



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5L5L / pdb_00005151
Title : Plexin A4 full extracellular region, domains 1 to 8 modeled, data to 8 angstrom, spacegroup P2(1)
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Deposited on : 2016-05-28
Resolution : 8.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

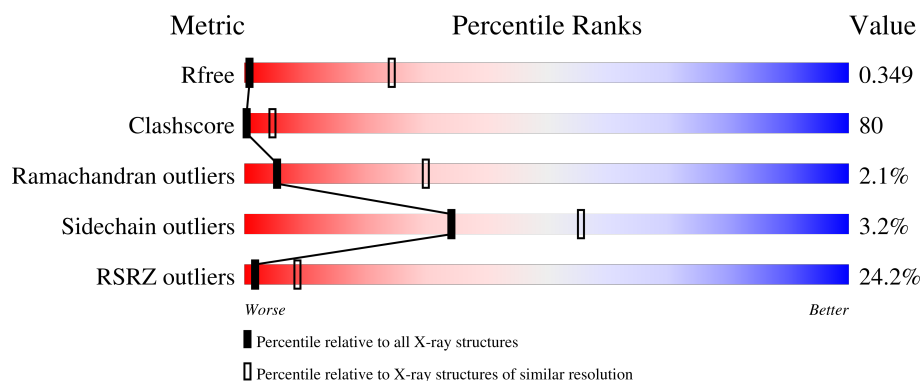
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1207	21% 24% 50% 8% 17%
1	B	1207	17% 23% 45% 7% 24%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15030 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1000	Total	C	N	O	S	0	0	0
			7841	4938	1356	1482	65			
1	B	915	Total	C	N	O	S	0	0	0
			7189	4533	1239	1357	60			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2
B	33	GLU	-	expression tag	UNP Q80UG2
B	34	THR	-	expression tag	UNP Q80UG2
B	35	GLY	-	expression tag	UNP Q80UG2
B	1230	GLY	-	expression tag	UNP Q80UG2
B	1231	ARG	-	expression tag	UNP Q80UG2
B	1232	THR	-	expression tag	UNP Q80UG2
B	1233	LYS	-	expression tag	UNP Q80UG2
B	1234	HIS	-	expression tag	UNP Q80UG2
B	1235	HIS	-	expression tag	UNP Q80UG2
B	1236	HIS	-	expression tag	UNP Q80UG2
B	1237	HIS	-	expression tag	UNP Q80UG2
B	1238	HIS	-	expression tag	UNP Q80UG2

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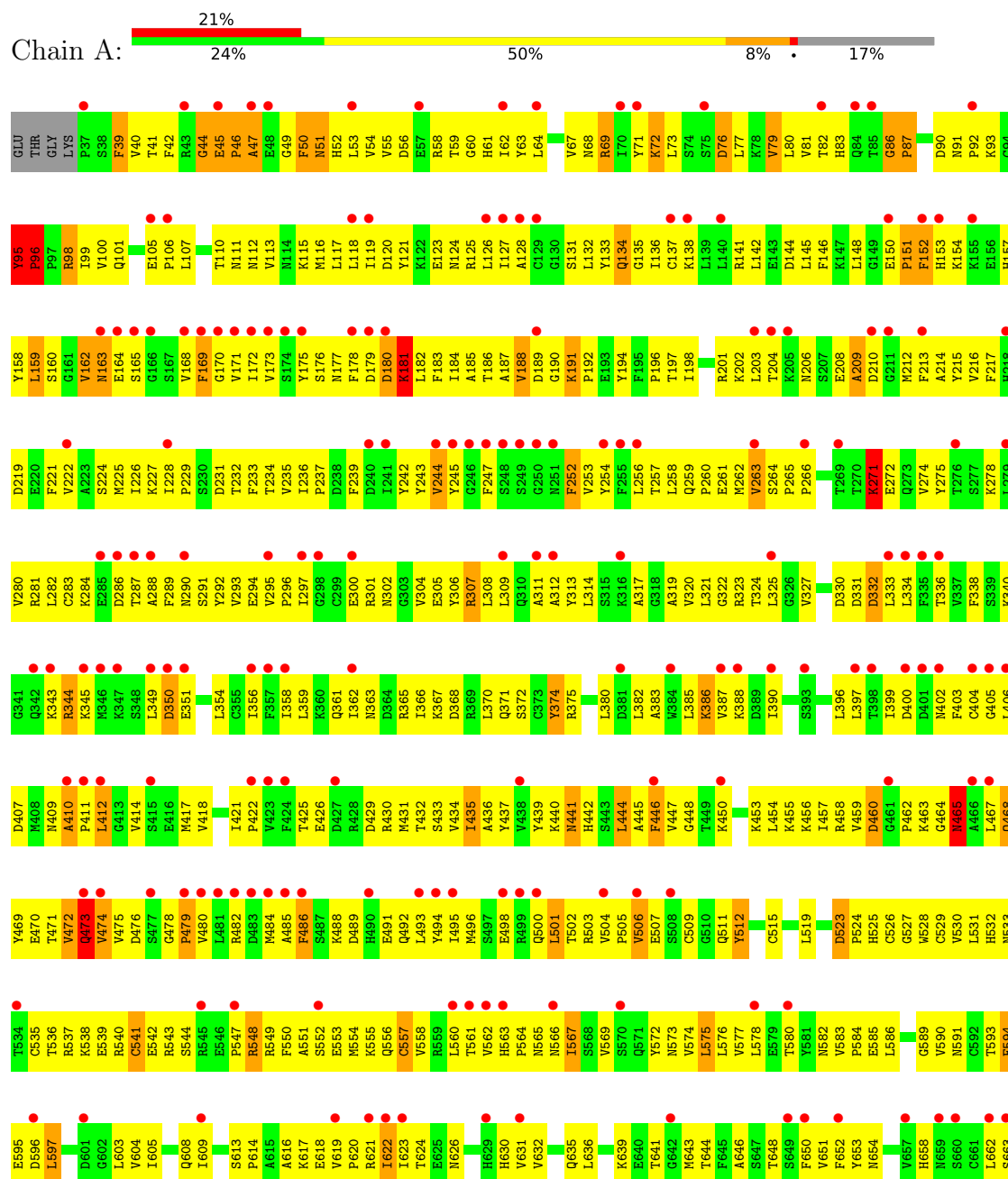
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP Q80UG2

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Plexin-A4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	142.18Å 241.00Å 144.07Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	47.74 – 8.00 47.74 – 8.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.74-8.00) 99.0 (47.74-8.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 8.32Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.349 , 0.349 0.348 , 0.349	Depositor DCC
R_{free} test set	489 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	450.9	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 289.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.043 for l,-k,h	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	15030	wwPDB-VP
Average B, all atoms (Å ²)	264.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.46	11/8007 (0.1%)	1.89	136/10846 (1.3%)
1	B	1.43	11/7344 (0.1%)	1.82	124/9943 (1.2%)
All	All	1.44	22/15351 (0.1%)	1.86	260/20789 (1.3%)

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	3
1	B	0	4
All	All	0	7

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	VAL	C-N	38.26	1.87	1.33
1	B	506	VAL	C-N	36.83	1.82	1.33
1	B	557	CYS	C-N	-29.46	0.94	1.33
1	A	700	CYS	C-N	-28.95	1.04	1.33
1	A	557	CYS	C-N	-27.90	0.86	1.33
1	B	700	CYS	C-N	12.79	1.63	1.33
1	A	49	GLY	C-N	9.86	1.45	1.33
1	B	49	GLY	C-N	9.84	1.45	1.33
1	A	653	TYR	C-N	8.06	1.45	1.33
1	B	180	ASP	C-N	7.58	1.44	1.33
1	A	180	ASP	C-N	7.48	1.44	1.33
1	B	49	GLY	CA-C	7.28	1.62	1.51
1	A	49	GLY	CA-C	7.26	1.62	1.51
1	B	50	PHE	N-CA	6.90	1.53	1.46
1	A	50	PHE	N-CA	6.77	1.53	1.46
1	B	46	PRO	N-CA	-6.44	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	46	PRO	N-CA	-6.42	1.41	1.47
1	A	465	ASN	C-N	5.23	1.41	1.33
1	B	465	ASN	C-N	5.17	1.41	1.33
1	A	711	VAL	CA-CB	-5.14	1.50	1.54
1	B	434	VAL	CA-CB	-5.03	1.50	1.55
1	B	711	VAL	CA-CB	-5.01	1.50	1.54

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	653	TYR	O-C-N	-45.82	69.23	123.29
1	B	747	GLN	CG-CD-OE1	-38.43	43.94	120.80
1	A	747	GLN	CG-CD-OE1	-38.41	43.98	120.80
1	B	557	CYS	O-C-N	-38.27	71.68	122.59
1	A	653	TYR	CA-C-N	27.60	163.37	123.07
1	A	653	TYR	C-N-CA	27.60	163.37	123.07
1	A	557	CYS	CA-C-N	-27.60	86.77	122.37
1	A	557	CYS	C-N-CA	-27.60	86.77	122.37
1	B	506	VAL	O-C-N	24.71	150.23	122.06
1	A	854	CYS	O-C-N	-24.61	85.56	122.96
1	B	506	VAL	CA-C-N	-22.48	84.57	122.33
1	B	506	VAL	C-N-CA	-22.48	84.57	122.33
1	A	557	CYS	O-C-N	22.38	152.35	122.59
1	A	854	CYS	CA-C-N	21.98	163.51	121.54
1	A	854	CYS	C-N-CA	21.98	163.51	121.54
1	B	557	CYS	CA-C-N	19.50	150.09	122.99
1	B	557	CYS	C-N-CA	19.50	150.09	122.99
1	A	506	VAL	O-C-N	-18.87	98.98	122.57
1	A	747	GLN	OE1-CD-NE2	15.14	137.74	122.60
1	B	747	GLN	CG-CD-NE2	-15.13	93.70	116.40
1	A	747	GLN	CG-CD-NE2	-15.09	93.76	116.40
1	B	747	GLN	OE1-CD-NE2	15.03	137.63	122.60
1	A	700	CYS	O-C-N	-14.88	104.76	121.43
1	B	700	CYS	CA-C-N	-12.28	104.49	119.84
1	B	700	CYS	C-N-CA	-12.28	104.49	119.84
1	A	843	ARG	CA-C-N	11.65	141.10	122.81
1	A	843	ARG	C-N-CA	11.65	141.10	122.81
1	B	843	ARG	CA-C-N	11.63	141.07	122.81
1	B	843	ARG	C-N-CA	11.63	141.07	122.81
1	B	892	HIS	CA-CB-CG	11.01	124.81	113.80
1	A	892	HIS	CA-CB-CG	10.97	124.77	113.80
1	B	700	CYS	C-N-CD	-10.70	81.14	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	700	CYS	CA-C-N	10.29	132.88	120.23
1	A	700	CYS	C-N-CA	10.29	132.88	120.23
1	B	478	GLY	CA-C-N	10.17	132.55	119.84
1	B	478	GLY	C-N-CA	10.17	132.55	119.84
1	A	479	PRO	N-CA-C	10.14	133.37	112.47
1	B	479	PRO	N-CA-C	10.12	133.31	112.47
1	A	478	GLY	CA-C-N	10.10	132.46	119.84
1	A	478	GLY	C-N-CA	10.10	132.46	119.84
1	B	473	GLN	CA-C-N	-9.46	104.95	121.97
1	B	473	GLN	C-N-CA	-9.46	104.95	121.97
1	A	473	GLN	CA-C-N	-9.45	104.97	121.97
1	A	473	GLN	C-N-CA	-9.45	104.97	121.97
1	B	700	CYS	O-C-N	-9.36	110.55	121.32
1	A	478	GLY	CA-C-O	-9.30	108.23	121.52
1	B	478	GLY	CA-C-O	-9.27	108.27	121.52
1	A	221	PHE	CA-CB-CG	-9.13	104.67	113.80
1	A	940	PHE	CA-CB-CG	-9.12	104.68	113.80
1	B	221	PHE	CA-CB-CG	-9.09	104.71	113.80
1	B	940	PHE	CA-CB-CG	-9.09	104.72	113.80
1	A	594	PHE	CA-CB-CG	-8.82	104.98	113.80
1	B	594	PHE	CA-CB-CG	-8.82	104.98	113.80
1	B	446	PHE	CA-CB-CG	-8.40	105.40	113.80
1	A	446	PHE	CA-CB-CG	-8.39	105.41	113.80
1	B	45	GLU	N-CA-C	-8.03	101.83	112.75
1	A	45	GLU	N-CA-C	-7.98	101.90	112.75
1	B	754	PHE	CA-CB-CG	-7.92	105.88	113.80
1	A	754	PHE	CA-CB-CG	-7.90	105.90	113.80
1	B	46	PRO	N-CA-CB	7.80	107.29	102.92
1	A	46	PRO	N-CA-CB	7.75	107.26	102.92
1	A	330	ASP	CA-CB-CG	-7.72	104.88	112.60
1	B	330	ASP	CA-CB-CG	-7.71	104.89	112.60
1	A	473	GLN	N-CA-C	-7.51	103.38	112.54
1	B	473	GLN	N-CA-C	-7.47	103.43	112.54
1	B	844	TRP	N-CA-C	-7.44	97.82	109.72
1	A	844	TRP	N-CA-C	-7.41	97.86	109.72
1	A	45	GLU	CA-C-N	-7.34	111.25	120.79
1	A	45	GLU	C-N-CA	-7.34	111.25	120.79
1	B	45	GLU	CA-C-N	-7.33	111.26	120.79
1	B	45	GLU	C-N-CA	-7.33	111.26	120.79
1	A	188	VAL	N-CA-C	7.15	117.96	111.81
1	B	188	VAL	N-CA-C	7.15	117.96	111.81
1	A	152	PHE	CA-CB-CG	-7.09	106.71	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	PHE	CA-CB-CG	-7.08	106.72	113.80
1	A	169	PHE	CA-CB-CG	-6.88	106.92	113.80
1	A	46	PRO	CB-CA-C	6.86	117.63	111.87
1	B	169	PHE	CA-CB-CG	-6.86	106.94	113.80
1	A	46	PRO	N-CA-C	-6.77	99.50	110.74
1	A	988	PHE	CA-CB-CG	-6.75	107.05	113.80
1	B	46	PRO	N-CA-C	-6.74	99.55	110.74
1	B	46	PRO	CB-CA-C	6.71	117.50	111.87
1	A	47	ALA	N-CA-C	-6.68	104.23	112.38
1	A	486	PHE	CA-CB-CG	-6.66	107.14	113.80
1	B	486	PHE	CA-CB-CG	-6.65	107.15	113.80
1	A	1023	ASP	CA-CB-CG	-6.64	105.95	112.60
1	A	1011	GLU	N-CA-C	-6.64	104.08	111.71
1	A	363	ASN	CA-CB-CG	-6.63	105.97	112.60
1	B	47	ALA	N-CA-C	-6.60	104.33	112.38
1	B	363	ASN	CA-CB-CG	-6.59	106.01	112.60
1	B	596	ASP	CA-CB-CG	-6.59	106.01	112.60
1	A	596	ASP	CA-CB-CG	-6.56	106.04	112.60
1	B	919	GLU	CA-C-N	6.47	134.88	121.94
1	B	919	GLU	C-N-CA	6.47	134.88	121.94
1	A	95	TYR	N-CA-C	-6.47	102.55	110.31
1	B	95	TYR	N-CA-C	-6.46	102.56	110.31
1	A	49	GLY	CA-C-N	6.45	135.74	121.81
1	A	49	GLY	C-N-CA	6.45	135.74	121.81
1	A	973	ILE	CB-CA-C	-6.44	103.16	110.96
1	A	919	GLU	CA-C-N	6.43	134.81	121.94
1	A	919	GLU	C-N-CA	6.43	134.81	121.94
1	A	39	PHE	CA-CB-CG	-6.40	107.40	113.80
1	B	49	GLY	CA-C-N	6.40	135.63	121.81
1	B	49	GLY	C-N-CA	6.40	135.63	121.81
1	A	134	GLN	N-CA-C	-6.39	104.01	113.40
1	B	134	GLN	N-CA-C	-6.38	104.02	113.40
1	B	39	PHE	CA-CB-CG	-6.35	107.45	113.80
1	B	741	ASN	CA-CB-CG	-6.35	106.25	112.60
1	B	476	ASP	CA-C-N	-6.34	113.75	123.14
1	B	476	ASP	C-N-CA	-6.34	113.75	123.14
1	A	741	ASN	CA-CB-CG	-6.34	106.26	112.60
1	A	476	ASP	CA-C-N	-6.34	113.76	123.14
1	A	476	ASP	C-N-CA	-6.34	113.76	123.14
1	A	79	VAL	CB-CA-C	-6.33	104.39	111.23
1	B	79	VAL	CB-CA-C	-6.32	104.41	111.23
1	B	928	PHE	CA-CB-CG	-6.26	107.54	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	928	PHE	CA-CB-CG	-6.23	107.57	113.80
1	B	183	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	183	PHE	CA-CB-CG	-6.19	107.61	113.80
1	B	441	ASN	CA-CB-CG	-6.17	106.43	112.60
1	B	622	ILE	CB-CA-C	-6.12	104.00	112.02
1	A	622	ILE	CB-CA-C	-6.08	104.06	112.02
1	A	441	ASN	CA-CB-CG	-6.08	106.53	112.60
1	A	573	ASN	CA-CB-CG	-6.04	106.56	112.60
1	A	209	ALA	CA-C-N	6.04	129.49	120.31
1	A	209	ALA	C-N-CA	6.04	129.49	120.31
1	B	573	ASN	CA-CB-CG	-6.01	106.58	112.60
1	A	307	ARG	N-CA-C	6.01	120.61	113.28
1	B	51	ASN	CA-CB-CG	-6.01	106.59	112.60
1	A	51	ASN	CA-CB-CG	-6.00	106.60	112.60
1	B	209	ALA	CA-C-N	5.99	129.41	120.31
1	B	209	ALA	C-N-CA	5.99	129.41	120.31
1	B	307	ARG	N-CA-C	5.98	120.58	113.28
1	A	512	TYR	CA-C-N	5.96	128.76	120.29
1	A	512	TYR	C-N-CA	5.96	128.76	120.29
1	B	512	TYR	CA-C-N	5.96	128.76	120.29
1	B	512	TYR	C-N-CA	5.96	128.76	120.29
1	B	86	GLY	O-C-N	5.96	127.73	121.77
1	A	86	GLY	O-C-N	5.91	127.68	121.77
1	A	924	GLN	N-CA-C	5.91	117.72	111.28
1	A	803	CYS	CA-C-N	5.90	132.98	121.41
1	A	803	CYS	C-N-CA	5.90	132.98	121.41
1	B	803	CYS	CA-C-N	5.89	132.96	121.41
1	B	803	CYS	C-N-CA	5.89	132.96	121.41
1	B	924	GLN	N-CA-C	5.89	117.70	111.28
1	B	805	ALA	CA-C-N	5.85	130.62	120.68
1	B	805	ALA	C-N-CA	5.85	130.62	120.68
1	A	290	ASN	CA-CB-CG	-5.83	106.77	112.60
1	A	244	VAL	N-CA-C	5.82	116.04	110.74
1	A	805	ALA	CA-C-N	5.81	130.56	120.68
1	A	805	ALA	C-N-CA	5.81	130.56	120.68
1	B	244	VAL	N-CA-C	5.79	116.01	110.74
1	B	290	ASN	CA-CB-CG	-5.78	106.83	112.60
1	A	409	ASN	CA-C-N	5.77	135.87	121.80
1	A	409	ASN	C-N-CA	5.77	135.87	121.80
1	B	409	ASN	CA-C-N	5.76	135.85	121.80
1	B	409	ASN	C-N-CA	5.76	135.85	121.80
1	A	805	ALA	N-CA-C	-5.75	104.61	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CA-CB-CG	-5.72	106.88	112.60
1	B	805	ALA	N-CA-C	-5.72	104.65	111.69
1	A	60	GLY	N-CA-C	-5.71	107.44	115.32
1	B	331	ASP	CA-CB-CG	-5.71	106.89	112.60
1	B	60	GLY	N-CA-C	-5.70	107.45	115.32
1	B	676	TYR	CA-CB-CG	-5.68	103.67	113.90
1	A	676	TYR	CA-CB-CG	-5.67	103.70	113.90
1	B	829	GLY	N-CA-C	-5.66	106.36	115.08
1	B	621	ARG	N-CA-C	-5.64	105.14	111.28
1	A	829	GLY	N-CA-C	-5.63	106.40	115.08
1	A	153	HIS	N-CA-C	5.63	117.09	111.07
1	A	699	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	476	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	332	ASP	CA-CB-CG	-5.60	107.00	112.60
1	B	460	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	460	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	621	ARG	N-CA-C	-5.60	105.18	111.28
1	B	476	ASP	CA-CB-CG	-5.60	107.00	112.60
1	B	332	ASP	CA-CB-CG	-5.58	107.02	112.60
1	B	153	HIS	N-CA-C	5.56	117.02	111.07
1	B	699	ASP	CA-CB-CG	-5.56	107.04	112.60
1	A	840	HIS	N-CA-C	-5.55	105.31	111.36
1	B	840	HIS	N-CA-C	-5.53	105.33	111.36
1	A	541	CYS	CB-CA-C	-5.53	101.22	110.29
1	B	541	CYS	CB-CA-C	-5.52	101.23	110.29
1	A	683	ASP	CA-CB-CG	-5.52	107.08	112.60
1	B	252	PHE	CA-CB-CG	-5.50	108.30	113.80
1	B	683	ASP	CA-CB-CG	-5.46	107.14	112.60
1	B	76	ASP	CA-CB-CG	-5.46	107.14	112.60
1	A	76	ASP	CA-CB-CG	-5.45	107.15	112.60
1	A	252	PHE	CA-CB-CG	-5.43	108.37	113.80
1	B	95	TYR	N-CA-CB	5.41	115.89	109.72
1	B	96	PRO	N-CA-CB	5.39	108.31	103.08
1	A	95	TYR	N-CA-CB	5.37	115.84	109.72
1	A	237	PRO	CA-C-N	5.36	132.03	121.58
1	A	237	PRO	C-N-CA	5.36	132.03	121.58
1	A	977	ASN	CA-CB-CG	-5.35	107.25	112.60
1	B	881	ASN	CB-CA-C	-5.35	103.89	111.76
1	A	96	PRO	N-CA-CB	5.34	108.26	103.08
1	B	237	PRO	CA-C-N	5.34	131.99	121.58
1	B	237	PRO	C-N-CA	5.34	131.99	121.58
1	A	881	ASN	CB-CA-C	-5.33	103.93	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASN	CA-CB-CG	-5.32	107.28	112.60
1	B	302	ASN	CA-CB-CG	-5.32	107.28	112.60
1	A	956	ALA	N-CA-C	5.32	118.23	111.69
1	A	1006	ASN	CA-CB-CG	-5.30	107.30	112.60
1	B	350	ASP	CA-CB-CG	-5.30	107.30	112.60
1	A	350	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	691	GLU	CA-C-N	5.28	130.18	120.79
1	A	691	GLU	C-N-CA	5.28	130.18	120.79
1	B	152	PHE	N-CA-C	5.27	119.83	113.41
1	A	565	ASN	CA-CB-CG	-5.26	107.34	112.60
1	B	565	ASN	CA-CB-CG	-5.25	107.34	112.60
1	B	691	GLU	CA-C-N	5.25	130.14	120.79
1	B	691	GLU	C-N-CA	5.25	130.14	120.79
1	A	152	PHE	N-CA-C	5.23	119.79	113.41
1	A	159	LEU	N-CA-C	5.17	117.71	111.40
1	A	287	THR	CA-C-N	5.16	128.16	120.31
1	A	287	THR	C-N-CA	5.16	128.16	120.31
1	A	1029	GLN	CA-C-N	5.16	127.71	120.28
1	A	1029	GLN	C-N-CA	5.16	127.71	120.28
1	B	151	PRO	CA-C-N	5.16	131.32	122.09
1	B	151	PRO	C-N-CA	5.16	131.32	122.09
1	B	886	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	886	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	774	ASN	CB-CA-C	-5.14	102.80	110.88
1	B	159	LEU	N-CA-C	5.14	117.67	111.40
1	A	151	PRO	CA-C-N	5.14	131.29	122.09
1	A	151	PRO	C-N-CA	5.14	131.29	122.09
1	B	287	THR	CA-C-N	5.13	128.10	120.31
1	B	287	THR	C-N-CA	5.13	128.10	120.31
1	A	855	THR	CA-C-N	5.12	128.35	122.83
1	A	855	THR	C-N-CA	5.12	128.35	122.83
1	B	774	ASN	CB-CA-C	-5.11	102.86	110.88
1	A	472	VAL	CA-C-N	-5.10	112.20	120.72
1	A	472	VAL	C-N-CA	-5.10	112.20	120.72
1	B	512	TYR	CA-CB-CG	-5.10	104.71	113.90
1	B	215	TYR	CA-CB-CG	-5.10	104.72	113.90
1	A	215	TYR	CA-CB-CG	-5.09	104.73	113.90
1	A	512	TYR	CA-CB-CG	-5.09	104.73	113.90
1	B	855	THR	CA-C-N	5.09	128.33	122.83
1	B	855	THR	C-N-CA	5.09	128.33	122.83
1	B	472	VAL	CA-C-N	-5.08	112.23	120.72
1	B	472	VAL	C-N-CA	-5.08	112.23	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	181	LYS	N-CA-C	5.08	121.61	110.80
1	B	844	TRP	CA-C-N	-5.06	116.02	123.00
1	B	844	TRP	C-N-CA	-5.06	116.02	123.00
1	A	163	ASN	CA-CB-CG	-5.05	107.55	112.60
1	B	181	LYS	N-CA-C	5.05	121.55	110.80
1	A	844	TRP	CA-C-N	-5.04	116.04	123.00
1	A	844	TRP	C-N-CA	-5.04	116.04	123.00
1	A	50	PHE	N-CA-C	5.03	116.05	108.46
1	B	523	ASP	CB-CA-C	-5.02	102.01	109.60
1	B	162	VAL	CA-C-N	5.02	129.93	121.14
1	B	162	VAL	C-N-CA	5.02	129.93	121.14
1	B	851	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	374	TYR	CA-CB-CG	-5.01	104.87	113.90
1	A	162	VAL	CA-C-N	5.00	129.90	121.14
1	A	162	VAL	C-N-CA	5.00	129.90	121.14
1	B	374	TYR	CA-CB-CG	-5.00	104.89	113.90
1	A	523	ASP	CB-CA-C	-5.00	102.05	109.60

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	854	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	Peptide
1	B	557	CYS	Mainchain
1	B	700	CYS	Mainchain
1	B	863	ILE	Peptide
1	B	95	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7711	1271	34
1	B	7189	0	7050	1099	67

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15030	0	14761	2370	69

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 80.

