



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 08:21 am BST

PDB ID : 3AOA
Title : Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors : Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on : 2010-09-23
Resolution : 3.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

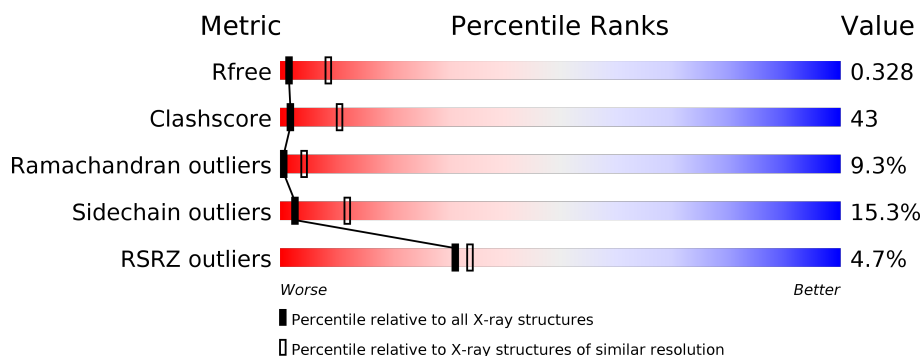
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 on 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	1053	<div> <div>4%</div> <div> <div></div> <div>37%</div> <div>45%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	1053	<div> <div>4%</div> <div> <div></div> <div>37%</div> <div>45%</div> <div>14%</div> <div>• •</div> </div> </div>
1	C	1053	<div> <div>5%</div> <div> <div></div> <div>37%</div> <div>47%</div> <div>11%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23325 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	EXPRESSION TAG	UNP P31224
A	1051	HIS	-	EXPRESSION TAG	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	HIS	-	EXPRESSION TAG	UNP P31224
B	1051	HIS	-	EXPRESSION TAG	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	HIS	-	EXPRESSION TAG	UNP P31224
C	1051	HIS	-	EXPRESSION TAG	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224

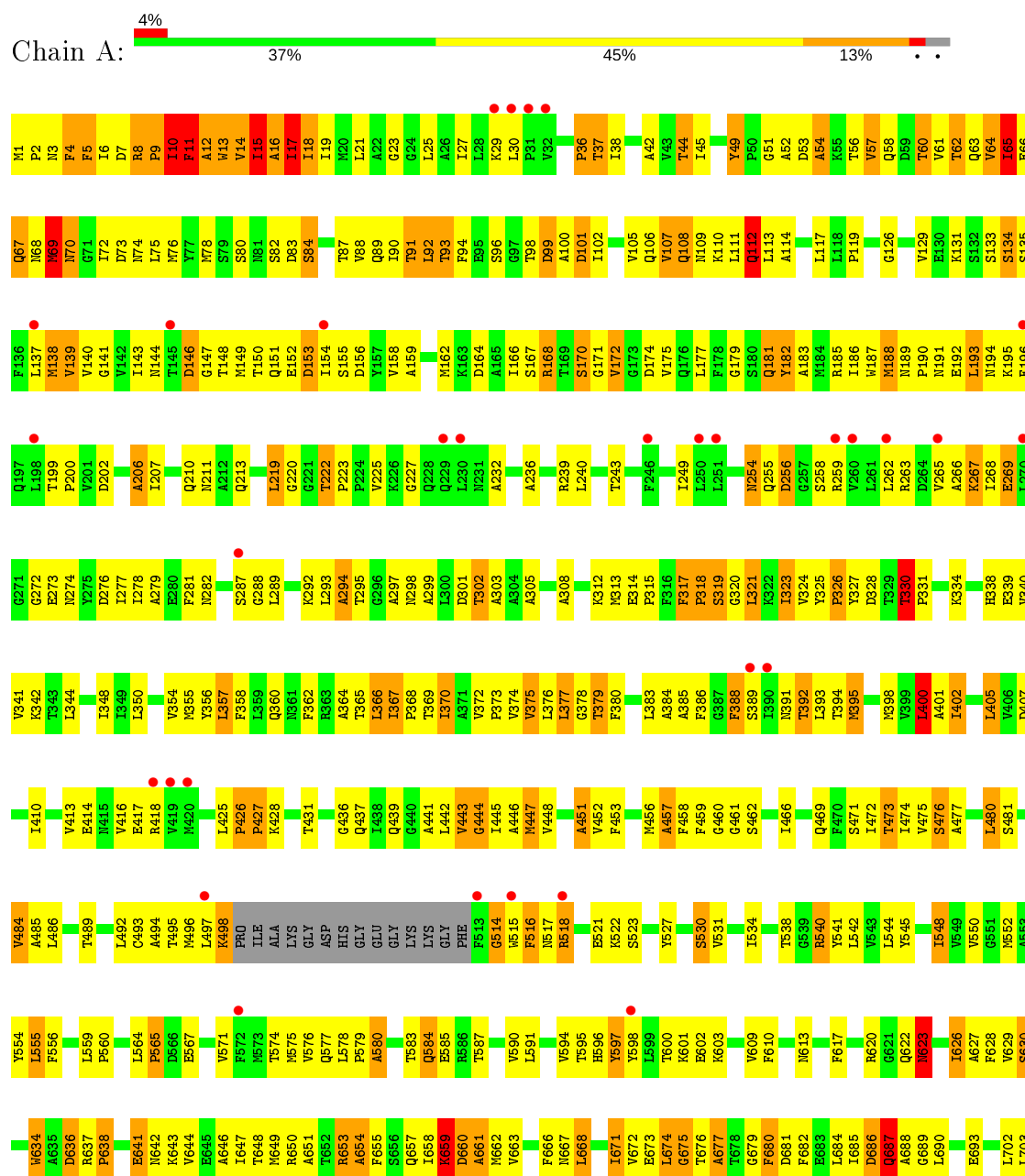
- Molecule 2 is water.

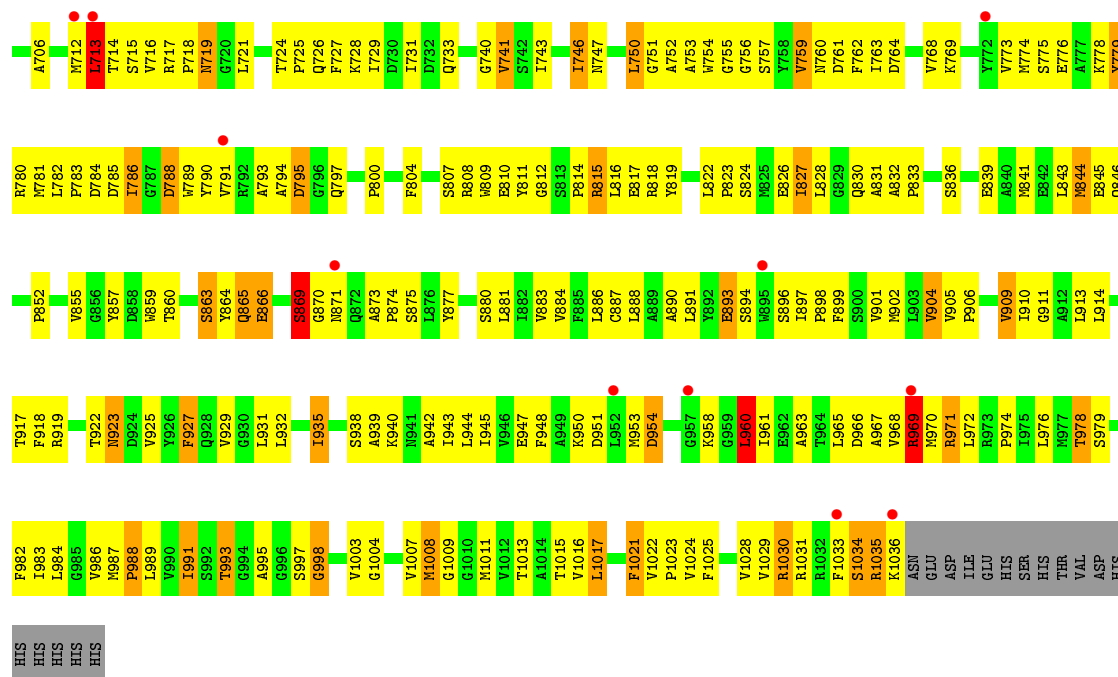
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		
2	B	1	Total	O	0	0
			1	1		
2	C	1	Total	O	0	0
			1	1		

3 Residue-property plots

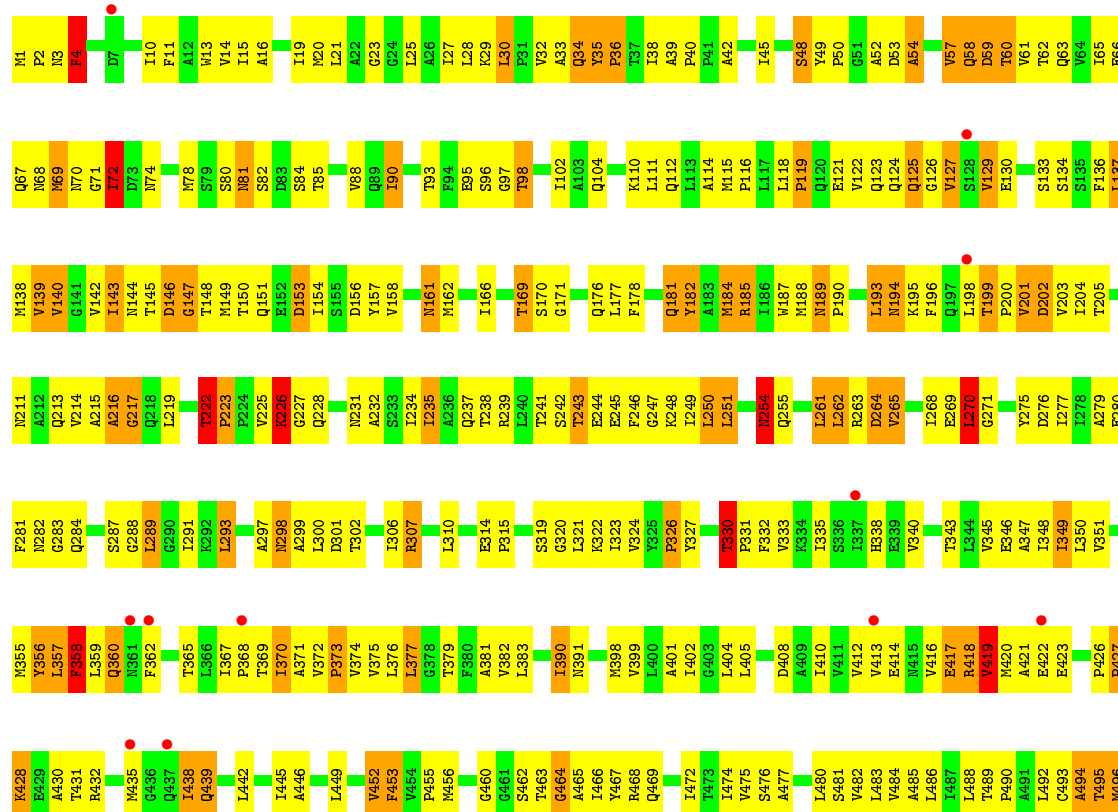
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

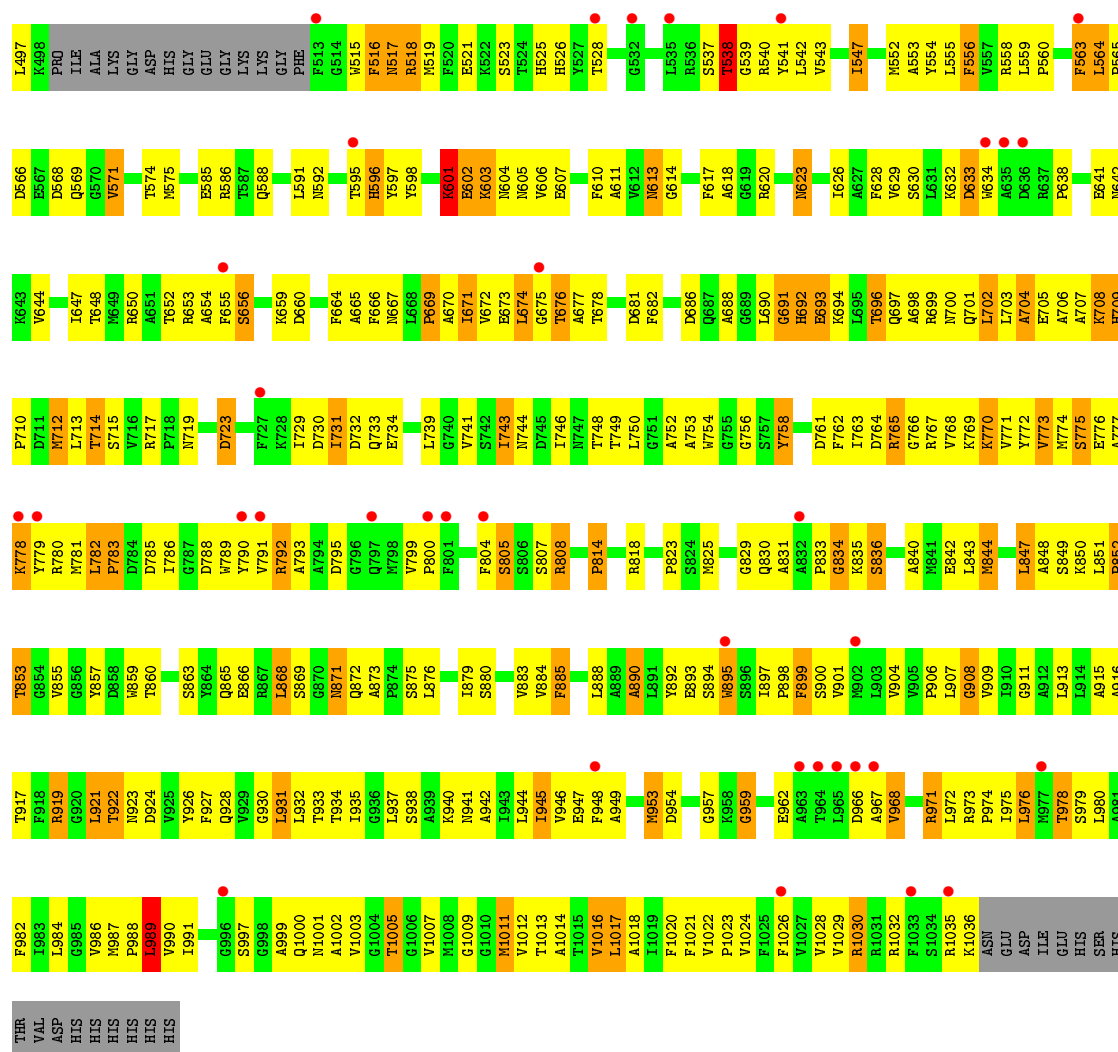
• Molecule 1: Acriflavine resistance protein B



