	0.55
1:B:217:GLU:HA	1:B:220:ILE:CD1	2.37	0.55
1:B:247:PHE:O	1:B:263:ILE:HA	2.07	0.55
1:B:418:GLN:O	1:B:421:ILE:HG12	2.07	0.55
1:B:633:LYS:CB	1:B:642:SER:N	2.70	0.55
2:D:154:ARG:HB2	2:D:169:VAL:HG11	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:78:ASN:H	3:E:81:VAL:CG1	2.16	0.55
1:B:355:ALA:O	1:B:359:PHE:CD2	2.60	0.55
1:B:752:ASP:HB2	1:B:769:LEU:HD11	1.87	0.55
2:C:147:THR:HG22	2:C:184:ASN:HD21	1.70	0.55
1:A:787:ARG:NH1	2:C:126:ASP:OD1	2.40	0.54
1:B:804:LEU:HD11	2:D:75:GLN:HE22	1.67	0.54
3:F:120:ARG:NH2	3:F:139:PHE:CE1	2.74	0.54
1:B:283:TYR:CE2	1:B:432:TYR:CE2	2.96	0.54
1:B:390:LEU:HD13	1:B:609:TYR:CD1	2.42	0.54
1:B:526:LYS:HB3	1:B:527:PRO:HD3	1.88	0.54
1:B:725:LEU:HG	1:B:781:LEU:HD21	1.89	0.54
1:B:869:ARG:CD	2:D:177:GLU:CD	2.66	0.54
2:D:100:ARG:HD2	2:D:103:GLU:OE1	2.07	0.54
1:A:73:GLU:O	1:A:76:VAL:HG12	2.07	0.54
1:A:218:ASP:O	1:A:222:GLN:HG2	2.07	0.54
1:B:36:ASP:C	1:B:48:LYS:HZ2	2.15	0.54
1:B:114:ILE:H	1:B:114:ILE:HD12	1.72	0.54
1:B:173:SER:O	1:B:668:HIS:HB2	2.08	0.54
1:B:233:ALA:HB1	1:B:281:ARG:O	2.08	0.54
3:E:118:TYR:O	3:E:122:MET:HG2	2.08	0.54
1:B:33:LEU:O	1:B:33:LEU:HD23	2.07	0.54
1:B:183:GLY:O	1:B:186:VAL:HG12	2.07	0.54
1:A:370:GLU:CB	1:A:372:GLN:H	2.21	0.54
1:B:61:ALA:O	1:B:69:VAL:HG12	2.07	0.54
1:A:549:LYS:CD	1:A:575:ALA:HB1	2.37	0.54
1:A:835:LYS:CE	3:E:165:LYS:HZ2	2.18	0.54
1:B:45:GLU:OE2	1:B:102:LEU:HD11	2.07	0.54
1:B:348:SER:HA	1:B:351:LYS:HD2	1.90	0.54
1:B:352:LEU:HD12	1:B:617:LEU:HG	1.90	0.54
1:B:603:GLU:CG	1:B:604:THR:H	2.10	0.54
2:C:141:ASP:HB2	2:C:185:TYR:HE2	1.72	0.54
3:F:72:GLU:C	3:F:85:MET:HE1	2.32	0.54
1:A:367:LYS:HE2	1:A:370:GLU:CB	2.24	0.54
1:A:835:LYS:HB2	3:E:164:GLU:HB3	1.90	0.54
1:B:190:ARG:C	1:B:193:GLN:HG2	2.33	0.54
1:B:404:VAL:HG12	1:B:411:VAL:C	2.32	0.54
1:B:483:GLU:HG2	1:B:521:ILE:HG12	1.89	0.54
1:B:787:ARG:NH1	2:D:127:THR:HA	2.23	0.54
1:A:39:VAL:HB	1:A:49:ALA:HB2	1.90	0.54
1:B:160:ASN:HA	1:B:163:GLN:HG2	1.89	0.54
2:C:46:PHE:HD1	2:C:119:GLN:NE2	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:118:LEU:N	2:C:118:LEU:HD12	2.23	0.54
1:A:38:PHE:CE2	1:A:99:PRO:HB2	2.43	0.54
1:A:709:PHE:HB3	1:A:764:PHE:HB3	1.89	0.54
1:A:805:LEU:HD13	2:C:60:LEU:HD13	1.89	0.54
1:B:115:TYR:CD2	1:B:124:THR:HG21	2.43	0.54
1:B:124:THR:OG1	1:B:672:CYS:SG	2.66	0.54
1:B:147:ARG:HG2	1:B:150:ALA:HB3	1.89	0.54
1:B:147:ARG:HH11	1:B:160:ASN:HD22	1.56	0.54
1:A:390:LEU:HD22	1:A:609:TYR:CE2	2.42	0.54
1:B:249:ARG:HA	1:B:457:ILE:O	2.08	0.54
2:C:154:ARG:HG3	2:C:169:VAL:HG11	1.90	0.54
2:D:46:PHE:CD2	2:D:54:PHE:CE2	2.96	0.54
3:F:142:PHE:O	3:F:144:PRO:HD3	2.08	0.54
3:F:152:TYR:CD2	3:F:153:LYS:HG3	2.43	0.54
1:A:133:VAL:HG22	1:A:153:HIS:CE1	2.43	0.53
1:A:316:GLY:O	1:A:364:PHE:HB3	2.08	0.53
2:C:134:VAL:O	2:C:138:ARG:HG2	2.08	0.53
2:D:134:VAL:O	2:D:138:ARG:HG3	2.09	0.53
1:A:213:LYS:HE2	1:A:221:ILE:CD1	2.38	0.53
1:A:810:SER:HB2	3:E:105:VAL:HG13	1.86	0.53
1:A:841:LYS:HG2	1:A:842:SER:H	1.73	0.53
1:B:141:ALA:O	1:B:145:LYS:HD3	2.08	0.53
1:B:417:VAL:HG13	1:B:418:GLN:N	2.22	0.53
1:B:788:ILE:HG22	2:D:133:PHE:CD2	2.43	0.53
1:B:870:ARG:HB3	1:B:871:LYS:HD3	1.89	0.53
2:D:151:ALA:O	2:D:154:ARG:HG2	2.08	0.53
3:E:21:PHE:CA	3:E:26:ILE:HG13	2.38	0.53
1:A:872:GLU:HG2	1:A:875:GLU:OE2	2.09	0.53
1:A:882:GLN:NE2	1:B:454:GLN:HB3	2.23	0.53
1:B:172:GLN:NE2	1:B:666:HIS:HB2	2.23	0.53
1:A:67:LYS:HG2	1:A:68:THR:N	2.19	0.53
2:C:46:PHE:HA	2:C:50:GLN:OE1	2.08	0.53
3:E:96:GLU:HA	3:E:159:ILE:CD1	2.38	0.53
1:B:176:ILE:HG12	1:B:670:VAL:HB	1.91	0.53
1:B:289:ILE:HD11	1:B:357:MET:CE	2.38	0.53
1:B:415:GLN:HB2	1:B:420:VAL:HG22	1.90	0.53
1:B:808:ARG:NH1	2:D:62:ASP:OD2	2.40	0.53
1:B:931:GLU:O	1:B:935:GLU:HG3	2.09	0.53
2:C:46:PHE:CD1	2:C:119:GLN:NE2	2.76	0.53
1:A:18:LYS:CE	1:A:86:LYS:HD3	2.38	0.53
1:A:798:ARG:NH1	2:C:82:ALA:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:MET:SD	1:B:99:PRO:CD	2.97	0.53
1:B:827:TRP:NE1	1:B:828:PRO:HD2	2.22	0.53
1:A:190:ARG:HA	1:A:193:GLN:HG2	1.91	0.53
1:A:451:GLN:CB	1:A:452:PRO:HD2	2.39	0.53
1:A:569:ILE:C	1:A:571:GLY:N	2.65	0.53
1:B:173:SER:HA	1:B:458:GLY:O	2.09	0.53
1:B:781:LEU:CD1	1:B:785:ILE:HD12	2.35	0.53
3:E:8:LYS:HD2	3:F:59:VAL:CA	2.31	0.53
3:F:145:ASP:HB3	3:F:150:LEU:CD2	2.38	0.53
1:A:631:ILE:HD11	1:A:639:LYS:CB	2.34	0.53
1:A:657:LYS:HG2	1:A:661:ASN:ND2	2.24	0.53
1:A:827:TRP:O	3:E:166:ASP:CG	2.51	0.53
1:A:950:LEU:HD11	1:B:951:LYS:HE3	1.91	0.53
1:B:147:ARG:NH1	1:B:160:ASN:HB2	2.24	0.53
1:B:826:ASN:CB	3:F:59:VAL:CG1	2.85	0.53
2:D:96:LEU:HG	2:D:98:LYS:O	2.09	0.53
1:A:44:GLN:O	1:A:45:GLU:HB3	2.09	0.53
1:A:780:ARG:HH21	2:C:135:GLU:CD	2.17	0.53
1:A:883:GLU:HA	1:A:886:ASP:HB2	1.90	0.53
1:B:45:GLU:CD	1:B:690:MET:HA	2.34	0.53
1:B:155:PHE:CE1	1:B:193:GLN:HG3	2.44	0.53
1:A:93:LEU:N	1:A:93:LEU:HD12	2.24	0.53
1:A:425:GLY:N	1:A:426:ALA:HB3	2.24	0.53
1:B:209:GLN:O	1:B:209:GLN:HG2	2.09	0.53
3:F:155:LEU:O	3:F:158:ILE:HG13	2.09	0.53
1:A:146:LYS:NZ	1:A:775:GLU:CA	2.72	0.52
1:A:713:ILE:O	1:A:762:LYS:HD2	2.09	0.52
1:B:55:GLU:OE1	1:B:58:LYS:HB3	2.09	0.52
1:B:439:MET:O	1:B:443:ILE:HG23	2.09	0.52
2:D:109:MET:CE	2:D:113:THR:HB	2.37	0.52
3:F:150:LEU:HG	3:F:152:TYR:HE1	1.73	0.52
1:A:549:LYS:HG3	1:A:590:ILE:HD12	1.91	0.52
1:B:251:HIS:ND1	1:B:456:PHE:HB3	2.24	0.52
1:B:533:ILE:HD12	1:B:533:ILE:N	2.25	0.52
1:B:633:LYS:N	1:B:641:GLY:N	2.57	0.52
1:B:686:ASN:HB2	1:B:687:PRO:HD3	1.90	0.52
1:B:726:ASN:HD21	1:B:730:ILE:CD1	2.21	0.52
2:C:172:LEU:HD23	2:C:172:LEU:C	2.35	0.52
2:D:76:CYS:HA	2:D:79:VAL:HG12	1.91	0.52
1:A:45:GLU:C	1:A:46:PHE:HD1	2.18	0.52
1:A:298:LEU:HG	1:A:303:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:LYS:O	1:A:349:MET:HG2	2.08	0.52
1:B:135:THR:OG1	1:B:136:PRO:HD2	2.08	0.52
1:B:380:GLU:H	1:B:380:GLU:CD	2.18	0.52
1:B:828:PRO:HG2	1:B:829:TRP:H	1.74	0.52
2:C:101:GLN:CB	2:C:102:GLU:HB2	2.38	0.52
1:A:235:THR:O	1:A:239:ASP:HA	2.08	0.52
1:A:298:LEU:HG	1:A:303:ILE:CD1	2.39	0.52
1:B:286:PHE:O	1:B:290:LEU:HD13	2.09	0.52
1:B:566:PRO:HB3	1:B:576:HIS:O	2.10	0.52
1:A:48:LYS:HE2	1:A:79:GLN:HE21	1.73	0.52
1:B:714:LEU:HD23	1:B:716:GLY:N	2.25	0.52
1:A:872:GLU:HA	1:A:875:GLU:CD	2.34	0.52
1:B:84:PHE:HE2	1:B:104:ASN:ND2	2.07	0.52
1:B:290:LEU:HG	1:B:303:ILE:CD1	2.30	0.52
1:B:633:LYS:CA	1:B:641:GLY:CA	2.87	0.52
1:B:732:GLU:CG	2:D:132:ASP:O	2.58	0.52
1:A:756:TYR:HB3	1:A:769:LEU:CD1	2.39	0.52
1:A:853:LYS:HZ3	1:B:841:LYS:HZ3	1.38	0.52
1:B:366:LEU:C	1:B:366:LEU:HD23	2.35	0.52
1:B:517:LEU:O	1:B:520:CYS:HB3	2.09	0.52
1:B:913:ILE:HG13	1:B:914:GLN:N	2.23	0.52
1:A:39:VAL:HG13	1:A:47:VAL:HG13	1.92	0.52
1:A:391:ASN:HB2	1:A:394:ASP:OD2	2.10	0.52
1:B:218:ASP:O	1:B:222:GLN:HG2	2.09	0.52
1:B:504:GLU:O	1:B:760:HIS:CD2	2.63	0.52
1:B:635:LYS:HB3	1:B:640:LYS:H	1.74	0.52
1:B:783:ARG:NH1	2:D:126:ASP:CG	2.57	0.52
2:C:153:LEU:HD22	2:C:183:ILE:CD1	2.40	0.52
2:D:98:LYS:HG2	2:D:106:THR:CG2	2.40	0.52
3:E:44:ILE:HG23	3:E:48:ASP:HB2	1.92	0.52
3:E:107:ASP:HB2	3:E:108:PRO:HD2	1.92	0.52
3:E:149:ASN:ND2	3:E:151:ASP:HA	2.25	0.52
1:A:356:ILE:HG22	1:A:431:VAL:HG11	1.92	0.52
1:A:922:MET:SD	1:B:919:VAL:HG13	2.50	0.52
1:B:124:THR:O	1:B:672:CYS:HA	2.10	0.52
1:B:164:TYR:CE1	1:B:762:LYS:HE3	2.45	0.52
1:B:251:HIS:HA	1:B:455:TYR:O	2.08	0.52
1:B:735:PHE:HA	2:D:138:ARG:HE	1.74	0.52
1:B:815:GLN:NE2	2:D:66:LYS:HB3	2.25	0.52
3:E:8:LYS:HG2	3:F:59:VAL:N	2.25	0.52
3:F:113:VAL:CG2	3:F:150:LEU:HD12	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:HD11	1:A:153:HIS:HB2	1.92	0.51
1:B:18:LYS:HZ3	1:B:88:GLU:HA	1.75	0.51
1:B:47:VAL:HG22	1:B:48:LYS:N	2.21	0.51
1:B:65:TYR:HE1	1:B:67:LYS:HE2	1.75	0.51
1:B:84:PHE:CE1	1:B:90:MET:O	2.63	0.51
1:B:115:TYR:CD2	1:B:124:THR:CG2	2.93	0.51
1:B:336:PHE:CE1	1:B:349:MET:CE	2.92	0.51
1:B:364:PHE:HB2	1:B:421:ILE:HG22	1.91	0.51
1:B:679:LYS:HG3	1:B:679:LYS:O	2.09	0.51
1:B:713:ILE:HD12	1:B:718:PHE:CZ	2.45	0.51
1:A:222:GLN:CG	1:A:338:VAL:HG21	2.39	0.51
1:A:234:LYS:HA	1:A:239:ASP:O	2.11	0.51
1:B:804:LEU:HD21	2:D:63:ARG:NE	2.24	0.51
1:B:866:SER:HA	1:B:869:ARG:NH1	2.25	0.51
1:B:924:GLU:C	1:B:927:GLU:HG2	2.35	0.51
2:D:66:LYS:HG2	3:F:126:GLN:CG	2.39	0.51
1:A:201:ILE:HG13	1:A:201:ILE:O	2.10	0.51
1:A:720:GLN:HG3	1:A:723:ARG:HH12	1.75	0.51
1:A:944:GLU:HA	1:A:947:CYS:SG	2.50	0.51
1:B:873:LEU:CD2	1:B:876:LYS:HD3	2.33	0.51
3:E:152:TYR:O	3:E:156:VAL:HG23	2.11	0.51
3:F:22:GLU:HG3	3:F:26:ILE:CD1	2.41	0.51
1:B:37:VAL:HG11	1:B:76:VAL:CG2	2.40	0.51
1:B:245:GLY:O	1:B:265:THR:HA	2.11	0.51
1:B:286:PHE:HB3	1:B:357:MET:SD	2.51	0.51
1:B:563:PHE:CD2	1:B:579:LEU:HD13	2.46	0.51
1:B:939:LYS:HZ2	1:B:943:LEU:HD21	1.73	0.51
1:A:146:LYS:NZ	1:A:775:GLU:HA	2.25	0.51
1:A:908:LEU:HD13	1:B:908:LEU:CB	2.21	0.51
1:B:472:SER:HB2	1:B:474:GLU:OE1	2.11	0.51
1:B:755:GLN:CD	1:B:766:LYS:HG3	2.36	0.51
3:E:31:GLU:OE2	3:F:30:LYS:NZ	2.44	0.51
1:A:109:TYR:HD1	1:A:125:VAL:HG13	1.69	0.51
1:A:735:PHE:HA	1:A:736:ILE:CB	2.40	0.51
1:A:859:LEU:HD11	1:B:860:LYS:HA	1.88	0.51
1:B:47:VAL:CG2	1:B:48:LYS:H	2.18	0.51
1:B:803:LYS:NZ	3:F:108:PRO:HA	2.25	0.51
2:D:109:MET:HE3	2:D:113:THR:CB	2.39	0.51
1:A:637:LYS:CG	1:A:638:ALA:H	2.23	0.51
1:A:805:LEU:HD13	2:C:60:LEU:HB3	1.93	0.51
1:B:164:TYR:CE1	1:B:762:LYS:CE	2.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LEU:CD1	1:B:609:TYR:HA	2.39	0.51
1:B:713:ILE:HD12	1:B:718:PHE:HZ	1.74	0.51
1:A:31:PHE:CE2	1:A:34:LYS:HB3	2.44	0.51
1:A:804:LEU:HD22	1:A:807:ARG:NH2	2.23	0.51
1:A:874:GLU:O	1:A:878:VAL:HG23	2.11	0.51
1:B:65:TYR:CD1	1:B:67:LYS:HB3	2.45	0.51
1:B:173:SER:OG	1:B:667:PRO:HA	2.10	0.51
1:A:215:THR:HG22	1:A:219:GLN:OE1	2.11	0.51
3:E:21:PHE:CB	3:F:31:GLU:HG2	2.41	0.51
1:B:147:ARG:HH21	1:B:156:SER:HB2	1.75	0.50
1:B:933:ASN:O	1:B:937:THR:HG23	2.11	0.50
1:A:455:TYR:CE1	1:B:403:ARG:CZ	2.79	0.50
1:A:515:MET:HE1	1:A:697:GLY:CA	2.41	0.50
1:A:788:ILE:HD13	2:C:133:PHE:CE2	1.89	0.50
1:B:36:ASP:HB3	1:B:48:LYS:HZ1	1.68	0.50
1:B:260:SER:HB3	1:B:449:THR:HA	1.91	0.50
1:B:281:ARG:HD2	1:B:318:THR:O	2.10	0.50
1:B:746:LEU:HB3	1:B:751:ILE:HD13	1.92	0.50
2:D:63:ARG:CZ	2:D:75:GLN:HE22	2.25	0.50
3:E:106:PHE:CE1	3:E:114:LEU:HD11	2.46	0.50
1:A:898:LEU:HD11	1:B:897:ASN:CG	2.36	0.50
1:B:84:PHE:CD2	1:B:84:PHE:O	2.64	0.50
1:B:159:ASP:HA	1:B:194:TYR:CZ	2.46	0.50
1:A:472:SER:HB2	1:A:596:LYS:NZ	2.27	0.50
1:A:872:GLU:HA	1:A:875:GLU:OE1	2.11	0.50
1:A:950:LEU:HD11	1:B:951:LYS:HE2	1.94	0.50
1:B:44:GLN:O	1:B:45:GLU:CB	2.59	0.50
1:B:65:TYR:OH	1:B:67:LYS:HE2	2.12	0.50
1:B:274:ILE:HA	1:B:312:PHE:CE1	2.46	0.50
1:B:726:ASN:HD21	1:B:730:ILE:CG1	2.24	0.50
1:A:357:MET:HE1	1:A:361:ASN:HD22	1.76	0.50
1:B:242:SER:HB2	1:B:463:ALA:CB	2.41	0.50
1:B:685:ASP:OD2	1:B:687:PRO:HD2	2.11	0.50
1:B:821:PHE:CD2	3:F:138:MET:HG3	2.44	0.50
1:A:43:LYS:O	1:A:687:PRO:HD3	2.11	0.50
1:A:378:THR:HA	1:A:380:GLU:HG3	1.93	0.50
1:A:684:MET:CE	1:A:689:VAL:HG22	2.34	0.50
1:A:908:LEU:CD1	1:B:908:LEU:C	2.76	0.50
1:B:154:ILE:HD11	1:B:191:VAL:HG22	1.93	0.50
1:A:609:TYR:HD2	1:A:617:LEU:HD11	1.77	0.50
1:B:142:TYR:HA	1:B:145:LYS:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:94:ARG:NH2	2:C:124:ASN:ND2	2.58	0.50
1:A:77:MET:SD	1:A:99:PRO:CD	2.99	0.50
1:A:303:ILE:HG13	1:A:303:ILE:O	2.12	0.50
1:A:367:LYS:HG2	1:A:368:GLN:N	2.25	0.50
1:A:580:ILE:HG22	1:A:585:ILE:HG22	1.92	0.50