All (2370) 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:868:PRO:HD2	1:A:981:GLY:CA	1.32	1.52
1:A:868:PRO:CD	1:A:981:GLY:CA	1.87	1.50
1:A:873:THR:CA	1:A:982:SER:HB2	1.46	1.43
1:A:873:THR:HA	1:A:982:SER:CB	1.48	1.40
1:A:870:GLU:CD	1:A:1025:ALA:HB2	1.46	1.38
1:B:506:VAL:HG22	1:B:525:HIS:NE2	1.33	1.38
1:B:629:HIS:CE1	1:B:669:TYR:OH	1.76	1.37
1:B:629:HIS:ND1	1:B:669:TYR:OH	1.56	1.34
1:A:868:PRO:HD3	1:A:981:GLY:N	1.06	1.33
1:B:506:VAL:C	1:B:507:GLU:N	1.82	1.33
1:A:506:VAL:C	1:A:507:GLU:N	1.87	1.31
1:B:506:VAL:N	1:B:507:GLU:N	1.77	1.29
1:A:868:PRO:CD	1:A:981:GLY:N	1.88	1.27
1:B:809:SER:HB2	1:B:881:ASN:CG	1.62	1.23
1:B:700:CYS:O	1:B:725:ASN:HB2	1.38	1.23
1:A:870:GLU:HB3	1:A:1024:ARG:CG	1.70	1.22
1:A:868:PRO:HD3	1:A:980:ALA:C	1.63	1.21
1:A:440:LYS:HB2	1:A:538:LYS:HZ2	1.04	1.19
1:B:809:SER:CB	1:B:881:ASN:OD1	1.89	1.19
1:B:802:LYS:C	1:B:803:CYS:N	2.01	1.19
1:A:569:VAL:CG2	1:A:654:ASN:HB2	1.71	1.18
1:A:867:GLY:HA2	1:A:981:GLY:N	1.59	1.17
1:A:359:LEU:HD12	1:A:362:ILE:HD11	1.24	1.17
1:B:118:LEU:HD12	1:B:172:ILE:HD12	1.17	1.17
1:B:456:LYS:HD2	1:B:523:ASP:OD2	1.44	1.17
1:B:676:TYR:CE1	1:B:730:GLN:HG2	1.80	1.15
1:B:295:VAL:HG12	1:B:414:VAL:HG11	1.27	1.14
1:A:453:LYS:HG2	1:A:472:VAL:HG22	1.25	1.14
1:B:359:LEU:HD12	1:B:362:ILE:HD11	1.24	1.14
1:B:506:VAL:CG2	1:B:525:HIS:NE2	2.11	1.14
1:A:324:THR:HB	1:A:462:PRO:HB3	1.27	1.13
1:A:118:LEU:HD12	1:A:172:ILE:HD12	1.17	1.12
1:A:458:ARG:HD2	1:A:524:PRO:HB3	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:MET:HE1	1:A:227:LYS:HG3	1.31	1.12
1:A:435:ILE:HG22	1:A:446:PHE:HB2	1.22	1.12
1:A:295:VAL:HG12	1:A:414:VAL:HG11	1.27	1.12
1:B:453:LYS:HG2	1:B:472:VAL:HG22	1.25	1.12
1:B:435:ILE:HG22	1:B:446:PHE:HB2	1.22	1.11
1:B:809:SER:HB2	1:B:881:ASN:OD1	0.95	1.11
1:A:533:ASN:ND2	1:A:644:THR:O	1.83	1.11
1:A:595:GLU:HB2	1:A:597:LEU:HD23	1.32	1.11
1:B:506:VAL:C	1:B:507:GLU:CA	2.21	1.11
1:B:676:TYR:CD1	1:B:730:GLN:CG	2.33	1.11
1:B:469:TYR:HB2	1:B:523:ASP:OD1	1.50	1.10
1:B:595:GLU:HB2	1:B:597:LEU:HD23	1.32	1.10
1:B:324:THR:HB	1:B:462:PRO:HB3	1.27	1.09
1:A:868:PRO:CD	1:A:981:GLY:HA3	1.61	1.09
1:A:871:GLY:O	1:A:1023:ASP:CB	2.00	1.09
1:A:1017:LYS:H	1:A:1017:LYS:HE2	1.18	1.08
1:B:444:LEU:HD23	1:B:524:PRO:CG	1.83	1.08
1:B:676:TYR:CE1	1:B:730:GLN:CG	2.37	1.08
1:A:474:VAL:HG12	1:A:475:VAL:HG23	1.33	1.08
1:A:868:PRO:HD2	1:A:981:GLY:HA2	1.17	1.08
1:B:468:GLN:HG3	1:B:523:ASP:HA	1.16	1.07
1:B:469:TYR:CB	1:B:523:ASP:OD1	2.02	1.07
1:A:870:GLU:CB	1:A:1024:ARG:HG2	1.84	1.07
1:B:474:VAL:HG12	1:B:475:VAL:HG23	1.33	1.07
1:A:439:TYR:CE2	1:A:538:LYS:NZ	2.23	1.06
1:A:871:GLY:O	1:A:1023:ASP:CG	1.98	1.06
1:A:1016:MET:HE2	1:A:1033:PHE:HB3	1.35	1.06
1:A:549:ARG:HD3	1:A:584:PRO:CB	1.84	1.06
1:A:440:LYS:HB2	1:A:538:LYS:NZ	1.68	1.06
1:A:806:MET:H	1:A:806:MET:HE3	1.16	1.05
1:B:506:VAL:CA	1:B:507:GLU:N	2.17	1.05
1:B:676:TYR:CD1	1:B:730:GLN:HG3	1.91	1.05
1:B:225:MET:HE1	1:B:227:LYS:HG3	1.32	1.04
1:A:569:VAL:HG21	1:A:654:ASN:HB2	1.32	1.04
1:B:506:VAL:HG22	1:B:525:HIS:CE1	1.92	1.04
1:B:444:LEU:HD23	1:B:524:PRO:HG3	1.37	1.03
1:B:301:ARG:HD2	1:B:425:THR:HG21	1.37	1.03
1:B:494:TYR:HB3	1:B:501:LEU:HD21	1.40	1.03
1:B:548:ARG:HG3	1:B:583:VAL:C	1.84	1.03
1:B:620:PRO:HA	1:B:623:ILE:HG13	1.41	1.03
1:B:806:MET:HE3	1:B:806:MET:H	1.16	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:PRO:HG2	1:A:69:ARG:HG3	1.41	1.02
1:A:301:ARG:HD2	1:A:425:THR:HG21	1.37	1.02
1:A:560:LEU:HD23	1:A:648:THR:HG23	1.37	1.02
1:A:440:LYS:HD2	1:A:538:LYS:HD3	1.37	1.02
1:A:620:PRO:HA	1:A:623:ILE:HG13	1.41	1.01
1:A:867:GLY:CA	1:A:981:GLY:H	1.72	1.01
1:A:494:TYR:HB3	1:A:501:LEU:HD21	1.40	1.01
1:A:870:GLU:CD	1:A:1025:ALA:CB	2.33	1.01
1:B:676:TYR:CD1	1:B:730:GLN:HG2	1.94	1.00
1:B:560:LEU:HD23	1:B:648:THR:HG23	1.37	1.00
1:B:46:PRO:HG2	1:B:69:ARG:HG3	1.41	1.00
1:A:873:THR:OG1	1:A:981:GLY:HA2	1.60	0.99
1:B:117:LEU:HD11	1:B:126:LEU:HD21	1.45	0.99
1:B:505:PRO:C	1:B:507:GLU:N	2.19	0.99
1:A:117:LEU:HD11	1:A:126:LEU:HD21	1.45	0.99
1:A:870:GLU:CB	1:A:1024:ARG:CG	2.40	0.99
1:B:623:ILE:HA	1:B:626:ASN:HD21	1.28	0.99
1:A:868:PRO:HD3	1:A:981:GLY:CA	1.73	0.99
1:A:870:GLU:HB3	1:A:1024:ARG:HG2	1.01	0.99
1:B:506:VAL:C	1:B:507:GLU:HA	1.84	0.98
1:A:458:ARG:HD2	1:A:524:PRO:CB	1.92	0.98
1:B:444:LEU:HD12	1:B:446:PHE:CE1	1.98	0.98
1:B:862:ILE:HG22	1:B:877:ILE:HA	1.46	0.98
1:A:444:LEU:HD12	1:A:446:PHE:CE1	1.98	0.97
1:A:870:GLU:OE1	1:A:1025:ALA:HB2	1.62	0.97
1:A:563:HIS:HB3	1:A:564:PRO:HD3	1.44	0.97
1:B:563:HIS:HB3	1:B:564:PRO:HD3	1.44	0.97
1:A:623:ILE:HA	1:A:626:ASN:HD21	1.28	0.96
1:A:862:ILE:HG22	1:A:877:ILE:HA	1.46	0.96
1:A:870:GLU:HG2	1:A:1024:ARG:C	1.91	0.96
1:B:662:LEU:HD23	1:B:791:ASP:OD2	1.65	0.96
1:B:949:TYR:HE2	1:B:951:MET:HE2	1.31	0.95
1:B:566:ASN:HA	1:B:651:VAL:HG23	1.49	0.95
1:B:458:ARG:HD2	1:B:524:PRO:HB3	1.45	0.95
1:B:629:HIS:CG	1:B:669:TYR:OH	2.15	0.95
1:A:566:ASN:HA	1:A:651:VAL:HG23	1.49	0.95
1:A:1016:MET:HE2	1:A:1033:PHE:CB	1.97	0.94
1:A:949:TYR:HE2	1:A:951:MET:HE2	1.31	0.94
1:A:42:PHE:HE1	1:A:79:VAL:HG22	1.31	0.94
1:A:868:PRO:HD2	1:A:981:GLY:HA3	1.16	0.94
1:A:870:GLU:OE2	1:A:1025:ALA:HB2	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:LEU:HD11	1:A:1006:ASN:HD22	1.31	0.94
1:A:72:LYS:HE3	1:A:80:LEU:HD13	1.49	0.94
1:A:871:GLY:O	1:A:1023:ASP:HB3	1.68	0.93
1:A:873:THR:C	1:A:982:SER:HB2	1.91	0.93
1:B:62:ILE:CG1	1:B:73:LEU:HB2	1.98	0.93
1:B:42:PHE:HE1	1:B:79:VAL:HG22	1.31	0.93
1:A:297:ILE:HG22	1:A:418:VAL:CG1	1.97	0.93
1:A:870:GLU:CG	1:A:1024:ARG:HG3	1.97	0.93
1:B:456:LYS:CD	1:B:523:ASP:OD2	2.15	0.93
1:B:297:ILE:HG22	1:B:418:VAL:HG12	1.49	0.93
1:B:804:GLY:HA2	1:B:806:MET:SD	2.09	0.93
1:A:62:ILE:CG1	1:A:73:LEU:HB2	1.98	0.93
1:B:225:MET:HE1	1:B:227:LYS:CG	1.99	0.93
1:A:440:LYS:HD2	1:A:538:LYS:CD	1.98	0.93
1:A:804:GLY:HA2	1:A:806:MET:SD	2.09	0.93
1:B:297:ILE:HG22	1:B:418:VAL:CG1	1.97	0.93
1:B:865:VAL:HG13	1:B:866:THR:HG23	1.50	0.93
1:A:297:ILE:HG22	1:A:418:VAL:HG12	1.49	0.93
1:B:863:ILE:HG22	1:B:876:THR:HB	1.48	0.92
1:A:863:ILE:HG22	1:A:876:THR:HB	1.48	0.92
1:A:39:PHE:CE2	1:A:473:GLN:HG3	2.05	0.92
1:B:72:LYS:HE3	1:B:80:LEU:HD13	1.49	0.92
1:B:271:LYS:HG3	1:B:272:GLU:H	1.34	0.92
1:A:225:MET:HE1	1:A:227:LYS:CG	1.99	0.92
1:A:435:ILE:HD13	1:A:436:ALA:H	1.34	0.92
1:B:527:GLY:HA3	1:B:550:PHE:CZ	2.04	0.92
1:A:239:PHE:HA	1:A:260:PRO:HG2	1.51	0.92
1:A:865:VAL:HG13	1:A:866:THR:HG23	1.50	0.92
1:B:39:PHE:CE2	1:B:473:GLN:HG3	2.05	0.92
1:A:933:VAL:HG23	1:A:934:ALA:H	1.35	0.91
1:B:239:PHE:HA	1:B:260:PRO:HG2	1.51	0.91
1:B:806:MET:SD	1:B:807:ARG:HG3	2.11	0.91
1:B:435:ILE:HD13	1:B:436:ALA:H	1.34	0.91
1:A:806:MET:SD	1:A:807:ARG:HG3	2.11	0.91
1:B:196:PRO:HB3	1:B:225:MET:HE2	1.53	0.90
1:A:527:GLY:HA3	1:A:550:PHE:CZ	2.05	0.90
1:A:447:VAL:HG22	1:A:455:LYS:HB2	1.53	0.90
1:A:549:ARG:HD3	1:A:584:PRO:HB2	1.53	0.90
1:B:933:VAL:HG23	1:B:934:ALA:H	1.36	0.90
1:A:271:LYS:HG3	1:A:272:GLU:H	1.34	0.90
1:A:359:LEU:CD1	1:A:362:ILE:HD11	2.02	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:CG2	1:A:455:LYS:HB2	2.03	0.89
1:A:972:THR:HG23	1:A:1002:TYR:CE1	2.07	0.89
1:B:653:TYR:HE2	1:B:682:HIS:ND1	1.69	0.89
1:A:453:LYS:CG	1:A:472:VAL:HG22	2.03	0.88
1:B:447:VAL:CG2	1:B:455:LYS:HB2	2.03	0.88
1:B:453:LYS:CG	1:B:472:VAL:HG22	2.03	0.88
1:B:95:TYR:CD2	1:B:96:PRO:HD3	2.08	0.88
1:B:447:VAL:HG22	1:B:455:LYS:HB2	1.53	0.88
1:B:802:LYS:O	1:B:803:CYS:N	2.06	0.88
1:B:181:LYS:CD	1:B:202:LYS:HA	2.04	0.88
1:A:870:GLU:OE2	1:A:1025:ALA:CB	2.22	0.88
1:B:359:LEU:CD1	1:B:362:ILE:HD11	2.02	0.88
1:A:863:ILE:HG23	1:A:864:PRO:HD2	1.55	0.88
1:B:892:HIS:HB2	1:B:932:CYS:O	1.74	0.88
1:A:446:PHE:HD2	1:A:454:LEU:HD21	1.38	0.87
1:B:847:LEU:HG	1:B:850:ALA:H	1.39	0.87
1:A:951:MET:C	1:A:952:THR:N	2.32	0.87
1:B:486:PHE:CD1	1:B:493:LEU:HD13	2.09	0.87
1:B:653:TYR:C	1:B:654:ASN:N	2.31	0.87
1:A:95:TYR:CD2	1:A:96:PRO:HD3	2.08	0.87
1:A:532:HIS:HA	1:A:641:THR:OG1	1.73	0.87
1:A:892:HIS:HB2	1:A:932:CYS:O	1.73	0.87
1:A:867:GLY:HA2	1:A:981:GLY:H	0.77	0.87
1:A:486:PHE:CD1	1:A:493:LEU:HD13	2.09	0.87
1:B:468:GLN:HG3	1:B:523:ASP:CA	2.03	0.87
1:B:863:ILE:HG23	1:B:864:PRO:HD2	1.56	0.86
1:B:110:THR:CG2	1:B:132:LEU:HD21	2.05	0.86
1:B:439:TYR:CE2	1:B:538:LYS:NZ	2.42	0.86
1:A:39:PHE:CE1	1:A:505:PRO:HD2	2.10	0.86
1:A:959:LYS:HB2	1:A:972:THR:HB	1.57	0.86
1:A:110:THR:CG2	1:A:132:LEU:HD21	2.05	0.86
1:A:181:LYS:CD	1:A:202:LYS:HA	2.04	0.86
1:A:833:LEU:HB2	1:A:836:HIS:HD2	1.39	0.86
1:B:446:PHE:HD2	1:B:454:LEU:HD21	1.38	0.86
1:B:603:LEU:HD23	1:B:604:VAL:N	1.90	0.86
1:B:699:ASP:HA	1:B:725:ASN:OD1	1.74	0.86
1:A:370:LEU:CD1	1:A:399:ILE:HD12	2.06	0.86
1:B:256:LEU:HB3	1:B:309:LEU:HD22	1.56	0.86
1:B:435:ILE:CG2	1:B:446:PHE:HB2	2.06	0.86
1:A:196:PRO:HB3	1:A:225:MET:HE2	1.53	0.86
1:B:833:LEU:HB2	1:B:836:HIS:HD2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:HA	1:B:414:VAL:CG2	2.05	0.86
1:A:118:LEU:HD13	1:A:119:ILE:N	1.91	0.86
1:A:295:VAL:HA	1:A:414:VAL:CG2	2.05	0.86
1:B:100:VAL:HG12	1:B:101:GLN:HG3	1.58	0.86
1:B:473:GLN:CG	1:B:504:VAL:HG22	2.06	0.86
1:B:700:CYS:HB3	1:B:701:PRO:CD	1.92	0.86
1:B:847:LEU:HD12	1:B:852:SER:HB3	1.58	0.86
1:A:603:LEU:HD23	1:A:604:VAL:N	1.90	0.85
1:B:370:LEU:CD1	1:B:399:ILE:HD12	2.05	0.85
1:B:531:LEU:O	1:B:641:THR:OG1	1.94	0.85
1:B:847:LEU:HD11	1:B:850:ALA:HA	1.58	0.85
1:A:100:VAL:HG12	1:A:101:GLN:HG3	1.58	0.85
1:B:676:TYR:HE1	1:B:730:GLN:HG2	1.41	0.85
1:B:133:TYR:CG	1:B:136:ILE:HG12	2.12	0.85
1:A:882:LEU:HB2	1:A:910:ALA:HA	1.58	0.85
1:A:847:LEU:HD12	1:A:852:SER:HB3	1.58	0.85
1:A:133:TYR:CG	1:A:136:ILE:HG12	2.12	0.85
1:A:706:VAL:HG22	1:A:707:ASP:H	1.42	0.85
1:A:473:GLN:CG	1:A:504:VAL:HG22	2.06	0.85
1:A:42:PHE:CZ	1:A:45:GLU:HB2	2.12	0.84
1:A:847:LEU:HG	1:A:850:ALA:H	1.39	0.84
1:B:118:LEU:HD13	1:B:119:ILE:N	1.91	0.84
1:B:39:PHE:CE1	1:B:505:PRO:HD2	2.11	0.84
1:A:256:LEU:HB3	1:A:309:LEU:HD22	1.56	0.84
1:B:548:ARG:HG3	1:B:583:VAL:O	1.77	0.84
1:A:989:GLY:HA2	1:A:1017:LYS:HE3	1.57	0.84
1:B:42:PHE:CZ	1:B:45:GLU:HB2	2.12	0.84
1:B:356:ILE:CG2	1:B:421:ILE:HB	2.07	0.84
1:B:295:VAL:CG1	1:B:414:VAL:HG11	2.07	0.84
1:A:951:MET:HG2	1:A:977:ASN:CG	2.03	0.84
1:B:50:PHE:HB2	1:B:498:GLU:O	1.78	0.84
1:B:40:VAL:CG1	1:B:503:ARG:HB3	2.08	0.84
1:B:809:SER:CB	1:B:881:ASN:CG	2.47	0.83
1:A:40:VAL:CG1	1:A:503:ARG:HB3	2.08	0.83
1:B:295:VAL:HA	1:B:414:VAL:HG22	1.60	0.83
1:A:229:PRO:O	1:A:232:THR:HG22	1.79	0.83
1:A:356:ILE:CG2	1:A:421:ILE:HB	2.07	0.83
1:A:336:THR:O	1:A:354:LEU:HD12	1.78	0.83
1:A:863:ILE:CG2	1:A:876:THR:HB	2.07	0.83
1:A:971:VAL:HG22	1:A:1005:CYS:O	1.78	0.83
1:B:706:VAL:HG22	1:B:707:ASP:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD12	1:A:172:ILE:CD1	2.05	0.83
1:B:830:GLN:HG2	1:B:831:CYS:H	1.43	0.83
1:B:474:VAL:HG22	1:B:495:ILE:HG21	1.61	0.83
1:B:118:LEU:HD12	1:B:172:ILE:CD1	2.05	0.83
1:B:336:THR:O	1:B:354:LEU:HD12	1.78	0.83
1:B:358:ILE:HG23	1:B:361:GLN:H	1.44	0.83
1:A:42:PHE:CE1	1:A:79:VAL:HG22	2.14	0.83
1:A:397:LEU:HD23	1:A:399:ILE:HD13	1.61	0.83
1:A:847:LEU:HD11	1:A:850:ALA:HA	1.58	0.83
1:A:996:HIS:HB3	1:A:1004:ILE:HG23	1.59	0.83
1:B:53:LEU:HB2	1:B:496:MET:HE3	1.61	0.83
1:B:229:PRO:O	1:B:232:THR:HG22	1.79	0.83
1:A:295:VAL:CG1	1:A:414:VAL:HG11	2.07	0.83
1:B:133:TYR:CB	1:B:136:ILE:HG12	2.09	0.83
1:A:440:LYS:CD	1:A:538:LYS:HD3	2.08	0.82
1:A:474:VAL:HG22	1:A:495:ILE:HG21	1.61	0.82
1:B:53:LEU:HD23	1:B:54:VAL:N	1.94	0.82
1:B:397:LEU:HD23	1:B:399:ILE:HD13	1.61	0.82
1:A:358:ILE:HG23	1:A:361:GLN:H	1.44	0.82
1:B:295:VAL:HG12	1:B:414:VAL:CG1	2.09	0.82
1:A:435:ILE:CG2	1:A:446:PHE:HB2	2.06	0.82
1:A:548:ARG:HG3	1:A:583:VAL:O	1.79	0.82
1:B:785:ASN:HB3	1:B:788:PHE:CD2	2.14	0.82
1:B:863:ILE:CG2	1:B:876:THR:HB	2.07	0.82
1:A:987:MET:HB2	1:A:1019:THR:CG2	2.09	0.82
1:A:44:GLY:HA2	1:A:50:PHE:CE2	2.15	0.82
1:A:53:LEU:HD23	1:A:54:VAL:N	1.94	0.82
1:A:44:GLY:HA2	1:A:50:PHE:HE2	1.44	0.82
1:B:44:GLY:HA2	1:B:50:PHE:CE2	2.15	0.82
1:B:949:TYR:CE2	1:B:951:MET:HE2	2.15	0.82
1:A:133:TYR:CB	1:A:136:ILE:HG12	2.09	0.82
1:A:785:ASN:HB3	1:A:788:PHE:CD2	2.14	0.82
1:A:50:PHE:HB2	1:A:498:GLU:O	1.78	0.82
1:A:295:VAL:HA	1:A:414:VAL:HG22	1.60	0.82
1:A:439:TYR:CE2	1:A:538:LYS:CE	2.63	0.82
1:A:991:GLN:CG	1:A:1008:THR:HG21	2.10	0.82
1:B:185:ALA:HB1	1:B:243:TYR:CE1	2.15	0.82
1:A:397:LEU:HD23	1:A:399:ILE:CD1	2.10	0.81
1:A:994:LEU:HD11	1:A:1006:ASN:HB2	1.63	0.81
1:B:356:ILE:HG22	1:B:421:ILE:HB	1.61	0.81
1:B:882:LEU:HB2	1:B:910:ALA:HA	1.58	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:TYR:CE2	1:A:951:MET:HE2	2.15	0.81
1:B:62:ILE:HG13	1:B:73:LEU:HB2	1.62	0.81
1:A:889:ILE:HG23	1:A:892:HIS:CE1	2.16	0.81
1:B:154:LYS:HD3	1:B:210:ASP:OD1	1.81	0.81
1:B:397:LEU:HD23	1:B:399:ILE:CD1	2.11	0.81
1:B:863:ILE:HG13	1:B:864:PRO:HD3	1.62	0.81
1:A:458:ARG:HD2	1:A:524:PRO:CG	2.10	0.81
1:B:42:PHE:CE1	1:B:79:VAL:HG22	2.14	0.81
1:A:1016:MET:O	1:A:1016:MET:HE3	1.80	0.81
1:A:440:LYS:CB	1:A:538:LYS:NZ	2.44	0.81
1:A:154:LYS:HD3	1:A:210:ASP:OD1	1.81	0.80
1:B:154:LYS:HB2	1:B:157:HIS:CD2	2.16	0.80
1:B:324:THR:HB	1:B:462:PRO:CB	2.10	0.80
1:A:185:ALA:HB1	1:A:243:TYR:CE1	2.15	0.80
1:A:623:ILE:HD12	1:A:624:THR:N	1.96	0.80
1:B:486:PHE:CE1	1:B:493:LEU:HD13	2.16	0.80
1:B:889:ILE:HG23	1:B:892:HIS:CE1	2.16	0.80
1:A:53:LEU:HB2	1:A:496:MET:HE3	1.61	0.80
1:A:830:GLN:HG2	1:A:831:CYS:H	1.43	0.80
1:A:356:ILE:HG22	1:A:421:ILE:HB	1.61	0.80
1:A:486:PHE:CE1	1:A:493:LEU:HD13	2.16	0.80
1:B:444:LEU:HD13	1:B:445:ALA:N	1.97	0.80
1:B:623:ILE:HD12	1:B:624:THR:N	1.96	0.80
1:A:620:PRO:HA	1:A:623:ILE:CG1	2.12	0.80
1:B:314:LEU:HD11	1:B:332:ASP:HB3	1.64	0.80
1:B:192:PRO:HB3	1:B:233:PHE:CE1	2.17	0.80
1:B:653:TYR:HE2	1:B:682:HIS:HD1	1.27	0.80
1:A:994:LEU:CD1	1:A:1006:ASN:HB2	2.12	0.79
1:B:620:PRO:HA	1:B:623:ILE:CG1	2.12	0.79
1:B:699:ASP:C	1:B:725:ASN:OD1	2.26	0.79
1:A:192:PRO:HB3	1:A:233:PHE:CE1	2.17	0.79
1:B:239:PHE:CE1	1:B:260:PRO:HD2	2.17	0.79
1:B:317:ALA:HB1	1:B:321:LEU:HB3	1.64	0.79
1:B:380:LEU:HD12	1:B:386:LYS:HE3	1.64	0.79
1:A:321:LEU:HD12	1:A:462:PRO:HG2	1.64	0.79
1:A:591:ASN:OD1	1:A:639:LYS:HE2	1.83	0.79
1:A:926:ALA:HB1	1:A:947:LEU:HD12	1.63	0.79
1:B:699:ASP:CA	1:B:725:ASN:OD1	2.29	0.79
1:A:154:LYS:HB2	1:A:157:HIS:CD2	2.16	0.79
1:A:370:LEU:HD12	1:A:399:ILE:HD12	1.64	0.79
1:B:370:LEU:HD12	1:B:399:ILE:HD12	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:CE1	1:A:260:PRO:HD2	2.17	0.79
1:A:244:VAL:HG13	1:A:482:ARG:NH1	1.98	0.79
1:B:244:VAL:HG13	1:B:482:ARG:NH1	1.98	0.79
1:A:324:THR:HB	1:A:462:PRO:CB	2.10	0.79
1:A:444:LEU:HD13	1:A:445:ALA:N	1.97	0.79
1:A:863:ILE:HG13	1:A:864:PRO:HD3	1.62	0.79
1:B:591:ASN:OD1	1:B:639:LYS:HE2	1.83	0.79
1:A:62:ILE:HG13	1:A:73:LEU:HB2	1.62	0.79
1:B:44:GLY:HA2	1:B:50:PHE:HE2	1.44	0.79
1:B:319:ALA:H	1:B:441:ASN:HD22	1.31	0.79
1:B:926:ALA:HB1	1:B:947:LEU:HD12	1.63	0.79
1:A:715:VAL:HG21	1:A:717:LYS:HD2	1.65	0.78
1:B:453:LYS:HE3	1:B:472:VAL:CG2	2.13	0.78
1:B:715:VAL:HG21	1:B:717:LYS:HD2	1.65	0.78
1:A:181:LYS:HZ3	1:A:216:VAL:HG23	1.48	0.78
1:A:319:ALA:H	1:A:441:ASN:HD22	1.31	0.78
1:A:231:ASP:O	1:A:234:THR:HG22	1.84	0.78
1:A:295:VAL:HG12	1:A:414:VAL:CG1	2.09	0.78
1:A:847:LEU:CG	1:A:850:ALA:HA	2.13	0.78
1:B:320:VAL:HG21	1:B:442:HIS:CD2	2.19	0.78
1:A:453:LYS:HE3	1:A:472:VAL:CG2	2.13	0.78
1:A:320:VAL:HG21	1:A:442:HIS:CD2	2.19	0.78
1:A:742:ILE:HB	1:A:745:ILE:O	1.84	0.78
1:A:873:THR:HA	1:A:982:SER:HB2	0.82	0.78
1:B:469:TYR:HB3	1:B:523:ASP:OD1	1.81	0.78
1:B:742:ILE:HB	1:B:745:ILE:O	1.84	0.78
1:A:380:LEU:HD12	1:A:386:LYS:HE3	1.64	0.78
1:A:868:PRO:CG	1:A:981:GLY:HA3	2.12	0.78
1:B:56:ASP:OD2	1:B:142:LEU:HD11	1.83	0.78
1:B:321:LEU:HD12	1:B:462:PRO:HG2	1.64	0.78
1:A:181:LYS:NZ	1:A:216:VAL:HG23	1.98	0.78
1:A:327:VAL:HG12	1:A:358:ILE:HD11	1.66	0.78
1:A:972:THR:HA	1:A:1002:TYR:HE1	1.47	0.78
1:B:439:TYR:OH	1:B:538:LYS:HE3	1.83	0.78
1:A:439:TYR:CZ	1:A:538:LYS:CE	2.67	0.78
1:A:870:GLU:HG2	1:A:1025:ALA:N	1.98	0.78
1:A:51:ASN:HD21	1:A:67:VAL:HG23	1.49	0.78
1:A:994:LEU:HD12	1:A:994:LEU:O	1.84	0.78
1:B:847:LEU:CG	1:B:850:ALA:HA	2.13	0.78
1:A:314:LEU:HD11	1:A:332:ASP:HB3	1.64	0.77
1:A:710:LEU:O	1:A:710:LEU:HD12	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:O	1:A:284:LYS:HD3	1.84	0.77
1:B:51:ASN:HD21	1:B:67:VAL:HG23	1.50	0.77
1:B:168:VAL:HG23	1:B:185:ALA:O	1.84	0.77
1:B:917:MET:HE1	1:B:948:TYR:OH	1.84	0.77
1:A:327:VAL:CG1	1:A:358:ILE:HD11	2.14	0.77
1:A:1014:LEU:H	1:A:1014:LEU:HD22	1.48	0.77
1:A:1016:MET:HG2	1:A:1035:TYR:CE2	2.19	0.77
1:B:327:VAL:CG1	1:B:358:ILE:HD11	2.14	0.77
1:A:56:ASP:OD2	1:A:142:LEU:HD11	1.83	0.77
1:B:710:LEU:HD12	1:B:710:LEU:O	1.84	0.77
1:B:595:GLU:CB	1:B:597:LEU:HD23	2.14	0.77
1:B:231:ASP:O	1:B:234:THR:HG22	1.84	0.77
1:B:327:VAL:HG12	1:B:358:ILE:HD11	1.65	0.77
1:B:567:ILE:HD13	1:B:567:ILE:H	1.50	0.77
1:A:168:VAL:HG23	1:A:185:ALA:O	1.84	0.77
1:A:917:MET:HE1	1:A:948:TYR:OH	1.84	0.77
1:B:662:LEU:HD11	1:B:702:GLN:NE2	1.99	0.77
1:A:317:ALA:HB1	1:A:321:LEU:HB3	1.64	0.77
1:A:547:PRO:O	1:A:548:ARG:HG2	1.84	0.77
1:A:870:GLU:HG3	1:A:1024:ARG:HG3	1.64	0.77
1:B:181:LYS:NZ	1:B:216:VAL:HG23	1.98	0.77
1:B:204:THR:HG21	1:B:209:ALA:HB3	1.66	0.77
1:B:359:LEU:HD12	1:B:362:ILE:CD1	2.10	0.77
1:A:1021:GLN:HG2	1:A:1026:ARG:HG3	1.67	0.77
1:B:403:PHE:CE1	1:B:406:LEU:HD23	2.20	0.77
1:A:549:ARG:HD3	1:A:584:PRO:HB3	1.66	0.76
1:A:567:ILE:H	1:A:567:ILE:HD13	1.50	0.76
1:B:284:LYS:O	1:B:284:LYS:HD3	1.84	0.76
1:A:120:ASP:OD2	1:A:123:GLU:HG3	1.86	0.76
1:A:403:PHE:CE1	1:A:406:LEU:HD23	2.20	0.76
1:A:439:TYR:OH	1:A:538:LYS:HE3	1.84	0.76
1:A:460:ASP:HB3	1:A:464:GLY:N	2.00	0.76
1:B:780:LEU:HD12	1:B:780:LEU:O	1.86	0.76
1:B:847:LEU:CD1	1:B:850:ALA:HA	2.16	0.76
1:A:873:THR:HA	1:A:982:SER:CA	2.15	0.76
1:B:172:ILE:HG12	1:B:182:LEU:HD13	1.68	0.76
1:B:616:ALA:O	1:B:620:PRO:HD2	1.85	0.76
1:A:359:LEU:HD12	1:A:362:ILE:CD1	2.09	0.76
1:A:616:ALA:O	1:A:620:PRO:HD2	1.85	0.76
1:A:780:LEU:HD12	1:A:780:LEU:O	1.86	0.76
1:B:120:ASP:OD2	1:B:123:GLU:HG3	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:LEU:HD12	1:B:496:MET:CE	2.16	0.76
1:B:460:ASP:HB3	1:B:464:GLY:N	2.00	0.76
1:A:873:THR:OG1	1:A:981:GLY:CA	2.34	0.76
1:A:42:PHE:HZ	1:A:45:GLU:HB2	1.50	0.75
1:A:256:LEU:CB	1:A:309:LEU:HD22	2.16	0.75
1:A:869:ARG:O	1:A:920:ALA:HB3	1.86	0.75
1:A:1010:SER:HB2	1:A:1035:TYR:CE2	2.20	0.75
1:A:172:ILE:HG12	1:A:182:LEU:HD13	1.68	0.75
1:A:458:ARG:CD	1:A:524:PRO:HB3	2.12	0.75
1:A:868:PRO:HG2	1:A:1022:VAL:HG22	1.65	0.75
1:A:919:GLU:HB3	1:A:1024:ARG:HH11	1.51	0.75
1:B:278:LYS:HE3	1:B:296:PRO:HG3	1.67	0.75
1:B:547:PRO:O	1:B:548:ARG:HG2	1.84	0.75
1:A:987:MET:HE2	1:A:990:SER:HA	1.65	0.75
1:B:847:LEU:HD12	1:B:852:SER:CB	2.16	0.75
1:A:874:LYS:N	1:A:982:SER:HB2	2.02	0.75
1:B:506:VAL:HG22	1:B:525:HIS:CD2	2.21	0.75
1:B:785:ASN:HB3	1:B:788:PHE:HD2	1.48	0.75
1:B:873:THR:HB	1:B:917:MET:CE	2.17	0.75
1:A:204:THR:HG21	1:A:209:ALA:HB3	1.66	0.75
1:A:806:MET:H	1:A:806:MET:CE	1.97	0.75
1:A:847:LEU:CD1	1:A:850:ALA:HA	2.16	0.75
1:A:873:THR:HG23	1:A:981:GLY:C	2.11	0.75
1:A:278:LYS:HE3	1:A:296:PRO:HG3	1.67	0.75
1:A:473:GLN:CB	1:A:504:VAL:HG22	2.17	0.75
1:B:323:ARG:HG3	1:B:324:THR:N	2.02	0.75
1:B:473:GLN:CB	1:B:504:VAL:HG22	2.17	0.75
1:B:784:TRP:HD1	1:B:790:ILE:HD11	1.51	0.75
1:B:806:MET:H	1:B:806:MET:CE	1.97	0.75
1:B:446:PHE:HB3	1:B:454:LEU:HD11	1.69	0.75
1:B:448:GLY:HA3	1:B:480:VAL:HG21	1.68	0.75
1:A:63:TYR:C	1:A:64:LEU:HD22	2.12	0.75
1:A:64:LEU:HD12	1:A:496:MET:CE	2.16	0.75
1:A:188:VAL:HG22	1:A:191:LYS:H	1.52	0.75
1:A:278:LYS:HG2	1:A:296:PRO:HA	1.69	0.75
1:A:739:ILE:CD1	1:A:748:ARG:HG2	2.17	0.75
1:A:847:LEU:HD12	1:A:852:SER:CB	2.16	0.75
1:B:700:CYS:CB	1:B:701:PRO:CD	2.50	0.75
1:A:323:ARG:HG3	1:A:324:THR:N	2.02	0.74
1:A:623:ILE:HA	1:A:626:ASN:ND2	2.01	0.74
1:A:683:ASP:O	1:A:686:THR:HG22	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:THR:HB	1:A:917:MET:CE	2.17	0.74
1:A:321:LEU:CD1	1:A:462:PRO:HG2	2.17	0.74
1:B:42:PHE:HZ	1:B:45:GLU:HB2	1.50	0.74
1:B:202:LYS:HD3	1:B:214:ALA:HB3	1.69	0.74
1:B:256:LEU:CB	1:B:309:LEU:HD22	2.16	0.74
1:B:321:LEU:CD1	1:B:462:PRO:HG2	2.17	0.74
1:B:869:ARG:O	1:B:920:ALA:HB3	1.86	0.74
1:A:99:ILE:HD11	1:A:152:PHE:HB2	1.69	0.74
1:A:785:ASN:HB3	1:A:788:PHE:HD2	1.48	0.74
1:A:151:PRO:HB2	1:A:157:HIS:ND1	2.02	0.74
1:B:623:ILE:HA	1:B:626:ASN:ND2	2.01	0.74
1:A:868:PRO:HG2	1:A:1022:VAL:CG2	2.17	0.74
1:A:448:GLY:HA3	1:A:480:VAL:HG21	1.68	0.74
1:B:151:PRO:HB2	1:B:157:HIS:ND1	2.03	0.74
1:B:188:VAL:HG22	1:B:191:LYS:H	1.52	0.74
1:A:1010:SER:HB2	1:A:1035:TYR:CZ	2.23	0.74
1:B:806:MET:HE3	1:B:806:MET:N	1.99	0.74
1:B:814:LEU:HB3	1:B:847:LEU:HB2	1.70	0.74
1:A:567:ILE:HD12	1:A:650:PHE:CZ	2.22	0.74
1:B:185:ALA:HB1	1:B:243:TYR:CZ	2.23	0.74
1:B:548:ARG:CG	1:B:584:PRO:HA	2.16	0.74
1:A:324:THR:HG21	1:A:462:PRO:HA	1.70	0.73
1:B:278:LYS:HG2	1:B:296:PRO:HA	1.68	0.73
1:B:739:ILE:CD1	1:B:748:ARG:HG2	2.17	0.73
1:A:185:ALA:HB1	1:A:243:TYR:CZ	2.23	0.73
1:A:569:VAL:CB	1:A:654:ASN:HB2	2.17	0.73
1:B:548:ARG:HG3	1:B:584:PRO:N	2.03	0.73
1:B:562:VAL:HG22	1:B:578:LEU:CD2	2.18	0.73
1:A:562:VAL:HG22	1:A:578:LEU:CD2	2.18	0.73
1:A:814:LEU:HB3	1:A:847:LEU:HB2	1.70	0.73
1:B:324:THR:HG21	1:B:462:PRO:HA	1.70	0.73
1:A:435:ILE:HD13	1:A:436:ALA:N	2.03	0.73
1:A:802:LYS:C	1:A:803:CYS:N	2.46	0.73
1:A:1016:MET:HE3	1:A:1016:MET:C	2.12	0.73
1:A:446:PHE:HB3	1:A:454:LEU:HD11	1.69	0.73
1:A:704:LEU:HD11	1:A:724:LYS:HE3	1.69	0.73
1:B:439:TYR:OH	1:B:538:LYS:CE	2.37	0.73
1:A:154:LYS:H	1:A:157:HIS:HD2	1.36	0.73
1:A:958:LEU:HD22	1:A:960:PRO:O	1.87	0.73
1:B:683:ASP:O	1:B:686:THR:HG22	1.88	0.73
1:B:468:GLN:CG	1:B:523:ASP:HA	2.08	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:PHE:CD2	1:A:454:LEU:HD21	2.24	0.73
1:B:46:PRO:HG2	1:B:69:ARG:CG	2.17	0.73
1:B:63:TYR:C	1:B:64:LEU:HD22	2.12	0.73
1:B:435:ILE:HD13	1:B:436:ALA:N	2.03	0.73
1:A:548:ARG:O	1:A:584:PRO:HD3	1.88	0.73
1:B:39:PHE:CD2	1:B:473:GLN:HG3	2.23	0.73
1:B:567:ILE:HD12	1:B:650:PHE:CZ	2.22	0.73
1:B:704:LEU:HD11	1:B:724:LYS:HE3	1.69	0.73
1:A:46:PRO:HG2	1:A:69:ARG:CG	2.17	0.72
1:A:670:ARG:HA	1:A:670:ARG:HE	1.54	0.72
1:B:184:ILE:O	1:B:184:ILE:HD12	1.89	0.72
1:A:1030:ASP:O	1:A:1032:VAL:HG23	1.89	0.72
1:A:73:LEU:HD22	1:A:79:VAL:HA	1.72	0.72
1:A:184:ILE:HD12	1:A:184:ILE:O	1.89	0.72
1:A:784:TRP:HD1	1:A:790:ILE:HD11	1.51	0.72
1:B:99:ILE:HD11	1:B:152:PHE:HB2	1.69	0.72
1:A:867:GLY:C	1:A:980:ALA:HB1	2.14	0.72
1:B:670:ARG:HA	1:B:670:ARG:HE	1.55	0.72
1:A:822:CYS:HA	1:A:833:LEU:HD23	1.70	0.72
1:A:994:LEU:HD11	1:A:1006:ASN:ND2	2.05	0.72
1:B:181:LYS:HD2	1:B:202:LYS:HA	1.71	0.72
1:B:822:CYS:HA	1:B:833:LEU:HD23	1.70	0.72
1:A:558:VAL:HG11	1:A:646:ALA:HB2	1.71	0.72
1:B:261:GLU:HA	1:B:264:SER:O	1.89	0.72
1:A:202:LYS:HD3	1:A:214:ALA:HB3	1.69	0.72
1:B:115:LYS:HB3	1:B:168:VAL:HG11	1.71	0.72
1:A:39:PHE:CD2	1:A:473:GLN:HG3	2.23	0.72
1:A:619:VAL:HB	1:A:620:PRO:HD3	1.72	0.72
1:A:832:THR:CG2	1:A:836:HIS:HB2	2.20	0.72
1:B:458:ARG:HG3	1:B:468:GLN:OE1	1.90	0.72
1:B:704:LEU:HB2	1:B:722:LYS:HG3	1.72	0.72
1:A:261:GLU:HA	1:A:264:SER:O	1.89	0.71
1:A:595:GLU:CB	1:A:597:LEU:HD23	2.14	0.71
1:A:937:ARG:CG	1:A:938:PRO:HD2	2.20	0.71
1:B:93:LYS:HD2	1:B:105:GLU:OE1	1.90	0.71
1:B:446:PHE:HZ	1:B:506:VAL:HG23	1.55	0.71
1:B:595:GLU:HG2	1:B:632:VAL:HG13	1.72	0.71
1:A:519:LEU:HD12	1:A:552:SER:O	1.90	0.71
1:B:380:LEU:HB2	1:B:386:LYS:CE	2.20	0.71
1:B:471:THR:HG23	1:B:473:GLN:HE22	1.55	0.71
1:A:321:LEU:HG	1:A:325:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LYS:H	1:A:1017:LYS:CE	2.01	0.71
1:B:832:THR:CG2	1:B:836:HIS:HB2	2.20	0.71
1:A:595:GLU:HG2	1:A:632:VAL:HG13	1.72	0.71
1:A:847:LEU:CD1	1:A:852:SER:HB3	2.20	0.71
1:B:937:ARG:CG	1:B:938:PRO:HD2	2.20	0.71
1:A:370:LEU:HD21	1:A:374:TYR:HE1	1.55	0.71
1:A:989:GLY:HA2	1:A:1017:LYS:CE	2.20	0.71
1:B:563:HIS:HB2	1:B:577:VAL:CG1	2.21	0.71
1:B:619:VAL:HB	1:B:620:PRO:HD3	1.72	0.71
1:B:847:LEU:CD1	1:B:852:SER:HB3	2.20	0.71
1:A:321:LEU:HG	1:A:325:LEU:HD11	1.71	0.71
1:B:188:VAL:HG13	1:B:190:GLY:H	1.56	0.71
1:B:321:LEU:HG	1:B:325:LEU:CD1	2.20	0.71
1:A:40:VAL:HG12	1:A:503:ARG:HB3	1.73	0.71
1:A:304:VAL:HG11	1:A:351:GLU:OE2	1.91	0.71
1:A:1016:MET:O	1:A:1032:VAL:HG13	1.91	0.71
1:B:450:LYS:HA	1:B:479:PRO:HB3	1.73	0.71
1:A:380:LEU:HB2	1:A:386:LYS:CE	2.20	0.71
1:A:474:VAL:HG21	1:A:495:ILE:HD13	1.72	0.71
1:A:515:CYS:O	1:A:519:LEU:HD23	1.91	0.71
1:A:704:LEU:HB2	1:A:722:LYS:HG3	1.71	0.71
1:A:1004:ILE:HD13	1:A:1005:CYS:N	2.06	0.71
1:B:474:VAL:HG21	1:B:495:ILE:HD13	1.72	0.71
1:B:575:LEU:HD22	1:B:575:LEU:H	1.56	0.71
1:A:962:ARG:HB3	1:A:1034:GLN:HG3	1.73	0.70
1:B:72:LYS:HE3	1:B:80:LEU:CD1	2.21	0.70
1:B:154:LYS:H	1:B:157:HIS:HD2	1.36	0.70
1:A:458:ARG:HG3	1:A:468:GLN:OE1	1.90	0.70
1:B:321:LEU:HG	1:B:325:LEU:HD11	1.71	0.70
1:A:115:LYS:HB3	1:A:168:VAL:HG11	1.71	0.70
1:A:446:PHE:HZ	1:A:506:VAL:HG23	1.55	0.70
1:A:480:VAL:HB	1:A:484:MET:CE	2.21	0.70
1:A:507:GLU:HG3	1:A:537:ARG:HG3	1.74	0.70
1:A:556:GLN:O	1:A:582:ASN:HB3	1.91	0.70
1:B:281:ARG:HB3	1:B:293:VAL:CG1	2.22	0.70
1:B:304:VAL:HG11	1:B:351:GLU:OE2	1.91	0.70
1:A:281:ARG:HB3	1:A:293:VAL:CG1	2.22	0.70
1:A:563:HIS:HB2	1:A:577:VAL:CG1	2.21	0.70
1:B:519:LEU:HD12	1:B:552:SER:O	1.90	0.70
1:B:854:CYS:C	1:B:855:THR:N	2.49	0.70
1:A:261:GLU:HG2	1:A:264:SER:C	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:THR:HG23	1:A:473:GLN:HE22	1.55	0.70
1:B:261:GLU:HG2	1:B:264:SER:C	2.17	0.70
1:B:370:LEU:HD21	1:B:374:TYR:HE1	1.55	0.70
1:A:39:PHE:HE1	1:A:505:PRO:HD2	1.56	0.70
1:A:93:LYS:HD2	1:A:105:GLU:OE1	1.91	0.70
1:A:181:LYS:HD2	1:A:202:LYS:HA	1.71	0.70
1:B:847:LEU:HD21	1:B:850:ALA:HA	1.73	0.70
1:A:42:PHE:HE1	1:A:79:VAL:CG2	2.05	0.70
1:B:216:VAL:HG12	1:B:224:SER:OG	1.92	0.70
1:B:480:VAL:HB	1:B:484:MET:CE	2.21	0.70
1:B:551:ALA:HA	1:B:556:GLN:OE1	1.92	0.70
1:A:367:LYS:HE2	1:A:399:ILE:O	1.91	0.69
1:A:450:LYS:HA	1:A:479:PRO:HB3	1.73	0.69
1:A:474:VAL:CG1	1:A:475:VAL:HG23	2.18	0.69
1:A:551:ALA:HA	1:A:556:GLN:OE1	1.92	0.69
1:A:806:MET:HE3	1:A:806:MET:N	1.99	0.69
1:B:73:LEU:HD22	1:B:79:VAL:HA	1.72	0.69
1:B:558:VAL:HG11	1:B:646:ALA:HB2	1.71	0.69
1:A:72:LYS:HE3	1:A:80:LEU:CD1	2.22	0.69
1:A:739:ILE:HB	1:A:781:THR:CG2	2.22	0.69
1:B:110:THR:HG22	1:B:132:LEU:HD21	1.73	0.69
1:B:807:ARG:HD3	1:B:812:LEU:C	2.17	0.69
1:A:807:ARG:HD3	1:A:812:LEU:C	2.18	0.69