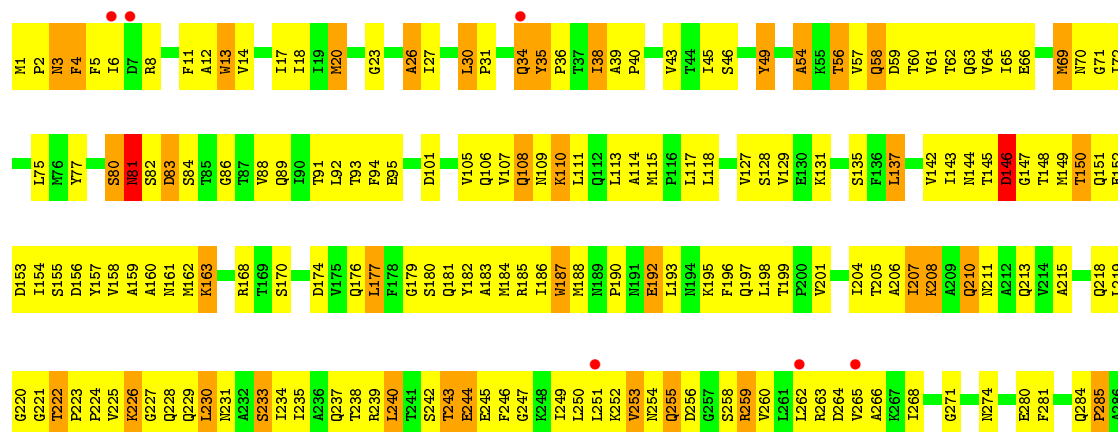


• Molecule 1: Acriflavine resistance protein B





• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	226.53Å 134.44Å 162.78Å 90.00° 97.73° 90.00°	Depositor
Resolution (Å)	49.30 – 3.35 48.52 – 3.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.30-3.35) 97.0 (48.52-3.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.271 , 0.326 0.272 , 0.328	Depositor DCC
R_{free} test set	3411 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	105.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 68.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23325	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/7920	0.76	5/10756 (0.0%)
1	B	0.57	0/7920	0.74	4/10756 (0.0%)
1	C	0.62	0/7920	0.75	3/10756 (0.0%)
All	All	0.60	0/23760	0.75	12/32268 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	LEU	CA-CB-CG	8.63	135.15	115.30
1	B	989	LEU	CA-CB-CG	7.46	132.46	115.30
1	B	563	PHE	CB-CA-C	7.28	124.95	110.40
1	A	400	LEU	CA-CB-CG	6.22	129.60	115.30
1	B	868	LEU	CA-CB-CG	5.67	128.35	115.30
1	C	35	TYR	N-CA-C	-5.59	95.91	111.00
1	C	767	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	B	377	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	8	ARG	C-N-CD	-5.38	108.75	120.60
1	C	972	LEU	CA-CB-CG	5.31	127.50	115.30
1	A	542	LEU	CA-CB-CG	5.24	127.36	115.30
1	A	972	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7774	0	7931	726	0
1	B	7774	0	7931	686	0
1	C	7774	0	7931	672	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	23325	0	23793	2013	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (2013) 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:C:669:PRO:HB2	1:C:672:VAL:CG2	1.38	1.52
1:A:7:ASP:C	1:A:9:PRO:HD2	1.43	1.38
1:A:6:ILE:HD12	1:A:7:ASP:N	1.40	1.34
1:C:669:PRO:CB	1:C:672:VAL:HG21	1.68	1.24
1:A:11:PHE:O	1:A:14:VAL:HG22	1.38	1.21
1:B:222:THR:HB	1:B:223:PRO:HD3	1.19	1.19
1:A:13:TRP:O	1:A:17:ILE:HG12	1.43	1.17
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.24	1.14
1:A:14:VAL:HA	1:A:17:ILE:HG13	1.29	1.13
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.31	1.12
1:A:14:VAL:CG2	1:A:15:ILE:H	1.58	1.12
1:A:69:MET:CE	1:A:69:MET:HA	1.78	1.12
1:A:69:MET:CA	1:A:69:MET:HE2	1.79	1.12
1:B:226:LYS:HA	1:B:226:LYS:HE3	1.17	1.12
1:B:59:ASP:OD2	1:B:60:THR:HG22	1.50	1.11
1:A:14:VAL:HG23	1:A:15:ILE:N	1.54	1.10
1:A:69:MET:CA	1:A:69:MET:CE	2.30	1.10
1:A:44:THR:HG23	1:A:91:THR:HG23	1.26	1.10
1:A:8:ARG:N	1:A:9:PRO:HD2	1.60	1.10
1:A:447:MET:HB3	1:A:887:CYS:SG	1.92	1.09
1:A:668:LEU:H	1:A:668:LEU:HD12	1.16	1.08
1:B:226:LYS:CE	1:B:226:LYS:HA	1.80	1.08
1:B:222:THR:HB	1:B:223:PRO:CD	1.83	1.08
1:B:709:HIS:H	1:B:710:PRO:HD3	1.12	1.07
1:A:69:MET:N	1:A:69:MET:HE3	1.69	1.06
1:A:367:ILE:HG13	1:A:368:PRO:N	1.71	1.06
1:B:54:ALA:HA	1:B:57:VAL:CG1	1.86	1.06
1:C:673:GLU:O	1:C:674:LEU:HB2	1.50	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:713:LEU:HD11	1:C:835:LYS:H	1.18	1.05
1:B:54:ALA:CA	1:B:57:VAL:CG1	2.36	1.04
1:C:246:PHE:O	1:C:249:ILE:HG12	1.56	1.04
1:B:54:ALA:CA	1:B:57:VAL:HG13	1.87	1.04
1:C:767:ARG:HG2	1:C:767:ARG:HH11	1.13	1.04
1:B:1:MET:HB3	1:B:2:PRO:HD2	1.40	1.03
1:B:127:VAL:HG12	1:B:127:VAL:O	1.54	1.02
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.40	1.02
1:A:69:MET:HA	1:A:69:MET:HE2	1.03	1.01
1:A:7:ASP:O	1:A:9:PRO:HG2	1.62	1.00
1:A:6:ILE:CD1	1:A:7:ASP:CG	2.30	1.00
1:A:661:ALA:O	1:A:663:VAL:HG23	1.61	1.00
1:B:54:ALA:O	1:B:57:VAL:HG13	1.61	1.00
1:A:14:VAL:CA	1:A:17:ILE:HG13	1.92	1.00
1:C:190:PRO:CD	1:C:779:TYR:HD1	1.74	1.00
1:A:7:ASP:C	1:A:9:PRO:CD	2.30	0.99
1:B:54:ALA:C	1:B:57:VAL:HG13	1.82	0.98
1:C:669:PRO:HG2	1:C:672:VAL:HB	1.44	0.98
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.44	0.98
1:A:6:ILE:HD11	1:A:7:ASP:OD2	1.61	0.98
1:B:516:PHE:N	1:B:516:PHE:CD1	2.30	0.97
1:A:112:GLN:HA	1:A:112:GLN:HE21	1.28	0.96
1:B:213:GLN:HG3	1:C:56:THR:HG23	1.47	0.96
1:C:211:ASN:HD22	1:C:240:LEU:HG	1.29	0.96
1:A:298:ASN:HD22	1:A:301:ASP:H	1.09	0.95
1:A:472:ILE:O	1:A:476:SER:HB2	1.66	0.95
1:C:669:PRO:CB	1:C:672:VAL:CG2	2.35	0.95
1:A:10:ILE:HD13	1:B:893:GLU:HA	1.47	0.95
1:C:702:LEU:HD12	1:C:851:LEU:HD11	1.48	0.95
1:A:11:PHE:HE1	1:B:890:ALA:HB1	1.29	0.95
1:B:145:THR:HG22	1:B:146:ASP:OD2	1.67	0.94
1:B:57:VAL:HG22	1:B:58:GLN:N	1.79	0.94
1:C:901:VAL:HG11	1:C:943:ILE:HG13	1.49	0.94
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.48	0.94
1:A:328:ASP:OD1	1:A:330:THR:HB	1.68	0.94
1:B:228:GLN:NE2	1:C:781:MET:SD	2.40	0.93
1:B:525:HIS:HA	1:B:528:THR:HG22	1.51	0.93
1:C:34:GLN:HG2	1:C:333:VAL:HG21	1.50	0.93
1:A:69:MET:N	1:A:69:MET:CE	2.30	0.93
1:A:367:ILE:HG13	1:A:368:PRO:CD	1.98	0.93
1:A:901:VAL:O	1:A:904:VAL:HG23	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:VAL:O	1:B:60:THR:HG23	1.69	0.93
1:B:213:GLN:CG	1:C:56:THR:HG23	1.98	0.92
1:A:6:ILE:CD1	1:A:7:ASP:N	2.30	0.92
1:A:14:VAL:O	1:A:17:ILE:HG12	1.69	0.92
1:B:971:ARG:HG3	1:B:971:ARG:HH11	1.33	0.92
1:C:190:PRO:HD2	1:C:779:TYR:HD1	1.33	0.92
1:B:650:ARG:O	1:B:654:ALA:HB2	1.70	0.91
1:C:672:VAL:HG12	1:C:672:VAL:O	1.70	0.91
1:B:54:ALA:HA	1:B:57:VAL:HG13	1.48	0.91
1:B:792:ARG:HG2	1:B:793:ALA:H	1.36	0.91
1:B:57:VAL:HG22	1:B:58:GLN:H	1.35	0.91
1:A:674:LEU:HD22	1:A:675:GLY:H	1.35	0.90
1:C:669:PRO:HB2	1:C:672:VAL:CB	2.00	0.90
1:A:151:GLN:NE2	1:A:279:ALA:H	1.68	0.90
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.71	0.89
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.36	0.89
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.54	0.89
1:C:66:GLU:OE2	1:C:80:SER:HB2	1.72	0.89
1:C:355:MET:HB3	1:C:365:THR:HG23	1.52	0.89
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.51	0.89
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.54	0.88
1:C:459:PHE:HB2	1:C:871:ASN:HB3	1.53	0.88
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.72	0.88
1:B:59:ASP:HA	1:B:63:GLN:CG	2.03	0.88
1:C:444:GLY:O	1:C:448:VAL:HG23	1.73	0.88
1:A:574:THR:HB	1:A:627:ALA:HB3	1.54	0.88
1:A:63:GLN:O	1:A:67:GLN:HG3	1.73	0.87
1:B:222:THR:CB	1:B:223:PRO:HD3	2.03	0.87
1:A:364:ALA:HB2	1:A:497:LEU:HD22	1.55	0.87
1:B:54:ALA:N	1:B:57:VAL:CG1	2.37	0.87
1:B:555:LEU:HB3	1:B:558:ARG:HH21	1.39	0.86
1:B:262:LEU:HA	1:B:265:VAL:HG12	1.57	0.86
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.57	0.86
1:B:709:HIS:H	1:B:710:PRO:CD	1.88	0.86
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.58	0.86
1:A:623:ASN:C	1:A:623:ASN:HD22	1.78	0.85
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.76	0.85
1:B:709:HIS:N	1:B:710:PRO:HD3	1.89	0.85
1:B:54:ALA:HA	1:B:57:VAL:HG11	1.57	0.85
1:A:6:ILE:HD12	1:A:7:ASP:H	1.05	0.85
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HD22	1:C:434:SER:HB2	1.41	0.85
1:C:952:LEU:O	1:C:953:MET:HB2	1.75	0.84
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.57	0.84
1:A:12:ALA:O	1:A:14:VAL:HG22	1.77	0.84
1:A:317:PHE:HB3	1:A:321:LEU:HD21	1.58	0.84
1:A:14:VAL:CA	1:A:17:ILE:CG1	2.55	0.84
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.42	0.84
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.41	0.84
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.42	0.84
1:C:690:LEU:HD23	1:C:694:LYS:HD2	1.60	0.84
1:C:721:LEU:HD21	1:C:813:SER:OG	1.77	0.84
1:B:269:GLU:O	1:B:270:LEU:HB2	1.77	0.84
1:C:767:ARG:HH11	1:C:767:ARG:CG	1.90	0.84
1:A:10:ILE:CD1	1:B:893:GLU:HA	2.07	0.83
1:C:54:ALA:HB2	1:C:84:SER:HB2	1.59	0.83
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.60	0.83
1:A:69:MET:O	1:C:168:ARG:HG2	1.79	0.83
1:B:226:LYS:HE3	1:B:226:LYS:CA	2.05	0.83
1:A:6:ILE:O	1:A:9:PRO:HG3	1.79	0.83
1:C:190:PRO:HD2	1:C:779:TYR:CD1	2.13	0.83
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.61	0.83
1:C:713:LEU:HD11	1:C:835:LYS:N	1.94	0.83
1:A:62:THR:O	1:A:66:GLU:HG3	1.79	0.82
1:C:669:PRO:HB2	1:C:672:VAL:HG21	0.83	0.82
1:C:81:ASN:C	1:C:81:ASN:HD22	1.82	0.82
1:A:1029:VAL:O	1:A:1030:ARG:HB2	1.76	0.82
1:A:365:THR:O	1:A:368:PRO:HG2	1.79	0.82
1:A:644:VAL:HG11	1:A:667:ASN:HD22	1.44	0.82
1:B:139:VAL:HG12	1:B:139:VAL:O	1.76	0.82
1:A:129:VAL:H	1:B:112:GLN:HE22	1.24	0.82
1:C:953:MET:HG3	1:C:959:GLY:HA2	1.59	0.82
1:C:554:TYR:HB3	1:C:558:ARG:HH21	1.44	0.82
1:A:8:ARG:O	1:A:10:ILE:HG13	1.80	0.82
1:C:778:LYS:HE3	1:C:779:TYR:HE2	1.44	0.82
1:C:829:GLY:O	1:C:830:GLN:HB3	1.78	0.82
1:B:57:VAL:HG22	1:B:82:SER:HB2	1.60	0.82
1:B:58:GLN:HB2	1:B:82:SER:HB3	1.62	0.81
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.61	0.81
1:B:988:PRO:O	1:B:989:LEU:HB3	1.80	0.81
1:A:66:GLU:C	1:A:68:ASN:H	1.79	0.81
1:C:204:ILE:HG23	1:C:759:VAL:CG1	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:HE2	1:B:118:LEU:HD22	1.61	0.81
1:A:11:PHE:CE1	1:B:890:ALA:HB1	2.15	0.81
1:A:171:GLY:O	1:A:294:ALA:HB2	1.81	0.81
1:B:516:PHE:HD1	1:B:516:PHE:H	0.91	0.81
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.61	0.81
1:C:38:ILE:HD13	1:C:38:ILE:H	1.45	0.81
1:A:785:ASP:O	1:A:788:ASP:HB2	1.81	0.81
1:B:767:ARG:HA	1:C:63:GLN:HE22	1.46	0.81
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.62	0.81
1:B:346:GLU:O	1:B:988:PRO:HG3	1.80	0.81
1:A:298:ASN:O	1:A:302:THR:HG23	1.81	0.81
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.63	0.80
1:C:901:VAL:O	1:C:904:VAL:HG23	1.80	0.80
1:A:364:ALA:HB2	1:A:497:LEU:CD2	2.12	0.80
1:A:12:ALA:O	1:A:14:VAL:CG2	2.30	0.80
1:A:367:ILE:N	1:A:368:PRO:HD2	1.95	0.80
1:A:6:ILE:O	1:A:9:PRO:CD	2.30	0.80
1:B:145:THR:CG2	1:B:146:ASP:OD2	2.30	0.80
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.62	0.80
1:C:760:ASN:O	1:C:771:VAL:HG23	1.82	0.80
1:B:516:PHE:O	1:B:517:ASN:ND2	2.15	0.80
1:A:13:TRP:HB3	1:A:17:ILE:HD11	1.64	0.80
1:A:278:ILE:HB	1:A:613:ASN:OD1	1.81	0.80
1:A:14:VAL:O	1:A:17:ILE:CG1	2.30	0.80
1:A:367:ILE:CG1	1:A:368:PRO:HD3	2.12	0.79
1:A:6:ILE:O	1:A:9:PRO:CG	2.30	0.79
1:A:395:MET:HA	1:A:395:MET:CE	2.11	0.79
1:C:721:LEU:CD2	1:C:721:LEU:O	2.30	0.79
1:C:655:PHE:C	1:C:657:GLN:H	1.86	0.79
1:A:365:THR:O	1:A:368:PRO:CG	2.30	0.79
1:A:74:ASN:HB3	1:A:98:THR:HG21	1.62	0.79
1:B:291:ILE:HG21	1:B:306:ILE:CD1	2.13	0.79
1:A:668:LEU:CD1	1:A:668:LEU:H	1.94	0.79
1:A:888:LEU:HD11	1:A:943:ILE:CD1	2.12	0.79
1:C:415:ASN:ND2	1:C:434:SER:HB2	1.96	0.79
1:A:266:ALA:O	1:A:267:LYS:HB2	1.81	0.79
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.64	0.78
1:A:712:MET:O	1:A:832:ALA:HB2	1.83	0.78
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.62	0.78
1:C:355:MET:SD	1:C:410:ILE:HD11	2.22	0.78
1:A:726:GLN:OE1	1:A:812:GLY:HA3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ALA:HB2	1:B:93:THR:HG22	1.64	0.78
1:A:317:PHE:HB3	1:A:321:LEU:CD2	2.13	0.78
1:A:597:TYR:C	1:A:597:TYR:CD1	2.57	0.78
1:A:75:LEU:HD11	1:A:92:LEU:HB3	1.64	0.78
1:A:7:ASP:O	1:A:9:PRO:CG	2.30	0.78
1:C:35:TYR:CD2	1:C:671:ILE:HD11	2.18	0.78
1:A:6:ILE:CD1	1:A:7:ASP:OD2	2.30	0.78
1:B:57:VAL:CG2	1:B:58:GLN:N	2.46	0.78
1:A:13:TRP:C	1:A:17:ILE:HD11	2.04	0.78
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.64	0.78
1:B:58:GLN:CB	1:B:82:SER:HB3	2.13	0.78
1:C:554:TYR:C	1:C:556:PHE:H	1.86	0.78
1:C:767:ARG:HG2	1:C:767:ARG:NH1	1.96	0.77
1:C:577:GLN:H	1:C:577:GLN:HE21	1.28	0.77
1:A:14:VAL:HG23	1:A:15:ILE:H	0.70	0.77
1:C:669:PRO:CG	1:C:672:VAL:HB	2.13	0.77
1:B:767:ARG:HA	1:C:63:GLN:NE2	2.00	0.77
1:B:276:ASP:O	1:B:614:GLY:HA3	1.84	0.77
1:C:457:ALA:H	1:C:459:PHE:HE2	1.31	0.77
1:A:8:ARG:N	1:A:9:PRO:CD	2.45	0.77
1:C:972:LEU:H	1:C:974:PRO:HD2	1.48	0.77
1:A:369:THR:O	1:A:373:PRO:CD	2.32	0.76
1:A:634:TRP:CE3	1:A:995:ALA:HB1	2.21	0.76
1:C:673:GLU:O	1:C:674:LEU:CB	2.32	0.76
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.15	0.76
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.20	0.76
1:A:686:ASP:O	1:A:687:GLN:HB2	1.86	0.76
1:A:750:LEU:HD23	1:A:754:TRP:CD1	2.19	0.76
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.51	0.76
1:A:498:LYS:HE2	1:A:498:LYS:O	1.85	0.76
1:B:130:GLU:OE1	1:C:110:LYS:HE2	1.85	0.76
1:A:5:PHE:O	1:A:9:PRO:HD3	1.85	0.76
1:B:767:ARG:O	1:B:769:LYS:HG3	1.84	0.76
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.67	0.76
1:C:686:ASP:OD1	1:C:687:GLN:N	2.19	0.76
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.67	0.76
1:A:13:TRP:C	1:A:17:ILE:HG12	2.06	0.75
1:C:686:ASP:OD2	1:C:690:LEU:HB2	1.86	0.75
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.67	0.75
1:A:790:TYR:HE1	1:A:800:PRO:HG3	1.49	0.75
1:B:307:ARG:HB2	1:B:307:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLY:HA3	1:B:302:THR:CB	2.17	0.75
1:C:721:LEU:HD23	1:C:721:LEU:O	1.86	0.75
1:A:193:LEU:HB2	1:A:265:VAL:HB	1.67	0.75
1:B:690:LEU:HD22	1:B:694:LYS:HD2	1.68	0.75
1:A:13:TRP:O	1:A:17:ILE:CG1	2.30	0.75
1:A:11:PHE:C	1:A:14:VAL:HG22	2.06	0.75
1:B:171:GLY:HA3	1:B:302:THR:HB	1.67	0.75
1:B:897:ILE:O	1:B:901:VAL:HG23	1.87	0.75
1:B:792:ARG:HB2	1:B:792:ARG:HH11	1.51	0.75
1:C:568:ASP:OD1	1:C:634:TRP:CD1	2.40	0.75
1:A:151:GLN:NE2	1:A:279:ALA:N	2.36	0.74
1:C:144:ASN:HD21	1:C:148:THR:N	1.85	0.74
1:C:80:SER:HB3	1:C:818:ARG:HB2	1.67	0.74
1:C:721:LEU:HG	1:C:815:ARG:O	1.85	0.74
1:C:831:ALA:HB2	1:C:840:ALA:HB2	1.69	0.74
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.69	0.74
1:C:945:ILE:HD13	1:C:1022:VAL:HG11	1.69	0.74
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.23	0.74
1:B:28:LEU:HD12	1:B:29:LYS:HG2	1.70	0.74
1:C:317:PHE:HD2	1:C:321:LEU:HB3	1.51	0.74
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.69	0.74
1:C:247:GLY:HA3	1:C:263:ARG:CZ	2.18	0.73
1:B:743:ILE:H	1:B:743:ILE:HD12	1.52	0.73
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.71	0.73
1:A:243:THR:HB	1:A:268:ILE:HG22	1.69	0.73
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.71	0.73
1:C:184:MET:HE3	1:C:184:MET:HA	1.70	0.73
1:B:1016:VAL:HG12	1:B:1017:LEU:HD12	1.70	0.72
1:A:880:SER:O	1:A:884:VAL:HG23	1.89	0.72
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.04	0.72
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.70	0.72
1:A:634:TRP:HE3	1:A:995:ALA:HB1	1.55	0.72
1:C:779:TYR:HD2	1:C:779:TYR:N	1.88	0.72
1:A:375:VAL:HG22	1:A:484:VAL:HG11	1.71	0.72
1:A:68:ASN:ND2	1:A:114:ALA:HB2	2.04	0.72
1:B:986:VAL:HG12	1:B:990:VAL:HG23	1.71	0.72
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.70	0.72
1:A:911:GLY:H	1:A:914:LEU:HD13	1.55	0.72
1:B:773:VAL:O	1:B:773:VAL:HG12	1.89	0.72
1:B:84:SER:HB3	1:B:814:PRO:HA	1.72	0.72
1:A:781:MET:HE2	1:C:225:VAL:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLN:HE22	1:C:620:ARG:HH11	1.37	0.72
1:A:140:VAL:HG12	1:A:141:GLY:H	1.53	0.72
1:A:298:ASN:ND2	1:A:301:ASP:H	1.84	0.72
1:B:126:GLY:O	1:B:127:VAL:HB	1.88	0.72
1:A:759:VAL:HG12	1:A:760:ASN:N	2.05	0.71
1:A:437:GLN:HB3	1:A:948:PHE:HE2	1.55	0.71
1:C:686:ASP:O	1:C:687:GLN:HG2	1.89	0.71
1:C:714:THR:HG22	1:C:715:SER:H	1.54	0.71
1:A:11:PHE:O	1:A:12:ALA:C	2.29	0.71
1:A:686:ASP:HB2	1:A:823:PRO:HG2	1.72	0.71
1:B:731:ILE:HD11	1:B:746:ILE:HG21	1.71	0.71
1:A:950:LYS:O	1:A:954:ASP:HB2	1.89	0.71
1:B:516:PHE:N	1:B:516:PHE:HD1	1.74	0.71
1:B:601:LYS:NZ	1:B:601:LYS:HB2	2.06	0.71
1:B:851:LEU:N	1:B:852:PRO:HD3	2.05	0.71
1:C:672:VAL:CG1	1:C:672:VAL:O	2.37	0.71
1:C:688:ALA:HB3	1:C:690:LEU:HD12	1.73	0.71
1:C:713:LEU:CD1	1:C:835:LYS:H	2.01	0.71
1:A:112:GLN:CA	1:A:112:GLN:HE21	2.03	0.71
1:A:137:LEU:O	1:A:138:MET:HB3	1.90	0.71
1:A:14:VAL:C	1:A:17:ILE:HG12	2.12	0.71
1:C:38:ILE:H	1:C:38:ILE:CD1	2.04	0.71
1:C:674:LEU:CD1	1:C:862:MET:HA	2.21	0.71
1:B:428:LYS:O	1:B:432:ARG:HG3	1.90	0.71
1:C:115:MET:SD	1:C:127:VAL:HG11	2.31	0.71
1:B:58:GLN:HG3	1:B:59:ASP:N	2.03	0.70
1:C:23:GLY:HA3	1:C:377:LEU:O	1.91	0.70
1:C:575:MET:O	1:C:576:VAL:HG13	1.91	0.70
1:A:27:ILE:HG12	1:A:380:PHE:HD2	1.56	0.70
1:B:974:PRO:O	1:B:978:THR:HB	1.91	0.70
1:C:759:VAL:C	1:C:760:ASN:HD22	1.94	0.70
1:A:991:ILE:HD13	1:A:1008:MET:HG3	1.74	0.70
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.74	0.70
1:A:11:PHE:O	1:A:14:VAL:CG2	2.30	0.70
1:A:659:LYS:HG2	1:A:660:ASP:N	2.06	0.70
1:B:149:MET:HB3	1:B:154:ILE:CG2	2.21	0.70
1:B:1:MET:HB3	1:B:2:PRO:CD	2.19	0.70
1:A:13:TRP:C	1:A:17:ILE:CD1	2.60	0.70
1:A:10:ILE:HG22	1:B:895:TRP:HD1	1.55	0.70
1:B:987:MET:O	1:B:991:ILE:HG12	1.92	0.70
1:C:674:LEU:HD11	1:C:861:GLY:C	2.12	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.21	0.70
1:B:145:THR:C	1:B:146:ASP:OD2	2.30	0.70
1:B:563:PHE:HD1	1:B:866:GLU:HG2	1.55	0.70
1:A:12:ALA:O	1:A:13:TRP:C	2.29	0.70
1:B:177:LEU:HD12	1:B:178:PHE:N	2.06	0.70
1:C:463:THR:O	1:C:465:ALA:N	2.25	0.70
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.27	0.70
1:A:16:ALA:O	1:A:17:ILE:C	2.29	0.70
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.74	0.70
1:A:13:TRP:O	1:A:14:VAL:C	2.30	0.69
1:A:931:LEU:O	1:A:935:ILE:HG12	1.91	0.69
1:A:15:ILE:O	1:A:16:ALA:C	2.30	0.69
1:A:13:TRP:O	1:A:16:ALA:HB3	1.92	0.69
1:A:395:MET:HA	1:A:395:MET:HE2	1.73	0.69
1:B:552:MET:SD	1:B:909:VAL:HG23	2.31	0.69
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.73	0.69
1:B:145:THR:O	1:B:146:ASP:CG	2.30	0.69
1:B:25:LEU:O	1:B:28:LEU:HG	1.92	0.69
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.22	0.69
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.22	0.69
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.28	0.69
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.27	0.69
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.75	0.69
1:C:741:VAL:HG11	1:C:746:ILE:HD11	1.75	0.69
1:C:778:LYS:C	1:C:779:TYR:HD2	1.96	0.69
1:B:968:VAL:O	1:B:972:LEU:HB2	1.92	0.69
1:C:748:THR:O	1:C:752:ALA:N	2.26	0.69
1:A:36:PRO:O	1:A:38:ILE:HG23	1.93	0.69
1:A:740:GLY:CA	1:A:793:ALA:HB1	2.23	0.69
1:C:204:ILE:CG1	1:C:773:VAL:HG21	2.23	0.69
1:A:883:VAL:O	1:A:887:CYS:HB2	1.92	0.69
1:C:378:GLY:O	1:C:382:VAL:HG23	1.93	0.69
1:C:474:ILE:O	1:C:478:MET:HB2	1.92	0.69
1:C:973:ARG:O	1:C:977:MET:HB2	1.93	0.69
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.74	0.69
1:A:584:GLN:H	1:A:622:GLN:HG2	1.57	0.69
1:A:418:ARG:HD3	1:A:970:MET:HG3	1.74	0.69
1:A:9:PRO:O	1:A:10:ILE:C	2.29	0.69
1:B:979:SER:HA	1:B:1011:MET:HE3	1.74	0.69
1:B:145:THR:C	1:B:146:ASP:CG	2.51	0.68
1:A:13:TRP:C	1:A:17:ILE:CG1	2.61	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:H	1:A:394:THR:HG22	1.56	0.68
1:A:576:VAL:HG21	1:A:591:LEU:HD23	1.75	0.68
1:A:893:GLU:O	1:A:893:GLU:HG3	1.92	0.68
1:C:115:MET:CE	1:C:118:LEU:HD23	2.23	0.68
1:C:210:GLN:HB3	1:C:249:ILE:HD12	1.75	0.68
1:C:58:GLN:HG3	1:C:59:ASP:OD2	1.92	0.68
1:A:42:ALA:HB2	1:A:93:THR:HA	1.75	0.68
1:B:198:LEU:HD13	1:B:251:LEU:HD23	1.74	0.68
1:B:681:ASP:HB3	1:B:860:THR:CG2	2.22	0.68
1:B:947:GLU:HA	1:B:947:GLU:OE1	1.92	0.68
1:B:213:GLN:HG2	1:C:56:THR:HG23	1.74	0.68
1:C:779:TYR:CD2	1:C:779:TYR:N	2.60	0.68
1:A:355:MET:CE	1:A:410:ILE:HG12	2.23	0.68
