



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:31 AM GMT

PDB ID : 3M8L
Title : Crystal Structure Analysis of the Feline Calicivirus Capsid Protein
Authors : Zhou, Y.; Prasad, B.V.V.
Deposited on : 2010-03-18
Resolution : 3.40 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

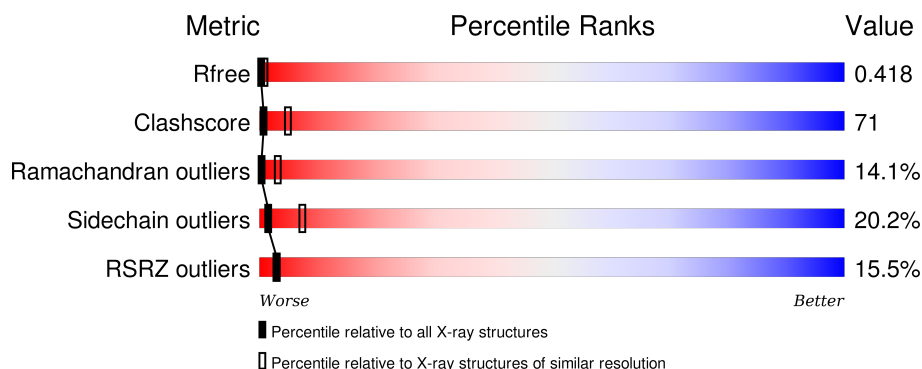
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

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. 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	534	<div> <div>13%</div> <div>25%</div> <div>52%</div> <div>20%</div> <div>.</div> </div>
1	C	534	<div> <div>16%</div> <div>23%</div> <div>56%</div> <div>19%</div> <div>.</div> </div>
2	B	530	<div> <div>18%</div> <div>20%</div> <div>55%</div> <div>21%</div> <div>.</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12360 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	534	Total	C	N	O	S	0	0	0
			4129	2632	687	796	14			
1	C	534	Total	C	N	O	S	0	0	0
			4130	2632	687	797	14			

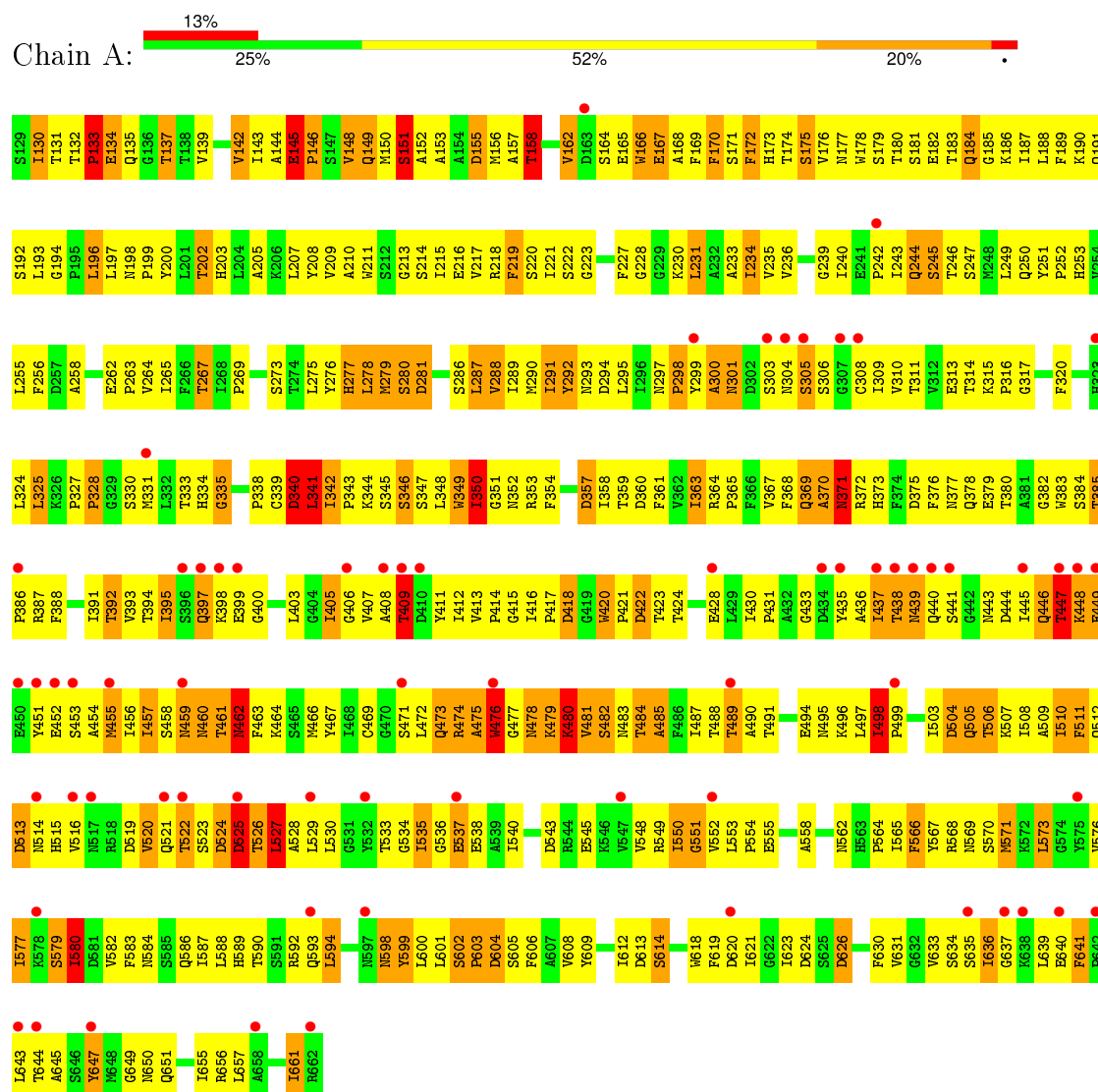
- Molecule 2 is a protein called Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4101	2615	683	789	14			

3 Residue-property plots

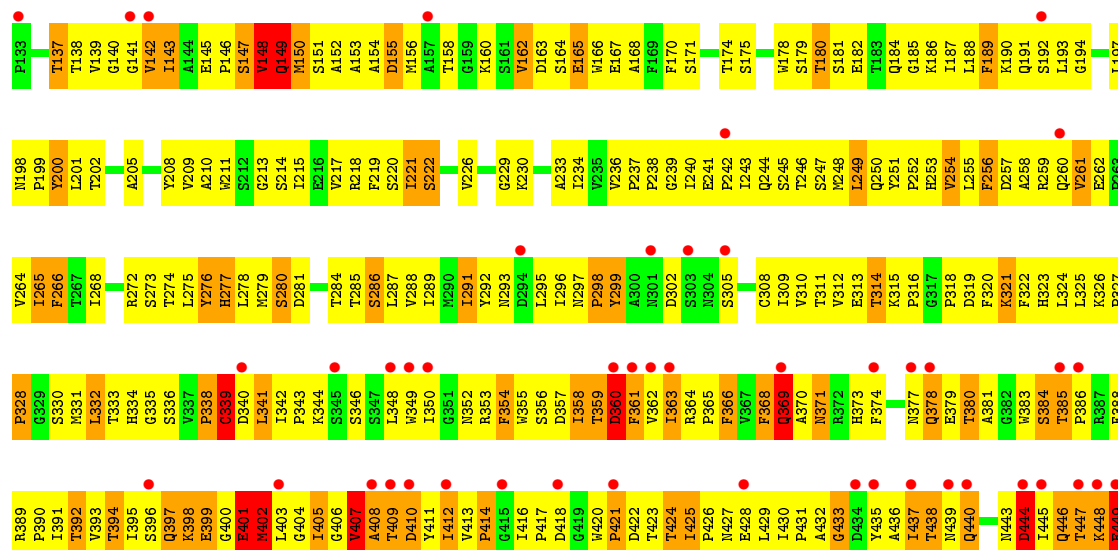
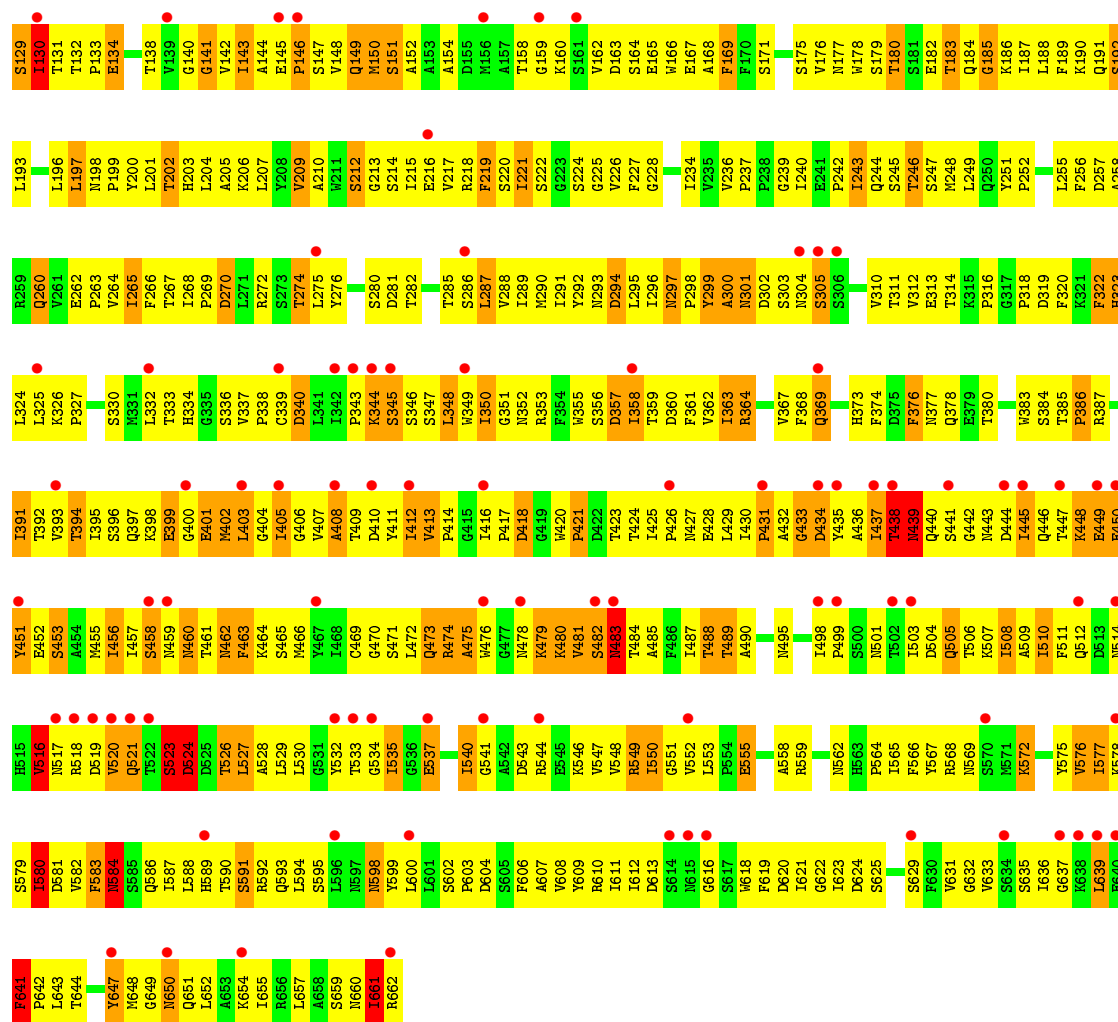
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

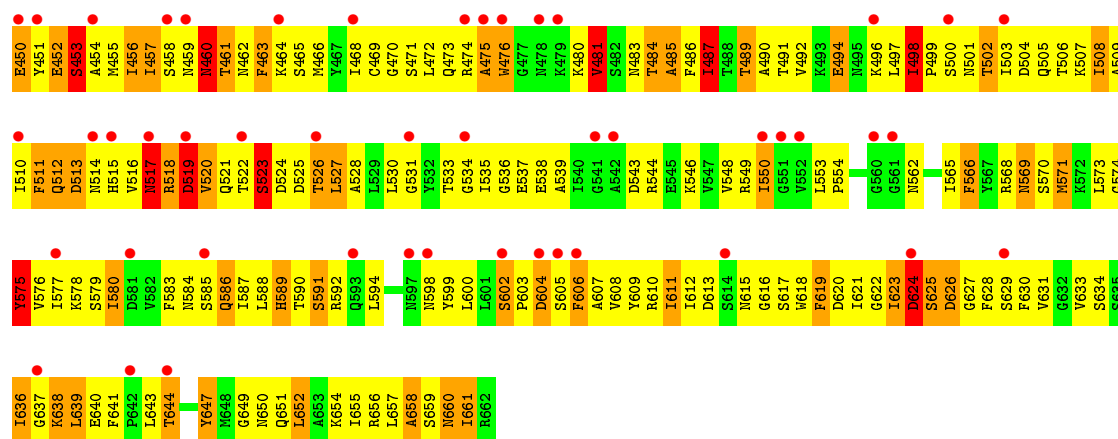
• Molecule 1: Capsid protein



• Molecule 1: Capsid protein







4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	427.08Å 450.73Å 467.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.40 29.98 – 3.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.40) 89.1 (29.98-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 3.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.390 , 0.370 0.419 , 0.418	Depositor DCC
R_{free} test set	27284 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	85.6	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , -9.8	EDS
Estimated twinning fraction	0.017 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	4 of 542437 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	12360	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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, 0.375 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	0.68	1/4229 (0.0%)	0.84	4/5759 (0.1%)
1	C	0.71	1/4230 (0.0%)	0.89	7/5759 (0.1%)
2	B	1.17	11/4201 (0.3%)	0.89	6/5719 (0.1%)
All	All	0.88	13/12660 (0.1%)	0.87	17/17237 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	624	ASP	CB-CG	33.85	2.22	1.51
2	B	606	PHE	CE1-CZ	24.62	1.84	1.37
2	B	606	PHE	CE2-CZ	22.49	1.80	1.37
2	B	606	PHE	CD2-CE2	20.22	1.79	1.39
2	B	606	PHE	CD1-CE1	20.20	1.79	1.39
2	B	606	PHE	CG-CD1	13.98	1.59	1.38
2	B	606	PHE	CG-CD2	13.53	1.59	1.38
2	B	361	PHE	CB-CG	6.29	1.62	1.51
1	C	476	TRP	CB-CG	6.03	1.61	1.50
2	B	444	ASP	CB-CG	5.90	1.64	1.51
2	B	437	ILE	CA-CB	5.74	1.68	1.54
1	A	476	TRP	CB-CG	5.61	1.60	1.50
2	B	476	TRP	CB-CG	5.60	1.60	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	THR	CB-CA-C	13.09	146.94	111.60
1	A	439	ASN	N-CA-CB	-13.07	87.07	110.60
2	B	624	ASP	CB-CG-OD1	9.58	126.92	118.30
1	C	451	TYR	CB-CA-C	-8.87	92.67	110.40
2	B	360	ASP	N-CA-C	8.51	133.98	111.00
2	B	624	ASP	OD1-CG-OD2	-8.27	107.59	123.30
2	B	624	ASP	CB-CG-OD2	7.79	125.31	118.30
1	C	145	GLU	N-CA-C	7.08	130.11	111.00
1	C	145	GLU	C-N-CD	-6.88	105.47	120.60
2	B	517	ASN	N-CA-C	6.21	127.76	111.00
1	C	480	LYS	N-CA-C	5.73	126.48	111.00
1	C	439	ASN	N-CA-C	5.70	126.38	111.00
1	C	438	THR	N-CA-C	-5.68	95.65	111.00
1	A	438	THR	N-CA-C	-5.58	95.93	111.00
1	C	483	ASN	N-CA-C	5.53	125.93	111.00
1	A	151	SER	N-CA-C	-5.39	96.44	111.00
2	B	361	PHE	N-CA-C	5.17	124.97	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	200	TYR	Sidechain

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	4129	0	4062	602	0
1	C	4130	0	4062	563	7
2	B	4101	0	4033	615	6
All	All	12360	0	12157	1731	7

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 71.