1:B:367:LYS:HE2	1:B:399:ILE:O	1.91	0.69
1:B:515:CYS:O	1:B:519:LEU:HD23	1.91	0.69
1:A:847:LEU:HD21	1:A:850:ALA:HA	1.73	0.69
1:B:40:VAL:HG12	1:B:503:ARG:HB3	1.73	0.69
1:A:216:VAL:HG12	1:A:224:SER:OG	1.92	0.69
1:A:380:LEU:HB2	1:A:386:LYS:HE3	1.74	0.69
1:A:439:TYR:CZ	1:A:538:LYS:HE3	2.28	0.69
1:A:560:LEU:CD2	1:A:648:THR:HG23	2.19	0.69
1:A:1016:MET:HG2	1:A:1035:TYR:HE2	1.57	0.69
1:A:188:VAL:HG13	1:A:190:GLY:H	1.56	0.69
1:A:435:ILE:HD12	1:A:486:PHE:CD1	2.27	0.69
1:A:473:GLN:OE1	1:A:504:VAL:HG13	1.93	0.69
1:A:873:THR:HG23	1:A:982:SER:N	2.07	0.69
1:B:473:GLN:OE1	1:B:504:VAL:HG13	1.93	0.69
1:A:595:GLU:CG	1:A:632:VAL:HG13	2.22	0.69
1:A:959:LYS:CB	1:A:972:THR:HB	2.21	0.69
1:A:988:PHE:HB3	1:A:1016:MET:SD	2.33	0.69
1:B:453:LYS:HE3	1:B:472:VAL:HG21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TYR:HB3	1:B:523:ASP:CG	2.18	0.69
1:A:958:LEU:HD23	1:A:959:LYS:N	2.08	0.69
1:B:380:LEU:HB2	1:B:386:LYS:HE3	1.74	0.69
1:A:133:TYR:CD2	1:A:136:ILE:HG12	2.28	0.69
1:A:133:TYR:HB2	1:A:136:ILE:HG12	1.75	0.69
1:B:133:TYR:CD2	1:B:136:ILE:HG12	2.28	0.69
1:B:446:PHE:CD2	1:B:454:LEU:HD21	2.24	0.68
1:B:507:GLU:HG3	1:B:537:ARG:HG3	1.74	0.68
1:A:453:LYS:HE3	1:A:472:VAL:HG21	1.73	0.68
1:B:46:PRO:HG3	1:B:69:ARG:HD2	1.75	0.68
1:A:440:LYS:CB	1:A:538:LYS:HZ2	1.95	0.68
1:A:972:THR:HG23	1:A:1002:TYR:CD1	2.28	0.68
1:B:739:ILE:HB	1:B:781:THR:CG2	2.23	0.68
1:B:412:LEU:HD13	1:B:412:LEU:H	1.59	0.68
1:A:773:ILE:HD13	1:A:773:ILE:H	1.59	0.68
1:B:405:GLY:C	1:B:406:LEU:HD22	2.19	0.68
1:B:474:VAL:CG1	1:B:475:VAL:HG23	2.18	0.68
1:B:773:ILE:HD13	1:B:773:ILE:H	1.59	0.68
1:A:110:THR:HG22	1:A:132:LEU:HD21	1.74	0.68
1:A:323:ARG:HG3	1:A:324:THR:H	1.58	0.68
1:A:689:PHE:CD1	1:A:691:GLU:HG2	2.28	0.68
1:A:703:LEU:HD13	1:A:723:ALA:HB2	1.76	0.68
1:B:435:ILE:HD12	1:B:486:PHE:CD1	2.27	0.68
1:A:594:PHE:O	1:A:595:GLU:HG2	1.94	0.68
1:A:867:GLY:HA3	1:A:948:TYR:OH	1.94	0.68
1:B:190:GLY:HA2	1:B:233:PHE:CE2	2.29	0.68
1:B:548:ARG:NE	1:B:583:VAL:O	2.26	0.68
1:B:595:GLU:CG	1:B:632:VAL:HG13	2.22	0.68
1:A:405:GLY:C	1:A:406:LEU:HD22	2.19	0.68
1:B:594:PHE:O	1:B:595:GLU:HG2	1.94	0.68
1:B:700:CYS:O	1:B:725:ASN:CB	2.30	0.68
1:A:40:VAL:HG11	1:A:503:ARG:NE	2.09	0.68
1:A:190:GLY:HA2	1:A:233:PHE:CE2	2.29	0.68
1:A:555:LYS:HG3	1:A:556:GLN:N	2.09	0.68
1:A:830:GLN:HG2	1:A:831:CYS:N	2.09	0.68
1:B:98:ARG:HE	1:B:107:LEU:CD1	2.07	0.68
1:B:689:PHE:CD1	1:B:691:GLU:HG2	2.28	0.68
1:B:830:GLN:HG2	1:B:831:CYS:N	2.09	0.68
1:A:73:LEU:CD2	1:A:79:VAL:HA	2.23	0.68
1:A:575:LEU:HD22	1:A:575:LEU:H	1.56	0.68
1:B:62:ILE:HG13	1:B:62:ILE:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:HD11	1:B:73:LEU:HD12	1.76	0.68
1:B:323:ARG:HG3	1:B:324:THR:H	1.58	0.68
1:A:962:ARG:HB3	1:A:1034:GLN:CG	2.23	0.67
1:B:548:ARG:HG3	1:B:584:PRO:CA	2.25	0.67
1:A:532:HIS:O	1:A:641:THR:HG21	1.94	0.67
1:A:1013:VAL:HG22	1:A:1014:LEU:H	1.60	0.67
1:B:42:PHE:HE1	1:B:79:VAL:CG2	2.05	0.67
1:B:560:LEU:CD2	1:B:648:THR:HG23	2.19	0.67
1:B:863:ILE:HG23	1:B:864:PRO:CD	2.23	0.67
1:A:46:PRO:HG3	1:A:69:ARG:HD2	1.75	0.67
1:B:460:ASP:HB3	1:B:463:LYS:HB3	1.77	0.67
1:B:867:GLY:HA3	1:B:948:TYR:OH	1.94	0.67
1:A:98:ARG:HE	1:A:107:LEU:HD11	1.60	0.67
1:A:225:MET:CE	1:A:227:LYS:HG3	2.19	0.67
1:A:531:LEU:HG	1:A:584:PRO:HG2	1.77	0.67
1:A:951:MET:HG3	1:A:952:THR:N	2.09	0.67
1:B:98:ARG:HE	1:B:107:LEU:HD11	1.60	0.67
1:A:137:CYS:HB2	1:A:213:PHE:CZ	2.30	0.67
1:A:321:LEU:O	1:A:325:LEU:HG	1.95	0.67
1:A:458:ARG:HG3	1:A:468:GLN:CD	2.20	0.67
1:B:458:ARG:HG3	1:B:468:GLN:CD	2.20	0.67
1:A:460:ASP:HB3	1:A:463:LYS:HB3	1.77	0.67
1:B:555:LYS:HG3	1:B:556:GLN:N	2.09	0.67
1:A:863:ILE:HG23	1:A:864:PRO:CD	2.23	0.67
1:A:994:LEU:CD1	1:A:1006:ASN:HD22	2.07	0.67
1:B:62:ILE:HD12	1:B:64:LEU:HD21	1.75	0.67
1:B:73:LEU:CD2	1:B:79:VAL:HA	2.24	0.67
1:B:321:LEU:O	1:B:325:LEU:HG	1.95	0.67
1:B:595:GLU:HG2	1:B:632:VAL:CG1	2.25	0.67
1:A:62:ILE:HD11	1:A:73:LEU:HD12	1.76	0.67
1:A:62:ILE:HD12	1:A:64:LEU:HD21	1.76	0.66
1:B:325:LEU:CD1	1:B:333:LEU:HD11	2.25	0.66
1:A:98:ARG:HE	1:A:107:LEU:CD1	2.07	0.66
1:A:595:GLU:HG2	1:A:632:VAL:CG1	2.25	0.66
1:A:847:LEU:HG	1:A:850:ALA:N	2.10	0.66
1:B:703:LEU:HD13	1:B:723:ALA:HB2	1.76	0.66
1:B:847:LEU:HG	1:B:850:ALA:N	2.10	0.66
1:A:532:HIS:HA	1:A:641:THR:CG2	2.25	0.66
1:A:873:THR:HG1	1:A:981:GLY:HA2	1.61	0.66
1:B:133:TYR:HB2	1:B:136:ILE:HG12	1.75	0.66
1:B:863:ILE:HG13	1:B:864:PRO:CD	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HG11	1:B:503:ARG:NE	2.09	0.66
1:B:98:ARG:HH21	1:B:107:LEU:HD12	1.60	0.66
1:A:98:ARG:HH21	1:A:107:LEU:HD12	1.59	0.66
1:A:239:PHE:CD1	1:A:260:PRO:HD2	2.30	0.66
1:A:566:ASN:HA	1:A:651:VAL:CG2	2.25	0.66
1:A:955:LEU:HG	1:A:973:ILE:CG2	2.24	0.66
1:B:133:TYR:HB2	1:B:136:ILE:H	1.61	0.66
1:A:446:PHE:CZ	1:A:486:PHE:HZ	2.13	0.66
1:B:739:ILE:HD12	1:B:748:ARG:HG2	1.76	0.66
1:A:325:LEU:CD1	1:A:333:LEU:HD11	2.25	0.66
1:A:739:ILE:HD12	1:A:748:ARG:HG2	1.76	0.66
1:A:863:ILE:HG13	1:A:864:PRO:CD	2.25	0.66
1:A:567:ILE:HD13	1:A:651:VAL:O	1.96	0.66
1:B:137:CYS:HB2	1:B:213:PHE:CZ	2.30	0.66
1:B:181:LYS:HD3	1:B:202:LYS:HA	1.78	0.66
1:B:410:ALA:HB1	1:B:411:PRO:HD2	1.78	0.66
1:B:548:ARG:HG3	1:B:584:PRO:HA	1.78	0.66
1:A:892:HIS:NE2	1:A:931:ILE:HB	2.11	0.66
1:B:110:THR:HB	1:B:132:LEU:CD2	2.26	0.66
1:B:629:HIS:CE1	1:B:669:TYR:CZ	2.69	0.66
1:A:296:PRO:HD2	1:A:414:VAL:CG2	2.27	0.65
1:A:216:VAL:HG12	1:A:224:SER:CB	2.26	0.65
1:A:257:THR:C	1:A:258:LEU:HD12	2.21	0.65
1:A:412:LEU:HD13	1:A:412:LEU:H	1.59	0.65
1:A:474:VAL:HG12	1:A:475:VAL:CG2	2.21	0.65
1:A:782:VAL:HG23	1:A:790:ILE:HB	1.78	0.65
1:A:797:LYS:N	1:A:797:LYS:HD2	2.11	0.65
1:A:870:GLU:CB	1:A:1024:ARG:HG3	2.17	0.65
1:B:239:PHE:CD1	1:B:260:PRO:HD2	2.30	0.65
1:B:782:VAL:HG23	1:B:790:ILE:HB	1.78	0.65
1:A:62:ILE:HG13	1:A:62:ILE:O	1.94	0.65
1:A:133:TYR:HB2	1:A:136:ILE:H	1.61	0.65
1:A:432:THR:OG1	1:A:480:VAL:HG23	1.96	0.65
1:A:473:GLN:HG2	1:A:504:VAL:HG22	1.79	0.65
1:B:257:THR:C	1:B:258:LEU:HD12	2.21	0.65
1:B:676:TYR:HD1	1:B:730:GLN:CG	2.08	0.65
1:B:847:LEU:CD2	1:B:850:ALA:HA	2.27	0.65
1:A:181:LYS:HD3	1:A:202:LYS:HA	1.78	0.65
1:A:154:LYS:H	1:A:157:HIS:CD2	2.15	0.65
1:B:265:PRO:HD3	1:B:274:VAL:CG2	2.27	0.65
1:B:446:PHE:CZ	1:B:486:PHE:HZ	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:675:LYS:HE3	1:B:694:VAL:HG22	1.79	0.65
1:A:110:THR:HB	1:A:132:LEU:CD2	2.26	0.65
1:A:453:LYS:HG2	1:A:472:VAL:CG2	2.16	0.65
1:A:706:VAL:HG13	1:A:707:ASP:O	1.96	0.65
1:B:216:VAL:HG12	1:B:224:SER:CB	2.26	0.65
1:A:872:GLY:HA3	1:A:1023:ASP:OD1	1.97	0.65
1:B:653:TYR:OH	1:B:682:HIS:CE1	2.50	0.65
1:A:368:ASP:O	1:A:371:GLN:HG2	1.97	0.64
1:A:675:LYS:HE3	1:A:694:VAL:HG22	1.79	0.64
1:B:432:THR:OG1	1:B:480:VAL:HG23	1.96	0.64
1:A:405:GLY:O	1:A:406:LEU:HD22	1.98	0.64
1:A:410:ALA:HB1	1:A:411:PRO:HD2	1.78	0.64
1:B:39:PHE:HE1	1:B:505:PRO:HD2	1.57	0.64
1:B:405:GLY:O	1:B:406:LEU:HD22	1.98	0.64
1:A:105:GLU:HB3	1:A:106:PRO:HD2	1.80	0.64
1:A:265:PRO:HD3	1:A:274:VAL:CG2	2.27	0.64
1:A:309:LEU:HD11	1:A:311:ALA:O	1.98	0.64
1:A:926:ALA:HB1	1:A:947:LEU:CD1	2.27	0.64
1:B:320:VAL:O	1:B:323:ARG:HG2	1.98	0.64
1:B:474:VAL:HG12	1:B:475:VAL:CG2	2.21	0.64
1:B:567:ILE:HD13	1:B:651:VAL:O	1.96	0.64
1:A:53:LEU:HB2	1:A:496:MET:CE	2.28	0.64
1:A:53:LEU:HG	1:A:64:LEU:CD1	2.28	0.64
1:A:620:PRO:CA	1:A:623:ILE:HG13	2.23	0.64
1:B:53:LEU:HB2	1:B:496:MET:CE	2.28	0.64
1:B:797:LYS:HD2	1:B:797:LYS:N	2.11	0.64
1:B:926:ALA:HB1	1:B:947:LEU:CD1	2.27	0.64
1:A:175:TYR:HD2	1:A:179:ASP:HB3	1.63	0.64
1:A:460:ASP:CB	1:A:463:LYS:HB3	2.28	0.64
1:A:868:PRO:CD	1:A:980:ALA:C	2.54	0.64
1:B:473:GLN:HG2	1:B:504:VAL:HG22	1.79	0.64
1:B:175:TYR:HD2	1:B:179:ASP:HB3	1.63	0.64
1:B:186:THR:HG22	1:B:187:ALA:N	2.12	0.64
1:B:296:PRO:HD2	1:B:414:VAL:CG2	2.27	0.64
1:B:460:ASP:CB	1:B:463:LYS:HB3	2.28	0.64
1:B:505:PRO:CB	1:B:507:GLU:O	2.46	0.64
1:A:566:ASN:HB3	1:A:651:VAL:HG21	1.80	0.64
1:A:847:LEU:CD2	1:A:850:ALA:HA	2.27	0.64
1:B:56:ASP:OD1	1:B:119:ILE:HD12	1.98	0.64
1:A:741:ASN:O	1:A:778:VAL:HG13	1.98	0.64
1:B:105:GLU:HB3	1:B:106:PRO:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:GLN:HB2	1:B:504:VAL:HG22	1.80	0.64
1:B:566:ASN:HA	1:B:651:VAL:CG2	2.25	0.64
1:A:56:ASP:OD1	1:A:119:ILE:HD12	1.98	0.64
1:B:53:LEU:HG	1:B:64:LEU:CD1	2.28	0.64
1:B:118:LEU:HG	1:B:172:ILE:HG13	1.80	0.64
1:B:154:LYS:H	1:B:157:HIS:CD2	2.15	0.64
1:B:309:LEU:HD11	1:B:311:ALA:O	1.98	0.64
1:B:706:VAL:HG13	1:B:707:ASP:O	1.96	0.64
1:B:713:VAL:HG12	1:B:714:GLU:HG3	1.79	0.64
1:B:806:MET:HG2	1:B:807:ARG:HG3	1.80	0.64
1:B:185:ALA:HB1	1:B:243:TYR:CD1	2.33	0.63
1:B:653:TYR:CE2	1:B:682:HIS:ND1	2.60	0.63
1:B:892:HIS:NE2	1:B:931:ILE:HB	2.11	0.63
1:B:368:ASP:O	1:B:371:GLN:HG2	1.97	0.63
1:B:446:PHE:CE1	1:B:486:PHE:HZ	2.16	0.63
1:B:480:VAL:HG11	1:B:495:ILE:HD11	1.81	0.63
1:B:653:TYR:CE2	1:B:682:HIS:CE1	2.87	0.63
1:B:894:LYS:HD3	1:B:899:GLU:HA	1.81	0.63
1:A:320:VAL:O	1:A:323:ARG:HG2	1.98	0.63
1:B:181:LYS:HE2	1:B:202:LYS:HG2	1.80	0.63
1:A:118:LEU:HG	1:A:172:ILE:HG13	1.80	0.63
1:A:713:VAL:HG12	1:A:714:GLU:HG3	1.79	0.63
1:A:978:LEU:O	1:A:998:ARG:HD2	1.98	0.63
1:A:1002:TYR:CZ	1:A:1004:ILE:HB	2.32	0.63
1:B:620:PRO:CA	1:B:623:ILE:HG13	2.23	0.63
1:A:806:MET:HG2	1:A:807:ARG:HG3	1.80	0.63
1:B:41:THR:HG22	1:B:502:THR:HA	1.81	0.63
1:B:446:PHE:CZ	1:B:506:VAL:HG23	2.33	0.63
1:B:566:ASN:HB3	1:B:651:VAL:HG21	1.79	0.63
1:A:186:THR:HG22	1:A:187:ALA:N	2.12	0.63
1:A:933:VAL:HG23	1:A:934:ALA:N	2.10	0.63
1:A:295:VAL:HA	1:A:414:VAL:HG21	1.81	0.63
1:A:446:PHE:CE1	1:A:486:PHE:HZ	2.16	0.63
1:A:894:LYS:HD3	1:A:899:GLU:HA	1.80	0.63
1:A:1014:LEU:HD22	1:A:1014:LEU:N	2.14	0.63
1:B:386:LYS:HG3	1:B:386:LYS:O	1.99	0.63
1:A:40:VAL:HG11	1:A:503:ARG:CZ	2.29	0.63
1:B:448:GLY:CA	1:B:480:VAL:HG21	2.29	0.63
1:B:575:LEU:HD22	1:B:575:LEU:N	2.14	0.63
1:A:197:THR:HG21	1:A:228:ILE:HD11	1.81	0.62
1:A:1015:ASP:O	1:A:1016:MET:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:ASN:O	1:B:778:VAL:HG13	1.98	0.62
1:A:180:ASP:O	1:A:181:LYS:HG2	1.99	0.62
1:A:185:ALA:HB1	1:A:243:TYR:CD1	2.33	0.62
1:A:372:SER:O	1:A:375:ARG:HB2	1.99	0.62
1:B:180:ASP:O	1:B:181:LYS:HG2	1.99	0.62
1:B:295:VAL:HA	1:B:414:VAL:HG21	1.81	0.62
1:B:474:VAL:CG2	1:B:495:ILE:HD13	2.29	0.62
1:A:382:LEU:HD23	1:A:385:LEU:HB3	1.81	0.62
1:A:439:TYR:OH	1:A:538:LYS:CE	2.47	0.62
1:A:492:GLN:HG2	1:A:503:ARG:CG	2.29	0.62
1:B:469:TYR:HE2	1:B:471:THR:HB	1.65	0.62
1:A:446:PHE:CZ	1:A:506:VAL:HG23	2.33	0.62
1:A:448:GLY:CA	1:A:480:VAL:HG21	2.28	0.62
1:B:320:VAL:HG21	1:B:442:HIS:HD2	1.64	0.62
1:A:575:LEU:HD22	1:A:575:LEU:N	2.14	0.62
1:B:296:PRO:HB2	1:B:417:MET:SD	2.39	0.62
1:A:480:VAL:CG2	1:A:484:MET:HE1	2.29	0.62
1:B:40:VAL:HG11	1:B:503:ARG:CZ	2.29	0.62
1:A:386:LYS:O	1:A:386:LYS:HG3	1.99	0.62
1:B:696:LEU:N	1:B:696:LEU:HD12	2.15	0.62
1:B:806:MET:CG	1:B:807:ARG:HG3	2.30	0.62
1:B:225:MET:CE	1:B:227:LYS:HG3	2.19	0.62
1:B:474:VAL:HG22	1:B:495:ILE:CG2	2.29	0.62
1:B:492:GLN:HG2	1:B:503:ARG:CG	2.29	0.62
1:B:855:THR:HG23	1:B:856:ASN:OD1	2.00	0.62
1:A:72:LYS:CD	1:A:80:LEU:HD12	2.30	0.61
1:A:182:LEU:HG	1:A:184:ILE:HG23	1.82	0.61
1:A:473:GLN:HB2	1:A:504:VAL:HG22	1.80	0.61
1:B:382:LEU:HD23	1:B:385:LEU:HB3	1.81	0.61
1:B:480:VAL:CG2	1:B:484:MET:HE1	2.30	0.61
1:B:715:VAL:CG2	1:B:717:LYS:HD2	2.30	0.61
1:A:855:THR:HG23	1:A:856:ASN:OD1	1.99	0.61
1:B:372:SER:O	1:B:375:ARG:HB2	1.99	0.61
1:A:110:THR:HG22	1:A:111:ASN:N	2.14	0.61
1:B:204:THR:HG22	1:B:212:MET:SD	2.40	0.61
1:A:181:LYS:HE2	1:A:202:LYS:HG2	1.80	0.61
1:A:296:PRO:HB2	1:A:417:MET:SD	2.39	0.61
1:A:41:THR:HG22	1:A:502:THR:HA	1.81	0.61
1:A:873:THR:HG23	1:A:982:SER:CA	2.30	0.61
1:B:110:THR:HG22	1:B:111:ASN:N	2.14	0.61
1:A:175:TYR:CD2	1:A:179:ASP:HB3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:THR:HG22	1:A:212:MET:SD	2.40	0.61
1:A:410:ALA:HB1	1:A:411:PRO:CD	2.30	0.61
1:A:474:VAL:CG2	1:A:495:ILE:HD13	2.29	0.61
1:A:480:VAL:HG11	1:A:495:ILE:HD11	1.81	0.61
1:A:488:LYS:HG3	1:A:489:ASP:N	2.14	0.61
1:A:712:PRO:HG3	1:A:801:TYR:OH	2.01	0.61
1:A:806:MET:CG	1:A:807:ARG:HG3	2.30	0.61
1:B:833:LEU:HB2	1:B:836:HIS:CD2	2.29	0.61
1:A:119:ILE:HD13	1:A:121:TYR:CZ	2.36	0.61
1:A:532:HIS:HA	1:A:641:THR:HG21	1.82	0.61
1:B:41:THR:HG22	1:B:502:THR:HG23	1.83	0.61
1:B:410:ALA:HB1	1:B:411:PRO:CD	2.30	0.61
1:B:933:VAL:HG23	1:B:934:ALA:N	2.10	0.61
1:A:696:LEU:HD12	1:A:696:LEU:N	2.15	0.61
1:B:46:PRO:HD2	1:B:71:TYR:CE1	2.35	0.61
1:B:175:TYR:CD2	1:B:179:ASP:HB3	2.36	0.61
1:B:181:LYS:HZ3	1:B:216:VAL:HG23	1.66	0.61
1:B:333:LEU:CD2	1:B:358:ILE:HG13	2.31	0.61
1:B:847:LEU:HD11	1:B:850:ALA:CA	2.29	0.61
1:A:474:VAL:HG22	1:A:495:ILE:CG2	2.29	0.60
1:A:569:VAL:HB	1:A:654:ASN:HB2	1.83	0.60
1:A:665:VAL:HG12	1:A:697:PRO:HG3	1.83	0.60
1:A:706:VAL:HG22	1:A:707:ASP:N	2.12	0.60
1:B:488:LYS:HG3	1:B:489:ASP:N	2.14	0.60
1:A:313:TYR:CE1	1:A:435:ILE:HG12	2.37	0.60
1:A:469:TYR:HE2	1:A:471:THR:HB	1.65	0.60
1:A:870:GLU:CG	1:A:1025:ALA:N	2.64	0.60
1:B:95:TYR:CG	1:B:96:PRO:HD3	2.36	0.60
1:B:444:LEU:CD2	1:B:524:PRO:HG3	2.23	0.60
1:B:548:ARG:HG2	1:B:584:PRO:HA	1.83	0.60
1:A:715:VAL:CG2	1:A:717:LYS:HD2	2.30	0.60
1:B:99:ILE:HG13	1:B:100:VAL:N	2.16	0.60
1:A:314:LEU:HD12	1:A:333:LEU:O	2.01	0.60
1:B:773:ILE:HD13	1:B:773:ILE:N	2.17	0.60
1:A:873:THR:HB	1:A:917:MET:HE2	1.82	0.60
1:A:919:GLU:HB3	1:A:1024:ARG:NH1	2.16	0.60
1:A:963:GLY:O	1:A:1036:VAL:HG22	2.01	0.60
1:B:313:TYR:CE1	1:B:435:ILE:HG12	2.37	0.60
1:B:314:LEU:HD12	1:B:333:LEU:O	2.01	0.60
1:B:712:PRO:HG3	1:B:801:TYR:OH	2.01	0.60
1:A:46:PRO:HD2	1:A:71:TYR:CE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:CD2	1:A:358:ILE:HG13	2.31	0.60
1:A:773:ILE:HD13	1:A:773:ILE:N	2.17	0.60
1:B:46:PRO:HD2	1:B:71:TYR:CZ	2.36	0.60
1:A:62:ILE:HD13	1:A:77:LEU:CD2	2.32	0.60
1:A:320:VAL:HG21	1:A:442:HIS:HD2	1.64	0.60
1:A:403:PHE:CZ	1:A:406:LEU:HD23	2.37	0.60
1:A:548:ARG:HG3	1:A:583:VAL:C	2.26	0.60
1:A:630:HIS:HD2	1:A:632:VAL:CG2	2.15	0.60
1:A:845:LEU:HD13	1:A:845:LEU:C	2.26	0.60
1:B:181:LYS:HZ2	1:B:216:VAL:HG23	1.64	0.60
1:B:495:ILE:CG2	1:B:502:THR:HB	2.32	0.60
1:B:873:THR:HB	1:B:917:MET:HE2	1.82	0.60
1:B:182:LEU:HG	1:B:184:ILE:HG23	1.82	0.60
1:B:323:ARG:HH21	1:B:463:LYS:HD2	1.67	0.60
1:A:91:ASN:CG	1:A:92:PRO:HD2	2.27	0.60
1:B:72:LYS:CD	1:B:80:LEU:HD12	2.30	0.60
1:B:91:ASN:CG	1:B:92:PRO:HD2	2.27	0.60
1:B:119:ILE:HD13	1:B:121:TYR:CZ	2.36	0.60
1:B:171:VAL:O	1:B:182:LEU:HD12	2.02	0.60
1:B:403:PHE:CZ	1:B:406:LEU:HD23	2.37	0.60
1:B:469:TYR:CE2	1:B:471:THR:HB	2.36	0.60
1:B:662:LEU:HD11	1:B:702:GLN:HE22	1.65	0.60
1:B:665:VAL:HG12	1:B:697:PRO:HG3	1.83	0.60
1:B:845:LEU:HD13	1:B:845:LEU:C	2.26	0.60
1:A:1029:GLN:HG2	1:A:1030:ASP:H	1.67	0.60
1:B:387:VAL:HG13	1:B:388:LYS:HG3	1.83	0.60
1:A:991:GLN:HG3	1:A:1008:THR:HG21	1.84	0.59
1:A:1002:TYR:CE2	1:A:1004:ILE:HB	2.37	0.59
1:B:154:LYS:N	1:B:157:HIS:HD2	2.00	0.59
1:A:95:TYR:CG	1:A:96:PRO:HD3	2.36	0.59
1:A:99:ILE:HG13	1:A:100:VAL:N	2.16	0.59
1:A:387:VAL:HG13	1:A:388:LYS:HG3	1.83	0.59
1:A:469:TYR:CE2	1:A:471:THR:HB	2.36	0.59
1:A:566:ASN:CA	1:A:651:VAL:HG23	2.28	0.59
1:B:243:TYR:CD2	1:B:257:THR:HG22	2.37	0.59
1:A:271:LYS:HG3	1:A:272:GLU:N	2.13	0.59
1:A:457:ILE:HG12	1:A:467:LEU:HD13	1.84	0.59
1:A:560:LEU:HD23	1:A:648:THR:CG2	2.25	0.59
1:A:847:LEU:HD11	1:A:850:ALA:CA	2.29	0.59
1:B:197:THR:HG21	1:B:228:ILE:HD11	1.82	0.59
1:B:239:PHE:CA	1:B:260:PRO:HG2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:VAL:HG13	1:B:388:LYS:N	2.18	0.59
1:B:665:VAL:HG11	1:B:697:PRO:HD3	1.84	0.59
1:B:706:VAL:HG22	1:B:707:ASP:N	2.12	0.59
1:A:46:PRO:HD2	1:A:71:TYR:CZ	2.37	0.59
1:A:243:TYR:CD2	1:A:257:THR:HG22	2.37	0.59
1:A:904:VAL:HG13	1:A:905:ASP:N	2.18	0.59
1:A:931:ILE:O	1:A:931:ILE:HG13	2.02	0.59
1:A:40:VAL:HG13	1:A:503:ARG:HB3	1.85	0.59
1:A:41:THR:HG22	1:A:502:THR:HG23	1.82	0.59
1:A:62:ILE:HD12	1:A:501:LEU:CD1	2.33	0.59
1:A:833:LEU:HB2	1:A:836:HIS:CD2	2.28	0.59
1:A:987:MET:HB2	1:A:1019:THR:HG23	1.83	0.59
1:A:994:LEU:CG	1:A:1006:ASN:HB2	2.31	0.59
1:B:453:LYS:HG2	1:B:472:VAL:CG2	2.16	0.59
1:B:548:ARG:CG	1:B:583:VAL:O	2.50	0.59
1:B:904:VAL:HG13	1:B:905:ASP:N	2.18	0.59
1:A:889:ILE:HD12	1:A:907:TYR:CZ	2.38	0.59
1:B:370:LEU:HD13	1:B:370:LEU:C	2.27	0.59
1:B:473:GLN:NE2	1:B:473:GLN:H	2.01	0.59
1:B:630:HIS:HD2	1:B:632:VAL:CG2	2.15	0.59
1:B:931:ILE:HG13	1:B:931:ILE:O	2.02	0.59
1:A:432:THR:HG1	1:A:480:VAL:HG23	1.65	0.59
1:A:972:THR:HA	1:A:1002:TYR:CE1	2.32	0.59
1:B:62:ILE:HD13	1:B:77:LEU:CD2	2.32	0.59
1:A:323:ARG:HH21	1:A:463:LYS:HD2	1.67	0.59
1:A:439:TYR:CZ	1:A:538:LYS:NZ	2.70	0.59
1:A:563:HIS:HB3	1:A:564:PRO:CD	2.28	0.59
1:B:349:LEU:HD22	1:B:349:LEU:N	2.18	0.59
1:B:578:LEU:HD13	1:B:636:LEU:HD21	1.85	0.59
1:A:814:LEU:HD22	1:A:847:LEU:N	2.18	0.59
1:A:959:LYS:CG	1:A:972:THR:HB	2.33	0.59
1:B:40:VAL:HG13	1:B:503:ARG:HB3	1.85	0.59
1:B:412:LEU:C	1:B:412:LEU:HD22	2.28	0.59
1:B:937:ARG:HG2	1:B:938:PRO:HD2	1.85	0.59
1:A:171:VAL:O	1:A:182:LEU:HD12	2.02	0.58
1:A:412:LEU:HD22	1:A:412:LEU:C	2.28	0.58
1:A:495:ILE:CG2	1:A:502:THR:HB	2.32	0.58
1:A:530:VAL:HG11	1:A:584:PRO:HD2	1.84	0.58
1:A:955:LEU:CD1	1:A:973:ILE:HG23	2.33	0.58
1:B:457:ILE:HG12	1:B:467:LEU:HD13	1.84	0.58
1:B:814:LEU:HD22	1:B:847:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG12	1:A:73:LEU:HB2	1.84	0.58
1:A:370:LEU:C	1:A:370:LEU:HD13	2.27	0.58
1:A:387:VAL:HG13	1:A:388:LYS:N	2.18	0.58
1:A:870:GLU:CG	1:A:1024:ARG:CG	2.69	0.58
1:B:271:LYS:HG3	1:B:272:GLU:N	2.13	0.58
1:A:349:LEU:HD22	1:A:349:LEU:N	2.18	0.58
1:A:780:LEU:HD12	1:A:780:LEU:C	2.27	0.58
1:B:780:LEU:HD12	1:B:780:LEU:C	2.27	0.58
1:A:665:VAL:HG11	1:A:697:PRO:HD3	1.84	0.58
1:B:560:LEU:HD23	1:B:648:THR:CG2	2.25	0.58
1:A:110:THR:HB	1:A:132:LEU:HD23	1.85	0.58
1:A:506:VAL:HG22	1:A:525:HIS:NE2	2.18	0.58
1:B:426:GLU:OE1	1:B:426:GLU:HA	2.04	0.58
1:B:198:ILE:HB	1:B:226:ILE:CG2	2.34	0.58
1:A:350:ASP:HA	1:A:430:ARG:HB2	1.86	0.58
1:A:473:GLN:NE2	1:A:473:GLN:H	2.01	0.58
1:B:188:VAL:HG22	1:B:191:LYS:N	2.18	0.58
1:B:653:TYR:HE2	1:B:682:HIS:CE1	2.21	0.58
1:B:832:THR:HG23	1:B:836:HIS:HB2	1.85	0.58
1:B:889:ILE:HD12	1:B:907:TYR:CZ	2.38	0.58
1:A:426:GLU:HA	1:A:426:GLU:OE1	2.04	0.58
1:A:430:ARG:HH21	1:A:432:THR:HG22	1.68	0.58
1:A:578:LEU:HD13	1:A:636:LEU:HD21	1.85	0.58
1:A:814:LEU:HD22	1:A:847:LEU:H	1.68	0.58
1:A:873:THR:HA	1:A:982:SER:N	2.17	0.58
1:B:51:ASN:HD21	1:B:67:VAL:CG2	2.15	0.58
1:B:110:THR:HB	1:B:132:LEU:HD23	1.85	0.58
1:B:623:ILE:HD12	1:B:623:ILE:C	2.28	0.58
1:B:759:VAL:HG12	1:B:760:GLN:N	2.18	0.58
1:A:456:LYS:O	1:A:468:GLN:HG2	2.04	0.58
1:A:585:GLU:OE1	1:A:585:GLU:HA	2.04	0.58
1:A:873:THR:HG23	1:A:982:SER:HA	1.86	0.58
1:A:1021:GLN:CG	1:A:1026:ARG:HG3	2.34	0.58
1:B:62:ILE:HD12	1:B:501:LEU:CD1	2.33	0.58
1:B:254:TYR:CZ	1:B:281:ARG:HD2	2.39	0.58
1:B:385:LEU:C	1:B:385:LEU:HD13	2.29	0.58
1:B:430:ARG:HH21	1:B:432:THR:HG22	1.68	0.58
1:A:623:ILE:HD12	1:A:623:ILE:C	2.29	0.58
1:A:759:VAL:HG12	1:A:760:GLN:N	2.18	0.58
1:A:972:THR:CA	1:A:1002:TYR:HE1	2.15	0.58
1:B:456:LYS:O	1:B:468:GLN:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ASN:CA	1:B:651:VAL:HG23	2.28	0.58
1:A:254:TYR:CZ	1:A:281:ARG:HD2	2.39	0.57
1:A:703:LEU:HD21	1:A:782:VAL:HG21	1.86	0.57
1:B:505:PRO:HB2	1:B:507:GLU:O	2.03	0.57
1:A:385:LEU:HD13	1:A:385:LEU:C	2.29	0.57
1:A:937:ARG:HG2	1:A:938:PRO:HD2	1.85	0.57
1:A:963:GLY:C	1:A:1036:VAL:HG22	2.29	0.57
1:A:458:ARG:HD2	1:A:524:PRO:HG3	1.86	0.57
1:A:994:LEU:HG	1:A:1006:ASN:HB2	1.87	0.57
1:A:874:LYS:N	1:A:982:SER:CB	2.66	0.57
1:A:892:HIS:CE1	1:A:931:ILE:HB	2.40	0.57
1:A:1018:VAL:HG13	1:A:1018:VAL:O	2.04	0.57
1:B:350:ASP:HA	1:B:430:ARG:HB2	1.86	0.57
1:A:154:LYS:N	1:A:157:HIS:HD2	2.00	0.57
1:A:265:PRO:HD3	1:A:274:VAL:HG21	1.87	0.57
1:B:370:LEU:HD21	1:B:374:TYR:CE1	2.39	0.57
1:A:198:ILE:HB	1:A:226:ILE:CG2	2.34	0.57
1:A:262:MET:O	1:A:262:MET:HG3	2.05	0.57
1:A:532:HIS:HA	1:A:641:THR:CB	2.35	0.57
1:A:51:ASN:HD21	1:A:67:VAL:CG2	2.15	0.57
1:A:188:VAL:HG22	1:A:191:LYS:N	2.18	0.57
1:A:263:VAL:O	1:A:263:VAL:HG12	2.04	0.57
1:A:324:THR:CG2	1:A:462:PRO:HA	2.34	0.57
1:A:370:LEU:HD21	1:A:374:TYR:CE1	2.39	0.57
1:A:458:ARG:CG	1:A:524:PRO:HG3	2.34	0.57
1:A:832:THR:HG23	1:A:836:HIS:HB2	1.85	0.57
1:B:42:PHE:CE2	1:B:50:PHE:HZ	2.23	0.57
1:B:265:PRO:HD3	1:B:274:VAL:HG21	1.87	0.57
1:B:433:SER:HB3	1:B:484:MET:SD	2.45	0.57
1:A:45:GLU:HB3	1:A:46:PRO:CD	2.35	0.57
1:A:239:PHE:CA	1:A:260:PRO:HG2	2.30	0.57
1:B:434:VAL:HG22	1:B:435:ILE:N	2.20	0.57
1:B:459:VAL:HG23	1:B:459:VAL:O	2.05	0.57
1:A:446:PHE:CE1	1:A:486:PHE:CZ	2.93	0.57
1:B:262:MET:HG3	1:B:262:MET:O	2.05	0.57
1:A:926:ALA:CB	1:A:947:LEU:HD12	2.35	0.56
1:A:1013:VAL:HG22	1:A:1014:LEU:N	2.19	0.56
1:B:396:LEU:C	1:B:396:LEU:HD13	2.30	0.56
1:B:665:VAL:CG1	1:B:697:PRO:HD3	2.35	0.56
1:A:435:ILE:CG2	1:A:486:PHE:HE1	2.19	0.56
1:A:501:LEU:HD23	1:A:502:THR:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:820:PHE:O	1:A:821:GLU:HB3	2.05	0.56
1:B:444:LEU:HD23	1:B:524:PRO:CD	2.35	0.56
1:A:305:GLU:O	1:A:340:LYS:HG3	2.06	0.56
1:A:434:VAL:HG22	1:A:435:ILE:N	2.20	0.56
1:A:459:VAL:HG23	1:A:459:VAL:O	2.05	0.56
1:A:882:LEU:HD12	1:A:882:LEU:N	2.21	0.56
1:B:41:THR:CG2	1:B:502:THR:HG23	2.36	0.56
1:B:53:LEU:HG	1:B:64:LEU:HD13	1.87	0.56
1:B:116:MET:HG3	1:B:117:LEU:N	2.20	0.56
1:B:882:LEU:N	1:B:882:LEU:HD12	2.21	0.56
1:A:42:PHE:CE2	1:A:50:PHE:HZ	2.23	0.56
1:A:473:GLN:CD	1:A:504:VAL:HG13	2.31	0.56
1:A:873:THR:CG2	1:A:981:GLY:C	2.78	0.56
1:A:955:LEU:HG	1:A:973:ILE:HG23	1.86	0.56
1:B:45:GLU:HB3	1:B:46:PRO:CD	2.35	0.56
1:B:263:VAL:O	1:B:263:VAL:HG12	2.04	0.56
1:B:305:GLU:O	1:B:340:LYS:HG3	2.06	0.56
1:B:785:ASN:HD22	1:B:788:PHE:HE2	1.54	0.56
1:B:885:GLU:HG3	1:B:887:ARG:H	1.70	0.56
1:A:665:VAL:CG1	1:A:697:PRO:HD3	2.35	0.56
1:A:870:GLU:CD	1:A:1025:ALA:CA	2.78	0.56
1:A:949:TYR:HE2	1:A:951:MET:CE	2.12	0.56
1:B:585:GLU:OE1	1:B:585:GLU:HA	2.04	0.56
1:B:700:CYS:HB3	1:B:701:PRO:HD2	1.81	0.56
1:B:710:LEU:HB2	1:B:801:TYR:HE1	1.70	0.56
1:B:814:LEU:HD22	1:B:847:LEU:H	1.69	0.56
1:A:480:VAL:HG21	1:A:484:MET:HE1	1.87	0.56
1:B:468:GLN:HB2	1:B:522:GLY:C	2.30	0.56
1:B:892:HIS:CE1	1:B:931:ILE:HB	2.40	0.56
1:A:474:VAL:CG2	1:A:495:ILE:HG21	2.35	0.56
1:A:785:ASN:ND2	1:A:788:PHE:HE2	2.03	0.56
1:B:324:THR:CG2	1:B:462:PRO:HA	2.34	0.56
1:B:446:PHE:CE1	1:B:486:PHE:CZ	2.93	0.56
1:B:526:CYS:HB3	1:B:535:CYS:SG	2.46	0.56
1:B:804:GLY:HA2	1:B:806:MET:CE	2.36	0.56
1:A:41:THR:CG2	1:A:502:THR:HG23	2.35	0.56
1:A:226:ILE:HG23	1:A:226:ILE:O	2.06	0.56
1:A:321:LEU:HD12	1:A:462:PRO:CG	2.34	0.56
1:A:549:ARG:HA	1:A:584:PRO:HB3	1.88	0.56
1:A:569:VAL:HB	1:A:654:ASN:CB	2.36	0.56
1:A:885:GLU:HG3	1:A:887:ARG:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HB3	1:B:127:ILE:CG2	2.36	0.56
1:B:435:ILE:CG2	1:B:486:PHE:HE1	2.19	0.56
1:B:567:ILE:HD13	1:B:567:ILE:N	2.20	0.56
1:B:569:VAL:HG21	1:B:654:ASN:HB2	1.87	0.56
1:A:42:PHE:HE2	1:A:50:PHE:HZ	1.54	0.56
1:A:118:LEU:HB3	1:A:127:ILE:CG2	2.36	0.56
1:A:526:CYS:HB3	1:A:535:CYS:SG	2.46	0.56
1:A:567:ILE:HD13	1:A:567:ILE:N	2.20	0.56
1:A:983:ASN:O	1:A:1022:VAL:HG23	2.06	0.56
1:B:53:LEU:HD23	1:B:53:LEU:C	2.31	0.56
1:B:184:ILE:HD12	1:B:184:ILE:C	2.31	0.56
1:A:46:PRO:CG	1:A:69:ARG:HD2	2.36	0.56
1:A:53:LEU:HG	1:A:64:LEU:HD13	1.87	0.56
1:A:447:VAL:HG23	1:A:447:VAL:O	2.06	0.56
1:B:505:PRO:HB3	1:B:507:GLU:O	2.04	0.56
1:B:785:ASN:ND2	1:B:788:PHE:HE2	2.03	0.56
1:B:865:VAL:HG13	1:B:866:THR:N	2.21	0.56
1:A:396:LEU:HD13	1:A:396:LEU:C	2.30	0.55
1:A:433:SER:HB3	1:A:484:MET:SD	2.45	0.55
1:A:704:LEU:HD11	1:A:724:LYS:CE	2.35	0.55
1:A:710:LEU:HB2	1:A:801:TYR:HE1	1.70	0.55
1:A:1022:VAL:O	1:A:1022:VAL:HG13	2.06	0.55
1:B:284:LYS:HD3	1:B:284:LYS:C	2.31	0.55
1:B:480:VAL:HG21	1:B:484:MET:HE1	1.87	0.55
1:A:460:ASP:OD2	1:A:463:LYS:HB3	2.06	0.55
1:B:46:PRO:CG	1:B:69:ARG:HD2	2.36	0.55
1:A:435:ILE:HD12	1:A:486:PHE:HD1	1.70	0.55
1:A:474:VAL:HG12	1:A:475:VAL:N	2.21	0.55
1:A:619:VAL:CB	1:A:620:PRO:HD3	2.36	0.55
1:B:62:ILE:HG12	1:B:73:LEU:HB2	1.84	0.55
1:B:412:LEU:HD13	1:B:412:LEU:N	2.21	0.55
1:B:501:LEU:HD23	1:B:502:THR:H	1.70	0.55
1:B:807:ARG:HD3	1:B:812:LEU:O	2.07	0.55
1:A:382:LEU:HD23	1:A:385:LEU:CB	2.36	0.55
1:B:110:THR:HG22	1:B:111:ASN:H	1.72	0.55
1:B:190:GLY:O	1:B:192:PRO:HD3	2.07	0.55
1:B:359:LEU:HA	1:B:362:ILE:HG12	1.89	0.55
1:B:447:VAL:HG23	1:B:447:VAL:O	2.06	0.55
1:B:474:VAL:CG2	1:B:495:ILE:HG21	2.34	0.55
1:B:703:LEU:HD21	1:B:782:VAL:HG21	1.86	0.55
1:B:713:VAL:HG13	1:B:766:TYR:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:GLY:HA3	1:A:480:VAL:CG2	2.37	0.55
1:B:51:ASN:ND2	1:B:67:VAL:HG23	2.20	0.55
1:B:710:LEU:HB2	1:B:801:TYR:CE1	2.42	0.55
1:B:820:PHE:O	1:B:821:GLU:HB3	2.06	0.55
1:A:284:LYS:HD3	1:A:284:LYS:C	2.31	0.55
1:A:713:VAL:HG13	1:A:766:TYR:O	2.06	0.55
1:A:825:CYS:HB3	1:A:828:PRO:HG2	1.89	0.55
1:A:861:GLU:HG3	1:A:862:ILE:N	2.21	0.55
1:A:1004:ILE:HD13	1:A:1004:ILE:C	2.32	0.55
1:A:1014:LEU:H	1:A:1014:LEU:CD2	2.17	0.55
1:B:72:LYS:HD2	1:B:80:LEU:HB2	1.87	0.55
1:B:280:VAL:HG12	1:B:281:ARG:N	2.22	0.55
1:A:53:LEU:HD23	1:A:53:LEU:C	2.31	0.55
1:A:168:VAL:HG22	1:A:169:PHE:N	2.22	0.55
1:A:190:GLY:O	1:A:192:PRO:HD3	2.07	0.55
1:A:509:CYS:HB3	1:A:535:CYS:SG	2.47	0.55
1:B:42:PHE:HE2	1:B:50:PHE:HZ	1.54	0.55
1:B:226:ILE:HG23	1:B:226:ILE:O	2.06	0.55
1:B:380:LEU:HB2	1:B:386:LYS:HE2	1.87	0.55
1:A:116:MET:HG3	1:A:117:LEU:N	2.21	0.55
1:B:242:TYR:CD1	1:B:345:LYS:HE2	2.41	0.55
1:B:473:GLN:CD	1:B:504:VAL:HG13	2.31	0.55
1:B:480:VAL:HB	1:B:484:MET:HE2	1.89	0.55
1:B:619:VAL:CB	1:B:620:PRO:HD3	2.36	0.55
1:B:937:ARG:HG3	1:B:938:PRO:HD2	1.89	0.55
1:A:184:ILE:HD12	1:A:184:ILE:C	2.31	0.55
1:A:242:TYR:CD1	1:A:345:LYS:HE2	2.41	0.55
1:A:380:LEU:HB2	1:A:386:LYS:HE2	1.87	0.55
1:A:988:PHE:HD2	1:A:1016:MET:SD	2.30	0.55
1:B:380:LEU:CD1	1:B:386:LYS:HE3	2.37	0.55
1:B:501:LEU:HD23	1:B:502:THR:N	2.22	0.55
1:A:72:LYS:HD2	1:A:80:LEU:HB2	1.87	0.55
1:A:196:PRO:HB3	1:A:225:MET:CE	2.33	0.55
1:A:239:PHE:HA	1:A:260:PRO:CG	2.32	0.55
1:A:370:LEU:HD13	1:A:370:LEU:O	2.07	0.55
1:A:501:LEU:HD23	1:A:502:THR:N	2.22	0.55
1:A:804:GLY:HA2	1:A:806:MET:CE	2.36	0.55
1:A:597:LEU:HD22	1:A:597:LEU:N	2.21	0.54
1:B:168:VAL:HG22	1:B:169:PHE:N	2.22	0.54
1:B:370:LEU:HD13	1:B:370:LEU:O	2.07	0.54
1:B:597:LEU:N	1:B:597:LEU:HD22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:704:LEU:HD11	1:B:724:LYS:CE	2.35	0.54