1:B:219:LEU:HD12	1:B:234:ILE:HG12	1.74	0.68
1:B:592:ASN:HA	1:B:595:THR:HG22	1.75	0.68
1:C:699:ARG:NH2	1:C:722:GLU:OE2	2.26	0.68
1:A:466:ILE:O	1:A:469:GLN:HB2	1.93	0.68
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.75	0.68
1:B:648:THR:HG23	1:B:665:ALA:O	1.93	0.68
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.74	0.68
1:C:552:MET:SD	1:C:909:VAL:HG21	2.34	0.68
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.75	0.68
1:A:6:ILE:HD12	1:A:7:ASP:CA	2.24	0.68
1:A:778:LYS:HD2	1:A:779:TYR:CZ	2.29	0.68
1:C:54:ALA:HB2	1:C:84:SER:CB	2.23	0.68
1:A:886:LEU:HG	1:C:14:VAL:HG23	1.76	0.68
1:C:210:GLN:O	1:C:240:LEU:HD21	1.94	0.68
1:A:14:VAL:O	1:A:15:ILE:C	2.30	0.68
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.76	0.68
1:C:155:SER:OG	1:C:179:GLY:HA3	1.94	0.68
1:C:925:VAL:HG23	1:C:926:TYR:H	1.56	0.68
1:C:962:GLU:HA	1:C:965:LEU:HD13	1.76	0.68
1:A:140:VAL:HG12	1:A:141:GLY:N	2.09	0.67
1:A:6:ILE:HD12	1:A:7:ASP:CG	2.13	0.67
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.30	0.67
1:B:731:ILE:CD1	1:B:746:ILE:HG21	2.25	0.67
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.75	0.67
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.24	0.67
1:C:62:THR:OG1	1:C:88:VAL:HG13	1.95	0.67
1:C:26:ALA:O	1:C:30:LEU:HB2	1.93	0.67
1:C:577:GLN:N	1:C:577:GLN:HE21	1.91	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.24	0.67
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.77	0.67
1:C:672:VAL:C	1:C:674:LEU:H	1.97	0.67
1:A:134:SER:HB2	1:A:673:GLU:OE2	1.95	0.67
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.94	0.67
1:B:944:LEU:HB3	1:B:971:ARG:HD3	1.77	0.67
1:C:674:LEU:HB3	1:C:865:GLN:OE1	1.95	0.66
1:C:326:PRO:O	1:C:630:SER:HB2	1.94	0.66
1:B:575:MET:HA	1:B:626:ILE:HG22	1.77	0.66
1:C:911:GLY:H	1:C:1013:THR:HG21	1.59	0.66
1:C:280:GLU:HB2	1:C:611:ALA:HB3	1.75	0.66
1:C:454:VAL:HG23	1:C:475:VAL:HG21	1.77	0.66
1:C:657:GLN:HG3	1:C:658:ILE:HG13	1.77	0.66
1:C:753:ALA:O	1:C:775:SER:HB3	1.95	0.66
1:A:1033:PHE:O	1:A:1034:SER:HB2	1.94	0.66
1:A:355:MET:HE1	1:A:410:ILE:HG12	1.76	0.66
1:B:880:SER:O	1:B:884:VAL:HG23	1.94	0.66
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.10	0.66
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.10	0.66
1:A:367:ILE:CG1	1:A:368:PRO:CD	2.70	0.66
1:A:852:PRO:O	1:A:855:VAL:HG22	1.94	0.66
1:A:7:ASP:O	1:A:9:PRO:CD	2.42	0.66
1:B:225:VAL:O	1:B:225:VAL:HG23	1.94	0.66
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.26	0.66
1:A:153:ASP:HA	1:A:182:TYR:CE1	2.31	0.66
1:A:671:ILE:HD13	1:A:674:LEU:HB3	1.76	0.66
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.60	0.65
1:A:299:ALA:O	1:A:303:ALA:HB2	1.95	0.65
1:A:365:THR:C	1:A:368:PRO:HD2	2.17	0.65
1:A:540:ARG:HD3	1:A:541:TYR:CD2	2.30	0.65
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.25	0.65
1:A:102:ILE:O	1:A:106:GLN:HG3	1.96	0.65
1:A:5:PHE:O	1:A:9:PRO:CD	2.44	0.65
1:C:144:ASN:HA	1:C:320:GLY:O	1.95	0.65
1:A:268:ILE:HG22	1:A:269:GLU:N	2.10	0.65
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.78	0.65
1:B:188:MET:H	1:B:775:SER:HA	1.60	0.65
1:C:13:TRP:HE1	1:C:492:LEU:HD21	1.62	0.65
1:C:160:ALA:HA	1:C:767:ARG:NH1	2.11	0.65
1:B:650:ARG:O	1:B:654:ALA:CB	2.43	0.65
1:C:459:PHE:HD2	1:C:459:PHE:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ASP:OD1	1:C:634:TRP:NE1	2.29	0.65
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.31	0.65
1:A:7:ASP:O	1:A:9:PRO:HD2	1.95	0.65
1:B:61:VAL:HG13	1:B:88:VAL:HG21	1.78	0.65
1:A:64:VAL:O	1:A:66:GLU:N	2.30	0.65
1:A:13:TRP:O	1:A:17:ILE:N	2.30	0.65
1:A:901:VAL:O	1:A:904:VAL:CG2	2.43	0.65
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.26	0.65
1:C:679:GLY:HA2	1:C:830:GLN:HA	1.79	0.65
1:A:518:ARG:HA	1:A:521:GLU:HB2	1.79	0.65
1:B:127:VAL:O	1:B:127:VAL:CG1	2.30	0.65
1:B:416:VAL:HG21	1:B:431:THR:HG22	1.77	0.65
1:B:59:ASP:OD2	1:B:60:THR:N	2.30	0.65
1:A:9:PRO:O	1:A:11:PHE:N	2.30	0.64
1:A:66:GLU:C	1:A:68:ASN:N	2.47	0.64
1:B:146:ASP:O	1:B:148:THR:N	2.30	0.64
1:B:145:THR:CB	1:B:146:ASP:OD2	2.45	0.64
1:B:602:GLU:OE2	1:B:650:ARG:NH2	2.30	0.64
1:C:655:PHE:O	1:C:657:GLN:N	2.30	0.64
1:A:637:ARG:HH11	1:A:643:LYS:HA	1.60	0.64
1:C:45:ILE:HD13	1:C:111:LEU:HD23	1.78	0.64
1:A:12:ALA:O	1:A:15:ILE:N	2.30	0.64
1:A:68:ASN:O	1:A:70:ASN:N	2.30	0.64
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.79	0.64
1:B:150:THR:H	1:B:153:ASP:HB3	1.62	0.64
1:B:177:LEU:HD12	1:B:178:PHE:H	1.59	0.64
1:C:218:GLN:HB3	1:C:233:SER:HA	1.80	0.64
1:B:465:ALA:HA	1:B:468:ARG:HG3	1.79	0.64
1:C:144:ASN:HD21	1:C:148:THR:H	1.45	0.64
1:C:901:VAL:HG11	1:C:943:ILE:CG1	2.25	0.64
1:A:610:PHE:HB3	1:A:628:PHE:HB2	1.79	0.64
1:A:66:GLU:O	1:A:68:ASN:N	2.29	0.64
1:A:746:ILE:HG12	1:A:804:PHE:CE1	2.33	0.64
1:B:516:PHE:O	1:B:517:ASN:CG	2.36	0.64
1:B:653:ARG:HA	1:B:656:SER:HB3	1.79	0.64
1:C:956:GLU:HB3	1:C:958:LYS:HD2	1.80	0.64
1:A:989:LEU:HB3	1:A:993:THR:HG23	1.80	0.64
1:B:664:PHE:HB3	1:B:666:PHE:CE1	2.33	0.64
1:C:686:ASP:C	1:C:687:GLN:HG2	2.17	0.64
1:A:74:ASN:CB	1:A:98:THR:HG21	2.28	0.64
1:B:59:ASP:OD2	1:B:59:ASP:C	2.34	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:ARG:O	1:B:780:ARG:HG2	1.97	0.64
1:C:181:GLN:OE1	1:C:767:ARG:NH1	2.27	0.64
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.33	0.64
1:C:190:PRO:HD3	1:C:779:TYR:CD1	2.33	0.64
1:A:44:THR:CG2	1:A:91:THR:HG23	2.16	0.64
1:B:227:GLY:HA2	1:C:585:GLU:OE2	1.97	0.64
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.33	0.64
1:A:51:GLY:O	1:C:215:ALA:HB1	1.97	0.64
1:C:162:MET:HG2	1:C:313:MET:SD	2.38	0.64
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.16	0.64
1:A:150:THR:O	1:A:154:ILE:HG13	1.98	0.64
1:B:150:THR:HB	1:B:153:ASP:HB2	1.79	0.64
1:C:911:GLY:N	1:C:1013:THR:HG21	2.13	0.64
1:C:459:PHE:CB	1:C:871:ASN:HB3	2.27	0.64
1:A:10:ILE:HD13	1:B:893:GLU:CA	2.24	0.63
1:C:204:ILE:HG12	1:C:773:VAL:HG21	1.79	0.63
1:A:365:THR:O	1:A:368:PRO:HD2	1.98	0.63
1:A:597:TYR:HD1	1:A:598:TYR:N	1.97	0.63
1:B:708:LYS:HB2	1:B:708:LYS:NZ	2.13	0.63
1:C:193:LEU:HB3	1:C:198:LEU:O	1.99	0.63
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.33	0.63
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.13	0.63
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.79	0.63
1:B:780:ARG:O	1:B:780:ARG:CG	2.46	0.63
1:A:389:SER:O	1:A:394:THR:HG21	1.97	0.63
1:A:747:ASN:HD21	1:C:237:GLN:NE2	1.97	0.63
1:A:6:ILE:C	1:A:9:PRO:CD	2.67	0.63
1:A:367:ILE:O	1:A:370:ILE:HG22	1.99	0.63
1:A:731:ILE:HD12	1:A:731:ILE:H	1.63	0.63
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.34	0.63
1:C:459:PHE:CD2	1:C:459:PHE:N	2.66	0.63
1:A:298:ASN:HB3	1:A:301:ASP:CB	2.24	0.63
1:B:741:VAL:HG22	1:B:792:ARG:O	1.98	0.63
1:A:100:ALA:HB1	1:A:131:LYS:HE3	1.81	0.62
1:A:99:ASP:OD1	1:A:102:ILE:HG22	1.99	0.62
1:B:370:ILE:CG2	1:B:370:ILE:O	2.47	0.62
1:C:192:GLU:HG2	1:C:264:ASP:O	1.98	0.62
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.34	0.62
1:B:699:ARG:HG2	1:B:700:ASN:H	1.64	0.62
1:B:945:ILE:HD13	1:B:946:VAL:HG23	1.81	0.62
1:B:54:ALA:N	1:B:57:VAL:HG11	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASP:CG	1:B:634:TRP:H	2.03	0.62
1:C:118:LEU:HD22	1:C:118:LEU:H	1.62	0.62
1:C:600:THR:O	1:C:603:LYS:HB2	1.99	0.62
1:C:662:MET:N	1:C:662:MET:SD	2.72	0.62
1:C:672:VAL:O	1:C:674:LEU:N	2.30	0.62
1:A:268:ILE:O	1:A:269:GLU:HB3	1.99	0.62
1:A:367:ILE:N	1:A:368:PRO:CD	2.62	0.62
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.82	0.62
1:A:317:PHE:HB3	1:A:321:LEU:CG	2.29	0.62
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.29	0.62
1:C:413:VAL:HA	1:C:493:CYS:SG	2.40	0.62
1:B:115:MET:HA	1:B:115:MET:CE	2.30	0.62
1:B:185:ARG:CG	1:B:185:ARG:HH11	2.10	0.62
1:C:713:LEU:HD12	1:C:834:GLY:HA3	1.81	0.62
1:C:925:VAL:HG23	1:C:926:TYR:N	2.14	0.62
1:A:188:MET:SD	1:A:200:PRO:HB3	2.40	0.62
1:A:728:LYS:HD3	1:C:235:ILE:HG22	1.82	0.62
1:B:351:VAL:HG12	1:B:351:VAL:O	1.99	0.62
1:A:199:THR:HB	1:A:200:PRO:HD2	1.82	0.62
1:A:141:GLY:HA2	1:A:288:GLY:CA	2.29	0.62
1:A:741:VAL:HG21	1:A:791:VAL:HG23	1.82	0.62
1:B:298:ASN:O	1:B:300:LEU:N	2.33	0.62
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.35	0.62
1:A:369:THR:O	1:A:373:PRO:CG	2.48	0.61
1:B:792:ARG:HG2	1:B:793:ALA:N	2.12	0.61
1:B:713:LEU:HD21	1:B:844:MET:HG2	1.81	0.61
1:C:144:ASN:ND2	1:C:148:THR:N	2.47	0.61
1:A:129:VAL:H	1:B:112:GLN:NE2	1.95	0.61
1:A:367:ILE:HG22	1:A:496:MET:CE	2.29	0.61
1:B:493:CYS:O	1:B:497:LEU:HB2	2.01	0.61
1:C:186:ILE:HD12	1:C:262:LEU:HD21	1.82	0.61
1:C:66:GLU:OE2	1:C:80:SER:CB	2.48	0.61
1:C:690:LEU:HD23	1:C:694:LYS:CD	2.29	0.61
1:A:3:ASN:O	1:A:6:ILE:HG13	1.98	0.61
1:A:447:MET:CB	1:A:887:CYS:SG	2.82	0.61
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.81	0.61
1:C:669:PRO:CB	1:C:672:VAL:CB	2.73	0.61
1:B:150:THR:CB	1:B:153:ASP:HB2	2.30	0.61
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.01	0.61
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.66	0.61
1:A:688:ALA:C	1:A:690:LEU:H	2.03	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ALA:O	1:A:943:ILE:HG12	2.01	0.61
1:C:247:GLY:HA3	1:C:263:ARG:NH2	2.15	0.61
1:A:719:ASN:HB2	1:A:828:LEU:HD22	1.81	0.61
1:B:158:VAL:HA	1:B:162:MET:HG2	1.82	0.61
1:C:418:ARG:HH21	1:C:971:ARG:HH12	1.46	0.61
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.83	0.61
1:A:1:MET:O	1:A:5:PHE:HB2	2.01	0.61
1:A:73:ASP:H	1:A:106:GLN:HE22	1.47	0.61
1:B:484:VAL:HG13	1:B:488:LEU:HB3	1.82	0.61
1:C:5:PHE:HD2	1:C:12:ALA:HB2	1.66	0.61
1:C:358:PHE:HB3	1:C:977:MET:CE	2.27	0.61
1:C:669:PRO:HG2	1:C:672:VAL:CB	2.27	0.61
1:C:872:GLN:O	1:C:875:SER:HB3	2.00	0.61
1:A:388:PHE:H	1:A:388:PHE:HD1	1.49	0.61
1:B:178:PHE:HD2	1:B:288:GLY:O	1.84	0.61
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.21	0.61
1:B:568:ASP:OD1	1:B:644:VAL:HG22	2.01	0.61
1:C:668:LEU:H	1:C:668:LEU:HD23	1.65	0.61
1:C:903:LEU:HB3	1:C:1025:PHE:CE1	2.35	0.61
1:A:12:ALA:O	1:A:14:VAL:N	2.34	0.60
1:A:199:THR:HB	1:A:200:PRO:CD	2.31	0.60
1:A:369:THR:O	1:A:373:PRO:HG2	2.01	0.60
1:C:204:ILE:HG23	1:C:759:VAL:HG13	1.82	0.60
1:C:758:TYR:HE2	1:C:770:LYS:HZ3	1.48	0.60
1:A:726:GLN:HB2	1:C:235:ILE:HD13	1.82	0.60
1:B:189:ASN:O	1:B:193:LEU:HB2	2.00	0.60
1:B:241:THR:HG22	1:B:763:ILE:O	2.00	0.60
1:C:110:LYS:HA	1:C:113:LEU:HD12	1.83	0.60
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.83	0.60
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.83	0.60
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.01	0.60
1:A:367:ILE:HG22	1:A:496:MET:HE3	1.83	0.60
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.82	0.60
1:A:13:TRP:CB	1:A:17:ILE:HD11	2.31	0.60
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.83	0.60
1:A:339:GLU:O	1:A:340:VAL:HB	2.02	0.60
1:A:688:ALA:O	1:A:690:LEU:N	2.34	0.60
1:B:355:MET:SD	1:B:410:ILE:HD11	2.40	0.60
1:A:112:GLN:HA	1:A:112:GLN:NE2	2.09	0.60
1:A:365:THR:O	1:A:368:PRO:CD	2.50	0.60
1:B:254:ASN:HD22	1:B:255:GLN:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:763:ILE:HG22	1:C:764:ASP:O	2.01	0.60
1:C:899:PHE:H	1:C:899:PHE:HD1	1.49	0.60
1:A:18:ILE:O	1:A:21:LEU:N	2.35	0.60
1:A:986:VAL:HG13	1:A:1008:MET:HG2	1.82	0.60
1:C:184:MET:CE	1:C:184:MET:HA	2.31	0.60
1:C:220:GLY:H	1:C:231:ASN:HD22	1.49	0.60
1:A:14:VAL:C	1:A:17:ILE:CG1	2.70	0.60
1:A:188:MET:HA	1:A:266:ALA:HA	1.84	0.60
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.65	0.60
1:C:448:VAL:HG22	1:C:887:CYS:HB3	1.83	0.60
1:C:685:ILE:O	1:C:685:ILE:HG13	2.01	0.60
1:C:702:LEU:CD1	1:C:851:LEU:HD11	2.27	0.60
1:A:211:ASN:ND2	1:A:760:ASN:OD1	2.31	0.60
1:A:890:ALA:HB1	1:C:11:PHE:HD1	1.66	0.60
1:B:58:GLN:HA	1:B:62:THR:OG1	2.01	0.60
1:B:953:MET:HA	1:B:957:GLY:O	2.01	0.60
1:A:314:GLU:HA	1:A:317:PHE:CZ	2.36	0.60
1:B:123:GLN:O	1:B:125:GLN:N	2.29	0.60
1:B:476:SER:O	1:B:480:LEU:HB2	2.02	0.60
1:A:137:LEU:O	1:A:137:LEU:HG	2.00	0.60
1:A:741:VAL:HG21	1:A:791:VAL:CG2	2.32	0.60
1:A:888:LEU:HD11	1:A:943:ILE:HD12	1.82	0.60
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.29	0.60
1:B:235:ILE:CD1	1:B:235:ILE:N	2.65	0.60
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.31	0.59
1:A:6:ILE:O	1:A:9:PRO:HD3	2.02	0.59
1:A:530:SER:O	1:A:534:ILE:HB	2.02	0.59
1:B:193:LEU:CD1	1:B:198:LEU:O	2.50	0.59
1:B:834:GLY:O	1:B:835:LYS:HD3	2.02	0.59
1:B:885:PHE:CD1	1:B:885:PHE:C	2.74	0.59
1:C:554:TYR:C	1:C:556:PHE:N	2.55	0.59
1:C:777:ALA:O	1:C:781:MET:CE	2.49	0.59
1:A:790:TYR:CE1	1:A:800:PRO:HG3	2.34	0.59
1:B:750:LEU:HD23	1:B:750:LEU:C	2.22	0.59
1:A:102:ILE:HD11	1:C:101:ASP:HB3	1.84	0.59
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.84	0.59
1:B:144:ASN:OD1	1:B:320:GLY:O	2.20	0.59
1:A:276:ASP:CB	1:C:222:THR:HG23	2.21	0.59
1:A:471:SER:O	1:A:475:VAL:HG12	2.01	0.59
1:A:901:VAL:HG11	1:A:943:ILE:HD13	1.82	0.59
1:B:247:GLY:O	1:B:263:ARG:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:699:ARG:O	1:B:701:GLN:N	2.35	0.59
1:B:770:LYS:HB3	1:B:772:TYR:HE2	1.67	0.59
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.84	0.59
1:C:778:LYS:HE3	1:C:779:TYR:CE2	2.34	0.59
1:A:913:LEU:HD22	1:A:927:PHE:HZ	1.65	0.59
1:B:773:VAL:O	1:B:773:VAL:CG1	2.51	0.59
1:C:228:GLN:NE2	1:C:230:LEU:O	2.32	0.59
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.84	0.59
1:B:847:LEU:H	1:B:847:LEU:HD23	1.67	0.59
1:C:514:GLY:HA2	1:C:518:ARG:HG3	1.85	0.59
1:C:754:TRP:CZ3	1:C:780:ARG:HA	2.38	0.59
1:C:894:SER:HB2	1:C:897:ILE:HD12	1.84	0.59
1:A:6:ILE:C	1:A:9:PRO:HD3	2.22	0.59
1:B:195:LYS:HG2	1:B:195:LYS:O	2.03	0.59
1:B:30:LEU:HD13	1:B:390:ILE:HD11	1.85	0.59
1:C:456:MET:O	1:C:457:ALA:HB3	2.03	0.59
1:C:513:PHE:CD2	1:C:517:ASN:HB3	2.38	0.59
1:A:68:ASN:HD22	1:A:114:ALA:HB2	1.67	0.59
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.31	0.59
1:C:66:GLU:O	1:C:69:MET:HB2	2.02	0.59
1:C:847:LEU:HA	1:C:850:LYS:CG	2.33	0.59
1:A:3:ASN:O	1:A:6:ILE:CG1	2.51	0.59
1:A:740:GLY:C	1:A:793:ALA:HB1	2.23	0.59
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.85	0.59
1:C:427:PRO:HB3	1:C:498:LYS:HD2	1.84	0.59
1:C:939:ALA:O	1:C:943:ILE:HG13	2.03	0.59
1:C:674:LEU:HD11	1:C:862:MET:N	2.18	0.58
1:A:609:VAL:HG12	1:A:629:VAL:HB	1.85	0.58
1:B:463:THR:HG21	1:B:869:SER:HB2	1.85	0.58
1:B:808:ARG:HH21	1:B:808:ARG:HB2	1.68	0.58
1:C:688:ALA:O	1:C:690:LEU:N	2.29	0.58
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.68	0.58
1:A:68:ASN:C	1:A:70:ASN:OD1	2.41	0.58
1:B:193:LEU:HD22	1:B:198:LEU:HB2	1.85	0.58
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.85	0.58
1:B:843:LEU:HD23	1:B:847:LEU:HD21	1.85	0.58
1:C:681:ASP:HB3	1:C:860:THR:HG22	1.85	0.58
1:B:1001:ASN:O	1:B:1005:THR:HB	2.03	0.58
1:C:368:PRO:HG3	1:C:413:VAL:HG11	1.83	0.58
1:C:445:ILE:HG13	1:C:446:ALA:H	1.66	0.58
1:C:778:LYS:HB2	1:C:779:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:158:VAL:HG23	2.03	0.58
1:A:181:GLN:O	1:A:181:GLN:HG2	2.03	0.58
1:A:441:ALA:O	1:A:445:ILE:HG23	2.03	0.58
1:A:69:MET:C	1:A:70:ASN:OD1	2.42	0.58
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.39	0.58
1:B:959:GLY:HA2	1:B:962:GLU:HB3	1.84	0.58
1:C:144:ASN:ND2	1:C:149:MET:H	2.02	0.58
1:A:780:ARG:NH2	1:C:223:PRO:O	2.37	0.58
1:A:677:ALA:C	1:A:679:GLY:H	2.06	0.58
1:A:971:ARG:O	1:A:974:PRO:HD2	2.03	0.58
1:B:356:TYR:O	1:B:360:GLN:N	2.36	0.58
1:B:452:VAL:O	1:B:453:PHE:HD2	1.87	0.58
1:B:585:GLU:O	1:B:588:GLN:N	2.36	0.58
1:B:693:GLU:HG3	1:B:694:LYS:H	1.68	0.58
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.12	0.58
1:B:871:ASN:N	1:B:871:ASN:HD22	2.00	0.58
1:A:584:GLN:H	1:A:622:GLN:CG	2.16	0.58
1:B:154:ILE:C	1:B:156:ASP:N	2.57	0.58
1:C:476:SER:O	1:C:478:MET:N	2.36	0.58
1:A:323:ILE:O	1:A:323:ILE:HG12	2.02	0.58
1:A:597:TYR:C	1:A:597:TYR:HD1	2.07	0.58
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.85	0.58
1:A:747:ASN:HD21	1:C:237:GLN:HE21	1.49	0.58
1:C:13:TRP:NE1	1:C:492:LEU:HD21	2.18	0.58
1:C:669:PRO:CG	1:C:672:VAL:CB	2.82	0.58
1:C:713:LEU:HD13	1:C:713:LEU:N	2.18	0.58
1:A:733:GLN:OE1	1:A:743:ILE:CD1	2.48	0.58
1:A:7:ASP:CA	1:A:9:PRO:HD2	2.30	0.58
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.33	0.58
1:A:108:GLN:OE1	1:B:112:GLN:HB2	2.03	0.58
1:A:172:VAL:O	1:A:172:VAL:HG23	2.04	0.58
1:A:151:GLN:HE22	1:A:279:ALA:N	2.01	0.58
1:A:376:LEU:O	1:A:378:GLY:N	2.37	0.58
1:A:818:ARG:HG2	1:A:823:PRO:HA	1.86	0.58
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.85	0.58
1:B:247:GLY:HA2	1:B:268:ILE:HG13	1.84	0.58
1:B:54:ALA:CA	1:B:57:VAL:HG11	2.22	0.58
1:B:158:VAL:HA	1:B:162:MET:CG	2.34	0.57
1:B:140:VAL:HG11	1:B:310:LEU:HD11	1.86	0.57
1:A:156:ASP:OD1	1:A:182:TYR:HB2	2.03	0.57
1:A:815:ARG:HB3	1:A:815:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.69	0.57
1:C:777:ALA:C	1:C:781:MET:HE3	2.25	0.57
1:C:875:SER:C	1:C:877:TYR:H	2.07	0.57
1:A:6:ILE:HD11	1:A:7:ASP:CG	2.08	0.57
1:B:591:LEU:CD1	1:B:611:ALA:HB1	2.26	0.57
1:B:358:PHE:HE1	1:B:973:ARG:HB2	1.68	0.57
1:C:17:ILE:HA	1:C:20:MET:HB2	1.86	0.57
1:B:144:ASN:ND2	1:B:149:MET:HG3	2.19	0.57
1:C:187:TRP:CZ3	1:C:774:MET:HB3	2.39	0.57
1:C:941:ASN:HB2	1:C:975:ILE:HG12	1.85	0.57
1:C:418:ARG:HH21	1:C:971:ARG:NH1	2.02	0.57
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.86	0.57
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.85	0.57
1:B:571:VAL:HG12	1:B:630:SER:HA	1.86	0.57
1:B:54:ALA:N	1:B:57:VAL:HG12	2.19	0.57
1:B:45:ILE:HD13	1:B:65:ILE:HG21	1.86	0.57
1:C:544:LEU:HD12	1:C:1021:PHE:HZ	1.69	0.57
1:A:405:LEU:HD21	1:A:477:ALA:HB1	1.87	0.57
1:B:65:ILE:HB	1:B:90:ILE:HD12	1.86	0.57
1:B:927:PHE:CE2	1:B:931:LEU:HG	2.39	0.57
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.34	0.57
1:A:574:THR:HG1	1:A:598:TYR:HE1	1.50	0.57
1:A:841:MET:O	1:A:845:GLU:HG3	2.05	0.57
1:B:289:LEU:HD12	1:B:289:LEU:N	2.19	0.57
1:C:307:ARG:NE	1:C:325:TYR:HE2	2.01	0.57
1:C:690:LEU:CD2	1:C:694:LYS:HD2	2.34	0.57
1:C:80:SER:O	1:C:81:ASN:HB3	2.05	0.57
1:A:1017:LEU:O	1:A:1021:PHE:HB2	2.03	0.57
1:A:590:VAL:O	1:A:594:VAL:HG23	2.05	0.57
1:A:836:SER:OG	1:A:839:GLU:HG3	2.03	0.57
1:A:904:VAL:HG11	1:A:938:SER:O	2.05	0.57
1:B:988:PRO:O	1:B:989:LEU:CB	2.50	0.57
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.69	0.57
1:A:646:ALA:O	1:A:649:MET:HB2	2.05	0.57
1:B:300:LEU:HD21	1:B:333:VAL:HG11	1.86	0.57
1:B:518:ARG:HA	1:B:521:GLU:CG	2.35	0.57
1:C:721:LEU:HD22	1:C:721:LEU:O	2.03	0.57
1:C:727:PHE:CZ	1:C:807:SER:CB	2.88	0.57
1:A:601:LYS:O	1:A:602:GLU:HG2	2.05	0.57
1:A:643:LYS:O	1:A:647:ILE:HG13	2.04	0.57
1:B:237:GLN:HG2	1:B:238:THR:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:O	1:B:453:PHE:HB2	2.05	0.57
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.34	0.57
1:C:575:MET:HB3	1:C:577:GLN:NE2	2.20	0.57
1:C:847:LEU:HA	1:C:850:LYS:HG3	1.87	0.57
1:A:395:MET:HE3	1:A:395:MET:HA	1.87	0.56
