Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:08 AM GMT

PDB ID	:	3O4Z
Title	:	Tel2 structure and function in the Hsp90-dependent maturation of mTOR and ATR complexes
Authors	:	Xie, Y.; Pavletich, N.P.
Deposited on	:	2010-07-27
Resolution	:	3.10 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

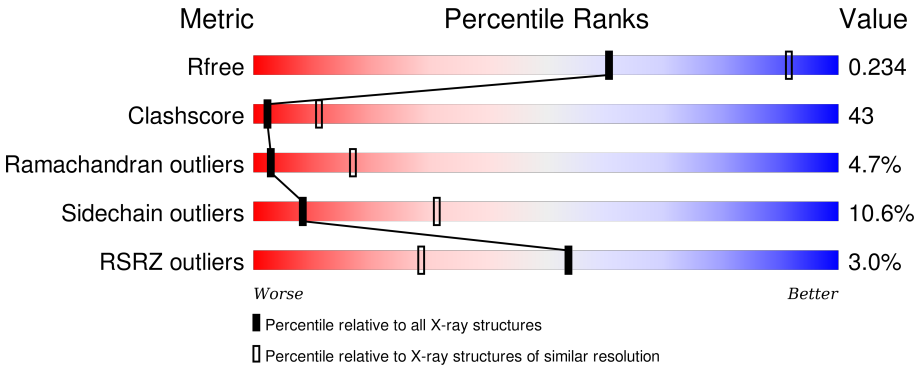
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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 <=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	647	2% 42% 38% 7% • 12%
1	B	647	% 43% 37% 8% • 12%
1	C	647	5% 43% 37% 7% • 12%
1	D	647	3% 42% 38% 8% • 12%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 18452 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 Telomere length regulation protein TEL2.

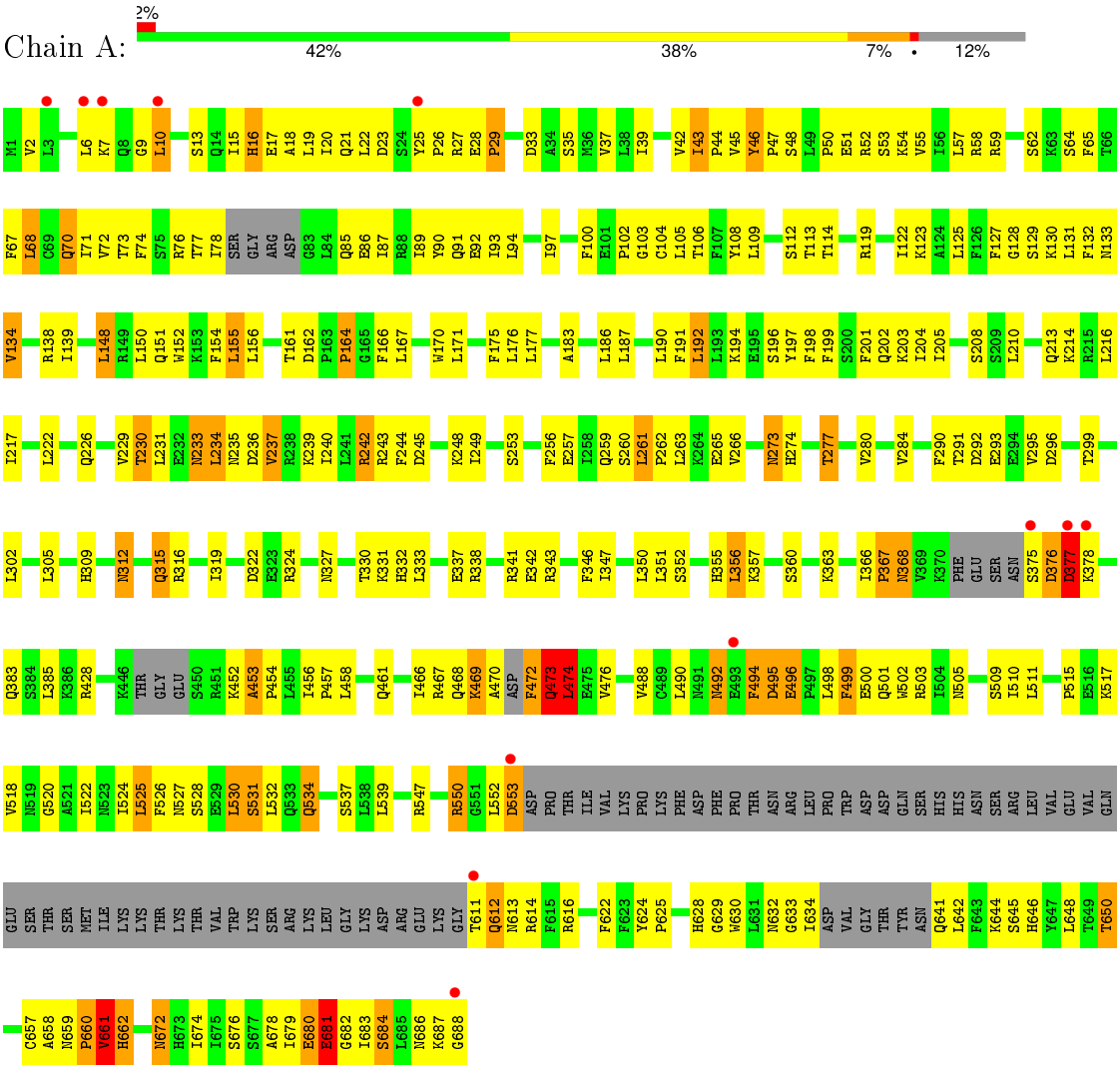
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	B	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	C	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			
1	D	572	Total	C	N	O	S	0	0	0
			4613	2995	769	834	15			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

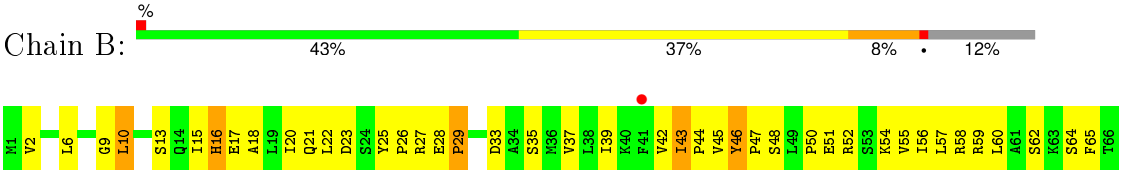
- Molecule 1: Telomere length regulation protein TEL2

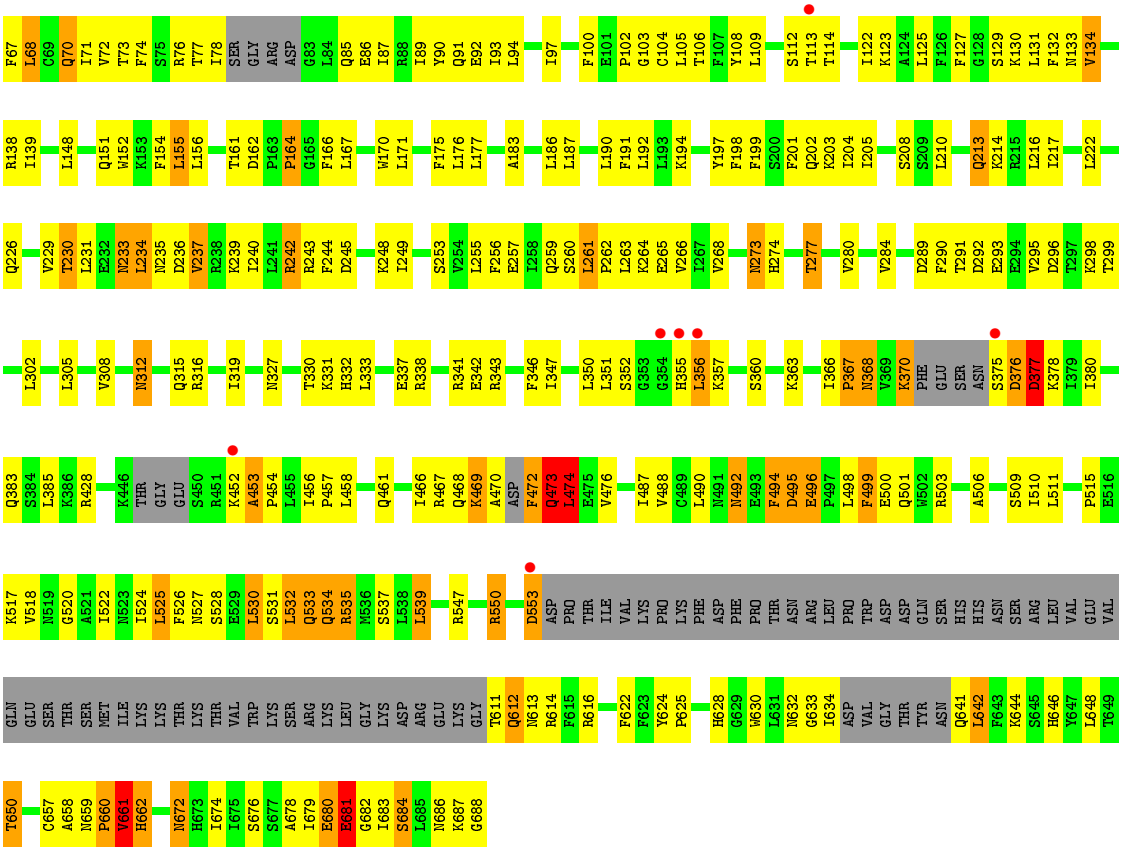
Chain A:



- Molecule 1: Telomere length regulation protein TEL2

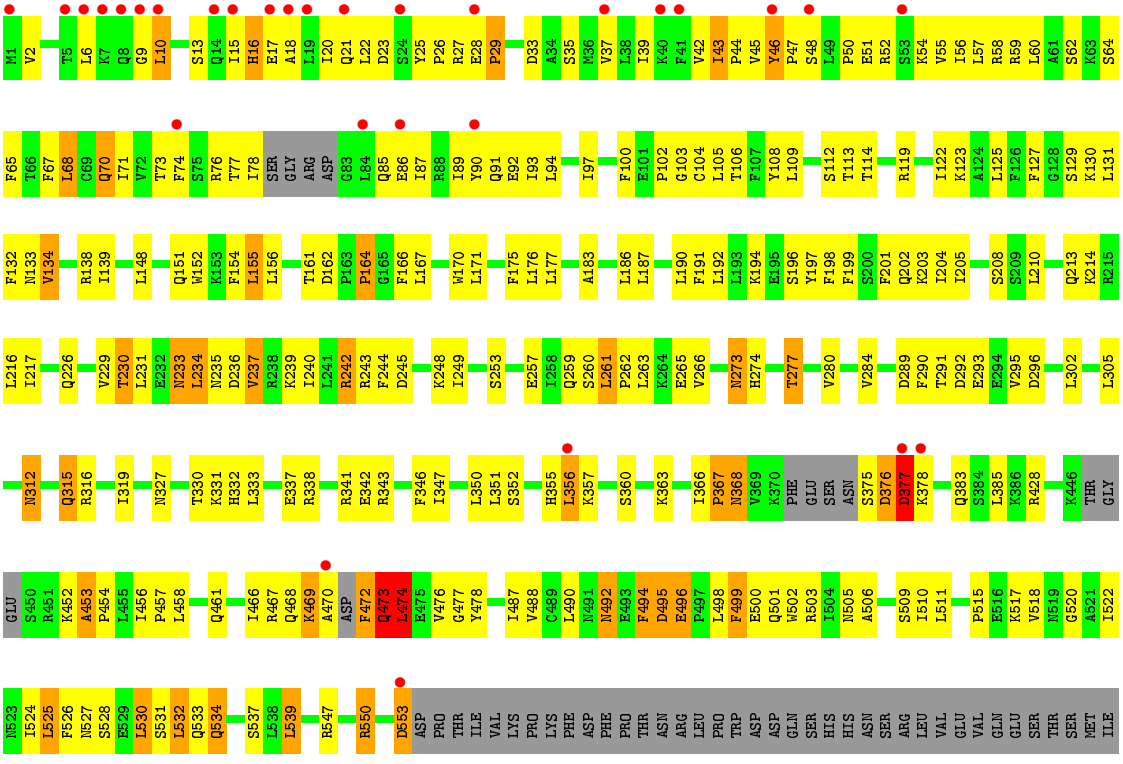
Chain B:

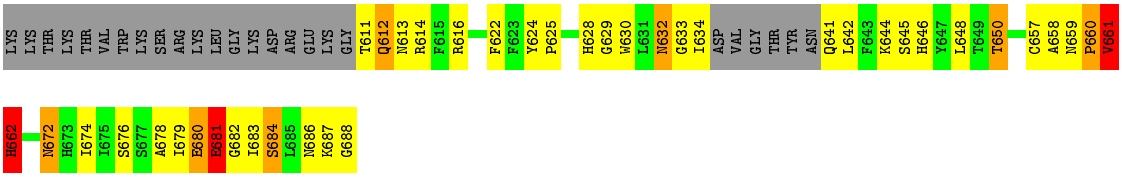


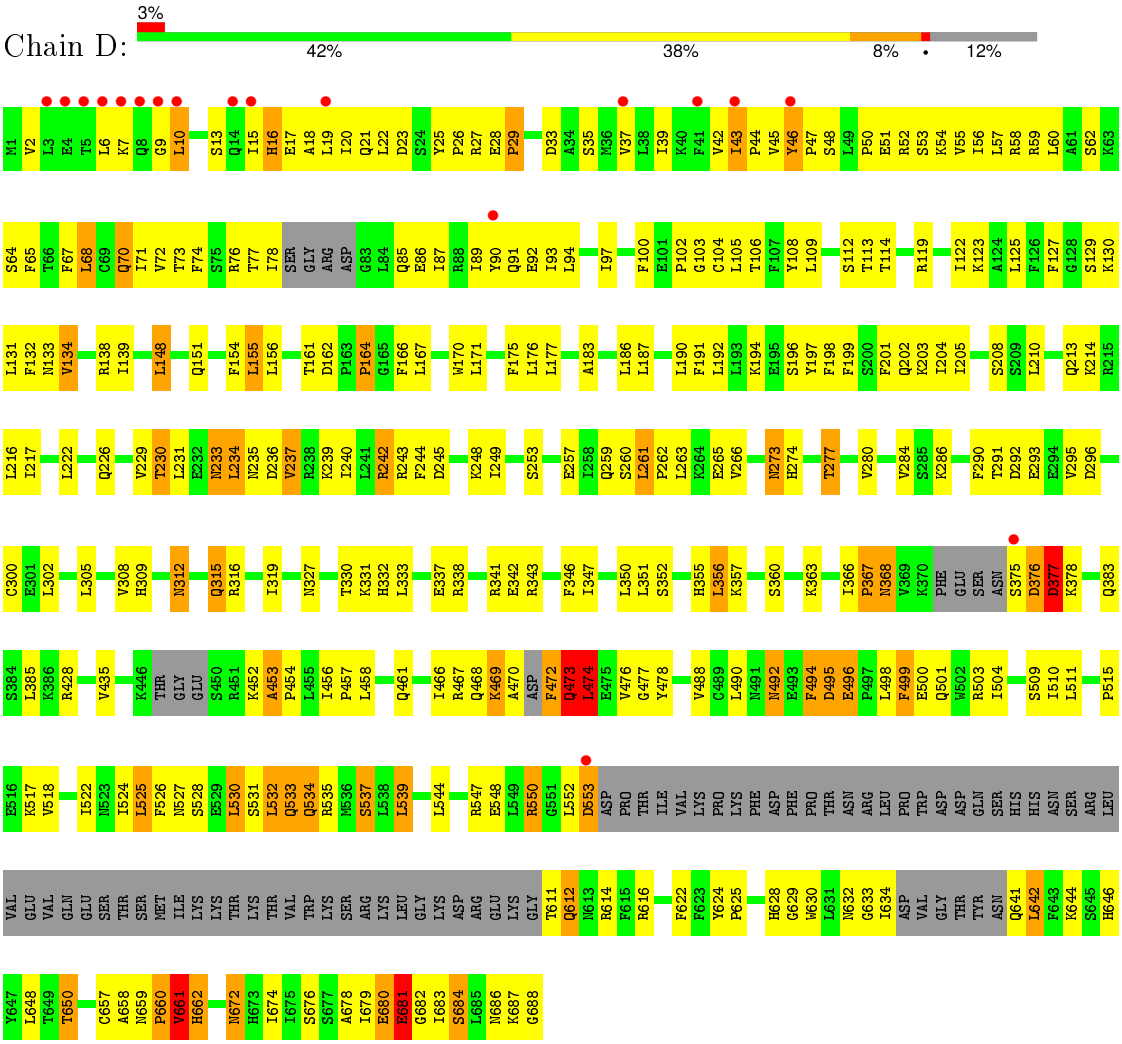


• Molecule 1: Telomere length regulation protein TEL2

Chain C:







• Molecule 1: Telomere length regulation protein TEL2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	91.40Å 123.30Å 162.30Å 90.00° 95.17° 90.00°	Depositor
Resolution (Å)	39.20 – 3.10 39.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	96.2 (39.20-3.10) 95.8 (39.14-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.222 , 0.239 0.221 , 0.234	Depositor DCC
R_{free} test set	2622 reflections (4.35%)	DCC
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 65609 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18452	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.46	0/4696	0.59	1/6331 (0.0%)
1	B	0.43	0/4696	0.57	0/6331
1	C	0.43	0/4696	0.58	0/6331
1	D	0.46	1/4696 (0.0%)	0.59	0/6331
All	All	0.45	1/18784 (0.0%)	0.58	1/25324 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	300	CYS	CB-SG	-5.24	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	GLY	N-CA-C	-5.17	100.19	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4613	0	4747	402	0
1	B	4613	0	4747	419	0
1	C	4613	0	4747	401	0
1	D	4613	0	4747	420	0
All	All	18452	0	18988	1605	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 (1605) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:HIS:NE2	1:B:20:ILE:HD11	1.26	1.46
1:C:16:HIS:NE2	1:C:20:ILE:HD11	1.27	1.46
1:D:16:HIS:NE2	1:D:20:ILE:HD11	1.27	1.45
1:A:16:HIS:NE2	1:A:20:ILE:HD11	1.27	1.44
1:B:305:LEU:HD23	1:B:366:ILE:CD1	1.47	1.43
1:C:305:LEU:HD23	1:C:366:ILE:CD1	1.50	1.41
1:D:305:LEU:HD23	1:D:366:ILE:CD1	1.49	1.39
1:A:305:LEU:HD23	1:A:366:ILE:CD1	1.52	1.38
1:A:6:LEU:HD22	1:A:10:LEU:CD1	1.55	1.36
1:D:6:LEU:HD22	1:D:10:LEU:CD1	1.54	1.36
1:B:6:LEU:HD22	1:B:10:LEU:CD1	1.56	1.35
1:C:6:LEU:HD22	1:C:10:LEU:CD1	1.54	1.35
1:D:9:GLY:O	1:D:10:LEU:HG	1.15	1.32
1:A:6:LEU:CD2	1:A:10:LEU:HD11	1.62	1.30
1:C:9:GLY:O	1:C:10:LEU:HG	1.14	1.29
1:D:6:LEU:CD2	1:D:10:LEU:HD11	1.61	1.29
1:C:6:LEU:CD2	1:C:10:LEU:HD11	1.62	1.29
1:B:9:GLY:O	1:B:10:LEU:HG	1.15	1.28
1:B:6:LEU:CD2	1:B:10:LEU:HD11	1.63	1.26
1:A:9:GLY:O	1:A:10:LEU:HG	1.15	1.23
1:C:472:PHE:HD2	1:C:473:GLN:N	1.36	1.23
1:B:472:PHE:HD2	1:B:473:GLN:N	1.35	1.22
1:A:472:PHE:HD2	1:A:473:GLN:N	1.35	1.21
1:D:472:PHE:HD2	1:D:473:GLN:N	1.34	1.20
1:C:611:THR:O	1:C:612:GLN:HB2	1.36	1.18
1:B:453:ALA:HB1	1:B:454:PRO:CD	1.74	1.18
1:D:155:LEU:O	1:D:155:LEU:HD23	1.44	1.17
1:C:453:ALA:HB1	1:C:454:PRO:CD	1.74	1.17
1:A:453:ALA:HB1	1:A:454:PRO:CD	1.75	1.16
1:B:357:LYS:HB2	1:D:684:SER:HB3	1.19	1.15
1:C:155:LEU:HD23	1:C:155:LEU:O	1.46	1.15
1:D:453:ALA:HB1	1:D:454:PRO:CD	1.75	1.14
1:B:687:LYS:HE2	1:D:338:ARG:HH22	1.10	1.14
1:A:155:LEU:HD23	1:A:155:LEU:O	1.45	1.14
1:B:611:THR:O	1:B:612:GLN:HB2	1.36	1.13
1:B:155:LEU:O	1:B:155:LEU:HD23	1.45	1.13
1:D:51:GLU:O	1:D:55:VAL:HG23	1.50	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HD22	1:B:10:LEU:HD11	1.14	1.11
1:A:611:THR:O	1:A:612:GLN:HB2	1.37	1.11
1:D:611:THR:O	1:D:612:GLN:HB2	1.36	1.11
1:A:51:GLU:O	1:A:55:VAL:HG23	1.51	1.11
1:C:51:GLU:O	1:C:55:VAL:HG23	1.52	1.10
1:B:16:HIS:HE2	1:B:20:ILE:CD1	1.65	1.09
1:C:305:LEU:HD23	1:C:366:ILE:HD11	1.12	1.08
1:D:9:GLY:O	1:D:10:LEU:CG	2.01	1.08
1:A:9:GLY:O	1:A:10:LEU:CG	2.01	1.08
1:D:6:LEU:HD22	1:D:10:LEU:HD11	1.13	1.08
1:C:9:GLY:O	1:C:10:LEU:CG	2.00	1.08
1:C:16:HIS:HE2	1:C:20:ILE:CD1	1.66	1.08
1:B:9:GLY:O	1:B:10:LEU:CG	2.01	1.08
1:B:51:GLU:O	1:B:55:VAL:HG23	1.52	1.08
1:B:367:PRO:O	1:B:368:ASN:HB2	1.54	1.07
1:A:550:ARG:HH22	1:A:660:PRO:HD3	1.18	1.07
1:C:367:PRO:O	1:C:368:ASN:HB2	1.54	1.07
1:D:16:HIS:HE2	1:D:20:ILE:CD1	1.67	1.07
1:B:2:VAL:HB	1:B:22:LEU:HD21	1.37	1.07
1:A:16:HIS:HE2	1:A:20:ILE:CD1	1.66	1.06
1:A:305:LEU:HD23	1:A:366:ILE:HD11	1.11	1.06
1:A:2:VAL:HB	1:A:22:LEU:HD21	1.37	1.06
1:D:305:LEU:HD23	1:D:366:ILE:HD11	1.13	1.06
1:D:533:GLN:HA	1:D:533:GLN:OE1	1.49	1.06
1:A:367:PRO:O	1:A:368:ASN:HB2	1.56	1.06
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.20	1.05
1:D:2:VAL:HB	1:D:22:LEU:HD21	1.35	1.05
1:D:550:ARG:HH11	1:D:550:ARG:HG2	1.17	1.05
1:B:550:ARG:HH11	1:B:550:ARG:HG2	1.19	1.05
1:A:687:LYS:HE2	1:C:338:ARG:HH22	0.97	1.05
1:C:16:HIS:CD2	1:C:20:ILE:HD11	1.91	1.04
1:C:550:ARG:HH22	1:C:660:PRO:HD3	1.20	1.04
1:D:16:HIS:CD2	1:D:20:ILE:HD11	1.91	1.04
1:B:16:HIS:CD2	1:B:20:ILE:HD11	1.91	1.04
1:D:550:ARG:HH22	1:D:660:PRO:HD3	1.19	1.04
1:D:6:LEU:HD22	1:D:10:LEU:HD13	1.39	1.04
1:D:453:ALA:CB	1:D:454:PRO:HD2	1.88	1.04
1:B:550:ARG:HH22	1:B:660:PRO:HD3	1.20	1.04
1:C:16:HIS:NE2	1:C:20:ILE:CD1	2.21	1.04
1:B:305:LEU:HD23	1:B:366:ILE:HD11	1.08	1.04
1:A:16:HIS:CD2	1:A:20:ILE:HD11	1.92	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:533:GLN:OE1	1:B:533:GLN:HA	1.53	1.03
1:B:6:LEU:CD2	1:B:10:LEU:CD1	2.30	1.03
1:C:2:VAL:HB	1:C:22:LEU:HD21	1.35	1.03
1:B:453:ALA:CB	1:B:454:PRO:HD2	1.88	1.03
1:C:632:ASN:C	1:C:632:ASN:HD22	1.53	1.03
1:C:453:ALA:CB	1:C:454:PRO:HD2	1.87	1.03
1:D:156:LEU:HD23	1:D:197:TYR:CD2	1.94	1.03
1:A:202:GLN:HE22	1:A:243:ARG:NH1	1.58	1.02
1:D:6:LEU:CD2	1:D:10:LEU:CD1	2.28	1.02
1:A:453:ALA:CB	1:A:454:PRO:HD2	1.90	1.02
1:C:550:ARG:HH11	1:C:550:ARG:HG2	1.20	1.02
1:D:273:ASN:O	1:D:277:THR:HG22	1.59	1.02
1:D:367:PRO:O	1:D:368:ASN:HB2	1.55	1.02
1:A:6:LEU:HD22	1:A:10:LEU:HD13	1.40	1.02
1:C:6:LEU:HD22	1:C:10:LEU:HD11	1.13	1.02
1:D:16:HIS:NE2	1:D:20:ILE:CD1	2.21	1.01
1:B:273:ASN:O	1:B:277:THR:HG22	1.60	1.01
1:B:16:HIS:NE2	1:B:20:ILE:CD1	2.20	1.01
1:B:156:LEU:HD23	1:B:197:TYR:CD2	1.96	1.01
1:C:6:LEU:CD2	1:C:10:LEU:CD1	2.28	1.01
1:C:156:LEU:HD23	1:C:197:TYR:CD2	1.96	1.01
1:A:6:LEU:CD2	1:A:10:LEU:CD1	2.28	1.00
1:B:6:LEU:HD22	1:B:10:LEU:HD13	1.41	1.00
1:C:453:ALA:CB	1:C:454:PRO:CD	2.38	1.00
1:C:273:ASN:O	1:C:277:THR:HG22	1.59	1.00
1:A:687:LYS:HE2	1:C:338:ARG:NH2	1.75	1.00
1:C:6:LEU:HD22	1:C:10:LEU:HD13	1.39	1.00
1:A:6:LEU:HD22	1:A:10:LEU:HD11	1.13	1.00
1:A:338:ARG:HH22	1:C:687:LYS:HE2	1.21	1.00
1:A:156:LEU:HD23	1:A:197:TYR:CD2	1.97	1.00
1:C:226:GLN:HE22	1:C:259:GLN:N	1.59	0.99
1:A:16:HIS:NE2	1:A:20:ILE:CD1	2.21	0.99
1:A:453:ALA:CB	1:A:454:PRO:CD	2.40	0.99
1:A:466:ILE:HD13	1:A:510:ILE:HG12	1.44	0.99
1:B:453:ALA:CB	1:B:454:PRO:CD	2.38	0.99
1:B:226:GLN:HE22	1:B:259:GLN:N	1.61	0.99
1:A:226:GLN:HE22	1:A:259:GLN:N	1.59	0.99
1:D:468:GLN:O	1:D:468:GLN:HG3	1.63	0.99
1:C:106:THR:HG21	1:C:154:PHE:CD1	1.99	0.98
1:A:453:ALA:HB1	1:A:454:PRO:HD3	1.45	0.98
1:D:550:ARG:HH11	1:D:550:ARG:CG	1.74	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:HD23	1:C:366:ILE:CG1	1.93	0.98
1:A:273:ASN:O	1:A:277:THR:HG22	1.61	0.98
1:B:305:LEU:HD23	1:B:366:ILE:CG1	1.93	0.97
1:D:106:THR:HG21	1:D:154:PHE:CD1	1.99	0.97
1:D:466:ILE:HD13	1:D:510:ILE:HG12	1.43	0.97
1:A:205:ILE:HD11	1:A:244:PHE:CE1	1.99	0.97
1:D:305:LEU:HD23	1:D:366:ILE:CG1	1.94	0.97
1:B:466:ILE:HD13	1:B:510:ILE:HG12	1.43	0.97
1:A:550:ARG:CG	1:A:550:ARG:HH11	1.78	0.97
1:C:16:HIS:CD2	1:C:20:ILE:CD1	2.48	0.97
1:B:453:ALA:HB1	1:B:454:PRO:HD3	1.44	0.97
1:B:305:LEU:CD2	1:B:366:ILE:HD11	1.94	0.97
1:B:16:HIS:CD2	1:B:20:ILE:CD1	2.48	0.97
1:D:226:GLN:HE22	1:D:259:GLN:N	1.61	0.97
1:C:453:ALA:HB1	1:C:454:PRO:HD3	1.45	0.96
1:B:106:THR:HG21	1:B:154:PHE:CD1	1.99	0.96
1:B:468:GLN:O	1:B:468:GLN:HG3	1.62	0.96
1:A:106:THR:HG21	1:A:154:PHE:CD1	2.00	0.96
1:C:466:ILE:HD13	1:C:510:ILE:HG12	1.43	0.96
1:A:468:GLN:HG3	1:A:468:GLN:O	1.62	0.96
1:A:305:LEU:HD23	1:A:366:ILE:CG1	1.95	0.96
1:C:226:GLN:HE22	1:C:259:GLN:H	0.96	0.96
1:A:226:GLN:HE22	1:A:259:GLN:H	0.97	0.96
1:D:16:HIS:CD2	1:D:20:ILE:CD1	2.48	0.95
1:D:453:ALA:HB1	1:D:454:PRO:HD3	1.45	0.95
1:A:16:HIS:CD2	1:A:20:ILE:CD1	2.48	0.95
1:D:205:ILE:HG22	1:D:216:LEU:HD13	1.47	0.95
1:D:226:GLN:HE22	1:D:259:GLN:H	0.96	0.95
1:C:550:ARG:HH11	1:C:550:ARG:CG	1.78	0.94
1:C:2:VAL:CB	1:C:22:LEU:HD21	1.97	0.94
1:D:305:LEU:CD2	1:D:366:ILE:HD11	1.98	0.94
1:B:226:GLN:HE22	1:B:259:GLN:H	0.99	0.94
1:C:205:ILE:HG22	1:C:216:LEU:HD13	1.49	0.94
1:C:202:GLN:HE22	1:C:243:ARG:HH11	0.98	0.94
1:C:468:GLN:HG3	1:C:468:GLN:O	1.63	0.93
1:B:305:LEU:CD2	1:B:366:ILE:CD1	2.44	0.93
1:D:453:ALA:CB	1:D:454:PRO:CD	2.38	0.93
1:B:2:VAL:CB	1:B:22:LEU:HD21	1.98	0.93
1:C:312:ASN:H	1:C:315:GLN:HE21	1.16	0.93
1:B:550:ARG:HH11	1:B:550:ARG:CG	1.79	0.93
1:D:202:GLN:HE22	1:D:243:ARG:HH11	0.97	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:LEU:CD2	1:C:366:ILE:HD11	1.98	0.93
1:B:205:ILE:HG22	1:B:216:LEU:HD13	1.48	0.93
1:D:2:VAL:CB	1:D:22:LEU:HD21	1.97	0.92
1:D:205:ILE:HD11	1:D:244:PHE:CE1	2.04	0.92
1:B:202:GLN:HE22	1:B:243:ARG:HH11	0.92	0.92
1:A:113:THR:HG21	1:A:166:PHE:CZ	2.04	0.92
1:D:6:LEU:HD23	1:D:10:LEU:HD21	1.52	0.92
1:B:256:PHE:HZ	1:B:299:THR:HG1	0.97	0.92
1:A:305:LEU:CD2	1:A:366:ILE:HD11	1.98	0.92
1:A:2:VAL:CB	1:A:22:LEU:HD21	1.99	0.92
1:D:78:ILE:HG22	1:D:87:ILE:CG1	2.00	0.92
1:C:113:THR:HG21	1:C:166:PHE:CZ	2.05	0.91
1:D:113:THR:HG21	1:D:166:PHE:CZ	2.04	0.91
1:A:155:LEU:HD23	1:A:155:LEU:C	1.90	0.91
1:A:312:ASN:H	1:A:315:GLN:HE21	1.13	0.91
1:B:472:PHE:CD2	1:B:473:GLN:N	2.21	0.91
1:C:472:PHE:CD2	1:C:473:GLN:N	2.20	0.91
1:A:202:GLN:NE2	1:A:243:ARG:HH11	1.69	0.91
1:B:155:LEU:C	1:B:155:LEU:HD23	1.91	0.91
1:B:360:SER:HB2	1:D:687:LYS:NZ	1.85	0.91
1:D:155:LEU:C	1:D:155:LEU:HD23	1.92	0.91
1:A:205:ILE:HG22	1:A:216:LEU:HD13	1.53	0.90
1:B:113:THR:HG21	1:B:166:PHE:CZ	2.06	0.90
1:D:661:VAL:O	1:D:662:HIS:HB3	1.71	0.90
1:A:472:PHE:CD2	1:A:473:GLN:N	2.20	0.90
1:B:202:GLN:HE22	1:B:243:ARG:NH1	1.68	0.90
1:D:240:ILE:HD11	1:D:385:LEU:HD11	1.54	0.90
1:A:661:VAL:O	1:A:662:HIS:HB3	1.71	0.90
1:B:305:LEU:HA	1:B:366:ILE:CD1	2.02	0.89
1:B:240:ILE:HD11	1:B:385:LEU:HD11	1.53	0.89
1:B:312:ASN:H	1:B:315:GLN:HE21	1.16	0.89
1:C:474:LEU:HG	1:C:476:VAL:HG23	1.54	0.89
1:C:155:LEU:HD23	1:C:155:LEU:C	1.91	0.89
1:C:13:SER:O	1:C:17:GLU:HG3	1.73	0.89
1:C:6:LEU:HD23	1:C:10:LEU:HD21	1.52	0.89
1:B:205:ILE:HD11	1:B:244:PHE:CE1	2.08	0.89
1:A:468:GLN:O	1:A:468:GLN:CG	2.21	0.89
1:D:305:LEU:HA	1:D:366:ILE:CD1	2.02	0.88
1:B:658:ALA:O	1:B:661:VAL:HG23	1.72	0.88
1:B:106:THR:HG21	1:B:154:PHE:HD1	1.39	0.88
1:A:171:LEU:HD21	1:A:175:PHE:HE2	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:SER:O	1:B:17:GLU:HG3	1.73	0.88
1:C:661:VAL:O	1:C:662:HIS:HB3	1.70	0.88
1:A:13:SER:O	1:A:17:GLU:HG3	1.74	0.88
1:C:305:LEU:HA	1:C:366:ILE:CD1	2.01	0.88
1:C:658:ALA:O	1:C:661:VAL:HG23	1.73	0.88
1:D:312:ASN:H	1:D:315:GLN:HE21	1.17	0.88
1:D:202:GLN:HE22	1:D:243:ARG:NH1	1.71	0.88
1:C:112:SER:OG	1:C:122:ILE:HD11	1.74	0.88
1:B:6:LEU:HD23	1:B:10:LEU:HD21	1.56	0.87
1:D:13:SER:O	1:D:17:GLU:HG3	1.73	0.87
1:B:474:LEU:HG	1:B:476:VAL:HG23	1.57	0.87
1:B:687:LYS:HE2	1:D:338:ARG:NH2	1.88	0.87
1:B:202:GLN:NE2	1:B:243:ARG:HH11	1.72	0.87
1:D:474:LEU:HG	1:D:476:VAL:HG23	1.55	0.87
1:C:468:GLN:CG	1:C:468:GLN:O	2.22	0.87
1:D:112:SER:OG	1:D:122:ILE:HD11	1.74	0.87
1:D:171:LEU:HD21	1:D:175:PHE:HE2	1.38	0.86
1:A:474:LEU:HG	1:A:476:VAL:HG23	1.56	0.86
1:B:370:LYS:CD	1:B:370:LYS:N	2.36	0.86
1:B:468:GLN:O	1:B:468:GLN:CG	2.23	0.86
1:A:305:LEU:HA	1:A:366:ILE:CD1	2.05	0.86
1:B:210:LEU:HD23	1:B:210:LEU:C	1.96	0.86
1:C:90:TYR:O	1:C:93:ILE:HG22	1.75	0.86
1:A:112:SER:OG	1:A:122:ILE:HD11	1.76	0.86
1:D:90:TYR:O	1:D:93:ILE:HG22	1.75	0.85
1:A:453:ALA:HB1	1:A:454:PRO:HD2	1.55	0.85
1:B:112:SER:OG	1:B:122:ILE:HD11	1.76	0.85
1:A:106:THR:HG21	1:A:154:PHE:HD1	1.39	0.85
1:B:171:LEU:HD21	1:B:175:PHE:HE2	1.40	0.85
1:B:338:ARG:HH22	1:D:687:LYS:HE2	1.41	0.85
1:A:16:HIS:ND1	1:A:50:PRO:CG	2.39	0.85
1:D:468:GLN:O	1:D:468:GLN:CG	2.22	0.85
1:C:171:LEU:HD21	1:C:175:PHE:HE2	1.40	0.85
1:C:205:ILE:HD11	1:C:244:PHE:CE1	2.12	0.85
1:D:106:THR:HG21	1:D:154:PHE:HD1	1.39	0.85
1:A:20:ILE:HG23	1:A:52:ARG:HH12	1.42	0.84
1:B:661:VAL:O	1:B:662:HIS:HB3	1.74	0.84
1:C:632:ASN:HD22	1:C:633:GLY:N	1.74	0.84
1:D:210:LEU:HD23	1:D:210:LEU:O	1.76	0.84
1:C:106:THR:HG21	1:C:154:PHE:HD1	1.39	0.84
1:D:658:ALA:O	1:D:661:VAL:HG23	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD23	1:A:10:LEU:HD21	1.56	0.84
1:D:472:PHE:CD2	1:D:473:GLN:N	2.20	0.84
1:A:202:GLN:HE22	1:A:243:ARG:HH11	0.88	0.84
1:C:210:LEU:O	1:C:210:LEU:HD23	1.76	0.84
1:C:210:LEU:HD23	1:C:210:LEU:C	1.97	0.84
1:C:202:GLN:NE2	1:C:243:ARG:HH11	1.74	0.84
1:D:305:LEU:CD2	1:D:366:ILE:CD1	2.46	0.84
1:C:632:ASN:C	1:C:632:ASN:ND2	2.30	0.84
1:B:210:LEU:HD23	1:B:210:LEU:O	1.77	0.84
1:D:65:PHE:HB2	1:D:108:TYR:CD2	2.13	0.84
1:D:202:GLN:NE2	1:D:243:ARG:HH11	1.75	0.84
1:A:550:ARG:HH22	1:A:660:PRO:CD	1.91	0.84
1:B:90:TYR:O	1:B:93:ILE:HG22	1.78	0.84
1:A:240:ILE:HD11	1:A:385:LEU:HD11	1.59	0.84
1:D:210:LEU:HD23	1:D:210:LEU:C	1.97	0.83
1:C:202:GLN:HE22	1:C:243:ARG:NH1	1.75	0.83
1:A:518:VAL:HG21	1:A:622:PHE:CZ	2.14	0.83
1:A:90:TYR:O	1:A:93:ILE:HG22	1.77	0.83
1:C:305:LEU:CD2	1:C:366:ILE:HG13	2.09	0.83
1:A:492:ASN:ND2	1:A:495:ASP:HA	1.93	0.83
1:D:550:ARG:HH22	1:D:660:PRO:CD	1.91	0.83
1:A:210:LEU:C	1:A:210:LEU:HD23	1.99	0.83
1:C:518:VAL:HG21	1:C:622:PHE:CZ	2.14	0.83
1:D:492:ASN:ND2	1:D:495:ASP:HA	1.94	0.82
1:D:2:VAL:HB	1:D:22:LEU:CD2	2.08	0.82
1:A:113:THR:O	1:A:113:THR:HG22	1.79	0.82
1:B:65:PHE:CE2	1:B:122:ILE:HG12	2.14	0.82
1:B:2:VAL:HB	1:B:22:LEU:CD2	2.09	0.82
1:D:518:VAL:HG21	1:D:622:PHE:CE1	2.14	0.82
1:B:644:LYS:HB3	1:B:683:ILE:HD13	1.60	0.82
1:D:518:VAL:HG21	1:D:622:PHE:CZ	2.14	0.82
1:A:210:LEU:O	1:A:210:LEU:HD23	1.79	0.82
1:C:550:ARG:HH22	1:C:660:PRO:CD	1.92	0.82
1:A:658:ALA:O	1:A:661:VAL:HG23	1.79	0.82
1:B:518:VAL:HG21	1:B:622:PHE:CZ	2.15	0.82
1:A:644:LYS:HB3	1:A:683:ILE:HD13	1.62	0.82
1:C:644:LYS:HB3	1:C:683:ILE:HD13	1.62	0.82
1:B:305:LEU:CD2	1:B:366:ILE:HG13	2.09	0.82
1:C:65:PHE:HB2	1:C:108:TYR:CD2	2.15	0.82
1:C:492:ASN:ND2	1:C:495:ASP:HA	1.95	0.81
1:D:305:LEU:CD2	1:D:366:ILE:HG13	2.09	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:THR:HB	1:B:155:LEU:HB2	1.63	0.81
1:A:2:VAL:HB	1:A:22:LEU:CD2	2.10	0.81
1:C:2:VAL:HB	1:C:22:LEU:CD2	2.08	0.81
1:B:376:ASP:OD1	1:B:376:ASP:N	2.12	0.81
1:D:65:PHE:CE2	1:D:122:ILE:HG12	2.15	0.81
1:D:230:THR:H	1:D:233:ASN:HB2	1.45	0.81
1:C:376:ASP:N	1:C:376:ASP:OD1	2.13	0.81
1:B:113:THR:O	1:B:113:THR:HG22	1.81	0.81
1:B:492:ASN:ND2	1:B:495:ASP:HA	1.94	0.81
1:C:78:ILE:HG22	1:C:87:ILE:CG1	2.11	0.80
1:A:106:THR:HB	1:A:155:LEU:HB2	1.64	0.80
1:B:230:THR:H	1:B:233:ASN:HB2	1.45	0.80
1:A:230:THR:H	1:A:233:ASN:HB2	1.46	0.80