1:A:480:VAL:HB	1:A:484:MET:HE2	1.88	0.54
1:A:785:ASN:HD22	1:A:788:PHE:HE2	1.54	0.54
1:A:797:LYS:HD2	1:A:797:LYS:H	1.72	0.54
1:A:865:VAL:HG13	1:A:866:THR:N	2.21	0.54
1:B:382:LEU:HD23	1:B:385:LEU:CB	2.37	0.54
1:B:435:ILE:HD12	1:B:486:PHE:HD1	1.71	0.54
1:B:930:GLU:OE2	1:B:941:MET:HG3	2.07	0.54
1:A:46:PRO:CG	1:A:69:ARG:HG3	2.27	0.54
1:A:72:LYS:HD2	1:A:80:LEU:HD12	1.90	0.54
1:A:471:THR:CG2	1:A:473:GLN:HE22	2.20	0.54
1:A:709:ILE:O	1:A:799:TYR:HD1	1.91	0.54
1:A:710:LEU:HB2	1:A:801:TYR:CE1	2.41	0.54
1:A:874:LYS:H	1:A:982:SER:CB	2.20	0.54
1:B:72:LYS:HD2	1:B:80:LEU:HD12	1.90	0.54
1:B:236:ILE:HG23	1:B:236:ILE:O	2.07	0.54
1:B:440:LYS:HB2	1:B:538:LYS:NZ	2.22	0.54
1:A:301:ARG:CD	1:A:425:THR:HG21	2.26	0.54
1:A:556:GLN:O	1:A:582:ASN:CB	2.56	0.54
1:A:947:LEU:H	1:A:947:LEU:CD2	2.21	0.54
1:B:460:ASP:OD2	1:B:463:LYS:HB3	2.06	0.54
1:A:63:TYR:CE2	1:A:72:LYS:HG2	2.43	0.54
1:A:151:PRO:O	1:A:157:HIS:HB3	2.07	0.54
1:A:359:LEU:HA	1:A:362:ILE:HG12	1.89	0.54
1:B:474:VAL:HG12	1:B:475:VAL:N	2.21	0.54
1:B:509:CYS:HB3	1:B:535:CYS:SG	2.47	0.54
1:A:994:LEU:HD11	1:A:1006:ASN:CB	2.37	0.54
1:B:426:GLU:HG2	1:B:429:ASP:O	2.08	0.54
1:A:699:ASP:HA	1:A:725:ASN:OD1	2.07	0.54
1:A:739:ILE:HB	1:A:781:THR:HG22	1.90	0.54
1:B:151:PRO:O	1:B:157:HIS:HB3	2.08	0.54
1:B:154:LYS:HB2	1:B:157:HIS:HD2	1.70	0.54
1:B:471:THR:CG2	1:B:473:GLN:HE22	2.20	0.54
1:A:429:ASP:OD1	1:A:450:LYS:HB3	2.08	0.54
1:A:930:GLU:OE2	1:A:941:MET:HG3	2.07	0.54
1:B:190:GLY:C	1:B:192:PRO:HD3	2.33	0.54
1:B:196:PRO:CB	1:B:225:MET:HE2	2.34	0.54
1:B:370:LEU:HD11	1:B:399:ILE:HD12	1.88	0.54
1:B:797:LYS:HD2	1:B:797:LYS:H	1.72	0.54
1:A:135:GLY:O	1:A:159:LEU:HD13	2.08	0.54
1:A:175:TYR:HB3	1:A:179:ASP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:HD13	1:A:412:LEU:N	2.21	0.54
1:A:531:LEU:O	1:A:641:THR:OG1	2.25	0.54
1:A:662:LEU:HD23	1:A:791:ASP:OD2	2.08	0.54
1:B:861:GLU:HG3	1:B:862:ILE:N	2.21	0.54
1:A:51:ASN:ND2	1:A:67:VAL:HG23	2.20	0.54
1:A:370:LEU:HD11	1:A:399:ILE:HD12	1.88	0.54
1:B:175:TYR:HB3	1:B:179:ASP:HB3	1.89	0.54
1:B:716:ILE:HG12	1:B:763:ASN:HB3	1.90	0.54
1:B:825:CYS:HB3	1:B:828:PRO:HG2	1.89	0.54
1:B:301:ARG:CD	1:B:425:THR:HG21	2.26	0.53
1:B:921:LYS:N	1:B:922:PRO:HD2	2.23	0.53
1:B:947:LEU:H	1:B:947:LEU:CD2	2.21	0.53
1:A:110:THR:HG22	1:A:111:ASN:H	1.72	0.53
1:A:280:VAL:HG12	1:A:281:ARG:N	2.22	0.53
1:A:955:LEU:CG	1:A:973:ILE:HG23	2.38	0.53
1:A:957:ASP:O	1:A:974:THR:HG22	2.08	0.53
1:B:63:TYR:CE2	1:B:72:LYS:HG2	2.43	0.53
1:B:662:LEU:HD23	1:B:791:ASP:CG	2.32	0.53
1:B:925:HIS:O	1:B:950:PHE:HD2	1.91	0.53
1:B:926:ALA:CB	1:B:947:LEU:HD12	2.35	0.53
1:A:473:GLN:CD	1:A:504:VAL:HG22	2.33	0.53
1:A:603:LEU:HD23	1:A:603:LEU:C	2.33	0.53
1:A:739:ILE:HB	1:A:781:THR:HG23	1.90	0.53
1:A:921:LYS:N	1:A:922:PRO:HD2	2.23	0.53
1:A:924:GLN:O	1:A:925:HIS:HB2	2.09	0.53
1:A:236:ILE:HG23	1:A:236:ILE:O	2.07	0.53
1:A:426:GLU:HG2	1:A:429:ASP:O	2.08	0.53
1:A:589:GLY:HA3	1:A:639:LYS:HG3	1.90	0.53
1:A:807:ARG:HD3	1:A:812:LEU:O	2.07	0.53
1:A:867:GLY:CA	1:A:981:GLY:N	2.49	0.53
1:B:429:ASP:OD1	1:B:450:LYS:HB3	2.08	0.53
1:B:924:GLN:O	1:B:925:HIS:HB2	2.09	0.53
1:A:321:LEU:CD2	1:A:325:LEU:HD11	2.39	0.53
1:A:495:ILE:HG23	1:A:495:ILE:O	2.08	0.53
1:A:533:ASN:HD22	1:A:643:MET:HB3	1.73	0.53
1:A:827:SER:HB2	1:A:828:PRO:HD3	1.91	0.53
1:B:181:LYS:CE	1:B:202:LYS:HG2	2.39	0.53
1:B:371:GLN:O	1:B:375:ARG:HG3	2.09	0.53
1:B:578:LEU:HB2	1:B:609:ILE:HB	1.91	0.53
1:B:603:LEU:HD23	1:B:603:LEU:C	2.33	0.53
1:B:709:ILE:O	1:B:799:TYR:HD1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB3	1:A:243:TYR:CG	2.44	0.53
1:A:509:CYS:HB2	1:A:536:THR:HA	1.91	0.53
1:A:679:VAL:HG12	1:A:680:CYS:N	2.23	0.53
1:A:716:ILE:HG12	1:A:763:ASN:HB3	1.90	0.53
1:B:278:LYS:HG2	1:B:296:PRO:CA	2.38	0.53
1:B:321:LEU:CD2	1:B:325:LEU:HD11	2.39	0.53
1:B:563:HIS:HB3	1:B:564:PRO:CD	2.28	0.53
1:A:190:GLY:HA2	1:A:233:PHE:HE2	1.73	0.53
1:A:549:ARG:CD	1:A:584:PRO:HB2	2.33	0.53
1:A:805:ALA:H	1:A:806:MET:CE	2.22	0.53
1:B:39:PHE:CD1	1:B:505:PRO:HD2	2.44	0.53
1:B:356:ILE:HG22	1:B:421:ILE:O	2.09	0.53
1:B:448:GLY:HA3	1:B:480:VAL:CG2	2.37	0.53
1:B:739:ILE:HB	1:B:781:THR:HG22	1.90	0.53
1:B:947:LEU:O	1:B:947:LEU:HD23	2.09	0.53
1:A:119:ILE:HG23	1:A:119:ILE:O	2.09	0.53
1:A:356:ILE:HG22	1:A:421:ILE:O	2.09	0.53
1:A:925:HIS:O	1:A:950:PHE:HD2	1.91	0.53
1:A:958:LEU:HD23	1:A:959:LYS:H	1.73	0.53
1:A:997:ARG:H	1:A:1004:ILE:CG2	2.22	0.53
1:B:198:ILE:HB	1:B:226:ILE:HG22	1.91	0.53
1:B:308:LEU:O	1:B:338:PHE:HA	2.09	0.53
1:B:716:ILE:HG23	1:B:716:ILE:O	2.09	0.53
1:A:190:GLY:C	1:A:192:PRO:HD3	2.33	0.53
1:A:575:LEU:H	1:A:575:LEU:CD2	2.22	0.53
1:A:937:ARG:HG3	1:A:938:PRO:HD2	1.89	0.53
1:A:40:VAL:HG11	1:A:503:ARG:NH2	2.24	0.53
1:A:308:LEU:O	1:A:338:PHE:HA	2.09	0.53
1:A:578:LEU:HB2	1:A:609:ILE:HB	1.91	0.53
1:A:807:ARG:HD2	1:A:813:CYS:HA	1.90	0.53
1:A:1032:VAL:HG12	1:A:1033:PHE:N	2.23	0.53
1:B:882:LEU:HD13	1:B:910:ALA:O	2.09	0.53
1:A:181:LYS:CE	1:A:202:LYS:HG2	2.39	0.52
1:A:580:THR:HG21	1:A:583:VAL:HG11	1.91	0.52
1:A:806:MET:HG2	1:A:807:ARG:CG	2.39	0.52
1:A:875:VAL:HG22	1:A:915:CYS:O	2.09	0.52
1:A:933:VAL:HG22	1:A:940:PHE:HB3	1.91	0.52
1:B:40:VAL:HG11	1:B:503:ARG:NH2	2.24	0.52
1:A:716:ILE:HG23	1:A:716:ILE:O	2.09	0.52
1:A:947:LEU:HD23	1:A:947:LEU:O	2.09	0.52
1:A:952:THR:HG23	1:A:952:THR:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LYS:HG2	1:A:972:THR:CG2	2.39	0.52
1:A:1019:THR:HG23	1:A:1019:THR:O	2.10	0.52
1:B:64:LEU:HD22	1:B:64:LEU:N	2.24	0.52
1:B:439:TYR:CZ	1:B:538:LYS:CE	2.92	0.52
1:B:495:ILE:O	1:B:495:ILE:HG23	2.08	0.52
1:B:807:ARG:HD2	1:B:813:CYS:HA	1.90	0.52
1:A:281:ARG:O	1:A:282:LEU:HD23	2.09	0.52
1:A:827:SER:HB2	1:A:828:PRO:CD	2.39	0.52
1:A:1004:ILE:HG23	1:A:1004:ILE:O	2.08	0.52
1:B:135:GLY:O	1:B:159:LEU:HD13	2.08	0.52
1:B:321:LEU:HD12	1:B:462:PRO:CG	2.34	0.52
1:B:679:VAL:HG12	1:B:680:CYS:N	2.23	0.52
1:B:185:ALA:HB3	1:B:243:TYR:CG	2.44	0.52
1:B:589:GLY:HA3	1:B:639:LYS:HG3	1.90	0.52
1:B:739:ILE:HB	1:B:781:THR:HG23	1.90	0.52
1:B:827:SER:HB2	1:B:828:PRO:CD	2.40	0.52
1:A:42:PHE:HZ	1:A:45:GLU:CB	2.22	0.52
1:B:127:ILE:O	1:B:127:ILE:HG23	2.09	0.52
1:B:281:ARG:O	1:B:282:LEU:HD23	2.09	0.52
1:B:473:GLN:CD	1:B:504:VAL:HG22	2.34	0.52
1:B:783:VAL:HG12	1:B:784:TRP:N	2.25	0.52
1:A:296:PRO:HD2	1:A:414:VAL:HG22	1.92	0.52
1:A:371:GLN:O	1:A:375:ARG:HG3	2.09	0.52
1:A:868:PRO:CG	1:A:1022:VAL:HG21	2.40	0.52
1:A:882:LEU:HD13	1:A:910:ALA:O	2.09	0.52
1:B:630:HIS:HD2	1:B:632:VAL:HG23	1.73	0.52
1:B:875:VAL:HG22	1:B:915:CYS:O	2.09	0.52
1:A:560:LEU:HG	1:A:648:THR:HG21	1.92	0.52
1:B:118:LEU:HD13	1:B:118:LEU:C	2.34	0.52
1:B:439:TYR:CZ	1:B:538:LYS:NZ	2.75	0.52
1:A:64:LEU:HD22	1:A:64:LEU:N	2.24	0.52
1:A:566:ASN:HB3	1:A:651:VAL:CG2	2.40	0.52
1:A:593:THR:HG23	1:A:593:THR:O	2.10	0.52
1:B:59:THR:HB	1:B:61:HIS:CE1	2.45	0.52
1:B:228:ILE:HG22	1:B:233:PHE:CE1	2.45	0.52
1:B:472:VAL:O	1:B:472:VAL:HG12	2.09	0.52
1:B:575:LEU:H	1:B:575:LEU:CD2	2.22	0.52
1:A:39:PHE:CD1	1:A:505:PRO:HD2	2.44	0.52
1:A:198:ILE:HB	1:A:226:ILE:HG22	1.91	0.52
1:A:472:VAL:HG12	1:A:472:VAL:O	2.09	0.52
1:A:553:GLU:HG3	1:A:554:MET:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:GLY:CA	1:B:327:VAL:HG22	2.40	0.52
1:B:560:LEU:HG	1:B:648:THR:HG21	1.92	0.52
1:B:806:MET:HG2	1:B:807:ARG:CG	2.39	0.52
1:A:322:GLY:CA	1:A:327:VAL:HG22	2.40	0.52
1:A:712:PRO:O	1:A:715:VAL:HG22	2.09	0.52
1:A:956:ALA:O	1:A:1031:LEU:HD11	2.10	0.52
1:B:64:LEU:HD11	1:B:501:LEU:HD12	1.92	0.52
1:B:171:VAL:HG12	1:B:172:ILE:N	2.25	0.52
1:B:509:CYS:HB2	1:B:536:THR:HA	1.91	0.52
1:B:580:THR:HG21	1:B:583:VAL:HG11	1.92	0.52
1:B:827:SER:HB2	1:B:828:PRO:HD3	1.91	0.52
1:A:54:VAL:HG22	1:A:55:VAL:N	2.25	0.51
1:A:64:LEU:HD11	1:A:501:LEU:HD12	1.92	0.51
1:A:171:VAL:HG12	1:A:172:ILE:N	2.26	0.51
1:A:716:ILE:CG1	1:A:763:ASN:HB3	2.41	0.51
1:A:986:VAL:HG12	1:A:988:PHE:CE1	2.45	0.51
1:B:444:LEU:HD12	1:B:446:PHE:CZ	2.44	0.51
1:A:127:ILE:HG23	1:A:127:ILE:O	2.09	0.51
1:A:154:LYS:HB2	1:A:157:HIS:HD2	1.71	0.51
1:A:185:ALA:CB	1:A:243:TYR:CG	2.94	0.51
1:A:228:ILE:HG22	1:A:233:PHE:CE1	2.45	0.51
1:B:712:PRO:O	1:B:715:VAL:HG22	2.09	0.51
1:B:805:ALA:H	1:B:806:MET:CE	2.22	0.51
1:A:93:LYS:HD3	1:A:105:GLU:OE2	2.10	0.51
1:A:118:LEU:HD13	1:A:118:LEU:C	2.34	0.51
1:A:712:PRO:HG3	1:A:801:TYR:CZ	2.45	0.51
1:B:119:ILE:HG23	1:B:119:ILE:O	2.09	0.51
1:B:553:GLU:HG3	1:B:554:MET:N	2.24	0.51
1:B:567:ILE:CD1	1:B:650:PHE:CE2	2.94	0.51
1:A:468:GLN:HG3	1:A:523:ASP:HA	1.92	0.51
1:B:418:VAL:HG13	1:B:418:VAL:O	2.11	0.51
1:B:519:LEU:N	1:B:519:LEU:HD22	2.26	0.51
1:B:695:LYS:CB	1:B:696:LEU:HD12	2.41	0.51
1:B:727:PRO:O	1:B:729:PRO:HD3	2.10	0.51
1:A:53:LEU:HG	1:A:64:LEU:HD11	1.92	0.51
1:A:196:PRO:CB	1:A:225:MET:HE2	2.34	0.51
1:A:216:VAL:HG13	1:A:217:PHE:N	2.26	0.51
1:A:695:LYS:CB	1:A:696:LEU:HD12	2.41	0.51
1:A:984:VAL:HG11	1:A:998:ARG:HD3	1.91	0.51
1:B:265:PRO:HD3	1:B:274:VAL:HG22	1.92	0.51
1:B:541:CYS:SG	1:B:550:PHE:HD2	2.33	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:PRO:HG3	1:B:801:TYR:CZ	2.45	0.51
1:B:716:ILE:CG1	1:B:763:ASN:HB3	2.40	0.51
1:B:933:VAL:HG22	1:B:940:PHE:HB3	1.91	0.51
1:B:54:VAL:HG22	1:B:55:VAL:N	2.25	0.51
1:A:278:LYS:HG2	1:A:296:PRO:CA	2.39	0.51
1:A:370:LEU:HD11	1:A:374:TYR:CE1	2.46	0.51
1:A:790:ILE:HD12	1:A:790:ILE:N	2.25	0.51
1:A:889:ILE:CD1	1:A:907:TYR:CE1	2.94	0.51
1:A:997:ARG:H	1:A:1004:ILE:HG23	1.75	0.51
1:B:426:GLU:HG3	1:B:429:ASP:H	1.75	0.51
1:B:548:ARG:O	1:B:584:PRO:HD3	2.11	0.51
1:B:823:GLY:HA3	1:B:844:TRP:CZ2	2.46	0.51
1:B:930:GLU:HG3	1:B:941:MET:SD	2.51	0.51
1:A:133:TYR:O	1:A:134:GLN:HB2	2.11	0.51
1:A:439:TYR:CD2	1:A:538:LYS:NZ	2.77	0.51
1:A:473:GLN:HB2	1:A:504:VAL:CG2	2.40	0.51
1:B:239:PHE:HA	1:B:260:PRO:CG	2.33	0.51
1:B:370:LEU:HD11	1:B:374:TYR:CE1	2.46	0.51
1:B:505:PRO:HB2	1:B:507:GLU:C	2.35	0.51
1:A:59:THR:HB	1:A:61:HIS:CE1	2.45	0.51
1:A:76:ASP:O	1:A:77:LEU:HB2	2.11	0.51
1:A:418:VAL:O	1:A:418:VAL:HG13	2.10	0.51
1:A:519:LEU:HD22	1:A:519:LEU:N	2.26	0.51
1:A:567:ILE:CD1	1:A:650:PHE:CE2	2.94	0.51
1:A:630:HIS:HD2	1:A:632:VAL:HG23	1.73	0.51
1:A:727:PRO:O	1:A:729:PRO:HD3	2.10	0.51
1:A:847:LEU:HG	1:A:850:ALA:HA	1.91	0.51
1:B:53:LEU:HG	1:B:64:LEU:HD11	1.92	0.51
1:B:296:PRO:HD2	1:B:414:VAL:HG22	1.92	0.51
1:B:527:GLY:HA3	1:B:550:PHE:CE1	2.45	0.51
1:B:703:LEU:HD22	1:B:703:LEU:N	2.26	0.51
1:B:847:LEU:HG	1:B:850:ALA:HA	1.91	0.51
1:A:507:GLU:HG3	1:A:537:ARG:CG	2.41	0.51
1:A:807:ARG:HD3	1:A:812:LEU:HB3	1.93	0.51
1:B:93:LYS:HD3	1:B:105:GLU:OE2	2.10	0.51
1:B:185:ALA:CB	1:B:243:TYR:CG	2.94	0.51
1:A:358:ILE:CG2	1:A:361:GLN:HB2	2.41	0.50
1:A:541:CYS:SG	1:A:550:PHE:HD2	2.33	0.50
1:A:823:GLY:HA3	1:A:844:TRP:CZ2	2.46	0.50
1:A:870:GLU:OE2	1:A:1025:ALA:CA	2.58	0.50
1:A:987:MET:HB2	1:A:1019:THR:HG22	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:THR:HG23	1:B:206:ASN:O	2.11	0.50
1:B:228:ILE:CG2	1:B:233:PHE:CE1	2.94	0.50
1:B:566:ASN:HB3	1:B:651:VAL:CG2	2.40	0.50
1:B:689:PHE:CE1	1:B:691:GLU:CG	2.94	0.50
1:B:790:ILE:HD12	1:B:790:ILE:N	2.25	0.50
1:B:807:ARG:HD3	1:B:812:LEU:HB3	1.93	0.50
1:B:895:VAL:O	1:B:896:ALA:HB3	2.11	0.50
1:A:204:THR:HG23	1:A:206:ASN:O	2.11	0.50
1:A:469:TYR:HB2	1:A:523:ASP:OD2	2.11	0.50
1:A:783:VAL:HG12	1:A:784:TRP:N	2.25	0.50
1:A:798:VAL:O	1:A:798:VAL:HG13	2.10	0.50
1:A:930:GLU:HG3	1:A:941:MET:SD	2.51	0.50
1:B:119:ILE:CG2	1:B:121:TYR:CE1	2.95	0.50
1:B:300:GLU:HG2	1:B:305:GLU:HA	1.93	0.50
1:B:400:ASP:HB2	1:B:402:ASN:OD1	2.11	0.50
1:A:228:ILE:CG2	1:A:233:PHE:CE1	2.94	0.50
1:A:265:PRO:HD3	1:A:274:VAL:HG22	1.92	0.50
1:A:703:LEU:N	1:A:703:LEU:HD22	2.26	0.50
1:A:785:ASN:HB3	1:A:788:PHE:CE2	2.46	0.50
1:A:1029:GLN:HG2	1:A:1030:ASP:N	2.26	0.50
1:B:370:LEU:CD1	1:B:374:TYR:CD1	2.95	0.50
1:B:370:LEU:HD13	1:B:374:TYR:CD1	2.46	0.50
1:B:473:GLN:HB2	1:B:504:VAL:CG2	2.40	0.50
1:B:949:TYR:HE2	1:B:951:MET:CE	2.12	0.50
1:A:185:ALA:CB	1:A:243:TYR:CD2	2.94	0.50
1:A:261:GLU:HG2	1:A:265:PRO:N	2.25	0.50
1:A:689:PHE:CE1	1:A:691:GLU:CG	2.94	0.50
1:A:782:VAL:CG2	1:A:790:ILE:HB	2.41	0.50
1:A:894:LYS:CD	1:A:899:GLU:HA	2.41	0.50
1:B:295:VAL:HG23	1:B:295:VAL:O	2.12	0.50
1:B:785:ASN:HB3	1:B:788:PHE:CE2	2.46	0.50
1:B:853:LYS:H	1:B:853:LYS:HD2	1.76	0.50
1:A:370:LEU:CD1	1:A:374:TYR:CD1	2.95	0.50
1:A:439:TYR:CE2	1:A:538:LYS:HE2	2.43	0.50
1:B:76:ASP:O	1:B:77:LEU:HB2	2.11	0.50
1:B:196:PRO:HB3	1:B:225:MET:CE	2.33	0.50
1:B:412:LEU:HD22	1:B:412:LEU:O	2.11	0.50
1:B:541:CYS:CB	1:B:544:SER:HB3	2.42	0.50
1:B:695:LYS:C	1:B:696:LEU:HD12	2.37	0.50
1:A:662:LEU:CD2	1:A:791:ASP:OD2	2.60	0.50
1:A:895:VAL:O	1:A:896:ALA:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1029:GLN:CG	1:A:1030:ASP:H	2.24	0.50
1:B:64:LEU:HB2	1:B:71:TYR:HD2	1.77	0.50
1:B:133:TYR:O	1:B:134:GLN:HB2	2.11	0.50
1:B:185:ALA:CB	1:B:243:TYR:CD2	2.94	0.50
1:B:261:GLU:HG2	1:B:265:PRO:N	2.25	0.50
1:B:403:PHE:CE1	1:B:406:LEU:CD2	2.94	0.50
1:B:491:GLU:O	1:B:506:VAL:HG12	2.11	0.50
1:A:39:PHE:CD2	1:A:473:GLN:CG	2.95	0.50
1:A:81:VAL:HG12	1:A:82:THR:N	2.26	0.50
1:A:110:THR:CB	1:A:132:LEU:HD21	2.42	0.50
1:A:185:ALA:HB1	1:A:243:TYR:CE2	2.47	0.50
1:A:440:LYS:CB	1:A:538:LYS:HZ3	2.23	0.50
1:A:491:GLU:O	1:A:506:VAL:HG12	2.11	0.50
1:A:527:GLY:HA3	1:A:550:PHE:CE1	2.45	0.50
1:A:532:HIS:C	1:A:641:THR:HG21	2.36	0.50
1:A:673:TRP:HB3	1:A:694:VAL:HB	1.94	0.50
1:B:358:ILE:CG2	1:B:361:GLN:HB2	2.41	0.50
1:B:457:ILE:HG12	1:B:467:LEU:CD1	2.42	0.50
1:B:798:VAL:HG13	1:B:798:VAL:O	2.10	0.50
1:A:40:VAL:HG21	1:A:76:ASP:O	2.12	0.50
1:A:320:VAL:HG23	1:A:441:ASN:HB3	1.94	0.50
1:A:736:TYR:CD2	1:A:784:TRP:HB3	2.47	0.50
1:B:889:ILE:CD1	1:B:907:TYR:CE1	2.94	0.50
1:A:119:ILE:CG2	1:A:121:TYR:CE1	2.95	0.50
1:A:300:GLU:HG2	1:A:305:GLU:HA	1.93	0.50
1:A:370:LEU:HD13	1:A:374:TYR:CD1	2.46	0.50
1:A:695:LYS:C	1:A:696:LEU:HD12	2.37	0.50
1:A:892:HIS:HD2	1:A:893:VAL:N	2.10	0.50
1:A:986:VAL:CG1	1:A:988:PHE:CE1	2.94	0.50
1:B:81:VAL:HG12	1:B:82:THR:N	2.26	0.50
1:B:593:THR:O	1:B:593:THR:HG23	2.10	0.50
1:B:736:TYR:CD2	1:B:784:TRP:HB3	2.47	0.50
1:B:841:GLU:HG3	1:B:842:SER:H	1.77	0.50
1:A:380:LEU:CD1	1:A:386:LYS:HE3	2.37	0.49
1:A:457:ILE:HG12	1:A:467:LEU:CD1	2.42	0.49
1:A:597:LEU:HD22	1:A:597:LEU:H	1.78	0.49
1:B:278:LYS:CE	1:B:296:PRO:HG3	2.41	0.49
1:B:882:LEU:HD23	1:B:913:ILE:HD11	1.94	0.49
1:A:265:PRO:CD	1:A:274:VAL:HG22	2.42	0.49
1:A:426:GLU:HG3	1:A:429:ASP:H	1.75	0.49
1:A:444:LEU:HD12	1:A:446:PHE:CZ	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:ILE:HD12	1:A:624:THR:CA	2.42	0.49
1:A:976:THR:HG22	1:A:977:ASN:N	2.27	0.49
1:B:623:ILE:HD12	1:B:624:THR:CA	2.42	0.49
1:B:790:ILE:HD12	1:B:790:ILE:H	1.77	0.49
1:B:856:ASN:N	1:B:857:PRO:HD3	2.27	0.49
1:B:892:HIS:HD2	1:B:893:VAL:N	2.10	0.49
1:A:105:GLU:CB	1:A:106:PRO:HD2	2.42	0.49
1:A:234:THR:HG23	1:A:235:VAL:N	2.26	0.49
1:A:400:ASP:HB2	1:A:402:ASN:OD1	2.11	0.49
1:B:59:THR:HB	1:B:61:HIS:ND1	2.27	0.49
1:B:234:THR:HG23	1:B:235:VAL:N	2.27	0.49
1:B:333:LEU:HD21	1:B:358:ILE:HG13	1.94	0.49
1:B:597:LEU:H	1:B:597:LEU:CD2	2.26	0.49
1:B:792:ASN:HD21	1:B:796:ASN:N	2.10	0.49
1:B:894:LYS:CD	1:B:899:GLU:HA	2.41	0.49
1:A:333:LEU:HD21	1:A:358:ILE:HG13	1.94	0.49
1:A:792:ASN:HD21	1:A:796:ASN:N	2.10	0.49
1:B:185:ALA:HB1	1:B:243:TYR:CE2	2.47	0.49
1:B:265:PRO:HB2	1:B:266:PRO:HD2	1.94	0.49
1:B:713:VAL:HG13	1:B:767:SER:HA	1.94	0.49
1:A:412:LEU:HD22	1:A:412:LEU:O	2.11	0.49
1:A:790:ILE:HD12	1:A:790:ILE:H	1.77	0.49
1:A:955:LEU:HD11	1:A:973:ILE:HG23	1.94	0.49
1:B:40:VAL:HG21	1:B:76:ASP:O	2.12	0.49
1:B:312:ALA:HB1	1:B:334:LEU:HD11	1.94	0.49
1:B:475:VAL:HG22	1:B:500:GLN:OE1	2.13	0.49
1:A:132:LEU:HD11	1:A:163:ASN:HD22	1.77	0.49
1:A:185:ALA:HA	1:A:197:THR:O	2.13	0.49
1:A:475:VAL:HG22	1:A:500:GLN:OE1	2.13	0.49
1:A:532:HIS:CA	1:A:641:THR:HG21	2.43	0.49
1:A:597:LEU:H	1:A:597:LEU:CD2	2.26	0.49
1:A:782:VAL:HG23	1:A:782:VAL:O	2.12	0.49
1:B:110:THR:CB	1:B:132:LEU:HD21	2.42	0.49
1:B:133:TYR:HB3	1:B:136:ILE:HG23	1.94	0.49
1:B:265:PRO:CD	1:B:274:VAL:HG22	2.42	0.49
1:B:374:TYR:CE2	1:B:397:LEU:HD22	2.48	0.49
1:A:254:TYR:CE2	1:A:281:ARG:HD2	2.48	0.49
1:A:295:VAL:O	1:A:295:VAL:HG23	2.12	0.49
1:A:374:TYR:CE2	1:A:397:LEU:HD22	2.48	0.49
1:A:995:PHE:HZ	1:A:998:ARG:HB2	1.77	0.49
1:A:1002:TYR:OH	1:A:1004:ILE:HB	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1021:GLN:HG2	1:A:1026:ARG:CG	2.41	0.49
1:B:444:LEU:CD2	1:B:524:PRO:CD	2.91	0.49
1:B:548:ARG:CD	1:B:583:VAL:O	2.60	0.49
1:A:541:CYS:CB	1:A:544:SER:HB3	2.42	0.49
1:A:841:GLU:HG3	1:A:842:SER:H	1.78	0.49
1:A:889:ILE:O	1:A:892:HIS:HB3	2.13	0.49
1:B:132:LEU:HD11	1:B:163:ASN:HD22	1.77	0.49
1:B:216:VAL:HG13	1:B:217:PHE:N	2.26	0.49
1:B:889:ILE:O	1:B:892:HIS:HB3	2.13	0.49
1:A:265:PRO:HB2	1:A:266:PRO:HD2	1.94	0.49
1:A:991:GLN:CB	1:A:1008:THR:HG21	2.42	0.49
1:B:473:GLN:HB3	1:B:502:THR:HG21	1.94	0.49
1:B:590:VAL:HG12	1:B:591:ASN:N	2.27	0.49
1:B:847:LEU:HG	1:B:850:ALA:CA	2.42	0.49
1:A:133:TYR:HB3	1:A:136:ILE:HG23	1.94	0.49
1:A:853:LYS:H	1:A:853:LYS:HD2	1.76	0.49
1:A:868:PRO:HG2	1:A:981:GLY:HA3	1.91	0.49
1:B:182:LEU:HD21	1:B:184:ILE:HG21	1.94	0.49
1:B:190:GLY:HA2	1:B:233:PHE:HE2	1.73	0.49
1:B:809:SER:CB	1:B:881:ASN:ND2	2.75	0.49
1:A:99:ILE:HD11	1:A:152:PHE:CB	2.41	0.48
1:A:856:ASN:N	1:A:857:PRO:HD3	2.27	0.48
1:A:863:ILE:HG13	1:A:864:PRO:N	2.28	0.48
1:B:39:PHE:CD2	1:B:473:GLN:CG	2.95	0.48
1:B:506:VAL:O	1:B:525:HIS:CE1	2.66	0.48
1:B:541:CYS:SG	1:B:550:PHE:CD2	3.06	0.48
1:B:676:TYR:CE1	1:B:730:GLN:CD	2.90	0.48
1:B:863:ILE:HG13	1:B:864:PRO:N	2.28	0.48
1:B:907:TYR:CZ	1:B:909:PRO:HA	2.48	0.48
1:A:59:THR:HB	1:A:61:HIS:ND1	2.27	0.48
1:A:790:ILE:HG22	1:A:791:ASP:N	2.29	0.48
1:A:847:LEU:HG	1:A:850:ALA:CA	2.42	0.48
1:A:868:PRO:CG	1:A:1022:VAL:CG2	2.88	0.48
1:B:160:SER:OG	1:B:162:VAL:HG23	2.13	0.48
1:A:590:VAL:HG12	1:A:591:ASN:N	2.27	0.48
1:A:713:VAL:HG13	1:A:767:SER:HA	1.94	0.48
1:A:743:GLN:H	1:A:743:GLN:CD	2.22	0.48
1:A:882:LEU:HD23	1:A:913:ILE:HD11	1.94	0.48
1:A:1020:VAL:O	1:A:1020:VAL:HG13	2.13	0.48
1:B:185:ALA:HA	1:B:197:THR:O	2.13	0.48
1:B:435:ILE:HG21	1:B:486:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:673:TRP:HB3	1:B:694:VAL:HB	1.94	0.48
1:B:743:GLN:CD	1:B:743:GLN:H	2.21	0.48
1:A:239:PHE:CD1	1:A:260:PRO:HG2	2.48	0.48
1:A:321:LEU:CG	1:A:325:LEU:HD11	2.40	0.48
1:A:991:GLN:HB3	1:A:1008:THR:HG21	1.96	0.48
1:B:239:PHE:CD1	1:B:260:PRO:HG2	2.48	0.48
1:B:254:TYR:CE2	1:B:281:ARG:HD2	2.48	0.48
1:B:320:VAL:HG23	1:B:441:ASN:HB3	1.94	0.48
1:B:781:THR:HG23	1:B:781:THR:O	2.12	0.48
1:B:807:ARG:HB3	1:B:812:LEU:HB2	1.95	0.48
1:A:435:ILE:HG21	1:A:486:PHE:CE1	2.48	0.48
1:A:473:GLN:HB3	1:A:502:THR:HG21	1.94	0.48
1:A:681:THR:HG21	1:A:686:THR:HG21	1.94	0.48
1:A:716:ILE:HD11	1:A:763:ASN:HB3	1.95	0.48
1:A:740:LEU:HD12	1:A:740:LEU:N	2.29	0.48
1:A:781:THR:HG23	1:A:781:THR:O	2.12	0.48
1:B:258:LEU:HD12	1:B:258:LEU:N	2.29	0.48
1:B:453:LYS:HE3	1:B:472:VAL:HG22	1.94	0.48
1:B:715:VAL:HG23	1:B:715:VAL:O	2.13	0.48
1:A:182:LEU:HD21	1:A:184:ILE:HG21	1.94	0.48
1:A:567:ILE:HD12	1:A:650:PHE:CE2	2.49	0.48
1:A:589:GLY:C	1:A:639:LYS:HG2	2.39	0.48
1:B:716:ILE:HD11	1:B:763:ASN:HB3	1.95	0.48
1:B:935:VAL:HG12	1:B:936:CYS:N	2.28	0.48
1:A:312:ALA:HB1	1:A:334:LEU:HD11	1.94	0.48
1:A:64:LEU:HB2	1:A:71:TYR:HD2	1.77	0.48
1:A:144:ASP:O	1:A:145:LEU:HB2	2.13	0.48
1:A:543:ARG:HH11	1:A:549:ARG:HH22	1.62	0.48
1:A:626:ASN:ND2	1:A:630:HIS:HB2	2.29	0.48
1:A:807:ARG:HB3	1:A:812:LEU:HB2	1.95	0.48
1:A:935:VAL:HG12	1:A:936:CYS:N	2.28	0.48
1:B:42:PHE:HZ	1:B:45:GLU:CB	2.22	0.48
1:B:144:ASP:O	1:B:145:LEU:HB2	2.13	0.48
1:B:626:ASN:ND2	1:B:630:HIS:HB2	2.29	0.48
1:B:782:VAL:CG2	1:B:790:ILE:HB	2.41	0.48
1:B:783:VAL:HG13	1:B:788:PHE:O	2.13	0.48
1:B:471:THR:HG23	1:B:473:GLN:NE2	2.27	0.48
1:A:710:LEU:HD13	1:A:801:TYR:OH	2.13	0.48
1:B:460:ASP:CG	1:B:463:LYS:HB3	2.39	0.48
1:B:782:VAL:HG23	1:B:782:VAL:O	2.12	0.48
1:A:361:GLN:HE21	1:A:365:ARG:HH21	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TYR:CB	1:A:523:ASP:OD2	2.62	0.47
1:A:704:LEU:H	1:A:723:ALA:HA	1.79	0.47
1:A:1010:SER:HB2	1:A:1035:TYR:CD2	2.49	0.47
1:B:440:LYS:HG2	1:B:440:LYS:O	2.14	0.47
1:B:561:THR:HG22	1:B:562:VAL:N	2.29	0.47
1:B:681:THR:HG21	1:B:686:THR:HG21	1.95	0.47
1:B:710:LEU:HD13	1:B:801:TYR:OH	2.13	0.47
1:A:124:ASN:OD1	1:A:142:LEU:HB3	2.14	0.47
1:A:258:LEU:HD12	1:A:258:LEU:N	2.28	0.47
1:A:440:LYS:O	1:A:440:LYS:HG2	2.14	0.47
1:A:541:CYS:SG	1:A:550:PHE:CD2	3.07	0.47
1:A:862:ILE:CG2	1:A:877:ILE:HG23	2.44	0.47
1:A:907:TYR:CZ	1:A:909:PRO:HA	2.48	0.47
1:A:991:GLN:OE1	1:A:991:GLN:HA	2.13	0.47
1:B:124:ASN:OD1	1:B:142:LEU:HB3	2.15	0.47
1:B:430:ARG:HG2	1:B:431:MET:O	2.14	0.47
1:B:589:GLY:C	1:B:639:LYS:HG2	2.39	0.47
1:B:814:LEU:HD11	1:B:845:LEU:CD1	2.44	0.47
1:A:468:GLN:HE21	1:A:468:GLN:HB3	1.47	0.47
1:A:695:LYS:HB2	1:A:696:LEU:HD12	1.97	0.47
1:A:728:GLN:HA	1:A:753:ARG:NH2	2.30	0.47
1:A:953:LEU:HB3	1:A:977:ASN:O	2.14	0.47
1:B:113:VAL:HG11	1:B:165:SER:HB3	1.97	0.47
1:B:361:GLN:HE21	1:B:365:ARG:HH21	1.61	0.47
1:B:507:GLU:HG3	1:B:537:ARG:CG	2.40	0.47
1:B:698:GLU:O	1:B:725:ASN:OD1	2.32	0.47
1:B:728:GLN:HA	1:B:753:ARG:NH2	2.29	0.47
1:A:90:ASP:C	1:A:107:LEU:HD22	2.39	0.47
1:A:783:VAL:HG13	1:A:788:PHE:O	2.14	0.47
1:A:984:VAL:O	1:A:984:VAL:HG23	2.14	0.47
1:A:991:GLN:HG2	1:A:1008:THR:HG21	1.96	0.47
1:A:997:ARG:HG2	1:A:998:ARG:N	2.30	0.47
1:B:52:HIS:O	1:B:496:MET:HE1	2.15	0.47
1:B:98:ARG:NH2	1:B:107:LEU:HD12	2.29	0.47
1:B:175:TYR:CG	1:B:176:SER:N	2.82	0.47
1:B:543:ARG:HH11	1:B:549:ARG:HH22	1.62	0.47
1:A:40:VAL:HG11	1:A:503:ARG:HE	1.79	0.47
1:A:264:SER:HA	1:A:265:PRO:HA	1.53	0.47
1:A:458:ARG:CD	1:A:524:PRO:HG3	2.44	0.47
1:A:702:GLN:O	1:A:723:ALA:HB1	2.14	0.47
1:A:715:VAL:HG23	1:A:715:VAL:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:ILE:CG1	1:A:864:PRO:HD3	2.39	0.47
1:A:68:ASN:ND2	1:A:87:PRO:HD3	2.29	0.47
1:A:77:LEU:HD22	1:A:501:LEU:HD13	1.96	0.47
1:A:175:TYR:CG	1:A:176:SER:N	2.82	0.47
1:A:430:ARG:HG2	1:A:431:MET:O	2.14	0.47
1:B:380:LEU:HD12	1:B:390:ILE:CG2	2.45	0.47
1:B:469:TYR:HB3	1:B:523:ASP:OD2	2.15	0.47
1:B:597:LEU:HD22	1:B:597:LEU:H	1.78	0.47
1:B:699:ASP:O	1:B:725:ASN:CB	2.63	0.47
1:B:745:ILE:O	1:B:745:ILE:HG23	2.14	0.47
1:A:72:LYS:O	1:A:80:LEU:HB2	2.15	0.47
1:A:333:LEU:CD2	1:A:358:ILE:HA	2.45	0.47
1:A:448:GLY:HA3	1:A:484:MET:HE1	1.97	0.47
1:A:569:VAL:HG23	1:A:654:ASN:HB2	1.80	0.47
1:A:710:LEU:HD12	1:A:710:LEU:C	2.40	0.47
1:A:745:ILE:O	1:A:745:ILE:HG23	2.15	0.47
1:A:814:LEU:HD11	1:A:845:LEU:CD1	2.44	0.47
1:B:90:ASP:C	1:B:107:LEU:HD22	2.39	0.47
1:B:262:MET:O	1:B:263:VAL:HB	2.14	0.47
1:B:372:SER:HA	1:B:375:ARG:NE	2.29	0.47
1:B:569:VAL:CG1	1:B:620:PRO:HG3	2.45	0.47
1:B:702:GLN:O	1:B:723:ALA:HB1	2.14	0.47
1:B:704:LEU:H	1:B:723:ALA:HA	1.79	0.47
1:B:884:LEU:HD23	1:B:884:LEU:HA	1.75	0.47
1:B:947:LEU:H	1:B:947:LEU:HD23	1.80	0.47
1:A:253:VAL:HG23	1:A:253:VAL:O	2.15	0.47
1:A:453:LYS:HE3	1:A:472:VAL:HG22	1.94	0.47
1:A:843:ARG:HB2	1:A:843:ARG:NH1	2.30	0.47
1:A:892:HIS:CD2	1:A:893:VAL:CG2	2.98	0.47
1:A:958:LEU:HD13	1:A:1033:PHE:HD1	1.79	0.47
1:B:45:GLU:HB3	1:B:46:PRO:HD3	1.97	0.47
1:B:253:VAL:HG23	1:B:253:VAL:O	2.15	0.47
1:B:403:PHE:HE1	1:B:406:LEU:HD23	1.75	0.47
1:B:740:LEU:N	1:B:740:LEU:HD12	2.29	0.47
1:B:790:ILE:HG22	1:B:791:ASP:N	2.28	0.47
1:A:52:HIS:O	1:A:496:MET:HE1	2.15	0.47
1:A:245:TYR:CE2	1:A:247:PHE:HD2	2.33	0.47
1:A:460:ASP:CG	1:A:463:LYS:HB3	2.39	0.47
1:A:569:VAL:CG1	1:A:620:PRO:HG3	2.45	0.47
1:A:873:THR:CG2	1:A:982:SER:N	2.78	0.47
1:B:68:ASN:ND2	1:B:87:PRO:HD3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:SER:OG	1:A:162:VAL:HG23	2.14	0.47
1:A:495:ILE:HG22	1:A:502:THR:HB	1.96	0.47
1:A:561:THR:HG22	1:A:562:VAL:N	2.28	0.47
1:A:947:LEU:HD23	1:A:947:LEU:N	2.30	0.47
1:A:1020:VAL:HG13	1:A:1027:ILE:HG12	1.96	0.47
1:B:82:THR:HG23	1:B:82:THR:O	2.14	0.47
1:B:105:GLU:CB	1:B:106:PRO:HD2	2.42	0.47
1:B:333:LEU:CD2	1:B:358:ILE:HA	2.45	0.47
1:B:343:LYS:HG2	1:B:344:ARG:HG2	1.97	0.47
1:A:372:SER:HA	1:A:375:ARG:NE	2.30	0.46
1:B:244:VAL:HB	1:B:309:LEU:HD23	1.97	0.46
1:B:783:VAL:HG11	1:B:786:GLY:O	2.15	0.46
1:B:843:ARG:NH1	1:B:843:ARG:HB2	2.30	0.46
1:B:862:ILE:CG2	1:B:877:ILE:HG23	2.44	0.46
1:B:863:ILE:CG1	1:B:864:PRO:HD3	2.39	0.46
1:A:68:ASN:HB3	1:A:86:GLY:HA3	1.97	0.46
1:A:403:PHE:HE1	1:A:406:LEU:HD23	1.75	0.46
1:A:873:THR:HG23	1:A:981:GLY:O	2.14	0.46
1:B:72:LYS:O	1:B:80:LEU:HB2	2.15	0.46
1:B:448:GLY:HA3	1:B:484:MET:HE1	1.97	0.46
1:B:567:ILE:HD12	1:B:650:PHE:CE2	2.49	0.46
1:B:805:ALA:H	1:B:806:MET:HE1	1.79	0.46
1:A:244:VAL:HB	1:A:309:LEU:HD23	1.97	0.46
1:B:286:ASP:OD1	1:B:288:ALA:HB3	2.15	0.46
1:B:380:LEU:CB	1:B:386:LYS:HE3	2.44	0.46
1:A:82:THR:O	1:A:82:THR:HG23	2.14	0.46
1:A:532:HIS:CA	1:A:641:THR:OG1	2.57	0.46
1:A:1007:THR:HG22	1:A:1008:THR:O	2.15	0.46
1:B:321:LEU:CG	1:B:325:LEU:HD11	2.40	0.46
1:A:252:PHE:CD1	1:A:283:CYS:HA	2.50	0.46
1:A:503:ARG:O	1:A:505:PRO:HD3	2.15	0.46
1:A:549:ARG:HA	1:A:584:PRO:HG3	1.97	0.46
1:A:549:ARG:CD	1:A:584:PRO:CB	2.76	0.46
1:A:569:VAL:HB	1:A:654:ASN:CG	2.41	0.46
1:A:862:ILE:HG22	1:A:877:ILE:CA	2.32	0.46
1:A:873:THR:HG22	1:A:874:LYS:N	2.31	0.46
1:B:68:ASN:HB3	1:B:86:GLY:HA3	1.97	0.46
1:B:159:LEU:HG	1:B:201:ARG:HH12	1.81	0.46
1:B:245:TYR:CD2	1:B:312:ALA:HB3	2.51	0.46
1:B:296:PRO:CD	1:B:414:VAL:HG22	2.45	0.46
1:B:468:GLN:O	1:B:521:SER:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:SER:HB2	1:B:791:ASP:OD1	2.16	0.46
1:B:892:HIS:CD2	1:B:893:VAL:CG2	2.98	0.46
1:A:265:PRO:CB	1:A:266:PRO:HD2	2.45	0.46
1:A:296:PRO:CD	1:A:414:VAL:HG22	2.46	0.46
1:A:492:GLN:HG2	1:A:503:ARG:HG2	1.98	0.46
1:A:1015:ASP:H	1:A:1035:TYR:H	1.63	0.46
1:B:46:PRO:CG	1:B:69:ARG:HG3	2.27	0.46
1:B:77:LEU:HD22	1:B:501:LEU:HD13	1.96	0.46
1:B:99:ILE:HD11	1:B:152:PHE:CB	2.41	0.46
1:B:902:PRO:HA	1:B:915:CYS:HA	1.97	0.46
1:A:62:ILE:HD11	1:A:73:LEU:CD1	2.45	0.46
1:A:62:ILE:CD1	1:A:77:LEU:CD2	2.94	0.46
1:A:113:VAL:HG11	1:A:165:SER:HB3	1.96	0.46
1:A:226:ILE:HD11	1:A:385:LEU:CD2	2.46	0.46
1:A:444:LEU:HD13	1:A:445:ALA:H	1.79	0.46
1:A:805:ALA:H	1:A:806:MET:HE1	1.79	0.46
1:A:873:THR:OG1	1:A:982:SER:N	2.48	0.46
1:B:295:VAL:CA	1:B:414:VAL:HG21	2.45	0.46
1:B:920:ALA:C	1:B:922:PRO:HD2	2.40	0.46
1:A:262:MET:O	1:A:263:VAL:HB	2.14	0.46
1:A:274:VAL:HG23	1:A:275:TYR:N	2.30	0.46