1:B:418:GLN:C	1:B:421:ILE:HG12	2.36	0.50
1:B:633:LYS:HG3	1:B:634:GLY:H	1.77	0.50
1:B:827:TRP:HB2	3:F:58:ARG:NH1	2.27	0.50
1:B:827:TRP:CE2	1:B:828:PRO:HD2	2.47	0.50
3:E:135:VAL:O	3:E:138:MET:HG2	2.12	0.50
1:A:31:PHE:CZ	1:A:34:LYS:HB2	2.47	0.50
1:A:316:GLY:CA	1:A:317:GLU:HB2	2.42	0.50
1:A:870:ARG:HB2	1:B:870:ARG:HB2	1.93	0.50
1:B:29:ARG:HB2	1:B:30:PRO:HD3	1.93	0.50
1:B:289:ILE:HD11	1:B:357:MET:HE1	1.93	0.50
1:B:771:GLY:O	1:B:774:GLU:HB3	2.12	0.50
1:B:777:ARG:O	1:B:781:LEU:HB2	2.12	0.50
2:D:46:PHE:N	2:D:46:PHE:CD1	2.80	0.50
1:A:99:PRO:HA	1:A:102:LEU:HB3	1.94	0.49
1:A:784:ILE:HA	1:A:785:ILE:HB	1.94	0.49
1:B:735:PHE:CA	2:D:138:ARG:HE	2.24	0.49
1:B:804:LEU:CD1	2:D:63:ARG:HD3	2.41	0.49
1:B:783:ARG:O	1:B:787:ARG:HG3	2.11	0.49
1:B:896:ASP:HA	1:B:899:ALA:CB	2.42	0.49
2:C:79:VAL:O	2:C:83:LEU:HG	2.12	0.49
3:F:73:ALA:HB1	3:F:77:ILE:HD11	1.94	0.49
1:A:472:SER:CB	1:A:596:LYS:NZ	2.75	0.49
1:A:755:GLN:CG	1:A:769:LEU:HD12	2.38	0.49
1:B:829:TRP:CE2	3:F:89:LYS:HD3	2.47	0.49
2:D:57:ALA:O	2:D:61:PHE:CD1	2.65	0.49
3:E:151:ASP:O	3:E:155:LEU:HD13	2.11	0.49
1:A:715:TYR:CE1	1:A:758:PHE:HD1	2.30	0.49
1:A:859:LEU:CD1	1:B:860:LYS:CA	2.80	0.49
1:B:84:PHE:CE1	1:B:87:ILE:CD1	2.89	0.49
1:B:815:GLN:HE22	2:D:66:LYS:HB3	1.76	0.49
1:A:106:LYS:HD2	1:A:686:ASN:HD21	1.78	0.49
1:A:849:MET:SD	1:B:852:MET:HE3	2.53	0.49
1:B:143:ARG:HA	1:B:198:ILE:HG23	1.94	0.49
1:B:801:TYR:OH	1:B:804:LEU:HD12	2.12	0.49
3:E:78:ASN:N	3:E:81:VAL:HG12	2.23	0.49
1:A:293:LYS:HD3	1:A:298:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLU:HB3	1:A:371:GLU:CB	2.41	0.49
1:A:601:LEU:HD22	1:A:606:VAL:CG2	2.41	0.49
1:B:803:LYS:HZ3	3:F:108:PRO:HA	1.77	0.49
2:D:66:LYS:CG	3:F:126:GLN:CG	2.89	0.49
3:E:42:GLY:O	3:E:78:ASN:HA	2.12	0.49
1:A:714:LEU:CD2	1:B:396:LEU:HD13	2.29	0.49
1:B:146:LYS:HB3	1:B:774:GLU:HB3	1.95	0.49
1:B:304:THR:HG23	1:B:310:TYR:CE1	2.47	0.49
1:B:732:GLU:CD	2:D:135:GLU:OE1	2.56	0.49
1:A:173:SER:O	1:A:667:PRO:HA	2.12	0.49
1:A:434:ARG:NH1	1:A:623:ASN:ND2	2.55	0.49
1:B:38:PHE:HD2	1:B:99:PRO:CB	2.25	0.49
1:B:45:GLU:C	1:B:46:PHE:HD1	2.21	0.49
1:B:498:GLN:HA	1:B:501:TYR:CD2	2.48	0.49
1:B:783:ARG:NH1	2:D:126:ASP:OD2	2.45	0.49
1:A:352:LEU:O	1:A:355:ALA:HB3	2.13	0.49
1:A:714:LEU:HD12	1:B:396:LEU:O	2.11	0.49
1:B:164:TYR:CZ	1:B:762:LYS:NZ	2.76	0.49
1:B:292:ASN:CB	1:B:329:LEU:HD23	2.42	0.49
3:E:124:THR:O	3:E:129:ARG:HD2	2.13	0.49
1:A:78:GLN:HG2	1:A:95:PHE:CZ	2.46	0.49
1:A:112:TRP:O	1:A:114:ILE:HG23	2.12	0.49
1:A:292:ASN:HD22	1:A:326:ALA:CB	2.25	0.49
1:A:568:ASN:OD1	1:A:569:ILE:HG23	2.13	0.49
1:A:781:LEU:HD13	2:C:139:VAL:HB	1.94	0.49
1:B:65:TYR:CZ	1:B:67:LYS:HE2	2.48	0.49
1:B:290:LEU:HD11	1:B:357:MET:HE1	1.95	0.49
1:B:730:ILE:CG2	1:B:736:ILE:HD13	2.42	0.49
1:B:735:PHE:HB3	2:D:138:ARG:CD	2.41	0.49
2:C:44:ILE:HD11	2:C:123:LYS:CG	2.40	0.49
2:C:46:PHE:CD2	2:C:51:ILE:HG22	2.48	0.49
1:A:38:PHE:HB2	1:A:77:MET:HB2	1.94	0.48
1:A:275:PHE:CG	1:A:276:GLN:N	2.78	0.48
1:A:735:PHE:HB3	1:A:741:GLY:HA3	1.95	0.48
1:B:769:LEU:C	1:B:769:LEU:HD23	2.38	0.48
3:E:80:THR:CB	3:F:40:ARG:CD	2.86	0.48
1:A:549:LYS:HD3	1:A:575:ALA:CB	2.41	0.48
1:B:533:ILE:HD12	1:B:533:ILE:H	1.79	0.48
1:B:549:LYS:CE	1:B:553:PHE:HZ	2.26	0.48
1:B:569:ILE:HG22	1:B:574:GLU:H	1.78	0.48
1:B:580:ILE:HG23	1:B:580:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:ARG:O	2:D:63:ARG:HG3	2.13	0.48
3:F:120:ARG:NH2	3:F:139:PHE:HE1	2.09	0.48
3:F:145:ASP:HB3	3:F:150:LEU:HD13	1.95	0.48
1:A:298:LEU:HD21	1:A:303:ILE:O	2.12	0.48
1:B:18:LYS:HE3	1:B:87:ILE:O	2.14	0.48
1:B:175:LEU:O	1:B:669:PHE:HA	2.13	0.48
1:B:507:GLU:HB2	1:B:758:PHE:CZ	2.49	0.48
1:B:841:LYS:HG3	1:B:842:SER:N	2.28	0.48
1:B:846:GLU:O	1:B:849:MET:HB3	2.12	0.48
1:B:868:ALA:C	1:B:871:LYS:HB2	2.38	0.48
1:A:44:GLN:HE22	1:A:106:LYS:NZ	2.11	0.48
1:A:553:PHE:HE1	1:A:566:PRO:HD3	1.75	0.48
1:A:673:ILE:HG23	1:A:692:GLN:OE1	2.14	0.48
1:A:872:GLU:C	1:A:875:GLU:HG2	2.38	0.48
1:B:201:ILE:O	1:B:201:ILE:HG13	2.13	0.48
1:B:534:LEU:C	1:B:538:CYS:HG	2.18	0.48
1:B:563:PHE:HA	1:B:579:LEU:HD12	1.95	0.48
1:B:755:GLN:CB	1:B:769:LEU:HD13	2.34	0.48
1:A:204:ARG:HD2	1:A:206:LYS:O	2.14	0.48
1:A:274:ILE:O	1:A:282:ASP:OD1	2.31	0.48
1:A:293:LYS:HZ3	1:A:303:ILE:HG12	1.79	0.48
1:A:425:GLY:C	1:A:429:LYS:HB2	2.39	0.48
1:A:688:LEU:HG	1:A:692:GLN:HE21	1.79	0.48
1:A:795:VAL:HG21	2:C:195:SER:C	2.39	0.48
1:B:217:GLU:HA	1:B:220:ILE:HD11	1.94	0.48
1:B:834:PHE:CE1	3:F:164:GLU:CD	2.54	0.48
1:A:216:LEU:O	1:A:220:ILE:HG23	2.14	0.48
1:A:417:VAL:HG23	1:A:418:GLN:N	2.28	0.48
1:A:724:ILE:HG23	2:C:135:GLU:HA	1.95	0.48
1:A:730:ILE:O	1:A:730:ILE:HG13	2.13	0.48
1:B:155:PHE:CE1	1:B:193:GLN:NE2	2.71	0.48
1:B:209:GLN:C	1:B:211:PRO:HD2	2.39	0.48
1:B:268:LEU:HD21	1:B:432:TYR:CD2	2.48	0.48
1:B:599:ASP:HB3	1:B:645:GLN:HB2	1.94	0.48
1:B:784:ILE:O	1:B:788:ILE:HG23	2.12	0.48
1:B:826:ASN:O	3:F:59:VAL:HG11	2.14	0.48
2:D:134:VAL:HG22	2:D:138:ARG:NH1	2.27	0.48
3:F:94:ASP:N	3:F:95:PRO:HD3	2.29	0.48
1:A:139:VAL:HG13	1:A:194:TYR:HE1	1.77	0.48
1:A:366:LEU:HD11	1:A:417:VAL:HB	1.96	0.48
1:A:736:ILE:HG13	1:A:737:ASP:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:MET:HE1	1:B:923:ASN:OD1	2.08	0.48
1:B:869:ARG:HG3	1:B:871:LYS:HE2	1.95	0.48
2:D:46:PHE:CZ	2:D:119:GLN:HA	2.49	0.48
2:D:101:GLN:NE2	2:D:103:GLU:HG3	2.28	0.48
2:D:134:VAL:HG13	2:D:138:ARG:NH1	2.24	0.48
3:E:106:PHE:CZ	3:E:114:LEU:CD1	2.96	0.48
2:D:61:PHE:CE2	2:D:79:VAL:CB	2.96	0.48
2:D:64:THR:HB	2:D:67:CYS:CA	2.44	0.48
3:F:49:LEU:HD23	3:F:53:PHE:CE1	2.49	0.48
1:A:720:GLN:O	1:A:723:ARG:HG2	2.14	0.48
1:B:194:TYR:O	1:B:198:ILE:HG12	2.14	0.48
1:A:416:ASN:O	1:A:420:VAL:HG13	2.13	0.48
1:A:805:LEU:CD1	2:C:60:LEU:CD2	2.71	0.48
1:A:922:MET:HE2	1:B:923:ASN:HD21	1.79	0.48
1:B:45:GLU:OE2	1:B:102:LEU:HD21	2.13	0.48
1:B:190:ARG:O	1:B:193:GLN:HG2	2.13	0.48
1:B:750:ASP:O	1:B:751:ILE:HG12	2.13	0.48
2:D:131:GLU:O	2:D:135:GLU:HG3	2.14	0.48
3:E:20:MET:HG3	3:E:90:LEU:CD1	2.44	0.48
1:A:17:ARG:CD	1:A:151:PRO:HG3	2.34	0.47
1:B:432:TYR:CA	1:B:435:MET:HE3	2.44	0.47
1:B:836:ILE:HD12	1:B:839:LEU:HD12	1.96	0.47
2:D:46:PHE:N	2:D:46:PHE:HD1	2.13	0.47
3:E:8:LYS:HD3	3:F:59:VAL:CG2	2.43	0.47
1:A:123:VAL:HG12	1:A:671:ARG:HB3	1.95	0.47
1:B:130:TRP:O	1:B:130:TRP:CD1	2.67	0.47
1:B:368:GLN:HG3	1:B:368:GLN:O	2.14	0.47
1:B:404:VAL:HG12	1:B:411:VAL:O	2.13	0.47
2:C:114:PHE:CD1	2:C:118:LEU:HD11	2.48	0.47
2:D:65:PRO:HD2	3:F:126:GLN:NE2	2.27	0.47
2:D:73:TYR:CZ	2:D:106:THR:HB	2.49	0.47
1:A:67:LYS:CG	1:A:68:THR:H	2.22	0.47
1:A:169:ARG:CB	1:B:403:ARG:NH2	2.57	0.47
1:A:359:PHE:CD1	1:A:384:SER:HB2	2.50	0.47
1:A:834:PHE:O	1:A:838:PRO:HD2	2.14	0.47
1:B:616:LEU:H	1:B:616:LEU:HD12	1.79	0.47
2:D:76:CYS:C	2:D:79:VAL:HG12	2.39	0.47
3:E:81:VAL:HG13	3:E:82:PHE:N	2.28	0.47
3:E:95:PRO:HG2	3:E:98:THR:CG2	2.44	0.47
1:A:553:PHE:HZ	1:A:576:HIS:O	1.97	0.47
1:A:714:LEU:HD23	1:A:715:TYR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:LEU:HD23	1:A:769:LEU:C	2.40	0.47
1:A:891:VAL:O	1:A:895:GLN:HG3	2.13	0.47
1:B:38:PHE:CD2	1:B:99:PRO:CG	2.97	0.47
1:B:139:VAL:HG11	1:B:197:VAL:HG11	1.95	0.47
1:B:207:LYS:HG3	1:B:207:LYS:O	2.14	0.47
1:B:826:ASN:OD1	3:E:8:LYS:HD2	2.14	0.47
2:D:107:LYS:HG2	2:D:108:MET:N	2.30	0.47
3:E:142:PHE:CE2	3:E:144:PRO:HG3	2.49	0.47
1:A:58:LYS:HE3	1:A:70:THR:HB	1.94	0.47
1:A:549:LYS:HG2	1:A:553:PHE:CE2	2.49	0.47
1:A:719:ARG:HH12	1:B:386:TYR:HB2	1.78	0.47
1:B:46:PHE:CB	1:B:99:PRO:HB3	2.43	0.47
1:B:162:TYR:CE1	1:B:166:LEU:HD11	2.48	0.47
1:B:810:SER:O	1:B:814:ILE:HG13	2.14	0.47
3:E:21:PHE:HA	3:E:26:ILE:HG13	1.95	0.47
1:A:609:TYR:CD2	1:A:617:LEU:HD11	2.50	0.47
1:A:617:LEU:C	1:A:617:LEU:HD23	2.39	0.47
1:A:735:PHE:HB3	1:A:741:GLY:N	2.30	0.47
1:B:39:VAL:HG23	1:B:47:VAL:HG13	1.95	0.47
1:B:624:TYR:HE2	1:B:626:GLY:HA2	1.79	0.47
2:D:61:PHE:CZ	2:D:79:VAL:HA	2.49	0.47
1:A:45:GLU:CB	1:A:686:ASN:HB3	2.45	0.47
1:A:546:MET:SD	1:A:575:ALA:HB2	2.55	0.47
1:A:793:ARG:NE	2:C:162:GLU:OE1	2.45	0.47
1:B:125:VAL:HG13	1:B:125:VAL:O	2.15	0.47
1:B:142:TYR:HA	1:B:145:LYS:CG	2.45	0.47
1:B:143:ARG:HH22	2:D:166:GLU:CG	2.28	0.47
1:B:209:GLN:O	1:B:211:PRO:HD2	2.14	0.47
1:B:427:LEU:CA	1:B:601:LEU:HD11	2.39	0.47
1:B:575:ALA:HB3	1:B:590:ILE:HB	1.97	0.47
1:B:631:ILE:HG13	1:B:631:ILE:O	2.15	0.47
1:B:783:ARG:CZ	2:D:126:ASP:OD2	2.62	0.47
2:C:54:PHE:CE1	2:C:83:LEU:HD13	2.49	0.47
2:C:95:VAL:HG22	2:C:117:MET:SD	2.55	0.47
2:C:137:LEU:HD22	2:C:185:TYR:HB2	1.97	0.47
3:E:24:THR:CB	3:E:161:HIS:NE2	2.75	0.47
1:A:26:ALA:HA	1:A:29:ARG:HH11	1.80	0.47
3:F:59:VAL:CG2	3:F:60:ASN:HD22	2.27	0.47
1:A:39:VAL:HG21	1:A:69:VAL:HG11	1.95	0.47
1:A:90:MET:O	1:A:93:LEU:HD13	2.15	0.47
1:B:18:LYS:HG2	1:B:113:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PHE:CE1	1:B:79:GLN:CD	2.93	0.47
1:B:352:LEU:CD1	1:B:620:LEU:HD12	2.38	0.47
1:A:352:LEU:HD22	1:A:435:MET:CE	2.41	0.47
1:A:713:ILE:HB	1:A:765:PHE:HE2	1.79	0.47
1:B:190:ARG:HG2	1:B:193:GLN:OE1	2.15	0.47
1:B:713:ILE:CG2	1:B:714:LEU:H	2.11	0.47
2:D:68:GLU:O	2:D:69:MET:HB3	2.14	0.47
2:D:114:PHE:O	2:D:117:MET:HB2	2.15	0.47
1:A:352:LEU:HD23	1:A:352:LEU:C	2.40	0.46
1:A:908:LEU:C	1:B:908:LEU:HD11	2.40	0.46
1:B:487:GLN:OE1	1:B:487:GLN:HA	2.15	0.46
1:B:827:TRP:H	3:F:58:ARG:HH11	1.53	0.46
1:B:898:LEU:O	1:B:898:LEU:HD23	2.14	0.46
3:E:26:ILE:HG23	3:E:86:PHE:HE2	1.79	0.46
1:A:38:PHE:HE1	1:A:79:GLN:HA	1.77	0.46
1:B:84:PHE:HE2	1:B:104:ASN:HD22	1.62	0.46
1:B:162:TYR:CZ	1:B:199:ALA:CB	2.94	0.46
1:B:413:LYS:HG3	1:B:414:GLY:O	2.16	0.46
1:B:520:CYS:SG	1:B:579:LEU:CD1	2.98	0.46
1:B:888:GLN:CA	1:B:891:VAL:HG12	2.44	0.46
2:D:111:PHE:CZ	2:D:115:LEU:HD21	2.51	0.46
3:E:77:ILE:HA	3:E:81:VAL:HG11	1.96	0.46
1:A:416:ASN:H	1:A:419:GLN:HB2	1.80	0.46
1:B:829:TRP:CB	3:F:89:LYS:HE2	2.45	0.46
1:B:883:GLU:O	1:B:887:LEU:HG	2.15	0.46
1:B:888:GLN:HA	1:B:891:VAL:CG1	2.46	0.46
1:A:591:ILE:HG13	1:A:591:ILE:O	2.16	0.46
1:A:637:LYS:HG3	1:A:638:ALA:N	2.26	0.46
1:A:714:LEU:HD23	1:A:716:GLY:N	2.31	0.46
1:A:715:TYR:CE1	1:A:758:PHE:CD1	3.02	0.46
1:A:822:MET:SD	3:E:138:MET:CE	3.00	0.46
1:A:827:TRP:O	3:E:166:ASP:OD1	2.33	0.46
1:A:908:LEU:HD11	1:B:908:LEU:HD23	0.60	0.46
1:B:139:VAL:HG12	1:B:198:ILE:HD11	1.96	0.46
1:A:292:ASN:HD22	1:A:326:ALA:HA	1.81	0.46
1:A:312:PHE:O	1:A:313:ILE:HG23	2.16	0.46
1:B:115:TYR:HD2	1:B:124:THR:HG21	1.78	0.46
1:B:440:VAL:O	1:B:443:ILE:HG12	2.15	0.46
1:B:633:LYS:C	1:B:640:LYS:O	2.59	0.46
1:B:638:ALA:HA	1:B:639:LYS:HA	1.76	0.46
2:C:131:GLU:O	2:C:134:VAL:HG12	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:119:VAL:O	3:E:123:LEU:HD13	2.15	0.46
1:A:38:PHE:HD2	1:A:99:PRO:HB2	1.73	0.46
1:A:908:LEU:HB3	1:B:908:LEU:HD13	1.83	0.46
2:C:147:THR:HG22	2:C:184:ASN:ND2	2.30	0.46
2:D:73:TYR:CE1	2:D:106:THR:CB	2.95	0.46
3:F:22:GLU:CG	3:F:26:ILE:HG12	2.46	0.46
1:A:367:LYS:CG	1:A:368:GLN:N	2.78	0.46
1:A:383:LYS:O	1:A:387:LEU:HD13	2.15	0.46
1:A:841:LYS:HG2	1:A:842:SER:N	2.30	0.46
1:B:63:THR:HG22	1:B:64:GLU:H	1.81	0.46
1:B:532:SER:HB2	1:B:533:ILE:HD12	1.96	0.46
1:B:813:VAL:HA	1:B:816:TRP:CD1	2.49	0.46
2:C:133:PHE:O	2:C:137:LEU:HG	2.16	0.46
1:A:154:ILE:HG23	1:A:155:PHE:CD1	2.51	0.46
1:A:352:LEU:HD21	1:A:431:VAL:HG22	1.96	0.46
1:A:417:VAL:O	1:A:420:VAL:HG22	2.15	0.46
1:A:855:GLU:HB3	1:B:856:PHE:CE1	2.43	0.46
1:B:613:SER:HA	2:C:145:ASN:ND2	2.31	0.46