1:B:156:ASP:OD2	1:B:182:TYR:HB2	2.05	0.56
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.87	0.56
1:C:115:MET:CE	1:C:127:VAL:HG11	2.35	0.56
1:C:213:GLN:NE2	1:C:238:THR:HA	2.20	0.56
1:C:188:MET:HG3	1:C:774:MET:O	2.05	0.56
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.39	0.56
1:A:99:ASP:OD1	1:A:101:ASP:N	2.37	0.56
1:A:298:ASN:HD22	1:A:301:ASP:N	1.91	0.56
1:A:595:THR:HA	1:A:609:VAL:HG21	1.86	0.56
1:A:894:SER:OG	1:A:897:ILE:HB	2.05	0.56
1:B:228:GLN:OE1	1:C:781:MET:HB3	2.05	0.56
1:A:54:ALA:HA	1:A:83:ASP:O	2.04	0.56
1:B:214:VAL:HG12	1:B:215:ALA:O	2.06	0.56
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.86	0.56
1:B:944:LEU:HD13	1:B:975:ILE:HG13	1.85	0.56
1:A:545:TYR:HB2	1:A:1021:PHE:CE1	2.40	0.56
1:A:14:VAL:N	1:A:17:ILE:HD11	2.20	0.56
1:A:344:LEU:HD23	1:A:402:ILE:CD1	2.34	0.56
1:A:69:MET:O	1:C:168:ARG:CG	2.53	0.56
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.87	0.56
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.86	0.56
1:B:219:LEU:HD21	1:C:783:PRO:HB3	1.88	0.56
1:C:380:PHE:HE2	1:C:395:MET:HE3	1.69	0.56
1:A:443:VAL:HG22	1:A:486:LEU:HD11	1.87	0.56
1:A:591:LEU:CD1	1:A:613:ASN:HB3	2.35	0.56
1:B:676:THR:HG22	1:B:676:THR:O	2.04	0.56
1:B:847:LEU:N	1:B:847:LEU:HD23	2.20	0.56
1:C:62:THR:HA	1:C:88:VAL:HG11	1.88	0.56
1:C:914:LEU:O	1:C:915:ALA:HB3	2.06	0.56
1:A:73:ASP:H	1:A:106:GLN:NE2	2.03	0.56
1:A:729:ILE:HD11	1:A:786:ILE:HD12	1.88	0.56
1:A:6:ILE:CD1	1:A:7:ASP:H	1.98	0.56
1:A:897:ILE:N	1:A:898:PRO:HD2	2.21	0.56
1:C:190:PRO:HB3	1:C:789:TRP:CE3	2.41	0.56
1:A:191:ASN:C	1:A:193:LEU:H	2.09	0.56
1:A:886:LEU:O	1:C:14:VAL:HG21	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.35	0.56
1:B:946:VAL:HG21	1:B:1026:PHE:CZ	2.41	0.56
1:C:983:ILE:HD11	1:C:1011:MET:HB3	1.87	0.56
1:C:1022:VAL:HA	1:C:1025:PHE:CE2	2.41	0.56
1:C:183:ALA:HB1	1:C:770:LYS:O	2.05	0.56
1:C:835:LYS:HG3	1:C:836:SER:N	2.20	0.56
1:A:555:LEU:HB3	1:A:913:LEU:HD12	1.88	0.56
1:C:564:LEU:HD23	1:C:565:PRO:HD2	1.87	0.56
1:C:57:VAL:HG13	1:C:88:VAL:HG22	1.87	0.56
1:C:712:MET:HB2	1:C:713:LEU:HD13	1.87	0.56
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.40	0.56
1:B:115:MET:HE2	1:B:115:MET:HA	1.87	0.56
1:B:149:MET:HB3	1:B:154:ILE:HG22	1.88	0.56
1:A:164:ASP:OD2	1:B:67:GLN:HG3	2.05	0.56
1:C:137:LEU:HD13	1:C:293:LEU:HD13	1.88	0.56
1:A:190:PRO:HD3	1:A:789:TRP:CZ2	2.41	0.56
1:A:330:THR:H	1:A:331:PRO:HD2	1.70	0.56
1:B:145:THR:HB	1:B:146:ASP:OD2	2.06	0.56
1:B:641:GLU:HB3	1:B:650:ARG:HH12	1.69	0.56
1:C:595:THR:HG21	1:C:611:ALA:HB2	1.88	0.56
1:C:743:ILE:HD13	1:C:743:ILE:H	1.71	0.56
1:C:865:GLN:C	1:C:867:ARG:H	2.08	0.56
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.71	0.55
1:B:307:ARG:HB2	1:B:307:ARG:NH1	2.21	0.55
1:B:419:VAL:O	1:B:419:VAL:HG13	2.07	0.55
1:A:10:ILE:HG22	1:B:895:TRP:CD1	2.39	0.55
1:C:150:THR:H	1:C:153:ASP:HB2	1.70	0.55
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.41	0.55
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.88	0.55
1:A:843:LEU:HA	1:A:846:GLN:NE2	2.17	0.55
1:B:446:ALA:HB2	1:B:482:VAL:HB	1.88	0.55
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.70	0.55
1:B:705:GLU:O	1:B:706:ALA:HB3	2.06	0.55
1:C:81:ASN:C	1:C:81:ASN:ND2	2.56	0.55
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.88	0.55
1:A:57:VAL:HG12	1:A:82:SER:HB3	1.87	0.55
1:B:982:PHE:HE2	1:B:1007:VAL:O	1.90	0.55
1:B:453:PHE:HA	1:B:456:MET:SD	2.46	0.55
1:B:971:ARG:NH1	1:B:971:ARG:HG3	2.09	0.55
1:B:412:VAL:HG21	1:B:485:ALA:HB1	1.88	0.55
1:B:885:PHE:HD1	1:B:885:PHE:C	2.09	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:THR:O	1:C:493:CYS:HB3	2.07	0.55
1:B:251:LEU:HD13	1:B:262:LEU:H	1.71	0.55
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.87	0.55
1:C:731:ILE:HD13	1:C:746:ILE:HG21	1.89	0.55
1:A:3:ASN:O	1:A:6:ILE:HD11	2.07	0.55
1:B:419:VAL:CG1	1:B:419:VAL:O	2.55	0.55
1:B:326:PRO:O	1:B:630:SER:HB2	2.06	0.55
1:B:945:ILE:HD12	1:B:1022:VAL:HB	1.88	0.55
1:A:13:TRP:O	1:A:16:ALA:N	2.39	0.55
1:A:428:LYS:HA	1:A:494:ALA:HB1	1.89	0.55
1:A:746:ILE:HG22	1:A:747:ASN:N	2.22	0.55
1:A:948:PHE:HA	1:A:951:ASP:HB2	1.89	0.55
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.88	0.55
1:B:370:ILE:O	1:B:370:ILE:HG22	2.06	0.55
1:B:791:VAL:O	1:B:799:VAL:HG12	2.07	0.55
1:C:115:MET:HA	1:C:118:LEU:HD23	1.87	0.55
1:C:155:SER:HB3	1:C:180:SER:O	2.05	0.55
1:C:950:LYS:O	1:C:954:ASP:HB2	2.07	0.55
1:A:146:ASP:O	1:A:148:THR:N	2.40	0.55
1:A:282:ASN:HD21	1:A:609:VAL:H	1.53	0.55
1:A:370:ILE:O	1:A:374:VAL:HG23	2.06	0.55
1:A:578:LEU:HG	1:A:587:THR:HG23	1.88	0.55
1:A:591:LEU:HD11	1:A:613:ASN:HB3	1.89	0.55
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.89	0.55
1:B:537:SER:HA	1:B:540:ARG:HH21	1.71	0.55
1:C:644:VAL:O	1:C:648:THR:HG22	2.07	0.55
1:C:701:GLN:NE2	1:C:852:PRO:HD3	2.22	0.55
1:A:706:ALA:HB1	1:A:716:VAL:HG11	1.88	0.55
1:A:945:ILE:HG13	1:A:971:ARG:CG	2.33	0.55
1:B:193:LEU:HD13	1:B:198:LEU:O	2.06	0.55
1:B:452:VAL:O	1:B:453:PHE:CD2	2.60	0.55
1:B:492:LEU:O	1:B:496:MET:HB2	2.07	0.55
1:C:435:MET:HA	1:C:438:ILE:HG22	1.88	0.55
1:B:219:LEU:HD12	1:B:234:ILE:CG1	2.37	0.54
1:B:326:PRO:HG3	1:B:610:PHE:CD1	2.42	0.54
1:B:485:ALA:HA	1:B:489:THR:HB	1.88	0.54
1:C:759:VAL:HG23	1:C:771:VAL:O	2.07	0.54
1:A:317:PHE:CD2	1:A:317:PHE:N	2.74	0.54
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.37	0.54
1:C:545:TYR:OH	1:C:1021:PHE:HB3	2.08	0.54
1:C:213:GLN:HE22	1:C:238:THR:HA	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:VAL:HG11	1:C:746:ILE:CD1	2.36	0.54
1:C:721:LEU:CD2	1:C:813:SER:OG	2.51	0.54
1:A:426:PRO:CB	1:A:427:PRO:HD2	2.36	0.54
1:B:61:VAL:CG1	1:B:88:VAL:HG21	2.36	0.54
1:C:489:THR:O	1:C:493:CYS:CB	2.56	0.54
1:C:736:ALA:HB1	1:C:741:VAL:HB	1.89	0.54
1:B:730:ASP:O	1:B:805:SER:HA	2.08	0.54
1:B:58:GLN:HB3	1:B:82:SER:HB3	1.87	0.54
1:B:879:ILE:O	1:B:883:VAL:HG23	2.08	0.54
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.89	0.54
1:B:623:ASN:OD1	1:B:623:ASN:N	2.41	0.54
1:B:399:VAL:HG11	1:B:989:LEU:HD23	1.90	0.54
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.90	0.54
1:C:669:PRO:CB	1:C:672:VAL:HB	2.36	0.54
1:C:749:THR:O	1:C:753:ALA:CB	2.55	0.54
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.88	0.54
1:B:921:LEU:HD21	1:B:1001:ASN:O	2.08	0.54
1:B:57:VAL:C	1:B:60:THR:HG23	2.27	0.54
1:B:188:MET:H	1:B:775:SER:CA	2.20	0.54
1:C:115:MET:HA	1:C:115:MET:HE2	1.89	0.54
1:C:61:VAL:O	1:C:64:VAL:HG12	2.08	0.54
1:A:376:LEU:O	1:A:377:LEU:C	2.44	0.54
1:A:818:ARG:HA	1:A:824:SER:H	1.73	0.54
1:B:460:GLY:HA3	1:B:464:GLY:HA3	1.90	0.54
1:B:908:GLY:HA2	1:B:1013:THR:HG23	1.90	0.54
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.42	0.54
1:C:704:ALA:O	1:C:707:ALA:HB3	2.07	0.54
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.90	0.54
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.90	0.54
1:B:463:THR:HA	1:B:466:ILE:HG13	1.90	0.54
1:B:518:ARG:HG3	1:B:521:GLU:HB2	1.90	0.54
1:A:14:VAL:N	1:A:17:ILE:CG1	2.71	0.54
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.43	0.54
1:B:289:LEU:CD1	1:B:289:LEU:N	2.71	0.54
1:B:53:ASP:C	1:B:57:VAL:HG12	2.27	0.54
1:B:563:PHE:CD1	1:B:866:GLU:HG2	2.40	0.54
1:B:919:ARG:HG3	1:B:1005:THR:HG21	1.89	0.54
1:C:795:ASP:OD2	1:C:797:GLN:HB2	2.08	0.54
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.43	0.54
1:A:751:GLY:O	1:A:755:GLY:N	2.39	0.54
1:C:253:VAL:HG12	1:C:259:ARG:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:LEU:HD13	1:C:825:MET:HG3	1.90	0.54
1:C:894:SER:OG	1:C:895:TRP:N	2.40	0.54
1:A:268:ILE:CG2	1:A:269:GLU:N	2.71	0.53
1:A:317:PHE:HB3	1:A:321:LEU:HG	1.90	0.53
1:A:366:LEU:C	1:A:368:PRO:HD2	2.29	0.53
1:B:157:TYR:O	1:B:161:ASN:ND2	2.32	0.53
1:C:492:LEU:C	1:C:494:ALA:H	2.12	0.53
1:A:375:VAL:O	1:A:379:THR:HG23	2.07	0.53
1:B:538:THR:H	1:B:540:ARG:NH2	2.06	0.53
1:C:115:MET:HE3	1:C:127:VAL:HG11	1.90	0.53
1:C:1:MET:HB2	1:C:2:PRO:CD	2.37	0.53
1:C:36:PRO:HG3	1:C:469:GLN:HG3	1.90	0.53
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.90	0.53
1:A:649:MET:HA	1:A:653:ARG:NH1	2.24	0.53
1:A:70:ASN:OD1	1:A:70:ASN:N	2.41	0.53
1:A:781:MET:CE	1:C:225:VAL:HG22	2.38	0.53
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.90	0.53
1:C:146:ASP:HB3	1:C:148:THR:OG1	2.08	0.53
1:C:244:GLU:O	1:C:263:ARG:NH2	2.41	0.53
1:C:355:MET:HG2	1:C:368:PRO:HG2	1.89	0.53
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.43	0.53
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.23	0.53
1:B:709:HIS:N	1:B:710:PRO:CD	2.61	0.53
1:C:114:ALA:O	1:C:117:LEU:N	2.38	0.53
1:A:728:LYS:CD	1:C:235:ILE:HG22	2.39	0.53
1:C:571:VAL:HG12	1:C:630:SER:HA	1.91	0.53
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.24	0.53
1:B:613:ASN:C	1:B:613:ASN:HD22	2.11	0.53
1:B:681:ASP:CB	1:B:860:THR:HG23	2.38	0.53
1:A:243:THR:HB	1:A:268:ILE:CG2	2.36	0.53
1:A:590:VAL:HG11	1:A:661:ALA:HB1	1.91	0.53
1:A:282:ASN:ND2	1:A:609:VAL:H	2.06	0.53
1:B:762:PHE:CZ	1:B:764:ASP:HB2	2.44	0.53
1:C:420:MET:SD	1:C:498:LYS:HD3	2.49	0.53
1:C:683:GLU:HG3	1:C:819:TYR:CE2	2.44	0.53
1:C:829:GLY:O	1:C:830:GLN:CB	2.53	0.53
1:A:379:THR:HG21	1:A:477:ALA:HA	1.90	0.53
1:B:376:LEU:HD22	1:B:398:MET:HE3	1.90	0.53
1:B:555:LEU:HB2	1:B:913:LEU:HD23	1.91	0.53
1:C:197:GLN:HB3	1:C:792:ARG:HD3	1.91	0.53
1:C:707:ALA:O	1:C:710:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CG1	1:A:141:GLY:H	2.22	0.53
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.91	0.53
1:A:740:GLY:HA3	1:A:793:ALA:HB1	1.90	0.53
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.89	0.53
1:B:681:ASP:HB3	1:B:860:THR:HG22	1.89	0.53
1:C:30:LEU:HD22	1:C:390:ILE:H	1.74	0.53
1:B:228:GLN:O	1:C:583:THR:HG21	2.09	0.53
1:C:669:PRO:HB2	1:C:672:VAL:HG23	1.71	0.53
1:A:68:ASN:C	1:A:69:MET:HE3	2.27	0.53
1:B:348:ILE:HG23	1:B:372:VAL:HG21	1.91	0.53
1:B:332:PHE:HB2	1:B:569:GLN:O	2.08	0.53
1:B:984:LEU:HA	1:B:987:MET:HB2	1.91	0.53
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.91	0.53
1:A:623:ASN:C	1:A:623:ASN:ND2	2.51	0.53
1:A:685:ILE:CG2	1:A:686:ASP:N	2.72	0.53
1:B:346:GLU:HG2	1:B:346:GLU:O	2.08	0.53
1:B:776:GLU:HG2	1:B:777:ALA:H	1.74	0.53
1:B:778:LYS:NZ	1:B:778:LYS:HB3	2.24	0.53
1:B:57:VAL:CG2	1:B:82:SER:HB2	2.35	0.53
1:C:156:ASP:CG	1:C:182:TYR:CD2	2.83	0.53
1:C:690:LEU:HD23	1:C:694:LYS:CB	2.38	0.53
1:A:14:VAL:CG2	1:A:15:ILE:N	2.30	0.52
1:A:668:LEU:HD12	1:A:668:LEU:N	2.02	0.52
1:B:516:PHE:O	1:B:517:ASN:CB	2.55	0.52
1:A:11:PHE:HD1	1:B:890:ALA:HA	1.74	0.52
1:B:921:LEU:HD21	1:B:1002:ALA:HA	1.91	0.52
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.92	0.52
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.75	0.52
1:B:972:LEU:N	1:B:974:PRO:HD2	2.24	0.52
1:C:2:PRO:O	1:C:6:ILE:HG13	2.08	0.52
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.59	0.52
1:C:43:VAL:HG23	1:C:94:PHE:CE1	2.44	0.52
1:A:457:ALA:O	1:A:458:PHE:HD2	1.92	0.52
1:A:530:SER:HA	1:A:534:ILE:HD12	1.91	0.52
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.09	0.52
1:A:552:MET:HG3	1:A:909:VAL:HG11	1.92	0.52
1:C:1007:VAL:O	1:C:1011:MET:HB2	2.10	0.52
1:A:492:LEU:HG	1:A:496:MET:CE	2.38	0.52
1:A:44:THR:HA	1:A:90:ILE:O	2.10	0.52
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.92	0.52
1:C:897:ILE:N	1:C:898:PRO:HD2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HG12	1:A:368:PRO:HD3	1.88	0.52
1:B:601:LYS:HB2	1:B:601:LYS:HZ3	1.73	0.52
1:B:693:GLU:CG	1:B:694:LYS:H	2.22	0.52
1:B:694:LYS:HA	1:B:697:GLN:HE21	1.73	0.52
1:B:708:LYS:HZ3	1:B:708:LYS:HB2	1.75	0.52
1:B:190:PRO:HG3	1:B:789:TRP:CZ2	2.45	0.52
1:C:457:ALA:HB1	1:C:468:ARG:HA	1.92	0.52
1:C:777:ALA:O	1:C:781:MET:HE3	2.09	0.52
1:C:953:MET:CG	1:C:959:GLY:HA2	2.34	0.52
1:A:222:THR:HB	1:A:223:PRO:HD2	1.92	0.52
1:A:302:THR:HA	1:A:305:ALA:HB3	1.91	0.52
1:A:498:LYS:HG2	1:A:498:LYS:O	2.09	0.52
1:A:638:PRO:HD2	1:A:642:ASN:ND2	2.23	0.52
1:B:144:ASN:HD21	1:B:148:THR:H	1.57	0.52
1:B:375:VAL:HG13	1:B:480:LEU:HB3	1.92	0.52
1:A:965:LEU:O	1:A:969:ARG:HB2	2.09	0.52
1:B:307:ARG:CB	1:B:307:ARG:HH11	2.23	0.52
1:B:754:TRP:CZ2	1:B:786:ILE:HD13	2.44	0.52
1:B:758:TYR:CE1	1:B:770:LYS:HG3	2.45	0.52
1:C:990:VAL:HG13	1:C:1005:THR:HG22	1.92	0.52
1:A:74:ASN:H	1:C:170:SER:HB2	1.73	0.52
1:C:356:TYR:O	1:C:360:GLN:HG2	2.10	0.52
1:A:1015:THR:O	1:A:1017:LEU:N	2.37	0.52
1:A:442:LEU:C	1:A:444:GLY:H	2.12	0.52
1:B:185:ARG:HH12	1:B:774:MET:HG3	1.74	0.52
1:B:231:ASN:ND2	1:B:232:ALA:N	2.57	0.52
1:B:58:GLN:CB	1:B:82:SER:CB	2.86	0.52
1:B:901:VAL:HG22	1:B:1026:PHE:HZ	1.75	0.52
1:C:355:MET:HG3	1:C:359:LEU:HD23	1.90	0.52
1:C:777:ALA:O	1:C:781:MET:HE2	2.10	0.52
1:A:268:ILE:O	1:A:269:GLU:CB	2.58	0.52
1:A:583:THR:HG22	1:A:585:GLU:N	2.24	0.52
1:B:330:THR:N	1:B:331:PRO:CD	2.73	0.52
1:B:226:LYS:CE	1:B:226:LYS:CA	2.66	0.52
1:B:468:ARG:O	1:B:469:GLN:C	2.48	0.52
1:C:1018:ALA:HA	1:C:1021:PHE:HB2	1.92	0.52
1:B:763:ILE:HG12	1:C:59:ASP:OD1	2.10	0.52
1:C:841:MET:CE	1:C:866:GLU:HG3	2.40	0.52
1:A:685:ILE:HG22	1:A:686:ASP:N	2.25	0.51
1:A:740:GLY:O	1:A:794:ALA:N	2.43	0.51
1:B:349:ILE:HG22	1:B:350:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:LEU:HB2	1:B:898:PRO:HG3	1.91	0.51
1:C:595:THR:CG2	1:C:611:ALA:HB2	2.40	0.51
1:C:670:ALA:O	1:C:672:VAL:N	2.42	0.51
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.92	0.51
1:B:150:THR:H	1:B:153:ASP:CB	2.22	0.51
1:B:314:GLU:N	1:B:315:PRO:CD	2.74	0.51
1:B:474:ILE:HG22	1:B:475:VAL:N	2.25	0.51
1:B:859:TRP:HB3	1:B:863:SER:CB	2.40	0.51
1:B:900:SER:HB3	1:B:1029:VAL:HG11	1.92	0.51
1:A:183:ALA:HB2	1:A:273:GLU:HG2	1.91	0.51
1:A:456:MET:HA	1:A:459:PHE:CE1	2.46	0.51
1:B:216:ALA:O	1:B:217:GLY:O	2.27	0.51
1:B:58:GLN:HB3	1:B:82:SER:CB	2.40	0.51
1:C:672:VAL:C	1:C:674:LEU:N	2.64	0.51
1:C:749:THR:O	1:C:753:ALA:HB3	2.10	0.51
1:A:133:SER:O	1:A:135:SER:N	2.43	0.51
1:A:199:THR:HG22	1:A:791:VAL:HA	1.93	0.51
1:A:380:PHE:HE1	1:A:398:MET:SD	2.33	0.51
1:B:517:ASN:H	1:B:519:MET:HG2	1.76	0.51
1:B:973:ARG:CG	1:B:974:PRO:HD3	2.41	0.51
1:C:331:PRO:O	1:C:335:ILE:HG12	2.10	0.51
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	2.99	0.51
1:B:330:THR:N	1:B:331:PRO:HD2	2.26	0.51
1:B:924:ASP:HB3	1:B:926:TYR:H	1.75	0.51
1:A:721:LEU:HD23	1:A:721:LEU:N	2.25	0.51
1:A:841:MET:HE1	1:A:866:GLU:HG3	1.92	0.51
1:B:271:GLY:HA3	1:B:275:TYR:OH	2.10	0.51
1:B:413:VAL:O	1:B:417:GLU:HB2	2.10	0.51
1:B:681:ASP:CB	1:B:860:THR:CG2	2.86	0.51
1:C:247:GLY:HA3	1:C:263:ARG:NE	2.25	0.51
1:C:576:VAL:O	1:C:577:GLN:C	2.48	0.51
1:A:117:LEU:HD12	1:A:117:LEU:N	2.26	0.51
1:A:167:SER:HA	1:A:175:VAL:HG21	1.93	0.51
1:B:1035:ARG:HG3	1:B:1036:LYS:N	2.25	0.51
1:B:326:PRO:HB3	1:B:610:PHE:HB2	1.93	0.51
1:B:356:TYR:O	1:B:358:PHE:N	2.44	0.51
1:B:68:ASN:ND2	1:B:114:ALA:HB2	2.26	0.51
1:B:701:GLN:CB	1:B:851:LEU:HD22	2.41	0.51
1:C:252:LYS:HG2	1:C:260:VAL:CG1	2.40	0.51
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.45	0.51
1:C:655:PHE:C	1:C:657:GLN:N	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASN:C	1:A:193:LEU:N	2.63	0.51
1:A:268:ILE:CG2	1:A:269:GLU:H	2.24	0.51
1:B:282:ASN:C	1:B:284:GLN:H	2.14	0.51
1:B:428:LYS:HA	1:B:494:ALA:HB1	1.93	0.51
1:B:924:ASP:O	1:B:928:GLN:HG3	2.11	0.51
1:C:115:MET:HE2	1:C:118:LEU:HD23	1.91	0.51
1:C:137:LEU:CD1	1:C:293:LEU:HD13	2.41	0.51
1:A:166:ILE:O	1:A:172:VAL:HG21	2.10	0.51
1:A:15:ILE:HG22	1:A:16:ALA:N	2.26	0.51
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.92	0.51
1:A:431:THR:CB	1:A:494:ALA:HB2	2.41	0.51
1:B:291:ILE:HG21	1:B:306:ILE:HD12	1.91	0.51
1:C:352:PHE:HD1	1:C:365:THR:HG22	1.76	0.51
1:C:713:LEU:O	1:C:713:LEU:HD22	2.11	0.51
1:C:58:GLN:HE21	1:C:816:LEU:HB3	1.76	0.51
1:A:727:PHE:HE2	1:A:786:ILE:HG13	1.76	0.51
1:B:489:THR:N	1:B:490:PRO:HD2	2.26	0.51
1:B:58:GLN:CG	1:B:59:ASP:N	2.72	0.51
1:A:12:ALA:O	1:A:14:VAL:HG23	2.09	0.50
1:A:151:GLN:HB3	1:A:152:GLU:OE2	2.11	0.50
1:A:227:GLY:HA2	1:B:585:GLU:OE1	2.11	0.50
1:B:399:VAL:O	1:B:402:ILE:HG22	2.11	0.50
1:B:492:LEU:O	1:B:496:MET:N	2.41	0.50
1:B:602:GLU:C	1:B:604:ASN:H	2.14	0.50
1:B:973:ARG:HG2	1:B:974:PRO:HD3	1.93	0.50
1:C:533:GLY:C	1:C:535:LEU:H	2.13	0.50
1:C:721:LEU:CG	1:C:815:ARG:O	2.55	0.50
1:A:426:PRO:CB	1:A:427:PRO:CD	2.90	0.50
1:B:517:ASN:C	1:B:519:MET:H	2.14	0.50
1:C:989:LEU:HD22	1:C:1000:GLN:HB3	1.93	0.50
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.93	0.50
1:C:753:ALA:O	1:C:775:SER:CB	2.59	0.50
1:C:727:PHE:CE2	1:C:807:SER:CB	2.94	0.50
1:C:841:MET:HE3	1:C:866:GLU:HG3	1.93	0.50
1:C:885:PHE:HE2	1:C:899:PHE:CE1	2.29	0.50
1:A:658:ILE:HG22	1:A:659:LYS:HD3	1.93	0.50
1:B:652:THR:O	1:B:656:SER:HB3	2.11	0.50
1:C:137:LEU:HD13	1:C:293:LEU:HB2	1.93	0.50
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.92	0.50
1:C:363:ARG:C	1:C:365:THR:H	2.14	0.50
1:C:38:ILE:N	1:C:38:ILE:CD1	2.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:HD22	1:C:496:MET:SD	2.51	0.50
1:C:61:VAL:HB	1:C:88:VAL:HG21	1.93	0.50
1:A:171:GLY:O	1:A:294:ALA:CB	2.55	0.50
1:B:39:ALA:HB1	1:B:40:PRO:HD2	1.92	0.50
1:B:469:GLN:O	1:B:472:ILE:HG22	2.12	0.50
1:C:576:VAL:H	1:C:577:GLN:NE2	2.09	0.50
1:C:945:ILE:HD13	1:C:1022:VAL:CG1	2.38	0.50
1:A:456:MET:O	1:A:458:PHE:N	2.44	0.50
1:A:476:SER:O	1:A:480:LEU:HB2	2.10	0.50
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.93	0.50
1:A:65:ILE:O	1:A:65:ILE:HG22	2.11	0.50
1:A:776:GLU:O	1:A:780:ARG:HG2	2.12	0.50
1:A:14:VAL:O	1:A:15:ILE:O	2.30	0.50
1:A:575:MET:SD	1:A:626:ILE:HG13	2.52	0.50
1:B:144:ASN:OD1	1:B:145:THR:O	2.30	0.50
1:C:578:LEU:CB	1:C:579:PRO:HD2	2.36	0.50
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.92	0.50
1:A:15:ILE:O	1:A:16:ALA:O	2.30	0.50
1:A:469:GLN:O	1:A:473:THR:OG1	2.29	0.50
1:A:636:ASP:OD2	1:A:636:ASP:N	2.45	0.50
1:B:123:GLN:C	1:B:125:GLN:H	2.13	0.50
1:A:10:ILE:O	1:A:11:PHE:O	2.30	0.50
1:A:354:VAL:O	1:A:355:MET:CB	2.59	0.50
1:A:584:GLN:N	1:A:622:GLN:HG2	2.26	0.50
1:B:254:ASN:ND2	1:B:255:GLN:H	2.10	0.50
1:B:399:VAL:HG11	1:B:989:LEU:CD2	2.42	0.50
1:B:539:GLY:C	1:B:541:TYR:H	2.14	0.50
1:B:58:GLN:O	1:B:59:ASP:OD2	2.30	0.50
1:C:831:ALA:HB2	1:C:840:ALA:CB	2.41	0.50
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.93	0.50
1:A:684:LEU:HB2	1:A:827:ILE:HD11	1.92	0.50
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.92	0.50
1:C:354:VAL:HG12	1:C:354:VAL:O	2.10	0.50
1:C:722:GLU:HA	1:C:722:GLU:OE1	2.12	0.50
1:C:417:GLU:HB2	1:C:973:ARG:HH12	1.77	0.50
1:A:11:PHE:O	1:A:12:ALA:O	2.30	0.49
1:A:782:LEU:O	1:A:785:ASP:HB2	2.11	0.49
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.92	0.49
1:A:418:ARG:HG2	1:A:970:MET:SD	2.52	0.49
1:B:517:ASN:O	1:B:519:MET:N	2.45	0.49
1:B:915:ALA:O	1:B:917:THR:N	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:CD1	1:A:7:ASP:OD1	2.60	0.49
1:A:702:LEU:HD11	1:A:844:MET:CE	2.42	0.49