1:A:295:VAL:CA	1:A:414:VAL:HG21	2.45	0.46
1:A:343:LYS:HG2	1:A:344:ARG:HG2	1.97	0.46
1:A:920:ALA:C	1:A:922:PRO:HD2	2.41	0.46
1:A:947:LEU:H	1:A:947:LEU:HD23	1.80	0.46
1:B:495:ILE:HG22	1:B:502:THR:HB	1.96	0.46
1:B:594:PHE:CZ	1:B:614:PRO:HD3	2.51	0.46
1:A:403:PHE:CE1	1:A:406:LEU:CD2	2.94	0.46
1:A:437:TYR:CE2	1:A:439:TYR:HB2	2.51	0.46
1:B:46:PRO:HD2	1:B:71:TYR:OH	2.16	0.46
1:B:91:ASN:OD1	1:B:92:PRO:HD2	2.16	0.46
1:B:245:TYR:CE2	1:B:247:PHE:HD2	2.34	0.46
1:B:278:LYS:HD3	1:B:294:GLU:HG2	1.98	0.46
1:A:286:ASP:OD1	1:A:288:ALA:HB3	2.16	0.46
1:A:380:LEU:HD12	1:A:390:ILE:CG2	2.45	0.46
1:A:531:LEU:C	1:A:641:THR:HG1	2.21	0.46
1:A:870:GLU:CA	1:A:1024:ARG:HG2	2.43	0.46
1:A:902:PRO:HA	1:A:915:CYS:HA	1.98	0.46
1:B:118:LEU:CD1	1:B:172:ILE:HD12	2.12	0.46
1:B:361:GLN:O	1:B:365:ARG:HG2	2.16	0.46
1:B:710:LEU:HD12	1:B:710:LEU:C	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HG11	1:A:358:ILE:HD11	1.97	0.45
1:A:624:THR:HG23	1:A:624:THR:O	2.15	0.45
1:A:828:PRO:HG3	1:A:837:CYS:SG	2.56	0.45
1:A:892:HIS:CD2	1:A:893:VAL:HG22	2.51	0.45
1:B:62:ILE:CD1	1:B:73:LEU:HB2	2.47	0.45
1:B:252:PHE:CD1	1:B:283:CYS:HA	2.50	0.45
1:B:435:ILE:HG23	1:B:486:PHE:HE1	1.81	0.45
1:B:439:TYR:CE2	1:B:538:LYS:CE	2.99	0.45
1:B:689:PHE:CE1	1:B:691:GLU:HG2	2.50	0.45
1:B:743:GLN:HG2	1:B:744:GLY:N	2.31	0.45
1:A:110:THR:CB	1:A:132:LEU:CD2	2.95	0.45
1:A:435:ILE:HG23	1:A:486:PHE:HE1	1.81	0.45
1:A:563:HIS:CB	1:A:577:VAL:HG12	2.46	0.45
1:A:870:GLU:OE2	1:A:1025:ALA:HA	2.16	0.45
1:A:890:ALA:O	1:A:891:SER:HB2	2.17	0.45
1:B:265:PRO:CB	1:B:266:PRO:HD2	2.45	0.45
1:A:45:GLU:HB3	1:A:46:PRO:HD3	1.97	0.45
1:A:203:LEU:HD22	1:A:212:MET:HE1	1.98	0.45
1:A:380:LEU:CB	1:A:386:LYS:HE3	2.43	0.45
1:A:1020:VAL:CG1	1:A:1027:ILE:CG1	2.95	0.45
1:B:118:LEU:HB3	1:B:127:ILE:HG22	1.98	0.45
1:B:663:SER:O	1:B:667:SER:HB2	2.17	0.45
1:B:695:LYS:HB2	1:B:696:LEU:HD12	1.96	0.45
1:A:361:GLN:O	1:A:365:ARG:HG2	2.16	0.45
1:A:458:ARG:HG3	1:A:468:GLN:NE2	2.32	0.45
1:A:469:TYR:CG	1:A:470:GLU:N	2.84	0.45
1:A:689:PHE:CE1	1:A:691:GLU:HG2	2.50	0.45
1:A:783:VAL:HG11	1:A:786:GLY:O	2.16	0.45
1:B:58:ARG:HG2	1:B:58:ARG:NH1	2.31	0.45
1:B:62:ILE:HD11	1:B:73:LEU:CD1	2.45	0.45
1:B:256:LEU:HD22	1:B:256:LEU:N	2.31	0.45
1:B:435:ILE:HG21	1:B:486:PHE:HE1	1.81	0.45
1:B:828:PRO:HG3	1:B:837:CYS:SG	2.56	0.45
1:B:892:HIS:CD2	1:B:893:VAL:N	2.85	0.45
1:A:159:LEU:HG	1:A:201:ARG:HH12	1.81	0.45
1:A:256:LEU:HD22	1:A:256:LEU:N	2.31	0.45
1:A:288:ALA:O	1:A:289:PHE:HB2	2.17	0.45
1:A:322:GLY:HA2	1:A:327:VAL:HG22	1.99	0.45
1:A:511:GLN:HG3	1:A:512:TYR:CD2	2.51	0.45
1:A:743:GLN:HG2	1:A:744:GLY:N	2.31	0.45
1:A:873:THR:OG1	1:A:981:GLY:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ILE:CD1	1:B:77:LEU:CD2	2.94	0.45
1:B:563:HIS:CB	1:B:577:VAL:HG12	2.46	0.45
1:B:624:THR:O	1:B:624:THR:HG23	2.15	0.45
1:A:118:LEU:HB3	1:A:127:ILE:HG22	1.98	0.45
1:A:245:TYR:CD2	1:A:312:ALA:HB3	2.51	0.45
1:A:278:LYS:CE	1:A:296:PRO:HG3	2.41	0.45
1:A:506:VAL:O	1:A:507:GLU:N	2.39	0.45
1:A:1014:LEU:HD12	1:A:1035:TYR:O	2.16	0.45
1:B:203:LEU:HD22	1:B:212:MET:HE1	1.98	0.45
1:B:442:HIS:CD2	1:B:458:ARG:HH21	2.35	0.45
1:B:503:ARG:O	1:B:505:PRO:HD3	2.15	0.45
1:B:671:CYS:HB3	1:B:680:CYS:SG	2.57	0.45
1:B:873:THR:HG22	1:B:874:LYS:N	2.31	0.45
1:B:892:HIS:CD2	1:B:893:VAL:HG22	2.51	0.45
1:B:947:LEU:HD23	1:B:947:LEU:N	2.30	0.45
1:A:46:PRO:HD2	1:A:71:TYR:OH	2.16	0.45
1:A:53:LEU:HD12	1:A:501:LEU:HG	1.99	0.45
1:A:358:ILE:CG2	1:A:361:GLN:CB	2.95	0.45
1:A:539:GLU:HG3	1:A:540:ARG:N	2.31	0.45
1:A:594:PHE:CZ	1:A:614:PRO:HD3	2.51	0.45
1:B:40:VAL:HG11	1:B:503:ARG:HE	1.80	0.45
1:B:62:ILE:CD1	1:B:501:LEU:CD1	2.95	0.45
1:B:118:LEU:O	1:B:127:ILE:HG22	2.17	0.45
1:B:226:ILE:HD11	1:B:385:LEU:CD2	2.46	0.45
1:B:635:GLN:HB3	1:B:644:THR:HB	1.99	0.45
1:B:890:ALA:O	1:B:891:SER:HB2	2.17	0.45
1:A:62:ILE:CD1	1:A:501:LEU:CD1	2.95	0.45
1:A:182:LEU:HB2	1:A:203:LEU:HD11	1.99	0.45
1:A:663:SER:O	1:A:667:SER:HB2	2.16	0.45
1:A:715:VAL:HG21	1:A:717:LYS:CD	2.44	0.45
1:A:841:GLU:HG3	1:A:842:SER:N	2.32	0.45
1:A:955:LEU:CD1	1:A:973:ILE:CG2	2.94	0.45
1:B:133:TYR:CG	1:B:136:ILE:CG1	2.94	0.45
1:B:464:GLY:O	1:B:465:ASN:HB3	2.17	0.45
1:A:492:GLN:HG2	1:A:503:ARG:HD2	1.98	0.45
1:A:873:THR:CB	1:A:982:SER:N	2.80	0.45
1:B:192:PRO:HB3	1:B:233:PHE:CZ	2.51	0.45
1:B:288:ALA:O	1:B:289:PHE:HB2	2.17	0.45
1:B:492:GLN:HG2	1:B:503:ARG:HG2	1.98	0.45
1:B:511:GLN:HG3	1:B:512:TYR:CD2	2.51	0.45
1:B:539:GLU:HG3	1:B:540:ARG:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:814:LEU:HB2	1:B:884:LEU:HD11	1.98	0.45
1:A:91:ASN:OD1	1:A:92:PRO:HD2	2.16	0.45
1:A:118:LEU:CD1	1:A:172:ILE:HD12	2.12	0.45
1:A:531:LEU:HG	1:A:584:PRO:CG	2.46	0.45
1:A:847:LEU:HD11	1:A:850:ALA:C	2.42	0.45
1:A:955:LEU:HD23	1:A:955:LEU:C	2.41	0.45
1:B:327:VAL:HG11	1:B:358:ILE:HD11	1.97	0.45
1:B:440:LYS:HB2	1:B:538:LYS:HZ2	1.82	0.45
1:B:468:GLN:HE21	1:B:468:GLN:HB3	1.47	0.45
1:B:862:ILE:HG22	1:B:877:ILE:CA	2.32	0.45
1:A:464:GLY:O	1:A:465:ASN:HB3	2.17	0.44
1:A:703:LEU:CD2	1:A:790:ILE:CG2	2.95	0.44
1:A:778:VAL:O	1:A:797:LYS:HB2	2.17	0.44
1:B:295:VAL:CB	1:B:414:VAL:HG21	2.48	0.44
1:B:469:TYR:CG	1:B:470:GLU:N	2.84	0.44
1:B:586:LEU:HD13	1:B:590:VAL:HG21	1.99	0.44
1:B:703:LEU:CD2	1:B:790:ILE:CG2	2.95	0.44
1:B:832:THR:HG21	1:B:836:HIS:CB	2.48	0.44
1:A:151:PRO:HB2	1:A:157:HIS:CE1	2.52	0.44
1:A:247:PHE:CD1	1:A:314:LEU:HD22	2.52	0.44
1:A:252:PHE:HD1	1:A:283:CYS:HA	1.82	0.44
1:A:278:LYS:HD3	1:A:294:GLU:HG2	1.98	0.44
1:A:471:THR:HG23	1:A:473:GLN:NE2	2.27	0.44
1:A:564:PRO:HB2	1:A:576:LEU:CD2	2.48	0.44
1:A:567:ILE:HD11	1:A:652:PHE:CD1	2.53	0.44
1:A:892:HIS:CD2	1:A:893:VAL:N	2.85	0.44
1:B:53:LEU:HD12	1:B:501:LEU:HG	1.99	0.44
1:B:162:VAL:HG21	1:B:187:ALA:HB3	1.99	0.44
1:B:252:PHE:HD1	1:B:283:CYS:HA	1.82	0.44
1:B:291:SER:HB3	1:B:404:CYS:O	2.18	0.44
1:B:305:GLU:HG2	1:B:307:ARG:HG2	1.99	0.44
1:B:458:ARG:HG3	1:B:468:GLN:NE2	2.32	0.44
1:B:492:GLN:HG2	1:B:503:ARG:HD2	1.98	0.44
1:B:531:LEU:HD13	1:B:640:GLU:CD	2.42	0.44
1:B:566:ASN:CB	1:B:651:VAL:CG2	2.95	0.44
1:A:189:ASP:HB3	1:A:191:LYS:HD3	1.99	0.44
1:B:597:LEU:HG	1:B:622:ILE:HG12	1.99	0.44
1:A:291:SER:HB3	1:A:404:CYS:O	2.18	0.44
1:A:566:ASN:CB	1:A:651:VAL:CG2	2.94	0.44
1:A:572:TYR:CD2	1:A:572:TYR:C	2.96	0.44
1:A:868:PRO:HG2	1:A:1022:VAL:HG21	1.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:PHE:CZ	1:A:998:ARG:HB2	2.52	0.44
1:B:182:LEU:HB2	1:B:203:LEU:HD11	1.99	0.44
1:B:247:PHE:CD1	1:B:314:LEU:HD22	2.52	0.44
1:B:264:SER:HA	1:B:265:PRO:HA	1.53	0.44
1:B:370:LEU:CD2	1:B:374:TYR:HE1	2.27	0.44
1:B:437:TYR:CE2	1:B:439:TYR:HB2	2.51	0.44
1:B:567:ILE:HD11	1:B:652:PHE:CD1	2.53	0.44
1:A:53:LEU:CG	1:A:64:LEU:CD1	2.96	0.44
1:A:58:ARG:HG2	1:A:58:ARG:NH1	2.31	0.44
1:A:68:ASN:CG	1:A:87:PRO:HD3	2.43	0.44
1:A:116:MET:SD	1:A:169:PHE:HA	2.57	0.44
1:A:262:MET:SD	1:A:383:ALA:HB3	2.57	0.44
1:A:541:CYS:HB3	1:A:544:SER:HB3	1.99	0.44
1:A:889:ILE:CD1	1:A:907:TYR:CZ	3.01	0.44
1:A:958:LEU:HD13	1:A:1033:PHE:CD1	2.53	0.44
1:A:991:GLN:CD	1:A:992:PRO:HD2	2.42	0.44
1:B:116:MET:SD	1:B:169:PHE:HA	2.57	0.44
1:B:572:TYR:CD2	1:B:572:TYR:C	2.96	0.44
1:A:281:ARG:NH1	1:A:366:ILE:HG21	2.33	0.44
1:A:306:TYR:HE1	1:A:351:GLU:HG2	1.83	0.44
1:A:635:GLN:HB3	1:A:644:THR:HB	1.99	0.44
1:A:671:CYS:HB3	1:A:680:CYS:SG	2.57	0.44
1:B:179:ASP:O	1:B:180:ASP:HB3	2.17	0.44
1:B:185:ALA:CB	1:B:243:TYR:CD1	3.00	0.44
1:B:262:MET:SD	1:B:383:ALA:HB3	2.58	0.44
1:A:40:VAL:HG13	1:A:40:VAL:O	2.17	0.44
1:A:72:LYS:CE	1:A:80:LEU:CD1	2.95	0.44
1:A:98:ARG:NH2	1:A:107:LEU:HD12	2.29	0.44
1:A:179:ASP:O	1:A:180:ASP:HB3	2.17	0.44
1:A:421:ILE:HA	1:A:422:PRO:HD2	1.84	0.44
1:A:586:LEU:HD13	1:A:590:VAL:HG21	1.99	0.44
1:A:597:LEU:HG	1:A:622:ILE:HG12	1.99	0.44
1:B:62:ILE:CD1	1:B:73:LEU:HD12	2.45	0.44
1:B:117:LEU:HD11	1:B:126:LEU:CD2	2.31	0.44
1:B:119:ILE:HG23	1:B:121:TYR:CE1	2.53	0.44
1:B:173:VAL:HG23	1:B:173:VAL:O	2.18	0.44
1:B:256:LEU:CB	1:B:309:LEU:CD2	2.94	0.44
1:B:281:ARG:NH1	1:B:366:ILE:HG21	2.33	0.44
1:B:699:ASP:O	1:B:725:ASN:HB3	2.18	0.44
1:A:118:LEU:O	1:A:127:ILE:HG22	2.17	0.44
1:A:133:TYR:CG	1:A:136:ILE:CG1	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:VAL:HG21	1:A:187:ALA:HB3	1.99	0.44
1:A:217:PHE:CE2	1:A:219:ASP:HB2	2.53	0.44
1:A:889:ILE:HA	1:A:892:HIS:ND1	2.33	0.44
1:B:42:PHE:CZ	1:B:45:GLU:CB	2.95	0.44
1:B:55:VAL:HG22	1:B:62:ILE:HG22	2.00	0.44
1:B:110:THR:CB	1:B:132:LEU:CD2	2.95	0.44
1:B:274:VAL:HG23	1:B:275:TYR:N	2.30	0.44
1:B:322:GLY:HA2	1:B:327:VAL:HG22	1.99	0.44
1:B:332:ASP:O	1:B:333:LEU:HD23	2.18	0.44
1:B:547:PRO:C	1:B:548:ARG:HG2	2.43	0.44
1:B:564:PRO:HB2	1:B:576:LEU:CD2	2.48	0.44
1:A:442:HIS:CD2	1:A:458:ARG:HH21	2.35	0.44
1:A:528:TRP:HZ2	1:A:533:ASN:OD1	2.01	0.44
1:A:569:VAL:CG2	1:A:654:ASN:CB	2.65	0.44
1:A:574:VAL:HG22	1:A:613:SER:OG	2.17	0.44
1:A:713:VAL:O	1:A:714:GLU:HB2	2.18	0.44
1:B:358:ILE:CG2	1:B:361:GLN:CB	2.95	0.44
1:B:778:VAL:O	1:B:797:LYS:HB2	2.17	0.44
1:B:863:ILE:HG22	1:B:876:THR:CB	2.35	0.44
1:B:889:ILE:CD1	1:B:907:TYR:CZ	3.01	0.44
1:A:53:LEU:HD11	1:A:501:LEU:HD11	2.00	0.43
1:A:62:ILE:CD1	1:A:73:LEU:HD12	2.45	0.43
1:A:332:ASP:O	1:A:333:LEU:HD23	2.18	0.43
1:A:567:ILE:HD11	1:A:650:PHE:CE2	2.53	0.43
1:A:574:VAL:CG2	1:A:613:SER:HB3	2.48	0.43
1:A:764:THR:CG2	1:A:766:TYR:CZ	3.01	0.43
1:A:774:ASN:OD1	1:A:806:MET:HE2	2.18	0.43
1:A:874:LYS:H	1:A:982:SER:HB2	1.80	0.43
1:B:53:LEU:HD11	1:B:501:LEU:HD11	2.00	0.43
1:B:189:ASP:HB3	1:B:191:LYS:HD3	1.99	0.43
1:B:306:TYR:HE1	1:B:351:GLU:HG2	1.83	0.43
1:B:711:VAL:HG21	1:B:798:VAL:CG2	2.48	0.43
1:B:841:GLU:HG3	1:B:842:SER:N	2.32	0.43
1:B:847:LEU:HD11	1:B:850:ALA:C	2.42	0.43
1:A:711:VAL:HG21	1:A:798:VAL:CG2	2.48	0.43
1:A:832:THR:HG21	1:A:836:HIS:CB	2.48	0.43
1:B:541:CYS:HB3	1:B:544:SER:HB3	1.99	0.43
1:A:119:ILE:HG23	1:A:121:TYR:CE1	2.53	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HG13	2.00	0.43
1:B:151:PRO:HB2	1:B:157:HIS:CE1	2.52	0.43
1:B:324:THR:O	1:B:324:THR:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:LYS:NZ	1:B:556:GLN:HG2	2.33	0.43
1:B:574:VAL:HG22	1:B:613:SER:OG	2.17	0.43
1:B:764:THR:CG2	1:B:766:TYR:CZ	3.01	0.43
1:B:889:ILE:HA	1:B:892:HIS:ND1	2.33	0.43
1:A:62:ILE:CD1	1:A:501:LEU:HD13	2.49	0.43
1:A:435:ILE:CD1	1:A:486:PHE:HD1	2.31	0.43
1:A:590:VAL:CG1	1:A:591:ASN:N	2.82	0.43
1:A:839:ALA:HB1	1:A:841:GLU:O	2.18	0.43
1:A:1014:LEU:HA	1:A:1035:TYR:HB2	2.00	0.43
1:A:1031:LEU:HD22	1:A:1031:LEU:N	2.34	0.43
1:B:296:PRO:HB2	1:B:417:MET:CE	2.48	0.43
1:B:370:LEU:HD12	1:B:399:ILE:HG23	2.00	0.43
1:B:456:LYS:HD3	1:B:523:ASP:OD2	2.10	0.43
1:B:527:GLY:HA3	1:B:550:PHE:HZ	1.72	0.43
1:B:528:TRP:HZ2	1:B:533:ASN:OD1	2.01	0.43
1:B:563:HIS:CB	1:B:577:VAL:CG1	2.95	0.43
1:A:173:VAL:HG23	1:A:173:VAL:O	2.18	0.43
1:A:224:SER:HA	1:A:289:PHE:CD1	2.54	0.43
1:A:501:LEU:CD2	1:A:502:THR:N	2.81	0.43
1:A:832:THR:CG2	1:A:836:HIS:CB	2.95	0.43
1:B:68:ASN:CG	1:B:87:PRO:HD3	2.43	0.43
1:B:333:LEU:HD23	1:B:358:ILE:HG13	2.00	0.43
1:B:458:ARG:HB2	1:B:468:GLN:HE22	1.83	0.43
1:B:574:VAL:CG2	1:B:613:SER:HB3	2.48	0.43
1:B:839:ALA:HB1	1:B:841:GLU:O	2.18	0.43
1:A:100:VAL:HG21	1:A:158:TYR:OH	2.19	0.43
1:A:128:ALA:O	1:A:138:LYS:HG2	2.19	0.43
1:A:162:VAL:HG12	1:A:164:GLU:H	1.84	0.43
1:A:295:VAL:CB	1:A:414:VAL:HG21	2.48	0.43
1:A:296:PRO:HB2	1:A:417:MET:CE	2.48	0.43
1:A:716:ILE:CD1	1:A:763:ASN:HB3	2.49	0.43
1:A:962:ARG:HD3	1:A:1034:GLN:HE21	1.83	0.43
1:A:978:LEU:HD13	1:A:1003:ILE:HG13	2.01	0.43
1:B:40:VAL:HG13	1:B:40:VAL:O	2.17	0.43
1:B:95:TYR:HD1	1:B:95:TYR:HA	1.70	0.43
1:B:117:LEU:HG	1:B:126:LEU:HD11	2.01	0.43
1:B:217:PHE:CE2	1:B:219:ASP:HB2	2.53	0.43
1:B:281:ARG:HB3	1:B:293:VAL:HG11	1.97	0.43
1:B:435:ILE:CD1	1:B:486:PHE:HD1	2.31	0.43
1:B:764:THR:HG23	1:B:766:TYR:CZ	2.54	0.43
1:A:185:ALA:CB	1:A:243:TYR:CE2	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:HG2	1:A:307:ARG:HG2	1.99	0.43
1:A:764:THR:HG23	1:A:766:TYR:CZ	2.54	0.43
1:A:962:ARG:CB	1:A:1034:GLN:HG3	2.45	0.43
1:A:965:MET:HG3	1:A:1010:SER:O	2.18	0.43
1:B:119:ILE:HG21	1:B:121:TYR:CE1	2.54	0.43
1:B:542:GLU:HG2	1:B:543:ARG:HG3	2.01	0.43
1:B:549:ARG:HD3	1:B:584:PRO:CB	2.48	0.43
1:A:72:LYS:CD	1:A:80:LEU:CD1	2.97	0.43
1:A:555:LYS:NZ	1:A:556:GLN:HG2	2.33	0.43
1:A:562:VAL:HG22	1:A:578:LEU:HD22	1.98	0.43
1:A:620:PRO:O	1:A:623:ILE:HG13	2.18	0.43
1:A:1010:SER:HB2	1:A:1035:TYR:CE1	2.52	0.43
1:B:484:MET:HE2	1:B:495:ILE:HG13	2.01	0.43
1:B:506:VAL:CG2	1:B:525:HIS:CE1	2.81	0.43
1:A:62:ILE:CD1	1:A:64:LEU:HD21	2.46	0.43
1:A:333:LEU:HD23	1:A:358:ILE:HA	2.01	0.43
1:A:484:MET:HE2	1:A:495:ILE:HG13	2.01	0.43
1:A:789:ASN:HD22	1:A:790:ILE:N	2.17	0.43
1:A:951:MET:HG2	1:A:977:ASN:OD1	2.17	0.43
1:B:100:VAL:HG21	1:B:158:TYR:OH	2.19	0.43
1:B:234:THR:CG2	1:B:235:VAL:N	2.82	0.43
1:B:358:ILE:HG23	1:B:358:ILE:O	2.18	0.43
1:B:506:VAL:HG21	1:B:525:HIS:NE2	2.22	0.43
1:B:620:PRO:O	1:B:623:ILE:HG13	2.18	0.43
1:A:55:VAL:HG22	1:A:62:ILE:HG22	2.00	0.43
1:A:112:ASN:ND2	1:A:133:TYR:HE2	2.17	0.43
1:A:117:LEU:HG	1:A:126:LEU:HD11	2.01	0.43
1:A:186:THR:CG2	1:A:187:ALA:N	2.81	0.43
1:A:281:ARG:HB3	1:A:293:VAL:HG11	1.97	0.43
1:A:617:LYS:HG3	1:A:618:GLU:N	2.34	0.43
1:A:805:ALA:N	1:A:806:MET:CE	2.82	0.43
1:A:885:GLU:HG3	1:A:886:PHE:N	2.34	0.43
1:B:123:GLU:HB2	1:B:125:ARG:HG2	2.01	0.43
1:B:501:LEU:CD2	1:B:502:THR:N	2.82	0.43
1:B:617:LYS:HG3	1:B:618:GLU:N	2.34	0.43
1:B:789:ASN:HD22	1:B:790:ILE:N	2.17	0.43
1:A:98:ARG:HE	1:A:107:LEU:HD12	1.83	0.42
1:A:665:VAL:HG11	1:A:697:PRO:CD	2.48	0.42
1:A:917:MET:HE1	1:A:948:TYR:CZ	2.54	0.42
1:B:62:ILE:CD1	1:B:501:LEU:HD13	2.49	0.42
1:B:128:ALA:O	1:B:138:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:VAL:O	1:B:714:GLU:HB2	2.18	0.42
1:A:192:PRO:HB3	1:A:233:PHE:CZ	2.51	0.42
1:A:972:THR:HG23	1:A:1002:TYR:HE1	1.72	0.42
1:B:133:TYR:CB	1:B:136:ILE:HG23	2.49	0.42
1:B:178:PHE:HD1	1:B:178:PHE:O	2.02	0.42
1:B:469:TYR:CB	1:B:523:ASP:CG	2.79	0.42
1:B:543:ARG:HB2	1:B:549:ARG:NH1	2.34	0.42
1:B:567:ILE:HD11	1:B:650:PHE:CE2	2.53	0.42
1:B:665:VAL:HG11	1:B:697:PRO:CD	2.48	0.42
1:A:110:THR:HG21	1:A:132:LEU:HD21	1.97	0.42
1:A:458:ARG:HB2	1:A:468:GLN:HE22	1.83	0.42
1:A:541:CYS:HB2	1:A:544:SER:HB3	2.01	0.42
1:A:630:HIS:CD2	1:A:632:VAL:CG2	3.00	0.42
1:A:889:ILE:HG23	1:A:892:HIS:NE2	2.33	0.42
1:A:1032:VAL:CG1	1:A:1033:PHE:N	2.82	0.42
1:B:185:ALA:CB	1:B:243:TYR:CE2	3.02	0.42
1:B:358:ILE:HG23	1:B:361:GLN:N	2.24	0.42
1:B:605:ILE:O	1:B:608:GLN:HG2	2.20	0.42
1:B:689:PHE:HD1	1:B:691:GLU:HG2	1.80	0.42
1:A:119:ILE:HG21	1:A:121:TYR:CE1	2.54	0.42
1:A:370:LEU:HD12	1:A:399:ILE:HG23	2.00	0.42
1:A:471:THR:HG21	1:A:473:GLN:OE1	2.19	0.42
1:A:567:ILE:N	1:A:567:ILE:CD1	2.82	0.42
1:A:865:VAL:CG1	1:A:866:THR:N	2.82	0.42
1:A:868:PRO:CD	1:A:981:GLY:HA2	1.99	0.42
1:A:953:LEU:HD12	1:A:978:LEU:HD23	2.01	0.42
1:A:1029:GLN:CG	1:A:1030:ASP:N	2.83	0.42
1:B:224:SER:HA	1:B:289:PHE:CD1	2.54	0.42
1:B:662:LEU:HD23	1:B:791:ASP:CB	2.48	0.42
1:A:169:PHE:CD2	1:A:170:GLY:N	2.84	0.42
1:A:178:PHE:O	1:A:178:PHE:HD1	2.02	0.42
1:A:358:ILE:HG23	1:A:358:ILE:O	2.18	0.42
1:A:358:ILE:HG23	1:A:361:GLN:N	2.24	0.42
1:A:955:LEU:CG	1:A:973:ILE:CG2	2.95	0.42
1:A:962:ARG:HD3	1:A:1034:GLN:NE2	2.34	0.42
1:B:216:VAL:CG1	1:B:217:PHE:N	2.82	0.42
1:B:333:LEU:HD23	1:B:358:ILE:HA	2.01	0.42
1:B:567:ILE:N	1:B:567:ILE:CD1	2.82	0.42
1:B:590:VAL:CG1	1:B:591:ASN:N	2.82	0.42
1:B:759:VAL:CG1	1:B:760:GLN:N	2.81	0.42
1:B:885:GLU:HG3	1:B:886:PHE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889:ILE:HG23	1:B:892:HIS:NE2	2.33	0.42
1:A:123:GLU:HB2	1:A:125:ARG:HG2	2.01	0.42
1:A:435:ILE:HG21	1:A:486:PHE:HE1	1.81	0.42
1:A:543:ARG:HB2	1:A:549:ARG:NH1	2.34	0.42
1:A:547:PRO:C	1:A:548:ARG:HG2	2.43	0.42
1:A:959:LYS:HG2	1:A:972:THR:HG21	2.01	0.42
1:A:1007:THR:HG22	1:A:1008:THR:N	2.33	0.42
1:B:68:ASN:CB	1:B:86:GLY:HA3	2.50	0.42
1:B:112:ASN:ND2	1:B:133:TYR:HE2	2.17	0.42
1:B:186:THR:CG2	1:B:187:ALA:N	2.81	0.42
1:B:470:GLU:HG2	1:B:471:THR:N	2.34	0.42
1:B:471:THR:HG21	1:B:473:GLN:OE1	2.19	0.42
1:B:917:MET:HE1	1:B:948:TYR:CZ	2.54	0.42
1:A:256:LEU:CB	1:A:309:LEU:CD2	2.94	0.42
1:A:549:ARG:CD	1:A:584:PRO:HB3	2.42	0.42
1:A:830:GLN:CG	1:A:831:CYS:H	2.24	0.42
1:B:321:LEU:HD23	1:B:333:LEU:CD1	2.50	0.42
1:A:542:GLU:HG2	1:A:543:ARG:HG3	2.00	0.42
1:A:845:LEU:HD11	1:A:852:SER:OG	2.20	0.42
1:A:917:MET:HE3	1:A:917:MET:HB2	1.84	0.42
1:B:458:ARG:HD2	1:B:524:PRO:CB	2.31	0.42
1:B:653:TYR:CZ	1:B:682:HIS:CE1	3.07	0.42
1:B:700:CYS:HA	1:B:701:PRO:HD3	1.45	0.42
1:A:234:THR:CG2	1:A:235:VAL:N	2.82	0.42
1:A:324:THR:O	1:A:324:THR:HG22	2.18	0.42
1:A:370:LEU:CD2	1:A:374:TYR:HE1	2.28	0.42
1:A:562:VAL:HG22	1:A:578:LEU:HD23	1.99	0.42
1:A:566:ASN:CA	1:A:651:VAL:CG2	2.95	0.42
1:A:783:VAL:CG1	1:A:784:TRP:N	2.83	0.42
1:B:385:LEU:C	1:B:385:LEU:CD1	2.93	0.42
1:B:446:PHE:CB	1:B:454:LEU:HD11	2.43	0.42
1:B:562:VAL:HG22	1:B:578:LEU:HD23	1.99	0.42
1:B:563:HIS:HB2	1:B:577:VAL:HG13	2.01	0.42
1:B:892:HIS:CD2	1:B:892:HIS:C	2.98	0.42
1:A:62:ILE:CD1	1:A:73:LEU:HB2	2.47	0.42
1:A:380:LEU:HD22	1:A:412:LEU:HB3	2.02	0.42
1:A:662:LEU:O	1:A:666:GLU:HB3	2.20	0.42
1:A:888:ASP:OD1	1:A:889:ILE:HG13	2.20	0.42
1:A:987:MET:CE	1:A:990:SER:HA	2.45	0.42
1:B:39:PHE:CZ	1:B:473:GLN:HG3	2.53	0.42
1:B:80:LEU:C	1:B:81:VAL:HG23	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:LEU:HD13	1:B:444:LEU:C	2.44	0.42
1:B:528:TRP:CZ2	1:B:533:ASN:OD1	2.73	0.42
1:B:783:VAL:CG1	1:B:784:TRP:N	2.83	0.42
1:B:926:ALA:HB2	1:B:949:TYR:CD1	2.55	0.42
1:A:67:VAL:CG1	1:A:111:ASN:HB3	2.50	0.41
1:A:412:LEU:N	1:A:412:LEU:CD1	2.83	0.41
1:A:440:LYS:HD2	1:A:538:LYS:HD2	1.93	0.41
1:A:605:ILE:O	1:A:608:GLN:HG2	2.19	0.41
1:B:162:VAL:HG12	1:B:164:GLU:H	1.84	0.41
1:B:177:ASN:O	1:B:178:PHE:CG	2.73	0.41
1:B:256:LEU:HD12	1:B:297:ILE:HD11	2.02	0.41
1:B:575:LEU:N	1:B:575:LEU:CD2	2.83	0.41
1:B:623:ILE:HD12	1:B:624:THR:HA	2.02	0.41
1:B:817:ASP:OD1	1:B:820:PHE:CD2	2.73	0.41
1:A:44:GLY:O	1:A:47:ALA:HA	2.20	0.41
1:A:68:ASN:CB	1:A:86:GLY:HA3	2.50	0.41
1:A:216:VAL:CG1	1:A:217:PHE:N	2.82	0.41
1:A:817:ASP:OD1	1:A:820:PHE:CD2	2.73	0.41
1:A:892:HIS:CD2	1:A:892:HIS:C	2.98	0.41
1:A:955:LEU:C	1:A:955:LEU:CD2	2.93	0.41
1:A:959:LYS:CG	1:A:972:THR:CB	2.97	0.41
1:B:72:LYS:CE	1:B:80:LEU:CD1	2.95	0.41
1:B:159:LEU:HG	1:B:201:ARG:NH1	2.35	0.41
1:B:403:PHE:CE2	1:B:405:GLY:HA2	2.55	0.41
1:B:492:GLN:HB3	1:B:503:ARG:HG3	2.02	0.41
1:B:716:ILE:CD1	1:B:763:ASN:HB3	2.49	0.41
1:B:728:GLN:HG3	1:B:753:ARG:NH2	2.35	0.41
1:A:177:ASN:O	1:A:178:PHE:CG	2.73	0.41
1:A:387:VAL:CG1	1:A:388:LYS:N	2.82	0.41
1:A:446:PHE:CD1	1:A:446:PHE:N	2.88	0.41
1:A:470:GLU:HG2	1:A:471:THR:N	2.34	0.41
1:A:728:GLN:HG3	1:A:753:ARG:NH2	2.35	0.41
1:B:412:LEU:N	1:B:412:LEU:CD1	2.83	0.41
1:B:444:LEU:HD23	1:B:524:PRO:HG2	1.91	0.41
1:B:619:VAL:HB	1:B:620:PRO:CD	2.47	0.41
1:B:865:VAL:CG1	1:B:866:THR:N	2.82	0.41
1:A:80:LEU:C	1:A:81:VAL:HG23	2.45	0.41
1:A:111:ASN:O	1:A:132:LEU:HD13	2.20	0.41
1:A:188:VAL:HG22	1:A:188:VAL:O	2.21	0.41
1:A:307:ARG:HD3	1:A:307:ARG:HA	1.88	0.41
1:A:349:LEU:N	1:A:349:LEU:CD2	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:PHE:CE2	1:A:405:GLY:HA2	2.55	0.41
1:A:563:HIS:HB2	1:A:577:VAL:HG13	2.01	0.41
1:A:631:VAL:O	1:A:631:VAL:HG13	2.19	0.41
1:A:711:VAL:HB	1:A:800:LEU:HD23	2.02	0.41
1:A:926:ALA:HB2	1:A:949:TYR:CD1	2.55	0.41
1:A:978:LEU:HD23	1:A:978:LEU:HA	1.93	0.41
1:B:110:THR:HG21	1:B:132:LEU:HD21	1.97	0.41
1:B:446:PHE:CD1	1:B:446:PHE:N	2.89	0.41
1:B:555:LYS:HZ2	1:B:556:GLN:HG2	1.86	0.41
1:B:562:VAL:HG22	1:B:578:LEU:HD22	1.98	0.41
1:B:679:VAL:CG1	1:B:680:CYS:N	2.82	0.41
1:B:862:ILE:HG21	1:B:877:ILE:HG12	2.03	0.41
1:B:909:PRO:C	1:B:911:GLU:H	2.29	0.41
1:A:133:TYR:CB	1:A:136:ILE:HG23	2.49	0.41
1:A:159:LEU:HG	1:A:201:ARG:NH1	2.36	0.41
1:A:226:ILE:HD11	1:A:385:LEU:HD23	2.03	0.41
1:A:385:LEU:C	1:A:385:LEU:CD1	2.93	0.41
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.91	0.41
1:A:988:PHE:CB	1:A:1016:MET:SD	3.06	0.41
1:A:1004:ILE:C	1:A:1004:ILE:CD1	2.93	0.41
1:A:1031:LEU:HD22	1:A:1031:LEU:H	1.84	0.41
1:B:137:CYS:SG	1:B:159:LEU:CD1	3.09	0.41
1:B:280:VAL:CG1	1:B:281:ARG:N	2.83	0.41
1:B:380:LEU:HD22	1:B:412:LEU:HB3	2.02	0.41
1:B:631:VAL:O	1:B:631:VAL:HG13	2.19	0.41
1:B:803:CYS:SG	1:B:832:THR:HA	2.61	0.41
1:A:446:PHE:CB	1:A:454:LEU:HD11	2.43	0.41
1:A:555:LYS:HZ1	1:A:556:GLN:HG2	1.85	0.41
1:A:703:LEU:HD13	1:A:723:ALA:CB	2.47	0.41
1:A:862:ILE:HG21	1:A:877:ILE:HG12	2.03	0.41
1:A:958:LEU:HD22	1:A:960:PRO:N	2.35	0.41
1:A:959:LYS:CG	1:A:972:THR:HG21	2.51	0.41
1:B:185:ALA:HB3	1:B:243:TYR:CD2	2.56	0.41
1:B:444:LEU:HD12	1:B:446:PHE:CD1	2.51	0.41
1:B:444:LEU:HD13	1:B:445:ALA:H	1.79	0.41
1:B:453:LYS:CE	1:B:472:VAL:HG22	2.51	0.41
1:B:506:VAL:CG1	1:B:507:GLU:N	2.84	0.41
1:B:541:CYS:HB2	1:B:544:SER:HB3	2.01	0.41
1:B:551:ALA:HB1	1:B:556:GLN:HB2	2.03	0.41
1:B:778:VAL:HG12	1:B:779:GLU:O	2.20	0.41
1:B:805:ALA:N	1:B:806:MET:CE	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:ASP:OD1	1:B:889:ILE:HG13	2.20	0.41
1:A:95:TYR:CG	1:A:96:PRO:CD	3.03	0.41
1:A:380:LEU:CB	1:A:386:LYS:CE	2.95	0.41
1:A:492:GLN:HB3	1:A:503:ARG:HG3	2.02	0.41
1:A:679:VAL:CG1	1:A:680:CYS:N	2.82	0.41
1:A:759:VAL:CG1	1:A:760:GLN:N	2.81	0.41
1:B:44:GLY:O	1:B:47:ALA:HA	2.20	0.41
1:B:67:VAL:CG1	1:B:111:ASN:HB3	2.50	0.41
1:B:137:CYS:O	1:B:150:GLU:HG3	2.20	0.41
1:B:387:VAL:CG1	1:B:388:LYS:N	2.82	0.41
1:B:658:HIS:ND1	1:B:663:SER:HB3	2.36	0.41
1:B:699:ASP:O	1:B:725:ASN:CG	2.63	0.41
1:A:137:CYS:O	1:A:150:GLU:HG3	2.20	0.41
1:A:185:ALA:HB3	1:A:243:TYR:CD2	2.56	0.41
1:A:188:VAL:CG2	1:A:191:LYS:HB2	2.51	0.41
1:A:280:VAL:CG1	1:A:281:ARG:N	2.83	0.41
1:A:396:LEU:C	1:A:396:LEU:CD1	2.94	0.41
1:A:909:PRO:C	1:A:911:GLU:H	2.29	0.41
1:A:972:THR:CG2	1:A:1002:TYR:CE1	2.93	0.41
1:A:988:PHE:CD2	1:A:1016:MET:SD	3.12	0.41
1:B:95:TYR:CG	1:B:96:PRO:CD	3.03	0.41
1:B:492:GLN:CG	1:B:503:ARG:HD2	2.51	0.41
1:A:117:LEU:HD11	1:A:126:LEU:CD2	2.31	0.41
1:A:137:CYS:SG	1:A:159:LEU:CD1	3.09	0.41
1:A:180:ASP:C	1:A:181:LYS:HG2	2.46	0.41
1:A:236:ILE:CG2	1:A:239:PHE:HB2	2.51	0.41
1:A:444:LEU:HD13	1:A:444:LEU:C	2.44	0.41
1:A:492:GLN:CG	1:A:503:ARG:HD2	2.51	0.41
1:A:528:TRP:CZ2	1:A:533:ASN:OD1	2.73	0.41
1:A:619:VAL:HB	1:A:620:PRO:CD	2.47	0.41
1:A:623:ILE:HD12	1:A:624:THR:HA	2.01	0.41
1:A:953:LEU:HA	1:A:977:ASN:HB2	2.02	0.41
1:A:959:LYS:HG2	1:A:972:THR:HB	2.02	0.41
1:B:93:LYS:HD2	1:B:105:GLU:CD	2.45	0.41
1:B:111:ASN:O	1:B:132:LEU:HD13	2.20	0.41
1:B:188:VAL:CG2	1:B:191:LYS:HB2	2.51	0.41
1:B:226:ILE:HD11	1:B:385:LEU:HD23	2.03	0.41
1:B:236:ILE:CG2	1:B:239:PHE:HB2	2.51	0.41
1:B:239:PHE:CD1	1:B:260:PRO:CD	3.03	0.41
1:B:349:LEU:N	1:B:349:LEU:CD2	2.84	0.41
1:B:535:CYS:C	1:B:536:THR:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:560:LEU:CG	1:B:648:THR:CG2	2.98	0.41
1:B:660:SER:HB2	1:B:791:ASP:CG	2.46	0.41
1:B:683:ASP:HA	1:B:684:PRO:HD3	1.83	0.41
1:B:696:LEU:HA	1:B:697:PRO:HD3	1.87	0.41
1:B:703:LEU:HD13	1:B:723:ALA:CB	2.47	0.41
1:B:832:THR:HG21	1:B:836:HIS:HB2	1.99	0.41
1:B:843:ARG:CZ	1:B:843:ARG:CB	2.99	0.41
1:B:901:SER:HA	1:B:902:PRO:HD2	1.89	0.41
1:A:95:TYR:CE2	1:A:194:TYR:CD1	3.09	0.41
1:A:111:ASN:O	1:A:132:LEU:HD22	2.21	0.41
1:A:181:LYS:HZ2	1:A:216:VAL:HG23	1.83	0.41
1:A:252:PHE:HE1	1:A:283:CYS:SG	2.44	0.41
1:A:256:LEU:HD12	1:A:297:ILE:HD11	2.01	0.41
1:A:321:LEU:HD23	1:A:333:LEU:CD1	2.50	0.41
1:A:551:ALA:HB1	1:A:556:GLN:HB2	2.03	0.41
1:A:560:LEU:CG	1:A:648:THR:CG2	2.98	0.41
1:A:658:HIS:ND1	1:A:663:SER:HB3	2.36	0.41
1:A:778:VAL:HG12	1:A:779:GLU:O	2.20	0.41
1:A:832:THR:HG21	1:A:836:HIS:HB2	1.99	0.41
1:B:180:ASP:C	1:B:181:LYS:HG2	2.46	0.41
1:B:469:TYR:CZ	1:B:470:GLU:O	2.74	0.41
1:B:560:LEU:HB3	1:B:648:THR:CG2	2.51	0.41
1:B:623:ILE:C	1:B:623:ILE:CD1	2.94	0.41
1:B:711:VAL:HB	1:B:800:LEU:HD23	2.02	0.41
1:A:93:LYS:HD2	1:A:105:GLU:CD	2.45	0.40
1:A:313:TYR:CZ	1:A:435:ILE:CD1	3.05	0.40
1:A:485:ALA:C	1:A:493:LEU:HD12	2.46	0.40
1:B:53:LEU:C	1:B:53:LEU:CD2	2.94	0.40
1:B:141:ARG:HB3	1:B:144:ASP:OD1	2.21	0.40
1:B:188:VAL:HG22	1:B:188:VAL:O	2.21	0.40
1:B:473:GLN:CD	1:B:504:VAL:CG1	2.95	0.40
1:B:667:SER:HB3	1:B:668:PRO:CD	2.51	0.40
1:B:832:THR:CG2	1:B:836:HIS:CB	2.95	0.40
1:A:45:GLU:CB	1:A:46:PRO:CD	3.00	0.40
1:A:185:ALA:CB	1:A:243:TYR:CD1	3.00	0.40
1:A:469:TYR:CZ	1:A:470:GLU:O	2.74	0.40
1:A:473:GLN:CD	1:A:504:VAL:CG1	2.95	0.40
1:A:667:SER:HB3	1:A:668:PRO:CD	2.51	0.40
1:A:955:LEU:HD23	1:A:957:ASP:N	2.37	0.40
1:B:44:GLY:CA	1:B:50:PHE:HE2	2.23	0.40
1:B:169:PHE:CD2	1:B:170:GLY:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASP:HB3	1:B:222:VAL:H	1.86	0.40
1:B:242:TYR:CE1	1:B:345:LYS:HE2	2.56	0.40
1:B:284:LYS:C	1:B:284:LYS:CD	2.94	0.40
1:B:949:TYR:CE2	1:B:951:MET:CE	2.95	0.40
1:A:131:SER:O	1:A:133:TYR:CD2	2.74	0.40
1:A:453:LYS:CE	1:A:472:VAL:HG22	2.51	0.40
1:A:527:GLY:HA3	1:A:550:PHE:HZ	1.72	0.40
1:A:589:GLY:C	1:A:639:LYS:CG	2.95	0.40
1:A:780:LEU:C	1:A:780:LEU:CD1	2.94	0.40
1:B:62:ILE:CD1	1:B:64:LEU:HD21	2.46	0.40
1:B:95:TYR:CE2	1:B:194:TYR:CD1	3.09	0.40
1:B:172:ILE:CG1	1:B:182:LEU:HD13	2.46	0.40
1:B:282:LEU:HD23	1:B:292:TYR:HA	2.03	0.40
1:B:450:LYS:CA	1:B:479:PRO:HB3	2.49	0.40
1:B:589:GLY:C	1:B:639:LYS:CG	2.95	0.40
1:B:662:LEU:O	1:B:666:GLU:HB3	2.20	0.40
1:A:188:VAL:HG13	1:A:189:ASP:N	2.36	0.40
1:A:219:ASP:HB3	1:A:222:VAL:H	1.86	0.40
1:A:259:GLN:HA	1:A:260:PRO:HD3	1.82	0.40
1:A:433:SER:HB3	1:A:484:MET:CE	2.52	0.40
1:A:455:LYS:HB3	1:A:467:LEU:CD1	2.52	0.40
1:A:773:ILE:N	1:A:773:ILE:CD1	2.82	0.40
1:A:803:CYS:SG	1:A:832:THR:HA	2.61	0.40
1:A:896:ALA:HB1	1:A:924:GLN:OE1	2.22	0.40
1:A:904:VAL:CG1	1:A:905:ASP:N	2.82	0.40
1:B:313:TYR:CZ	1:B:435:ILE:CD1	3.04	0.40
1:B:410:ALA:CB	1:B:411:PRO:CD	2.98	0.40
1:B:660:SER:HB2	1:B:791:ASP:OD2	2.22	0.40
1:B:904:VAL:CG1	1:B:905:ASP:N	2.82	0.40
1:A:53:LEU:C	1:A:53:LEU:CD2	2.94	0.40
1:A:242:TYR:CE1	1:A:345:LYS:HE2	2.56	0.40
1:A:282:LEU:HD23	1:A:292:TYR:HA	2.03	0.40
1:A:535:CYS:C	1:A:536:THR:HG23	2.46	0.40
1:A:847:LEU:CD1	1:A:850:ALA:CA	2.94	0.40
1:A:943:ARG:CZ	1:A:943:ARG:HB2	2.51	0.40
1:B:53:LEU:CG	1:B:64:LEU:CD1	2.96	0.40
1:B:81:VAL:CG1	1:B:82:THR:N	2.85	0.40
1:B:131:SER:O	1:B:133:TYR:CD2	2.74	0.40
1:B:681:THR:OG1	1:B:686:THR:HG21	2.21	0.40
1:B:889:ILE:HD12	1:B:907:TYR:CE1	2.56	0.40
1:B:943:ARG:CZ	1:B:943:ARG:HB2	2.51	0.40