1:B:635:LYS:CE	1:B:650:LEU:HB2	2.46	0.46
1:B:723:ARG:NH2	1:B:785:ILE:CA	2.69	0.46
2:C:68:GLU:HB3	2:C:70:LYS:HD2	1.97	0.46
1:A:31:PHE:CE2	1:A:34:LYS:HE3	2.51	0.46
1:A:768:GLY:O	1:A:772:LEU:HG	2.15	0.46
1:A:925:ARG:O	1:A:928:ASP:HB3	2.16	0.46
1:B:106:LYS:HE3	1:B:686:ASN:OD1	2.15	0.46
1:B:153:HIS:NE2	1:B:154:ILE:HG22	2.31	0.46
1:B:233:ALA:HB3	1:B:243:ARG:HE	1.80	0.46
1:B:601:LEU:HD23	1:B:602:ASN:O	2.16	0.46
1:B:738:SER:OG	2:D:142:LYS:HA	2.16	0.46
1:B:871:LYS:HD3	1:B:871:LYS:N	2.31	0.46
1:B:871:LYS:H	1:B:871:LYS:CD	2.28	0.46
2:D:48:PRO:O	2:D:51:ILE:HG12	2.16	0.46
3:E:8:LYS:HG2	3:F:59:VAL:O	2.16	0.46
1:A:43:LYS:O	1:A:687:PRO:CD	2.63	0.46
1:A:139:VAL:HG13	1:A:194:TYR:CE1	2.51	0.46
1:A:439:MET:O	1:A:443:ILE:HG12	2.16	0.46
1:A:472:SER:HB2	1:A:596:LYS:HZ3	1.81	0.46
1:B:38:PHE:CE1	1:B:79:GLN:OE1	2.68	0.46
1:B:197:VAL:O	1:B:204:ARG:NH2	2.49	0.46
1:B:352:LEU:CD2	1:B:435:MET:HE2	2.46	0.46
1:B:492:HIS:ND1	1:B:667:PRO:HB3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:GLY:HA3	1:B:760:HIS:CD2	2.51	0.46
1:B:716:GLY:HA2	1:B:719:ARG:HH21	1.79	0.46
1:A:723:ARG:HE	2:C:138:ARG:NH1	2.14	0.45
1:A:735:PHE:CD2	1:A:735:PHE:O	2.69	0.45
1:B:229:ALA:O	1:B:284:HIS:HB2	2.16	0.45
2:D:48:PRO:HA	2:D:51:ILE:HG12	1.97	0.45
3:F:16:ASN:HB3	3:F:90:LEU:CD1	2.46	0.45
3:F:64:GLU:HG3	3:F:65:GLU:HG3	1.98	0.45
1:A:60:THR:HA	1:A:70:THR:HA	1.98	0.45
1:A:147:ARG:HH22	1:A:157:ILE:HA	1.80	0.45
1:A:608:LEU:HD23	1:A:608:LEU:C	2.41	0.45
1:A:675:PRO:CB	1:A:684:MET:SD	3.04	0.45
1:B:38:PHE:HD2	1:B:99:PRO:CG	2.29	0.45
1:B:121:PHE:HD1	1:B:705:CYS:HG	1.64	0.45
1:B:193:GLN:O	1:B:197:VAL:CG1	2.63	0.45
1:B:476:LEU:HD22	1:B:593:TRP:CH2	2.51	0.45
2:C:85:GLN:HE21	2:C:121:ILE:HG22	1.81	0.45
3:F:49:LEU:HD11	3:F:70:ILE:CD1	2.46	0.45
1:A:464:GLY:HA2	1:A:482:ASN:OD1	2.16	0.45
1:A:735:PHE:HB3	1:A:741:GLY:CA	2.46	0.45
1:B:134:TYR:CB	1:B:193:GLN:HE22	2.29	0.45
1:B:520:CYS:SG	1:B:579:LEU:CG	3.04	0.45
1:B:632:GLU:O	1:B:633:LYS:CG	2.64	0.45
2:D:46:PHE:CE1	2:D:119:GLN:HA	2.51	0.45
3:E:8:LYS:CE	3:F:60:ASN:HD21	2.28	0.45
1:A:379:GLU:HB3	1:A:383:LYS:HD3	1.99	0.45
1:A:390:LEU:HD21	1:A:609:TYR:CD2	2.51	0.45
1:A:596:LYS:HA	1:A:600:PRO:HD3	1.99	0.45
1:B:298:LEU:C	1:B:298:LEU:HD23	2.41	0.45
1:B:494:PHE:HE2	1:B:515:MET:HB2	1.82	0.45
1:B:534:LEU:HB2	1:B:548:PHE:CE1	2.51	0.45
1:B:867:GLU:HB2	1:B:871:LYS:HG2	1.98	0.45
3:E:80:THR:CA	3:F:40:ARG:CD	2.95	0.45
1:A:52:VAL:HB	1:A:60:THR:O	2.17	0.45
1:A:283:TYR:HE2	1:A:432:TYR:CZ	2.35	0.45
1:B:146:LYS:NZ	1:B:721:ARG:NH1	2.65	0.45
1:B:263:ILE:H	1:B:444:ASN:ND2	2.14	0.45
1:B:499:GLU:O	1:B:502:LYS:HB3	2.16	0.45
1:B:734:GLN:OE1	2:D:135:GLU:OE2	2.33	0.45
1:B:826:ASN:O	3:F:59:VAL:CG1	2.65	0.45
1:B:898:LEU:HD23	1:B:898:LEU:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:16:ASN:HB3	3:F:90:LEU:HD12	1.97	0.45
3:F:97:GLU:O	3:F:101:ASN:HB2	2.16	0.45
1:A:25:GLU:O	1:A:29:ARG:NH1	2.50	0.45
1:A:498:GLN:O	1:A:502:LYS:HG3	2.17	0.45
1:B:520:CYS:SG	1:B:579:LEU:CD2	3.03	0.45
1:B:544:THR:HG23	1:B:547:THR:H	1.79	0.45
1:B:836:ILE:CG2	3:F:28:GLU:OE1	2.60	0.45
2:D:69:MET:O	2:D:69:MET:HG3	2.16	0.45
3:E:8:LYS:CD	3:F:59:VAL:N	2.79	0.45
3:E:103:PHE:O	3:E:106:PHE:HB2	2.17	0.45
1:A:367:LYS:O	1:A:368:GLN:HB2	2.16	0.45
1:A:735:PHE:CD2	1:B:379:GLU:CD	2.93	0.45
1:A:882:GLN:CD	1:B:454:GLN:HB3	2.42	0.45
1:B:16:LEU:CD2	1:B:133:VAL:HG23	2.46	0.45
1:B:114:ILE:HD12	1:B:114:ILE:N	2.31	0.45
1:B:139:VAL:HG12	1:B:139:VAL:O	2.16	0.45
1:B:324:ASP:OD2	1:B:326:ALA:HB3	2.17	0.45
1:B:388:MET:CA	1:B:617:LEU:HD23	2.27	0.45
2:D:48:PRO:HA	2:D:51:ILE:CD1	2.46	0.45
3:E:33:PHE:HA	3:E:36:MET:HE3	1.98	0.45
3:E:100:LEU:HD23	3:E:100:LEU:C	2.42	0.45
1:A:45:GLU:OE2	1:A:690:MET:HB2	2.16	0.45
1:A:143:ARG:NH2	1:A:197:VAL:HG22	2.31	0.45
1:A:426:ALA:N	1:A:429:LYS:HB2	2.32	0.45
1:A:715:TYR:HE1	1:A:763:VAL:HB	1.82	0.45
1:B:45:GLU:HG3	1:B:690:MET:CG	2.46	0.45
1:B:268:LEU:CD2	1:B:432:TYR:CE2	2.94	0.45
1:B:277:LEU:HD23	1:B:278:LYS:HB2	1.98	0.45
1:B:342:THR:OG1	1:B:345:GLU:HG3	2.16	0.45
1:B:534:LEU:HD12	1:B:538:CYS:SG	2.56	0.45
1:B:637:LYS:HB3	1:B:637:LYS:HE3	1.78	0.45
1:B:870:ARG:NE	1:B:871:LYS:HD3	2.32	0.45
1:B:888:GLN:O	1:B:891:VAL:HG12	2.17	0.45
1:B:924:GLU:O	1:B:927:GLU:CG	2.63	0.45
2:D:100:ARG:HD3	2:D:101:GLN:OE1	2.17	0.45
3:F:62:LYS:HB3	3:F:64:GLU:HG2	1.99	0.45
1:A:55:GLU:HG3	1:A:55:GLU:O	2.17	0.45
1:A:571:GLY:O	1:A:573:PRO:N	2.50	0.45
1:A:922:MET:HE2	1:B:923:ASN:CG	2.42	0.45
1:B:147:ARG:HD3	1:B:711:ASN:OD1	2.17	0.45
1:B:168:ASP:OD2	1:B:762:LYS:CG	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASN:O	1:B:228:GLU:HG3	2.17	0.45
1:B:356:ILE:HA	1:B:359:PHE:HD2	1.82	0.45
1:B:723:ARG:NE	1:B:785:ILE:HG12	2.32	0.45
2:C:67:CYS:SG	2:C:68:GLU:HA	2.57	0.45
3:F:66:ILE:HG13	3:F:67:ASP:N	2.20	0.45
1:A:431:VAL:HG13	1:A:432:TYR:N	2.32	0.45
1:B:283:TYR:CE2	1:B:432:TYR:CZ	3.05	0.45
1:B:505:GLY:HA3	1:B:760:HIS:NE2	2.32	0.45
1:B:832:LEU:HD23	3:F:164:GLU:HG3	1.98	0.45
3:F:38:GLN:OE1	3:F:48:ASP:HB2	2.17	0.45
1:A:39:VAL:CB	1:A:49:ALA:HB2	2.46	0.44
1:A:515:MET:HE1	1:A:697:GLY:HA2	1.99	0.44
1:B:267:LEU:HG	1:B:268:LEU:N	2.32	0.44
1:B:283:TYR:CD2	1:B:432:TYR:CZ	3.05	0.44
1:B:417:VAL:O	1:B:421:ILE:HG23	2.17	0.44
1:B:494:PHE:O	1:B:498:GLN:HG2	2.17	0.44
2:D:61:PHE:CE2	2:D:79:VAL:HA	2.52	0.44
2:D:111:PHE:CZ	2:D:115:LEU:HD11	2.52	0.44
3:E:101:ASN:O	3:E:105:VAL:HG12	2.16	0.44
1:A:171:ASN:ND2	1:A:665:THR:HG22	2.33	0.44
1:A:275:PHE:HB2	1:A:421:ILE:CG1	2.47	0.44
1:A:549:LYS:CG	1:A:553:PHE:HE2	2.31	0.44
1:B:168:ASP:O	1:B:168:ASP:OD1	2.36	0.44
1:B:196:ALA:HA	1:B:217:GLU:OE1	2.17	0.44
1:A:190:ARG:C	1:A:193:GLN:HG2	2.43	0.44
1:A:500:GLU:O	1:A:504:GLU:HG2	2.17	0.44
1:B:145:LYS:HA	1:B:145:LYS:HD2	1.81	0.44
1:B:165:MET:HG3	1:B:166:LEU:N	2.32	0.44
1:B:197:VAL:HG22	1:B:204:ARG:NH2	2.33	0.44
1:B:345:GLU:O	1:B:349:MET:HG2	2.16	0.44
1:B:834:PHE:CE2	1:B:835:LYS:HB2	2.52	0.44
1:B:869:ARG:C	1:B:871:LYS:N	2.74	0.44
1:B:899:ALA:O	1:B:902:GLU:HB2	2.16	0.44
2:C:93:LEU:HD11	2:C:101:GLN:HG3	1.99	0.44
3:E:22:GLU:CG	3:E:25:GLN:HE21	2.27	0.44
1:A:285:ILE:HA	1:A:288:GLN:OE1	2.17	0.44
1:A:357:MET:C	1:A:357:MET:SD	3.01	0.44
1:A:815:GLN:NE2	3:E:127:ALA:HB3	2.31	0.44
1:B:126:ASN:OD1	1:B:127:PRO:HD2	2.17	0.44
1:B:276:GLN:NE2	1:B:276:GLN:H	2.15	0.44
1:B:355:ALA:C	1:B:359:PHE:CE2	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:869:ARG:HG3	1:B:870:ARG:N	2.30	0.44
2:C:109:MET:HE3	2:C:113:THR:CB	2.44	0.44
3:F:59:VAL:HG13	3:F:60:ASN:H	1.81	0.44
1:A:124:THR:OG1	1:A:672:CYS:SG	2.75	0.44
1:B:293:LYS:CE	1:B:298:LEU:HA	2.48	0.44
1:B:631:ILE:HG22	1:B:637:LYS:O	2.16	0.44
3:E:8:LYS:HD3	3:F:59:VAL:HG23	2.00	0.44
1:A:388:MET:HB3	1:A:390:LEU:HD13	1.99	0.44
1:A:642:SER:OG	1:A:645:GLN:HB2	2.17	0.44
1:A:730:ILE:CB	1:A:734:GLN:HG3	2.42	0.44
1:A:735:PHE:CE2	1:B:379:GLU:OE2	2.70	0.44
1:B:76:VAL:HG13	1:B:76:VAL:O	2.17	0.44
1:B:726:ASN:ND2	1:B:730:ILE:HG13	2.33	0.44
1:B:804:LEU:HD11	2:D:75:GLN:HE21	1.74	0.44
2:C:63:ARG:HG3	2:C:63:ARG:O	2.17	0.44
2:D:65:PRO:CD	3:F:126:GLN:NE2	2.75	0.44
1:A:915:LEU:O	1:A:919:VAL:HG23	2.17	0.44
1:B:98:GLU:HB2	1:B:99:PRO:HD3	1.99	0.44
1:B:195:PHE:HE2	1:B:457:ILE:HD12	1.82	0.44
1:B:302:LEU:HD13	1:B:383:LYS:HA	1.98	0.44
2:D:194:SER:O	2:D:195:SER:HB3	2.17	0.44
1:A:65:TYR:N	1:A:65:TYR:CD1	2.86	0.44
1:A:146:LYS:NZ	1:A:775:GLU:CB	2.80	0.44
1:B:18:LYS:CE	1:B:88:GLU:HA	2.47	0.44
1:B:652:ARG:HA	1:B:652:ARG:NE	2.29	0.44
1:B:950:LEU:O	1:B:954:ILE:HG13	2.17	0.44
2:C:54:PHE:CE1	2:C:118:LEU:HD23	2.53	0.44
2:C:88:THR:OG1	2:C:91:GLU:HG3	2.17	0.44
2:D:63:ARG:CZ	2:D:75:GLN:NE2	2.81	0.44
3:F:73:ALA:N	3:F:74:PRO:HD3	2.32	0.44
1:A:31:PHE:CZ	1:A:34:LYS:CB	3.01	0.44
1:A:33:LEU:CB	1:A:50:LYS:HZ3	2.27	0.44
1:A:746:LEU:HB3	1:A:751:ILE:HD11	1.99	0.44
1:B:136:PRO:HA	1:B:139:VAL:HB	2.00	0.44
1:B:139:VAL:CG1	1:B:197:VAL:HG13	2.42	0.44
1:B:789:GLN:NE2	2:D:160:LEU:O	2.47	0.44
2:C:50:GLN:O	2:C:54:PHE:CD2	2.71	0.44
2:D:155:HIS:O	2:D:159:THR:HG23	2.18	0.44
3:E:159:ILE:O	3:E:159:ILE:HG13	2.17	0.44
3:F:22:GLU:HB3	3:F:26:ILE:HG12	1.99	0.44
1:A:362:MET:HE3	1:A:421:ILE:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:GLU:HG3	1:B:25:GLU:O	2.18	0.43
1:B:45:GLU:OE2	1:B:102:LEU:CD1	2.66	0.43
1:B:472:SER:HB3	1:B:596:LYS:HZ2	1.82	0.43
1:B:751:ILE:HD12	1:B:756:TYR:CE2	2.53	0.43
1:B:781:LEU:HD23	1:B:781:LEU:HA	1.87	0.43
1:B:818:ILE:CD1	3:F:130:PHE:CE2	2.97	0.43
1:B:832:LEU:CD2	3:F:164:GLU:HG2	2.38	0.43
2:D:66:LYS:CD	3:F:126:GLN:C	2.89	0.43
3:E:125:THR:O	3:E:129:ARG:NH1	2.50	0.43
3:E:158:ILE:HG22	3:E:159:ILE:HG23	2.00	0.43
3:F:159:ILE:HG13	3:F:160:THR:H	1.82	0.43
1:A:286:PHE:HE1	1:A:356:ILE:HG13	1.83	0.43
1:A:735:PHE:CD1	1:A:741:GLY:CA	2.83	0.43
1:A:837:LYS:HE3	3:E:28:GLU:HB2	1.99	0.43
1:A:841:LYS:NZ	3:F:21:PHE:HB3	2.33	0.43
1:B:114:ILE:HG23	1:B:125:VAL:O	2.18	0.43
3:E:110:GLY:O	3:E:111:LYS:HB3	2.18	0.43
1:A:174:ILE:HD12	1:A:668:HIS:HB2	1.98	0.43
1:A:515:MET:HE1	1:A:697:GLY:HA3	2.01	0.43
1:A:714:LEU:HD23	1:A:716:GLY:H	1.84	0.43
1:A:930:GLU:O	1:A:933:ASN:HB3	2.18	0.43
1:B:112:TRP:O	1:B:114:ILE:HD12	2.19	0.43
1:B:155:PHE:HE1	1:B:193:GLN:HE21	1.58	0.43
1:B:162:TYR:HA	1:B:165:MET:HG2	2.00	0.43
1:B:355:ALA:HB1	1:B:359:PHE:CE2	2.54	0.43
1:B:411:VAL:HG12	1:B:412:THR:N	2.33	0.43
1:B:540:PHE:CE1	1:B:913:ILE:HD13	2.53	0.43
1:B:699:LEU:HG	1:B:703:ARG:NH1	2.34	0.43
1:B:699:LEU:HG	1:B:703:ARG:HH11	1.83	0.43
3:E:125:THR:O	3:E:129:ARG:NH2	2.52	0.43
1:A:417:VAL:O	1:A:421:ILE:HG12	2.18	0.43
1:B:136:PRO:O	1:B:140:ALA:HB2	2.17	0.43
1:B:471:ASN:HB3	1:B:588:TYR:CD1	2.53	0.43
1:B:733:GLY:H	2:D:135:GLU:HA	1.09	0.43
2:C:141:ASP:HB2	2:C:185:TYR:CE2	2.53	0.43
1:A:635:LYS:O	1:A:637:LYS:N	2.52	0.43
1:A:831:LYS:HB3	3:E:163:GLU:O	2.16	0.43
1:B:98:GLU:N	1:B:99:PRO:HD2	2.33	0.43
1:B:332:THR:O	1:B:335:ALA:HB3	2.19	0.43
1:B:824:VAL:HG13	1:B:825:LYS:N	2.32	0.43
2:C:109:MET:CE	2:C:113:THR:HB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:45:ASP:CG	3:F:46:LYS:H	2.27	0.43
3:F:88:GLU:OE1	3:F:91:LYS:HD2	2.19	0.43
1:B:233:ALA:HB3	1:B:243:ARG:NE	2.33	0.43
1:B:352:LEU:HD21	1:B:435:MET:HE2	2.00	0.43
1:B:724:ILE:HG12	1:B:784:ILE:HB	2.00	0.43
2:C:172:LEU:HD21	2:C:188:PHE:HE1	1.81	0.43
2:D:101:GLN:O	2:D:102:GLU:CG	2.67	0.43
2:D:115:LEU:HD23	2:D:118:LEU:HD12	2.00	0.43
3:E:51:ASP:O	3:E:54:ALA:HB3	2.18	0.43
3:E:139:PHE:CE2	3:E:142:PHE:CE1	3.07	0.43
1:A:54:ARG:HG3	1:A:54:ARG:O	2.18	0.43
1:A:106:LYS:HD2	1:A:686:ASN:ND2	2.33	0.43
1:A:134:TYR:CG	1:A:190:ARG:HD3	2.50	0.43
1:A:834:PHE:CE1	1:A:835:LYS:HG2	2.54	0.43
1:A:898:LEU:C	1:A:898:LEU:HD23	2.43	0.43
1:B:251:HIS:CE1	1:B:456:PHE:HB3	2.53	0.43
1:A:45:GLU:HB2	1:A:686:ASN:HB3	1.99	0.43
1:A:190:ARG:HA	1:A:193:GLN:CD	2.44	0.43
1:B:46:PHE:CG	1:B:99:PRO:HB3	2.52	0.43
1:B:63:THR:CG2	1:B:64:GLU:N	2.82	0.43
1:B:63:THR:CG2	1:B:65:TYR:CE2	2.96	0.43
1:B:750:ASP:O	1:B:751:ILE:CG1	2.67	0.43
1:B:815:GLN:C	1:B:818:ILE:HG12	2.44	0.43
1:B:865:LYS:O	1:B:867:GLU:O	2.37	0.43
2:D:76:CYS:HA	2:D:79:VAL:CG1	2.48	0.43
1:A:43:LYS:HD3	1:A:43:LYS:N	2.33	0.43
1:A:503:LYS:NZ	1:B:372:GLN:HB2	2.34	0.43
1:A:596:LYS:C	1:A:598:LYS:H	2.27	0.43
1:B:48:LYS:HZ3	1:B:79:GLN:CB	2.31	0.43
1:B:84:PHE:CD1	1:B:87:ILE:HD11	2.50	0.43
1:B:151:PRO:HB2	1:B:152:PRO:CD	2.42	0.43