1:A:305:LEU:CD2	1:A:366:ILE:HG13	2.11	0.80
1:B:533:GLN:CA	1:B:533:GLN:OE1	2.30	0.80
1:C:453:ALA:HB3	1:C:454:PRO:HD2	1.64	0.80
1:B:531:SER:H	1:B:534:GLN:HG3	1.46	0.80
1:D:453:ALA:HB1	1:D:454:PRO:HD2	1.54	0.80
1:B:68:LEU:HD22	1:B:125:LEU:HD21	1.64	0.80
1:C:230:THR:H	1:C:233:ASN:HB2	1.46	0.80
1:D:644:LYS:HB3	1:D:683:ILE:HD13	1.62	0.79
1:A:376:ASP:OD1	1:A:376:ASP:N	2.13	0.79
1:C:305:LEU:CD2	1:C:366:ILE:CD1	2.47	0.79
1:C:226:GLN:NE2	1:C:259:GLN:H	1.78	0.79
1:C:518:VAL:HG21	1:C:622:PHE:CE1	2.17	0.79
1:D:6:LEU:HD23	1:D:10:LEU:HD11	1.65	0.79
1:C:113:THR:O	1:C:113:THR:HG22	1.80	0.79
1:A:518:VAL:HG21	1:A:622:PHE:CE1	2.18	0.79
1:B:550:ARG:HH22	1:B:660:PRO:CD	1.93	0.79
1:D:226:GLN:NE2	1:D:259:GLN:H	1.79	0.79
1:D:113:THR:HG22	1:D:113:THR:O	1.81	0.79
1:D:453:ALA:HB3	1:D:454:PRO:HD2	1.63	0.79
1:D:533:GLN:CA	1:D:533:GLN:OE1	2.30	0.79
1:A:65:PHE:CE2	1:A:122:ILE:HG12	2.18	0.79
1:B:531:SER:O	1:B:532:LEU:C	2.20	0.78
1:A:357:LYS:HB2	1:C:684:SER:HB3	1.62	0.78
1:B:518:VAL:HG21	1:B:622:PHE:CE1	2.19	0.78
1:B:205:ILE:HD11	1:B:244:PHE:CD1	2.18	0.78
1:A:205:ILE:HD11	1:A:244:PHE:CD1	2.18	0.78
1:B:453:ALA:HB3	1:B:454:PRO:HD2	1.64	0.78
1:D:550:ARG:CG	1:D:550:ARG:NH1	2.42	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:LEU:HD23	1:B:10:LEU:HD11	1.66	0.78
1:D:492:ASN:CG	1:D:495:ASP:HA	2.04	0.78
1:B:467:ARG:NH1	1:B:509:SER:HB3	1.99	0.78
1:A:467:ARG:NH1	1:A:509:SER:HB3	1.99	0.77
1:A:468:GLN:O	1:A:469:LYS:CB	2.32	0.77
1:C:472:PHE:O	1:C:474:LEU:HD23	1.85	0.77
1:A:492:ASN:CG	1:A:495:ASP:HA	2.04	0.77
1:D:376:ASP:N	1:D:376:ASP:OD1	2.15	0.77
1:B:468:GLN:O	1:B:469:LYS:CB	2.33	0.77
1:B:305:LEU:CD2	1:B:366:ILE:CG1	2.63	0.77
1:A:226:GLN:NE2	1:A:259:GLN:H	1.80	0.76
1:D:65:PHE:CZ	1:D:122:ILE:HG12	2.20	0.76
1:C:492:ASN:CG	1:C:495:ASP:HA	2.04	0.76
1:B:42:VAL:C	1:B:44:PRO:HD2	2.06	0.76
1:B:226:GLN:NE2	1:B:259:GLN:H	1.81	0.76
1:C:65:PHE:CE2	1:C:122:ILE:HG12	2.21	0.76
1:A:6:LEU:HD23	1:A:10:LEU:HD11	1.64	0.76
1:A:202:GLN:NE2	1:A:243:ARG:NH1	2.27	0.76
1:D:205:ILE:HD11	1:D:244:PHE:CD1	2.20	0.76
1:C:467:ARG:NH1	1:C:509:SER:HB3	2.01	0.76
1:A:550:ARG:NH2	1:A:660:PRO:HD3	2.00	0.76
1:D:106:THR:HB	1:D:155:LEU:HB2	1.66	0.76
1:B:492:ASN:CG	1:B:495:ASP:HA	2.05	0.76
1:D:467:ARG:NH1	1:D:509:SER:HB3	2.01	0.76
1:A:453:ALA:HB3	1:A:454:PRO:HD2	1.66	0.76
1:D:472:PHE:O	1:D:474:LEU:HD23	1.85	0.75
1:C:106:THR:HB	1:C:155:LEU:HB2	1.66	0.75
1:A:42:VAL:C	1:A:44:PRO:HD2	2.06	0.75
1:C:42:VAL:C	1:C:44:PRO:HD2	2.06	0.75
1:D:20:ILE:HG23	1:D:52:ARG:HH12	1.52	0.75
1:C:305:LEU:CD2	1:C:366:ILE:CG1	2.64	0.75
1:B:628:HIS:O	1:B:632:ASN:ND2	2.20	0.75
1:A:16:HIS:ND1	1:A:50:PRO:HG2	2.01	0.74
1:D:74:PHE:CE1	1:D:78:ILE:CD1	2.71	0.74
1:A:74:PHE:CE1	1:A:78:ILE:CD1	2.69	0.74
1:B:16:HIS:ND1	1:B:50:PRO:CG	2.50	0.74
1:A:16:HIS:ND1	1:A:50:PRO:HG3	2.02	0.74
1:B:472:PHE:O	1:B:474:LEU:HD23	1.87	0.74
1:B:74:PHE:CE1	1:B:78:ILE:CD1	2.70	0.74
1:A:472:PHE:O	1:A:474:LEU:HD23	1.87	0.74
1:C:73:THR:O	1:C:77:THR:HG23	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:CD2	1:A:366:ILE:CD1	2.49	0.74
1:B:375:SER:C	1:B:376:ASP:OD1	2.26	0.74
1:C:658:ALA:O	1:C:661:VAL:CG2	2.36	0.74
1:C:74:PHE:CE1	1:C:78:ILE:CD1	2.70	0.74
1:D:280:VAL:HG11	1:D:319:ILE:HD11	1.70	0.74
1:D:611:THR:O	1:D:612:GLN:CB	2.24	0.73
1:C:375:SER:C	1:C:376:ASP:OD1	2.27	0.73
1:B:330:THR:OG1	1:D:672:ASN:HB3	1.88	0.73
1:A:628:HIS:O	1:A:632:ASN:ND2	2.21	0.73
1:C:6:LEU:HD23	1:C:10:LEU:HD11	1.65	0.73
1:C:468:GLN:O	1:C:469:LYS:CB	2.34	0.73
1:B:74:PHE:CZ	1:B:78:ILE:HD11	2.24	0.73
1:B:20:ILE:HG23	1:B:52:ARG:HH12	1.51	0.73
1:C:550:ARG:HD2	1:C:550:ARG:O	1.88	0.73
1:D:42:VAL:C	1:D:44:PRO:HD2	2.08	0.73
1:B:684:SER:HB3	1:D:357:LYS:HB2	1.71	0.73
1:C:45:VAL:C	1:C:47:PRO:HD2	2.09	0.73
1:D:628:HIS:O	1:D:632:ASN:ND2	2.22	0.73
1:A:73:THR:O	1:A:77:THR:HG23	1.88	0.73
1:B:217:ILE:HD12	1:B:249:ILE:HD13	1.71	0.73
1:C:74:PHE:CZ	1:C:78:ILE:HD11	2.24	0.73
1:D:305:LEU:CD2	1:D:366:ILE:CG1	2.64	0.73
1:D:6:LEU:HD23	1:D:10:LEU:CD2	2.18	0.73
1:D:113:THR:HG21	1:D:166:PHE:HZ	1.54	0.73
1:C:515:PRO:O	1:C:518:VAL:HG23	1.89	0.73
1:B:611:THR:O	1:B:612:GLN:CB	2.24	0.73
1:A:550:ARG:CG	1:A:550:ARG:NH1	2.45	0.73
1:B:305:LEU:HA	1:B:366:ILE:HD12	1.70	0.73
1:B:550:ARG:CG	1:B:550:ARG:NH1	2.46	0.73
1:D:468:GLN:O	1:D:469:LYS:CB	2.36	0.73
1:A:210:LEU:HD21	1:A:214:LYS:HE3	1.70	0.73
1:D:74:PHE:CZ	1:D:78:ILE:HD11	2.24	0.73
1:D:68:LEU:HD12	1:D:108:TYR:OH	1.87	0.73
1:D:73:THR:O	1:D:77:THR:HG23	1.88	0.73
1:C:531:SER:O	1:C:533:GLN:N	2.21	0.73
1:A:74:PHE:CZ	1:A:78:ILE:HD11	2.24	0.73
1:D:45:VAL:C	1:D:47:PRO:HD2	2.09	0.73
1:C:305:LEU:HA	1:C:366:ILE:HD12	1.69	0.72
1:A:45:VAL:C	1:A:47:PRO:HD2	2.10	0.72
1:B:73:THR:O	1:B:77:THR:HG23	1.88	0.72
1:A:155:LEU:C	1:A:155:LEU:CD2	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:532:LEU:O	1:D:535:ARG:N	2.22	0.72
1:B:202:GLN:NE2	1:B:243:ARG:NH1	2.34	0.72
1:B:9:GLY:C	1:B:10:LEU:HG	2.08	0.72
1:C:6:LEU:HD23	1:C:10:LEU:CD2	2.19	0.72
1:D:305:LEU:HA	1:D:366:ILE:HD12	1.70	0.72
1:A:338:ARG:NH2	1:C:687:LYS:HE2	2.00	0.72
1:A:68:LEU:HD22	1:A:125:LEU:HD21	1.71	0.72
1:B:155:LEU:C	1:B:155:LEU:CD2	2.58	0.72
1:D:171:LEU:HD21	1:D:175:PHE:CE2	2.25	0.72
1:A:550:ARG:HD2	1:A:550:ARG:O	1.90	0.72
1:A:375:SER:C	1:A:376:ASP:OD1	2.28	0.72
1:B:45:VAL:C	1:B:47:PRO:HD2	2.10	0.72
1:D:92:GLU:HG2	1:D:138:ARG:NH2	2.06	0.71
1:B:198:PHE:CZ	1:B:240:ILE:HG23	2.25	0.71
1:B:280:VAL:HG11	1:B:319:ILE:HD11	1.71	0.71
1:C:155:LEU:CD2	1:C:155:LEU:C	2.58	0.71
1:D:550:ARG:HD2	1:D:550:ARG:O	1.89	0.71
1:B:171:LEU:HD22	1:B:216:LEU:HD22	1.73	0.71
1:D:155:LEU:CD2	1:D:155:LEU:C	2.58	0.71
1:C:65:PHE:CZ	1:C:122:ILE:HG12	2.25	0.71
1:C:2:VAL:CG1	1:C:22:LEU:HD21	2.21	0.71
1:B:113:THR:CG2	1:B:166:PHE:CZ	2.74	0.71
1:B:550:ARG:O	1:B:550:ARG:HD2	1.89	0.71
1:D:113:THR:CG2	1:D:166:PHE:CZ	2.73	0.71
1:A:74:PHE:CE1	1:A:78:ILE:HD11	2.26	0.71
1:A:305:LEU:HA	1:A:366:ILE:HD12	1.72	0.71
1:B:658:ALA:O	1:B:661:VAL:CG2	2.38	0.71
1:C:92:GLU:HG2	1:C:138:ARG:NH2	2.06	0.71
1:D:375:SER:C	1:D:376:ASP:OD1	2.29	0.71
1:C:9:GLY:C	1:C:10:LEU:HG	2.09	0.71
1:D:217:ILE:HD12	1:D:249:ILE:HD13	1.72	0.71
1:B:16:HIS:CD2	1:B:16:HIS:C	2.65	0.70
1:B:16:HIS:ND1	1:B:50:PRO:HG3	2.06	0.70
1:C:474:LEU:CG	1:C:476:VAL:HG23	2.21	0.70
1:B:2:VAL:CG1	1:B:22:LEU:HD21	2.21	0.70
1:A:217:ILE:HD12	1:A:249:ILE:HD13	1.72	0.70
1:A:6:LEU:HD23	1:A:10:LEU:CD2	2.22	0.70
1:B:357:LYS:CB	1:D:684:SER:HB3	2.11	0.70
1:A:113:THR:CG2	1:A:166:PHE:CZ	2.73	0.70
1:D:531:SER:O	1:D:532:LEU:C	2.30	0.70
1:D:78:ILE:HG22	1:D:87:ILE:HG12	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:GLU:HG2	1:B:138:ARG:NH2	2.06	0.70
1:D:16:HIS:C	1:D:16:HIS:CD2	2.65	0.70
1:D:532:LEU:O	1:D:533:GLN:C	2.29	0.70
1:C:217:ILE:HD12	1:C:249:ILE:HD13	1.72	0.70
1:A:280:VAL:HG11	1:A:319:ILE:HD11	1.72	0.70
1:C:305:LEU:HD21	1:C:366:ILE:HG13	1.74	0.70
1:C:611:THR:O	1:C:612:GLN:CB	2.24	0.70
1:C:113:THR:CG2	1:C:166:PHE:CZ	2.74	0.70
1:A:355:HIS:O	1:A:356:LEU:HB2	1.92	0.70
1:D:9:GLY:C	1:D:10:LEU:HG	2.09	0.70
1:D:474:LEU:CG	1:D:476:VAL:HG23	2.22	0.70
1:D:64:SER:HB3	1:D:67:PHE:HB3	1.74	0.70
1:C:280:VAL:HG11	1:C:319:ILE:HD11	1.72	0.70
1:C:64:SER:HB3	1:C:67:PHE:HB3	1.74	0.70
1:A:16:HIS:CD2	1:A:16:HIS:C	2.65	0.69
1:D:550:ARG:NH2	1:D:660:PRO:HD3	2.01	0.69
1:D:74:PHE:CE1	1:D:78:ILE:HD11	2.27	0.69
1:C:205:ILE:HD11	1:C:244:PHE:CD1	2.27	0.69
1:D:515:PRO:O	1:D:518:VAL:HG23	1.92	0.69
1:B:525:LEU:CD1	1:B:539:LEU:HD13	2.21	0.69
1:C:16:HIS:C	1:C:16:HIS:CD2	2.65	0.69
1:B:305:LEU:HD21	1:B:366:ILE:HG13	1.72	0.69
1:C:68:LEU:HD12	1:C:108:TYR:OH	1.92	0.69
1:C:511:LEU:HD22	1:C:518:VAL:HG22	1.74	0.69
1:B:74:PHE:CE1	1:B:78:ILE:HD11	2.27	0.69
1:B:550:ARG:NH2	1:B:660:PRO:HD3	2.03	0.69
1:D:2:VAL:CG1	1:D:22:LEU:HD21	2.21	0.69
1:B:64:SER:HB3	1:B:67:PHE:HB3	1.74	0.69
1:C:74:PHE:CE1	1:C:78:ILE:HD11	2.26	0.69
1:D:525:LEU:CD1	1:D:539:LEU:HD13	2.23	0.69
1:A:20:ILE:HG23	1:A:52:ARG:NH1	2.07	0.69
1:C:327:ASN:HD21	1:C:331:LYS:HE3	1.58	0.69
1:A:92:GLU:HG2	1:A:138:ARG:NH2	2.07	0.69
1:B:261:LEU:HD22	1:B:367:PRO:CD	2.23	0.69
1:A:2:VAL:CG1	1:A:22:LEU:HD21	2.23	0.69
1:D:210:LEU:HD21	1:D:214:LYS:HE3	1.73	0.69
1:B:171:LEU:HD21	1:B:175:PHE:CE2	2.27	0.69
1:B:210:LEU:HD21	1:B:214:LYS:HE3	1.74	0.69
1:D:305:LEU:HD21	1:D:366:ILE:HG13	1.74	0.69
1:B:205:ILE:HG22	1:B:216:LEU:CD1	2.20	0.69
1:B:515:PRO:O	1:B:518:VAL:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:OG1	1:C:672:ASN:HB3	1.93	0.69
1:A:474:LEU:CG	1:A:476:VAL:HG23	2.23	0.69
1:C:113:THR:HG21	1:C:166:PHE:HZ	1.56	0.69
1:C:93:ILE:O	1:C:97:ILE:HG13	1.93	0.68
1:A:9:GLY:C	1:A:10:LEU:HG	2.09	0.68
1:B:6:LEU:HD23	1:B:10:LEU:CD2	2.22	0.68
1:A:515:PRO:O	1:A:518:VAL:HG23	1.93	0.68
1:D:658:ALA:O	1:D:661:VAL:CG2	2.42	0.68
1:A:360:SER:HB2	1:C:687:LYS:NZ	2.08	0.68
1:D:23:ASP:OD1	1:D:23:ASP:O	2.12	0.68
1:B:305:LEU:HA	1:B:366:ILE:HD11	1.75	0.68
1:C:240:ILE:HD11	1:C:385:LEU:HD11	1.76	0.68
1:D:305:LEU:HA	1:D:366:ILE:HD11	1.76	0.68
1:A:305:LEU:CD2	1:A:366:ILE:CG1	2.66	0.68
1:C:210:LEU:HD21	1:C:214:LYS:HE3	1.75	0.68
1:D:93:ILE:O	1:D:97:ILE:HG13	1.94	0.68
1:A:64:SER:HB3	1:A:67:PHE:HB3	1.74	0.68
1:A:171:LEU:HD21	1:A:175:PHE:CE2	2.25	0.68
1:B:113:THR:HG21	1:B:166:PHE:HZ	1.56	0.68
1:B:33:ASP:O	1:B:37:VAL:HG23	1.94	0.67
1:C:305:LEU:HA	1:C:366:ILE:HD11	1.75	0.67
1:D:202:GLN:NE2	1:D:243:ARG:NH1	2.37	0.67
1:B:474:LEU:CG	1:B:476:VAL:HG23	2.23	0.67
1:D:205:ILE:HG22	1:D:216:LEU:CD1	2.21	0.67
1:D:467:ARG:HH11	1:D:509:SER:HB3	1.60	0.67
1:A:33:ASP:O	1:A:37:VAL:HG23	1.94	0.67
1:B:370:LYS:HD2	1:B:370:LYS:N	2.09	0.67
1:C:23:ASP:OD1	1:C:23:ASP:O	2.11	0.67
1:A:312:ASN:H	1:A:315:GLN:NE2	1.89	0.67
1:B:93:ILE:O	1:B:97:ILE:HG13	1.94	0.67
1:D:33:ASP:O	1:D:37:VAL:HG23	1.93	0.67
1:C:205:ILE:HG22	1:C:216:LEU:CD1	2.22	0.67
1:C:550:ARG:O	1:C:550:ARG:CD	2.43	0.67
1:B:312:ASN:H	1:B:315:GLN:NE2	1.90	0.67
1:C:33:ASP:O	1:C:37:VAL:HG23	1.94	0.67
1:A:23:ASP:O	1:A:23:ASP:OD1	2.13	0.67
1:B:68:LEU:HD12	1:B:108:TYR:OH	1.95	0.67
1:D:305:LEU:HD23	1:D:366:ILE:HD12	1.70	0.67
1:C:499:PHE:O	1:C:500:GLU:HB2	1.94	0.67
1:C:634:ILE:HG22	1:C:644:LYS:HE2	1.78	0.66
1:B:327:ASN:HD21	1:B:331:LYS:HE3	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:H	1:A:151:GLN:HE21	1.43	0.66
1:D:18:ALA:O	1:D:22:LEU:HG	1.95	0.66
1:D:171:LEU:HD22	1:D:216:LEU:HD22	1.77	0.66
1:C:171:LEU:HD21	1:C:175:PHE:CE2	2.26	0.66
1:A:78:ILE:HG22	1:A:87:ILE:CG1	2.25	0.66
1:D:327:ASN:HD21	1:D:331:LYS:HE3	1.60	0.66
1:D:499:PHE:O	1:D:500:GLU:HB2	1.95	0.66
1:D:355:HIS:O	1:D:356:LEU:HB2	1.94	0.66
1:C:18:ALA:O	1:C:22:LEU:HG	1.95	0.66
1:D:312:ASN:H	1:D:315:GLN:NE2	1.93	0.66
1:A:467:ARG:HH11	1:A:509:SER:HB3	1.57	0.66
1:C:20:ILE:HG23	1:C:52:ARG:HH12	1.61	0.66
1:D:16:HIS:ND1	1:D:50:PRO:CG	2.59	0.66
1:B:474:LEU:CD1	1:B:476:VAL:HG23	2.26	0.66
1:D:634:ILE:HG22	1:D:644:LYS:HE2	1.77	0.66
1:D:105:LEU:H	1:D:151:GLN:HE21	1.43	0.66
1:B:531:SER:N	1:B:534:GLN:HG3	2.11	0.66
1:A:525:LEU:CD1	1:A:539:LEU:HD13	2.26	0.66
1:C:525:LEU:CD1	1:C:539:LEU:HD13	2.26	0.66
1:A:312:ASN:N	1:A:315:GLN:HE21	1.91	0.66
1:B:360:SER:HB2	1:D:687:LYS:HZ2	1.58	0.66
1:C:65:PHE:HB2	1:C:108:TYR:CE2	2.31	0.66
1:C:453:ALA:HB1	1:C:454:PRO:HD2	1.52	0.66
1:B:467:ARG:HH11	1:B:509:SER:HB3	1.58	0.66
1:B:23:ASP:O	1:B:23:ASP:OD1	2.14	0.66
1:B:261:LEU:HD22	1:B:367:PRO:CG	2.25	0.65
1:B:634:ILE:HG22	1:B:644:LYS:HE2	1.78	0.65
1:A:78:ILE:HG22	1:A:87:ILE:HD11	1.78	0.65
1:C:355:HIS:O	1:C:356:LEU:HB2	1.95	0.65
1:A:305:LEU:HD21	1:A:366:ILE:HG13	1.76	0.65
1:B:532:LEU:O	1:B:533:GLN:C	2.34	0.65
1:C:202:GLN:NE2	1:C:243:ARG:NH1	2.39	0.65
1:A:113:THR:HG21	1:A:166:PHE:HZ	1.54	0.65
1:B:355:HIS:O	1:B:356:LEU:HB2	1.96	0.65
1:B:672:ASN:HB3	1:D:330:THR:OG1	1.96	0.65
1:B:261:LEU:HD22	1:B:367:PRO:HD3	1.77	0.65
1:A:511:LEU:HD22	1:A:518:VAL:HG22	1.79	0.65
1:A:474:LEU:CD1	1:A:476:VAL:HG23	2.27	0.65
1:A:18:ALA:O	1:A:22:LEU:HG	1.96	0.65
1:C:467:ARG:HH11	1:C:509:SER:HB3	1.60	0.65
1:B:133:ASN:ND2	1:C:478:TYR:OH	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:N	1:C:262:PRO:HD2	2.11	0.65
1:A:499:PHE:O	1:A:500:GLU:HB2	1.95	0.65
1:B:18:ALA:O	1:B:22:LEU:HG	1.96	0.65
1:A:93:ILE:O	1:A:97:ILE:HG13	1.97	0.65
1:C:21:GLN:O	1:C:25:TYR:CD1	2.50	0.65
1:B:305:LEU:HD23	1:B:366:ILE:HD12	1.69	0.65
1:D:261:LEU:N	1:D:262:PRO:HD2	2.12	0.65
1:C:474:LEU:CD1	1:C:476:VAL:HG23	2.27	0.65
1:C:550:ARG:NH1	1:C:550:ARG:CG	2.45	0.65
1:B:550:ARG:O	1:B:550:ARG:CD	2.45	0.65
1:B:240:ILE:CD1	1:B:385:LEU:HD11	2.27	0.65
1:B:16:HIS:CD2	1:B:16:HIS:O	2.50	0.64
1:D:531:SER:O	1:D:533:GLN:N	2.30	0.64
1:D:550:ARG:CD	1:D:550:ARG:O	2.45	0.64
1:C:312:ASN:H	1:C:315:GLN:NE2	1.90	0.64
1:C:105:LEU:H	1:C:151:GLN:HE21	1.45	0.64
1:A:261:LEU:N	1:A:262:PRO:HD2	2.12	0.64
1:A:305:LEU:HA	1:A:366:ILE:HD11	1.78	0.64
1:B:499:PHE:O	1:B:500:GLU:HB2	1.96	0.64
1:D:78:ILE:CG2	1:D:87:ILE:CG1	2.74	0.64
1:B:342:GLU:OE2	1:D:687:LYS:HE3	1.98	0.64
1:B:261:LEU:N	1:B:262:PRO:HD2	2.12	0.64
1:A:634:ILE:HG22	1:A:644:LYS:HE2	1.79	0.64
1:C:85:GLN:O	1:C:89:ILE:HG13	1.98	0.64
1:A:672:ASN:HB3	1:C:330:THR:OG1	1.97	0.64
1:C:210:LEU:CD2	1:C:210:LEU:C	2.66	0.64
1:A:16:HIS:O	1:A:16:HIS:CD2	2.51	0.64
1:A:198:PHE:CZ	1:A:240:ILE:HG23	2.33	0.64
1:D:21:GLN:O	1:D:25:TYR:CD1	2.50	0.64
1:A:658:ALA:O	1:A:661:VAL:CG2	2.45	0.64
1:C:261:LEU:HD22	1:C:367:PRO:CG	2.28	0.64
1:A:550:ARG:CD	1:A:550:ARG:O	2.46	0.63
1:B:525:LEU:HD11	1:B:539:LEU:HD13	1.79	0.63
1:D:210:LEU:CD2	1:D:210:LEU:C	2.66	0.63
1:D:85:GLN:O	1:D:89:ILE:HG13	1.98	0.63
1:A:468:GLN:O	1:A:469:LYS:HB2	1.98	0.63
1:D:65:PHE:HB2	1:D:108:TYR:CE2	2.33	0.63
1:A:42:VAL:O	1:A:44:PRO:N	2.32	0.63
1:D:474:LEU:CD1	1:D:476:VAL:HG23	2.27	0.63
1:A:355:HIS:O	1:A:356:LEU:CB	2.46	0.63
1:B:21:GLN:O	1:B:25:TYR:CD1	2.52	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:O	1:A:29:PRO:HD2	1.99	0.63
1:D:16:HIS:CD2	1:D:16:HIS:O	2.51	0.63
1:D:634:ILE:CG2	1:D:644:LYS:HE2	2.29	0.63
1:C:550:ARG:NH2	1:C:660:PRO:HD3	2.03	0.63
1:A:85:GLN:O	1:A:89:ILE:HG13	1.98	0.63
1:B:210:LEU:CD2	1:B:210:LEU:C	2.66	0.63
1:A:21:GLN:O	1:A:25:TYR:CD1	2.52	0.63
1:B:16:HIS:HD2	1:B:16:HIS:O	1.82	0.62
1:C:16:HIS:O	1:C:16:HIS:CD2	2.51	0.62
1:C:226:GLN:NE2	1:C:259:GLN:N	2.42	0.62
1:C:164:PRO:HB3	1:C:166:PHE:CE1	2.34	0.62
1:B:85:GLN:O	1:B:89:ILE:HG13	1.99	0.62
1:C:235:ASN:HD21	1:C:375:SER:HB3	1.64	0.62