All (1731) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:PHE:CE1	2:B:606:PHE:CZ	1.84	1.62
2:B:606:PHE:CD2	2:B:606:PHE:CE2	1.79	1.62
2:B:606:PHE:CD1	2:B:606:PHE:CE1	1.79	1.62
2:B:606:PHE:CZ	2:B:606:PHE:CE2	1.80	1.61
2:B:606:PHE:CZ	2:B:624:ASP:CB	1.88	1.51
2:B:606:PHE:CE2	2:B:624:ASP:CB	1.92	1.50
2:B:606:PHE:CZ	2:B:624:ASP:CG	1.87	1.47
2:B:606:PHE:CE1	2:B:624:ASP:CG	1.88	1.46
2:B:606:PHE:CE2	2:B:624:ASP:CG	1.97	1.37
2:B:606:PHE:CE1	2:B:624:ASP:CB	2.10	1.34
2:B:606:PHE:CD1	2:B:624:ASP:CG	2.02	1.32
2:B:606:PHE:CZ	2:B:624:ASP:HB3	1.53	1.30
2:B:606:PHE:CD1	2:B:624:ASP:HA	1.66	1.28
2:B:606:PHE:CD2	2:B:624:ASP:CB	2.20	1.24
2:B:606:PHE:CD2	2:B:624:ASP:CG	2.11	1.24
2:B:606:PHE:CE1	2:B:624:ASP:OD2	1.91	1.23
1:A:209:VAL:HG22	1:A:324:LEU:O	1.36	1.23
1:C:437:ILE:CD1	1:C:457:ILE:HD11	1.73	1.19
2:B:436:ALA:HB3	2:B:461:THR:HA	1.18	1.17
2:B:606:PHE:CG	2:B:624:ASP:CG	2.20	1.15
2:B:453:SER:CB	2:B:456:ILE:HD13	1.76	1.15
2:B:606:PHE:CD2	2:B:624:ASP:OD1	1.98	1.14
2:B:606:PHE:CD1	2:B:624:ASP:CA	2.32	1.13
1:C:358:ILE:HD12	1:C:358:ILE:H	1.07	1.11
2:B:606:PHE:CD2	2:B:624:ASP:HB2	1.84	1.11
1:A:405:ILE:HD12	1:A:510:ILE:HG12	1.28	1.11
1:A:474:ARG:HH21	1:A:523:SER:HB3	1.03	1.11
1:A:474:ARG:HD3	1:A:523:SER:HA	1.35	1.08
1:A:175:SER:HB3	1:A:311:THR:HG22	1.33	1.08
2:B:606:PHE:CD1	2:B:624:ASP:CB	2.37	1.07
2:B:624:ASP:CG	2:B:624:ASP:CB	2.22	1.07
2:B:396:SER:HA	2:B:521:GLN:HE21	1.14	1.07
1:A:439:ASN:HB2	1:A:456:ILE:HA	1.35	1.07
2:B:606:PHE:CE2	2:B:624:ASP:HB2	1.69	1.07
1:A:535:ILE:HG13	1:A:536:GLY:H	1.18	1.06
2:B:395:ILE:HG12	2:B:396:SER:H	1.04	1.06
2:B:623:ILE:H	2:B:623:ILE:HD12	1.15	1.06
2:B:606:PHE:CZ	2:B:624:ASP:OD2	2.09	1.05
1:A:456:ILE:O	1:A:458:SER:N	1.89	1.05
1:C:437:ILE:HD12	1:C:457:ILE:HD11	1.09	1.04
2:B:449:GLU:O	2:B:450:GLU:HB2	1.53	1.03
2:B:213:GLY:HA3	2:B:320:PHE:HA	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:TRP:HE3	2:B:358:ILE:HD13	1.23	1.02
1:C:448:LYS:HE3	1:C:537:GLU:OE2	1.60	1.02
1:A:399:GLU:HG3	1:A:516:VAL:HG21	1.40	1.01
2:B:185:GLY:H	2:B:291:ILE:HG13	1.24	1.01
1:A:438:THR:HG21	1:A:458:SER:HA	1.40	1.00
1:C:287:LEU:HD12	1:C:288:VAL:N	1.75	1.00
1:A:406:GLY:H	1:A:508:ILE:HD11	1.26	1.00
1:C:587:ILE:HD12	1:C:587:ILE:H	1.25	0.99
2:B:606:PHE:CG	2:B:624:ASP:CB	2.45	0.99
2:B:453:SER:HB3	2:B:456:ILE:HD13	1.40	0.99
1:C:550:ILE:O	1:C:550:ILE:HD13	1.61	0.98
2:B:393:VAL:HA	2:B:409:THR:HG21	1.43	0.98
1:A:130:ILE:HG13	1:A:131:THR:H	1.29	0.97
1:A:474:ARG:NH2	1:A:523:SER:HB3	1.78	0.97
1:A:438:THR:HG22	1:A:457:ILE:O	1.65	0.96
2:B:385:THR:HG22	2:B:386:PRO:HD2	1.45	0.96
1:C:149:GLN:O	1:C:152:ALA:HB2	1.65	0.96
2:B:190:LYS:HE3	2:B:242:PRO:HB2	1.43	0.96
2:B:452:GLU:O	2:B:453:SER:HB2	1.63	0.96
2:B:346:SER:HB3	2:B:643:LEU:HB2	1.48	0.95
1:A:189:PHE:CZ	1:A:191:GLN:HB2	2.01	0.95
1:A:405:ILE:HG13	1:A:509:ALA:HA	1.49	0.94
2:B:395:ILE:HG12	2:B:396:SER:N	1.82	0.94
1:C:416:ILE:HD12	1:C:503:ILE:HG12	1.50	0.94
2:B:358:ILE:HG13	2:B:359:THR:H	1.32	0.94
1:C:577:ILE:HG13	1:C:578:LYS:H	1.33	0.94
1:C:397:GLN:HB2	1:C:521:GLN:HA	1.47	0.94
1:A:148:VAL:HG22	1:A:149:GLN:H	1.33	0.94
2:B:636:ILE:HD13	2:B:636:ILE:H	1.28	0.93
2:B:638:LYS:H	2:B:638:LYS:HD2	1.33	0.93
2:B:446:GLN:NE2	2:B:447:THR:HG23	1.83	0.93
1:C:544:ARG:HD3	1:C:553:LEU:HD21	1.50	0.93
1:A:445:ILE:O	1:A:445:ILE:HG13	1.69	0.92
2:B:606:PHE:CG	2:B:624:ASP:OD1	2.21	0.92
1:A:506:THR:O	1:A:507:LYS:HD2	1.67	0.92
1:A:487:ILE:HG22	1:A:510:ILE:HA	1.50	0.92
2:B:661:ILE:HD13	2:B:661:ILE:H	1.33	0.91
1:C:221:ILE:HD13	1:C:221:ILE:H	1.34	0.91
2:B:353:ARG:H	2:B:584:ASN:ND2	1.68	0.91
1:C:352:ASN:ND2	1:C:586:GLN:H	1.67	0.91
1:C:219:PHE:HB3	1:C:312:VAL:HA	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:HD22	2:B:443:ASN:HD21	1.18	0.91
1:C:448:LYS:CE	1:C:537:GLU:OE2	2.19	0.91
2:B:470:GLY:H	2:B:528:ALA:H	1.13	0.91
1:A:350:ILE:HA	1:A:357:ASP:HA	1.52	0.91
1:A:246:THR:O	1:A:249:LEU:HB2	1.69	0.90
1:C:448:LYS:O	1:C:449:GLU:HB2	1.70	0.90
1:C:144:ALA:HB1	1:C:147:SER:HB3	1.52	0.90
2:B:352:ASN:HD21	2:B:369:GLN:HE22	1.17	0.90
2:B:349:TRP:CE3	2:B:358:ILE:HD13	2.07	0.90
1:C:474:ARG:H	1:C:524:ASP:HA	1.33	0.90
1:A:273:SER:O	2:B:275:LEU:HD12	1.71	0.90
2:B:226:VAL:HG12	2:B:298:PRO:HG2	1.51	0.90
1:C:437:ILE:CD1	1:C:457:ILE:CD1	2.51	0.89
1:C:451:TYR:H	1:C:458:SER:HB2	1.36	0.89
1:C:358:ILE:N	1:C:358:ILE:HD12	1.86	0.89
1:A:213:GLY:HA3	1:A:320:PHE:HA	1.54	0.89
1:A:405:ILE:HB	1:A:508:ILE:HG13	1.53	0.89
2:B:255:LEU:HB2	1:C:131:THR:HG23	1.55	0.89
1:C:236:VAL:HG23	1:C:286:SER:HB2	1.54	0.89
1:C:464:LYS:HA	1:C:533:THR:HG21	1.52	0.89
1:A:476:TRP:CD1	1:A:520:VAL:HB	2.09	0.88
1:A:148:VAL:HG13	1:A:149:GLN:HG3	1.56	0.88
2:B:623:ILE:HD12	2:B:623:ILE:N	1.89	0.88
1:C:437:ILE:HD12	1:C:457:ILE:CD1	2.02	0.87
1:A:454:ALA:O	1:A:455:MET:HG3	1.75	0.87
2:B:192:SER:HA	2:B:286:SER:HB3	1.57	0.86
1:A:503:ILE:HG22	1:A:549:ARG:O	1.76	0.86
2:B:210:ALA:HB3	2:B:323:HIS:HB2	1.54	0.86
1:C:349:TRP:HB3	1:C:358:ILE:HD13	1.55	0.86
2:B:146:PRO:HB2	2:B:149:GLN:CD	1.96	0.86
1:A:378:GLN:HG3	1:C:654:LYS:NZ	1.90	0.86
1:C:287:LEU:HD12	1:C:288:VAL:H	1.38	0.85
2:B:417:PRO:HB2	2:B:420:TRP:HB2	1.58	0.85
1:A:447:THR:HG22	1:A:447:THR:O	1.76	0.85
1:C:631:VAL:HG12	1:C:633:VAL:H	1.41	0.85
2:B:243:ILE:HG22	2:B:245:SER:H	1.40	0.85
1:C:358:ILE:CD1	1:C:358:ILE:H	1.89	0.85
1:C:391:ILE:N	1:C:391:ILE:HD12	1.90	0.85
1:A:438:THR:CG2	1:A:458:SER:HA	2.06	0.84
1:A:416:ILE:HD12	1:A:503:ILE:HG12	1.57	0.84
2:B:394:THR:HG22	2:B:522:THR:HG23	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:ARG:H	2:B:584:ASN:HD22	1.25	0.84
1:C:221:ILE:HG22	1:C:310:VAL:HG22	1.57	0.84
1:C:451:TYR:HD1	1:C:457:ILE:CA	1.91	0.84
2:B:451:TYR:HE1	2:B:457:ILE:HD11	1.43	0.84
2:B:521:GLN:HG2	2:B:522:THR:H	1.43	0.84
1:A:346:SER:HB3	1:A:643:LEU:HB2	1.58	0.84
2:B:606:PHE:CE1	2:B:624:ASP:CA	2.61	0.83
1:C:451:TYR:N	1:C:458:SER:HB2	1.91	0.83
2:B:490:ALA:HB1	2:B:498:ILE:O	1.78	0.83
2:B:623:ILE:H	2:B:623:ILE:CD1	1.81	0.83
1:A:394:THR:OG1	1:A:407:VAL:HG11	1.78	0.82
1:A:473:GLN:HB3	1:A:482:SER:HA	1.60	0.82
1:C:572:LYS:H	1:C:572:LYS:HD2	1.44	0.82
1:C:141:GLY:HA3	1:C:144:ALA:HB3	1.61	0.82
2:B:553:LEU:HD12	2:B:554:PRO:HD2	1.62	0.82
2:B:453:SER:CB	2:B:456:ILE:CD1	2.57	0.81
2:B:327:PRO:O	2:B:330:SER:HB2	1.79	0.81
1:A:397:GLN:HE22	1:A:520:VAL:HG23	1.44	0.81
2:B:397:GLN:OE1	2:B:521:GLN:HB3	1.80	0.81
2:B:533:THR:O	2:B:535:ILE:HG23	1.79	0.81
1:A:405:ILE:CD1	1:A:510:ILE:HG12	2.10	0.81
2:B:463:PHE:HB3	2:B:466:MET:HG3	1.62	0.81
1:A:234:ILE:HD13	1:A:234:ILE:N	1.96	0.81
1:C:608:VAL:HB	1:C:648:MET:HB2	1.63	0.81
1:A:535:ILE:HG13	1:A:536:GLY:N	1.94	0.81
1:C:424:THR:OG1	1:C:489:THR:HG23	1.80	0.80
2:B:411:TYR:CZ	2:B:417:PRO:HA	2.16	0.80
1:C:219:PHE:HB2	1:C:311:THR:O	1.79	0.80
1:A:459:ASN:O	1:A:460:ASN:CG	2.19	0.80
1:C:187:ILE:HG12	1:C:244:GLN:HG2	1.64	0.80
2:B:451:TYR:CE1	2:B:457:ILE:CD1	2.64	0.80
1:A:353:ARG:H	1:A:584:ASN:ND2	1.79	0.80
1:A:184:GLN:HE21	1:A:293:ASN:HA	1.47	0.80
2:B:439:ASN:ND2	2:B:456:ILE:HG13	1.97	0.80
2:B:402:MET:HE2	2:B:511:PHE:HA	1.64	0.79
1:C:221:ILE:CD1	1:C:221:ILE:H	1.95	0.79
1:C:210:ALA:HB3	1:C:324:LEU:H	1.46	0.79
2:B:606:PHE:CE1	2:B:624:ASP:HB3	2.17	0.79
1:A:476:TRP:CE3	1:A:522:THR:HB	2.17	0.79
2:B:171:SER:O	2:B:313:GLU:HB3	1.82	0.79
1:A:393:VAL:O	1:A:525:ASP:HB3	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:407:VAL:O	2:B:409:THR:HG22	1.82	0.79
1:C:532:TYR:OH	1:C:535:ILE:HD13	1.81	0.79
1:C:451:TYR:HD1	1:C:457:ILE:CB	1.95	0.79
2:B:174:THR:HG22	2:B:175:SER:H	1.45	0.79
1:A:566:PHE:CE2	1:A:583:PHE:HB3	2.18	0.79