1:B:155:PHE:HZ	1:B:193:GLN:HE21	1.55	0.43
1:B:260:SER:HB3	1:B:449:THR:CA	2.49	0.43
1:B:293:LYS:HZ1	1:B:303:ILE:CG2	2.31	0.43
1:B:303:ILE:HA	1:B:310:TYR:OH	2.18	0.43
1:B:723:ARG:HG3	1:B:724:ILE:N	2.25	0.43
1:A:388:MET:O	1:A:614:LEU:HD22	2.19	0.43
1:B:293:LYS:HE3	1:B:298:LEU:CA	2.48	0.43
1:B:335:ALA:O	1:B:339:LEU:HG	2.18	0.43
1:B:635:LYS:HB3	1:B:640:LYS:N	2.33	0.43
1:B:732:GLU:HG3	2:D:136:GLY:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:159:ILE:HG13	3:F:160:THR:N	2.34	0.43
1:A:113:MET:HB2	1:A:113:MET:HE3	1.77	0.42
1:A:293:LYS:NZ	1:A:303:ILE:HD13	2.34	0.42
1:A:713:ILE:HB	1:A:765:PHE:CE2	2.54	0.42
1:A:922:MET:HE2	1:B:923:ASN:ND2	2.33	0.42
1:B:59:VAL:O	1:B:70:THR:HA	2.19	0.42
1:B:174:ILE:O	1:B:459:VAL:HA	2.19	0.42
1:B:390:LEU:HD11	1:B:609:TYR:CD1	2.54	0.42
1:B:404:VAL:CG1	1:B:411:VAL:HB	2.49	0.42
1:B:534:LEU:HG	1:B:538:CYS:SG	2.59	0.42
1:B:720:GLN:NE2	2:D:137:LEU:HA	2.34	0.42
1:B:818:ILE:HG13	3:F:130:PHE:CZ	2.53	0.42
1:B:833:TYR:O	1:B:833:TYR:CG	2.71	0.42
1:B:849:MET:CA	1:B:852:MET:HG3	2.46	0.42
2:C:147:THR:CG2	2:C:184:ASN:HD21	2.32	0.42
1:B:48:LYS:NZ	1:B:79:GLN:CB	2.81	0.42
1:B:549:LYS:CE	1:B:566:PRO:HG3	2.48	0.42
1:B:834:PHE:CG	1:B:835:LYS:N	2.87	0.42
1:A:268:LEU:HD23	1:A:433:GLU:OE1	2.19	0.42
1:B:256:GLY:CA	2:D:154:ARG:NH2	2.75	0.42
1:B:286:PHE:HZ	1:B:356:ILE:HG13	1.81	0.42
3:E:8:LYS:CG	3:F:59:VAL:C	2.91	0.42
3:E:38:GLN:HB3	3:E:48:ASP:OD2	2.19	0.42
1:B:104:ASN:CG	1:B:108:ARG:HH22	2.28	0.42
1:B:172:GLN:HE22	1:B:666:HIS:CG	2.37	0.42
1:B:230:PHE:HZ	1:B:349:MET:HE2	1.83	0.42
1:B:562:ASN:HB3	1:B:580:ILE:HG22	2.01	0.42
1:B:633:LYS:CA	1:B:641:GLY:HA3	2.49	0.42
1:B:867:GLU:CB	1:B:871:LYS:HG2	2.49	0.42
2:C:153:LEU:HD22	2:C:183:ILE:HD12	1.99	0.42
1:A:472:SER:CB	1:A:596:LYS:HZ2	2.32	0.42
1:A:746:LEU:HD22	1:A:751:ILE:CD1	2.40	0.42
1:B:246:LYS:HA	1:B:264:GLU:O	2.20	0.42
1:B:685:ASP:CG	1:B:687:PRO:HD2	2.45	0.42
2:D:76:CYS:O	2:D:79:VAL:HG12	2.19	0.42
3:F:22:GLU:CB	3:F:26:ILE:HG12	2.49	0.42
3:F:156:VAL:HG23	3:F:159:ILE:CD1	2.45	0.42
1:A:65:TYR:N	1:A:65:TYR:HD1	2.17	0.42
1:A:133:VAL:CG2	1:A:138:VAL:HG11	2.49	0.42
1:A:717:ASP:HA	1:B:392:SER:HB3	2.01	0.42
1:B:139:VAL:O	1:B:204:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLU:HA	1:B:348:SER:HB2	2.00	0.42
1:B:403:ARG:HG3	1:B:403:ARG:O	2.19	0.42
1:B:793:ARG:NH2	2:D:162:GLU:OE2	2.52	0.42
1:B:871:LYS:CD	1:B:871:LYS:N	2.82	0.42
2:C:100:ARG:O	2:C:100:ARG:HG2	2.18	0.42
3:E:37:ASP:O	3:E:40:ARG:NH1	2.52	0.42
1:A:96:LEU:HD13	1:A:703:ARG:HG2	2.00	0.42
1:A:115:TYR:CD1	1:A:124:THR:CG2	3.02	0.42
1:A:366:LEU:HD11	1:A:417:VAL:CG1	2.50	0.42
1:A:549:LYS:HD3	1:A:576:HIS:N	2.34	0.42
1:A:791:GLN:NE2	2:C:193:MET:HE3	2.19	0.42
1:A:909:ILE:N	1:B:908:LEU:HD11	2.35	0.42
1:B:109:TYR:HE2	1:B:684:MET:HB3	1.85	0.42
1:B:227:LEU:HD21	1:B:443:ILE:HD13	2.00	0.42
1:B:432:TYR:HA	1:B:435:MET:CG	2.48	0.42
1:B:924:GLU:HA	1:B:927:GLU:CD	2.45	0.42
2:C:46:PHE:CE2	2:C:51:ILE:HG22	2.53	0.42
1:A:87:ILE:CG1	1:A:104:ASN:ND2	2.82	0.42
1:A:404:VAL:HG23	1:A:603:GLU:OE1	2.19	0.42
1:A:756:TYR:CE2	1:A:758:PHE:CZ	2.96	0.42
1:B:250:ILE:O	1:B:456:PHE:HA	2.19	0.42
1:B:431:VAL:HG22	1:B:435:MET:CE	2.48	0.42
1:B:628:ASP:OD1	1:B:628:ASP:O	2.37	0.42
3:E:33:PHE:CD1	3:E:36:MET:SD	3.13	0.42
1:A:714:LEU:HD22	1:B:396:LEU:HB2	1.85	0.42
1:A:745:LEU:HD23	1:A:745:LEU:C	2.44	0.42
1:A:908:LEU:HD13	1:B:908:LEU:HD22	0.86	0.42
1:A:944:GLU:O	1:A:947:CYS:SG	2.72	0.42
1:B:303:ILE:HG13	1:B:304:THR:O	2.20	0.42
1:B:440:VAL:CA	1:B:443:ILE:HG12	2.49	0.42
1:B:616:LEU:HD12	1:B:616:LEU:N	2.34	0.42
1:B:804:LEU:HD22	2:D:63:ARG:HD3	0.42	0.42
1:B:834:PHE:CD1	3:F:164:GLU:HG3	2.44	0.42
1:B:924:GLU:HA	1:B:927:GLU:HG2	2.01	0.42
1:B:944:GLU:O	1:B:947:CYS:SG	2.74	0.42
2:D:131:GLU:CA	2:D:134:VAL:HG12	2.46	0.42
1:A:98:GLU:N	1:A:99:PRO:CD	2.83	0.42
1:A:168:ASP:OD1	1:A:168:ASP:O	2.37	0.42
1:B:39:VAL:HG23	1:B:47:VAL:CG1	2.49	0.42
1:B:228:GLU:O	1:B:232:ASN:HB2	2.19	0.42
1:B:540:PHE:CE1	1:B:913:ILE:CD1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:LEU:CB	1:B:617:LEU:HD13	2.45	0.42
1:B:735:PHE:H	2:D:138:ARG:NH2	2.13	0.42
2:C:93:LEU:HD11	2:C:101:GLN:CG	2.50	0.42
2:C:172:LEU:HD21	2:C:188:PHE:HZ	1.82	0.42
3:E:56:LEU:HB3	3:E:165:LYS:CD	2.43	0.42
1:A:37:VAL:HG21	1:A:76:VAL:HG23	2.02	0.41
1:A:785:ILE:HG23	1:A:785:ILE:O	2.20	0.41
1:A:849:MET:CE	1:B:852:MET:SD	2.81	0.41
1:B:18:LYS:HG3	1:B:113:MET:CE	2.50	0.41
1:B:108:ARG:HA	1:B:108:ARG:HD3	1.84	0.41
1:B:292:ASN:CB	1:B:329:LEU:HB3	2.50	0.41
1:B:591:ILE:O	1:B:591:ILE:HG13	2.19	0.41
1:B:633:LYS:HA	1:B:642:SER:H	1.85	0.41
3:E:33:PHE:HA	3:E:36:MET:SD	2.60	0.41
1:A:680:SER:HA	1:A:681:PRO:HD2	1.91	0.41
1:A:785:ILE:HG23	1:A:788:ILE:HB	2.01	0.41
1:A:947:CYS:O	1:A:951:LYS:HB2	2.20	0.41
1:B:45:GLU:CD	1:B:690:MET:CB	2.94	0.41
1:B:243:ARG:HB2	1:B:283:TYR:HE1	1.85	0.41
1:B:256:GLY:H	2:D:154:ARG:NH2	2.08	0.41
1:B:524:ILE:O	1:B:527:PRO:HD2	2.20	0.41
2:D:66:LYS:HD3	3:F:126:GLN:O	2.20	0.41
2:D:183:ILE:HG22	2:D:184:ASN:N	2.35	0.41
1:A:37:VAL:C	1:A:38:PHE:HD1	2.28	0.41
1:A:160:ASN:OD1	1:A:164:TYR:CZ	2.73	0.41
1:A:246:LYS:HB3	1:A:461:ASP:HB3	2.02	0.41
1:A:390:LEU:HD11	1:A:612:SER:OG	2.20	0.41
1:B:285:ILE:O	1:B:289:ILE:HG23	2.20	0.41
1:B:888:GLN:C	1:B:891:VAL:HG12	2.44	0.41
2:C:81:ARG:HA	2:C:85:GLN:O	2.21	0.41
2:C:137:LEU:HD11	2:C:189:VAL:HG21	2.00	0.41
2:D:76:CYS:CA	2:D:79:VAL:HG12	2.50	0.41
3:E:33:PHE:HA	3:E:36:MET:CG	2.48	0.41
3:E:67:ASP:HA	3:E:70:ILE:HD13	2.02	0.41
1:A:735:PHE:CB	1:A:741:GLY:HA3	2.51	0.41
1:A:791:GLN:HB3	2:C:192:ILE:CG2	2.50	0.41
1:A:804:LEU:HD23	1:A:807:ARG:NE	2.31	0.41
1:A:827:TRP:CD1	1:A:829:TRP:H	2.38	0.41
1:A:929:GLU:HA	1:A:929:GLU:OE1	2.20	0.41
1:B:209:GLN:H	1:B:209:GLN:CD	2.28	0.41
1:B:293:LYS:HG3	1:B:297:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:812:LEU:O	1:B:816:TRP:CD1	2.73	0.41
3:E:96:GLU:HA	3:E:159:ILE:HD11	2.01	0.41
1:A:795:VAL:HG23	2:C:195:SER:OXT	2.21	0.41
1:B:113:MET:HG3	1:B:115:TYR:O	2.19	0.41
1:B:869:ARG:HG3	1:B:871:LYS:CE	2.51	0.41
2:C:61:PHE:HE2	2:C:79:VAL:HA	1.84	0.41
2:C:154:ARG:NH2	2:C:173:MET:SD	2.93	0.41
3:F:145:ASP:N	3:F:150:LEU:HD13	2.34	0.41
1:A:13:ALA:N	1:A:14:PRO:CD	2.83	0.41
1:A:18:LYS:CG	1:A:113:MET:SD	3.08	0.41
1:A:631:ILE:HG13	1:A:638:ALA:HA	2.03	0.41
1:A:643:SER:HB3	1:A:645:GLN:HG3	2.03	0.41
1:A:715:TYR:CE1	1:A:763:VAL:HB	2.56	0.41
1:A:879:SER:O	1:A:883:GLU:HG3	2.19	0.41
1:B:81:PRO:HA	1:B:82:PRO:HD3	1.85	0.41
2:C:66:LYS:HG3	2:C:66:LYS:O	2.20	0.41
2:D:173:MET:HG3	2:D:173:MET:O	2.20	0.41
1:A:428:ALA:C	1:A:431:VAL:HG12	2.45	0.41
1:A:549:LYS:O	1:A:553:PHE:CD2	2.74	0.41
1:B:217:GLU:HA	1:B:220:ILE:HG12	2.01	0.41
1:B:470:PHE:CE1	1:B:472:SER:OG	2.70	0.41
1:B:570:LYS:HA	1:B:573:PRO:HB3	2.02	0.41
1:B:811:LEU:HD11	2:D:65:PRO:HB3	0.77	0.41
2:C:114:PHE:O	2:C:118:LEU:HD13	2.20	0.41
3:F:72:GLU:O	3:F:85:MET:HE1	2.21	0.41
1:A:569:ILE:C	1:A:571:GLY:H	2.27	0.41
1:B:45:GLU:OE2	1:B:690:MET:CA	2.61	0.41
1:B:134:TYR:HB3	1:B:193:GLN:HE22	1.86	0.41
1:B:190:ARG:HG2	1:B:193:GLN:CD	2.46	0.41
1:B:370:GLU:HG3	1:B:372:GLN:HG3	2.02	0.41
1:B:504:GLU:CD	1:B:762:LYS:HD3	2.46	0.41
1:B:714:LEU:HD23	1:B:714:LEU:C	2.46	0.41
1:B:819:ARG:HH21	3:F:128:GLU:CD	2.29	0.41
1:B:826:ASN:HB3	3:F:58:ARG:HG3	1.98	0.41
1:A:18:LYS:HE3	1:A:18:LYS:HB3	1.82	0.41
1:A:35:LYS:HB3	1:A:51:ILE:HB	2.02	0.41
1:A:38:PHE:CE1	1:A:79:GLN:CA	2.98	0.41
1:A:106:LYS:HD2	1:A:686:ASN:OD1	2.20	0.41
1:A:293:LYS:HZ2	1:A:303:ILE:HD13	1.84	0.41
1:A:423:ALA:O	1:A:426:ALA:CB	2.69	0.41
1:A:516:ASP:OD2	1:A:518:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:PHE:CG	1:A:735:PHE:O	2.73	0.41
1:A:825:LYS:O	1:A:825:LYS:HG2	2.21	0.41
1:B:180:SER:O	1:B:237:ARG:NH1	2.53	0.41
1:B:208:ASP:C	1:B:210:SER:HA	2.43	0.41
1:B:348:SER:HB2	1:B:616:LEU:HD22	2.03	0.41
1:B:725:LEU:C	1:B:727:PRO:HD3	2.45	0.41
1:B:753:HIS:HA	1:B:756:TYR:CE2	2.56	0.41
1:B:818:ILE:HD12	3:F:130:PHE:HE2	1.77	0.41
1:B:939:LYS:O	1:B:943:LEU:HG	2.20	0.41
3:E:21:PHE:CB	3:E:26:ILE:HG13	2.51	0.41
3:F:116:ALA:HA	3:F:149:ASN:ND2	2.36	0.41
1:B:427:LEU:HD21	1:B:609:TYR:CZ	2.56	0.41
1:B:486:GLN:O	1:B:489:PHE:HB3	2.21	0.41
1:B:538:CYS:SG	1:B:597:ASN:ND2	2.94	0.41
1:B:715:TYR:CE1	1:B:719:ARG:HD3	2.56	0.41
2:C:93:LEU:CD2	2:C:101:GLN:HG3	2.50	0.41
2:C:114:PHE:CE2	2:C:118:LEU:CD2	3.00	0.41
2:C:183:ILE:HG13	2:C:183:ILE:O	2.21	0.41
2:D:134:VAL:HG23	2:D:185:TYR:CE2	2.56	0.41
1:A:188:THR:O	1:A:192:ILE:HG13	2.22	0.40
1:A:784:ILE:O	2:C:160:LEU:HB3	2.22	0.40
1:B:160:ASN:CA	1:B:163:GLN:HG2	2.51	0.40
1:B:276:GLN:CD	1:B:282:ASP:OD1	2.63	0.40
1:B:287:TYR:CD1	1:B:287:TYR:N	2.89	0.40
1:B:362:MET:SD	1:B:381:ALA:HB2	2.61	0.40
1:B:641:GLY:O	1:B:642:SER:HB2	2.21	0.40
1:B:734:GLN:C	1:B:735:PHE:HD1	2.28	0.40
3:F:49:LEU:HD11	3:F:70:ILE:CG1	2.51	0.40
3:F:62:LYS:CG	3:F:64:GLU:HG2	2.50	0.40
1:A:293:LYS:CG	1:A:297:LEU:HB2	2.51	0.40
1:A:714:LEU:CG	1:B:396:LEU:HD13	2.50	0.40
1:A:836:ILE:HG21	3:E:56:LEU:HA	2.03	0.40
1:B:18:LYS:HD3	1:B:108:ARG:CD	2.44	0.40
1:B:38:PHE:CZ	1:B:79:GLN:NE2	2.90	0.40
1:B:143:ARG:N	1:B:145:LYS:HG2	2.36	0.40
1:B:276:GLN:CG	1:B:282:ASP:OD1	2.68	0.40
1:B:292:ASN:HB2	1:B:326:ALA:O	2.21	0.40
1:B:313:ILE:HG23	1:B:313:ILE:O	2.22	0.40
1:B:438:TRP:HB2	1:B:620:LEU:HD23	2.02	0.40
1:B:549:LYS:CG	1:B:553:PHE:CE2	2.93	0.40
1:B:574:GLU:O	1:B:591:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:ILE:O	1:B:706:ARG:HB3	2.21	0.40
2:D:100:ARG:HD3	2:D:100:ARG:HA	1.89	0.40
3:F:62:LYS:HG3	3:F:64:GLU:H	1.87	0.40
3:F:103:PHE:CE1	3:F:114:LEU:HD22	2.54	0.40
3:F:106:PHE:CD2	3:F:114:LEU:HD12	2.56	0.40
1:A:109:TYR:CD1	1:A:125:VAL:CG1	3.01	0.40
1:A:298:LEU:HD23	1:A:298:LEU:C	2.46	0.40
1:A:810:SER:OG	3:E:102:ALA:C	2.63	0.40
1:A:872:GLU:HG2	1:A:875:GLU:CD	2.46	0.40
1:B:168:ASP:O	1:B:169:ARG:HB2	2.21	0.40
1:B:449:THR:O	1:B:452:PRO:HD3	2.21	0.40
1:B:623:ASN:OD1	1:B:624:TYR:CA	2.65	0.40
1:B:709:PHE:CZ	1:B:757:LYS:HG2	2.56	0.40
2:D:46:PHE:HZ	2:D:119:GLN:N	2.20	0.40
3:E:8:LYS:HG3	3:F:60:ASN:ND2	2.36	0.40
1:A:38:PHE:CD2	1:A:99:PRO:CB	2.99	0.40
1:A:43:LYS:HE2	1:A:43:LYS:HB2	1.94	0.40
1:A:316:GLY:HA2	1:A:317:GLU:HB2	2.02	0.40
1:B:146:LYS:NZ	1:B:721:ARG:HH12	2.18	0.40
1:B:244:PHE:HA	1:B:267:LEU:O	2.21	0.40
1:B:605:VAL:HG22	1:B:609:TYR:CZ	2.56	0.40
1:B:830:MET:O	1:B:831:LYS:HE3	2.21	0.40
1:A:329:LEU:HD13	1:A:329:LEU:O	2.22	0.40
1:A:405:LYS:HD2	1:A:410:TYR:CE1	2.56	0.40
1:A:818:ILE:O	1:A:822:MET:HG3	2.21	0.40
1:A:918:LYS:O	1:A:922:MET:HG3	2.21	0.40
1:A:931:GLU:O	1:A:935:GLU:HG3	2.21	0.40
1:B:63:THR:HG21	1:B:65:TYR:CD2	2.53	0.40
1:B:95:PHE:N	1:B:95:PHE:HD1	2.20	0.40
1:B:292:ASN:CG	1:B:329:LEU:HD23	2.47	0.40
1:B:344:GLU:CD	1:B:344:GLU:H	2.28	0.40
1:B:666:HIS:CE1	1:B:762:LYS:NZ	2.89	0.40
1:B:815:GLN:NE2	2:D:65:PRO:O	2.55	0.40
1:B:869:ARG:N	1:B:871:LYS:HE3	2.37	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	952/1935 (49%)	759 (80%)	141 (15%)	52 (6%)	1	15
1	B	948/1935 (49%)	781 (82%)	111 (12%)	56 (6%)	1	13
2	C	150/195 (77%)	132 (88%)	12 (8%)	6 (4%)	2	18
2	D	150/195 (77%)	133 (89%)	12 (8%)	5 (3%)	3	21
3	E	158/166 (95%)	111 (70%)	32 (20%)	15 (10%)	0	8
3	F	158/166 (95%)	115 (73%)	27 (17%)	16 (10%)	0	7
All	All	2516/4592 (55%)	2031 (81%)	335 (13%)	150 (6%)	2	13