All (69) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:CE1	1:B:730:GLN:CD[1_655]	0.64	1.56
1:B:287:THR:OG1	1:B:840:HIS:CG[1_655]	0.67	1.53
1:A:146:PHE:CE1	1:B:730:GLN:OE1[1_655]	0.77	1.43
1:A:146:PHE:CD1	1:B:730:GLN:OE1[1_655]	0.78	1.42
1:B:287:THR:CA	1:B:840:HIS:NE2[1_655]	0.79	1.41
1:B:287:THR:CB	1:B:840:HIS:CG[1_655]	0.85	1.35
1:B:287:THR:CB	1:B:840:HIS:CD2[1_655]	0.93	1.27
1:B:287:THR:CA	1:B:840:HIS:CD2[1_655]	1.03	1.17
1:A:731:SER:OG	1:B:83:HIS:CE1[2_646]	1.19	1.01
1:A:146:PHE:CZ	1:B:730:GLN:NE2[1_655]	1.20	1.00
1:A:146:PHE:CZ	1:B:730:GLN:CD[1_655]	1.29	0.91
1:A:730:GLN:OE1	1:B:146:PHE:CD1[2_646]	1.43	0.77
1:B:219:ASP:OD1	1:B:826:GLN:CD[1_655]	1.50	0.70
1:A:730:GLN:NE2	1:B:146:PHE:CE1[2_646]	1.52	0.68
1:B:287:THR:OG1	1:B:840:HIS:ND1[1_655]	1.52	0.68
1:A:407:ASP:OD2	1:A:926:ALA:O[1_554]	1.55	0.65
1:B:287:THR:C	1:B:840:HIS:NE2[1_655]	1.55	0.65
1:A:148:LEU:O	1:B:728:GLN:OE1[1_655]	1.56	0.64
1:B:220:GLU:OE2	1:B:939:GLU:OE1[1_655]	1.56	0.64
1:A:730:GLN:CD	1:B:146:PHE:CE1[2_646]	1.57	0.63
1:B:287:THR:OG1	1:B:840:HIS:CB[1_655]	1.58	0.62
1:B:287:THR:C	1:B:840:HIS:CD2[1_655]	1.60	0.60
1:B:287:THR:OG1	1:B:840:HIS:CD2[1_655]	1.61	0.59
1:A:83:HIS:CE1	1:B:731:SER:OG[1_655]	1.62	0.58
1:B:219:ASP:OD1	1:B:826:GLN:OE1[1_655]	1.68	0.52
1:B:288:ALA:CB	1:B:841:GLU:OE1[1_655]	1.71	0.49
1:B:287:THR:CA	1:B:840:HIS:CE1[1_655]	1.74	0.46
1:A:146:PHE:CE1	1:B:730:GLN:CG[1_655]	1.75	0.45
1:A:146:PHE:CZ	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:A:146:PHE:CG	1:B:730:GLN:OE1[1_655]	1.75	0.45
1:B:287:THR:CG2	1:B:840:HIS:CD2[1_655]	1.77	0.43
1:B:287:THR:CG2	1:B:840:HIS:C[1_655]	1.78	0.42
1:A:728:GLN:OE1	1:B:148:LEU:O[2_646]	1.83	0.37
1:A:730:GLN:OE1	1:B:146:PHE:CE1[2_646]	1.84	0.36
1:A:731:SER:OG	1:B:83:HIS:ND1[2_646]	1.85	0.35
1:B:219:ASP:OD1	1:B:826:GLN:CG[1_655]	1.86	0.34
1:A:146:PHE:CE1	1:B:730:GLN:NE2[1_655]	1.88	0.32
1:A:728:GLN:NE2	1:B:148:LEU:O[2_646]	1.89	0.31
1:B:217:PHE:CD1	1:B:827:SER:OG[1_655]	1.90	0.30
1:A:752:LEU:CD2	1:B:152:PHE:CE1[2_646]	1.91	0.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:CB	1:B:840:HIS:CB[1_655]	1.91	0.29
1:B:287:THR:CB	1:B:840:HIS:ND1[1_655]	1.92	0.28
1:A:208:GLU:OE2	1:B:728:GLN:NE2[1_655]	1.93	0.27
1:B:217:PHE:CE1	1:B:827:SER:OG[1_655]	1.93	0.27
1:A:146:PHE:CD1	1:B:730:GLN:CD[1_655]	1.94	0.26
1:B:220:GLU:OE2	1:B:939:GLU:CD[1_655]	1.96	0.24
1:B:287:THR:N	1:B:840:HIS:NE2[1_655]	1.98	0.22
1:A:148:LEU:O	1:B:728:GLN:CD[1_655]	1.99	0.21
1:B:220:GLU:OE1	1:B:939:GLU:OE2[1_655]	2.00	0.20
1:A:730:GLN:NE2	1:B:146:PHE:CZ[2_646]	2.01	0.19
1:B:219:ASP:OD2	1:B:826:GLN:OE1[1_655]	2.01	0.19
1:B:287:THR:CA	1:B:840:HIS:CG[1_655]	2.01	0.19
1:B:287:THR:CB	1:B:840:HIS:NE2[1_655]	2.01	0.19
1:A:731:SER:OG	1:B:83:HIS:NE2[2_646]	2.03	0.17
1:B:219:ASP:CG	1:B:826:GLN:OE1[1_655]	2.03	0.17
1:B:219:ASP:CG	1:B:826:GLN:CD[1_655]	2.04	0.16
1:B:287:THR:O	1:B:840:HIS:NE2[1_655]	2.05	0.15
1:A:141:ARG:NH2	1:B:691:GLU:OE2[1_655]	2.06	0.14
1:A:208:GLU:OE2	1:B:728:GLN:CD[1_655]	2.08	0.12
1:A:728:GLN:CD	1:B:148:LEU:O[2_646]	2.09	0.11
1:B:287:THR:CG2	1:B:840:HIS:O[1_655]	2.09	0.11
1:A:407:ASP:OD1	1:A:924:GLN:OE1[1_554]	2.11	0.09
1:A:730:GLN:CD	1:B:146:PHE:CD1[2_646]	2.11	0.09
1:B:287:THR:CG2	1:B:840:HIS:CG[1_655]	2.12	0.08
1:B:287:THR:CG2	1:B:841:GLU:N[1_655]	2.13	0.07
1:A:208:GLU:OE1	1:B:753:ARG:NH2[1_655]	2.15	0.05
1:B:219:ASP:OD2	1:B:826:GLN:NE2[1_655]	2.16	0.04
1:A:728:GLN:OE1	1:B:148:LEU:C[2_646]	2.18	0.02
1:A:728:GLN:OE1	1:B:149:GLY:CA[2_646]	2.19	0.01