1:A:447:THR:CG2	1:A:447:THR:O	2.31	0.79
2:B:146:PRO:O	2:B:149:GLN:HG2	1.84	0.78
1:A:571:MET:HB3	1:A:580:ILE:HD11	1.65	0.78
1:A:278:LEU:H	1:A:278:LEU:HD23	1.47	0.78
1:C:451:TYR:HD1	1:C:457:ILE:HA	1.47	0.78
2:B:451:TYR:HE1	2:B:457:ILE:CD1	1.96	0.78
1:C:471:SER:HB3	1:C:527:LEU:HB3	1.64	0.78
1:A:239:GLY:O	2:B:333:THR:HG22	1.83	0.78
1:C:473:GLN:HA	1:C:524:ASP:OD1	1.84	0.78
2:B:287:LEU:HD12	2:B:288:VAL:H	1.48	0.78
1:C:349:TRP:HB3	1:C:358:ILE:CD1	2.14	0.78
1:A:327:PRO:HG2	1:A:330:SER:OG	1.84	0.78
2:B:476:TRP:CD1	2:B:520:VAL:HB	2.20	0.77
1:A:406:GLY:N	1:A:508:ILE:HD11	1.99	0.77
1:C:487:ILE:HG22	1:C:510:ILE:HG22	1.66	0.77
2:B:424:THR:HG22	2:B:489:THR:HG23	1.67	0.77
1:A:130:ILE:CG1	1:A:131:THR:H	1.96	0.77
1:C:397:GLN:HG2	1:C:523:SER:HB2	1.64	0.77
1:A:631:VAL:HA	1:A:657:LEU:HD12	1.66	0.77
2:B:310:VAL:O	2:B:310:VAL:HG13	1.85	0.77
1:C:360:ASP:HB3	1:C:568:ARG:HB3	1.65	0.77
1:A:474:ARG:HD2	1:A:475:ALA:H	1.48	0.77
1:A:234:ILE:HD13	1:A:234:ILE:H	1.50	0.77
2:B:576:VAL:O	2:B:576:VAL:HG12	1.83	0.77
1:A:236:VAL:HG11	1:A:242:PRO:HG3	1.65	0.77
2:B:487:ILE:CG2	2:B:510:ILE:HG22	2.15	0.76
1:A:148:VAL:O	1:A:150:MET:N	2.18	0.76
1:A:459:ASN:O	1:A:460:ASN:CB	2.33	0.76
2:B:436:ALA:CB	2:B:461:THR:HA	2.10	0.76
2:B:370:ALA:HB2	2:B:554:PRO:HD3	1.67	0.76
1:A:342:ILE:HD12	1:A:609:TYR:HD2	1.48	0.76
1:C:398:LYS:N	1:C:403:LEU:HD23	2.00	0.76
1:C:352:ASN:HD22	1:C:586:GLN:H	1.33	0.76
2:B:425:ILE:HG12	2:B:499:PRO:HB3	1.67	0.76
2:B:606:PHE:CG	2:B:624:ASP:CA	2.67	0.76
1:C:451:TYR:CD1	1:C:457:ILE:HB	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLN:HB2	2:B:328:PRO:HG2	1.67	0.76
2:B:453:SER:HB3	2:B:456:ILE:CD1	2.16	0.75
2:B:341:LEU:HG	2:B:609:TYR:OH	1.86	0.75
1:A:221:ILE:HD12	1:A:221:ILE:O	1.86	0.75
1:C:363:ILE:HD13	1:C:363:ILE:H	1.50	0.75
2:B:606:PHE:CE2	2:B:624:ASP:HB3	2.16	0.75
1:A:608:VAL:HG23	1:A:650:ASN:HA	1.68	0.75
2:B:451:TYR:CE1	2:B:457:ILE:HD11	2.20	0.75
1:C:395:ILE:HG22	1:C:406:GLY:HA3	1.66	0.75
1:C:401:GLU:OE1	1:C:402:MET:HB3	1.85	0.75
1:A:394:THR:O	1:A:407:VAL:HB	1.85	0.75
1:C:587:ILE:HD12	1:C:587:ILE:N	2.01	0.75
1:A:333:THR:HG22	1:C:239:GLY:HA2	1.65	0.75
2:B:439:ASN:OD1	2:B:456:ILE:HA	1.87	0.75
2:B:383:TRP:O	2:B:412:ILE:HD11	1.87	0.75
1:A:149:GLN:O	1:A:153:ALA:HB3	1.86	0.75
2:B:456:ILE:HG23	2:B:457:ILE:N	2.02	0.74
1:A:352:ASN:HB2	1:A:372:ARG:HB3	1.68	0.74
2:B:253:HIS:O	1:C:133:PRO:HB3	1.87	0.74
1:C:350:ILE:HA	1:C:357:ASP:HA	1.69	0.74
2:B:158:THR:C	2:B:160:LYS:H	1.90	0.74
2:B:327:PRO:HG2	2:B:330:SER:HB2	1.70	0.74
1:A:624:ASP:OD2	1:A:626:ASP:HB2	1.87	0.74
1:C:297:ASN:HD22	1:C:298:PRO:CD	1.99	0.74
2:B:453:SER:HB3	2:B:456:ILE:HB	1.68	0.74
1:A:464:LYS:HA	1:A:533:THR:HG21	1.69	0.74
1:A:240:ILE:O	1:A:240:ILE:HD12	1.86	0.74
1:A:497:LEU:O	1:A:498:ILE:HG13	1.87	0.74
2:B:504:ASP:HB2	2:B:507:LYS:HD3	1.68	0.74
2:B:631:VAL:HG12	2:B:633:VAL:H	1.51	0.73
2:B:185:GLY:N	2:B:291:ILE:HG13	2.01	0.73
1:A:151:SER:O	1:A:152:ALA:HB3	1.88	0.73
1:A:197:LEU:HD12	1:A:215:ILE:HD12	1.69	0.73
1:C:535:ILE:HD12	1:C:546:LYS:NZ	2.03	0.73
2:B:427:ASN:O	2:B:499:PRO:HD3	1.86	0.73
2:B:606:PHE:CG	2:B:624:ASP:HA	2.23	0.73
1:A:535:ILE:HD11	1:A:538:GLU:HB2	1.71	0.73
1:C:150:MET:C	1:C:152:ALA:H	1.90	0.73
1:C:408:ALA:HB2	1:C:417:PRO:HG3	1.70	0.73
1:A:439:ASN:HB3	1:A:456:ILE:HG12	1.70	0.73
1:C:297:ASN:HD22	1:C:298:PRO:N	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:CYS:SG	1:A:647:TYR:HB2	2.28	0.73
1:A:185:GLY:H	1:A:291:ILE:HG13	1.53	0.73
1:A:133:PRO:HB3	1:A:134:GLU:OE2	1.87	0.73
1:A:472:LEU:O	1:A:473:GLN:HB3	1.87	0.72
1:A:287:LEU:HG	1:A:288:VAL:N	2.03	0.72
1:A:350:ILE:HG22	1:A:357:ASP:HB3	1.71	0.72
1:C:611:ILE:HD12	1:C:611:ILE:N	2.04	0.72
2:B:402:MET:CE	2:B:512:GLN:H	2.01	0.72
2:B:148:VAL:HG23	2:B:149:GLN:HE21	1.54	0.72
2:B:661:ILE:H	2:B:661:ILE:CD1	2.02	0.72
2:B:615:ASN:HB2	2:B:640:GLU:HG2	1.72	0.72
1:C:447:THR:O	1:C:448:LYS:HB3	1.88	0.72
1:C:339:CYS:SG	1:C:649:GLY:HA2	2.29	0.72
1:A:405:ILE:HD12	1:A:510:ILE:CG1	2.16	0.72
2:B:342:ILE:HD12	2:B:587:ILE:HD12	1.71	0.72
1:C:219:PHE:CB	1:C:312:VAL:HA	2.18	0.72
1:A:472:LEU:HD23	1:A:473:GLN:HG2	1.68	0.72
2:B:336:SER:H	2:B:599:TYR:HA	1.55	0.72
2:B:579:SER:O	2:B:580:ILE:HG13	1.90	0.72
1:C:490:ALA:HB1	1:C:498:ILE:O	1.90	0.71
1:A:438:THR:HG21	1:A:459:ASN:H	1.55	0.71
2:B:198:ASN:HB2	2:B:314:THR:OG1	1.90	0.71
2:B:656:ARG:O	2:B:657:LEU:HD23	1.89	0.71
1:A:335:GLY:HA3	1:A:600:LEU:H	1.54	0.71
2:B:397:GLN:CD	2:B:521:GLN:HB3	2.11	0.71
1:C:201:LEU:HD11	1:C:316:PRO:HB3	1.72	0.71
2:B:412:ILE:HD13	2:B:413:VAL:HG23	1.71	0.71
2:B:452:GLU:O	2:B:453:SER:CB	2.37	0.71
1:C:451:TYR:CD1	1:C:457:ILE:HA	2.25	0.71
2:B:409:THR:O	2:B:410:ASP:HB2	1.89	0.71
2:B:188:LEU:O	2:B:188:LEU:HD23	1.91	0.71
1:C:175:SER:HB3	1:C:311:THR:HA	1.73	0.71
1:A:562:ASN:OD1	1:A:657:LEU:HG	1.91	0.71
1:C:201:LEU:HD22	1:C:320:PHE:HE2	1.56	0.71
1:C:130:ILE:H	1:C:130:ILE:HD13	1.56	0.71
1:A:398:LYS:N	1:A:403:LEU:HD22	2.06	0.71
1:A:565:ILE:HD12	1:A:566:PHE:N	2.05	0.71
1:C:334:HIS:HB3	1:C:600:LEU:HD11	1.73	0.71
2:B:439:ASN:HD21	2:B:456:ILE:HD11	1.56	0.71
2:B:374:PHE:H	2:B:586:GLN:HE22	1.39	0.71
2:B:451:TYR:CE1	2:B:457:ILE:HD12	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ILE:HD12	2:B:289:ILE:N	2.06	0.70
1:A:474:ARG:HD3	1:A:523:SER:CA	2.16	0.70
2:B:350:ILE:HD12	2:B:588:LEU:HD23	1.72	0.70
1:A:131:THR:OG1	1:C:255:LEU:HB2	1.91	0.70
1:C:620:ASP:HB2	1:C:657:LEU:HB3	1.73	0.70
1:C:197:LEU:HD12	1:C:215:ILE:CD1	2.22	0.70
1:A:378:GLN:HG3	1:C:654:LYS:HZ1	1.55	0.70
1:A:405:ILE:CG2	1:A:510:ILE:HG23	2.21	0.70
1:C:471:SER:CB	1:C:527:LEU:HB3	2.21	0.70
2:B:580:ILE:O	2:B:580:ILE:HD12	1.91	0.70
1:C:189:PHE:HD1	1:C:289:ILE:HB	1.55	0.70
1:A:451:TYR:HA	1:A:452:GLU:HB2	1.72	0.70
1:A:461:THR:HG22	1:A:464:LYS:HB3	1.73	0.70
2:B:463:PHE:CB	2:B:466:MET:HG3	2.22	0.70
1:C:373:HIS:HA	1:C:586:GLN:OE1	1.92	0.70
2:B:178:TRP:CZ2	2:B:295:LEU:HB2	2.27	0.70
1:C:567:TYR:OH	1:C:587:ILE:HD11	1.91	0.70
2:B:221:ILE:H	2:B:221:ILE:HD12	1.57	0.70
1:A:655:ILE:HD12	1:A:655:ILE:O	1.90	0.70
1:A:164:SER:HA	1:A:166:TRP:CE3	2.27	0.70
1:A:175:SER:HB3	1:A:311:THR:CG2	2.15	0.69
1:C:425:ILE:HG13	1:C:499:PRO:HB3	1.74	0.69
2:B:210:ALA:CB	2:B:323:HIS:HB2	2.22	0.69
2:B:354:PHE:C	2:B:356:SER:H	1.95	0.69
2:B:425:ILE:HD13	2:B:425:ILE:N	2.07	0.69
1:C:508:ILE:N	1:C:508:ILE:HD13	2.07	0.69
1:C:397:GLN:HB2	1:C:520:VAL:O	1.92	0.69
1:A:420:TRP:CD1	1:A:421:PRO:HD2	2.26	0.69
2:B:453:SER:HB2	2:B:456:ILE:HD13	1.73	0.69
1:A:251:TYR:CG	1:A:252:PRO:HD2	2.28	0.69
1:C:577:ILE:HG13	1:C:578:LYS:N	2.06	0.69
2:B:606:PHE:CE2	2:B:624:ASP:OD1	2.45	0.69
1:A:406:GLY:H	1:A:508:ILE:CD1	2.04	0.69
1:A:460:ASN:O	1:A:462:ASN:N	2.26	0.69
2:B:503:ILE:HG22	2:B:549:ARG:O	1.93	0.69
1:C:578:LYS:O	1:C:579:SER:OG	2.09	0.69
1:A:221:ILE:HD12	1:A:221:ILE:C	2.12	0.69
1:A:231:LEU:CD1	1:A:291:ILE:HA	2.23	0.69
1:C:346:SER:HB2	1:C:643:LEU:HB2	1.75	0.69
2:B:513:ASP:HB2	2:B:515:HIS:NE2	2.08	0.69
1:C:587:ILE:H	1:C:587:ILE:CD1	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ARG:H	1:C:584:ASN:ND2	1.90	0.69
1:A:601:LEU:HD11	1:A:606:PHE:O	1.92	0.69
1:C:567:TYR:CZ	1:C:587:ILE:HD11	2.28	0.69
1:C:345:SER:HA	1:C:644:THR:HG22	1.75	0.69
1:C:376:PHE:HB2	1:C:625:SER:O	1.92	0.69
1:C:450:GLU:O	1:C:451:TYR:HB2	1.92	0.68
1:A:352:ASN:ND2	1:A:586:GLN:H	1.90	0.68
2:B:611:ILE:N	2:B:611:ILE:HD12	2.09	0.68
2:B:637:GLY:O	2:B:639:LEU:HD22	1.94	0.68
2:B:396:SER:HB2	2:B:404:GLY:HA2	1.75	0.68
1:A:350:ILE:CA	1:A:357:ASP:HA	2.22	0.68
1:A:360:ASP:HB2	1:A:568:ARG:HD2	1.75	0.68
1:A:398:LYS:H	1:A:403:LEU:HD22	1.58	0.68
2:B:425:ILE:HG22	2:B:465:SER:HB2	1.76	0.68