All (150) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	27	GLN
1	A	208	ASP
1	A	272	ARG
1	A	313	ILE
1	A	314	SER
1	A	367	LYS
1	A	368	GLN
1	A	396	LEU
1	A	397	LYS
1	A	452	PRO
1	A	463	ALA
1	A	572	LYS
1	A	599	ASP
1	A	605	VAL
1	A	636	GLY
1	A	844	GLU
1	B	45	GLU
1	B	91	ALA
1	B	147	ARG

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Mol	Chain	Res	Type
1	B	211	PRO
1	B	260	SER
1	B	277	LEU
1	B	370	GLU
1	B	452	PRO
1	B	615	LYS
1	B	623	ASN
1	B	635	LYS
1	B	641	GLY
1	B	643	SER
1	B	723	ARG
1	B	828	PRO
1	B	833	TYR
1	B	843	ALA
2	C	101	GLN
2	C	105	ASN
2	C	144	GLY
3	E	20	MET
3	E	28	GLU
3	E	127	ALA
3	F	23	GLN
3	F	76	PRO
3	F	96	GLU
3	F	116	ALA
1	A	64	GLU
1	A	143	ARG
1	A	274	ILE
1	A	302	LEU
1	A	307	PRO
1	A	369	ARG
1	A	370	GLU
1	A	371	GLU
1	A	395	LEU
1	A	571	GLY
1	A	623	ASN
1	A	635	LYS
1	A	736	ILE
1	A	785	ILE
1	A	830	MET
1	B	73	GLU
1	B	154	ILE
1	B	183	GLY