1:A:210:LEU:C	1:A:210:LEU:CD2	2.68	0.62
1:D:312:ASN:N	1:D:315:GLN:HE21	1.94	0.62
1:A:65:PHE:HB2	1:A:108:TYR:CD2	2.34	0.62
1:A:327:ASN:HD21	1:A:331:LYS:HE3	1.63	0.62
1:C:634:ILE:CG2	1:C:644:LYS:HE2	2.30	0.62
1:C:78:ILE:HG22	1:C:87:ILE:HG12	1.81	0.62
1:B:366:ILE:HG13	1:B:367:PRO:HD2	1.82	0.62
1:C:550:ARG:NH2	1:C:660:PRO:CD	2.62	0.62
1:B:687:LYS:O	1:B:687:LYS:HG2	2.00	0.62
1:D:16:HIS:HD2	1:D:16:HIS:O	1.83	0.62
1:A:16:HIS:HD2	1:A:16:HIS:O	1.82	0.62
1:D:217:ILE:HD12	1:D:249:ILE:CD1	2.30	0.62
1:B:312:ASN:N	1:B:315:GLN:HE21	1.93	0.62
1:C:16:HIS:HD2	1:C:16:HIS:O	1.83	0.61
1:A:550:ARG:NH2	1:A:660:PRO:CD	2.61	0.61
1:B:531:SER:O	1:B:534:GLN:N	2.26	0.61
1:B:360:SER:HB2	1:D:687:LYS:HZ1	1.61	0.61
1:C:123:LYS:HG3	1:C:170:TRP:CD1	2.35	0.61
1:B:123:LYS:HG3	1:B:170:TRP:CD1	2.35	0.61
1:D:550:ARG:NH2	1:D:660:PRO:CD	2.61	0.61
1:B:217:ILE:HD12	1:B:249:ILE:CD1	2.29	0.61
1:C:312:ASN:N	1:C:315:GLN:HE21	1.94	0.61
1:C:355:HIS:O	1:C:356:LEU:CB	2.48	0.61
1:D:366:ILE:HG13	1:D:367:PRO:HD2	1.83	0.61
1:B:453:ALA:HB1	1:B:454:PRO:HD2	1.54	0.61
1:D:355:HIS:O	1:D:356:LEU:CB	2.47	0.61
1:B:105:LEU:H	1:B:151:GLN:HE21	1.46	0.61
1:D:123:LYS:HG3	1:D:170:TRP:CD1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ILE:HD12	1:C:249:ILE:CD1	2.30	0.61
1:D:687:LYS:O	1:D:687:LYS:HG2	2.01	0.61
1:A:217:ILE:HD12	1:A:249:ILE:CD1	2.30	0.61
1:D:164:PRO:HB3	1:D:166:PHE:CE1	2.35	0.61
1:B:634:ILE:CG2	1:B:644:LYS:HE2	2.31	0.61
1:B:355:HIS:O	1:B:356:LEU:CB	2.48	0.61
1:B:205:ILE:CD1	1:B:217:ILE:HD11	2.31	0.61
1:C:488:VAL:HG12	1:C:530:LEU:HD22	1.82	0.61
1:B:164:PRO:HB3	1:B:166:PHE:CE1	2.36	0.60
1:C:42:VAL:O	1:C:44:PRO:N	2.34	0.60
1:C:687:LYS:HG2	1:C:687:LYS:O	2.00	0.60
1:D:525:LEU:HD11	1:D:539:LEU:HD13	1.81	0.60
1:B:646:HIS:O	1:B:650:THR:HG23	2.01	0.60
1:C:16:HIS:ND1	1:C:50:PRO:CG	2.64	0.60
1:B:171:LEU:HD22	1:B:216:LEU:CD2	2.31	0.60
1:A:65:PHE:CZ	1:A:122:ILE:HG12	2.36	0.60
1:A:634:ILE:CG2	1:A:644:LYS:HE2	2.31	0.60
1:D:511:LEU:HD22	1:D:518:VAL:HG22	1.83	0.60
1:A:123:LYS:HG3	1:A:170:TRP:CD1	2.37	0.60
1:B:205:ILE:HD12	1:B:217:ILE:HD11	1.83	0.60
1:A:171:LEU:HD22	1:A:216:LEU:HD22	1.82	0.60
1:D:78:ILE:HG22	1:D:87:ILE:CD1	2.30	0.60
1:D:376:ASP:O	1:D:377:ASP:C	2.40	0.60
1:A:164:PRO:HB3	1:A:166:PHE:CE1	2.37	0.60
1:B:42:VAL:O	1:B:44:PRO:N	2.34	0.60
1:C:305:LEU:HD23	1:C:366:ILE:HD12	1.73	0.60
1:A:205:ILE:HG22	1:A:216:LEU:CD1	2.29	0.60
1:A:68:LEU:HD12	1:A:108:TYR:OH	2.02	0.60
1:C:29:PRO:HD2	1:C:29:PRO:O	2.02	0.60
1:D:16:HIS:ND1	1:D:50:PRO:HG3	2.17	0.60
1:C:366:ILE:HG13	1:C:367:PRO:HD2	1.83	0.60
1:D:468:GLN:O	1:D:469:LYS:HB2	2.02	0.59
1:C:632:ASN:ND2	1:C:633:GLY:N	2.47	0.59
1:D:42:VAL:O	1:D:44:PRO:N	2.35	0.59
1:D:265:GLU:HG3	1:D:305:LEU:HD22	1.84	0.59
1:D:21:GLN:O	1:D:25:TYR:CE1	2.55	0.59
1:D:204:ILE:O	1:D:208:SER:HB2	2.03	0.59
1:B:687:LYS:HE3	1:D:342:GLU:OE2	2.02	0.59
1:D:198:PHE:CZ	1:D:240:ILE:HG23	2.37	0.59
1:A:240:ILE:CD1	1:A:385:LEU:HD11	2.32	0.59
1:A:687:LYS:HG2	1:A:687:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:LEU:HB3	1:A:534:GLN:HE21	1.68	0.59
1:C:21:GLN:O	1:C:25:TYR:CE1	2.55	0.59
1:C:494:PHE:O	1:C:495:ASP:C	2.41	0.59
1:D:530:LEU:HB3	1:D:534:GLN:HE21	1.68	0.58
1:D:466:ILE:CD1	1:D:510:ILE:HG12	2.27	0.58
1:C:468:GLN:O	1:C:469:LYS:HB2	2.02	0.58
1:B:612:GLN:O	1:B:614:ARG:N	2.36	0.58
1:B:494:PHE:O	1:B:495:ASP:C	2.42	0.58
1:B:204:ILE:O	1:B:208:SER:HB2	2.03	0.58
1:D:240:ILE:CD1	1:D:385:LEU:HD11	2.29	0.58
1:A:376:ASP:O	1:A:377:ASP:C	2.42	0.58
1:A:676:SER:HA	1:A:679:ILE:HD12	1.84	0.58
1:A:204:ILE:O	1:A:208:SER:HB2	2.04	0.58
1:A:226:GLN:NE2	1:A:259:GLN:N	2.43	0.58
1:B:65:PHE:CZ	1:B:122:ILE:HG12	2.39	0.58
1:A:494:PHE:O	1:A:495:ASP:C	2.42	0.58
1:C:530:LEU:HB3	1:C:534:GLN:HE21	1.68	0.58
1:A:646:HIS:O	1:A:650:THR:HG23	2.04	0.58
1:A:20:ILE:CG2	1:A:52:ARG:HH12	2.14	0.58
1:D:65:PHE:CZ	1:D:122:ILE:CG1	2.87	0.58
1:C:89:ILE:O	1:C:92:GLU:HB2	2.04	0.58
1:C:676:SER:HA	1:C:679:ILE:HD12	1.85	0.58
1:B:29:PRO:HD2	1:B:29:PRO:O	2.03	0.58
1:D:265:GLU:OE2	1:D:309:HIS:HE1	1.87	0.58
1:D:226:GLN:NE2	1:D:259:GLN:N	2.44	0.58
1:D:29:PRO:HD2	1:D:29:PRO:O	2.01	0.58
1:C:171:LEU:HD22	1:C:216:LEU:HD22	1.83	0.58
1:B:676:SER:HA	1:B:679:ILE:HD12	1.85	0.57
1:D:89:ILE:O	1:D:92:GLU:HB2	2.04	0.57
1:B:65:PHE:HB2	1:B:108:TYR:CD2	2.40	0.57
1:D:78:ILE:HG22	1:D:87:ILE:HD11	1.85	0.57
1:D:494:PHE:O	1:D:495:ASP:C	2.42	0.57
1:A:684:SER:HB3	1:C:357:LYS:HB2	1.86	0.57
1:B:89:ILE:O	1:B:92:GLU:HB2	2.04	0.57
1:C:525:LEU:HD11	1:C:539:LEU:HD13	1.86	0.57
1:B:468:GLN:O	1:B:469:LYS:HB3	2.04	0.57
1:B:256:PHE:HZ	1:B:299:THR:OG1	1.76	0.57
1:B:550:ARG:NH2	1:B:660:PRO:CD	2.64	0.57
1:B:466:ILE:CD1	1:B:510:ILE:HG12	2.28	0.57
1:C:376:ASP:O	1:C:377:ASP:C	2.41	0.57
1:C:531:SER:O	1:C:532:LEU:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:LEU:HD11	1:A:539:LEU:HD13	1.85	0.57
1:A:611:THR:O	1:A:612:GLN:CB	2.24	0.57
1:D:78:ILE:CG2	1:D:87:ILE:HG12	2.35	0.57
1:C:112:SER:OG	1:C:122:ILE:CD1	2.52	0.56
1:B:376:ASP:O	1:B:377:ASP:C	2.41	0.56
1:A:6:LEU:HD23	1:A:10:LEU:CD1	2.28	0.56
1:B:20:ILE:HG23	1:B:52:ARG:NH1	2.17	0.56
1:C:261:LEU:HD22	1:C:367:PRO:CD	2.35	0.56
1:B:468:GLN:O	1:B:469:LYS:HB2	2.03	0.56
1:C:198:PHE:CZ	1:C:240:ILE:HG23	2.41	0.56
1:A:21:GLN:O	1:A:25:TYR:CE1	2.58	0.56
1:C:204:ILE:O	1:C:208:SER:HB2	2.05	0.56
1:B:16:HIS:ND1	1:B:50:PRO:HG2	2.19	0.56
1:D:680:GLU:O	1:D:682:GLY:N	2.38	0.56
1:D:93:ILE:HG23	1:D:94:LEU:N	2.20	0.56
1:A:522:ILE:HG21	1:A:625:PRO:HB2	1.88	0.56
1:D:683:ILE:HG22	1:D:684:SER:N	2.21	0.56
1:A:687:LYS:HE3	1:C:342:GLU:OE2	2.05	0.56
1:C:93:ILE:HG23	1:C:94:LEU:N	2.20	0.56
1:A:305:LEU:HD23	1:A:366:ILE:HD12	1.75	0.56
1:D:6:LEU:CB	1:D:10:LEU:HD11	2.35	0.56
1:A:2:VAL:CG1	1:A:18:ALA:HB1	2.36	0.56
1:C:16:HIS:ND1	1:C:50:PRO:HG3	2.21	0.56
1:A:16:HIS:CE1	1:A:50:PRO:HG2	2.40	0.56
1:B:687:LYS:NZ	1:D:360:SER:HB2	2.20	0.56
1:C:468:GLN:O	1:C:469:LYS:HB3	2.07	0.56
1:D:676:SER:HA	1:D:679:ILE:HD12	1.86	0.56
1:D:16:HIS:ND1	1:D:50:PRO:HG2	2.21	0.55
1:B:680:GLU:O	1:B:682:GLY:N	2.39	0.55
1:A:16:HIS:CE1	1:A:50:PRO:CG	2.89	0.55
1:C:55:VAL:O	1:C:59:ARG:HG3	2.05	0.55
1:D:171:LEU:HD22	1:D:216:LEU:CD2	2.35	0.55
1:D:68:LEU:HD22	1:D:125:LEU:HD21	1.88	0.55
1:B:511:LEU:HD22	1:B:518:VAL:HG22	1.87	0.55
1:C:6:LEU:CB	1:C:10:LEU:HD11	2.36	0.55
1:A:612:GLN:O	1:A:614:ARG:N	2.38	0.55
1:B:205:ILE:O	1:B:213:GLN:NE2	2.36	0.55
1:A:495:ASP:OD1	1:A:495:ASP:N	2.38	0.55
1:A:78:ILE:HG22	1:A:87:ILE:CD1	2.36	0.55
1:B:522:ILE:HG21	1:B:625:PRO:HB2	1.87	0.55
1:A:93:ILE:HG23	1:A:94:LEU:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:VAL:CG1	1:D:18:ALA:HB1	2.36	0.55
1:B:531:SER:O	1:B:533:GLN:N	2.39	0.55
1:C:469:LYS:O	1:C:470:ALA:HB2	2.07	0.55
1:B:21:GLN:O	1:B:25:TYR:CE1	2.58	0.55
1:C:6:LEU:HD23	1:C:10:LEU:CD1	2.29	0.55
1:D:55:VAL:O	1:D:59:ARG:HG3	2.07	0.55
1:C:550:ARG:NH1	1:C:657:CYS:O	2.40	0.55
1:D:495:ASP:OD1	1:D:495:ASP:N	2.38	0.55
1:B:499:PHE:CD2	1:B:500:GLU:N	2.75	0.55
1:A:680:GLU:O	1:A:682:GLY:N	2.39	0.55
1:D:646:HIS:O	1:D:650:THR:HG23	2.06	0.55
1:A:468:GLN:O	1:A:469:LYS:HB3	2.06	0.55
1:A:377:ASP:O	1:A:378:LYS:HB2	2.06	0.55
1:D:672:ASN:ND2	1:D:672:ASN:H	2.05	0.55
1:C:199:PHE:HE2	1:C:203:LYS:HE3	1.71	0.55
1:B:357:LYS:HB2	1:D:684:SER:CB	2.12	0.55
1:A:205:ILE:HD12	1:A:217:ILE:HD11	1.89	0.55
1:B:338:ARG:NH2	1:D:687:LYS:HE2	2.19	0.55
1:A:6:LEU:CB	1:A:10:LEU:HD11	2.37	0.54
1:D:522:ILE:HG21	1:D:625:PRO:HB2	1.88	0.54
1:B:273:ASN:N	1:B:273:ASN:OD1	2.41	0.54
1:C:54:LYS:O	1:C:58:ARG:HG3	2.08	0.54
1:C:499:PHE:CD2	1:C:500:GLU:N	2.76	0.54
1:D:456:ILE:N	1:D:457:PRO:CD	2.70	0.54
1:D:114:THR:HG22	1:D:114:THR:O	2.07	0.54
1:C:2:VAL:CG1	1:C:18:ALA:HB1	2.37	0.54
1:C:16:HIS:HD2	1:C:16:HIS:C	2.11	0.54
1:A:499:PHE:CD2	1:A:500:GLU:N	2.75	0.54
1:B:333:LEU:HA	1:B:341:ARG:HG3	1.90	0.54
1:C:646:HIS:O	1:C:650:THR:HG23	2.07	0.54
1:D:16:HIS:C	1:D:16:HIS:HD2	2.10	0.54
1:B:55:VAL:O	1:B:59:ARG:HG3	2.06	0.54
1:A:2:VAL:CB	1:A:22:LEU:CD2	2.79	0.54
1:C:680:GLU:O	1:C:682:GLY:N	2.41	0.54
1:C:296:ASP:OD1	1:C:332:HIS:NE2	2.28	0.54
1:A:55:VAL:O	1:A:59:ARG:HG3	2.07	0.54
1:C:466:ILE:CD1	1:C:510:ILE:HG12	2.28	0.54
1:B:2:VAL:CB	1:B:22:LEU:CD2	2.77	0.54
1:B:113:THR:O	1:B:113:THR:CG2	2.54	0.54
1:B:199:PHE:HE2	1:B:203:LYS:HE3	1.73	0.54
1:B:112:SER:OG	1:B:122:ILE:CD1	2.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASP:OD1	1:C:23:ASP:C	2.46	0.54
1:C:522:ILE:HG21	1:C:625:PRO:HB2	1.89	0.54
1:B:114:THR:HG22	1:B:114:THR:O	2.07	0.54
1:B:2:VAL:CG1	1:B:18:ALA:HB1	2.37	0.54
1:C:2:VAL:CB	1:C:22:LEU:CD2	2.76	0.54
1:B:72:VAL:HG21	1:B:125:LEU:HD11	1.90	0.54
1:B:93:ILE:HG23	1:B:94:LEU:N	2.23	0.54
1:D:54:LYS:O	1:D:58:ARG:HG3	2.08	0.54
1:C:495:ASP:OD1	1:C:495:ASP:N	2.41	0.53
1:B:78:ILE:HG22	1:B:87:ILE:CG1	2.38	0.53
1:A:89:ILE:O	1:A:92:GLU:HB2	2.06	0.53
1:A:7:LYS:HG2	1:A:37:VAL:HG13	1.90	0.53
1:B:105:LEU:HB3	1:B:151:GLN:HG3	1.90	0.53
1:D:20:ILE:HG23	1:D:52:ARG:NH1	2.23	0.53
1:A:265:GLU:HG3	1:A:305:LEU:HD22	1.91	0.53
1:B:6:LEU:CB	1:B:10:LEU:HD11	2.38	0.53
1:C:612:GLN:O	1:C:614:ARG:N	2.40	0.53
1:D:106:THR:CG2	1:D:154:PHE:CD1	2.85	0.53
1:C:45:VAL:O	1:C:48:SER:N	2.37	0.53
1:A:253:SER:O	1:A:257:GLU:HG3	2.08	0.53
1:D:612:GLN:O	1:D:614:ARG:N	2.42	0.53
1:C:205:ILE:CG2	1:C:216:LEU:HD13	2.32	0.53
1:A:54:LYS:O	1:A:58:ARG:HG3	2.07	0.53
1:C:105:LEU:HB3	1:C:151:GLN:HG3	1.90	0.53
1:A:474:LEU:HD22	1:D:474:LEU:HD22	1.90	0.53
1:A:466:ILE:CD1	1:A:510:ILE:HG12	2.27	0.53
1:B:683:ILE:HG22	1:B:684:SER:N	2.23	0.53
1:A:127:PHE:O	1:A:177:LEU:HD21	2.09	0.53
1:C:114:THR:O	1:C:114:THR:HG22	2.08	0.53
1:C:683:ILE:HG22	1:C:684:SER:N	2.24	0.53
1:C:274:HIS:O	1:C:277:THR:HG23	2.09	0.53
1:A:105:LEU:CB	1:A:151:GLN:HG3	2.39	0.53
1:D:105:LEU:HB3	1:D:151:GLN:HG3	1.91	0.53
1:A:16:HIS:HD2	1:A:16:HIS:C	2.10	0.53
1:B:616:ARG:CG	1:B:661:VAL:HA	2.39	0.53
1:A:683:ILE:HG22	1:A:684:SER:N	2.23	0.53
1:C:672:ASN:ND2	1:C:672:ASN:H	2.07	0.53
1:C:498:LEU:C	1:C:499:PHE:O	2.46	0.53
1:D:105:LEU:CB	1:D:151:GLN:HG3	2.39	0.53
1:A:488:VAL:HG12	1:A:530:LEU:HD22	1.90	0.53
1:A:456:ILE:N	1:A:457:PRO:CD	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:GLN:HA	1:B:461:GLN:NE2	2.24	0.53
1:B:16:HIS:HD2	1:B:16:HIS:C	2.10	0.53
1:A:492:ASN:ND2	1:A:495:ASP:CA	2.70	0.53
1:C:377:ASP:O	1:C:378:LYS:HB2	2.09	0.53
1:A:105:LEU:HB3	1:A:151:GLN:HG3	1.90	0.53
1:B:105:LEU:CB	1:B:151:GLN:HG3	2.39	0.53
1:C:129:SER:OG	1:C:132:PHE:HB3	2.09	0.53
1:D:16:HIS:CD2	1:D:20:ILE:HD12	2.43	0.52
1:B:360:SER:HB3	1:D:687:LYS:HD2	1.91	0.52
1:D:23:ASP:C	1:D:23:ASP:OD1	2.47	0.52
1:D:2:VAL:HG13	1:D:18:ALA:HB1	1.91	0.52
1:D:550:ARG:NH1	1:D:657:CYS:O	2.43	0.52
1:A:616:ARG:CG	1:A:661:VAL:HA	2.39	0.52
1:A:46:TYR:N	1:A:47:PRO:HD2	2.24	0.52
1:B:133:ASN:HD22	1:B:133:ASN:N	2.07	0.52
1:C:105:LEU:CB	1:C:151:GLN:HG3	2.39	0.52
1:D:199:PHE:HE2	1:D:203:LYS:HE3	1.74	0.52
1:C:6:LEU:CD2	1:C:10:LEU:CD2	2.86	0.52
1:D:205:ILE:CD1	1:D:244:PHE:CE1	2.88	0.52
1:A:64:SER:O	1:A:65:PHE:HB3	2.10	0.52
1:D:171:LEU:CD2	1:D:175:PHE:CE2	2.92	0.52
1:D:112:SER:OG	1:D:122:ILE:CD1	2.52	0.52
1:A:42:VAL:O	1:A:43:ILE:C	2.46	0.52
1:A:498:LEU:C	1:A:499:PHE:O	2.47	0.52
1:A:29:PRO:O	1:A:29:PRO:CD	2.55	0.52
1:A:199:PHE:HE2	1:A:203:LYS:HE3	1.75	0.52
1:A:133:ASN:HD22	1:A:133:ASN:N	2.06	0.52
1:D:51:GLU:O	1:D:55:VAL:CG2	2.40	0.52
1:C:171:LEU:CD2	1:C:175:PHE:CE2	2.93	0.52
1:B:54:LYS:O	1:B:58:ARG:HG3	2.08	0.52
1:B:646:HIS:O	1:B:650:THR:CG2	2.58	0.52
1:D:129:SER:OG	1:D:132:PHE:HB3	2.10	0.52
1:C:16:HIS:O	1:C:20:ILE:HG13	2.10	0.52
1:D:6:LEU:CD2	1:D:10:LEU:CD2	2.86	0.52
1:C:106:THR:CG2	1:C:154:PHE:CD1	2.84	0.52
1:A:550:ARG:NH1	1:A:657:CYS:O	2.43	0.52
1:A:273:ASN:N	1:A:273:ASN:OD1	2.40	0.52
1:A:205:ILE:CD1	1:A:244:PHE:CE1	2.84	0.52
1:B:10:LEU:HD13	1:B:15:ILE:HG12	1.92	0.52
1:B:2:VAL:HG13	1:B:18:ALA:HB1	1.92	0.52
1:B:194:LYS:HD2	1:B:197:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:CD2	1:A:175:PHE:CE2	2.92	0.52
1:B:469:LYS:O	1:B:470:ALA:HB2	2.09	0.52
1:B:127:PHE:O	1:B:177:LEU:HD21	2.09	0.52
1:D:333:LEU:HA	1:D:341:ARG:HG3	1.92	0.52
1:D:274:HIS:O	1:D:277:THR:HG23	2.10	0.52
1:B:495:ASP:N	1:B:495:ASP:OD1	2.40	0.52
1:C:42:VAL:O	1:C:43:ILE:C	2.47	0.52
1:A:630:TRP:CH2	1:A:648:LEU:HD12	2.45	0.52
1:A:114:THR:HG22	1:A:114:THR:O	2.09	0.52
1:B:16:HIS:HE2	1:B:20:ILE:HD11	0.71	0.52
1:A:469:LYS:O	1:A:470:ALA:HB2	2.10	0.52
1:D:492:ASN:ND2	1:D:495:ASP:CA	2.70	0.52
1:B:377:ASP:O	1:B:378:LYS:HB2	2.09	0.52
1:C:46:TYR:N	1:C:47:PRO:HD2	2.24	0.52
1:B:46:TYR:O	1:B:54:LYS:HE2	2.10	0.52
1:B:46:TYR:N	1:B:47:PRO:HD2	2.25	0.52
1:C:456:ILE:N	1:C:457:PRO:CD	2.73	0.52
1:D:265:GLU:OE2	1:D:309:HIS:CE1	2.62	0.52
1:A:261:LEU:HD22	1:A:367:PRO:CD	2.40	0.52
1:D:499:PHE:CD2	1:D:500:GLU:N	2.78	0.52
1:D:46:TYR:N	1:D:47:PRO:HD2	2.25	0.51
1:B:630:TRP:CH2	1:B:648:LEU:HD12	2.45	0.51
1:B:456:ILE:N	1:B:457:PRO:CD	2.73	0.51
1:D:531:SER:O	1:D:534:GLN:N	2.42	0.51
1:B:532:LEU:O	1:B:534:GLN:N	2.43	0.51
1:B:672:ASN:ND2	1:B:672:ASN:H	2.08	0.51
1:D:29:PRO:O	1:D:29:PRO:CD	2.58	0.51
1:B:16:HIS:O	1:B:20:ILE:HG13	2.10	0.51
1:A:106:THR:CG2	1:A:154:PHE:CD1	2.85	0.51
1:C:645:SER:OG	1:C:686:ASN:OD1	2.29	0.51
1:D:42:VAL:O	1:D:43:ILE:C	2.49	0.51
1:B:23:ASP:OD1	1:B:23:ASP:C	2.48	0.51
1:C:293:GLU:OE1	1:C:343:ARG:NH2	2.43	0.51
1:B:2:VAL:HG11	1:B:22:LEU:HD21	1.93	0.51
1:D:498:LEU:C	1:D:499:PHE:O	2.48	0.51
1:C:133:ASN:N	1:C:133:ASN:HD22	2.07	0.51
1:D:292:ASP:HB3	1:D:295:VAL:HB	1.92	0.51
1:D:127:PHE:O	1:D:177:LEU:HD21	2.10	0.51
1:D:16:HIS:O	1:D:20:ILE:HG13	2.10	0.51
1:A:59:ARG:O	1:A:62:SER:HB2	2.10	0.51
1:A:2:VAL:HG13	1:A:18:ALA:HB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:CD2	1:B:175:PHE:CE2	2.93	0.51
1:A:342:GLU:OE2	1:C:687:LYS:HE3	2.09	0.51
1:D:468:GLN:O	1:D:469:LYS:HB3	2.10	0.51
1:D:78:ILE:CG2	1:D:87:ILE:HG13	2.41	0.51
1:A:7:LYS:HG2	1:A:37:VAL:CG1	2.41	0.51
1:D:490:LEU:O	1:D:503:ARG:NH1	2.44	0.51
1:C:333:LEU:HA	1:C:341:ARG:HG3	1.92	0.51
1:A:461:GLN:HA	1:A:461:GLN:NE2	2.26	0.51
1:D:78:ILE:HG22	1:D:87:ILE:HG13	1.89	0.51
1:D:630:TRP:CH2	1:D:648:LEU:HD12	2.46	0.51
1:C:261:LEU:HD22	1:C:367:PRO:HD3	1.93	0.51
1:B:106:THR:CG2	1:B:154:PHE:CD1	2.84	0.51
1:B:42:VAL:C	1:B:44:PRO:CD	2.79	0.51
1:B:296:ASP:OD1	1:B:332:HIS:NE2	2.29	0.51
1:C:461:GLN:NE2	1:C:461:GLN:HA	2.26	0.51
1:C:630:TRP:CH2	1:C:648:LEU:HD12	2.45	0.51