2:B:566:PHE:CD2	2:B:583:PHE:HB3	2.28	0.68
1:A:411:TYR:CD1	1:A:418:ASP:N	2.61	0.68
2:B:365:PRO:O	2:B:366:PHE:HD1	1.77	0.68
2:B:468:ILE:HB	2:B:531:GLY:H	1.57	0.68
1:A:656:ARG:O	1:A:657:LEU:HD23	1.94	0.67
1:C:431:PRO:HB3	1:C:511:PHE:CZ	2.28	0.67
1:A:438:THR:HG21	1:A:458:SER:CA	2.20	0.67
2:B:428:GLU:HG3	2:B:498:ILE:HG22	1.75	0.67
2:B:472:LEU:HD22	2:B:473:GLN:N	2.08	0.67
1:A:189:PHE:CE2	1:A:191:GLN:HB2	2.29	0.67
2:B:145:GLU:OE1	2:B:146:PRO:HD2	1.94	0.67
2:B:437:ILE:O	2:B:438:THR:HB	1.94	0.67
1:A:446:GLN:O	1:A:447:THR:C	2.33	0.67
2:B:368:PHE:O	2:B:369:GLN:HB3	1.95	0.67
1:C:412:ILE:HD12	1:C:413:VAL:HG22	1.77	0.67
1:A:408:ALA:HB2	1:A:417:PRO:HG3	1.77	0.67
1:C:463:PHE:HB2	1:C:466:MET:HG3	1.76	0.67
1:A:448:LYS:O	1:A:449:GLU:CB	2.42	0.67
1:A:535:ILE:CD1	1:A:538:GLU:HB2	2.25	0.67
2:B:624:ASP:O	2:B:627:GLY:N	2.20	0.67
1:A:352:ASN:H	1:A:584:ASN:HD22	1.41	0.67
2:B:473:GLN:HE21	2:B:475:ALA:N	1.92	0.67
1:C:470:GLY:H	1:C:530:LEU:HD13	1.58	0.67
1:C:287:LEU:CD1	1:C:288:VAL:N	2.56	0.67
1:C:296:ILE:HD12	1:C:296:ILE:O	1.95	0.67
1:A:472:LEU:HD22	1:A:524:ASP:HB3	1.77	0.66
1:C:540:ILE:HB	1:C:582:VAL:CG1	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LYS:O	1:C:345:SER:HB2	1.95	0.66
1:A:457:ILE:HG13	1:A:457:ILE:O	1.94	0.66
2:B:516:VAL:O	2:B:516:VAL:HG13	1.96	0.66
1:C:448:LYS:O	1:C:449:GLU:CB	2.41	0.66
1:C:408:ALA:HB1	1:C:411:TYR:CD2	2.29	0.66
1:A:341:LEU:HB2	1:A:609:TYR:OH	1.96	0.66
2:B:446:GLN:HE22	2:B:447:THR:HG23	1.60	0.66
1:A:197:LEU:HD12	1:A:215:ILE:CD1	2.26	0.66
1:C:529:LEU:C	1:C:530:LEU:HD12	2.16	0.66
2:B:158:THR:O	2:B:160:LYS:N	2.29	0.66
1:A:428:GLU:HG2	1:A:499:PRO:HD2	1.76	0.66
1:C:332:LEU:HD23	1:C:334:HIS:H	1.61	0.66
1:A:393:VAL:C	1:A:525:ASP:HB3	2.14	0.66
1:A:461:THR:CG2	1:A:464:LYS:HB3	2.26	0.66
1:A:490:ALA:HB1	1:A:498:ILE:O	1.95	0.66
1:A:469:CYS:O	1:A:485:ALA:CB	2.44	0.66
1:A:349:TRP:CE3	1:A:358:ILE:HD12	2.31	0.66
1:A:142:VAL:O	1:A:143:ILE:HG22	1.94	0.66
1:A:431:PRO:HB3	1:A:511:PHE:CE1	2.30	0.66
2:B:397:GLN:HE21	2:B:514:ASN:CG	1.99	0.66
2:B:385:THR:HG22	2:B:386:PRO:CD	2.24	0.66
1:A:189:PHE:HB3	1:A:289:ILE:CD1	2.26	0.66
1:A:367:VAL:HG13	1:A:566:PHE:CE1	2.31	0.66
2:B:366:PHE:CE2	1:C:414:PRO:HD3	2.31	0.66
2:B:425:ILE:HD11	2:B:490:ALA:HB2	1.78	0.65
1:A:342:ILE:HD12	1:A:609:TYR:CD2	2.30	0.65
2:B:439:ASN:CG	2:B:456:ILE:HG13	2.16	0.65
1:A:393:VAL:HA	1:A:409:THR:HG22	1.79	0.65
1:A:439:ASN:CB	1:A:456:ILE:HA	2.20	0.65
1:C:398:LYS:H	1:C:403:LEU:HD23	1.60	0.65
1:A:334:HIS:C	1:A:600:LEU:HD12	2.16	0.65
2:B:397:GLN:HA	2:B:398:LYS:HZ2	1.60	0.65
1:C:150:MET:C	1:C:152:ALA:N	2.49	0.65
1:A:378:GLN:HG3	1:C:654:LYS:HZ2	1.60	0.65
1:A:132:THR:O	1:A:133:PRO:C	2.35	0.65
2:B:656:ARG:C	2:B:657:LEU:HD23	2.15	0.65
1:C:387:ARG:HH21	1:C:592:ARG:HD3	1.61	0.65
2:B:439:ASN:HD21	2:B:456:ILE:CD1	2.09	0.65
1:A:456:ILE:HG22	1:A:456:ILE:O	1.96	0.65
2:B:363:ILE:O	2:B:363:ILE:HD13	1.96	0.65
2:B:453:SER:HB2	2:B:456:ILE:CG1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ARG:H	1:C:584:ASN:HD21	1.42	0.65
1:A:459:ASN:N	1:A:459:ASN:ND2	2.45	0.65
1:C:149:GLN:O	1:C:152:ALA:CB	2.42	0.65
2:B:251:TYR:CG	2:B:252:PRO:HD2	2.32	0.65
1:C:565:ILE:HD11	1:C:629:SER:HB3	1.78	0.65
1:A:209:VAL:CG2	1:A:324:LEU:O	2.30	0.65
1:A:170:PHE:CD1	1:A:170:PHE:N	2.65	0.65
2:B:633:VAL:HG12	2:B:634:SER:N	2.12	0.65
1:A:172:PHE:N	1:A:172:PHE:CD1	2.65	0.65
2:B:606:PHE:HB3	2:B:622:GLY:O	1.97	0.64
2:B:472:LEU:HD12	2:B:526:THR:HB	1.79	0.64
1:A:459:ASN:N	1:A:459:ASN:HD22	1.95	0.64
2:B:623:ILE:HA	2:B:628:PHE:O	1.97	0.64
1:A:148:VAL:HG22	1:A:149:GLN:N	2.11	0.64
1:A:498:ILE:HD12	1:A:499:PRO:O	1.96	0.64
1:C:661:ILE:HG12	1:C:662:ARG:N	2.12	0.64
1:A:407:VAL:HG12	1:A:408:ALA:N	2.13	0.64
1:A:469:CYS:HB3	1:A:527:LEU:HB2	1.79	0.64
1:A:278:LEU:N	1:A:278:LEU:HD23	2.11	0.64
2:B:453:SER:HB2	2:B:456:ILE:CD1	2.26	0.64
1:C:209:VAL:HG23	1:C:324:LEU:CB	2.27	0.64
2:B:544:ARG:HH22	1:C:505:GLN:HE22	1.45	0.64
1:C:439:ASN:HD21	1:C:440:GLN:HE22	1.46	0.64
1:A:145:GLU:O	1:A:146:PRO:C	2.35	0.64
2:B:550:ILE:HD13	2:B:550:ILE:O	1.97	0.64
1:A:405:ILE:N	1:A:405:ILE:HD13	2.13	0.64
1:A:334:HIS:HA	1:A:600:LEU:HD12	1.78	0.64
1:C:437:ILE:O	1:C:461:THR:HB	1.98	0.64
1:A:353:ARG:H	1:A:584:ASN:HD22	1.45	0.64
1:C:395:ILE:HD13	1:C:403:LEU:CD1	2.28	0.64
1:C:474:ARG:HB2	1:C:524:ASP:C	2.19	0.64
2:B:222:SER:O	2:B:308:CYS:HB2	1.97	0.64
1:A:461:THR:O	1:A:463:PHE:N	2.30	0.64
1:A:535:ILE:CG1	1:A:536:GLY:H	2.02	0.64
2:B:349:TRP:HB3	2:B:358:ILE:CG2	2.28	0.64
2:B:639:LEU:HD23	2:B:639:LEU:N	2.12	0.64
1:A:569:ASN:ND2	1:A:570:SER:H	1.96	0.64
1:C:435:TYR:CD1	1:C:435:TYR:O	2.50	0.64
1:A:353:ARG:HE	1:A:422:ASP:HB2	1.63	0.63
1:C:540:ILE:HB	1:C:582:VAL:HG13	1.78	0.63
1:C:613:ASP:HA	1:C:643:LEU:HD23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ILE:O	1:A:550:ILE:HD13	1.98	0.63
2:B:470:GLY:N	2:B:528:ALA:H	1.89	0.63
1:A:130:ILE:HG13	1:A:131:THR:N	2.09	0.63
1:A:571:MET:O	1:A:579:SER:O	2.16	0.63
1:C:297:ASN:HD22	1:C:298:PRO:HD2	1.62	0.63
1:A:277:HIS:CD2	1:A:277:HIS:H	2.16	0.63
1:A:424:THR:HG23	1:A:548:VAL:HG22	1.80	0.63
1:C:393:VAL:HG22	1:C:408:ALA:HA	1.81	0.63
1:C:473:GLN:HB3	1:C:482:SER:HA	1.80	0.63
1:C:288:VAL:C	1:C:289:ILE:HD12	2.19	0.63
1:C:300:ALA:O	1:C:301:ASN:HB2	1.98	0.63
2:B:437:ILE:HD11	2:B:440:GLN:HA	1.80	0.63
2:B:395:ILE:O	2:B:521:GLN:HG3	1.98	0.63
2:B:411:TYR:HD1	2:B:418:ASP:HB2	1.64	0.63
1:C:482:SER:O	1:C:483:ASN:HB3	1.99	0.63
2:B:251:TYR:CD1	1:C:327:PRO:HB3	2.33	0.63
1:A:590:THR:O	1:A:594:LEU:HB2	1.99	0.63
1:A:407:VAL:HG12	1:A:408:ALA:H	1.61	0.63
1:C:471:SER:O	1:C:482:SER:HB2	1.98	0.63
1:A:614:SER:HB2	1:A:640:GLU:OE1	1.97	0.63
1:C:504:ASP:O	1:C:506:THR:N	2.32	0.63
2:B:565:ILE:HD11	2:B:629:SER:HB2	1.79	0.63
1:C:451:TYR:CD1	1:C:457:ILE:CA	2.78	0.63
2:B:453:SER:O	2:B:456:ILE:CG2	2.46	0.63
1:A:512:GLN:OE1	1:A:514:ASN:HB2	1.98	0.63
1:C:481:VAL:O	1:C:481:VAL:HG13	1.97	0.63
1:C:391:ILE:N	1:C:391:ILE:CD1	2.60	0.63
2:B:256:PHE:CE1	2:B:264:VAL:HB	2.34	0.63
1:A:408:ALA:HB1	1:A:411:TYR:CD2	2.33	0.62
1:C:401:GLU:CD	1:C:402:MET:H	2.03	0.62
1:A:364:ARG:HB3	1:A:365:PRO:HD2	1.80	0.62
2:B:487:ILE:HG22	2:B:509:ALA:O	1.99	0.62
1:C:187:ILE:N	1:C:244:GLN:HE21	1.97	0.62
1:A:540:ILE:HB	1:A:582:VAL:HG13	1.80	0.62
2:B:384:SER:HA	2:B:418:ASP:OD1	1.99	0.62
1:C:607:ALA:HB3	1:C:623:ILE:HG12	1.81	0.62
2:B:437:ILE:CD1	2:B:440:GLN:HA	2.29	0.62
1:C:349:TRP:O	1:C:350:ILE:HG12	2.00	0.62
1:C:351:GLY:HA3	1:C:584:ASN:OD1	1.99	0.62
2:B:615:ASN:HB2	2:B:640:GLU:CG	2.30	0.62
2:B:453:SER:CB	2:B:456:ILE:HB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:LYS:HA	1:A:533:THR:CG2	2.29	0.62
1:A:152:ALA:O	1:A:155:ASP:HB2	2.00	0.62
1:A:580:ILE:HD12	1:A:580:ILE:C	2.20	0.62
2:B:611:ILE:CD1	2:B:621:ILE:HD13	2.29	0.62
1:C:447:THR:O	1:C:448:LYS:CB	2.48	0.62
1:A:297:ASN:ND2	1:A:298:PRO:HD2	2.15	0.62
2:B:238:PRO:HB3	2:B:284:THR:HA	1.82	0.62
2:B:636:ILE:CD1	2:B:636:ILE:H	2.06	0.62
2:B:420:TRP:CE2	2:B:508:ILE:HG22	2.34	0.62
1:C:236:VAL:HG11	1:C:242:PRO:HG3	1.80	0.62
1:C:472:LEU:HD13	1:C:472:LEU:C	2.20	0.62
1:C:327:PRO:HG2	1:C:330:SER:HB2	1.81	0.62
2:B:569:ASN:HD22	2:B:570:SER:N	1.97	0.62
2:B:402:MET:HE2	2:B:512:GLN:H	1.65	0.61
1:C:562:ASN:OD1	1:C:657:LEU:HG	2.01	0.61
1:C:187:ILE:O	1:C:188:LEU:HD23	1.99	0.61
1:A:310:VAL:HG12	1:A:311:THR:N	2.14	0.61
1:A:438:THR:HG21	1:A:459:ASN:N	2.15	0.61
2:B:586:GLN:OE1	2:B:591:SER:HB3	1.99	0.61
1:A:221:ILE:HD12	1:A:223:GLY:H	1.66	0.61
1:A:334:HIS:CA	1:A:600:LEU:HD12	2.30	0.61
1:A:439:ASN:CG	1:A:440:GLN:H	2.03	0.61
2:B:358:ILE:HG13	2:B:359:THR:N	2.07	0.61