1:A:8:ARG:O	1:A:10:ILE:N	2.44	0.49
1:B:20:MET:CG	1:B:374:VAL:HA	2.41	0.49
1:B:973:ARG:N	1:B:974:PRO:HD2	2.28	0.49
1:C:353:LEU:O	1:C:356:TYR:HB2	2.12	0.49
1:A:13:TRP:O	1:A:14:VAL:O	2.30	0.49
1:A:64:VAL:C	1:A:66:GLU:H	2.16	0.49
1:A:832:ALA:O	1:A:833:PRO:C	2.50	0.49
1:B:146:ASP:O	1:B:147:GLY:C	2.49	0.49
1:B:231:ASN:HD22	1:B:232:ALA:N	2.09	0.49
1:B:439:GLN:HA	1:B:442:LEU:HD12	1.95	0.49
1:B:518:ARG:CG	1:B:521:GLU:HB2	2.43	0.49
1:B:556:PHE:O	1:B:556:PHE:HD2	1.95	0.49
1:B:743:ILE:H	1:B:743:ILE:CD1	2.15	0.49
1:A:74:ASN:H	1:C:170:SER:CB	2.25	0.49
1:C:448:VAL:O	1:C:452:VAL:HG23	2.12	0.49
1:A:144:ASN:HB2	1:A:149:MET:HE3	1.94	0.49
1:A:254:ASN:N	1:A:258:SER:OG	2.45	0.49
1:A:437:GLN:HB3	1:A:948:PHE:CE2	2.42	0.49
1:A:550:VAL:O	1:A:550:VAL:HG12	2.13	0.49
1:A:902:MET:O	1:A:905:VAL:HG23	2.12	0.49
1:B:598:TYR:CD1	1:B:606:VAL:HG21	2.48	0.49
1:C:199:THR:OG1	1:C:201:VAL:HB	2.12	0.49
1:C:935:ILE:CG2	1:C:935:ILE:O	2.59	0.49
1:A:170:SER:OG	1:A:170:SER:O	2.26	0.49
1:A:775:SER:HB2	1:A:789:TRP:HZ2	1.77	0.49
1:B:201:VAL:O	1:B:202:ASP:C	2.50	0.49
1:C:409:ALA:O	1:C:413:VAL:HG12	2.12	0.49
1:C:695:LEU:HD13	1:C:825:MET:CG	2.43	0.49
1:C:831:ALA:HB3	1:C:837:THR:HG22	1.94	0.49
1:A:99:ASP:OD1	1:A:99:ASP:C	2.50	0.49
1:B:1005:THR:HG22	1:B:1005:THR:O	2.13	0.49
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.95	0.49
1:B:669:PRO:HG3	1:B:678:THR:HA	1.94	0.49
1:B:947:GLU:CA	1:B:947:GLU:OE1	2.60	0.49
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.43	0.49
1:C:693:GLU:O	1:C:694:LYS:C	2.51	0.49
1:A:294:ALA:O	1:A:295:THR:HB	2.13	0.49
1:A:481:SER:O	1:A:484:VAL:N	2.46	0.49
1:A:686:ASP:CB	1:A:823:PRO:HG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HD13	1:A:7:ASP:OD1	2.13	0.49
1:B:418:ARG:HH11	1:B:418:ARG:HB3	1.76	0.49
1:A:338:HIS:CD2	1:A:342:LYS:HE2	2.48	0.49
1:B:136:PHE:CE1	1:B:617:PHE:CZ	3.00	0.49
1:B:427:PRO:O	1:B:430:ALA:HB3	2.12	0.49
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.95	0.49
1:C:1028:VAL:HG13	1:C:1032:ARG:HH22	1.77	0.49
1:C:265:VAL:O	1:C:266:ALA:HB2	2.13	0.49
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.94	0.49
1:C:3:ASN:C	1:C:5:PHE:H	2.16	0.49
1:C:674:LEU:HD12	1:C:862:MET:HA	1.94	0.49
1:A:325:TYR:O	1:A:327:TYR:N	2.46	0.49
1:A:379:THR:CG2	1:A:477:ALA:HA	2.42	0.49
1:B:200:PRO:CD	1:B:749:THR:HG22	2.42	0.49
1:C:108:GLN:HG2	1:C:129:VAL:HG21	1.95	0.49
1:C:835:LYS:HD2	1:C:839:GLU:HG3	1.94	0.49
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.37	0.49
1:C:934:THR:HG22	1:C:1011:MET:SD	2.53	0.49
1:A:211:ASN:HA	1:A:240:LEU:HD13	1.95	0.49
1:A:682:PHE:CZ	1:A:857:TYR:CB	2.96	0.49
1:A:685:ILE:HG21	1:A:822:LEU:CD1	2.43	0.49
1:A:963:ALA:O	1:A:967:ALA:N	2.44	0.49
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.94	0.49
1:C:146:ASP:HB2	1:C:320:GLY:HA3	1.95	0.49
1:A:364:ALA:O	1:A:367:ILE:HG12	2.13	0.48
1:A:682:PHE:HD2	1:A:827:ILE:HG13	1.78	0.48
1:B:231:ASN:ND2	1:B:231:ASN:C	2.65	0.48
1:B:282:ASN:O	1:B:284:GLN:N	2.46	0.48
1:B:792:ARG:HH11	1:B:792:ARG:CB	2.24	0.48
1:C:218:GLN:HA	1:C:234:ILE:HG13	1.94	0.48
1:C:58:GLN:HA	1:C:62:THR:HB	1.94	0.48
1:C:721:LEU:HD13	1:C:825:MET:CE	2.43	0.48
1:A:451:ALA:O	1:A:453:PHE:N	2.46	0.48
1:A:6:ILE:HD12	1:A:7:ASP:CB	2.43	0.48
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.94	0.48
1:C:527:TYR:HE2	1:C:968:VAL:O	1.96	0.48
1:A:107:VAL:HG12	1:A:108:GLN:N	2.28	0.48
1:B:1016:VAL:HG12	1:B:1017:LEU:N	2.28	0.48
1:B:698:ALA:CB	1:B:855:VAL:HG21	2.42	0.48
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.95	0.48
1:A:211:ASN:CG	1:A:211:ASN:O	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:688:ALA:C	1:A:690:LEU:N	2.67	0.48
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.40	0.48
1:B:201:VAL:O	1:B:203:VAL:N	2.47	0.48
1:B:264:ASP:O	1:B:265:VAL:HB	2.14	0.48
1:B:762:PHE:CD2	1:B:771:VAL:HG22	2.44	0.48
1:C:488:LEU:HG	1:C:492:LEU:HD12	1.95	0.48
1:C:633:ASP:O	1:C:633:ASP:CG	2.52	0.48
1:C:43:VAL:HG23	1:C:94:PHE:HE1	1.79	0.48
1:A:3:ASN:O	1:A:6:ILE:CD1	2.61	0.48
1:A:552:MET:HG3	1:A:909:VAL:CG1	2.44	0.48
1:C:946:VAL:O	1:C:946:VAL:HG12	2.14	0.48
1:A:191:ASN:O	1:A:193:LEU:N	2.47	0.48
1:A:364:ALA:O	1:A:367:ILE:HG23	2.13	0.48
1:A:445:ILE:HG13	1:A:446:ALA:N	2.28	0.48
1:B:373:PRO:O	1:B:377:LEU:HG	2.14	0.48
1:B:423:GLU:HG3	1:B:426:PRO:HB3	1.96	0.48
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.43	0.48
1:B:765:ARG:HG3	1:B:765:ARG:HH21	1.79	0.48
1:C:445:ILE:HG13	1:C:446:ALA:N	2.29	0.48
1:C:879:ILE:O	1:C:883:VAL:HG23	2.13	0.48
1:C:898:PRO:O	1:C:900:SER:N	2.46	0.48
1:A:364:ALA:CB	1:A:497:LEU:CD2	2.89	0.48
1:A:68:ASN:C	1:A:69:MET:CE	2.80	0.48
1:A:418:ARG:CD	1:A:970:MET:HG3	2.44	0.48
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.14	0.48
1:B:115:MET:HE2	1:B:118:LEU:CD2	2.37	0.48
1:B:193:LEU:HD11	1:B:198:LEU:O	2.14	0.48
1:B:692:HIS:ND1	1:B:692:HIS:O	2.46	0.48
1:B:873:ALA:C	1:B:875:SER:H	2.17	0.48
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.42	0.48
1:A:187:TRP:HA	1:A:774:MET:O	2.13	0.48
1:A:966:ASP:HA	1:A:969:ARG:HB2	1.96	0.48
1:A:987:MET:O	1:A:988:PRO:O	2.32	0.48
1:B:681:ASP:HB3	1:B:860:THR:HG23	1.94	0.48
1:B:770:LYS:HB3	1:B:772:TYR:CE2	2.48	0.48
1:B:989:LEU:HD11	1:B:1003:VAL:HG13	1.95	0.48
1:C:394:THR:HG22	1:C:395:MET:HE2	1.95	0.48
1:C:524:THR:HA	1:C:527:TYR:HB3	1.95	0.48
1:A:896:SER:C	1:A:898:PRO:HD2	2.35	0.48
1:A:923:ASN:HD22	1:A:923:ASN:C	2.17	0.48
1:B:111:LEU:HD21	1:B:127:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:VAL:HG13	1:B:262:LEU:HD21	1.96	0.48
1:B:226:LYS:HE2	1:B:226:LYS:HA	1.87	0.48
1:B:190:PRO:HG3	1:B:789:TRP:CE2	2.48	0.48
1:B:898:PRO:O	1:B:900:SER:N	2.47	0.48
1:C:549:VAL:O	1:C:549:VAL:HG12	2.13	0.48
1:C:805:SER:O	1:C:806:SER:HB3	2.13	0.48
1:C:997:SER:O	1:C:999:ALA:N	2.47	0.48
1:A:376:LEU:C	1:A:378:GLY:N	2.67	0.48
1:A:56:THR:O	1:A:60:THR:HB	2.14	0.48
1:A:727:PHE:CE1	1:A:807:SER:HB3	2.49	0.48
1:B:764:ASP:HB3	1:B:769:LYS:HE3	1.95	0.48
1:B:785:ASP:O	1:B:786:ILE:C	2.51	0.48
1:C:754:TRP:CE3	1:C:780:ARG:HB2	2.49	0.48
1:C:681:ASP:OD2	1:C:826:GLU:OE2	2.32	0.48
1:A:139:VAL:HG13	1:A:327:TYR:HB3	1.93	0.47
1:A:400:LEU:HG	1:A:929:VAL:HG12	1.96	0.47
1:B:10:ILE:HD13	1:C:893:GLU:O	2.13	0.47
1:B:142:VAL:N	1:B:287:SER:O	2.43	0.47
1:B:338:HIS:C	1:B:340:VAL:H	2.17	0.47
1:B:696:THR:HG22	1:B:699:ARG:HH12	1.79	0.47
1:B:696:THR:HG22	1:B:699:ARG:NH1	2.29	0.47
1:B:732:ASP:O	1:B:734:GLU:HG2	2.14	0.47
1:C:552:MET:HB3	1:C:910:ILE:HG12	1.95	0.47
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.44	0.47
1:C:727:PHE:CE2	1:C:807:SER:HB2	2.49	0.47
1:C:898:PRO:C	1:C:900:SER:H	2.16	0.47
1:A:426:PRO:HB3	1:A:427:PRO:HD2	1.96	0.47
1:B:355:MET:CE	1:B:368:PRO:HB2	2.44	0.47
1:B:80:SER:HB2	1:B:90:ILE:HG23	1.96	0.47
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.14	0.47
1:C:251:LEU:HB2	1:C:260:VAL:O	2.14	0.47
1:C:183:ALA:N	1:C:271:GLY:O	2.43	0.47
1:C:943:ILE:O	1:C:947:GLU:HB2	2.14	0.47
1:C:983:ILE:HG23	1:C:1008:MET:HG3	1.96	0.47
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.39	0.47
1:A:268:ILE:HG22	1:A:269:GLU:H	1.74	0.47
1:A:385:ALA:C	1:A:386:PHE:HD1	2.17	0.47
1:B:140:VAL:O	1:B:140:VAL:HG23	2.14	0.47
1:A:686:ASP:O	1:A:687:GLN:CB	2.58	0.47
1:B:242:SER:O	1:B:244:GLU:N	2.47	0.47
1:B:307:ARG:HA	1:B:310:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:O	1:B:453:PHE:CB	2.62	0.47
1:B:455:PRO:HG3	1:B:880:SER:HA	1.94	0.47
1:B:596:HIS:O	1:B:597:TYR:C	2.53	0.47
1:B:633:ASP:CG	1:B:634:TRP:N	2.67	0.47
1:B:753:ALA:HA	1:B:774:MET:O	2.14	0.47
1:B:900:SER:CB	1:B:1029:VAL:HG11	2.45	0.47
1:C:211:ASN:ND2	1:C:240:LEU:H	2.12	0.47
1:A:583:THR:HG23	1:A:622:GLN:HE21	1.78	0.47
1:A:84:SER:HB2	1:A:814:PRO:HA	1.96	0.47
1:B:185:ARG:NH1	1:B:185:ARG:CG	2.74	0.47
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.49	0.47
1:C:801:PHE:CD1	1:C:804:PHE:CE1	2.99	0.47
1:A:917:THR:O	1:A:919:ARG:N	2.48	0.47
1:B:178:PHE:CD2	1:B:288:GLY:O	2.67	0.47
1:B:485:ALA:HA	1:B:489:THR:CB	2.44	0.47
1:B:692:HIS:HE1	1:B:723:ASP:OD1	1.98	0.47
1:C:997:SER:HA	1:C:1000:GLN:OE1	2.14	0.47
1:C:309:GLU:HG3	1:C:313:MET:CE	2.45	0.47
1:A:274:ASN:ND2	1:A:276:ASP:OD2	2.46	0.47
1:A:356:TYR:C	1:A:358:PHE:H	2.18	0.47
1:A:391:ASN:O	1:A:393:LEU:N	2.48	0.47
1:A:756:GLY:HA2	1:A:774:MET:HG3	1.96	0.47
1:A:987:MET:N	1:A:988:PRO:CD	2.78	0.47
1:B:946:VAL:HG11	1:B:1026:PHE:CE1	2.50	0.47
1:B:137:LEU:HD23	1:B:138:MET:HB2	1.96	0.47
1:B:185:ARG:HG2	1:B:187:TRP:CZ2	2.49	0.47
1:C:601:LYS:C	1:C:603:LYS:H	2.17	0.47
1:C:670:ALA:O	1:C:671:ILE:C	2.53	0.47
1:C:966:ASP:HA	1:C:969:ARG:HB3	1.97	0.47
1:A:219:LEU:HD12	1:A:232:ALA:HB3	1.96	0.47
1:B:701:GLN:HB3	1:B:851:LEU:HD22	1.96	0.47
1:C:240:LEU:HD23	1:C:240:LEU:N	2.30	0.47
1:C:949:ALA:HB1	1:C:1026:PHE:CZ	2.50	0.47
1:A:295:THR:HG22	1:A:295:THR:O	2.15	0.47
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.50	0.47
1:C:38:ILE:HD13	1:C:39:ALA:H	1.80	0.47
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.95	0.47
1:A:740:GLY:HA3	1:A:794:ALA:H	1.80	0.47
1:A:947:GLU:O	1:A:951:ASP:N	2.46	0.47
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.35	0.47
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:THR:C	1:C:368:PRO:HD2	2.35	0.47
1:C:489:THR:OG1	1:C:490:PRO:HD3	2.15	0.47
1:C:596:HIS:O	1:C:600:THR:HG23	2.15	0.47
1:A:819:TYR:H	1:A:824:SER:HB3	1.80	0.47
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.45	0.47
1:B:58:GLN:O	1:B:59:ASP:CG	2.53	0.47
1:C:240:LEU:CD1	1:C:249:ILE:HD11	2.44	0.47
1:A:207:ILE:CG2	1:A:759:VAL:HG11	2.45	0.46
1:A:917:THR:C	1:A:919:ARG:H	2.19	0.46
1:A:997:SER:OG	1:A:998:GLY:N	2.48	0.46
1:B:641:GLU:HB3	1:B:650:ARG:NH1	2.30	0.46
1:B:782:LEU:HD23	1:B:783:PRO:HD2	1.98	0.46
1:C:190:PRO:HB3	1:C:789:TRP:CD2	2.49	0.46
1:C:754:TRP:CZ3	1:C:780:ARG:CA	2.97	0.46
1:A:15:ILE:O	1:A:18:ILE:N	2.48	0.46
1:A:367:ILE:HD11	1:A:413:VAL:HB	1.97	0.46
1:A:367:ILE:HG22	1:A:496:MET:HE1	1.97	0.46
1:A:781:MET:HE2	1:C:225:VAL:N	2.23	0.46
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.30	0.46
1:B:1017:LEU:O	1:B:1021:PHE:HB2	2.15	0.46
1:B:34:GLN:HE21	1:B:332:PHE:HE2	1.62	0.46
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.97	0.46
1:C:144:ASN:HB2	1:C:154:ILE:HD11	1.97	0.46
1:C:250:LEU:HD13	1:C:259:ARG:NH1	2.31	0.46
1:A:583:THR:HA	1:A:622:GLN:HG2	1.98	0.46
1:B:538:THR:N	1:B:540:ARG:NH2	2.64	0.46
1:C:352:PHE:CD1	1:C:365:THR:HG22	2.50	0.46
1:C:351:VAL:HG12	1:C:369:THR:HG23	1.97	0.46
1:A:324:VAL:HG12	1:A:325:TYR:H	1.80	0.46
1:A:324:VAL:HG12	1:A:325:TYR:N	2.31	0.46
1:A:344:LEU:HD22	1:A:376:LEU:HD11	1.97	0.46
1:A:634:TRP:N	1:A:634:TRP:CD1	2.79	0.46
1:A:6:ILE:HD13	1:A:7:ASP:CG	2.32	0.46
1:B:238:THR:CG2	1:B:239:ARG:N	2.78	0.46
1:B:417:GLU:O	1:B:973:ARG:NH1	2.48	0.46
1:A:10:ILE:HD13	1:B:893:GLU:C	2.36	0.46
1:C:732:ASP:HB3	1:C:735:LYS:HB2	1.98	0.46
1:C:187:TRP:HZ3	1:C:774:MET:HB3	1.76	0.46
1:C:908:GLY:HA2	1:C:1013:THR:HG23	1.97	0.46
1:A:102:ILE:HA	1:A:105:VAL:CG2	2.43	0.46
1:A:369:THR:O	1:A:373:PRO:HD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:OD2	1:A:978:THR:HG21	2.15	0.46
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.97	0.46
1:B:181:GLN:HB3	1:B:181:GLN:HE21	1.51	0.46
1:C:379:THR:HB	1:C:398:MET:CE	2.45	0.46
1:C:633:ASP:O	1:C:634:TRP:HB2	2.16	0.46
1:C:685:ILE:HD11	1:C:687:GLN:OE1	2.15	0.46
1:C:778:LYS:HB2	1:C:779:TYR:CD2	2.51	0.46
1:C:58:GLN:HE21	1:C:816:LEU:CB	2.28	0.46
1:A:457:ALA:HB2	1:A:471:SER:HB3	1.98	0.46
1:A:498:LYS:C	1:A:498:LYS:HE2	2.35	0.46
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.97	0.46
1:B:199:THR:N	1:B:202:ASP:OD2	2.37	0.46
1:B:438:ILE:HD11	1:B:971:ARG:HH12	1.81	0.46
1:B:671:ILE:O	1:B:673:GLU:N	2.49	0.46
1:B:81:ASN:O	1:B:81:ASN:ND2	2.47	0.46
1:C:30:LEU:HA	1:C:31:PRO:HD3	1.79	0.46
1:C:314:GLU:HA	1:C:317:PHE:CE1	2.50	0.46
1:C:674:LEU:O	1:C:865:GLN:NE2	2.37	0.46
1:A:1033:PHE:O	1:A:1034:SER:CB	2.63	0.46
1:B:348:ILE:CG2	1:B:372:VAL:HG21	2.45	0.46
1:C:229:GLN:HG2	1:C:229:GLN:H	1.60	0.46
1:C:422:GLU:OE1	1:C:433:LYS:HE2	2.16	0.46
1:C:696:THR:HG22	1:C:699:ARG:NH1	2.30	0.46
1:C:782:LEU:HB2	1:C:784:ASP:OD2	2.16	0.46
1:A:960:LEU:HD22	1:A:1031:ARG:HH21	1.81	0.46
1:A:326:PRO:HG3	1:A:610:PHE:HD1	1.80	0.46
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.45	0.46
1:A:583:THR:HG22	1:A:585:GLU:H	1.81	0.46
1:A:126:GLY:HA3	1:B:116:PRO:CB	2.44	0.46
1:B:193:LEU:HD23	1:B:265:VAL:CG2	2.45	0.46
1:C:70:ASN:O	1:C:72:ILE:HG13	2.16	0.46
1:A:1013:THR:O	1:A:1017:LEU:HB3	2.15	0.46
1:A:597:TYR:HE2	1:A:654:ALA:HB1	1.81	0.46
1:A:965:LEU:HB3	1:A:969:ARG:HH11	1.81	0.46
1:B:715:SER:O	1:B:829:GLY:HA2	2.16	0.46
1:B:706:ALA:HB2	1:B:847:LEU:HD12	1.97	0.46
1:B:402:ILE:HA	1:B:402:ILE:HD12	1.83	0.46
1:B:932:LEU:HA	1:B:935:ILE:HD12	1.98	0.46
1:B:973:ARG:N	1:B:974:PRO:CD	2.78	0.46
1:C:57:VAL:HG21	1:C:86:GLY:CA	2.41	0.46
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:703:LEU:O	1:B:707:ALA:HB2	2.16	0.45
1:B:453:PHE:HZ	1:B:933:THR:HG23	1.80	0.45
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.15	0.45
1:C:568:ASP:OD2	1:C:644:VAL:HG23	2.17	0.45
1:C:633:ASP:O	1:C:635:ALA:N	2.44	0.45
1:C:738:ALA:C	1:C:740:GLY:H	2.19	0.45
1:C:979:SER:O	1:C:983:ILE:HG13	2.16	0.45
1:A:140:VAL:CG1	1:A:141:GLY:N	2.77	0.45
1:A:64:VAL:C	1:A:66:GLU:N	2.70	0.45
1:B:371:ALA:HA	1:B:374:VAL:CG1	2.46	0.45
1:B:463:THR:O	1:B:465:ALA:N	2.46	0.45
1:B:605:ASN:O	1:B:632:LYS:HG2	2.16	0.45
1:B:699:ARG:HA	1:B:702:LEU:HB2	1.98	0.45
1:B:763:ILE:HD11	1:C:59:ASP:HB3	1.98	0.45
1:C:84:SER:C	1:C:86:GLY:H	2.18	0.45
1:C:914:LEU:O	1:C:915:ALA:CB	2.64	0.45
1:C:945:ILE:HG13	1:C:971:ARG:HG3	1.96	0.45
1:A:83:ASP:HA	1:A:815:ARG:HA	1.97	0.45
1:B:938:SER:HB3	1:B:1014:ALA:HB1	1.97	0.45
1:B:445:ILE:HG12	1:B:940:LYS:HG3	1.99	0.45
1:B:57:VAL:O	1:B:61:VAL:HG12	2.17	0.45
1:B:699:ARG:HG2	1:B:700:ASN:N	2.30	0.45
1:C:253:VAL:CG1	1:C:259:ARG:HB3	2.47	0.45
1:C:254:ASN:OD1	1:C:258:SER:O	2.34	0.45
1:C:727:PHE:HD1	1:C:809:TRP:CE2	2.35	0.45
1:C:837:THR:O	1:C:841:MET:HG3	2.17	0.45
1:A:159:ALA:HB2	1:A:177:LEU:HD21	1.99	0.45
1:A:175:VAL:HG13	1:A:289:LEU:HD21	1.99	0.45
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.98	0.45
1:A:69:MET:O	1:C:168:ARG:CD	2.65	0.45
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.16	0.45
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.79	0.45
1:C:154:ILE:O	1:C:155:SER:C	2.55	0.45
1:C:254:ASN:O	1:C:256:ASP:N	2.50	0.45
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.41	0.45
1:A:37:THR:HG22	1:A:37:THR:O	2.15	0.45
1:A:733:GLN:CD	1:A:743:ILE:HD11	2.32	0.45
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.99	0.45
1:A:759:VAL:HG12	1:A:760:ASN:H	1.79	0.45
1:B:66:GLU:HG3	1:B:78:MET:SD	2.57	0.45
1:B:701:GLN:HA	1:B:704:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:ARG:HA	1:C:268:ILE:HD12	1.98	0.45
1:C:574:THR:HA	1:C:665:ALA:HA	1.99	0.45
1:C:735:LYS:O	1:C:739:LEU:HB2	2.16	0.45
1:A:23:GLY:HA3	1:A:377:LEU:O	2.17	0.45
1:A:199:THR:CG2	1:A:791:VAL:HA	2.45	0.45
1:B:922:THR:OG1	1:B:923:ASN:N	2.50	0.45
1:C:395:MET:O	1:C:398:MET:N	2.49	0.45
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.79	0.45
1:C:556:PHE:HD1	1:C:913:LEU:HD11	1.82	0.45
1:C:952:LEU:HA	1:C:956:GLU:HB2	1.98	0.45
1:A:367:ILE:HA	1:A:370:ILE:HG22	1.98	0.45
1:A:401:ALA:O	1:A:405:LEU:HD23	2.17	0.45
1:A:584:GLN:HB3	1:A:622:GLN:HG3	1.98	0.45
1:B:941:ASN:ND2	1:B:1014:ALA:O	2.49	0.45
1:B:452:VAL:HG11	1:B:932:LEU:O	2.16	0.45
1:B:474:ILE:O	1:B:477:ALA:HB3	2.16	0.45
1:C:607:GLU:HB2	1:C:631:LEU:O	2.17	0.45
1:C:674:LEU:CD1	1:C:862:MET:CA	2.94	0.45
1:C:776:GLU:O	1:C:780:ARG:HG2	2.17	0.45
1:A:317:PHE:CB	1:A:321:LEU:HD21	2.40	0.45
1:A:447:MET:HB3	1:A:887:CYS:HG	1.75	0.45
1:A:416:VAL:HG21	1:A:493:CYS:SG	2.57	0.45
1:A:495:THR:O	1:A:496:MET:HG3	2.17	0.45
1:B:367:ILE:HG13	1:B:492:LEU:HD13	1.98	0.45
1:A:768:VAL:CG2	1:B:60:THR:HA	2.46	0.45
1:B:460:GLY:HA2	1:B:872:GLN:OE1	2.17	0.45
1:B:934:THR:O	1:B:937:LEU:N	2.50	0.45
1:C:420:MET:HB2	1:C:498:LYS:HE2	1.99	0.45
1:C:513:PHE:CD1	1:C:516:PHE:HB3	2.52	0.45
1:C:719:ASN:HD22	1:C:719:ASN:HA	1.50	0.45
1:A:189:ASN:O	1:A:193:LEU:HB3	2.17	0.45
1:B:136:PHE:HE1	1:B:617:PHE:CZ	2.35	0.45
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.98	0.45
1:B:280:GLU:HB2	1:B:284:GLN:O	2.17	0.45
1:B:468:ARG:HG3	1:B:468:ARG:HH11	1.82	0.45
1:B:764:ASP:C	1:B:766:GLY:H	2.20	0.45
1:B:756:GLY:HA2	1:B:774:MET:HA	1.99	0.45
1:C:476:SER:O	1:C:477:ALA:HB3	2.17	0.45
1:C:463:THR:HG23	1:C:563:PHE:HE1	1.82	0.45
1:C:717:ARG:O	1:C:827:ILE:HG23	2.17	0.45
1:A:111:LEU:O	1:A:113:LEU:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:O	1:A:206:ALA:HB3	2.17	0.44
1:A:481:SER:O	1:A:484:VAL:HG12	2.17	0.44
1:A:49:TYR:O	1:A:52:ALA:HB2	2.17	0.44
1:A:66:GLU:HB3	1:A:78:MET:CE	2.47	0.44
1:A:725:PRO:HG3	1:A:811:TYR:CE1	2.52	0.44
1:A:753:ALA:HA	1:A:775:SER:HB3	1.99	0.44
1:A:75:LEU:HA	1:A:75:LEU:HD12	1.83	0.44
1:B:555:LEU:HB3	1:B:558:ARG:NH2	2.18	0.44
1:B:764:ASP:O	1:B:766:GLY:N	2.50	0.44
1:C:184:MET:N	1:C:770:LYS:O	2.49	0.44
1:C:914:LEU:HA	1:C:917:THR:OG1	2.17	0.44
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.99	0.44
1:C:941:ASN:HA	1:C:944:LEU:HD12	1.99	0.44
1:A:29:LYS:O	1:A:29:LYS:HG2	2.18	0.44
1:A:492:LEU:HG	1:A:496:MET:HE2	1.98	0.44
1:A:514:GLY:O	1:A:516:PHE:N	2.51	0.44
1:A:681:ASP:H	1:A:863:SER:HB2	1.82	0.44
1:A:729:ILE:HD11	1:A:786:ILE:CD1	2.47	0.44
1:A:807:SER:C	1:A:808:ARG:HG2	2.37	0.44
1:A:865:GLN:HB2	1:A:865:GLN:HE21	1.55	0.44
1:B:139:VAL:CG1	1:B:139:VAL:O	2.48	0.44
1:B:346:GLU:OE1	1:B:988:PRO:HB3	2.17	0.44
1:B:67:GLN:O	1:B:70:ASN:ND2	2.49	0.44
1:B:691:GLY:O	1:B:693:GLU:N	2.51	0.44
1:C:284:GLN:HA	1:C:285:PRO:HD2	1.81	0.44
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.48	0.44
1:C:524:THR:O	1:C:528:THR:OG1	2.29	0.44
1:C:763:ILE:N	1:C:763:ILE:HD12	2.31	0.44
1:C:57:VAL:CG1	1:C:88:VAL:HG22	2.47	0.44
1:A:141:GLY:HA2	1:A:288:GLY:HA3	1.97	0.44
1:A:495:THR:O	1:A:496:MET:CG	2.65	0.44
1:A:211:ASN:ND2	1:A:761:ASP:O	2.46	0.44
1:B:930:GLY:O	1:B:934:THR:HG23	2.17	0.44
1:C:968:VAL:HG21	1:C:1023:PRO:HG3	1.98	0.44
1:C:195:LYS:HE3	1:C:196:PHE:CE1	2.52	0.44
1:C:80:SER:OG	1:C:81:ASN:N	2.50	0.44
1:B:115:MET:O	1:B:118:LEU:HB2	2.17	0.44
1:B:404:LEU:HD13	1:B:449:LEU:HD13	1.99	0.44
1:B:613:ASN:C	1:B:613:ASN:ND2	2.71	0.44
1:B:607:GLU:HG2	1:B:632:LYS:HA	2.00	0.44
1:A:579:PRO:O	1:A:580:ALA:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.51	0.44
1:A:756:GLY:CA	1:A:774:MET:HG3	2.47	0.44
1:A:986:VAL:O	1:A:991:ILE:HD12	2.18	0.44
1:B:1016:VAL:C	1:B:1018:ALA:H	2.21	0.44
1:B:54:ALA:C	1:B:57:VAL:CG1	2.69	0.44
1:C:1017:LEU:HD23	1:C:1017:LEU:O	2.17	0.44
1:C:1027:VAL:HG12	1:C:1031:ARG:HD2	1.98	0.44