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Mol	Chain	Res	Type
1	B	315	GLN
1	B	450	LYS
1	B	454	GLN
1	B	520	CYS
1	B	634	GLY
1	B	644	PHE
1	B	802	LYS
1	B	824	VAL
1	B	841	LYS
1	B	869	ARG
2	D	102	GLU
2	D	105	ASN
3	E	17	VAL
3	E	25	GLN
3	E	29	PHE
3	E	111	LYS
3	F	27	GLN
3	F	33	PHE
3	F	66	ILE
1	A	182	ALA
1	A	842	SER
1	B	62	GLU
1	B	322	SER
1	B	378	THR
1	B	750	ASP
2	C	143	GLU
2	D	67	CYS
2	D	69	MET
3	F	42	GLY
3	F	159	ILE
3	F	161	HIS
1	A	16	LEU
1	A	211	PRO
1	A	267	LEU
1	A	317	GLU
1	A	628	ASP
1	A	826	ASN
1	B	205	SER
1	B	362	MET
1	B	417	VAL
1	B	449	THR
1	B	538	CYS

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Mol	Chain	Res	Type
1	B	624	TYR
1	B	633	LYS
1	B	678	THR
1	B	735	PHE
1	B	751	ILE
1	B	803	LYS
1	B	832	LEU
3	E	37	ASP
3	E	146	VAL
3	F	146	VAL
3	F	164	GLU
1	A	179	GLU
1	A	210	SER
1	A	231	GLY
1	A	273	VAL
1	A	824	VAL
1	B	114	ILE
1	B	532	SER
1	B	870	ARG
2	C	62	ASP
2	C	163	ARG
3	E	59	VAL
3	E	60	ASN
3	F	59	VAL
1	A	304	THR
3	E	110	GLY
3	F	14	ASN
1	A	285	ILE
1	A	838	PRO
1	B	505	GLY
1	B	713	ILE
2	D	181	GLY
3	E	77	ILE
3	F	162	GLY
1	A	71	VAL
1	A	407	GLY
1	B	82	PRO
1	B	569	ILE
1	A	414	GLY
1	A	713	ILE
1	B	76	VAL
1	B	580	ILE