1:A:210:ALA:CB	1:A:278:LEU:HA	2.31	0.61
1:A:641:PHE:O	1:A:643:LEU:HG	2.01	0.61
2:B:652:LEU:CD2	2:B:654:LYS:HD3	2.30	0.61
2:B:535:ILE:HG13	2:B:536:GLY:O	2.00	0.61
2:B:237:PRO:HD2	2:B:240:ILE:HD11	1.82	0.61
1:C:186:LYS:H	1:C:290:MET:HG3	1.66	0.61
1:A:411:TYR:CG	1:A:417:PRO:HA	2.36	0.61
1:A:484:THR:O	1:A:485:ALA:HB3	2.00	0.61
1:A:405:ILE:HG23	1:A:510:ILE:HG12	1.82	0.61
1:C:197:LEU:HD12	1:C:215:ILE:HD12	1.83	0.61
2:B:287:LEU:HD12	2:B:288:VAL:N	2.14	0.61
2:B:412:ILE:H	2:B:412:ILE:HD13	1.65	0.61
2:B:158:THR:C	2:B:160:LYS:N	2.55	0.61
1:A:399:GLU:HG3	1:A:516:VAL:CG2	2.24	0.61
1:A:171:SER:O	1:A:313:GLU:HA	2.01	0.61
2:B:373:HIS:CG	2:B:586:GLN:HE21	2.19	0.60
2:B:391:ILE:HD12	2:B:391:ILE:N	2.16	0.60
2:B:411:TYR:CE2	2:B:417:PRO:HA	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:251:TYR:HE1	1:C:325:LEU:O	1.84	0.60
1:C:205:ALA:HA	1:C:322:PHE:HE2	1.67	0.60
1:C:452:GLU:HB2	1:C:456:ILE:HD13	1.84	0.60
2:B:451:TYR:CD1	2:B:457:ILE:HD12	2.36	0.60
1:C:144:ALA:CB	1:C:147:SER:HB3	2.27	0.60
2:B:179:SER:HB3	2:B:182:GLU:OE1	2.01	0.60
2:B:602:SER:C	2:B:604:ASP:H	2.05	0.60
1:C:218:ARG:HB2	1:C:265:ILE:HG23	1.82	0.60
2:B:424:THR:HB	2:B:425:ILE:HD13	1.83	0.60
1:A:363:ILE:HD11	1:A:635:SER:HA	1.84	0.60
1:C:251:TYR:CG	1:C:252:PRO:HD2	2.36	0.60
1:C:166:TRP:C	1:C:168:ALA:H	2.04	0.60
1:A:474:ARG:C	1:A:524:ASP:HB2	2.22	0.60
2:B:394:THR:HG22	2:B:522:THR:CG2	2.32	0.60
2:B:661:ILE:N	2:B:661:ILE:HD13	2.12	0.60
1:A:454:ALA:O	1:A:455:MET:CG	2.48	0.60
2:B:160:LYS:HE3	2:B:163:ASP:HA	1.82	0.60
2:B:220:SER:O	2:B:310:VAL:HG23	2.02	0.60
1:C:451:TYR:CE1	1:C:457:ILE:HB	2.37	0.60
1:A:438:THR:CG2	1:A:458:SER:CA	2.79	0.60
2:B:412:ILE:CD1	2:B:413:VAL:HG23	2.32	0.60
1:C:362:VAL:HG12	1:C:364:ARG:HG2	1.83	0.60
1:C:180:THR:HA	1:C:295:LEU:HB3	1.83	0.60
2:B:472:LEU:HD13	2:B:472:LEU:C	2.21	0.60
2:B:141:GLY:O	2:B:143:ILE:HG12	2.01	0.60
2:B:443:ASN:ND2	2:B:447:THR:HG21	2.17	0.60
1:A:250:GLN:O	2:B:328:PRO:HD2	2.01	0.60
2:B:580:ILE:C	2:B:580:ILE:HD12	2.23	0.60
2:B:448:LYS:HA	2:B:448:LYS:NZ	2.17	0.60
1:C:464:LYS:HA	1:C:533:THR:CG2	2.31	0.59
1:C:532:TYR:CD2	1:C:540:ILE:HD11	2.37	0.59
1:C:612:ILE:HG22	1:C:618:TRP:HB3	1.84	0.59
1:C:162:VAL:HG12	1:C:164:SER:H	1.66	0.59
1:A:234:ILE:N	1:A:234:ILE:CD1	2.65	0.59
1:C:299:TYR:CD1	1:C:299:TYR:N	2.69	0.59
1:A:178:TRP:CZ2	1:A:295:LEU:HB2	2.37	0.59
1:C:166:TRP:HA	1:C:169:PHE:CE2	2.36	0.59
1:C:162:VAL:HG12	1:C:164:SER:OG	2.03	0.59
1:A:423:THR:HB	1:A:467:TYR:HE1	1.68	0.59
1:A:130:ILE:CG1	1:A:131:THR:N	2.65	0.59
2:B:574:GLY:O	2:B:575:TYR:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:HG12	2:B:262:GLU:N	2.17	0.59
1:A:190:LYS:HG3	1:A:651:GLN:HE22	1.68	0.59
1:A:474:ARG:CZ	1:A:521:GLN:O	2.51	0.59
1:C:221:ILE:N	1:C:221:ILE:CD1	2.62	0.59
1:C:535:ILE:HD12	1:C:546:LYS:HZ3	1.66	0.59
1:A:540:ILE:HG13	1:A:582:VAL:HG22	1.84	0.59
1:A:661:ILE:N	1:A:661:ILE:HD12	2.17	0.59
1:A:220:SER:HB3	1:A:263:PRO:HB3	1.84	0.59
1:A:392:THR:O	1:A:409:THR:HG23	2.01	0.59
2:B:398:LYS:H	2:B:398:LYS:HZ3	1.51	0.59
1:A:461:THR:O	1:A:461:THR:HG23	2.03	0.59
1:C:236:VAL:CG2	1:C:286:SER:HB2	2.29	0.59
2:B:449:GLU:HB3	2:B:452:GLU:HG2	1.84	0.59
1:A:411:TYR:HD1	1:A:418:ASP:HB3	1.67	0.59
2:B:210:ALA:HB3	2:B:324:LEU:H	1.66	0.59
2:B:237:PRO:CD	2:B:240:ILE:HD11	2.32	0.59
1:A:573:LEU:HG	1:A:580:ILE:HG23	1.84	0.59
1:A:256:PHE:HE1	1:A:264:VAL:HG23	1.67	0.59
2:B:184:GLN:HG3	2:B:292:TYR:O	2.02	0.59
1:A:457:ILE:CG1	1:A:460:ASN:HD22	2.16	0.59
1:C:474:ARG:HD3	1:C:523:SER:O	2.03	0.59
2:B:398:LYS:NZ	2:B:398:LYS:H	2.00	0.59
1:A:359:THR:CG2	1:A:568:ARG:HG2	2.32	0.59
1:C:288:VAL:HG12	1:C:289:ILE:N	2.17	0.59
1:A:193:LEU:HG	1:A:194:GLY:N	2.16	0.59
2:B:260:GLN:NE2	1:C:129:SER:HA	2.18	0.59
1:C:361:PHE:CE1	1:C:619:PHE:HZ	2.20	0.59
1:A:167:GLU:HA	1:A:316:PRO:HG2	1.85	0.59
2:B:453:SER:O	2:B:456:ILE:HG22	2.02	0.58
1:A:472:LEU:CD2	1:A:473:GLN:HG2	2.33	0.58
2:B:469:CYS:HB2	2:B:527:LEU:HB3	1.86	0.58
1:A:193:LEU:HD12	1:A:197:LEU:HD11	1.85	0.58
1:A:179:SER:N	1:A:182:GLU:OE1	2.34	0.58
2:B:214:SER:O	2:B:215:ILE:HD13	2.02	0.58
1:C:220:SER:HB3	1:C:263:PRO:HA	1.85	0.58
1:C:187:ILE:CG1	1:C:244:GLN:HG2	2.32	0.58
1:A:333:THR:CG2	1:C:239:GLY:HA2	2.33	0.58
1:A:231:LEU:HD12	1:A:291:ILE:HA	1.84	0.58
1:A:255:LEU:HD12	1:A:255:LEU:H	1.67	0.58
2:B:491:THR:O	2:B:497:LEU:HA	2.03	0.58
2:B:503:ILE:O	2:B:503:ILE:HG13	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ILE:HG22	1:C:310:VAL:HG13	1.85	0.58
1:A:415:GLY:HA3	1:A:505:GLN:HG3	1.85	0.58
1:A:474:ARG:HH21	1:A:523:SER:CB	1.96	0.58
2:B:395:ILE:CG1	2:B:396:SER:H	1.94	0.58
2:B:412:ILE:CD1	2:B:412:ILE:H	2.16	0.58
2:B:146:PRO:HB2	2:B:149:GLN:OE1	2.03	0.58
1:A:330:SER:HA	1:C:243:ILE:HD11	1.85	0.58
1:A:587:ILE:O	1:A:590:THR:HB	2.04	0.58
1:A:377:ASN:HB2	1:A:379:GLU:HG3	1.84	0.58
2:B:194:GLY:HA2	2:B:211:TRP:CH2	2.39	0.58
1:A:180:THR:HG23	1:A:306:SER:O	2.03	0.58
1:C:240:ILE:HG13	1:C:240:ILE:O	2.03	0.58
2:B:218:ARG:HD3	2:B:265:ILE:HG12	1.86	0.58
1:C:221:ILE:CG2	1:C:310:VAL:HG22	2.32	0.58
1:C:187:ILE:H	1:C:244:GLN:HE21	1.51	0.58
2:B:438:THR:HG23	2:B:457:ILE:CG2	2.32	0.58
1:A:433:GLY:HA3	1:A:462:ASN:CG	2.23	0.58
2:B:146:PRO:O	2:B:149:GLN:CG	2.49	0.58
1:C:661:ILE:HD13	1:C:661:ILE:H	1.68	0.58
1:C:349:TRP:CB	1:C:358:ILE:HD13	2.29	0.58
1:C:580:ILE:HD12	1:C:580:ILE:C	2.24	0.58
2:B:439:ASN:ND2	2:B:443:ASN:HD21	1.96	0.58
1:C:474:ARG:N	1:C:524:ASP:HA	2.13	0.58
1:C:404:GLY:HA2	1:C:510:ILE:HG12	1.84	0.58
2:B:178:TRP:CE2	2:B:295:LEU:HB2	2.39	0.58
2:B:400:GLY:C	2:B:401:GLU:HG3	2.23	0.58
1:A:391:ILE:HD12	1:A:391:ILE:N	2.19	0.58
1:A:408:ALA:HB1	1:A:411:TYR:HD2	1.69	0.58
1:A:433:GLY:HA3	1:A:462:ASN:ND2	2.19	0.58
1:C:399:GLU:HB2	1:C:519:ASP:OD1	2.04	0.58
2:B:146:PRO:O	2:B:149:GLN:NE2	2.37	0.58
2:B:151:SER:C	2:B:153:ALA:H	2.07	0.58
1:C:297:ASN:C	1:C:297:ASN:HD22	2.05	0.58
2:B:455:MET:O	2:B:455:MET:HG2	2.04	0.58
2:B:446:GLN:HE21	2:B:447:THR:HG23	1.64	0.57
2:B:402:MET:CE	2:B:511:PHE:HA	2.34	0.57
2:B:233:ALA:O	2:B:234:ILE:HG23	2.04	0.57
1:C:482:SER:O	1:C:483:ASN:CB	2.52	0.57
1:C:526:THR:C	1:C:527:LEU:HD23	2.23	0.57
1:A:353:ARG:N	1:A:584:ASN:ND2	2.49	0.57
1:A:457:ILE:HD11	1:A:460:ASN:ND2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:THR:HG23	1:C:485:ALA:H	1.69	0.57
2:B:237:PRO:HB2	1:C:324:LEU:HD13	1.86	0.57
2:B:611:ILE:H	2:B:611:ILE:HD12	1.67	0.57
1:A:377:ASN:HB3	1:C:559:ARG:HD3	1.85	0.57
1:C:257:ASP:OD1	1:C:258:ALA:N	2.37	0.57
1:C:214:SER:HB3	1:C:269:PRO:HA	1.86	0.57
1:A:205:ALA:C	1:A:207:LEU:H	2.07	0.57
1:A:438:THR:CG2	1:A:459:ASN:H	2.17	0.57
1:C:610:ARG:C	1:C:611:ILE:HD12	2.25	0.57
2:B:396:SER:HA	2:B:521:GLN:NE2	1.99	0.57
1:C:205:ALA:HA	1:C:322:PHE:CE2	2.39	0.57
1:C:580:ILE:HD12	1:C:581:ASP:N	2.20	0.57
1:C:598:ASN:HD22	1:C:598:ASN:C	2.07	0.57
1:C:439:ASN:CB	1:C:457:ILE:HG12	2.34	0.57
1:C:368:PHE:HB3	1:C:544:ARG:NH1	2.19	0.57
2:B:480:LYS:O	2:B:481:VAL:HG12	2.03	0.57
1:A:187:ILE:HD11	1:A:244:GLN:HA	1.85	0.57
2:B:591:SER:HA	2:B:594:LEU:HD12	1.85	0.57
2:B:633:VAL:HG12	2:B:634:SER:H	1.69	0.57
2:B:472:LEU:HD22	2:B:473:GLN:H	1.66	0.57
1:C:416:ILE:CD1	1:C:503:ILE:HG12	2.29	0.57
1:C:408:ALA:HB1	1:C:411:TYR:HD2	1.70	0.57
1:A:194:GLY:HA2	1:A:211:TRP:CZ2	2.40	0.57
1:C:591:SER:HA	1:C:594:LEU:HD12	1.86	0.57
1:A:474:ARG:O	1:A:524:ASP:HB2	2.05	0.57
1:A:459:ASN:O	1:A:460:ASN:HB2	2.04	0.57
1:A:460:ASN:O	1:A:461:THR:C	2.41	0.57
1:A:189:PHE:HB3	1:A:289:ILE:HD12	1.86	0.57
2:B:148:VAL:O	2:B:149:GLN:C	2.41	0.57
1:A:609:TYR:CE1	1:A:647:TYR:HB3	2.40	0.57
1:C:659:SER:OG	1:C:661:ILE:HD12	2.04	0.57