1:C:16:HIS:CD2	1:C:20:ILE:HD12	2.43	0.51
1:A:16:HIS:CD2	1:A:20:ILE:HD12	2.43	0.51
1:D:59:ARG:O	1:D:62:SER:HB2	2.11	0.51
1:C:59:ARG:O	1:C:62:SER:HB2	2.10	0.51
1:D:273:ASN:N	1:D:273:ASN:OD1	2.42	0.51
1:B:202:GLN:OE1	1:B:243:ARG:HG3	2.10	0.51
1:B:235:ASN:HD21	1:B:375:SER:HB3	1.75	0.51
1:B:492:ASN:ND2	1:B:495:ASP:CA	2.71	0.51
1:A:23:ASP:C	1:A:23:ASP:OD1	2.48	0.51
1:C:499:PHE:O	1:C:501:GLN:N	2.43	0.51
1:C:199:PHE:CE2	1:C:203:LYS:HE3	2.45	0.51
1:B:630:TRP:CD1	1:B:674:ILE:HG23	2.46	0.51
1:A:293:GLU:OE1	1:A:343:ARG:NH2	2.44	0.51
1:A:296:ASP:OD1	1:A:332:HIS:NE2	2.33	0.51
1:D:39:ILE:HD11	1:D:70:GLN:HB3	1.93	0.51
1:D:616:ARG:CG	1:D:661:VAL:HA	2.40	0.51
1:C:492:ASN:ND2	1:C:495:ASP:CA	2.71	0.51
1:C:74:PHE:CE1	1:C:78:ILE:HD12	2.47	0.51
1:A:45:VAL:O	1:A:48:SER:N	2.36	0.51
1:D:630:TRP:CD1	1:D:674:ILE:HG23	2.46	0.51
1:D:16:HIS:HE2	1:D:20:ILE:HD11	0.73	0.50
1:B:530:LEU:HB3	1:B:534:GLN:NE2	2.26	0.50
1:C:2:VAL:HG13	1:C:18:ALA:HB1	1.92	0.50
1:B:171:LEU:CD2	1:B:216:LEU:HD22	2.41	0.50
1:C:65:PHE:CZ	1:C:122:ILE:CG1	2.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:VAL:O	1:B:43:ILE:C	2.48	0.50
1:B:226:GLN:NE2	1:B:259:GLN:N	2.44	0.50
1:B:370:LYS:HD3	1:B:370:LYS:N	2.22	0.50
1:C:78:ILE:HG22	1:C:87:ILE:CD1	2.41	0.50
1:A:377:ASP:O	1:A:378:LYS:CB	2.59	0.50
1:C:236:ASP:O	1:C:240:ILE:HG13	2.11	0.50
1:A:499:PHE:O	1:A:501:GLN:N	2.41	0.50
1:D:472:PHE:O	1:D:474:LEU:N	2.45	0.50
1:B:550:ARG:NH1	1:B:657:CYS:O	2.45	0.50
1:A:171:LEU:HD22	1:A:216:LEU:CD2	2.41	0.50
1:D:113:THR:O	1:D:113:THR:CG2	2.54	0.50
1:B:226:GLN:NE2	1:B:260:SER:H	2.10	0.50
1:D:64:SER:O	1:D:65:PHE:HB3	2.11	0.50
1:C:93:ILE:CG2	1:C:94:LEU:N	2.74	0.50
1:C:127:PHE:O	1:C:177:LEU:HD21	2.12	0.50
1:D:261:LEU:HD22	1:D:367:PRO:CD	2.42	0.50
1:B:59:ARG:O	1:B:62:SER:HB2	2.11	0.50
1:D:2:VAL:CB	1:D:22:LEU:CD2	2.77	0.50
1:C:194:LYS:HD2	1:C:197:TYR:CE1	2.46	0.50
1:A:226:GLN:NE2	1:A:260:SER:H	2.10	0.50
1:D:133:ASN:HD22	1:D:133:ASN:N	2.09	0.50
1:A:16:HIS:HE2	1:A:20:ILE:HD11	0.72	0.50
1:B:261:LEU:CD2	1:B:367:PRO:HD3	2.41	0.50
1:A:10:LEU:HD13	1:A:15:ILE:HG12	1.93	0.50
1:D:93:ILE:CG2	1:D:94:LEU:N	2.74	0.50
1:B:65:PHE:CZ	1:B:122:ILE:CG1	2.94	0.50
1:A:42:VAL:C	1:A:44:PRO:CD	2.79	0.50
1:C:78:ILE:HG22	1:C:87:ILE:HD11	1.94	0.50
1:D:239:LYS:O	1:D:242:ARG:HG3	2.12	0.50
1:A:74:PHE:CE1	1:A:78:ILE:HD12	2.45	0.50
1:C:327:ASN:ND2	1:C:331:LYS:HE3	2.27	0.50
1:C:525:LEU:HD13	1:C:539:LEU:HD13	1.94	0.50
1:C:616:ARG:CG	1:C:661:VAL:HA	2.42	0.50
1:A:205:ILE:CD1	1:A:217:ILE:HD11	2.42	0.50
1:D:67:PHE:O	1:D:71:ILE:HG13	2.12	0.50
1:C:46:TYR:O	1:C:54:LYS:HE2	2.11	0.50
1:C:630:TRP:CD1	1:C:674:ILE:HG23	2.47	0.50
1:C:253:SER:O	1:C:257:GLU:HG3	2.11	0.50
1:B:130:LYS:O	1:B:134:VAL:HG12	2.12	0.50
1:D:10:LEU:HD13	1:D:15:ILE:HG12	1.94	0.50
1:D:194:LYS:HD2	1:D:197:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:ASP:O	1:D:378:LYS:HB2	2.12	0.50
1:B:45:VAL:O	1:B:48:SER:N	2.37	0.50
1:D:525:LEU:HD13	1:D:539:LEU:HD13	1.93	0.50
1:A:672:ASN:ND2	1:A:672:ASN:H	2.10	0.50
1:A:6:LEU:CG	1:A:10:LEU:HD11	2.39	0.49
1:A:6:LEU:CD2	1:A:10:LEU:CD2	2.90	0.49
1:B:171:LEU:CD2	1:B:216:LEU:CD2	2.89	0.49
1:D:469:LYS:O	1:D:470:ALA:HB2	2.11	0.49
1:C:500:GLU:OE1	1:C:503:ARG:NH2	2.43	0.49
1:A:16:HIS:O	1:A:20:ILE:HG13	2.11	0.49
1:D:156:LEU:HD11	1:D:191:PHE:HE1	1.77	0.49
1:B:256:PHE:CE1	1:B:298:LYS:HB2	2.46	0.49
1:A:67:PHE:O	1:A:71:ILE:HG13	2.11	0.49
1:B:67:PHE:O	1:B:71:ILE:HG13	2.13	0.49
1:C:239:LYS:O	1:C:242:ARG:HG3	2.12	0.49
1:A:547:ARG:CZ	1:A:553:ASP:OD1	2.60	0.49
1:B:474:LEU:HD22	1:C:474:LEU:HD22	1.94	0.49
1:C:469:LYS:O	1:C:470:ALA:CB	2.60	0.49
1:C:64:SER:O	1:C:65:PHE:HB3	2.11	0.49
1:D:46:TYR:O	1:D:54:LYS:HE2	2.12	0.49
1:B:672:ASN:O	1:B:676:SER:HB3	2.13	0.49
1:A:333:LEU:HA	1:A:341:ARG:HG3	1.94	0.49
1:B:274:HIS:O	1:B:277:THR:HG23	2.11	0.49
1:C:239:LYS:HE2	1:C:376:ASP:H	1.77	0.49
1:B:78:ILE:HG22	1:B:87:ILE:HD11	1.94	0.49
1:B:292:ASP:HB3	1:B:295:VAL:HB	1.93	0.49
1:A:630:TRP:CD1	1:A:674:ILE:HG23	2.46	0.49
1:C:477:GLY:O	1:C:517:LYS:HE3	2.13	0.49
1:A:130:LYS:O	1:A:134:VAL:HG12	2.13	0.49
1:A:366:ILE:HG13	1:A:367:PRO:HD2	1.95	0.49
1:D:6:LEU:CG	1:D:10:LEU:HD11	2.38	0.49
1:C:226:GLN:NE2	1:C:260:SER:H	2.11	0.49
1:A:65:PHE:CZ	1:A:122:ILE:CG1	2.96	0.49
1:B:64:SER:O	1:B:65:PHE:HB3	2.12	0.49
1:D:239:LYS:HE2	1:D:376:ASP:H	1.77	0.49
1:B:39:ILE:HD11	1:B:70:GLN:HB3	1.94	0.49
1:A:672:ASN:O	1:A:676:SER:HB3	2.12	0.49
1:D:261:LEU:HD22	1:D:367:PRO:HD3	1.94	0.49
1:B:525:LEU:HD13	1:B:539:LEU:HD13	1.94	0.49
1:B:498:LEU:C	1:B:499:PHE:O	2.44	0.49
1:B:199:PHE:CE2	1:B:203:LYS:HE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:SER:OG	1:C:132:PHE:CB	2.61	0.49
1:A:199:PHE:CE2	1:A:203:LYS:HE3	2.48	0.49
1:A:292:ASP:HB3	1:A:295:VAL:HB	1.95	0.49
1:A:46:TYR:O	1:A:54:LYS:HE2	2.12	0.49
1:B:253:SER:O	1:B:257:GLU:HG3	2.13	0.49
1:A:256:PHE:HZ	1:A:299:THR:OG1	1.96	0.49
1:C:16:HIS:HE2	1:C:20:ILE:HD11	0.72	0.49
1:D:205:ILE:HD12	1:D:217:ILE:HD11	1.94	0.49
1:B:205:ILE:CD1	1:B:244:PHE:CE1	2.91	0.49
1:D:74:PHE:CE1	1:D:78:ILE:HD12	2.47	0.49
1:C:42:VAL:HG12	1:C:43:ILE:N	2.27	0.49
1:B:293:GLU:OE1	1:B:343:ARG:NH2	2.45	0.49
1:D:19:LEU:HD12	1:D:53:SER:OG	2.12	0.49
1:B:16:HIS:CE1	1:B:50:PRO:CG	2.95	0.49
1:A:261:LEU:HD22	1:A:367:PRO:CG	2.43	0.49
1:C:156:LEU:HD11	1:C:191:PHE:HE1	1.77	0.49
1:A:360:SER:HB2	1:C:687:LYS:HZ2	1.76	0.49
1:A:492:ASN:HD21	1:A:496:GLU:H	1.61	0.49
1:D:230:THR:HG22	1:D:231:LEU:H	1.78	0.49
1:A:239:LYS:O	1:A:242:ARG:HG3	2.13	0.49
1:B:91:GLN:HB3	1:B:138:ARG:HD2	1.95	0.49
1:C:624:TYR:N	1:C:625:PRO:CD	2.76	0.49
1:D:199:PHE:CE2	1:D:203:LYS:HE3	2.47	0.49
1:A:524:ILE:HG23	1:A:528:SER:OG	2.13	0.49
1:B:532:LEU:O	1:B:535:ARG:N	2.45	0.48
1:B:156:LEU:HD11	1:B:191:PHE:HE1	1.78	0.48
1:B:492:ASN:HD21	1:B:496:GLU:H	1.61	0.48
1:D:646:HIS:O	1:D:650:THR:CG2	2.61	0.48
1:C:130:LYS:O	1:C:134:VAL:HG12	2.13	0.48
1:B:524:ILE:HG23	1:B:528:SER:OG	2.13	0.48
1:D:633:GLY:O	1:D:634:ILE:HB	2.14	0.48
1:D:39:ILE:CD1	1:D:70:GLN:HB3	2.43	0.48
1:C:39:ILE:HD11	1:C:70:GLN:HB3	1.94	0.48
1:D:7:LYS:HG2	1:D:37:VAL:HG13	1.93	0.48
1:D:499:PHE:O	1:D:501:GLN:N	2.45	0.48
1:A:646:HIS:O	1:A:650:THR:CG2	2.61	0.48
1:A:129:SER:OG	1:A:132:PHE:HB3	2.12	0.48
1:C:171:LEU:HD22	1:C:216:LEU:CD2	2.42	0.48
1:A:42:VAL:HG12	1:A:43:ILE:N	2.27	0.48
1:C:230:THR:HG22	1:C:231:LEU:H	1.77	0.48
1:A:461:GLN:HA	1:A:461:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:461:GLN:HE21	1:C:461:GLN:HA	1.78	0.48
1:D:186:LEU:O	1:D:190:LEU:HB3	2.12	0.48
1:C:292:ASP:HB3	1:C:295:VAL:HB	1.94	0.48
1:A:316:ARG:HG2	1:A:351:LEU:CD2	2.43	0.48
1:C:10:LEU:HD13	1:C:15:ILE:HG12	1.94	0.48
1:C:273:ASN:N	1:C:273:ASN:OD1	2.42	0.48
1:C:113:THR:O	1:C:113:THR:CG2	2.53	0.48
1:C:68:LEU:HD22	1:C:125:LEU:HD21	1.95	0.48
1:B:472:PHE:O	1:B:474:LEU:N	2.46	0.48
1:C:67:PHE:O	1:C:71:ILE:HG13	2.12	0.48
1:A:236:ASP:O	1:A:240:ILE:HG13	2.14	0.48
1:C:672:ASN:O	1:C:676:SER:HB3	2.12	0.48
1:B:461:GLN:HA	1:B:461:GLN:HE21	1.78	0.48
1:B:129:SER:OG	1:B:132:PHE:HB3	2.14	0.48
1:C:214:LYS:HA	1:C:249:ILE:HG23	1.96	0.48
1:A:39:ILE:HD11	1:A:70:GLN:HB3	1.95	0.48
1:A:93:ILE:CG2	1:A:94:LEU:N	2.76	0.48
1:B:74:PHE:CE1	1:B:78:ILE:HD12	2.46	0.48
1:D:7:LYS:HG2	1:D:37:VAL:CG1	2.43	0.48
1:D:130:LYS:O	1:D:134:VAL:HG12	2.14	0.48
1:D:524:ILE:HG23	1:D:528:SER:OG	2.13	0.48
1:B:16:HIS:CD2	1:B:20:ILE:HD12	2.43	0.48
1:A:51:GLU:O	1:A:55:VAL:CG2	2.41	0.48
1:A:2:VAL:HG11	1:A:22:LEU:HD21	1.95	0.48
1:B:488:VAL:HG12	1:B:530:LEU:HD22	1.96	0.48
1:B:214:LYS:HA	1:B:249:ILE:HG23	1.95	0.48
1:D:103:GLY:O	1:D:104:CYS:C	2.52	0.48
1:B:93:ILE:CG2	1:B:94:LEU:N	2.77	0.48
1:D:45:VAL:O	1:D:48:SER:N	2.36	0.48
1:D:253:SER:O	1:D:257:GLU:HG3	2.13	0.48
1:B:6:LEU:CD2	1:B:10:LEU:CD2	2.90	0.48
1:D:42:VAL:C	1:D:44:PRO:CD	2.81	0.48
1:D:236:ASP:O	1:D:240:ILE:HG13	2.13	0.48
1:B:236:ASP:O	1:B:240:ILE:HG13	2.14	0.48
1:A:230:THR:HG22	1:A:231:LEU:H	1.78	0.48
1:C:42:VAL:C	1:C:44:PRO:CD	2.80	0.48
1:A:525:LEU:HD13	1:A:539:LEU:HD13	1.94	0.48
1:A:624:TYR:N	1:A:625:PRO:CD	2.76	0.48
1:D:42:VAL:HG12	1:D:43:ILE:N	2.27	0.48
1:D:686:ASN:O	1:D:687:LYS:C	2.52	0.48
1:C:78:ILE:HG22	1:C:87:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:CG2	1:C:87:ILE:CG1	2.86	0.48
1:A:628:HIS:C	1:A:632:ASN:ND2	2.67	0.48
1:B:327:ASN:ND2	1:B:331:LYS:HE3	2.29	0.48
1:B:10:LEU:HB3	1:B:15:ILE:CG1	2.44	0.47
1:C:472:PHE:O	1:C:474:LEU:N	2.47	0.47
1:B:633:GLY:O	1:B:634:ILE:HB	2.14	0.47
1:D:672:ASN:O	1:D:676:SER:HB3	2.13	0.47
1:D:45:VAL:HB	1:D:48:SER:OG	2.14	0.47
1:B:499:PHE:O	1:B:501:GLN:N	2.44	0.47
1:B:239:LYS:O	1:B:242:ARG:HG3	2.14	0.47
1:B:642:LEU:HA	1:B:642:LEU:HD23	1.77	0.47
1:D:10:LEU:HB3	1:D:15:ILE:CG1	2.45	0.47
1:C:233:ASN:O	1:C:237:VAL:HG13	2.14	0.47
1:B:45:VAL:HB	1:B:48:SER:OG	2.14	0.47
1:D:296:ASP:OD1	1:D:332:HIS:NE2	2.32	0.47
1:B:265:GLU:HG3	1:B:305:LEU:HD22	1.97	0.47
1:A:274:HIS:O	1:A:277:THR:HG23	2.13	0.47
1:A:633:GLY:O	1:A:634:ILE:HB	2.14	0.47
1:B:39:ILE:CD1	1:B:70:GLN:HB3	2.45	0.47
1:B:25:TYR:HB3	1:B:26:PRO:HD2	1.96	0.47
1:B:131:LEU:O	1:B:134:VAL:HG13	2.15	0.47
1:D:229:VAL:O	1:D:229:VAL:HG13	2.14	0.47
1:C:10:LEU:HB3	1:C:15:ILE:CG1	2.45	0.47
1:D:214:LYS:HA	1:D:249:ILE:HG23	1.96	0.47
1:D:235:ASN:HD21	1:D:375:SER:HB3	1.80	0.47
1:C:39:ILE:CD1	1:C:70:GLN:HB3	2.44	0.47
1:C:45:VAL:HB	1:C:48:SER:OG	2.14	0.47
1:D:129:SER:OG	1:D:132:PHE:CB	2.62	0.47
1:D:293:GLU:OE1	1:D:343:ARG:NH2	2.47	0.47
1:D:641:GLN:OE1	1:D:641:GLN:HA	2.15	0.47
1:A:245:ASP:OD1	1:A:248:LYS:HE2	2.14	0.47
1:C:633:GLY:O	1:C:634:ILE:HB	2.14	0.47
1:D:156:LEU:CD2	1:D:197:TYR:CD2	2.84	0.47
1:B:469:LYS:HB3	1:B:470:ALA:H	1.45	0.47
1:A:103:GLY:O	1:A:104:CYS:C	2.52	0.47
1:B:103:GLY:O	1:B:104:CYS:C	2.53	0.47
1:A:78:ILE:CG2	1:A:87:ILE:CG1	2.92	0.47
1:D:456:ILE:N	1:D:457:PRO:HD2	2.30	0.47
1:A:229:VAL:O	1:A:229:VAL:HG13	2.15	0.47
1:A:156:LEU:HD11	1:A:191:PHE:HE1	1.79	0.47
1:A:191:PHE:CD1	1:A:201:PHE:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:ASN:HD21	1:C:496:GLU:H	1.62	0.47
1:B:42:VAL:HG12	1:B:43:ILE:N	2.30	0.47
1:B:43:ILE:N	1:B:44:PRO:HD2	2.30	0.47
1:D:327:ASN:ND2	1:D:331:LYS:HE3	2.28	0.47
1:B:624:TYR:N	1:B:625:PRO:CD	2.78	0.47
1:D:316:ARG:HG2	1:D:351:LEU:HD23	1.96	0.47
1:B:316:ARG:HG2	1:B:351:LEU:CD2	2.44	0.47
1:A:472:PHE:O	1:A:474:LEU:N	2.48	0.47
1:B:51:GLU:O	1:B:55:VAL:CG2	2.43	0.47
1:B:469:LYS:O	1:B:470:ALA:CB	2.62	0.47
1:C:103:GLY:O	1:C:104:CYS:C	2.52	0.47
1:A:35:SER:HB2	1:A:67:PHE:CD2	2.50	0.47
1:B:230:THR:HG22	1:B:231:LEU:H	1.78	0.47
1:D:45:VAL:O	1:D:46:TYR:C	2.52	0.47
1:A:45:VAL:HB	1:A:48:SER:OG	2.14	0.47
1:A:45:VAL:O	1:A:46:TYR:C	2.53	0.47
1:D:25:TYR:HB3	1:D:26:PRO:HD2	1.97	0.47
1:D:461:GLN:HA	1:D:461:GLN:NE2	2.30	0.47
1:D:366:ILE:O	1:D:367:PRO:O	2.33	0.47
1:C:51:GLU:O	1:C:55:VAL:CG2	2.42	0.47
1:D:2:VAL:HG11	1:D:22:LEU:HD21	1.94	0.47
1:B:233:ASN:O	1:B:237:VAL:HG13	2.14	0.47
1:B:490:LEU:O	1:B:503:ARG:NH1	2.46	0.47
1:A:641:GLN:O	1:A:645:SER:HB2	2.15	0.47
1:D:659:ASN:CG	1:D:659:ASN:O	2.53	0.47
1:A:16:HIS:CE1	1:A:50:PRO:HG3	2.50	0.47
1:A:469:LYS:O	1:A:470:ALA:CB	2.62	0.47
1:A:233:ASN:O	1:A:237:VAL:HG13	2.15	0.47
1:A:316:ARG:HG2	1:A:351:LEU:HD23	1.96	0.47
1:D:316:ARG:HG2	1:D:351:LEU:CD2	2.45	0.47
1:A:10:LEU:HB3	1:A:15:ILE:CG1	2.45	0.47
1:A:469:LYS:HB3	1:A:470:ALA:H	1.44	0.47
1:C:91:GLN:HB3	1:C:138:ARG:HD2	1.96	0.47
1:D:467:ARG:NH2	1:D:548:GLU:OE2	2.47	0.47
1:B:628:HIS:C	1:B:632:ASN:ND2	2.68	0.47
1:A:490:LEU:O	1:A:503:ARG:NH1	2.44	0.47
1:A:91:GLN:HB3	1:A:138:ARG:HD2	1.96	0.46
1:C:131:LEU:O	1:C:134:VAL:HG13	2.14	0.46
1:A:214:LYS:HA	1:A:249:ILE:HG23	1.97	0.46
1:D:91:GLN:HB3	1:D:138:ARG:HD2	1.96	0.46
1:D:686:ASN:O	1:D:688:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:ASP:O	1:C:378:LYS:CB	2.62	0.46
1:B:500:GLU:OE1	1:B:503:ARG:NH2	2.44	0.46
1:C:186:LEU:O	1:C:190:LEU:HB3	2.15	0.46
1:D:624:TYR:N	1:D:625:PRO:CD	2.79	0.46
1:C:646:HIS:O	1:C:650:THR:CG2	2.64	0.46
1:D:517:LYS:HD3	1:D:517:LYS:HA	1.65	0.46
1:B:530:LEU:HB3	1:B:534:GLN:HE21	1.81	0.46
1:C:191:PHE:CD1	1:C:201:PHE:HB2	2.50	0.46
1:A:39:ILE:HG23	1:A:90:TYR:HE2	1.81	0.46
1:D:628:HIS:C	1:D:632:ASN:ND2	2.68	0.46
1:B:316:ARG:HG2	1:B:351:LEU:HD23	1.98	0.46
1:A:641:GLN:OE1	1:A:641:GLN:HA	2.15	0.46
1:B:183:ALA:O	1:B:187:LEU:HB2	2.16	0.46
1:D:280:VAL:O	1:D:284:VAL:HG23	2.15	0.46
1:C:488:VAL:O	1:C:534:GLN:HG3	2.14	0.46
1:B:186:LEU:O	1:B:190:LEU:HB3	2.16	0.46
1:B:16:HIS:CE1	1:B:50:PRO:HG3	2.49	0.46
1:A:686:ASN:O	1:A:687:LYS:C	2.53	0.46
1:D:205:ILE:CD1	1:D:217:ILE:HD11	2.46	0.46
1:D:226:GLN:NE2	1:D:260:SER:H	2.13	0.46
1:C:25:TYR:HB3	1:C:26:PRO:HD2	1.97	0.46
1:C:316:ARG:HG2	1:C:351:LEU:CD2	2.45	0.46
1:D:74:PHE:HE1	1:D:90:TYR:CZ	2.34	0.46
1:C:86:GLU:O	1:C:90:TYR:HD1	1.99	0.46
1:B:35:SER:HB2	1:B:67:PHE:CD2	2.51	0.46
1:B:641:GLN:OE1	1:B:641:GLN:HA	2.15	0.46
1:C:16:HIS:ND1	1:C:50:PRO:HG2	2.30	0.46
1:A:261:LEU:HD22	1:A:367:PRO:HD3	1.97	0.46
1:C:64:SER:HB3	1:C:67:PHE:CB	2.45	0.46
1:B:280:VAL:HG11	1:B:319:ILE:CD1	2.43	0.46
1:C:29:PRO:CD	1:C:29:PRO:O	2.58	0.46
1:B:29:PRO:CD	1:B:29:PRO:O	2.58	0.46
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.75	0.46
1:A:78:ILE:HG22	1:A:87:ILE:HG12	1.97	0.46
1:C:45:VAL:O	1:C:46:TYR:C	2.54	0.46
1:A:25:TYR:HB3	1:A:26:PRO:HD2	1.97	0.46
1:B:648:LEU:HD11	1:B:678:ALA:HB2	1.98	0.46
1:C:377:ASP:C	1:C:378:LYS:HG3	2.36	0.46
1:D:648:LEU:HD11	1:D:678:ALA:HB2	1.98	0.46
1:C:547:ARG:CZ	1:C:553:ASP:OD1	2.64	0.46
1:C:2:VAL:HG11	1:C:22:LEU:HD21	1.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:LYS:O	1:D:687:LYS:CG	2.65	0.45
1:C:43:ILE:N	1:C:44:PRO:HD2	2.31	0.45
1:B:191:PHE:CD1	1:B:201:PHE:HB2	2.51	0.45
1:A:39:ILE:CD1	1:A:70:GLN:HB3	2.45	0.45
1:B:377:ASP:C	1:B:378:LYS:HG3	2.36	0.45
1:B:377:ASP:O	1:B:378:LYS:CB	2.62	0.45
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.83	0.45
1:D:672:ASN:ND2	1:D:672:ASN:N	2.61	0.45
1:C:648:LEU:HD11	1:C:678:ALA:HB2	1.98	0.45
1:B:686:ASN:O	1:B:687:LYS:C	2.54	0.45
1:A:194:LYS:HD2	1:A:197:TYR:CE1	2.50	0.45
1:C:35:SER:HB2	1:C:67:PHE:CD2	2.51	0.45
1:A:104:CYS:HB3	1:A:108:TYR:CE1	2.51	0.45
1:A:19:LEU:HD12	1:A:53:SER:OG	2.16	0.45
1:D:234:LEU:HA	1:D:234:LEU:HD23	1.75	0.45
1:C:641:GLN:OE1	1:C:641:GLN:HA	2.17	0.45
1:A:106:THR:HB	1:A:155:LEU:CB	2.42	0.45
1:D:488:VAL:HG12	1:D:530:LEU:HD22	1.98	0.45