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Mol	Chain	Res	Type
1	B	407	GLY
3	E	76	PRO
3	F	11	GLY
3	E	112	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	831/1695 (49%)	813 (98%)	18 (2%)	45	64
1	B	828/1695 (49%)	811 (98%)	17 (2%)	47	65
2	C	133/167 (80%)	132 (99%)	1 (1%)	73	80
2	D	133/167 (80%)	131 (98%)	2 (2%)	57	72
3	E	137/141 (97%)	136 (99%)	1 (1%)	76	81
3	F	137/141 (97%)	133 (97%)	4 (3%)	37	58
All	All	2199/4006 (55%)	2156 (98%)	43 (2%)	48	66

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	TYR
1	A	246	LYS
1	A	269	GLU
1	A	309	ASP
1	A	315	GLN
1	A	337	ASP
1	A	365	LYS
1	A	500	GLU
1	A	574	GLU
1	A	588	TYR
1	A	593	TRP
1	A	602	ASN
1	A	814	ILE
1	A	867	GLU

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Mol	Chain	Res	Type
1	A	870	ARG
1	A	871	LYS
1	A	874	GLU
1	A	886	ASP
1	B	96	LEU
1	B	139	VAL
1	B	151	PRO
1	B	177	THR
1	B	179	GLU
1	B	408	ASN
1	B	416	ASN
1	B	420	VAL
1	B	451	GLN
1	B	640	LYS
1	B	770	LEU
1	B	775	GLU
1	B	826	ASN
1	B	835	LYS
1	B	837	LYS
1	B	861	GLU
1	B	871	LYS
2	C	186	GLU
2	D	132	ASP
2	D	185	TYR
3	E	28	GLU
3	F	25	GLN
3	F	84	THR
3	F	95	PRO
3	F	145	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	78	GLN
1	A	79	GLN
1	A	153	HIS
1	A	160	ASN
1	A	288	GLN
1	A	292	ASN
1	A	361	ASN
1	A	401	HIS

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Mol	Chain	Res	Type
1	A	416	ASN
1	A	492	HIS
1	A	564	GLN
1	A	589	ASN
1	A	597	ASN
1	A	602	ASN
1	A	623	ASN
1	A	654	ASN
1	A	711	ASN
1	A	890	GLN
1	A	895	GLN
1	A	914	GLN
1	A	933	ASN
1	B	160	ASN
1	B	251	HIS
1	B	276	GLN
1	B	292	ASN
1	B	368	GLN
1	B	401	HIS
1	B	415	GLN
1	B	444	ASN
1	B	471	ASN
1	B	490	ASN
1	B	581	HIS
1	B	597	ASN
1	B	656	ASN
1	B	691	HIS
1	B	726	ASN
1	B	755	GLN
1	B	760	HIS
1	B	815	GLN
1	B	882	GLN
1	B	885	ASN
1	B	892	GLN
1	B	895	GLN
2	C	85	GLN
2	C	119	GLN
2	C	124	ASN
2	C	184	ASN
2	D	75	GLN
2	D	105	ASN
2	D	119	GLN

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Mol	Chain	Res	Type
2	D	145	ASN
2	D	180	ASN
2	D	184	ASN
2	D	191	HIS
3	E	25	GLN
3	E	149	ASN
3	E	157	HIS
3	F	60	ASN
3	F	149	ASN
3	F	154	ASN
3	F	161	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2240. These allow visual inspection of the internal detail of the map and identification of artifacts.

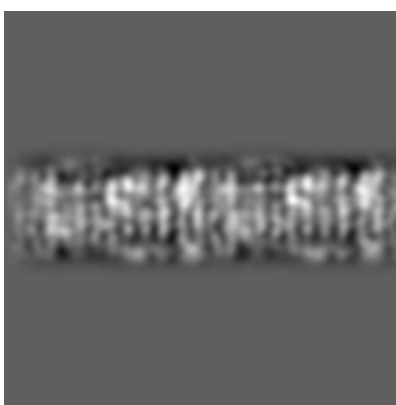
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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: 80



Y Index: 80



Z Index: 80

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

6.3 Largest variance slices [i](#)

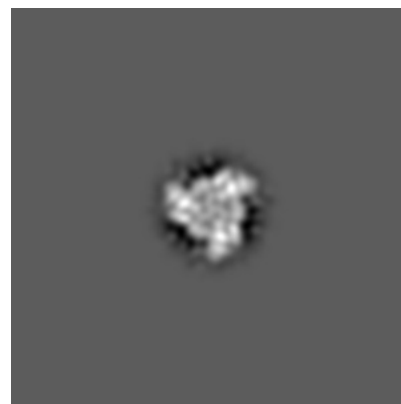
6.3.1 Primary map



X Index: 89



Y Index: 71

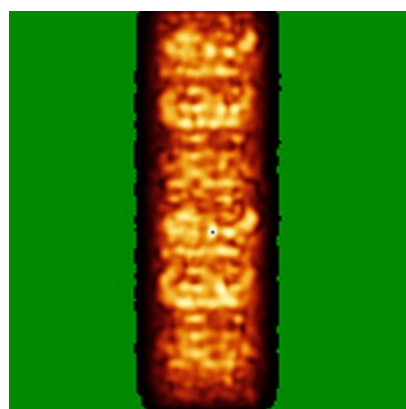


Z Index: 43

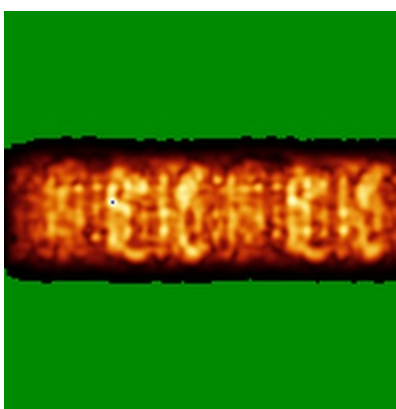
The images above show the largest variance slices of the map in three orthogonal directions.

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

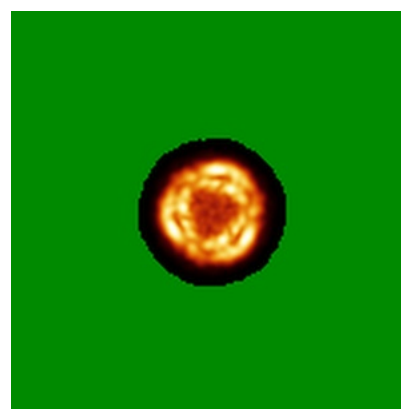
6.4.1 Primary map



X



Y

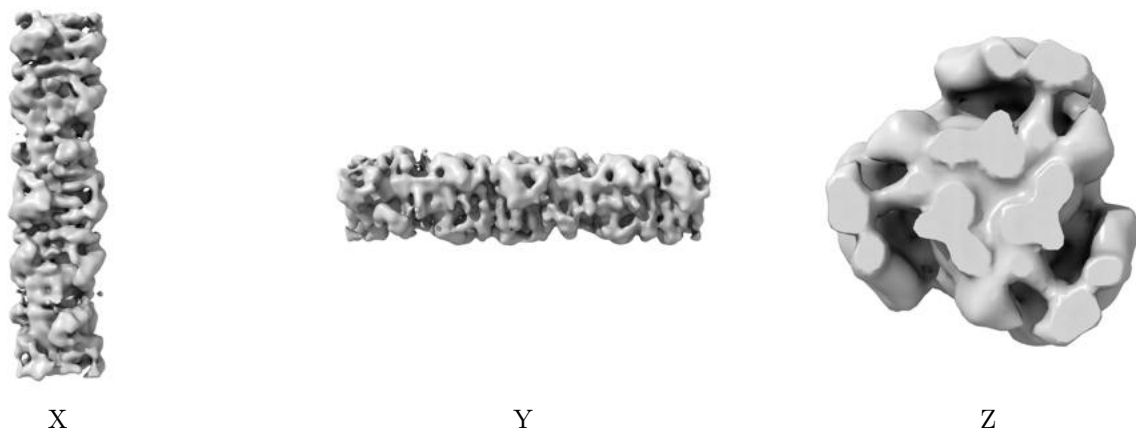


Z

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 1.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

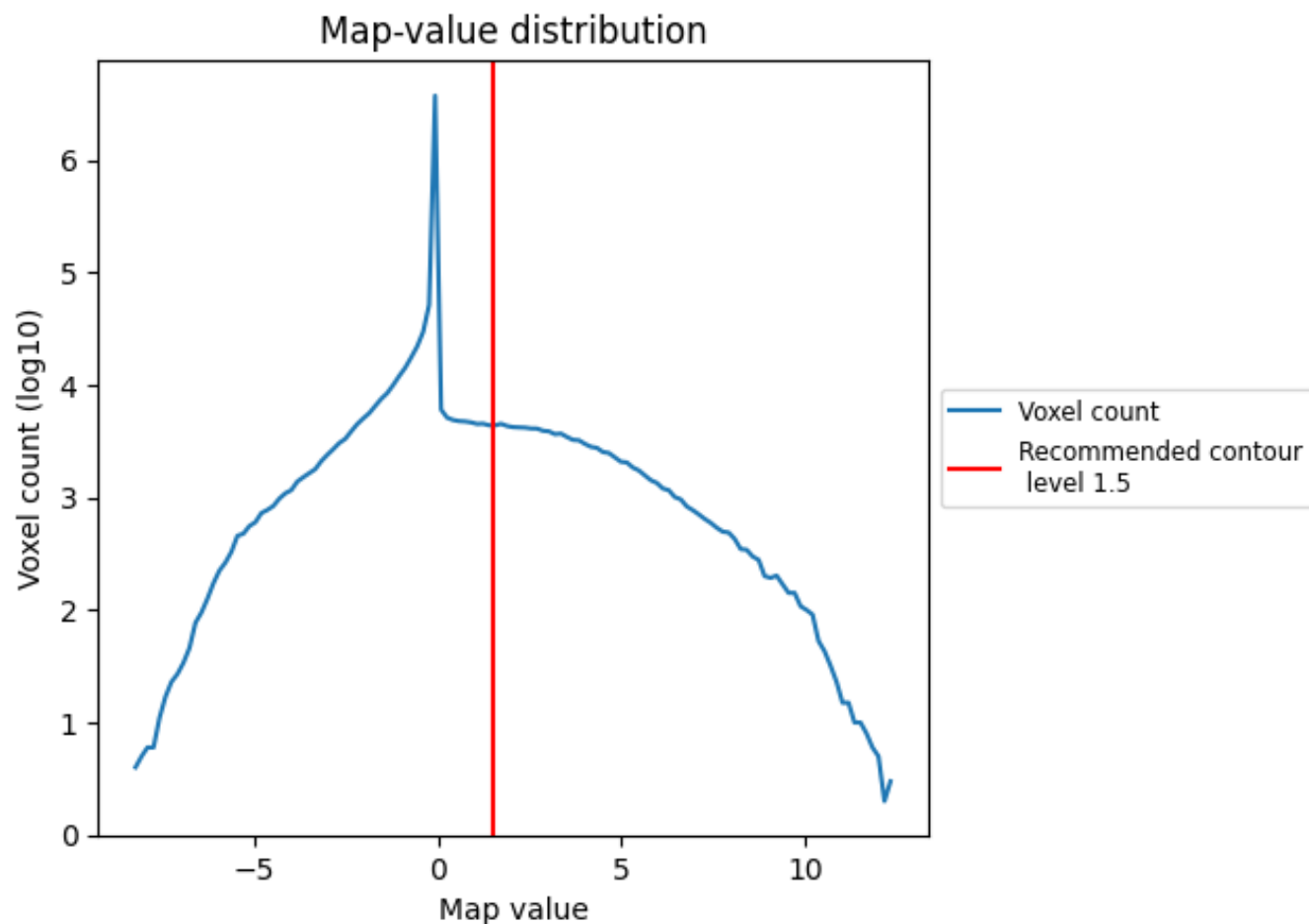
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

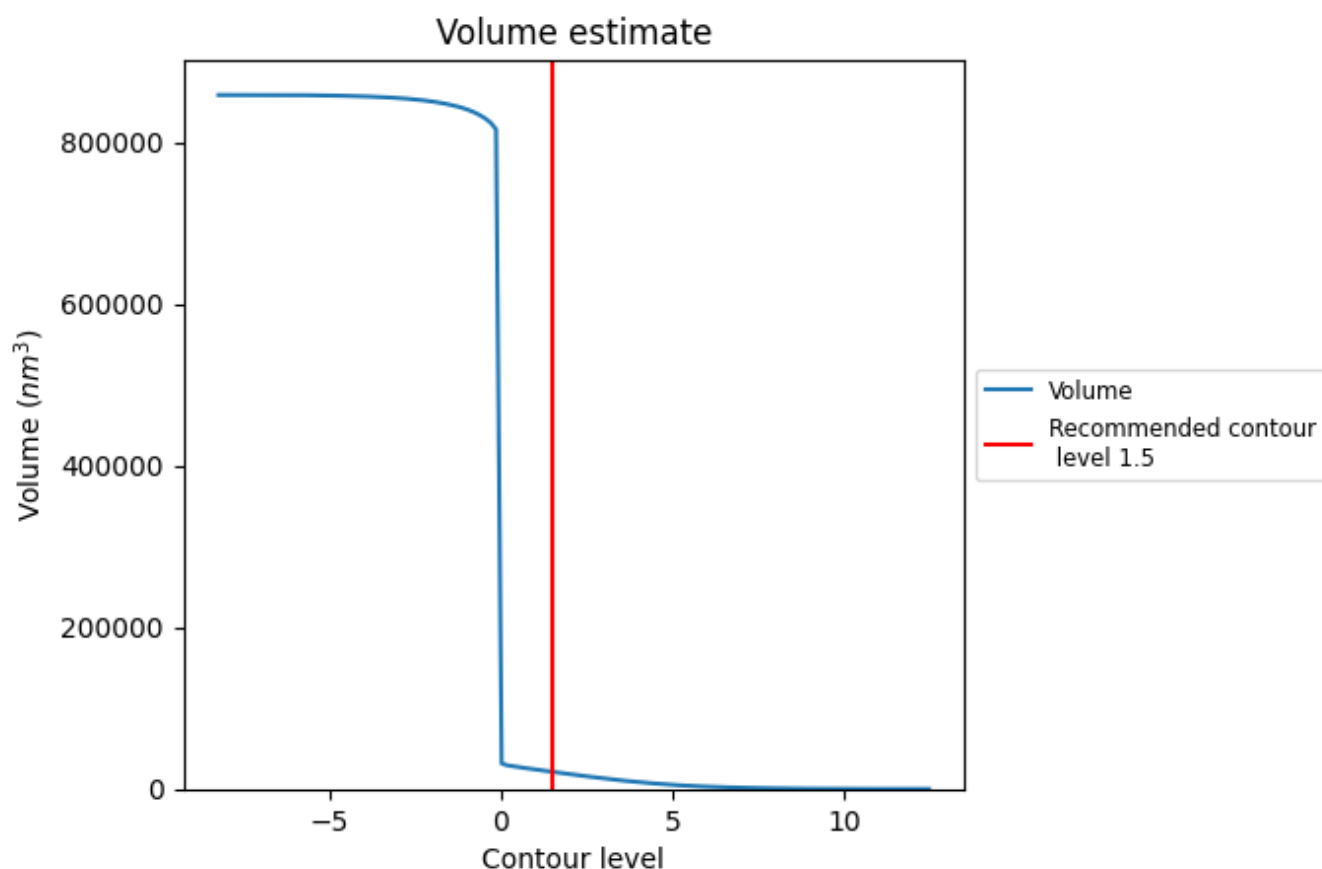
This section contains the results of statistical analysis of the map.