1:C:401:ALA:O	1:C:405:LEU:HG	2.16	0.44
1:C:4:PHE:O	1:C:8:ARG:NH1	2.49	0.44
1:C:935:ILE:O	1:C:935:ILE:HG22	2.17	0.44
1:A:194:ASN:C	1:A:196:PHE:H	2.21	0.44
1:A:314:GLU:HA	1:A:317:PHE:CE1	2.53	0.44
1:A:42:ALA:CB	1:A:93:THR:HA	2.45	0.44
1:B:211:ASN:ND2	1:B:246:PHE:HZ	2.15	0.44
1:B:262:LEU:HA	1:B:265:VAL:CG1	2.40	0.44
1:B:601:LYS:CB	1:B:601:LYS:NZ	2.79	0.44
1:C:188:MET:HA	1:C:266:ALA:CB	2.48	0.44
1:A:314:GLU:N	1:A:315:PRO:HD2	2.33	0.44
1:A:687:GLN:HE21	1:A:687:GLN:HB2	1.62	0.44
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.17	0.44
1:B:306:ILE:HG22	1:B:310:LEU:HD12	1.99	0.44
1:B:941:ASN:HA	1:B:944:LEU:HD12	1.99	0.44
1:C:157:TYR:O	1:C:161:ASN:HB2	2.18	0.44
1:C:463:THR:HG23	1:C:563:PHE:CE1	2.53	0.44
1:A:276:ASP:HB3	1:C:222:THR:CG2	2.23	0.44
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.53	0.44
1:A:819:TYR:N	1:A:824:SER:HB3	2.33	0.44
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.53	0.44
1:C:11:PHE:O	1:C:14:VAL:HG12	2.18	0.44
1:C:903:LEU:O	1:C:906:PRO:HD2	2.18	0.44
1:A:356:TYR:O	1:A:360:GLN:HA	2.17	0.44
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.18	0.44
1:B:369:THR:C	1:B:371:ALA:H	2.21	0.44
1:B:585:GLU:O	1:B:586:ARG:C	2.56	0.44
1:C:265:VAL:O	1:C:265:VAL:HG23	2.18	0.44
1:B:225:VAL:HG11	1:C:778:LYS:HG2	1.99	0.44
1:A:70:ASN:O	1:A:110:LYS:HG2	2.17	0.43
1:A:372:VAL:HA	1:A:375:VAL:HG23	1.99	0.43
1:A:564:LEU:O	1:A:565:PRO:C	2.56	0.43
1:A:714:THR:O	1:A:715:SER:HB2	2.18	0.43
1:B:144:ASN:CG	1:B:149:MET:HG3	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CB	1:B:2:PRO:HD2	2.27	0.43
1:B:42:ALA:CB	1:B:93:THR:HG22	2.40	0.43
1:C:131:LYS:O	1:C:295:THR:HG22	2.18	0.43
1:C:184:MET:HE3	1:C:185:ARG:H	1.83	0.43
1:C:252:LYS:O	1:C:260:VAL:HG12	2.18	0.43
1:C:644:VAL:HG11	1:C:667:ASN:HB2	2.00	0.43
1:A:9:PRO:C	1:A:11:PHE:N	2.72	0.43
1:A:367:ILE:HD12	1:A:489:THR:HG22	1.98	0.43
1:A:448:VAL:HG21	1:A:888:LEU:HD13	2.00	0.43
1:B:382:VAL:O	1:B:383:LEU:C	2.55	0.43
1:B:712:MET:HE2	1:B:835:LYS:H	1.82	0.43
1:C:159:ALA:HA	1:C:163:LYS:HB3	2.00	0.43
1:C:307:ARG:HH11	1:C:307:ARG:HG2	1.83	0.43
1:C:146:ASP:OD2	1:C:319:SER:HB3	2.18	0.43
1:C:450:SER:O	1:C:454:VAL:HB	2.17	0.43
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.52	0.43
1:A:149:MET:HE1	1:A:321:LEU:HD22	2.00	0.43
1:A:571:VAL:HG12	1:A:630:SER:HA	2.00	0.43
1:B:215:ALA:O	1:B:216:ALA:HB2	2.19	0.43
1:B:225:VAL:CG2	1:B:225:VAL:O	2.65	0.43
1:B:523:SER:HA	1:B:526:HIS:CD2	2.52	0.43
1:B:756:GLY:CA	1:B:774:MET:HG2	2.48	0.43
1:C:92:LEU:HD12	1:C:92:LEU:H	1.83	0.43
1:C:418:ARG:NH2	1:C:971:ARG:HH12	2.13	0.43
1:A:548:ILE:CG1	1:A:910:ILE:HD13	2.49	0.43
1:A:596:HIS:O	1:A:597:TYR:C	2.56	0.43
1:B:111:LEU:HD22	1:B:129:VAL:HG13	2.00	0.43
1:B:133:SER:OG	1:B:134:SER:N	2.51	0.43
1:B:144:ASN:ND2	1:B:149:MET:N	2.67	0.43
1:B:201:VAL:O	1:B:204:ILE:N	2.52	0.43
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.99	0.43
1:B:602:GLU:O	1:B:604:ASN:N	2.51	0.43
1:B:748:THR:O	1:B:752:ALA:HB2	2.19	0.43
1:B:189:ASN:ND2	1:B:779:TYR:OH	2.51	0.43
1:C:106:GLN:O	1:C:107:VAL:C	2.56	0.43
1:C:186:ILE:HG13	1:C:207:ILE:CD1	2.49	0.43
1:C:318:PRO:HD2	1:C:321:LEU:HG	2.00	0.43
1:C:575:MET:O	1:C:576:VAL:CG1	2.62	0.43
1:C:778:LYS:HB2	1:C:779:TYR:HE2	1.80	0.43
1:A:1029:VAL:HG13	1:A:1033:PHE:HD2	1.83	0.43
1:A:190:PRO:O	1:A:194:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LEU:O	1:A:379:THR:N	2.51	0.43
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.99	0.43
1:A:781:MET:HE1	1:C:228:GLN:HG2	1.99	0.43
1:B:463:THR:C	1:B:465:ALA:H	2.21	0.43
1:B:453:PHE:CD2	1:B:474:ILE:HG21	2.53	0.43
1:C:1016:VAL:HA	1:C:1019:ILE:HG22	1.99	0.43
1:A:783:PRO:HD3	1:C:219:LEU:HD13	2.01	0.43
1:C:489:THR:O	1:C:493:CYS:HB2	2.19	0.43
1:C:972:LEU:HA	1:C:1019:ILE:HD11	2.00	0.43
1:A:651:ALA:HA	1:A:654:ALA:HB3	2.01	0.43
1:A:731:ILE:HG12	1:A:746:ILE:HG21	2.00	0.43
1:A:754:TRP:CZ3	1:A:780:ARG:HA	2.53	0.43
1:A:76:MET:SD	1:A:864:TYR:HE2	2.42	0.43
1:A:961:ILE:HG22	1:A:961:ILE:O	2.18	0.43
1:A:953:MET:HB2	1:A:963:ALA:CB	2.48	0.43
1:B:300:LEU:CD2	1:B:333:VAL:HG11	2.47	0.43
1:B:36:PRO:HD2	1:B:38:ILE:HD11	2.01	0.43
1:B:477:ALA:O	1:B:481:SER:N	2.50	0.43
1:B:538:THR:H	1:B:540:ARG:HH21	1.66	0.43
1:B:618:ALA:HB1	1:B:719:ASN:O	2.17	0.43
1:B:669:PRO:HB2	1:B:670:ALA:H	1.61	0.43
1:A:167:SER:HB3	1:B:70:ASN:ND2	2.33	0.43
1:C:14:VAL:HG22	1:C:18:ILE:HG12	1.99	0.43
1:C:40:PRO:HB2	1:C:94:PHE:O	2.18	0.43
1:C:459:PHE:H	1:C:459:PHE:HD2	1.64	0.43
1:C:578:LEU:CB	1:C:579:PRO:CD	2.96	0.43
1:C:672:VAL:HG11	1:C:677:ALA:HA	2.01	0.43
1:C:700:ASN:HA	1:C:703:LEU:HD12	1.99	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.19	0.43
1:A:364:ALA:O	1:A:368:PRO:HD3	2.19	0.43
1:A:44:THR:CG2	1:A:89:GLN:HG2	2.48	0.43
1:A:894:SER:C	1:A:896:SER:H	2.21	0.43
1:B:154:ILE:O	1:B:157:TYR:N	2.50	0.43
1:B:242:SER:O	1:B:243:THR:C	2.56	0.43
1:B:675:GLY:C	1:B:677:ALA:H	2.22	0.43
1:C:367:ILE:HD11	1:C:489:THR:HA	1.99	0.43
1:C:679:GLY:HA2	1:C:830:GLN:CA	2.46	0.43
1:A:189:ASN:C	1:A:189:ASN:OD1	2.56	0.43
1:A:225:VAL:HG12	1:B:781:MET:CE	2.49	0.43
1:A:983:ILE:HA	1:A:986:VAL:HG12	2.00	0.43
1:B:462:SER:H	1:B:865:GLN:NE2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:VAL:O	1:B:990:VAL:HG23	2.18	0.43
1:C:206:ALA:O	1:C:208:LYS:N	2.51	0.43
1:C:49:TYR:HE1	1:C:60:THR:HG21	1.83	0.43
1:C:326:PRO:CG	1:C:610:PHE:CD1	3.02	0.43
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.39	0.43
1:C:959:GLY:H	1:C:962:GLU:HB2	1.83	0.43
1:A:1:MET:N	1:A:2:PRO:HD2	2.34	0.43
1:A:648:THR:O	1:A:649:MET:C	2.57	0.43
1:A:681:ASP:OD2	1:A:860:THR:HG23	2.19	0.43
1:A:62:THR:HG23	1:A:88:VAL:HG11	2.01	0.43
1:B:204:ILE:O	1:B:205:THR:C	2.57	0.43
1:B:674:LEU:C	1:B:676:THR:H	2.22	0.43
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.49	0.43
1:B:976:LEU:O	1:B:980:LEU:HD12	2.18	0.43
1:C:453:PHE:O	1:C:456:MET:HG3	2.19	0.43
1:C:577:GLN:HA	1:C:624:THR:HA	2.00	0.43
1:C:752:ALA:O	1:C:756:GLY:HA2	2.19	0.43
1:A:1022:VAL:N	1:A:1023:PRO:CD	2.80	0.43
1:A:108:GLN:OE1	1:B:112:GLN:CB	2.67	0.43
1:A:75:LEU:HD21	1:A:92:LEU:HD23	1.99	0.43
1:B:144:ASN:HD22	1:B:149:MET:N	2.17	0.43
1:B:566:ASP:HB3	1:B:667:ASN:HD22	1.84	0.43
1:B:574:THR:HA	1:B:664:PHE:O	2.19	0.43
1:B:68:ASN:O	1:B:110:LYS:HE3	2.19	0.43
1:B:686:ASP:HB3	1:B:823:PRO:O	2.19	0.43
1:C:115:MET:HA	1:C:115:MET:CE	2.48	0.43
1:C:145:THR:O	1:C:147:GLY:N	2.52	0.43
1:C:251:LEU:HD11	1:C:262:LEU:HA	2.01	0.43
1:C:470:PHE:O	1:C:471:SER:C	2.56	0.43
1:A:255:GLN:O	1:A:256:ASP:HB3	2.18	0.42
1:A:268:ILE:N	1:A:268:ILE:HD12	2.34	0.42
1:A:369:THR:O	1:A:373:PRO:HD3	2.17	0.42
1:A:779:TYR:N	1:A:779:TYR:CD1	2.86	0.42
1:B:15:ILE:O	1:B:19:ILE:HG12	2.19	0.42
1:B:293:LEU:CD1	1:B:297:ALA:HB3	2.49	0.42
1:B:345:VAL:C	1:B:347:ALA:H	2.23	0.42
1:B:990:VAL:HG22	1:B:1005:THR:N	2.33	0.42
1:C:576:VAL:HG11	1:C:591:LEU:HD22	2.01	0.42
1:C:832:ALA:CB	1:C:833:PRO:CD	2.90	0.42
1:C:847:LEU:HA	1:C:850:LYS:HG2	2.00	0.42
1:C:875:SER:C	1:C:877:TYR:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:THR:N	1:B:320:GLY:O	2.52	0.42
1:B:330:THR:H	1:B:331:PRO:CD	2.32	0.42
1:B:300:LEU:HD21	1:B:333:VAL:CG1	2.48	0.42
1:B:967:ALA:O	1:B:968:VAL:C	2.57	0.42
1:B:986:VAL:O	1:B:986:VAL:HG12	2.18	0.42
1:C:144:ASN:ND2	1:C:148:THR:H	2.12	0.42
1:A:171:GLY:O	1:A:172:VAL:C	2.58	0.42
1:A:318:PRO:HB2	1:A:319:SER:H	1.74	0.42
1:A:4:PHE:O	1:A:8:ARG:NH1	2.52	0.42
1:A:571:VAL:HG12	1:A:630:SER:HB3	2.01	0.42
1:B:355:MET:O	1:B:365:THR:OG1	2.28	0.42
1:B:602:GLU:C	1:B:604:ASN:N	2.73	0.42
1:C:146:ASP:HB3	1:C:148:THR:HG23	2.01	0.42
1:C:218:GLN:HA	1:C:234:ILE:H	1.84	0.42
1:C:372:VAL:HG13	1:C:373:PRO:HD3	2.01	0.42
1:C:410:ILE:O	1:C:414:GLU:HB2	2.19	0.42
1:C:684:LEU:HD13	1:C:685:ILE:N	2.34	0.42
1:C:978:THR:O	1:C:981:ALA:N	2.52	0.42
1:A:17:ILE:O	1:A:18:ILE:C	2.56	0.42
1:A:552:MET:CG	1:A:909:VAL:HG11	2.49	0.42
1:B:34:GLN:O	1:B:391:ASN:HB2	2.19	0.42
1:C:242:SER:O	1:C:243:THR:C	2.56	0.42
1:C:34:GLN:HG3	1:C:333:VAL:HG11	2.00	0.42
1:C:764:ASP:O	1:C:766:GLY:N	2.51	0.42
1:A:425:LEU:HB3	1:A:426:PRO:HD2	2.01	0.42
1:A:703:LEU:HD11	1:A:718:PRO:HG3	2.00	0.42
1:A:729:ILE:CD1	1:A:786:ILE:HD12	2.50	0.42
1:B:1020:PHE:CD2	1:B:1020:PHE:N	2.87	0.42
1:B:559:LEU:HA	1:B:560:PRO:HD3	1.87	0.42
1:B:698:ALA:O	1:B:702:LEU:HB2	2.19	0.42
1:B:906:PRO:HA	1:B:909:VAL:CG2	2.47	0.42
1:B:65:ILE:HB	1:B:90:ILE:CD1	2.48	0.42
1:C:686:ASP:C	1:C:686:ASP:OD1	2.56	0.42
1:C:204:ILE:HD11	1:C:773:VAL:HG21	2.01	0.42
1:C:77:TYR:N	1:C:77:TYR:CD2	2.87	0.42
1:C:83:ASP:HA	1:C:815:ARG:HA	2.01	0.42
1:C:950:LYS:HE3	1:C:954:ASP:OD1	2.20	0.42
1:C:958:LYS:HB3	1:C:962:GLU:HB3	2.02	0.42
1:A:10:ILE:O	1:A:11:PHE:C	2.57	0.42
1:A:655:PHE:C	1:A:657:GLN:H	2.23	0.42
1:A:713:LEU:HD21	1:A:843:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ALA:CA	1:A:83:ASP:O	2.68	0.42
1:B:123:GLN:C	1:B:125:GLN:N	2.72	0.42
1:B:420:MET:O	1:B:421:ALA:C	2.58	0.42
1:B:758:TYR:HD2	1:B:758:TYR:C	2.23	0.42
1:B:776:GLU:HG2	1:B:777:ALA:N	2.34	0.42
1:C:534:ILE:HG13	1:C:534:ILE:H	1.36	0.42
1:C:57:VAL:HG13	1:C:88:VAL:CG2	2.49	0.42
1:C:591:LEU:HD12	1:C:611:ALA:HB1	2.01	0.42
1:A:112:GLN:CA	1:A:112:GLN:NE2	2.76	0.42
1:A:134:SER:HB2	1:A:673:GLU:CD	2.40	0.42
1:A:164:ASP:O	1:A:168:ARG:HG2	2.20	0.42
1:B:182:TYR:HD1	1:B:182:TYR:HA	1.72	0.42
1:B:237:GLN:CG	1:B:238:THR:N	2.83	0.42
1:B:575:MET:N	1:B:664:PHE:O	2.52	0.42
1:C:225:VAL:O	1:C:226:LYS:C	2.57	0.42
1:C:295:THR:O	1:C:295:THR:HG23	2.19	0.42
1:C:327:TYR:O	1:C:328:ASP:HB2	2.19	0.42
1:C:338:HIS:HA	1:C:341:VAL:HG12	2.01	0.42
1:C:414:GLU:OE2	1:C:974:PRO:HA	2.19	0.42
1:A:117:LEU:N	1:A:117:LEU:CD1	2.82	0.42
1:A:11:PHE:HB3	1:A:12:ALA:H	1.49	0.42
1:A:314:GLU:HG2	1:A:314:GLU:O	2.19	0.42
1:A:425:LEU:HD12	1:A:425:LEU:H	1.84	0.42
1:A:817:GLU:OE1	1:A:826:GLU:N	2.45	0.42
1:B:136:PHE:CE1	1:B:617:PHE:HZ	2.37	0.42
1:B:190:PRO:O	1:B:193:LEU:HB3	2.19	0.42
1:C:340:VAL:HG12	1:C:395:MET:HB3	2.01	0.42
1:C:72:ILE:CG2	1:C:94:PHE:HE2	2.33	0.42
1:A:578:LEU:CD2	1:A:590:VAL:HG21	2.44	0.42
1:B:178:PHE:HA	1:B:277:ILE:HG21	2.00	0.42
1:A:11:PHE:CD1	1:B:890:ALA:HA	2.54	0.42
1:B:453:PHE:CZ	1:B:933:THR:HG23	2.55	0.42
1:C:219:LEU:O	1:C:221:GLY:N	2.52	0.42
1:C:204:ILE:CD1	1:C:773:VAL:HG21	2.50	0.42
1:C:775:SER:HG	1:C:789:TRP:HZ2	1.67	0.42
1:A:641:GLU:OE1	1:A:642:ASN:N	2.53	0.42
1:A:953:MET:HG2	1:A:953:MET:O	2.20	0.42
1:B:23:GLY:HA3	1:B:377:LEU:O	2.20	0.42
1:B:602:GLU:HG3	1:B:647:ILE:HG23	2.02	0.42
1:B:705:GLU:O	1:B:706:ALA:CB	2.67	0.42
1:B:184:MET:H	1:B:762:PHE:HE2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ASP:O	1:C:105:VAL:HG23	2.20	0.42
1:C:795:ASP:OD2	1:C:795:ASP:C	2.58	0.42
1:A:72:ILE:HD13	1:A:107:VAL:HA	2.02	0.41
1:A:13:TRP:O	1:A:16:ALA:CB	2.65	0.41
1:A:155:SER:OG	1:A:179:GLY:HA3	2.20	0.41
1:A:456:MET:HA	1:A:459:PHE:HE1	1.82	0.41
1:A:567:GLU:HG2	1:A:998:GLY:HA3	2.02	0.41
1:A:869:SER:HB2	1:A:870:GLY:H	1.70	0.41
1:A:76:MET:HG3	1:A:94:PHE:O	2.19	0.41
1:B:166:ILE:HA	1:B:169:THR:OG1	2.19	0.41
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.83	0.41
1:A:225:VAL:HG11	1:B:778:LYS:NZ	2.35	0.41
1:B:898:PRO:C	1:B:900:SER:N	2.74	0.41
1:C:456:MET:O	1:C:457:ALA:CB	2.67	0.41
1:C:684:LEU:CD1	1:C:684:LEU:C	2.88	0.41
1:C:885:PHE:CE2	1:C:899:PHE:CE1	3.07	0.41
1:A:189:ASN:OD1	1:A:191:ASN:N	2.53	0.41
1:A:1:MET:N	1:A:2:PRO:CD	2.83	0.41
1:A:927:PHE:CD2	1:A:927:PHE:C	2.93	0.41
1:A:978:THR:CG2	1:A:979:SER:N	2.84	0.41
1:B:949:ALA:HB3	1:B:1030:ARG:HH12	1.85	0.41
1:B:468:ARG:HG3	1:B:468:ARG:NH1	2.35	0.41
1:B:938:SER:HB3	1:B:1014:ALA:CB	2.50	0.41
1:B:948:PHE:HD2	1:B:967:ALA:HA	1.84	0.41
1:C:1030:ARG:C	1:C:1032:ARG:H	2.24	0.41
1:C:70:ASN:O	1:C:71:GLY:C	2.58	0.41
1:C:750:LEU:O	1:C:754:TRP:HD1	2.03	0.41
1:A:574:THR:OG1	1:A:598:TYR:HE1	2.01	0.41
1:B:3:ASN:O	1:B:4:PHE:C	2.58	0.41
1:B:48:SER:O	1:B:50:PRO:HD3	2.19	0.41
1:C:142:VAL:HG13	1:C:321:LEU:HD13	2.01	0.41
1:C:352:PHE:N	1:C:369:THR:HG21	2.34	0.41
1:C:670:ALA:C	1:C:672:VAL:N	2.74	0.41
1:A:185:ARG:HD3	1:A:272:GLY:O	2.20	0.41
1:A:674:LEU:HD22	1:A:675:GLY:N	2.18	0.41
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.20	0.41
1:A:888:LEU:HD21	1:A:901:VAL:HB	2.01	0.41
1:B:235:ILE:HD12	1:B:235:ILE:N	2.34	0.41
1:B:249:ILE:O	1:B:251:LEU:HD12	2.20	0.41
1:B:34:GLN:NE2	1:B:332:PHE:HE2	2.18	0.41
1:B:605:ASN:ND2	1:B:642:ASN:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:TYR:HB3	1:C:1003:VAL:HG22	2.02	0.41
1:C:27:ILE:HD11	1:C:380:PHE:CD1	2.56	0.41
1:C:394:THR:HG22	1:C:395:MET:CE	2.50	0.41
1:C:945:ILE:C	1:C:947:GLU:H	2.24	0.41
1:A:444:GLY:HA3	1:A:891:LEU:HD13	2.02	0.41
1:A:577:GLN:O	1:A:577:GLN:HG3	2.20	0.41
1:B:144:ASN:HB2	1:B:321:LEU:HD12	2.02	0.41
1:B:157:TYR:CA	1:B:161:ASN:ND2	2.81	0.41
1:B:34:GLN:HB2	1:B:333:VAL:HG22	2.02	0.41
1:B:35:TYR:HB3	1:B:36:PRO:HD2	2.01	0.41
1:B:701:GLN:HB2	1:B:851:LEU:HD22	2.03	0.41
1:B:97:GLY:O	1:B:98:THR:O	2.38	0.41
1:C:416:VAL:HA	1:C:419:VAL:HG22	2.02	0.41
1:C:713:LEU:O	1:C:713:LEU:CD2	2.68	0.41
1:C:774:MET:HG2	1:C:775:SER:N	2.35	0.41
1:A:23:GLY:O	1:A:27:ILE:HG13	2.20	0.41
1:A:323:ILE:O	1:A:325:TYR:CE1	2.74	0.41
1:A:367:ILE:CD1	1:A:413:VAL:HB	2.49	0.41
1:A:461:GLY:O	1:A:462:SER:C	2.59	0.41
1:A:911:GLY:HA2	1:A:914:LEU:HB2	2.02	0.41
1:B:895:TRP:O	1:B:899:PHE:CD2	2.74	0.41
1:A:728:LYS:HD2	1:C:235:ILE:O	2.21	0.41
1:C:240:LEU:HB3	1:C:245:GLU:HB2	2.02	0.41
1:A:1036:LYS:HB2	1:A:1036:LYS:NZ	2.36	0.41
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.88	0.41
1:A:308:ALA:O	1:A:312:LYS:HD3	2.20	0.41
1:A:591:LEU:HD12	1:A:613:ASN:HB3	2.03	0.41
1:A:726:GLN:N	1:A:810:GLU:O	2.49	0.41
1:A:682:PHE:CE1	1:A:857:TYR:HB2	2.55	0.41
1:B:194:ASN:C	1:B:196:PHE:H	2.24	0.41
1:B:58:GLN:HG3	1:B:59:ASP:H	1.84	0.41
1:B:671:ILE:C	1:B:673:GLU:H	2.24	0.41
1:B:758:TYR:CD2	1:B:758:TYR:C	2.94	0.41
1:C:293:LEU:HD22	1:C:299:ALA:HB2	2.03	0.41
1:C:597:TYR:CD1	1:C:601:LYS:HG3	2.56	0.41
1:C:714:THR:CG2	1:C:716:VAL:HG23	2.51	0.41
1:A:380:PHE:CE1	1:A:398:MET:SD	3.14	0.41
1:A:653:ARG:C	1:A:655:PHE:H	2.24	0.41
1:A:706:ALA:HB3	1:A:716:VAL:HG21	2.02	0.41
1:A:731:ILE:HG21	1:A:746:ILE:HG21	2.01	0.41
1:B:428:LYS:HA	1:B:494:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:676:THR:O	1:B:676:THR:CG2	2.69	0.41
1:B:774:MET:O	1:B:775:SER:HB3	2.20	0.41
1:B:852:PRO:HB2	1:B:853:THR:H	1.58	0.41
1:B:916:ALA:HA	1:B:919:ARG:HG2	2.03	0.41
1:B:986:VAL:O	1:B:990:VAL:CG2	2.69	0.41
1:C:69:MET:SD	1:C:92:LEU:HD21	2.60	0.41
1:C:728:LYS:HG3	1:C:729:ILE:N	2.35	0.41
1:C:947:GLU:O	1:C:950:LYS:HB2	2.21	0.41
1:A:111:LEU:C	1:A:113:LEU:H	2.24	0.41
1:A:442:LEU:C	1:A:444:GLY:N	2.73	0.41
1:B:119:PRO:HB2	1:B:122:VAL:HG23	2.02	0.41
1:B:150:THR:HG22	1:B:151:GLN:N	2.36	0.41
1:B:226:LYS:HB3	1:B:227:GLY:H	1.69	0.41
1:B:543:VAL:O	1:B:547:ILE:HD13	2.20	0.41
1:B:696:THR:HA	1:B:699:ARG:NH1	2.36	0.41
1:B:804:PHE:O	1:B:805:SER:CB	2.68	0.41
1:B:414:GLU:OE1	1:B:974:PRO:HG3	2.21	0.41
1:B:997:SER:C	1:B:999:ALA:H	2.24	0.41
1:C:713:LEU:HD23	1:C:832:ALA:N	2.35	0.41
1:A:1004:GLY:O	1:A:1007:VAL:N	2.54	0.41
1:A:162:MET:HA	1:A:313:MET:HE1	2.03	0.41
1:A:601:LYS:HG2	1:A:601:LYS:O	2.21	0.41
1:A:3:ASN:C	1:A:6:ILE:HG13	2.42	0.41
1:B:146:ASP:N	1:B:146:ASP:OD2	2.53	0.41
1:B:20:MET:HG2	1:B:374:VAL:HA	2.03	0.41
1:B:518:ARG:O	1:B:518:ARG:HG2	2.20	0.41
1:C:545:TYR:OH	1:C:1025:PHE:CZ	2.71	0.41
1:C:688:ALA:HB3	1:C:690:LEU:CD1	2.47	0.41
1:C:925:VAL:CG2	1:C:926:TYR:H	2.28	0.41
1:C:350:LEU:HD22	1:C:984:LEU:CD2	2.50	0.41
1:A:239:ARG:HD3	1:A:762:PHE:HA	2.03	0.41
1:A:644:VAL:HG11	1:A:667:ASN:ND2	2.23	0.41
1:A:775:SER:HB2	1:A:789:TRP:CZ2	2.53	0.41
1:A:548:ILE:HG12	1:A:910:ILE:HD13	2.02	0.41
1:B:146:ASP:O	1:B:148:THR:OG1	2.30	0.41
1:B:235:ILE:N	1:B:235:ILE:HD13	2.36	0.41
1:B:375:VAL:HB	1:B:405:LEU:HD22	2.03	0.41
1:B:372:VAL:O	1:B:376:LEU:HB2	2.21	0.41
1:B:574:THR:HA	1:B:665:ALA:HA	2.04	0.41
1:B:775:SER:HB2	1:B:789:TRP:HZ2	1.86	0.41
1:C:356:TYR:HA	1:C:356:TYR:HD1	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:724:THR:HG23	1:C:725:PRO:HD2	2.02	0.41
1:A:576:VAL:HG21	1:A:591:LEU:CD2	2.47	0.40
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.83	0.40
1:B:438:ILE:HD12	1:B:438:ILE:HA	1.84	0.40
1:B:71:GLY:O	1:B:72:ILE:C	2.59	0.40
1:B:848:ALA:C	1:B:850:LYS:H	2.24	0.40
1:B:900:SER:OG	1:B:1029:VAL:HG11	2.21	0.40
1:B:931:LEU:HA	1:B:931:LEU:HD23	1.97	0.40
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.55	0.40
1:C:155:SER:HB3	1:C:180:SER:H	1.86	0.40
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.51	0.40
1:C:574:THR:HG22	1:C:575:MET:N	2.36	0.40
1:C:759:VAL:O	1:C:760:ASN:HB3	2.21	0.40
1:C:959:GLY:O	1:C:960:LEU:C	2.59	0.40
1:A:1008:MET:HB3	1:A:1009:GLY:H	1.72	0.40
1:A:325:TYR:CD1	1:A:325:TYR:N	2.89	0.40
1:B:518:ARG:HA	1:B:521:GLU:HB2	2.03	0.40
1:B:871:ASN:N	1:B:871:ASN:ND2	2.67	0.40
1:C:531:VAL:HB	1:C:532:GLY:H	1.69	0.40
1:C:937:LEU:HD12	1:C:937:LEU:HA	1.83	0.40
1:C:418:ARG:CZ	1:C:974:PRO:HG3	2.50	0.40
1:A:187:TRP:O	1:A:188:MET:O	2.39	0.40
1:A:685:ILE:HG21	1:A:822:LEU:HD12	2.02	0.40
1:A:87:THR:HG21	1:A:620:ARG:NH1	2.36	0.40
1:A:970:MET:O	1:A:971:ARG:HB2	2.21	0.40
1:A:350:LEU:HD11	1:A:984:LEU:HB3	2.02	0.40
1:B:151:GLN:HE22	1:B:279:ALA:H	1.67	0.40
1:B:314:GLU:H	1:B:315:PRO:CD	2.34	0.40
1:B:439:GLN:O	1:B:439:GLN:HG2	2.22	0.40
1:B:327:TYR:HB2	1:B:628:PHE:HB3	2.04	0.40
1:B:692:HIS:HD2	1:B:825:MET:HE2	1.87	0.40
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.56	0.40
1:A:391:ASN:O	1:A:392:THR:C	2.60	0.40
1:A:485:ALA:HA	1:A:489:THR:OG1	2.21	0.40
1:A:493:CYS:O	1:A:497:LEU:HG	2.21	0.40
1:A:685:ILE:HG21	1:A:822:LEU:HD13	2.04	0.40
1:B:1007:VAL:O	1:B:1007:VAL:HG13	2.20	0.40
1:B:552:MET:C	1:B:554:TYR:H	2.24	0.40
1:C:343:THR:HA	1:C:346:GLU:HG2	2.02	0.40
1:C:350:LEU:HD13	1:C:984:LEU:HD23	2.04	0.40
1:C:636:ASP:O	1:C:638:PRO:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:HIS:C	1:C:711:ASP:H	2.25	0.40
1:C:751:GLY:O	1:C:755:GLY:N	2.47	0.40
1:C:905:VAL:HB	1:C:906:PRO:HD3	2.04	0.40
1:A:7:ASP:C	1:A:9:PRO:CG	2.82	0.40
1:A:886:LEU:HG	1:C:14:VAL:CG2	2.48	0.40
1:B:143:ILE:HD13	1:B:322:LYS:O	2.22	0.40
1:B:251:LEU:HD13	1:B:262:LEU:N	2.34	0.40
1:B:310:LEU:HD22	1:B:323:ILE:HD13	2.04	0.40
1:B:32:VAL:O	1:B:33:ALA:HB2	2.21	0.40
1:B:560:PRO:HB3	1:B:836:SER:CB	2.51	0.40
1:B:58:GLN:C	1:B:60:THR:H	2.25	0.40
1:B:659:LYS:HG2	1:B:660:ASP:H	1.87	0.40
1:B:741:VAL:HG21	1:B:799:VAL:HG11	2.02	0.40
1:C:361:ASN:HB2	1:C:364:ALA:HB3	2.02	0.40
1:C:1:MET:HG3	1:C:3:ASN:H	1.87	0.40
1:C:570:GLY:HA3	1:C:634:TRP:CZ2	2.57	0.40
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1018/1053 (97%)	713 (70%)	191 (19%)	114 (11%)	0	2
1	B	1018/1053 (97%)	695 (68%)	231 (23%)	92 (9%)	1	5
1	C	1018/1053 (97%)	728 (72%)	213 (21%)	77 (8%)	1	7
All	All	3054/3159 (97%)	2136 (70%)	635 (21%)	283 (9%)	0	4