1:A:144:ALA:C	1:A:145:GLU:HG3	2.25	0.57
2:B:439:ASN:ND2	2:B:456:ILE:CG1	2.68	0.57
1:A:412:ILE:HD12	1:A:413:VAL:HG23	1.86	0.57
2:B:407:VAL:HG13	2:B:408:ALA:N	2.19	0.57
1:A:183:THR:HA	1:A:294:ASP:OD1	2.05	0.57
2:B:655:ILE:HD12	2:B:655:ILE:O	2.05	0.57
1:C:399:GLU:CG	1:C:519:ASP:HA	2.33	0.57
2:B:344:LYS:NZ	2:B:647:TYR:OH	2.37	0.57
2:B:254:VAL:C	2:B:255:LEU:HD22	2.25	0.56
1:A:333:THR:HG22	1:C:239:GLY:CA	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASN:HD22	1:A:298:PRO:HD2	1.70	0.56
1:A:405:ILE:HG23	1:A:510:ILE:HG23	1.86	0.56
2:B:394:THR:CG2	2:B:522:THR:HG23	2.32	0.56
1:C:352:ASN:HB3	1:C:586:GLN:O	2.04	0.56
2:B:153:ALA:O	2:B:156:MET:HB2	2.06	0.56
1:C:391:ILE:HD12	1:C:391:ILE:H	1.66	0.56
1:A:360:ASP:HB2	1:A:568:ARG:CD	2.36	0.56
1:A:571:MET:HB2	1:A:582:VAL:HG23	1.88	0.56
1:A:325:LEU:H	1:A:325:LEU:HD12	1.70	0.56
2:B:517:ASN:CG	2:B:518:ARG:H	2.08	0.56
1:C:453:SER:O	1:C:456:ILE:O	2.24	0.56
1:A:567:TYR:CE1	1:A:586:GLN:HA	2.40	0.56
1:A:436:ALA:HB2	1:A:462:ASN:HB2	1.87	0.56
1:C:189:PHE:CD1	1:C:289:ILE:HB	2.38	0.56
2:B:390:PRO:C	2:B:391:ILE:HD12	2.26	0.56
2:B:453:SER:CB	2:B:456:ILE:CG1	2.84	0.56
1:A:397:GLN:NE2	1:A:520:VAL:HG23	2.18	0.56
2:B:487:ILE:HG22	2:B:510:ILE:HG22	1.88	0.56
2:B:411:TYR:CD1	2:B:418:ASP:HB2	2.41	0.56
2:B:423:THR:HA	2:B:546:LYS:O	2.05	0.56
1:C:484:THR:OG1	1:C:485:ALA:N	2.39	0.56
1:A:405:ILE:HG13	1:A:508:ILE:O	2.06	0.56
2:B:554:PRO:HB2	2:B:628:PHE:HZ	1.71	0.56
1:C:401:GLU:CD	1:C:402:MET:N	2.58	0.56
1:C:424:THR:HG22	1:C:425:ILE:N	2.20	0.56
1:C:533:THR:O	1:C:535:ILE:HG23	2.05	0.56
1:A:297:ASN:HD22	1:A:298:PRO:CD	2.18	0.56
2:B:652:LEU:HD23	2:B:654:LYS:HD3	1.87	0.56
1:C:176:VAL:HG12	1:C:177:ASN:N	2.20	0.56
1:C:199:PRO:O	1:C:202:THR:HG22	2.06	0.56
2:B:370:ALA:HB2	2:B:554:PRO:CD	2.35	0.56
1:C:403:LEU:CD2	1:C:514:ASN:HD21	2.18	0.56
1:A:256:PHE:CE1	1:A:264:VAL:HG23	2.41	0.56
1:C:297:ASN:C	1:C:297:ASN:ND2	2.59	0.56
2:B:179:SER:OG	2:B:180:THR:N	2.37	0.56
2:B:391:ILE:O	2:B:391:ILE:HG22	2.06	0.56
1:C:272:ARG:HD2	1:C:274:THR:O	2.04	0.56
1:A:397:GLN:HE22	1:A:520:VAL:CG2	2.18	0.56
1:C:474:ARG:O	1:C:475:ALA:HB2	2.06	0.56
1:C:439:ASN:ND2	1:C:440:GLN:HE22	2.03	0.56
2:B:353:ARG:N	2:B:584:ASN:ND2	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:SER:HA	2:B:286:SER:CB	2.31	0.56
1:C:504:ASP:C	1:C:506:THR:H	2.08	0.56
1:A:589:HIS:CD2	1:A:593:GLN:HE21	2.24	0.56
1:A:612:ILE:HG22	1:A:618:TRP:CB	2.36	0.56
2:B:449:GLU:CB	2:B:452:GLU:CG	2.84	0.56
2:B:424:THR:HG22	2:B:489:THR:O	2.06	0.56
1:C:236:VAL:HB	1:C:240:ILE:HD11	1.87	0.56
1:C:339:CYS:HB3	1:C:647:TYR:HB2	1.87	0.56
1:A:173:HIS:O	1:A:174:THR:HB	2.06	0.56
2:B:573:LEU:HD12	2:B:579:SER:OG	2.05	0.56
1:A:474:ARG:NH1	1:A:520:VAL:O	2.38	0.55
1:C:221:ILE:HG22	1:C:310:VAL:CG2	2.33	0.55
1:C:427:ASN:HB3	1:C:429:LEU:CD2	2.35	0.55
2:B:453:SER:HB2	2:B:456:ILE:HG12	1.87	0.55
1:A:422:ASP:O	1:A:548:VAL:HG23	2.06	0.55
1:A:399:GLU:O	1:A:516:VAL:HG11	2.05	0.55
2:B:327:PRO:HG2	2:B:330:SER:CB	2.36	0.55
1:A:183:THR:C	1:A:291:ILE:HD12	2.27	0.55
2:B:436:ALA:HB3	2:B:461:THR:CA	2.12	0.55
1:A:189:PHE:HB3	1:A:289:ILE:HD13	1.89	0.55
2:B:255:LEU:HB2	1:C:131:THR:CG2	2.32	0.55
1:C:610:ARG:HH21	1:C:648:MET:CE	2.18	0.55
1:A:428:GLU:CG	1:A:499:PRO:HD2	2.36	0.55
2:B:407:VAL:HG22	2:B:408:ALA:H	1.71	0.55
1:C:517:ASN:C	1:C:519:ASP:H	2.08	0.55
1:A:579:SER:O	1:A:580:ILE:HG13	2.06	0.55
1:A:498:ILE:C	1:A:498:ILE:HD12	2.27	0.55
2:B:354:PHE:O	2:B:356:SER:N	2.40	0.55
1:A:251:TYR:CD2	1:A:252:PRO:HD2	2.42	0.55
1:A:191:GLN:HE21	1:A:192:SER:H	1.54	0.55
2:B:148:VAL:HG23	2:B:149:GLN:NE2	2.21	0.55
1:A:134:GLU:CD	1:A:134:GLU:N	2.60	0.55
2:B:393:VAL:HG23	2:B:407:VAL:O	2.06	0.55
2:B:393:VAL:CA	2:B:409:THR:HG21	2.29	0.55
1:A:571:MET:HB2	1:A:582:VAL:CG2	2.37	0.55
2:B:168:ALA:HA	2:B:315:LYS:NZ	2.22	0.55
1:A:216:GLU:HG2	1:A:267:THR:HG23	1.87	0.55
1:A:469:CYS:O	1:A:485:ALA:HB1	2.05	0.55
1:A:391:ILE:O	1:A:527:LEU:HD12	2.06	0.55
1:C:401:GLU:OE1	1:C:402:MET:N	2.38	0.55
1:C:398:LYS:H	1:C:403:LEU:CD2	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:VAL:CG1	1:C:338:PRO:HD2	2.37	0.55
1:C:612:ILE:O	1:C:612:ILE:HG13	2.06	0.55
1:C:184:GLN:HG3	1:C:292:TYR:O	2.07	0.55
1:A:636:ILE:H	1:A:636:ILE:HD13	1.72	0.55
2:B:397:GLN:HE21	2:B:514:ASN:ND2	2.05	0.55
1:C:285:THR:HG22	1:C:286:SER:N	2.21	0.55
1:C:470:GLY:H	1:C:530:LEU:CD1	2.20	0.55
1:C:403:LEU:HD21	1:C:514:ASN:HD21	1.71	0.55
1:A:430:ILE:HG22	1:A:495:ASN:O	2.07	0.55
2:B:431:PRO:HB3	2:B:511:PHE:CZ	2.42	0.55
1:C:234:ILE:HD12	1:C:234:ILE:O	2.07	0.55
1:C:451:TYR:CD1	1:C:458:SER:N	2.72	0.55
2:B:438:THR:OG1	2:B:460:ASN:O	2.24	0.55
2:B:349:TRP:HB3	2:B:358:ILE:HG23	1.89	0.55
1:C:411:TYR:CD1	1:C:418:ASP:HB3	2.42	0.55
1:C:482:SER:OG	1:C:483:ASN:N	2.39	0.55
2:B:174:THR:HG22	2:B:175:SER:N	2.18	0.55
1:A:193:LEU:CD1	1:A:215:ILE:HD12	2.37	0.55
1:A:481:VAL:HG13	1:A:481:VAL:O	2.07	0.55
1:C:304:ASN:O	1:C:305:SER:C	2.44	0.55
1:C:443:ASN:ND2	1:C:446:GLN:HB3	2.22	0.54
1:C:451:TYR:CD1	1:C:457:ILE:CB	2.77	0.54
1:A:528:ALA:O	1:A:530:LEU:CD1	2.55	0.54
1:C:465:SER:HA	1:C:532:TYR:CZ	2.41	0.54
1:C:566:PHE:CD2	1:C:583:PHE:HB3	2.42	0.54
1:C:132:THR:HB	1:C:133:PRO:HD2	1.88	0.54
1:A:488:THR:H	1:A:509:ALA:HB3	1.72	0.54
1:C:237:PRO:O	1:C:240:ILE:HG12	2.08	0.54
1:C:395:ILE:HD13	1:C:403:LEU:HD11	1.89	0.54
1:A:601:LEU:HD21	1:A:605:SER:O	2.06	0.54
2:B:608:VAL:HG12	2:B:609:TYR:N	2.22	0.54
2:B:217:VAL:HG21	2:B:268:ILE:HD11	1.89	0.54
1:A:603:PRO:HG2	1:A:604:ASP:H	1.71	0.54
2:B:395:ILE:C	2:B:521:GLN:HG3	2.28	0.54
1:A:151:SER:O	1:A:152:ALA:CB	2.55	0.54
1:C:221:ILE:HD13	1:C:221:ILE:N	2.10	0.54
1:A:472:LEU:O	1:A:473:GLN:CB	2.55	0.54
2:B:339:CYS:SG	2:B:649:GLY:HA2	2.46	0.54
1:A:210:ALA:HB2	1:A:278:LEU:HA	1.88	0.54
1:A:573:LEU:HD21	1:A:580:ILE:HG21	1.88	0.54
1:A:236:VAL:HB	1:A:240:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:THR:HG22	2:B:295:LEU:O	2.08	0.54
1:C:397:GLN:HG2	1:C:523:SER:CB	2.36	0.54
1:A:222:SER:C	1:A:308:CYS:SG	2.86	0.54
1:C:451:TYR:O	1:C:456:ILE:O	2.24	0.54
1:C:216:GLU:HA	1:C:267:THR:HG22	1.90	0.54
1:C:448:LYS:NZ	1:C:537:GLU:OE2	2.40	0.54
1:A:469:CYS:HB2	1:A:485:ALA:HB1	1.89	0.54
1:A:550:ILE:HG23	1:A:551:GLY:N	2.22	0.54
1:A:598:ASN:HB2	1:C:654:LYS:HG3	1.90	0.54
1:A:383:TRP:HB2	1:A:413:VAL:HG21	1.88	0.54
1:A:148:VAL:HG13	1:A:149:GLN:N	2.23	0.54
1:C:392:THR:O	1:C:409:THR:HG22	2.08	0.54
1:C:501:ASN:O	1:C:548:VAL:HG13	2.08	0.54
2:B:565:ILE:HG12	2:B:629:SER:O	2.08	0.54
2:B:398:LYS:HG2	2:B:399:GLU:H	1.72	0.53
2:B:240:ILE:HB	1:C:330:SER:OG	2.08	0.53
1:A:335:GLY:HA3	1:A:600:LEU:N	2.23	0.53
2:B:239:GLY:HA2	1:C:333:THR:HG22	1.88	0.53
1:A:392:THR:HA	1:A:526:THR:HA	1.90	0.53
1:C:228:GLY:O	1:C:296:ILE:HG13	2.08	0.53
2:B:569:ASN:HD22	2:B:570:SER:H	1.56	0.53
2:B:339:CYS:SG	2:B:647:TYR:HB2	2.48	0.53
2:B:438:THR:HG23	2:B:457:ILE:HG22	1.90	0.53
1:C:439:ASN:HB3	1:C:457:ILE:HG12	1.91	0.53
1:A:234:ILE:O	1:A:288:VAL:HG23	2.08	0.53
1:C:426:PRO:O	1:C:427:ASN:HB2	2.08	0.53
1:C:398:LYS:HB2	1:C:403:LEU:HB3	1.91	0.53
1:C:469:CYS:O	1:C:485:ALA:HB3	2.08	0.53
2:B:333:THR:HG23	2:B:334:HIS:N	2.24	0.53
1:A:661:ILE:H	1:A:661:ILE:HD12	1.73	0.53
2:B:360:ASP:N	2:B:360:ASP:OD2	2.41	0.53
2:B:553:LEU:CD1	2:B:554:PRO:HD2	2.38	0.53
2:B:641:PHE:O	2:B:643:LEU:HG	2.09	0.53
2:B:621:ILE:HA	2:B:630:PHE:O	2.08	0.53
1:C:358:ILE:HG22	1:C:359:THR:N	2.24	0.53
2:B:588:LEU:C	2:B:590:THR:H	2.11	0.53
1:C:550:ILE:O	1:C:550:ILE:CD1	2.48	0.53
2:B:234:ILE:O	2:B:287:LEU:HD12	2.09	0.53
1:C:469:CYS:HA	1:C:530:LEU:HD13	1.89	0.53
1:C:641:PHE:N	1:C:642:PRO:HD3	2.23	0.53