1:D:171:LEU:CD2	1:D:216:LEU:HD22	2.47	0.45
1:B:202:GLN:CD	1:B:243:ARG:HG2	2.37	0.45
1:A:72:VAL:HG21	1:A:125:LEU:HD11	1.97	0.45
1:C:92:GLU:HG2	1:C:138:ARG:HH22	1.82	0.45
1:B:233:ASN:HA	1:B:233:ASN:HD22	1.58	0.45
1:C:233:ASN:HA	1:C:233:ASN:HD22	1.58	0.45
1:B:346:PHE:CD2	1:B:363:LYS:HA	2.52	0.45
1:C:183:ALA:O	1:C:187:LEU:HB2	2.15	0.45
1:A:265:GLU:OE2	1:A:309:HIS:CE1	2.70	0.45
1:C:316:ARG:HG2	1:C:351:LEU:HD23	1.97	0.45
1:A:186:LEU:O	1:A:190:LEU:HB3	2.16	0.45
1:B:234:LEU:HD22	1:B:266:VAL:HG21	1.99	0.45
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.79	0.45
1:D:191:PHE:CD1	1:D:201:PHE:HB2	2.51	0.45
1:C:156:LEU:CD2	1:C:197:TYR:CD2	2.86	0.45
1:D:616:ARG:HG2	1:D:661:VAL:HA	1.98	0.45
1:A:686:ASN:O	1:A:688:GLY:N	2.49	0.45
1:A:112:SER:OG	1:A:122:ILE:CD1	2.55	0.45
1:C:672:ASN:N	1:C:672:ASN:ND2	2.65	0.45
1:C:648:LEU:CD1	1:C:678:ALA:HB2	2.46	0.45
1:D:131:LEU:O	1:D:134:VAL:HG13	2.16	0.45
1:D:261:LEU:HD22	1:D:367:PRO:CG	2.47	0.45
1:B:6:LEU:CG	1:B:10:LEU:HD11	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:LYS:O	1:B:687:LYS:CG	2.63	0.45
1:C:686:ASN:O	1:C:687:LYS:C	2.55	0.45
1:B:240:ILE:HD11	1:B:385:LEU:CD1	2.37	0.45
1:D:377:ASP:C	1:D:378:LYS:HG3	2.37	0.45
1:B:347:ILE:O	1:B:351:LEU:HG	2.17	0.45
1:B:547:ARG:CZ	1:B:553:ASP:OD1	2.64	0.45
1:C:659:ASN:O	1:C:659:ASN:CG	2.55	0.45
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.82	0.45
1:D:469:LYS:HB3	1:D:470:ALA:H	1.43	0.45
1:A:616:ARG:HG2	1:A:661:VAL:HA	1.98	0.45
1:A:377:ASP:C	1:A:378:LYS:HG3	2.36	0.45
1:D:347:ILE:O	1:D:351:LEU:HG	2.17	0.45
1:C:245:ASP:OD1	1:C:248:LYS:HE2	2.16	0.45
1:D:642:LEU:HD23	1:D:642:LEU:HA	1.75	0.45
1:B:255:LEU:HD12	1:B:255:LEU:HA	1.83	0.45
1:B:16:HIS:CE1	1:B:50:PRO:HG2	2.51	0.45
1:D:64:SER:HB3	1:D:67:PHE:CB	2.45	0.45
1:B:45:VAL:O	1:B:46:TYR:C	2.56	0.45
1:C:490:LEU:O	1:C:503:ARG:NH1	2.45	0.45
1:B:672:ASN:ND2	1:B:672:ASN:N	2.65	0.45
1:A:456:ILE:N	1:A:457:PRO:HD2	2.32	0.45
1:B:648:LEU:CD1	1:B:678:ALA:HB2	2.47	0.45
1:C:346:PHE:CD2	1:C:363:LYS:HA	2.52	0.45
1:D:35:SER:HB2	1:D:67:PHE:CD2	2.51	0.44
1:B:86:GLU:O	1:B:90:TYR:HD1	2.00	0.44
1:D:492:ASN:HD22	1:D:492:ASN:C	2.21	0.44
1:C:280:VAL:O	1:C:284:VAL:HG23	2.17	0.44
1:A:648:LEU:HD11	1:A:678:ALA:HB2	1.98	0.44
1:C:517:LYS:HD3	1:C:517:LYS:HA	1.64	0.44
1:A:129:SER:OG	1:A:132:PHE:CB	2.66	0.44
1:D:183:ALA:O	1:D:187:LEU:HB2	2.17	0.44
1:D:469:LYS:O	1:D:470:ALA:CB	2.65	0.44
1:D:114:THR:O	1:D:114:THR:CG2	2.65	0.44
1:D:461:GLN:HA	1:D:461:GLN:HE21	1.82	0.44
1:C:524:ILE:HG23	1:C:528:SER:OG	2.17	0.44
1:D:547:ARG:CZ	1:D:553:ASP:OD1	2.65	0.44
1:D:92:GLU:HG2	1:D:138:ARG:HH22	1.80	0.44
1:C:164:PRO:CB	1:C:166:PHE:CE1	3.00	0.44
1:B:104:CYS:HB3	1:B:108:TYR:CE1	2.52	0.44
1:B:129:SER:OG	1:B:132:PHE:CB	2.65	0.44
1:D:176:LEU:HA	1:D:176:LEU:HD23	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ILE:O	1:B:367:PRO:O	2.35	0.44
1:B:106:THR:HB	1:B:155:LEU:CB	2.41	0.44
1:D:171:LEU:CD2	1:D:216:LEU:CD2	2.95	0.44
1:D:377:ASP:O	1:D:378:LYS:CB	2.65	0.44
1:D:648:LEU:CD1	1:D:678:ALA:HB2	2.47	0.44
1:A:131:LEU:O	1:A:134:VAL:HG13	2.17	0.44
1:B:229:VAL:O	1:B:229:VAL:HG13	2.16	0.44
1:A:265:GLU:OE2	1:A:309:HIS:HE1	2.00	0.44
1:B:64:SER:HB3	1:B:67:PHE:CB	2.45	0.44
1:A:43:ILE:N	1:A:44:PRO:HD2	2.32	0.44
1:C:78:ILE:CG2	1:C:87:ILE:HG12	2.47	0.44
1:B:456:ILE:N	1:B:457:PRO:HD2	2.33	0.44
1:B:245:ASP:OD1	1:B:248:LYS:HE2	2.16	0.44
1:C:289:ASP:O	1:C:289:ASP:CG	2.55	0.44
1:C:100:PHE:O	1:C:102:PRO:HD3	2.18	0.44
1:B:616:ARG:HG2	1:B:661:VAL:HA	1.99	0.44
1:D:86:GLU:O	1:D:90:TYR:HD1	2.00	0.44
1:D:233:ASN:O	1:D:237:VAL:HG13	2.18	0.44
1:B:686:ASN:O	1:B:688:GLY:N	2.51	0.44
1:C:687:LYS:CG	1:C:687:LYS:O	2.62	0.44
1:A:64:SER:HB3	1:A:67:PHE:CB	2.46	0.44
1:D:242:ARG:HB2	1:D:242:ARG:HE	1.60	0.44
1:A:7:LYS:HE2	1:A:37:VAL:CG2	2.47	0.44
1:C:114:THR:O	1:C:114:THR:CG2	2.66	0.44
1:B:161:THR:HG22	1:B:162:ASP:N	2.33	0.44
1:D:504:ILE:HD11	1:D:537:SER:HB3	2.00	0.44
1:B:659:ASN:O	1:B:659:ASN:CG	2.55	0.44
1:C:205:ILE:HD12	1:C:217:ILE:HD11	1.99	0.44
1:D:43:ILE:N	1:D:44:PRO:HD2	2.32	0.44
1:D:628:HIS:O	1:D:629:GLY:C	2.56	0.44
1:C:488:VAL:CG1	1:C:530:LEU:HD22	2.46	0.44
1:C:347:ILE:O	1:C:351:LEU:HG	2.18	0.44
1:A:687:LYS:NZ	1:C:360:SER:HB2	2.33	0.43
1:D:39:ILE:HG23	1:D:90:TYR:HE2	1.83	0.43
1:D:68:LEU:CD1	1:D:108:TYR:OH	2.61	0.43
1:A:86:GLU:O	1:A:90:TYR:HD1	2.00	0.43
1:B:644:LYS:CD	1:B:683:ILE:HD11	2.48	0.43
1:C:234:LEU:HD22	1:C:266:VAL:HG21	1.99	0.43
1:A:500:GLU:OE1	1:A:503:ARG:NH2	2.45	0.43
1:A:648:LEU:CD1	1:A:678:ALA:HB2	2.48	0.43
1:D:100:PHE:O	1:D:102:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:PRO:HB2	1:C:368:ASN:H	1.59	0.43
1:C:104:CYS:HB3	1:C:108:TYR:CE1	2.54	0.43
1:D:205:ILE:CG2	1:D:216:LEU:HD13	2.33	0.43
1:C:456:ILE:N	1:C:457:PRO:HD2	2.32	0.43
1:A:176:LEU:HA	1:A:176:LEU:HD23	1.85	0.43
1:B:350:LEU:O	1:B:350:LEU:HG	2.17	0.43
1:C:20:ILE:HG23	1:C:52:ARG:NH1	2.31	0.43
1:C:644:LYS:CD	1:C:683:ILE:HD11	2.48	0.43
1:C:205:ILE:CD1	1:C:217:ILE:HD11	2.49	0.43
1:A:520:GLY:O	1:A:524:ILE:HG13	2.17	0.43
1:A:552:LEU:HD12	1:A:552:LEU:HA	1.76	0.43
1:A:367:PRO:O	1:A:368:ASN:CB	2.41	0.43
1:B:152:TRP:O	1:B:156:LEU:HB2	2.18	0.43
1:B:256:PHE:HE1	1:B:298:LYS:HB2	1.83	0.43
1:A:35:SER:HB2	1:A:67:PHE:HD2	1.83	0.43
1:D:492:ASN:HD21	1:D:496:GLU:H	1.65	0.43
1:D:280:VAL:HG11	1:D:319:ILE:CD1	2.43	0.43
1:B:680:GLU:O	1:B:681:GLU:C	2.57	0.43
1:B:114:THR:O	1:B:114:THR:CG2	2.66	0.43
1:C:229:VAL:HG13	1:C:229:VAL:O	2.18	0.43
1:C:10:LEU:HB3	1:C:15:ILE:HG13	2.01	0.43
1:C:312:ASN:CG	1:C:315:GLN:HE21	2.22	0.43
1:B:35:SER:HB2	1:B:67:PHE:HD2	1.84	0.43
1:C:518:VAL:HG12	1:C:518:VAL:O	2.17	0.43
1:A:280:VAL:HG11	1:A:319:ILE:CD1	2.47	0.43
1:A:105:LEU:HB2	1:A:151:GLN:CG	2.49	0.43
1:A:327:ASN:ND2	1:A:331:LYS:HE3	2.32	0.43
1:B:234:LEU:HD23	1:B:234:LEU:HA	1.81	0.43
1:D:552:LEU:HD12	1:D:552:LEU:HA	1.75	0.43
1:C:350:LEU:O	1:C:350:LEU:HG	2.17	0.43
1:A:113:THR:O	1:A:113:THR:CG2	2.53	0.43
1:C:68:LEU:CD1	1:C:108:TYR:OH	2.63	0.43
1:B:65:PHE:CD2	1:B:122:ILE:HG12	2.52	0.43
1:B:92:GLU:HG2	1:B:138:ARG:HH22	1.81	0.43
1:A:346:PHE:CD2	1:A:363:LYS:HA	2.53	0.43
1:A:183:ALA:O	1:A:187:LEU:HB2	2.18	0.43
1:D:680:GLU:O	1:D:681:GLU:C	2.57	0.43
1:B:687:LYS:HZ1	1:D:360:SER:HB2	1.83	0.43
1:A:502:TRP:HA	1:A:505:ASN:HD22	1.84	0.43
1:C:366:ILE:O	1:C:367:PRO:O	2.37	0.43
1:D:10:LEU:HB3	1:D:15:ILE:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:CG	1:C:10:LEU:HD11	2.39	0.43
1:B:312:ASN:CG	1:B:315:GLN:HE21	2.22	0.43
1:A:461:GLN:CA	1:A:461:GLN:HE21	2.32	0.43
1:A:472:PHE:N	1:A:474:LEU:HD21	2.34	0.43
1:D:550:ARG:HG3	1:D:550:ARG:NH1	2.30	0.43
1:D:661:VAL:HB	1:D:662:HIS:H	1.61	0.43
1:D:518:VAL:O	1:D:518:VAL:HG12	2.19	0.43
1:A:233:ASN:HA	1:A:233:ASN:HD22	1.56	0.43
1:A:628:HIS:O	1:A:629:GLY:C	2.58	0.43
1:B:105:LEU:HB2	1:B:151:GLN:CG	2.48	0.43
1:D:367:PRO:HB2	1:D:368:ASN:H	1.58	0.42
1:D:644:LYS:CD	1:D:683:ILE:HD11	2.49	0.42
1:D:72:VAL:HG21	1:D:125:LEU:HD11	2.00	0.42
1:A:39:ILE:HA	1:A:43:ILE:HD12	2.01	0.42
1:B:520:GLY:O	1:B:524:ILE:HG13	2.19	0.42
1:A:659:ASN:CG	1:A:659:ASN:O	2.57	0.42
1:C:487:ILE:HD13	1:C:506:ALA:HB1	2.01	0.42
1:A:113:THR:HG23	1:A:119:ARG:HG2	2.01	0.42
1:D:164:PRO:CB	1:D:166:PHE:CE1	3.02	0.42
1:B:164:PRO:CB	1:B:166:PHE:CE1	3.03	0.42
1:A:644:LYS:CD	1:A:683:ILE:HD11	2.49	0.42
1:A:242:ARG:HB2	1:A:242:ARG:HE	1.61	0.42
1:B:280:VAL:O	1:B:284:VAL:HG23	2.19	0.42
1:C:105:LEU:HB2	1:C:151:GLN:CG	2.49	0.42
1:D:477:GLY:O	1:D:517:LYS:HE3	2.19	0.42
1:C:502:TRP:HA	1:C:505:ASN:HD22	1.84	0.42
1:D:350:LEU:O	1:D:350:LEU:HG	2.18	0.42
1:B:16:HIS:CD2	1:B:20:ILE:CG1	3.03	0.42
1:D:87:ILE:O	1:D:91:GLN:HG3	2.19	0.42
1:B:370:LYS:CD	1:B:370:LYS:H	2.28	0.42
1:D:532:LEU:HB3	1:D:533:GLN:H	1.68	0.42
1:A:360:SER:HB2	1:C:687:LYS:HZ1	1.80	0.42
1:A:65:PHE:HB2	1:A:108:TYR:CE2	2.54	0.42
1:A:511:LEU:HA	1:A:511:LEU:HD23	1.90	0.42
1:D:672:ASN:HD22	1:D:672:ASN:N	2.17	0.42
1:B:461:GLN:CA	1:B:461:GLN:HE21	2.31	0.42
1:D:346:PHE:CD2	1:D:363:LYS:HA	2.54	0.42
1:A:234:LEU:HD22	1:A:266:VAL:HG21	2.01	0.42
1:C:660:PRO:O	1:C:661:VAL:C	2.58	0.42
1:A:511:LEU:HD22	1:A:518:VAL:CG2	2.48	0.42
1:A:672:ASN:N	1:A:672:ASN:ND2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:LEU:HA	1:D:302:LEU:HD23	1.76	0.42
1:C:472:PHE:N	1:C:474:LEU:HD21	2.34	0.42
1:B:205:ILE:HD12	1:B:217:ILE:CD1	2.47	0.42
1:D:233:ASN:HD22	1:D:233:ASN:HA	1.55	0.42
1:C:280:VAL:HG11	1:C:319:ILE:CD1	2.45	0.42
1:A:161:THR:HG22	1:A:162:ASP:N	2.33	0.42
1:B:194:LYS:HD2	1:B:197:TYR:CD1	2.54	0.42
1:C:461:GLN:CA	1:C:461:GLN:HE21	2.32	0.42
1:D:20:ILE:CG2	1:D:52:ARG:HH12	2.27	0.42
1:C:550:ARG:HD3	1:C:550:ARG:O	2.17	0.42
1:A:492:ASN:C	1:A:492:ASN:HD22	2.22	0.42
1:B:289:ASP:O	1:B:289:ASP:CG	2.58	0.42
1:D:550:ARG:HD3	1:D:550:ARG:O	2.20	0.42
1:A:661:VAL:HB	1:A:662:HIS:H	1.62	0.42
1:A:100:PHE:O	1:A:102:PRO:HD3	2.19	0.42
1:D:683:ILE:CG2	1:D:684:SER:N	2.82	0.42
1:C:171:LEU:CD2	1:C:216:LEU:HD22	2.49	0.42
1:D:39:ILE:HA	1:D:43:ILE:HD12	2.01	0.42
1:C:39:ILE:HA	1:C:43:ILE:HD12	2.01	0.42
1:D:105:LEU:HB2	1:D:151:GLN:CG	2.49	0.42
1:A:114:THR:CG2	1:A:114:THR:O	2.67	0.42
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.75	0.42
1:B:100:PHE:O	1:B:102:PRO:HD3	2.20	0.42
1:C:16:HIS:CD2	1:C:20:ILE:CG1	3.03	0.41
1:B:261:LEU:N	1:B:262:PRO:CD	2.81	0.41
1:C:661:VAL:HB	1:C:662:HIS:H	1.62	0.41
1:B:156:LEU:CD2	1:B:197:TYR:CD2	2.86	0.41
1:C:686:ASN:O	1:C:688:GLY:N	2.53	0.41
1:D:104:CYS:HB3	1:D:108:TYR:CE1	2.54	0.41
1:B:39:ILE:HA	1:B:43:ILE:HD12	2.02	0.41
1:A:280:VAL:O	1:A:284:VAL:HG23	2.20	0.41
1:C:161:THR:HG22	1:C:162:ASP:N	2.35	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.79	0.41
1:A:261:LEU:N	1:A:262:PRO:CD	2.82	0.41
1:B:6:LEU:HD23	1:B:10:LEU:CD1	2.30	0.41
1:D:472:PHE:N	1:D:474:LEU:HD21	2.35	0.41
1:A:202:GLN:OE1	1:A:243:ARG:HG3	2.21	0.41
1:A:194:LYS:HD3	1:A:196:SER:HB3	2.03	0.41
1:C:469:LYS:HB3	1:C:470:ALA:H	1.44	0.41
1:C:35:SER:HB2	1:C:67:PHE:HD2	1.84	0.41
1:A:42:VAL:O	1:A:44:PRO:CD	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:531:SER:O	1:C:534:GLN:N	2.53	0.41
1:B:539:LEU:HA	1:B:539:LEU:HD12	1.84	0.41
1:C:520:GLY:O	1:C:524:ILE:HG13	2.20	0.41
1:B:56:ILE:O	1:B:60:LEU:HG	2.20	0.41
1:D:6:LEU:HA	1:D:10:LEU:HD11	2.02	0.41
1:B:10:LEU:HB3	1:B:15:ILE:HG13	2.00	0.41
1:B:357:LYS:HE3	1:D:682:GLY:O	2.21	0.41
1:D:194:LYS:HD3	1:D:196:SER:HB3	2.02	0.41
1:D:35:SER:HB2	1:D:67:PHE:HD2	1.85	0.41
1:B:492:ASN:C	1:B:492:ASN:HD22	2.23	0.41
1:B:106:THR:HG21	1:B:154:PHE:CE1	2.53	0.41
1:C:683:ILE:CG2	1:C:684:SER:N	2.84	0.41
1:B:43:ILE:N	1:B:44:PRO:CD	2.83	0.41
1:B:176:LEU:HD23	1:B:176:LEU:HA	1.85	0.41
1:A:10:LEU:HB3	1:A:15:ILE:HG13	2.01	0.41
1:C:194:LYS:HD3	1:C:196:SER:HB3	2.03	0.41
1:C:492:ASN:HD22	1:C:492:ASN:C	2.22	0.41
1:A:230:THR:HG22	1:A:231:LEU:N	2.35	0.41
1:B:42:VAL:O	1:B:44:PRO:CD	2.69	0.41
1:D:245:ASP:OD1	1:D:248:LYS:HE2	2.20	0.41
1:B:367:PRO:O	1:B:368:ASN:CB	2.40	0.41
1:D:171:LEU:HD11	1:D:191:PHE:CE2	2.56	0.41
1:B:683:ILE:CG2	1:B:684:SER:N	2.83	0.41
1:C:78:ILE:CG2	1:C:87:ILE:HG13	2.51	0.41
1:C:42:VAL:O	1:C:44:PRO:CD	2.69	0.41
1:A:150:LEU:HD23	1:A:150:LEU:HA	1.89	0.41
1:A:350:LEU:O	1:A:350:LEU:HG	2.20	0.41
1:D:16:HIS:CD2	1:D:20:ILE:CG1	3.03	0.41
1:B:171:LEU:HD11	1:B:191:PHE:CE2	2.55	0.41
1:C:87:ILE:O	1:C:91:GLN:HG3	2.21	0.41
1:D:234:LEU:HD22	1:D:266:VAL:HG21	2.03	0.41
1:C:628:HIS:O	1:C:629:GLY:C	2.58	0.41
1:D:435:VAL:O	1:D:435:VAL:HG12	2.21	0.41
1:C:6:LEU:HA	1:C:10:LEU:HD11	2.02	0.41
1:B:472:PHE:N	1:B:474:LEU:HD21	2.35	0.41
1:A:239:LYS:HE2	1:A:376:ASP:H	1.85	0.41
1:D:539:LEU:HA	1:D:539:LEU:HD12	1.81	0.41
1:A:680:GLU:O	1:A:681:GLU:C	2.58	0.41
1:D:148:LEU:HA	1:D:148:LEU:HD22	1.90	0.41
1:C:176:LEU:HA	1:C:176:LEU:HD23	1.89	0.41
1:D:6:LEU:HD23	1:D:10:LEU:CD1	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:PRO:O	1:B:661:VAL:C	2.60	0.41
1:C:152:TRP:O	1:C:156:LEU:HB2	2.20	0.41
1:A:152:TRP:O	1:A:156:LEU:HB2	2.21	0.41
1:A:164:PRO:CB	1:A:166:PHE:CE1	3.04	0.41
1:B:518:VAL:HG12	1:B:518:VAL:O	2.20	0.41
1:C:680:GLU:O	1:C:681:GLU:C	2.59	0.41
1:A:347:ILE:O	1:A:351:LEU:HG	2.21	0.41
1:D:286:LYS:HE2	1:D:286:LYS:HB2	1.75	0.41
1:A:517:LYS:HD3	1:A:517:LYS:HA	1.63	0.41
1:B:16:HIS:HD2	1:B:20:ILE:CD1	2.24	0.41
1:C:194:LYS:HD2	1:C:197:TYR:CD1	2.56	0.41
1:A:171:LEU:CD2	1:A:216:LEU:CD2	2.99	0.41
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.86	0.41
1:A:235:ASN:HD21	1:A:375:SER:HB3	1.85	0.41
1:A:92:GLU:HG2	1:A:138:ARG:HH22	1.81	0.41
1:C:648:LEU:HD11	1:C:678:ALA:CB	2.51	0.41
1:A:531:SER:O	1:A:532:LEU:C	2.59	0.41
1:C:56:ILE:O	1:C:60:LEU:HG	2.21	0.41
1:A:367:PRO:HB2	1:A:368:ASN:H	1.65	0.40
1:A:6:LEU:HA	1:A:10:LEU:HD11	2.03	0.40
1:D:113:THR:HG23	1:D:119:ARG:HG2	2.03	0.40
1:D:222:LEU:HA	1:D:222:LEU:HD23	1.81	0.40
1:A:192:LEU:HA	1:A:192:LEU:HD12	1.95	0.40
1:A:9:GLY:O	1:A:10:LEU:CD2	2.67	0.40
1:C:616:ARG:HG2	1:C:661:VAL:HA	2.02	0.40
1:C:113:THR:HG23	1:C:119:ARG:HG2	2.02	0.40
1:A:16:HIS:CD2	1:A:20:ILE:CG1	3.03	0.40
1:D:261:LEU:N	1:D:262:PRO:CD	2.80	0.40
1:B:240:ILE:HG12	1:B:380:ILE:HD13	2.03	0.40
1:A:43:ILE:N	1:A:44:PRO:CD	2.84	0.40
1:D:467:ARG:NH2	1:D:548:GLU:OE1	2.55	0.40
1:D:45:VAL:O	1:D:47:PRO:N	2.54	0.40
1:D:7:LYS:HE2	1:D:37:VAL:CG2	2.51	0.40
1:D:161:THR:HG22	1:D:162:ASP:N	2.35	0.40
1:C:265:GLU:HG3	1:C:305:LEU:HD22	2.02	0.40
1:C:71:ILE:HG13	1:C:71:ILE:H	1.72	0.40
1:A:511:LEU:O	1:A:515:PRO:HA	2.22	0.40
1:C:233:ASN:O	1:C:234:LEU:C	2.60	0.40
1:C:43:ILE:N	1:C:44:PRO:CD	2.84	0.40
1:C:488:VAL:O	1:C:534:GLN:CG	2.70	0.40
1:B:487:ILE:HD13	1:B:506:ALA:HB1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ILE:O	1:D:60:LEU:HG	2.22	0.40
1:D:544:LEU:HD23	1:D:544:LEU:HA	1.91	0.40
1:B:517:LYS:HA	1:B:517:LYS:HD3	1.66	0.40
1:A:322:ASP:OD2	1:A:324:ARG:HB2	2.21	0.40
1:D:194:LYS:HD2	1:D:197:TYR:CD1	2.57	0.40
1:A:683:ILE:CG2	1:A:684:SER:N	2.83	0.40
1:C:375:SER:CA	1:C:376:ASP:OD1	2.69	0.40
1:A:133:ASN:ND2	1:D:478:TYR:OH	2.47	0.40
1:B:264:LYS:O	1:B:268:VAL:HG23	2.21	0.40
1:A:148:LEU:HA	1:A:148:LEU:HD22	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	558/647 (86%)	486 (87%)	46 (8%)	26 (5%)	3 17
1	B	558/647 (86%)	482 (86%)	49 (9%)	27 (5%)	3 17
1	C	558/647 (86%)	485 (87%)	46 (8%)	27 (5%)	3 17
1	D	558/647 (86%)	489 (88%)	43 (8%)	26 (5%)	3 17
All	All	2232/2588 (86%)	1942 (87%)	184 (8%)	106 (5%)	3 17