All (283) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	PRO
1	A	11	PHE
1	A	12	ALA
1	A	13	TRP
1	A	14	VAL
1	A	15	ILE
1	A	134	SER
1	A	146	ASP
1	A	147	GLY
1	A	181	GLN
1	A	188	MET
1	A	206	ALA
1	A	256	ASP
1	A	267	LYS
1	A	269	GLU
1	A	293	LEU
1	A	388	PHE
1	A	392	THR
1	A	460	GLY
1	A	515	TRP
1	A	516	PHE
1	A	580	ALA
1	A	659	LYS
1	A	676	THR
1	A	746	ILE
1	A	831	ALA
1	A	958	LYS
1	A	960	LEU
1	A	1008	MET
1	A	1017	LEU
1	A	1030	ARG
1	A	1034	SER
1	B	52	ALA
1	B	54	ALA
1	B	72	ILE
1	B	98	THR
1	B	147	GLY
1	B	216	ALA
1	B	217	GLY
1	B	222	THR
1	B	254	ASN
1	B	265	VAL
1	B	270	LEU

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Mol	Chain	Res	Type
1	B	299	ALA
1	B	427	PRO
1	B	486	LEU
1	B	517	ASN
1	B	671	ILE
1	B	672	VAL
1	B	709	HIS
1	B	723	ASP
1	B	733	GLN
1	B	765	ARG
1	B	775	SER
1	B	852	PRO
1	B	1016	VAL
1	C	80	SER
1	C	146	ASP
1	C	226	LYS
1	C	255	GLN
1	C	295	THR
1	C	438	ILE
1	C	464	GLY
1	C	656	SER
1	C	674	LEU
1	C	678	THR
1	C	715	SER
1	C	806	SER
1	C	820	ASN
1	C	830	GLN
1	C	871	ASN
1	C	895	TRP
1	C	953	MET
1	C	960	LEU
1	C	965	LEU
1	A	10	ILE
1	A	16	ALA
1	A	17	ILE
1	A	18	ILE
1	A	37	THR
1	A	65	ILE
1	A	67	GLN
1	A	69	MET
1	A	112	GLN
1	A	138	MET