1:C:433:GLY:O	1:C:434:ASP:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:THR:HG21	1:A:512:GLN:NE2	2.24	0.53
1:C:367:VAL:HG22	1:C:566:PHE:CE1	2.44	0.53
1:C:187:ILE:HG21	1:C:190:LYS:HG3	1.91	0.53
1:A:339:CYS:O	1:A:340:ASP:HB3	2.08	0.53
2:B:354:PHE:C	2:B:356:SER:N	2.61	0.53
2:B:368:PHE:HA	2:B:554:PRO:O	2.09	0.53
1:A:612:ILE:HG22	1:A:618:TRP:HB3	1.91	0.53
1:A:209:VAL:O	1:A:279:MET:HG2	2.09	0.53
2:B:198:ASN:HB3	2:B:201:LEU:HD12	1.90	0.53
1:C:517:ASN:C	1:C:519:ASP:N	2.61	0.53
1:C:353:ARG:HH12	1:C:541:GLY:HA3	1.74	0.53
1:C:404:GLY:O	1:C:405:ILE:HD12	2.09	0.53
1:C:142:VAL:HG12	1:C:143:ILE:HD13	1.91	0.53
2:B:199:PRO:O	2:B:202:THR:HB	2.09	0.53
1:A:443:ASN:OD1	1:A:443:ASN:O	2.27	0.53
2:B:457:ILE:HG23	2:B:459:ASN:H	1.73	0.52
1:A:477:GLY:HA3	1:A:520:VAL:HG21	1.91	0.52
2:B:426:PRO:HB3	2:B:546:LYS:HE2	1.92	0.52
1:A:178:TRP:CZ3	1:A:231:LEU:HD22	2.44	0.52
1:C:249:LEU:C	1:C:251:TYR:H	2.13	0.52
2:B:214:SER:H	2:B:319:ASP:CG	2.12	0.52
1:A:438:THR:CG2	1:A:459:ASN:N	2.72	0.52
1:A:130:ILE:HA	1:C:260:GLN:OE1	2.09	0.52
2:B:476:TRP:NE1	2:B:520:VAL:HB	2.23	0.52
1:A:228:GLY:O	1:A:295:LEU:HD12	2.08	0.52
2:B:571:MET:O	2:B:579:SER:O	2.26	0.52
1:A:397:GLN:HA	1:A:403:LEU:HD13	1.92	0.52
2:B:607:ALA:O	2:B:623:ILE:HD12	2.09	0.52
1:C:481:VAL:O	1:C:482:SER:C	2.47	0.52
1:A:349:TRP:C	1:A:350:ILE:HG23	2.30	0.52
1:A:498:ILE:HD12	1:A:498:ILE:O	2.10	0.52
1:C:143:ILE:HD13	1:C:143:ILE:N	2.24	0.52
1:C:540:ILE:O	1:C:582:VAL:HG13	2.09	0.52
2:B:327:PRO:O	2:B:327:PRO:HG2	2.10	0.52
1:C:337:VAL:HG13	1:C:338:PRO:HD2	1.91	0.52
2:B:332:LEU:HB3	2:B:335:GLY:O	2.09	0.52
1:A:209:VAL:HG22	1:A:324:LEU:C	2.20	0.52
1:A:436:ALA:HB3	1:A:461:THR:HA	1.90	0.52
1:C:209:VAL:HG23	1:C:324:LEU:HB3	1.91	0.52
1:A:342:ILE:HG23	1:A:609:TYR:CE2	2.44	0.52
1:C:612:ILE:HG22	1:C:618:TRP:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:LEU:N	1:A:325:LEU:HD12	2.24	0.52
1:C:450:GLU:O	1:C:451:TYR:CB	2.57	0.52
2:B:449:GLU:HB2	2:B:452:GLU:CD	2.30	0.52
1:A:476:TRP:HD1	1:A:520:VAL:HB	1.72	0.52
1:A:550:ILE:C	1:A:550:ILE:HD13	2.29	0.52
2:B:394:THR:O	2:B:406:GLY:HA2	2.10	0.52
2:B:395:ILE:CG2	2:B:521:GLN:HB2	2.38	0.52
1:C:197:LEU:HD12	1:C:215:ILE:HD13	1.90	0.52
1:C:398:LYS:O	1:C:399:GLU:HB3	2.09	0.52
1:C:469:CYS:HB2	1:C:528:ALA:O	2.10	0.52
1:C:484:THR:HG21	1:C:512:GLN:HA	1.92	0.52
1:C:368:PHE:HB3	1:C:544:ARG:HH12	1.74	0.52
2:B:209:VAL:O	2:B:278:LEU:HA	2.09	0.52
1:C:334:HIS:HB3	1:C:600:LEU:CD1	2.38	0.52
1:C:427:ASN:HB3	1:C:429:LEU:HD21	1.92	0.52
1:A:576:VAL:HG12	1:A:577:ILE:N	2.24	0.52
1:A:300:ALA:O	1:A:301:ASN:HB2	2.10	0.52
1:A:461:THR:HG21	1:A:533:THR:HG22	1.92	0.52
2:B:374:PHE:H	2:B:586:GLN:NE2	2.06	0.52
1:A:149:GLN:HA	1:A:153:ALA:CB	2.40	0.52
1:A:240:ILE:HG22	2:B:332:LEU:HA	1.91	0.52
2:B:610:ARG:NH2	2:B:618:TRP:CH2	2.78	0.52
1:A:297:ASN:ND2	1:A:298:PRO:CD	2.72	0.52
1:C:602:SER:C	1:C:604:ASP:H	2.13	0.52
1:A:193:LEU:HD11	1:A:215:ILE:HD12	1.91	0.52
2:B:611:ILE:HD11	2:B:621:ILE:HD13	1.91	0.52
2:B:426:PRO:HD3	2:B:465:SER:OG	2.10	0.52
1:A:130:ILE:O	1:A:131:THR:HG23	2.10	0.52
2:B:481:VAL:O	2:B:481:VAL:HG13	2.10	0.52
1:C:216:GLU:HG2	1:C:267:THR:HG22	1.91	0.52
2:B:432:ALA:HB3	2:B:462:ASN:CB	2.40	0.52
1:C:221:ILE:HD13	1:C:221:ILE:O	2.09	0.51
1:A:230:LYS:HD2	1:A:293:ASN:HD22	1.75	0.51
1:A:491:THR:HG22	1:A:498:ILE:HG13	1.92	0.51
2:B:454:ALA:C	2:B:456:ILE:H	2.14	0.51
2:B:487:ILE:HG21	2:B:510:ILE:HG22	1.90	0.51
2:B:187:ILE:HB	2:B:244:GLN:NE2	2.24	0.51
1:A:571:MET:HG3	1:A:582:VAL:HG21	1.92	0.51
1:C:299:TYR:O	1:C:300:ALA:O	2.29	0.51
1:C:201:LEU:HD22	1:C:320:PHE:CE2	2.43	0.51
1:A:214:SER:OG	1:A:269:PRO:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:THR:HB	1:C:650:ASN:HD21	1.75	0.51
1:A:393:VAL:HG12	1:A:394:THR:O	2.09	0.51
1:A:439:ASN:HD22	1:A:456:ILE:CG1	2.23	0.51
1:C:217:VAL:HG12	1:C:219:PHE:CD2	2.45	0.51
1:C:144:ALA:HB1	1:C:147:SER:CB	2.34	0.51
1:C:540:ILE:HD12	1:C:582:VAL:HG21	1.91	0.51
1:C:608:VAL:O	1:C:609:TYR:HD1	1.94	0.51
1:A:327:PRO:HG2	1:A:330:SER:HG	1.74	0.51
2:B:292:TYR:HD2	2:B:293:ASN:ND2	2.09	0.51
1:C:437:ILE:HD11	1:C:457:ILE:CD1	2.40	0.51
2:B:349:TRP:HB3	2:B:358:ILE:HG21	1.92	0.51
2:B:393:VAL:HA	2:B:409:THR:CG2	2.29	0.51
1:C:148:VAL:O	1:C:150:MET:N	2.44	0.51
1:C:397:GLN:CB	1:C:520:VAL:O	2.59	0.51
2:B:146:PRO:HB2	2:B:149:GLN:NE2	2.26	0.51
1:A:641:PHE:O	1:A:643:LEU:N	2.44	0.51
2:B:600:LEU:HD13	2:B:600:LEU:C	2.30	0.51
1:A:145:GLU:H	1:A:146:PRO:CD	2.24	0.51
2:B:449:GLU:HB3	2:B:452:GLU:CG	2.40	0.51
1:A:474:ARG:O	1:A:475:ALA:HB2	2.10	0.51
2:B:411:TYR:CD1	2:B:418:ASP:N	2.73	0.51
1:C:150:MET:O	1:C:152:ALA:N	2.44	0.51
1:A:504:ASP:O	1:A:507:LYS:HB2	2.10	0.51
1:C:488:THR:OG1	1:C:489:THR:N	2.44	0.51
2:B:155:ASP:O	2:B:158:THR:N	2.38	0.51
2:B:620:ASP:C	2:B:621:ILE:HD12	2.31	0.51
1:C:198:ASN:O	1:C:202:THR:HB	2.11	0.51
2:B:247:SER:O	2:B:250:GLN:HB2	2.11	0.51
1:A:209:VAL:HG23	1:A:210:ALA:N	2.25	0.51
2:B:449:GLU:HB2	2:B:452:GLU:CG	2.41	0.51
1:A:287:LEU:HG	1:A:288:VAL:H	1.73	0.51
1:A:540:ILE:CG1	1:A:582:VAL:HG22	2.39	0.51
2:B:363:ILE:O	2:B:364:ARG:HD3	2.11	0.51
1:C:214:SER:HB2	1:C:268:ILE:O	2.11	0.51
1:A:478:ASN:O	1:A:479:LYS:O	2.29	0.51
1:A:471:SER:HB2	1:A:485:ALA:HB2	1.93	0.51
2:B:405:ILE:HA	2:B:508:ILE:O	2.11	0.51
1:C:463:PHE:O	1:C:466:MET:CG	2.59	0.51
1:C:466:MET:O	1:C:532:TYR:HA	2.11	0.51
1:A:335:GLY:HA3	1:A:600:LEU:HB2	1.92	0.51
1:C:641:PHE:C	1:C:643:LEU:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:LYS:O	1:A:449:GLU:HB3	2.11	0.51
2:B:647:TYR:N	2:B:647:TYR:CD1	2.78	0.51
1:C:452:GLU:HB2	1:C:456:ILE:CD1	2.40	0.51
2:B:288:VAL:HG12	2:B:289:ILE:N	2.26	0.51
1:C:622:GLY:O	1:C:623:ILE:HD13	2.11	0.51
1:C:187:ILE:HG22	1:C:188:LEU:N	2.26	0.51
2:B:539:ALA:HB3	2:B:583:PHE:HE1	1.75	0.51
1:C:402:MET:SD	1:C:403:LEU:N	2.84	0.51
1:C:228:GLY:HA3	1:C:296:ILE:HD11	1.93	0.51
1:A:405:ILE:HG21	1:A:509:ALA:C	2.31	0.51
1:C:383:TRP:HA	1:C:413:VAL:HG11	1.92	0.51
2:B:150:MET:O	2:B:153:ALA:HB3	2.11	0.51
1:A:227:PHE:HE1	1:A:308:CYS:HB2	1.76	0.51
1:A:526:THR:O	1:A:527:LEU:HG	2.11	0.50
1:C:578:LYS:C	1:C:579:SER:OG	2.49	0.50
1:C:440:GLN:HB3	1:C:443:ASN:HB3	1.91	0.50
1:A:393:VAL:HG22	1:A:411:TYR:HE2	1.76	0.50
1:A:399:GLU:HA	1:A:516:VAL:CG2	2.41	0.50
2:B:393:VAL:O	2:B:525:ASP:HB3	2.11	0.50
1:A:359:THR:O	1:A:641:PHE:CZ	2.64	0.50
1:A:363:ILE:HG22	1:A:565:ILE:HG22	1.93	0.50
1:C:420:TRP:CG	1:C:421:PRO:HD2	2.46	0.50
1:C:441:SER:C	1:C:443:ASN:H	2.15	0.50
2:B:525:ASP:O	2:B:526:THR:C	2.49	0.50
1:C:393:VAL:HG13	1:C:407:VAL:O	2.12	0.50
1:A:643:LEU:O	1:A:644:THR:HG23	2.11	0.50
1:A:277:HIS:CD2	1:A:277:HIS:N	2.80	0.50
1:C:293:ASN:O	1:C:294:ASP:O	2.29	0.50
1:A:157:ALA:O	1:A:158:THR:OG1	2.28	0.50
1:A:369:GLN:N	1:A:553:LEU:HD11	2.26	0.50
1:A:439:ASN:OD1	1:A:440:GLN:HG3	2.12	0.50
1:A:438:THR:HB	1:A:456:ILE:HG22	1.92	0.50
2:B:517:ASN:CG	2:B:518:ARG:N	2.64	0.50
1:A:133:PRO:CB	1:A:134:GLU:OE2	2.58	0.50
1:C:183:THR:O	1:C:291:ILE:HD11	2.11	0.50
1:A:392:THR:HB	1:A:526:THR:HG22	1.93	0.50
2:B:371:ASN:ND2	2:B:383:TRP:CZ2	2.80	0.50
2:B:190:LYS:HA	2:B:288:VAL:HG22	1.92	0.50
1:A:253:HIS:N	1:A:253:HIS:ND1	2.59	0.50
2:B:325:LEU:HD23	2:B:326:LYS:N	2.27	0.50
1:A:474:ARG:HA	1:A:524:ASP:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ALA:O	1:A:530:LEU:HD12	2.12	0.50
1:A:287:LEU:CG	1:A:288:VAL:N	2.74	0.50
1:A:343:PRO:C	1:A:345:SER:H	2.15	0.50
2:B:341:LEU:HG	2:B:609:TYR:HH	1.75	0.50
1:A:166:TRP:HE1	1:A:200:TYR:HB3	1.77	0.50
1:A:416:ILE:HG23	1:A:503:ILE:HD11	1.94	0.50
2:B:489:THR:HG21	2:B:548:VAL:HG21	1.93	0.50
1:C:193:LEU:HD12	1:C:215:ILE:HD12	1.94	0.50
1:A:375:ASP:CG	1:A:376:PHE:N	2.65	0.50