All (106) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	PRO
1	A	356	LEU
1	A	367	PRO
1	A	368	ASN
1	A	473	GLN

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Mol	Chain	Res	Type
1	A	527	ASN
1	A	612	GLN
1	A	661	VAL
1	A	681	GLU
1	B	29	PRO
1	B	356	LEU
1	B	367	PRO
1	B	368	ASN
1	B	473	GLN
1	B	527	ASN
1	B	612	GLN
1	B	661	VAL
1	B	681	GLU
1	C	29	PRO
1	C	356	LEU
1	C	367	PRO
1	C	368	ASN
1	C	473	GLN
1	C	527	ASN
1	C	532	LEU
1	C	612	GLN
1	C	661	VAL
1	C	681	GLU
1	D	29	PRO
1	D	356	LEU
1	D	367	PRO
1	D	368	ASN
1	D	377	ASP
1	D	473	GLN
1	D	527	ASN
1	D	532	LEU
1	D	612	GLN
1	D	661	VAL
1	D	681	GLU
1	A	10	LEU
1	A	28	GLU
1	A	164	PRO
1	A	377	ASP
1	A	452	LYS
1	A	469	LYS
1	A	474	LEU
1	A	495	ASP

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Mol	Chain	Res	Type
1	A	499	PHE
1	A	662	HIS
1	A	680	GLU
1	B	10	LEU
1	B	28	GLU
1	B	164	PRO
1	B	377	ASP
1	B	452	LYS
1	B	469	LYS
1	B	474	LEU
1	B	495	ASP
1	B	499	PHE
1	B	532	LEU
1	B	662	HIS
1	B	680	GLU
1	C	10	LEU
1	C	28	GLU
1	C	164	PRO
1	C	377	ASP
1	C	452	LYS
1	C	469	LYS
1	C	474	LEU
1	C	495	ASP
1	C	499	PHE
1	C	662	HIS
1	C	680	GLU
1	D	10	LEU
1	D	28	GLU
1	D	164	PRO
1	D	452	LYS
1	D	469	LYS
1	D	474	LEU
1	D	495	ASP
1	D	662	HIS
1	D	680	GLU
1	A	526	PHE
1	A	613	ASN
1	A	660	PRO
1	B	526	PHE
1	B	660	PRO
1	C	526	PHE
1	D	499	PHE