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 X-ray entries followed by that with respect to entries of similar resolution.

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	994/1207 (82%)	923 (93%)	51 (5%)	20 (2%)	6	31
1	B	907/1207 (75%)	845 (93%)	43 (5%)	19 (2%)	5	30
All	All	1901/2414 (79%)	1768 (93%)	94 (5%)	39 (2%)	5	30

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN
1	A	804	GLY
1	A	864	PRO
1	B	96	PRO
1	B	181	LYS
1	B	191	LYS
1	B	410	ALA
1	B	465	ASN
1	B	557	CYS
1	B	700	CYS
1	B	701	PRO
1	B	804	GLY
1	B	864	PRO
1	A	87	PRO
1	B	87	PRO
1	A	271	LYS
1	A	474	VAL
1	A	557	CYS
1	A	849	GLY
1	A	1015	ASP
1	A	1016	MET
1	B	271	LYS
1	B	474	VAL
1	B	849	GLY
1	A	263	VAL
1	B	263	VAL
1	A	344	ARG
1	B	344	ARG
1	A	933	VAL
1	A	1013	VAL
1	B	933	VAL

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Mol	Chain	Res	Type
1	A	44	GLY
1	A	921	LYS
1	B	921	LYS
1	B	44	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 X-ray entries followed by that with respect to entries of similar resolution.