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.

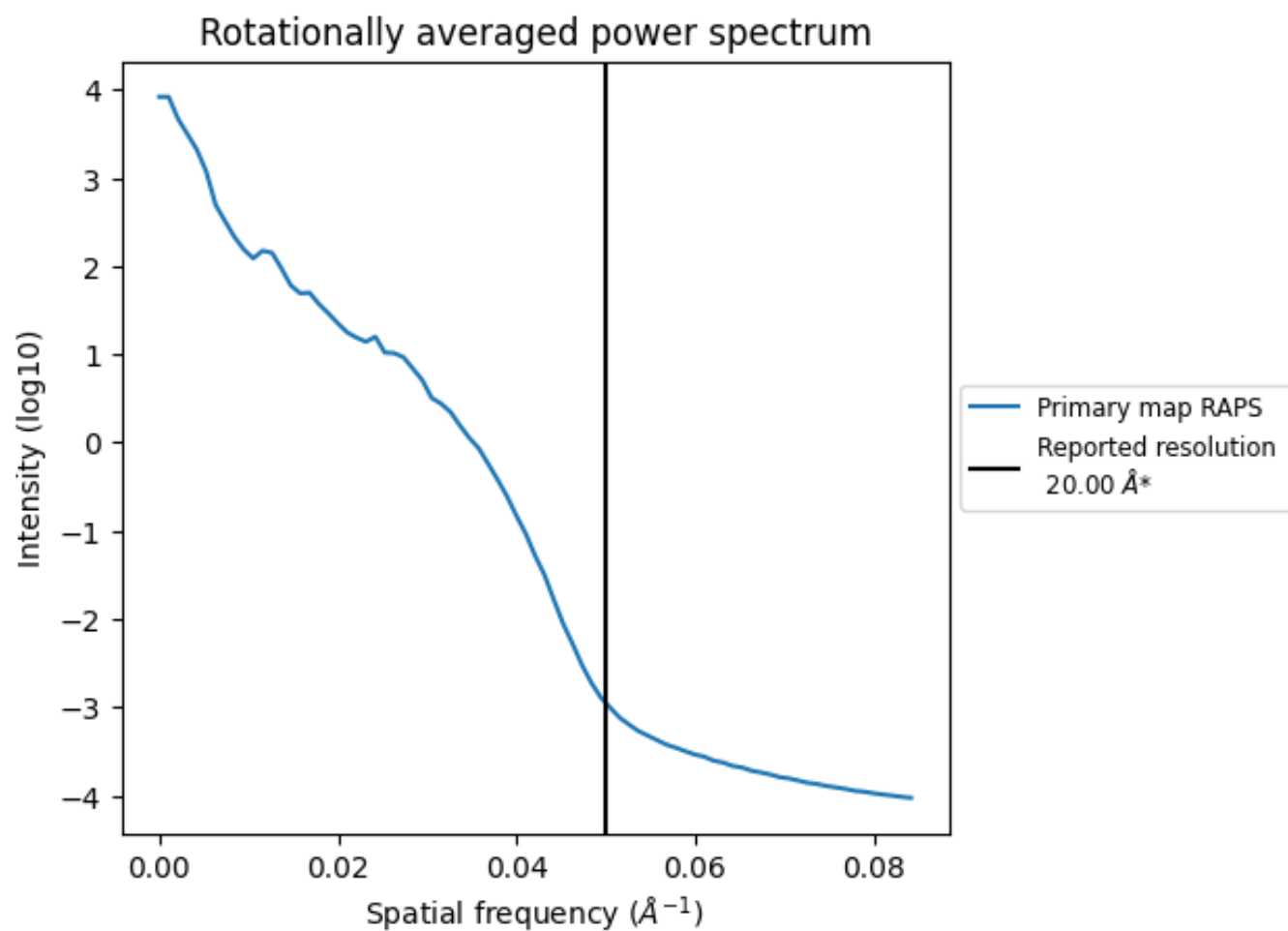
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 21179 nm^3 ; this corresponds to an approximate mass of 19131 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 0.050 Å⁻¹

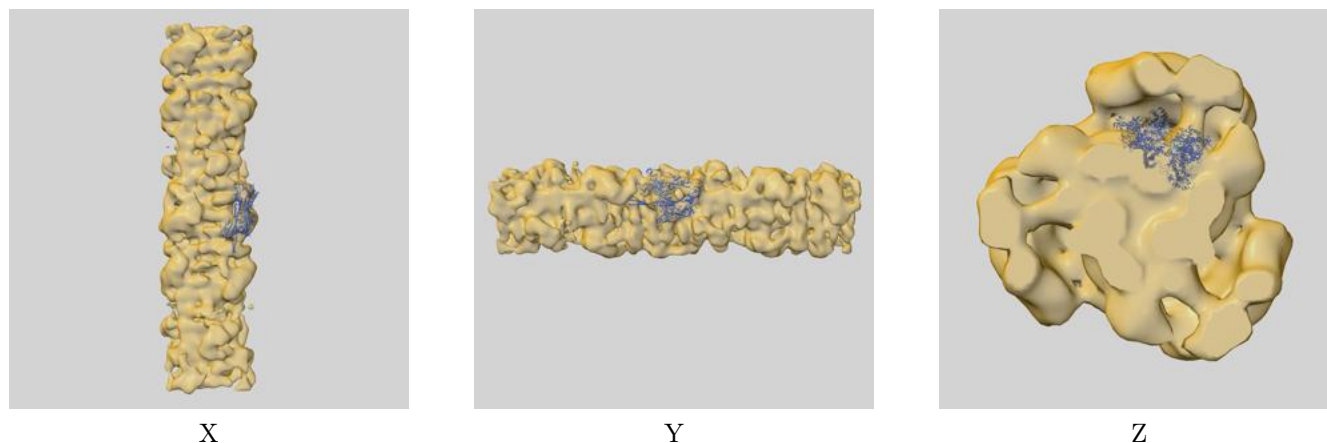
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

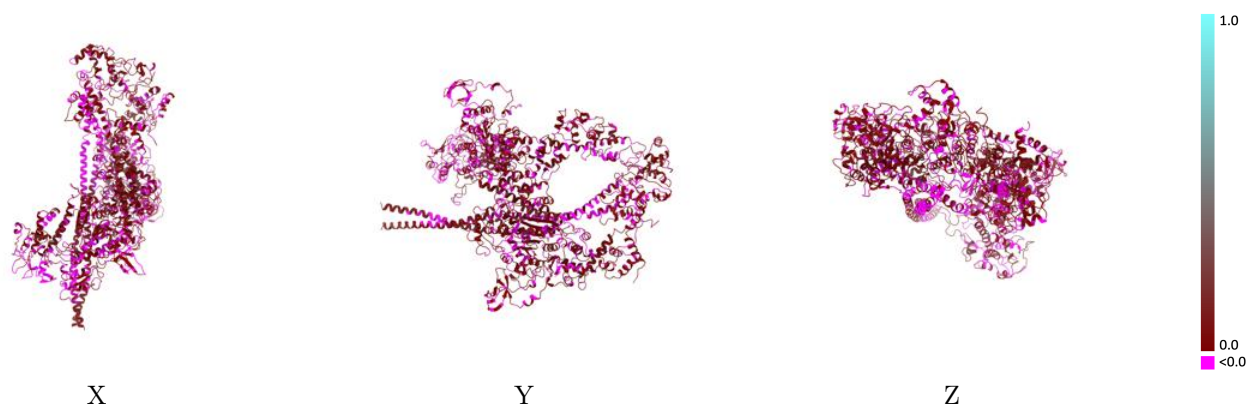
This section contains information regarding the fit between EMDB map EMD-2240 and PDB model 5TBY. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



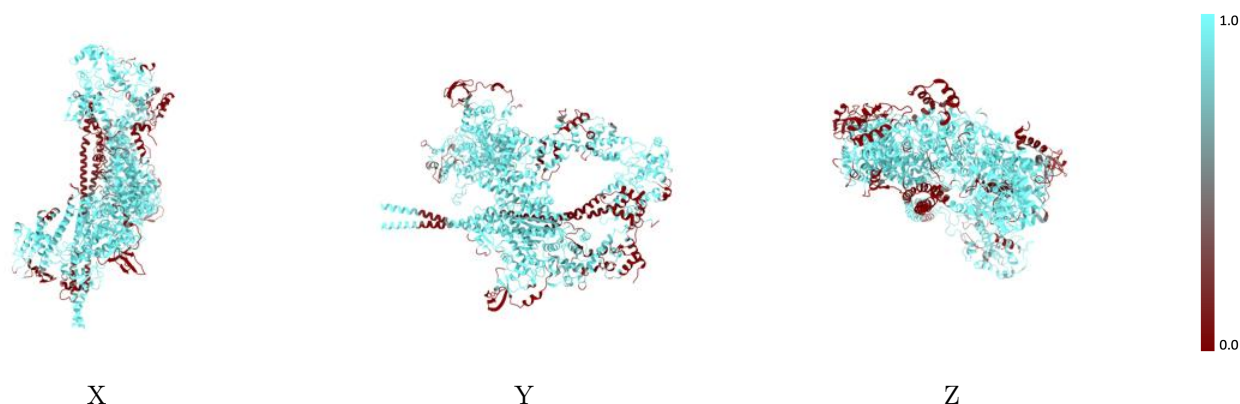
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



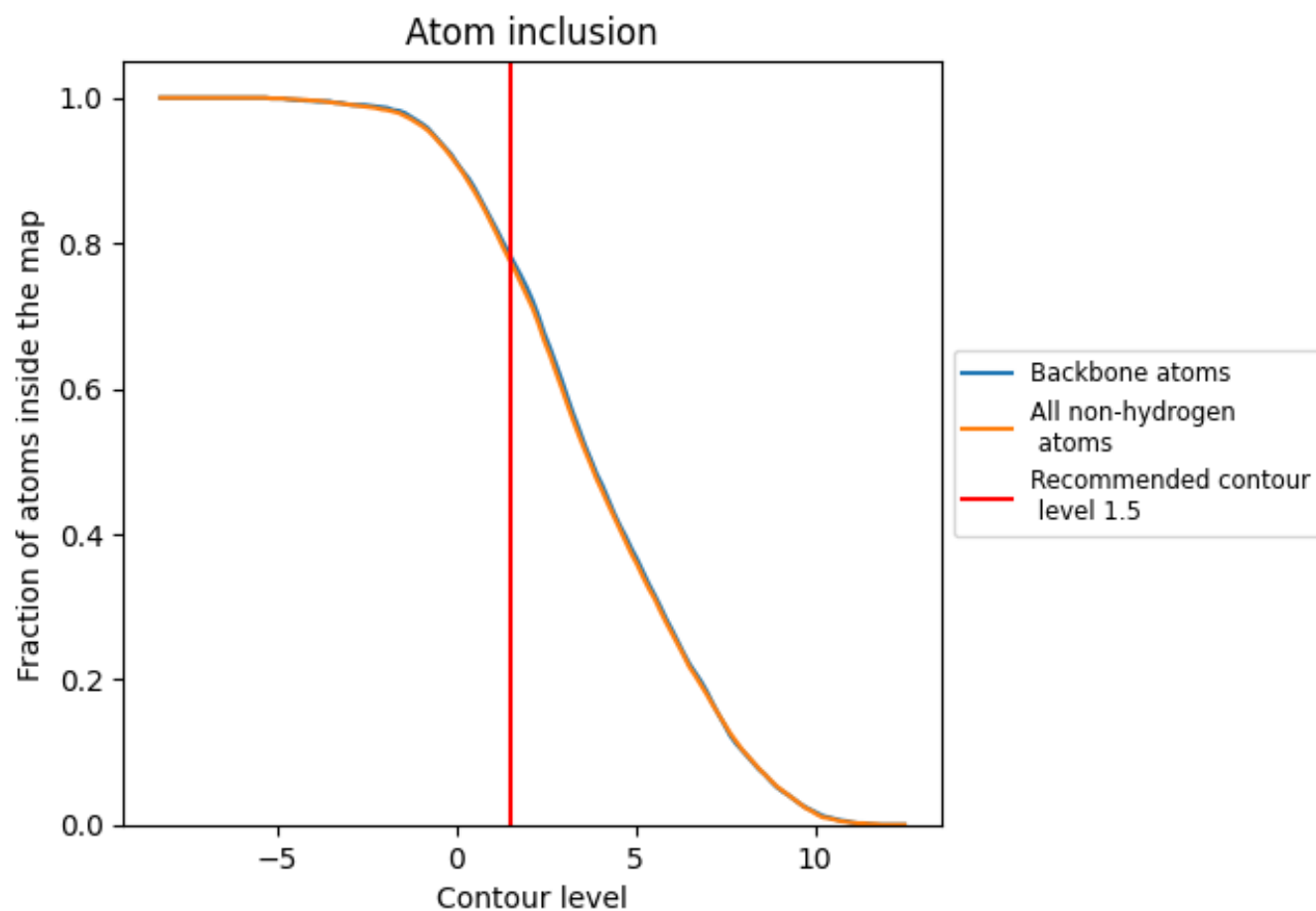
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7750	0.0320
A	0.8090	0.0230
B	0.8260	0.0380
C	0.5510	0.0350
D	0.4360	0.0430
E	0.9130	0.0340
F	0.6610	0.0420

1.0
0.0
-0.0