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Mol	Chain	Res	Type
1	D	526	PHE
1	D	660	PRO
1	A	453	ALA
1	B	453	ALA
1	B	613	ASN
1	C	453	ALA
1	C	613	ASN
1	C	660	PRO
1	D	453	ALA
1	A	43	ILE
1	B	43	ILE
1	C	43	ILE
1	D	43	ILE
1	D	46	TYR
1	A	46	TYR
1	B	46	TYR
1	C	46	TYR

5.3.2 Protein sidechains (i)

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	516/590 (88%)	463 (90%)	53 (10%)	9	32
1	B	516/590 (88%)	460 (89%)	56 (11%)	8	30
1	C	516/590 (88%)	461 (89%)	55 (11%)	8	31
1	D	516/590 (88%)	461 (89%)	55 (11%)	8	31
All	All	2064/2360 (88%)	1845 (89%)	219 (11%)	8	31

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	27	ARG
1	A	57	LEU
1	A	68	LEU

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Mol	Chain	Res	Type
1	A	70	GLN
1	A	76	ARG
1	A	109	LEU
1	A	134	VAL
1	A	139	ILE
1	A	148	LEU
1	A	155	LEU
1	A	167	LEU
1	A	192	LEU
1	A	213	GLN
1	A	230	THR
1	A	233	ASN
1	A	234	LEU
1	A	237	VAL
1	A	242	ARG
1	A	261	LEU
1	A	263	LEU
1	A	273	ASN
1	A	277	THR
1	A	290	PHE
1	A	291	THR
1	A	312	ASN
1	A	315	GLN
1	A	337	GLU
1	A	352	SER
1	A	376	ASP
1	A	377	ASP
1	A	383	GLN
1	A	428	ARG
1	A	458	LEU
1	A	472	PHE
1	A	473	GLN
1	A	474	LEU
1	A	492	ASN
1	A	494	PHE
1	A	496	GLU
1	A	525	LEU
1	A	530	LEU
1	A	531	SER
1	A	534	GLN
1	A	537	SER
1	A	550	ARG

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Mol	Chain	Res	Type
1	A	553	ASP
1	A	642	LEU
1	A	650	THR
1	A	661	VAL
1	A	672	ASN
1	A	681	GLU
1	A	684	SER
1	B	16	HIS
1	B	27	ARG
1	B	57	LEU
1	B	68	LEU
1	B	70	GLN
1	B	76	ARG
1	B	109	LEU
1	B	134	VAL
1	B	139	ILE
1	B	148	LEU
1	B	155	LEU
1	B	167	LEU
1	B	192	LEU
1	B	213	GLN
1	B	230	THR
1	B	233	ASN
1	B	234	LEU
1	B	237	VAL
1	B	242	ARG
1	B	261	LEU
1	B	263	LEU
1	B	273	ASN
1	B	277	THR
1	B	290	PHE
1	B	291	THR
1	B	308	VAL
1	B	312	ASN
1	B	337	GLU
1	B	352	SER
1	B	370	LYS
1	B	376	ASP
1	B	377	ASP
1	B	383	GLN
1	B	428	ARG
1	B	458	LEU

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Mol	Chain	Res	Type
1	B	472	PHE
1	B	473	GLN
1	B	474	LEU
1	B	492	ASN
1	B	494	PHE
1	B	496	GLU
1	B	525	LEU
1	B	530	LEU
1	B	533	GLN
1	B	534	GLN
1	B	535	ARG
1	B	537	SER
1	B	539	LEU
1	B	550	ARG
1	B	553	ASP
1	B	642	LEU
1	B	650	THR
1	B	661	VAL
1	B	672	ASN
1	B	681	GLU
1	B	684	SER
1	C	16	HIS
1	C	27	ARG
1	C	57	LEU
1	C	68	LEU
1	C	70	GLN
1	C	76	ARG
1	C	109	LEU
1	C	134	VAL
1	C	139	ILE
1	C	148	LEU
1	C	155	LEU
1	C	167	LEU
1	C	192	LEU
1	C	213	GLN
1	C	230	THR
1	C	233	ASN
1	C	234	LEU
1	C	237	VAL
1	C	242	ARG
1	C	261	LEU
1	C	263	LEU

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Mol	Chain	Res	Type
1	C	273	ASN
1	C	277	THR
1	C	290	PHE
1	C	291	THR
1	C	312	ASN
1	C	315	GLN
1	C	337	GLU
1	C	352	SER
1	C	376	ASP
1	C	377	ASP
1	C	383	GLN
1	C	428	ARG
1	C	458	LEU
1	C	472	PHE
1	C	473	GLN
1	C	474	LEU
1	C	492	ASN
1	C	494	PHE
1	C	496	GLU
1	C	525	LEU
1	C	530	LEU
1	C	534	GLN
1	C	537	SER
1	C	539	LEU
1	C	550	ARG
1	C	553	ASP
1	C	632	ASN
1	C	642	LEU
1	C	650	THR
1	C	661	VAL
1	C	662	HIS
1	C	672	ASN
1	C	681	GLU
1	C	684	SER
1	D	16	HIS
1	D	27	ARG
1	D	57	LEU
1	D	68	LEU
1	D	70	GLN
1	D	76	ARG
1	D	109	LEU
1	D	134	VAL

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Mol	Chain	Res	Type
1	D	139	ILE
1	D	148	LEU
1	D	155	LEU
1	D	167	LEU
1	D	192	LEU
1	D	213	GLN
1	D	230	THR
1	D	233	ASN
1	D	234	LEU
1	D	237	VAL
1	D	242	ARG
1	D	261	LEU
1	D	263	LEU
1	D	273	ASN
1	D	277	THR
1	D	290	PHE
1	D	291	THR
1	D	308	VAL
1	D	312	ASN
1	D	315	GLN
1	D	337	GLU
1	D	352	SER
1	D	376	ASP
1	D	377	ASP
1	D	383	GLN
1	D	428	ARG
1	D	458	LEU
1	D	472	PHE
1	D	473	GLN
1	D	474	LEU
1	D	492	ASN
1	D	494	PHE
1	D	496	GLU
1	D	525	LEU
1	D	530	LEU
1	D	533	GLN
1	D	534	GLN
1	D	537	SER
1	D	539	LEU
1	D	550	ARG
1	D	553	ASP
1	D	642	LEU

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Mol	Chain	Res	Type
1	D	650	THR
1	D	661	VAL
1	D	672	ASN
1	D	681	GLU
1	D	684	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	133	ASN
1	A	151	GLN
1	A	202	GLN
1	A	226	GLN
1	A	233	ASN
1	A	235	ASN
1	A	309	HIS
1	A	315	GLN
1	A	327	ASN
1	A	355	HIS
1	A	461	GLN
1	A	491	ASN
1	A	492	ASN
1	A	534	GLN
1	A	632	ASN
1	A	672	ASN
1	B	70	GLN
1	B	133	ASN
1	B	151	GLN
1	B	202	GLN
1	B	226	GLN
1	B	233	ASN
1	B	235	ASN
1	B	309	HIS
1	B	312	ASN
1	B	315	GLN
1	B	327	ASN
1	B	355	HIS
1	B	461	GLN
1	B	491	ASN
1	B	492	ASN
1	B	534	GLN

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Mol	Chain	Res	Type
1	B	632	ASN
1	B	672	ASN
1	C	70	GLN
1	C	133	ASN
1	C	151	GLN
1	C	202	GLN
1	C	226	GLN
1	C	233	ASN
1	C	235	ASN
1	C	309	HIS
1	C	315	GLN
1	C	327	ASN
1	C	355	HIS
1	C	461	GLN
1	C	491	ASN
1	C	492	ASN
1	C	534	GLN
1	C	632	ASN
1	D	70	GLN
1	D	133	ASN
1	D	151	GLN
1	D	202	GLN
1	D	226	GLN
1	D	233	ASN
1	D	235	ASN
1	D	309	HIS
1	D	315	GLN
1	D	327	ASN
1	D	355	HIS
1	D	461	GLN
1	D	491	ASN
1	D	492	ASN
1	D	534	GLN
1	D	632	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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, 95^{th} 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	572/647 (88%)	-0.07	12 (2%) 67 44	60, 88, 144, 185	0
1	B	572/647 (88%)	-0.07	8 (1%) 78 60	64, 100, 154, 194	0
1	C	572/647 (88%)	0.13	30 (5%) 31 13	62, 102, 210, 270	0
1	D	572/647 (88%)	-0.01	18 (3%) 52 28	52, 90, 197, 247	0
All	All	2288/2588 (88%)	-0.00	68 (2%) 54 29	52, 95, 181, 270	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	PHE	7.4
1	C	21	GLN	6.4
1	C	8	GLN	5.8
1	D	10	LEU	5.2
1	C	470	ALA	4.6
1	A	3	LEU	4.4
1	C	14	GLN	4.4
1	B	354	GLY	4.4
1	C	19	LEU	4.3
1	C	37	VAL	4.2
1	D	8	GLN	4.2
1	D	3	LEU	4.0
1	C	15	ILE	3.9
1	D	41	PHE	3.9
1	C	6	LEU	3.9
1	C	24	SER	3.8
1	D	6	LEU	3.6
1	B	355	HIS	3.6
1	D	15	ILE	3.5
1	A	375	SER	3.5
1	C	10	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	553	ASP	3.4
1	A	377	ASP	3.4
1	C	86	GLU	3.3
1	B	375	SER	3.3
1	C	46	TYR	3.3
1	A	10	LEU	3.2
1	C	5	THR	3.2
1	D	19	LEU	3.2
1	C	40	LYS	3.2
1	D	553	ASP	3.1
1	A	611	THR	3.0
1	D	375	SER	3.0
1	C	74	PHE	3.0
1	C	377	ASP	2.9
1	C	18	ALA	2.8
1	A	25	TYR	2.8
1	D	46	TYR	2.8
1	C	84	LEU	2.8
1	C	9	GLY	2.7
1	B	553	ASP	2.6
1	B	452	LYS	2.6
1	C	28	GLU	2.6
1	D	14	GLN	2.6
1	C	378	LYS	2.5
1	D	9	GLY	2.5
1	B	41	PHE	2.5
1	C	53	SER	2.5
1	B	356	LEU	2.4
1	C	17	GLU	2.4
1	A	7	LYS	2.4
1	C	90	TYR	2.4
1	C	7	LYS	2.3
1	D	37	VAL	2.3
1	C	1	MET	2.2
1	B	113	THR	2.2
1	A	688	GLY	2.2
1	C	356	LEU	2.2
1	D	43	ILE	2.1
1	C	48	SER	2.1
1	D	5	THR	2.1
1	A	493	GLU	2.1
1	C	553	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	2.1
1	D	4	GLU	2.0
1	D	7	LYS	2.0
1	D	90	TYR	2.0
1	A	378	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no 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.