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Mol	Chain	Res	Type
1	A	172	VAL
1	A	192	GLU
1	A	294	ALA
1	A	318	PRO
1	A	320	GLY
1	A	362	PHE
1	A	426	PRO
1	A	427	PRO
1	A	443	VAL
1	A	517	ASN
1	A	538	THR
1	A	617	PHE
1	A	650	ARG
1	A	660	ASP
1	A	661	ALA
1	A	662	MET
1	A	672	VAL
1	A	675	GLY
1	A	686	ASP
1	A	689	GLY
1	A	759	VAL
1	A	893	GLU
1	A	925	VAL
1	A	971	ARG
1	A	988	PRO
1	A	1016	VAL
1	B	36	PRO
1	B	140	VAL
1	B	201	VAL
1	B	243	THR
1	B	262	LEU
1	B	283	GLY
1	B	319	SER
1	B	357	LEU
1	B	358	PHE
1	B	360	GLN
1	B	370	ILE
1	B	418	ARG
1	B	453	PHE
1	B	518	ARG
1	B	633	ASP
1	B	656	SER

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Mol	Chain	Res	Type
1	B	669	PRO
1	B	704	ALA
1	B	807	SER
1	B	834	GLY
1	B	890	ALA
1	B	899	PHE
1	B	921	LEU
1	B	953	MET
1	C	285	PRO
1	C	404	LEU
1	C	427	PRO
1	C	534	ILE
1	C	576	VAL
1	C	577	GLN
1	C	673	GLU
1	C	872	GLN
1	C	893	GLU
1	C	899	PHE
1	C	998	GLY
1	A	96	SER
1	A	219	LEU
1	A	330	THR
1	A	357	LEU
1	A	377	LEU
1	A	439	GLN
1	A	444	GLY
1	A	457	ALA
1	A	687	GLN
1	A	809	TRP
1	A	844	MET
1	A	869	SER
1	A	875	SER
1	A	918	PHE
1	A	969	ARG
1	B	69	MET
1	B	124	GLN
1	B	202	ASP
1	B	226	LYS
1	B	251	LEU
1	B	439	GLN
1	B	495	THR
1	B	601	LYS

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Mol	Chain	Res	Type
1	B	603	LYS
1	B	692	HIS
1	B	849	SER
1	B	1005	THR
1	B	1017	LEU
1	C	4	PHE
1	C	54	ALA
1	C	69	MET
1	C	422	GLU
1	C	461	GLY
1	C	463	THR
1	C	602	GLU
1	C	718	PRO
1	C	720	GLY
1	C	808	ARG
1	C	832	ALA
1	C	892	TYR
1	A	19	ILE
1	A	54	ALA
1	A	287	SER
1	A	451	ALA
1	A	452	VAL
1	A	514	GLY
1	A	531	VAL
1	A	623	ASN
1	A	752	ALA
1	A	871	ASN
1	A	1035	ARG
1	B	184	MET
1	B	553	ALA
1	B	676	THR
1	B	693	GLU
1	B	814	PRO
1	B	959	GLY
1	C	26	ALA
1	C	81	ASN
1	C	207	ILE
1	C	222	THR
1	C	230	LEU
1	C	328	ASP
1	C	424	GLY
1	C	425	LEU

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Mol	Chain	Res	Type
1	C	693	GLU
1	C	765	ARG
1	C	802	SER
1	C	866	GLU
1	C	876	LEU
1	C	894	SER
1	C	915	ALA
1	C	1006	GLY
1	C	1017	LEU
1	A	36	PRO
1	A	53	ASP
1	A	220	GLY
1	A	236	ALA
1	A	326	PRO
1	A	436	GLY
1	A	565	PRO
1	A	638	PRO
1	A	654	ALA
1	A	677	ALA
1	A	784	ASP
1	A	788	ASP
1	A	866	GLU
1	A	991	ILE
1	B	4	PHE
1	B	223	PRO
1	B	250	LEU
1	B	428	LYS
1	B	542	LEU
1	B	688	ALA
1	B	805	SER
1	C	939	ALA
1	C	940	LYS
1	C	974	PRO
1	C	1016	VAL
1	C	1031	ARG
1	A	64	VAL
1	A	195	LYS
1	A	263	ARG
1	A	909	VAL
1	B	119	PRO
1	B	127	VAL
1	B	494	ALA

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Mol	Chain	Res	Type
1	B	538	THR
1	B	602	GLU
1	B	638	PRO
1	B	691	GLY
1	C	187	TRP
1	C	243	THR
1	C	531	VAL
1	C	712	MET
1	C	837	THR
1	A	107	VAL
1	A	998	GLY
1	B	773	VAL
1	B	326	PRO
1	B	783	PRO
1	C	675	GLY
1	C	975	ILE
1	B	390	ILE
1	B	419	VAL
1	B	464	GLY
1	B	908	GLY
1	B	968	VAL
1	C	372	VAL
1	B	330	THR
1	B	373	PRO
1	C	671	ILE
1	C	689	GLY
1	B	139	VAL
1	C	315	PRO
1	C	658	ILE
1	C	672	VAL

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	833/859 (97%)	706 (85%)	127 (15%)	3 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	833/859 (97%)	700 (84%)	133 (16%)	2	10
1	C	833/859 (97%)	711 (85%)	122 (15%)	3	13
All	All	2499/2577 (97%)	2117 (85%)	382 (15%)	2	12

All (382) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	5	PHE
1	A	10	ILE
1	A	11	PHE
1	A	15	ILE
1	A	17	ILE
1	A	25	LEU
1	A	44	THR
1	A	49	TYR
1	A	57	VAL
1	A	58	GLN
1	A	60	THR
1	A	62	THR
1	A	65	ILE
1	A	69	MET
1	A	70	ASN
1	A	80	SER
1	A	84	SER
1	A	91	THR
1	A	92	LEU
1	A	93	THR
1	A	99	ASP
1	A	101	ASP
1	A	108	GLN
1	A	109	ASN
1	A	112	GLN
1	A	139	VAL
1	A	153	ASP
1	A	168	ARG
1	A	170	SER
1	A	182	TYR
1	A	193	LEU
1	A	213	GLN
1	A	222	THR

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	259	ARG
1	A	277	ILE
1	A	302	THR
1	A	317	PHE
1	A	319	SER
1	A	321	LEU
1	A	323	ILE
1	A	330	THR
1	A	334	LYS
1	A	341	VAL
1	A	348	ILE
1	A	357	LEU
1	A	366	LEU
1	A	367	ILE
1	A	370	ILE
1	A	375	VAL
1	A	379	THR
1	A	395	MET
1	A	400	LEU
1	A	402	ILE
1	A	405	LEU
1	A	417	GLU
1	A	447	MET
1	A	473	THR
1	A	476	SER
1	A	480	LEU
1	A	484	VAL
1	A	498	LYS
1	A	518	ARG
1	A	522	LYS
1	A	523	SER
1	A	527	TYR
1	A	530	SER
1	A	540	ARG
1	A	544	LEU
1	A	548	ILE
1	A	554	TYR
1	A	555	LEU
1	A	556	PHE
1	A	584	GLN
1	A	597	TYR

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Mol	Chain	Res	Type
1	A	600	THR
1	A	603	LYS
1	A	623	ASN
1	A	626	ILE
1	A	630	SER
1	A	634	TRP
1	A	636	ASP
1	A	641	GLU
1	A	653	ARG
1	A	659	LYS
1	A	666	PHE
1	A	668	LEU
1	A	671	ILE
1	A	674	LEU
1	A	680	PHE
1	A	687	GLN
1	A	693	GLU
1	A	713	LEU
1	A	717	ARG
1	A	719	ASN
1	A	724	THR
1	A	741	VAL
1	A	750	LEU
1	A	757	SER
1	A	763	ILE
1	A	773	VAL
1	A	779	TYR
1	A	786	ILE
1	A	795	ASP
1	A	815	ARG
1	A	827	ILE
1	A	830	GLN
1	A	863	SER
1	A	865	GLN
1	A	869	SER
1	A	881	LEU
1	A	899	PHE
1	A	904	VAL
1	A	923	ASN
1	A	927	PHE
1	A	935	ILE
1	A	954	ASP

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Mol	Chain	Res	Type
1	A	960	LEU
1	A	969	ARG
1	A	976	LEU
1	A	978	THR
1	A	982	PHE
1	A	993	THR
1	A	1011	MET
1	A	1021	PHE
1	A	1035	ARG
1	B	4	PHE
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	27	ILE
1	B	30	LEU
1	B	34	GLN
1	B	35	TYR
1	B	48	SER
1	B	49	TYR
1	B	57	VAL
1	B	58	GLN
1	B	59	ASP
1	B	60	THR
1	B	69	MET
1	B	72	ILE
1	B	74	ASN
1	B	81	ASN
1	B	85	THR
1	B	90	ILE
1	B	95	GLU
1	B	96	SER
1	B	102	ILE
1	B	104	GLN
1	B	121	GLU
1	B	125	GLN
1	B	129	VAL
1	B	137	LEU
1	B	143	ILE
1	B	146	ASP
1	B	153	ASP
1	B	161	ASN
1	B	169	THR

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Mol	Chain	Res	Type
1	B	170	SER
1	B	176	GLN
1	B	181	GLN
1	B	182	TYR
1	B	185	ARG
1	B	189	ASN
1	B	193	LEU
1	B	194	ASN
1	B	199	THR
1	B	222	THR
1	B	226	LYS
1	B	235	ILE
1	B	248	LYS
1	B	254	ASN
1	B	261	LEU
1	B	264	ASP
1	B	270	LEU
1	B	289	LEU
1	B	293	LEU
1	B	298	ASN
1	B	307	ARG
1	B	330	THR
1	B	335	ILE
1	B	349	ILE
1	B	356	TYR
1	B	357	LEU
1	B	358	PHE
1	B	359	LEU
1	B	362	PHE
1	B	379	THR
1	B	408	ASP
1	B	417	GLU
1	B	419	VAL
1	B	422	GLU
1	B	435	MET
1	B	438	ILE
1	B	452	VAL
1	B	483	LEU
1	B	495	THR
1	B	496	MET
1	B	515	TRP
1	B	516	PHE

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Mol	Chain	Res	Type
1	B	538	THR
1	B	547	ILE
1	B	556	PHE
1	B	564	LEU
1	B	571	VAL
1	B	596	HIS
1	B	601	LYS
1	B	603	LYS
1	B	613	ASN
1	B	620	ARG
1	B	623	ASN
1	B	629	VAL
1	B	655	PHE
1	B	674	LEU
1	B	696	THR
1	B	702	LEU
1	B	708	LYS
1	B	712	MET
1	B	714	THR
1	B	717	ARG
1	B	729	ILE
1	B	731	ILE
1	B	739	LEU
1	B	743	ILE
1	B	744	ASN
1	B	758	TYR
1	B	761	ASP
1	B	770	LYS
1	B	778	LYS
1	B	782	LEU
1	B	788	ASP
1	B	792	ARG
1	B	795	ASP
1	B	808	ARG
1	B	818	ARG
1	B	836	SER
1	B	842	GLU
1	B	844	MET
1	B	847	LEU
1	B	853	THR
1	B	868	LEU
1	B	871	ASN

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Mol	Chain	Res	Type
1	B	876	LEU
1	B	885	PHE
1	B	895	TRP
1	B	919	ARG
1	B	922	THR
1	B	931	LEU
1	B	945	ILE
1	B	954	ASP
1	B	966	ASP
1	B	971	ARG
1	B	976	LEU
1	B	978	THR
1	B	989	LEU
1	B	1011	MET
1	B	1030	ARG
1	B	1032	ARG
1	C	3	ASN
1	C	13	TRP
1	C	20	MET
1	C	30	LEU
1	C	34	GLN
1	C	38	ILE
1	C	46	SER
1	C	49	TYR
1	C	56	THR
1	C	58	GLN
1	C	75	LEU
1	C	81	ASN
1	C	82	SER
1	C	83	ASP
1	C	89	GLN
1	C	91	THR
1	C	93	THR
1	C	95	GLU
1	C	108	GLN
1	C	109	ASN
1	C	110	LYS
1	C	128	SER
1	C	135	SER
1	C	137	LEU
1	C	146	ASP
1	C	150	THR

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Mol	Chain	Res	Type
1	C	151	GLN
1	C	152	GLU
1	C	163	LYS
1	C	177	LEU
1	C	192	GLU
1	C	205	THR
1	C	208	LYS
1	C	210	GLN
1	C	233	SER
1	C	239	ARG
1	C	240	LEU
1	C	244	GLU
1	C	253	VAL
1	C	255	GLN
1	C	259	ARG
1	C	274	ASN
1	C	319	SER
1	C	321	LEU
1	C	330	THR
1	C	339	GLU
1	C	355	MET
1	C	356	TYR
1	C	367	ILE
1	C	369	THR
1	C	372	VAL
1	C	379	THR
1	C	408	ASP
1	C	422	GLU
1	C	429	GLU
1	C	431	THR
1	C	456	MET
1	C	458	PHE
1	C	459	PHE
1	C	480	LEU
1	C	483	LEU
1	C	497	LEU
1	C	517	ASN
1	C	534	ILE
1	C	542	LEU
1	C	544	LEU
1	C	561	SER
1	C	564	LEU

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Mol	Chain	Res	Type
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	624	THR
1	C	656	SER
1	C	658	ILE
1	C	662	MET
1	C	668	LEU
1	C	671	ILE
1	C	674	LEU
1	C	676	THR
1	C	681	ASP
1	C	684	LEU
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	690	LEU
1	C	693	GLU
1	C	696	THR
1	C	713	LEU
1	C	719	ASN
1	C	739	LEU
1	C	743	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	760	ASN
1	C	767	ARG
1	C	770	LYS
1	C	779	TYR
1	C	808	ARG
1	C	825	MET
1	C	828	LEU
1	C	847	LEU
1	C	849	SER
1	C	877	TYR
1	C	895	TRP
1	C	899	PHE
1	C	907	LEU
1	C	909	VAL
1	C	910	ILE

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Mol	Chain	Res	Type
1	C	917	THR
1	C	921	LEU
1	C	941	ASN
1	C	950	LYS
1	C	954	ASP
1	C	958	LYS
1	C	960	LEU
1	C	965	LEU
1	C	993	THR
1	C	1011	MET
1	C	1017	LEU
1	C	1021	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	81	ASN
1	A	106	GLN
1	A	109	ASN
1	A	112	GLN
1	A	123	GLN
1	A	151	GLN
1	A	181	GLN
1	A	210	GLN
1	A	254	ASN
1	A	282	ASN
1	A	284	GLN
1	A	298	ASN
1	A	338	HIS
1	A	360	GLN
1	A	569	GLN
1	A	584	GLN
1	A	622	GLN
1	A	623	ASN
1	A	667	ASN
1	A	687	GLN
1	A	701	GLN
1	A	709	HIS
1	A	719	ASN
1	A	737	GLN
1	A	846	GLN

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Mol	Chain	Res	Type
1	A	865	GLN
1	A	923	ASN
1	B	34	GLN
1	B	63	GLN
1	B	67	GLN
1	B	68	ASN
1	B	104	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	125	GLN
1	B	144	ASN
1	B	151	GLN
1	B	161	ASN
1	B	189	ASN
1	B	194	ASN
1	B	213	GLN
1	B	231	ASN
1	B	254	ASN
1	B	437	GLN
1	B	526	HIS
1	B	569	GLN
1	B	613	ASN
1	B	692	HIS
1	B	697	GLN
1	B	700	ASN
1	B	726	GLN
1	B	744	ASN
1	B	760	ASN
1	B	820	ASN
1	B	846	GLN
1	B	865	GLN
1	B	871	ASN
1	C	3	ASN
1	C	58	GLN
1	C	63	GLN
1	C	81	ASN
1	C	104	GLN
1	C	144	ASN
1	C	176	GLN
1	C	211	ASN
1	C	213	GLN

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Mol	Chain	Res	Type
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	360	GLN
1	C	415	ASN
1	C	577	GLN
1	C	588	GLN
1	C	592	ASN
1	C	605	ASN
1	C	667	ASN
1	C	687	GLN
1	C	697	GLN
1	C	700	ASN
1	C	709	HIS
1	C	719	ASN
1	C	737	GLN
1	C	760	ASN
1	C	820	ASN
1	C	846	GLN
1	C	923	ASN
1	C	941	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	1022/1053 (97%)	0.18	42 (4%)	37	39	61, 117, 152, 178	0
1	B	1022/1053 (97%)	0.23	46 (4%)	33	36	78, 122, 158, 177	0
1	C	1022/1053 (97%)	0.24	57 (5%)	24	26	59, 113, 162, 190	0
All	All	3066/3159 (97%)	0.22	145 (4%)	31	34	59, 118, 158, 190	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	PHE	7.7
1	C	497	LEU	6.9
1	C	920	GLY	6.0
1	A	1036	LYS	5.4
1	B	963	ALA	5.0
1	C	515	TRP	5.0
1	A	265	VAL	4.5
1	C	7	ASP	4.3
1	B	964	THR	4.3
1	A	515	TRP	4.2
1	C	425	LEU	4.2
1	C	413	VAL	4.2
1	A	390	ILE	4.2
1	B	435	MET	4.1
1	A	497	LEU	4.0
1	B	1035	ARG	3.9
1	C	957	GLY	3.9
1	C	538	THR	3.8
1	B	804	PHE	3.8
1	C	921	LEU	3.7
1	C	541	TYR	3.7
1	A	259	ARG	3.7
1	B	513	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	337	ILE	3.6
1	A	32	VAL	3.5
1	C	416	VAL	3.5
1	C	496	MET	3.5
1	C	539	GLY	3.5
1	C	493	CYS	3.4
1	C	498	LYS	3.4
1	B	532	GLY	3.4
1	C	537	SER	3.3
1	A	230	LEU	3.3
1	A	198	LEU	3.3
1	B	966	ASP	3.3
1	B	7	ASP	3.2
1	B	634	TRP	3.2
1	B	791	VAL	3.2
1	B	801	PHE	3.1
1	C	671	ILE	3.1
1	A	871	ASN	3.1
1	B	779	TYR	3.1
1	B	635	ALA	3.1
1	C	676	THR	3.1
1	C	34	GLN	3.1
1	A	712	MET	3.1
1	B	1033	PHE	3.0
1	C	1033	PHE	3.0
1	C	536	ARG	2.9
1	C	574	THR	2.9
1	C	495	THR	2.9
1	B	535	LEU	2.9
1	C	424	GLY	2.9
1	B	832	ALA	2.8
1	C	540	ARG	2.8
1	C	970	MET	2.8
1	B	362	PHE	2.8
1	A	30	LEU	2.8
1	C	606	VAL	2.8
1	A	420	MET	2.8
1	A	145	THR	2.8
1	B	965	LEU	2.8
1	C	870	GLY	2.8
1	A	419	VAL	2.7
1	B	902	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	437	GLN	2.7
1	A	772	TYR	2.7
1	C	420	MET	2.7
1	C	418	ARG	2.7
1	C	832	ALA	2.7
1	C	560	PRO	2.7
1	A	31	PRO	2.6
1	C	951	ASP	2.6
1	A	287	SER	2.6
1	A	389	SER	2.6
1	C	713	LEU	2.6
1	A	791	VAL	2.5
1	B	368	PRO	2.5
1	B	948	PHE	2.5
1	A	952	LEU	2.5
1	A	246	PHE	2.5
1	A	572	PHE	2.5
1	B	996	GLY	2.5
1	A	251	LEU	2.4
1	C	532	GLY	2.4
1	A	1033	PHE	2.4
1	B	675	GLY	2.4
1	C	900	SER	2.4
1	C	1036	LYS	2.4
1	A	154	ILE	2.4
1	C	514	GLY	2.4
1	A	260	VAL	2.4
1	C	741	VAL	2.4
1	C	262	LEU	2.3
1	C	6	ILE	2.3
1	B	655	PHE	2.3
1	C	399	VAL	2.3
1	B	800	PRO	2.3
1	A	713	LEU	2.3
1	B	198	LEU	2.3
1	C	362	PHE	2.3
1	A	957	GLY	2.3
1	A	229	GLN	2.3
1	A	250	LEU	2.3
1	A	598	TYR	2.3
1	B	541	TYR	2.3
1	B	727	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1034	SER	2.3
1	A	969	ARG	2.2
1	B	895	TRP	2.2
1	B	797	GLN	2.2
1	B	636	ASP	2.2
1	C	492	LEU	2.2
1	B	1026	PHE	2.2
1	B	413	VAL	2.2
1	A	418	ARG	2.2
1	B	967	ALA	2.2
1	C	981	ALA	2.2
1	C	712	MET	2.2
1	A	137	LEU	2.1
1	C	994	GLY	2.1
1	A	196	PHE	2.1
1	C	1026	PHE	2.1
1	C	674	LEU	2.1
1	B	790	TYR	2.1
1	B	595	THR	2.1
1	A	262	LEU	2.1
1	A	518	ARG	2.1
1	B	778	LYS	2.1
1	B	422	GLU	2.1
1	C	919	ARG	2.1
1	B	361	ASN	2.1
1	B	977	MET	2.1
1	A	270	LEU	2.1
1	B	528	THR	2.1
1	C	406	VAL	2.1
1	C	980	LEU	2.1
1	B	563	PHE	2.1
1	A	29	LYS	2.0
1	A	895	TRP	2.0
1	C	641	GLU	2.0
1	C	419	VAL	2.0
1	C	251	LEU	2.0
1	C	265	VAL	2.0
1	B	128	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.