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	888/1067 (83%)	858 (97%)	30 (3%)	32	54
1	B	812/1067 (76%)	788 (97%)	24 (3%)	36	57
All	All	1700/2134 (80%)	1646 (97%)	54 (3%)	34	56

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	ARG
1	A	72	LYS
1	A	98	ARG
1	A	271	LYS
1	A	386	LYS
1	A	412	LEU
1	A	435	ILE
1	A	444	LEU
1	A	468	GLN
1	A	473	GLN
1	A	501	LEU
1	A	529	CYS
1	A	548	ARG
1	A	567	ILE
1	A	575	LEU
1	A	597	LEU
1	A	670	ARG
1	A	722	LYS
1	A	743	GLN

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Mol	Chain	Res	Type
1	A	773	ILE
1	A	797	LYS
1	A	853	LYS
1	A	854	CYS
1	A	892	HIS
1	A	955	LEU
1	A	1004	ILE
1	A	1014	LEU
1	A	1016	MET
1	A	1017	LYS
1	A	1024	ARG
1	B	69	ARG
1	B	72	LYS
1	B	98	ARG
1	B	271	LYS
1	B	386	LYS
1	B	412	LEU
1	B	435	ILE
1	B	444	LEU
1	B	468	GLN
1	B	473	GLN
1	B	501	LEU
1	B	529	CYS
1	B	548	ARG
1	B	567	ILE
1	B	575	LEU
1	B	597	LEU
1	B	670	ARG
1	B	722	LYS
1	B	743	GLN
1	B	773	ILE
1	B	797	LYS
1	B	853	LYS
1	B	854	CYS
1	B	892	HIS

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

Mol	Chain	Res	Type
1	A	51	ASN
1	A	52	HIS
1	A	101	GLN

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Mol	Chain	Res	Type
1	A	114	ASN
1	A	134	GLN
1	A	157	HIS
1	A	163	ASN
1	A	273	GLN
1	A	361	GLN
1	A	441	ASN
1	A	442	HIS
1	A	473	GLN
1	A	490	HIS
1	A	500	GLN
1	A	533	ASN
1	A	566	ASN
1	A	630	HIS
1	A	672	HIS
1	A	685	ASN
1	A	690	GLN
1	A	702	GLN
1	A	728	GLN
1	A	747	GLN
1	A	787	HIS
1	A	789	ASN
1	A	792	ASN
1	A	826	GLN
1	A	970	GLN
1	A	983	ASN
1	A	1006	ASN
1	B	51	ASN
1	B	52	HIS
1	B	101	GLN
1	B	114	ASN
1	B	134	GLN
1	B	157	HIS
1	B	163	ASN
1	B	273	GLN
1	B	361	GLN
1	B	441	ASN
1	B	442	HIS
1	B	473	GLN
1	B	500	GLN
1	B	566	ASN
1	B	629	HIS

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Mol	Chain	Res	Type
1	B	630	HIS
1	B	672	HIS
1	B	682	HIS
1	B	685	ASN
1	B	690	GLN
1	B	702	GLN
1	B	728	GLN
1	B	730	GLN
1	B	747	GLN
1	B	787	HIS
1	B	789	ASN
1	B	792	ASN
1	B	826	GLN
1	B	836	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	854:CYS	C	855:THR	N	2.49
1	A	802:LYS	C	803:CYS	N	2.46
1	A	951:MET	C	952:THR	N	2.32
1	B	653:TYR	C	654:ASN	N	2.31
1	B	802:LYS	C	803:CYS	N	2.01
1	A	506:VAL	C	507:GLU	N	1.87
1	B	506:VAL	C	507:GLU	N	1.82
1	B	700:CYS	C	701:PRO	N	1.63
1	A	700:CYS	C	701:PRO	N	1.04
1	B	557:CYS	C	558:VAL	N	0.94
1	A	557:CYS	C	558:VAL	N	0.86

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1000/1207 (82%)	1.30	256 (25%) 1 8	195, 258, 410, 410	0
1	B	915/1207 (75%)	1.16	208 (22%) 2 9	209, 257, 329, 329	0
All	All	1915/2414 (79%)	1.23	464 (24%) 2 9	195, 257, 329, 410	0

All (464) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	9.4
1	A	621	ARG	9.3
1	A	631	VAL	9.3
1	A	311	ALA	8.2
1	A	400	ASP	8.1
1	B	659	ASN	7.9
1	A	250	GLY	7.7
1	B	412	LEU	7.6
1	A	172	ILE	7.6
1	B	270	THR	7.5
1	A	410	ALA	7.3
1	B	43	ARG	7.0
1	B	842	SER	7.0
1	A	285	GLU	6.7
1	A	164	GLU	6.4
1	B	182	LEU	6.4
1	A	766	TYR	6.2
1	A	240	ASP	6.1
1	A	748	ARG	6.1
1	A	411	PRO	6.1
1	A	899	GLU	6.1
1	B	850	ALA	6.1
1	B	851	ASN	6.0
1	A	747	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	482	ARG	5.8
1	A	495	ILE	5.8
1	A	312	ALA	5.8
1	B	566	ASN	5.8
1	B	411	PRO	5.7
1	B	250	GLY	5.7
1	B	829	GLY	5.6
1	B	284	LYS	5.6
1	B	218	HIS	5.6
1	B	292	TYR	5.6
1	B	37	PRO	5.6
1	B	251	ASN	5.5
1	A	402	ASN	5.5
1	B	583	VAL	5.4
1	A	705	ARG	5.4
1	A	256	LEU	5.3
1	A	479	PRO	5.3
1	A	405	GLY	5.2
1	B	401	ASP	5.2
1	B	181	LYS	5.2
1	B	495	ILE	5.1
1	A	349	LEU	5.1
1	B	98	ARG	5.1
1	B	473	GLN	5.0
1	A	48	GLU	4.9
1	A	165	SER	4.9
1	B	172	ILE	4.9
1	A	388	LYS	4.8
1	A	962	ARG	4.8
1	A	1014	LEU	4.8
1	A	174	SER	4.8
1	A	350	ASP	4.8
1	A	245	TYR	4.7
1	A	92	PRO	4.7
1	A	47	ALA	4.7
1	A	499	ARG	4.7
1	A	709	ILE	4.7
1	A	398	THR	4.7
1	A	309	LEU	4.7
1	A	983	ASN	4.6
1	A	247	PHE	4.6
1	A	996	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	137	CYS	4.6
1	A	566	ASN	4.6
1	B	504	VAL	4.5
1	B	150	GLU	4.5
1	B	657	VAL	4.5
1	A	622	ILE	4.5
1	B	183	PHE	4.5
1	B	431	MET	4.4
1	A	64	LEU	4.4
1	A	140	LEU	4.4
1	A	412	LEU	4.4
1	A	138	LYS	4.4
1	A	601	ASP	4.4
1	B	656	SER	4.4
1	A	485	ALA	4.4
1	A	129	CYS	4.4
1	A	150	GLU	4.4
1	A	415	SER	4.3
1	A	578	LEU	4.3
1	B	203	LEU	4.3
1	A	279	LEU	4.3
1	B	479	PRO	4.2
1	A	609	ILE	4.2
1	A	504	VAL	4.2
1	B	410	ALA	4.2
1	A	649	SER	4.2
1	B	256	LEU	4.2
1	A	362	ILE	4.2
1	A	118	LEU	4.2
1	A	629	HIS	4.2
1	A	772	GLU	4.2
1	A	128	ALA	4.2
1	A	552	SER	4.1
1	A	484	MET	4.1
1	A	493	LEU	4.1
1	B	670	ARG	4.1
1	B	830	GLN	4.1
1	A	619	VAL	4.1
1	A	251	ASN	4.0
1	A	246	GLY	4.0
1	B	255	PHE	4.0
1	A	345	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	450	LYS	4.0
1	B	654	ASN	4.0
1	A	244	VAL	4.0
1	A	706	VAL	4.0
1	A	288	ALA	4.0
1	B	285	GLU	4.0
1	A	255	PHE	4.0
1	B	446	PHE	4.0
1	B	271	LYS	4.0
1	B	415	SER	4.0
1	A	163	ASN	4.0
1	A	966	SER	4.0
1	A	657	VAL	4.0
1	A	347	LYS	3.9
1	A	745	ILE	3.9
1	B	466	ALA	3.9
1	B	838	PRO	3.9
1	A	169	PHE	3.9
1	B	170	GLY	3.9
1	A	401	ASP	3.9
1	A	659	ASN	3.9
1	A	952	THR	3.8
1	B	913	ILE	3.8
1	B	649	SER	3.8
1	A	473	GLN	3.8
1	A	943	ARG	3.8
1	A	228	ILE	3.8
1	A	423	VAL	3.8
1	A	62	ILE	3.7
1	B	679	VAL	3.7
1	B	171	VAL	3.7
1	B	53	LEU	3.7
1	B	82	THR	3.7
1	A	498	GLU	3.7
1	B	584	PRO	3.7
1	A	486	PHE	3.7
1	B	163	ASN	3.7
1	B	423	VAL	3.6
1	A	210	ASP	3.6
1	B	45	GLU	3.6
1	A	222	VAL	3.6
1	B	222	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	LYS	3.6
1	B	625	GLU	3.6
1	B	805	ALA	3.6
1	A	346	MET	3.6
1	A	241	ILE	3.6
1	A	945	SER	3.6
1	A	928	PHE	3.6
1	B	631	VAL	3.6
1	A	815	LYS	3.6
1	B	388	LYS	3.6
1	B	766	TYR	3.6
1	B	772	GLU	3.6
1	A	126	LEU	3.5
1	A	168	VAL	3.5
1	B	711	VAL	3.5
1	A	846	GLU	3.5
1	A	357	PHE	3.5
1	B	570	SER	3.5
1	B	853	LYS	3.5
1	B	307	ARG	3.5
1	B	734	ARG	3.5
1	B	494	TYR	3.5
1	A	1024	ARG	3.5
1	B	675	LYS	3.5
1	B	843	ARG	3.5
1	A	563	HIS	3.4
1	B	143	GLU	3.4
1	A	71	TYR	3.4
1	A	707	ASP	3.4
1	A	931	ILE	3.4
1	A	1019	THR	3.4
1	A	316	LYS	3.4
1	A	734	ARG	3.4
1	B	239	PHE	3.4
1	B	156	GLU	3.4
1	A	660	SER	3.4
1	B	798	VAL	3.4
1	B	752	LEU	3.4
1	A	494	TYR	3.3
1	B	81	VAL	3.3
1	B	720	THR	3.3
1	A	384	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	92	PRO	3.3
1	A	732	GLY	3.3
1	B	276	THR	3.3
1	B	93	LYS	3.3
1	A	266	PRO	3.3
1	A	300	GLU	3.3
1	A	53	LEU	3.3
1	A	358	ILE	3.3
1	B	62	ILE	3.3
1	B	905	ASP	3.3
1	A	381	ASP	3.3
1	A	57	GLU	3.3
1	A	211	GLY	3.3
1	A	722	LYS	3.2
1	A	287	THR	3.2
1	A	719	ILE	3.2
1	B	889	ILE	3.2
1	A	180	ASP	3.2
1	A	685	ASN	3.2
1	A	390	ILE	3.2
1	A	735	GLY	3.2
1	B	152	PHE	3.2
1	B	467	LEU	3.2
1	B	360	LYS	3.2
1	A	424	PHE	3.2
1	B	740	LEU	3.2
1	A	155	LYS	3.1
1	B	364	ASP	3.2
1	A	290	ASN	3.1
1	B	64	LEU	3.1
1	A	642	GLY	3.1
1	A	490	HIS	3.1
1	B	474	VAL	3.1
1	B	756	SER	3.1
1	B	213	PHE	3.1
1	A	773	ILE	3.1
1	A	821	GLU	3.1
1	A	37	PRO	3.1
1	A	467	LEU	3.1
1	A	446	PHE	3.1
1	A	508	SER	3.1
1	A	938	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	663	SER	3.1
1	A	127	ILE	3.1
1	A	763	ASN	3.1
1	B	709	ILE	3.1
1	A	826	GLN	3.0
1	A	82	THR	3.0
1	A	481	LEU	3.0
1	B	140	LEU	3.0
1	B	852	SER	3.0
1	A	1020	VAL	3.0
1	B	54	VAL	3.0
1	A	356	ILE	3.0
1	B	402	ASN	3.0
1	B	856	ASN	3.0
1	A	336	THR	3.0
1	A	218	HIS	3.0
1	A	152	PHE	3.0
1	A	650	PHE	3.0
1	A	422	PRO	3.0
1	A	721	LEU	2.9
1	B	309	LEU	2.9
1	B	269	THR	2.9
1	B	705	ARG	2.9
1	A	500	GLN	2.9
1	A	404	CYS	2.9
1	A	688	SER	2.9
1	A	1009	SER	2.9
1	B	563	HIS	2.9
1	A	744	GLY	2.9
1	A	297	ILE	2.9
1	A	670	ARG	2.9
1	A	75	SER	2.9
1	B	238	ASP	2.9
1	B	787	HIS	2.9
1	A	166	GLY	2.9
1	B	552	SER	2.9
1	B	484	MET	2.8
1	A	596	ASP	2.8
1	B	481	LEU	2.8
1	A	921	LYS	2.8
1	B	440	LYS	2.8
1	A	213	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	901	SER	2.8
1	B	416	GLU	2.8
1	B	601	ASP	2.8
1	A	84	GLN	2.8
1	A	738	CYS	2.8
1	A	173	VAL	2.8
1	B	465	ASN	2.8
1	A	263	VAL	2.8
1	A	1011	GLU	2.8
1	B	732	GLY	2.8
1	B	755	ASN	2.8
1	B	77	LEU	2.8
1	B	493	LEU	2.8
1	A	1003	ILE	2.8
1	B	413	GLY	2.8
1	A	946	GLN	2.8
1	B	874	LYS	2.8
1	B	567	ILE	2.8
1	B	396	LEU	2.8
1	B	620	PRO	2.8
1	B	316	LYS	2.7
1	B	520	GLY	2.7
1	B	524	PRO	2.7
1	B	624	THR	2.7
1	B	349	LEU	2.7
1	B	849	GLY	2.7
1	B	839	ALA	2.7
1	A	106	PRO	2.7
1	A	534	THR	2.7
1	A	343	LYS	2.7
1	A	286	ASP	2.7
1	B	407	ASP	2.7
1	A	711	VAL	2.7
1	A	203	LEU	2.7
1	A	397	LEU	2.7
1	A	930	GLU	2.7
1	B	480	VAL	2.7
1	B	706	VAL	2.7
1	B	915	CYS	2.7
1	A	570	SER	2.7
1	B	75	SER	2.7
1	A	119	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	800	LEU	2.7
1	B	803	CYS	2.7
1	A	775	ASN	2.6
1	A	325	LEU	2.6
1	A	740	LEU	2.6
1	B	272	GLU	2.6
1	A	175	TYR	2.6
1	A	752	LEU	2.6
1	A	1004	ILE	2.6
1	A	254	TYR	2.6
1	B	345	LYS	2.6
1	A	720	THR	2.6
1	B	676	TYR	2.6
1	B	858	ARG	2.6
1	B	84	GLN	2.6
1	B	559	ARG	2.6
1	A	276	THR	2.6
1	B	315	SER	2.6
1	B	841	GLU	2.6
1	A	1036	VAL	2.6
1	A	269	THR	2.6
1	A	695	LYS	2.6
1	B	76	ASP	2.5
1	A	480	VAL	2.5
1	B	424	PHE	2.5
1	B	486	PHE	2.5
1	B	540	ARG	2.5
1	A	960	PRO	2.5
1	B	602	GLY	2.5
1	A	171	VAL	2.5
1	B	904	VAL	2.5
1	A	189	ASP	2.5
1	B	343	LYS	2.5
1	B	736	TYR	2.5
1	A	335	PHE	2.5
1	B	178	PHE	2.5
1	B	828	PRO	2.5
1	A	427	ASP	2.5
1	B	565	ASN	2.5
1	B	384	TRP	2.5
1	B	47	ALA	2.5
1	B	248	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLU	2.5
1	B	668	PRO	2.5
1	B	228	ILE	2.4
1	B	804	GLY	2.4
1	B	312	ALA	2.4
1	A	623	ILE	2.4
1	A	953	LEU	2.4
1	A	970	GLN	2.4
1	A	897	GLY	2.4
1	B	721	LEU	2.4
1	A	342	GLN	2.4
1	A	733	GLN	2.4
1	B	450	LYS	2.4
1	B	767	SER	2.4
1	A	178	PHE	2.4
1	A	817	ASP	2.4
1	B	144	ASP	2.4
1	B	532	HIS	2.4
1	A	204	THR	2.4
1	A	767	SER	2.4
1	A	545	ARG	2.4
1	B	660	SER	2.4
1	B	470	GLU	2.3
1	A	482	ARG	2.3
1	A	506	VAL	2.3
1	A	333	LEU	2.3
1	A	461	GLY	2.3
1	B	808	GLU	2.3
1	B	643	MET	2.3
1	B	406	LEU	2.3
1	B	273	GLN	2.3
1	A	43	ARG	2.3
1	A	731	SER	2.3
1	B	903	LEU	2.3
1	B	650	PHE	2.3
1	B	161	GLY	2.3
1	B	782	VAL	2.3
1	A	406	LEU	2.3
1	B	117	LEU	2.3
1	B	582	ASN	2.3
1	A	438	VAL	2.3
1	A	483	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	70	ILE	2.3
1	B	280	VAL	2.3
1	A	755	ASN	2.2
1	B	580	THR	2.2
1	B	745	ILE	2.2
1	B	731	SER	2.2
1	A	466	ALA	2.2
1	A	652	PHE	2.2
1	B	754	PHE	2.2
1	B	819	ASP	2.2
1	B	155	LYS	2.2
1	B	290	ASN	2.2
1	A	896	ALA	2.2
1	B	289	PHE	2.2
1	B	210	ASP	2.2
1	B	727	PRO	2.2
1	A	153	HIS	2.2
1	A	959	LYS	2.2
1	A	791	ASP	2.2
1	A	295	VAL	2.2
1	A	561	THR	2.2
1	A	249	SER	2.2
1	B	634	LEU	2.2
1	A	779	GLU	2.2
1	A	298	GLY	2.1
1	B	483	ASP	2.1
1	A	663	SER	2.1
1	B	310	GLN	2.1
1	B	636	LEU	2.1
1	B	240	ASP	2.1
1	B	476	ASP	2.1
1	A	387	VAL	2.1
1	A	562	VAL	2.1
1	B	387	VAL	2.1
1	A	393	SER	2.1
1	A	45	GLU	2.1
1	A	662	LEU	2.1
1	A	179	ASP	2.1
1	A	580	THR	2.1
1	A	746	GLU	2.1
1	A	547	PRO	2.1
1	A	248	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	477	SER	2.1
1	B	129	CYS	2.1
1	B	313	TYR	2.1
1	A	919	GLU	2.1
1	B	508	SER	2.1
1	A	834	ARG	2.0
1	A	334	LEU	2.0
1	A	819	ASP	2.0
1	B	442	HIS	2.0
1	B	678	HIS	2.0
1	A	105	GLU	2.0
1	A	474	VAL	2.0
1	A	560	LEU	2.0
1	B	501	LEU	2.0
1	B	892	HIS	2.0
1	B	253	VAL	2.0
1	B	875	VAL	2.0
1	A	85	THR	2.0
1	B	41	THR	2.0
1	B	111	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.