1:A:308:CYS:SG	1:A:309:ILE:N	2.84	0.50
1:A:200:TYR:CD1	1:A:200:TYR:N	2.80	0.50
1:C:439:ASN:ND2	1:C:440:GLN:NE2	2.60	0.50
1:A:246:THR:O	1:A:249:LEU:N	2.34	0.50
1:C:647:TYR:N	1:C:647:TYR:CD1	2.78	0.50
1:C:166:TRP:HA	1:C:169:PHE:HE2	1.77	0.50
1:C:196:LEU:HA	1:C:202:THR:OG1	2.12	0.50
1:C:349:TRP:C	1:C:350:ILE:HG12	2.32	0.49
2:B:473:GLN:HE21	2:B:474:ARG:C	2.15	0.49
1:A:292:TYR:HD1	1:A:292:TYR:O	1.93	0.49
1:A:222:SER:C	1:A:308:CYS:HG	2.15	0.49
2:B:342:ILE:HD12	2:B:587:ILE:CD1	2.40	0.49
1:A:370:ALA:HB2	1:A:554:PRO:HD2	1.93	0.49
2:B:334:HIS:O	2:B:600:LEU:HB2	2.13	0.49
1:C:393:VAL:CG1	1:C:394:THR:N	2.74	0.49
2:B:362:VAL:HG23	2:B:568:ARG:HB2	1.94	0.49
2:B:430:ILE:HG22	2:B:496:LYS:HA	1.94	0.49
1:A:350:ILE:HD12	1:A:351:GLY:O	2.13	0.49
1:C:633:VAL:HG12	1:C:635:SER:H	1.76	0.49
1:A:509:ALA:O	1:A:510:ILE:HG23	2.12	0.49
2:B:201:LEU:HD21	2:B:316:PRO:HB3	1.94	0.49
2:B:358:ILE:CG1	2:B:359:THR:H	2.16	0.49
1:A:399:GLU:CG	1:A:516:VAL:HG21	2.29	0.49
1:C:549:ARG:HD3	1:C:553:LEU:HD13	1.93	0.49
1:A:565:ILE:HD12	1:A:565:ILE:C	2.33	0.49
1:A:580:ILE:HD12	1:A:580:ILE:O	2.12	0.49
1:A:205:ALA:C	1:A:207:LEU:N	2.66	0.49
1:A:550:ILE:CG2	1:A:551:GLY:N	2.75	0.49
2:B:310:VAL:O	2:B:310:VAL:CG1	2.57	0.49
1:C:358:ILE:HG22	1:C:360:ASP:H	1.77	0.49
1:A:391:ILE:O	1:A:526:THR:HA	2.13	0.49
2:B:320:PHE:O	2:B:321:LYS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLN:NE2	1:A:192:SER:H	2.10	0.49
2:B:605:SER:HA	2:B:652:LEU:HA	1.94	0.49
1:C:162:VAL:CG1	1:C:164:SER:OG	2.60	0.49
1:A:479:LYS:C	1:A:480:LYS:HG3	2.32	0.49
1:A:287:LEU:O	1:A:288:VAL:HG13	2.13	0.49
1:C:352:ASN:HD22	1:C:586:GLN:N	2.05	0.49
2:B:295:LEU:HD12	2:B:296:ILE:H	1.78	0.49
1:A:200:TYR:HD1	1:A:200:TYR:H	1.60	0.49
1:A:243:ILE:O	1:A:245:SER:N	2.41	0.49
1:C:436:ALA:HB1	1:C:461:THR:HA	1.93	0.49
1:A:352:ASN:N	1:A:584:ASN:HD22	2.10	0.49
2:B:393:VAL:HG23	2:B:409:THR:CG2	2.43	0.49
2:B:187:ILE:HG21	2:B:190:LYS:HB2	1.95	0.49
1:C:506:THR:OG1	1:C:507:LYS:HD2	2.12	0.49
1:A:255:LEU:HD12	1:A:255:LEU:N	2.28	0.49
1:C:216:GLU:HG2	1:C:267:THR:CG2	2.42	0.49
2:B:625:SER:O	2:B:626:ASP:C	2.52	0.48
1:C:424:THR:HG1	1:C:489:THR:HG23	1.77	0.48
1:A:566:PHE:CD2	1:A:583:PHE:HB3	2.48	0.48
2:B:657:LEU:O	2:B:658:ALA:O	2.31	0.48
1:C:431:PRO:HD2	1:C:495:ASN:O	2.12	0.48
1:A:190:LYS:HG3	1:A:651:GLN:NE2	2.28	0.48
2:B:344:LYS:HE3	2:B:647:TYR:OH	2.13	0.48
2:B:521:GLN:HG2	2:B:522:THR:N	2.22	0.48
2:B:198:ASN:HB2	2:B:314:THR:HG1	1.78	0.48
1:A:130:ILE:HD11	1:C:255:LEU:O	2.12	0.48
1:C:487:ILE:CG2	1:C:510:ILE:HG22	2.40	0.48
1:C:374:PHE:CZ	1:C:386:PRO:HD3	2.48	0.48
1:C:203:HIS:O	1:C:206:LYS:HB2	2.13	0.48
2:B:624:ASP:O	2:B:625:SER:C	2.51	0.48
2:B:463:PHE:HB3	2:B:466:MET:CE	2.43	0.48
1:A:164:SER:HA	1:A:166:TRP:HE3	1.73	0.48
1:C:451:TYR:HB3	1:C:457:ILE:HA	1.96	0.48
2:B:398:LYS:HZ3	2:B:398:LYS:N	2.12	0.48
2:B:512:GLN:CD	2:B:513:ASP:H	2.16	0.48
1:C:526:THR:HG22	1:C:527:LEU:H	1.78	0.48
1:C:424:THR:CG2	1:C:425:ILE:N	2.76	0.48
1:A:565:ILE:HG21	1:A:631:VAL:HG23	1.95	0.48
1:C:618:TRP:CE2	1:C:660:ASN:HB2	2.49	0.48
2:B:200:TYR:O	2:B:201:LEU:C	2.52	0.48
1:A:273:SER:HA	2:B:276:TYR:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:611:ILE:HD13	2:B:621:ILE:HD13	1.94	0.48
1:C:661:ILE:H	1:C:661:ILE:CD1	2.25	0.48
1:C:440:GLN:OE1	1:C:456:ILE:HA	2.14	0.48
2:B:587:ILE:HB	2:B:590:THR:OG1	2.13	0.48
1:A:143:ILE:HG23	1:A:143:ILE:O	2.13	0.48
2:B:142:VAL:CG1	2:B:142:VAL:O	2.62	0.48
1:C:448:LYS:HE3	1:C:537:GLU:CD	2.33	0.48
2:B:588:LEU:O	2:B:590:THR:N	2.47	0.48
1:C:395:ILE:HD13	1:C:403:LEU:HD13	1.94	0.48
2:B:658:ALA:O	2:B:659:SER:HB3	2.12	0.48
1:C:270:ASP:OD2	1:C:272:ARG:NH1	2.47	0.48
2:B:273:SER:O	1:C:275:LEU:HG	2.14	0.48
1:C:437:ILE:O	1:C:438:THR:HB	2.13	0.48
1:A:417:PRO:HG2	1:A:508:ILE:HG21	1.95	0.48
1:A:464:LYS:HD2	1:A:535:ILE:HG22	1.96	0.48
2:B:405:ILE:HD13	2:B:405:ILE:N	2.29	0.48
1:C:393:VAL:HG12	1:C:394:THR:N	2.27	0.48
2:B:425:ILE:HD13	2:B:425:ILE:H	1.79	0.48
2:B:607:ALA:HA	2:B:650:ASN:CB	2.44	0.48
1:C:396:SER:O	1:C:403:LEU:CD2	2.62	0.48
1:C:403:LEU:CG	1:C:514:ASN:HD21	2.27	0.48
1:A:359:THR:HG23	1:A:360:ASP:N	2.28	0.48
2:B:325:LEU:C	2:B:325:LEU:HD23	2.34	0.48
1:A:142:VAL:HG22	1:A:142:VAL:O	2.13	0.48
1:A:145:GLU:N	1:A:146:PRO:HD2	2.28	0.48
2:B:402:MET:HB3	2:B:403:LEU:H	1.29	0.48
1:C:191:GLN:HE21	1:C:197:LEU:CD2	2.25	0.48
1:C:397:GLN:HA	1:C:403:LEU:HD21	1.96	0.48
1:A:506:THR:C	1:A:507:LYS:HD2	2.31	0.48
1:A:613:ASP:HB3	1:A:643:LEU:HD23	1.96	0.48
1:C:209:VAL:HG23	1:C:324:LEU:HB2	1.94	0.48
1:A:621:ILE:HA	1:A:630:PHE:O	2.13	0.48
2:B:562:ASN:OD1	2:B:657:LEU:HG	2.13	0.48
1:C:590:THR:O	1:C:591:SER:C	2.51	0.48
2:B:272:ARG:O	1:C:276:TYR:HE1	1.97	0.48
1:A:354:PHE:H	1:A:584:ASN:HD21	1.62	0.47
1:C:402:MET:C	1:C:402:MET:SD	2.92	0.47
1:C:298:PRO:HB2	1:C:299:TYR:CE1	2.49	0.47
1:C:332:LEU:CD2	1:C:334:HIS:H	2.26	0.47
1:C:346:SER:HB2	1:C:643:LEU:CB	2.42	0.47
2:B:610:ARG:HA	2:B:620:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:TRP:CZ3	1:A:522:THR:HB	2.49	0.47
2:B:395:ILE:HG23	2:B:521:GLN:HB2	1.97	0.47
2:B:373:HIS:HD2	2:B:585:SER:HB2	1.79	0.47
2:B:226:VAL:CG1	2:B:298:PRO:HG2	2.35	0.47
1:C:465:SER:HA	1:C:532:TYR:CE1	2.48	0.47
1:C:509:ALA:C	1:C:510:ILE:HG23	2.34	0.47
1:C:204:LEU:HD23	1:C:204:LEU:C	2.34	0.47
1:C:437:ILE:HD13	1:C:439:ASN:HB2	1.94	0.47
2:B:353:ARG:HG2	2:B:353:ARG:NH1	2.29	0.47
2:B:420:TRP:CG	2:B:421:PRO:HD2	2.49	0.47
2:B:353:ARG:N	2:B:584:ASN:HD22	2.03	0.47
1:A:342:ILE:HD13	1:A:342:ILE:O	2.14	0.47
1:A:451:TYR:HA	1:A:452:GLU:CB	2.37	0.47
1:A:155:ASP:O	1:A:156:MET:C	2.53	0.47
1:C:602:SER:O	1:C:604:ASP:N	2.47	0.47
1:C:451:TYR:CA	1:C:458:SER:HB2	2.45	0.47
2:B:402:MET:HE2	2:B:402:MET:HA	1.96	0.47
1:A:439:ASN:CB	1:A:456:ILE:HG12	2.41	0.47
1:C:362:VAL:HB	1:C:566:PHE:HB2	1.96	0.47
1:A:553:LEU:HD12	1:A:554:PRO:HD2	1.95	0.47
2:B:628:PHE:N	2:B:628:PHE:CD1	2.83	0.47
2:B:349:TRP:O	2:B:358:ILE:HG23	2.15	0.47
1:A:253:HIS:H	1:A:253:HIS:HD1	1.62	0.47
1:C:609:TYR:CE1	1:C:647:TYR:HB3	2.49	0.47
2:B:249:LEU:C	2:B:251:TYR:H	2.17	0.47
2:B:366:PHE:HE2	1:C:414:PRO:HD3	1.79	0.47
1:A:187:ILE:N	1:A:187:ILE:HD13	2.29	0.47
1:A:576:VAL:HG12	1:A:577:ILE:H	1.80	0.47
1:C:451:TYR:H	1:C:458:SER:CB	2.18	0.47
1:A:423:THR:HB	1:A:467:TYR:CE1	2.47	0.47
1:A:416:ILE:CD1	1:A:503:ILE:HG12	2.35	0.47
2:B:398:LYS:H	2:B:398:LYS:CD	2.27	0.47
1:A:466:MET:HB2	1:A:533:THR:OG1	2.14	0.47
2:B:368:PHE:O	2:B:369:GLN:CB	2.62	0.47
1:C:540:ILE:HB	1:C:582:VAL:CG2	2.45	0.47
1:A:236:VAL:HB	1:A:240:ILE:HD11	1.96	0.47
1:A:376:PHE:HE2	1:A:601:LEU:HD22	1.80	0.47
1:A:333:THR:HA	1:C:652:LEU:HD11	1.97	0.47
2:B:354:PHE:CE2	2:B:571:MET:HG2	2.49	0.47
1:C:130:ILE:CD1	1:C:130:ILE:H	2.25	0.47
1:C:385:THR:O	1:C:387:ARG:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:360:ASP:OD2	2:B:568:ARG:HB3	2.14	0.47
1:A:176:VAL:HG12	1:A:177:ASN:N	2.29	0.47
1:C:460:ASN:CG	1:C:461:THR:H	2.19	0.47
2:B:451:TYR:O	2:B:453:SER:N	2.44	0.47
1:A:439:ASN:HD22	1:A:456:ILE:HG12	1.79	0.47
2:B:533:THR:O	2:B:535:ILE:CG2	2.56	0.47
2:B:239:GLY:O	1:C:332:LEU:HA	2.15	0.47
1:C:618:TRP:NE1	1:C:660:ASN:HB2	2.30	0.47
1:C:246:THR:O	1:C:248:MET:N	2.47	0.47
1:A:338:PRO:HA	1:A:599:TYR:CD2	2.50	0.47
2:B:430:ILE:HG13	2:B:431:PRO:O	2.14	0.47
2:B:521:GLN:C	2:B:523:SER:N	2.66	0.47
2:B:587:ILE:O	2:B:590:THR:HB	2.15	0.47
1:A:193:LEU:HD12	1:A:197:LEU:CD1	2.44	0.47
1:C:385:THR:CG2	1:C:386:PRO:HD2	2.45	0.47
1:C:199:PRO:HG2	1:C:200:TYR:H	1.80	0.47
1:C:420:TRP:O	1:C:421:PRO:O	2.32	0.47
1:A:405:ILE:CG1	1:A:509:ALA:HA	2.32	0.47
1:A:373:HIS:HA	1:A:586:GLN:OE1	2.15	0.47
2:B:369:GLN:H	2:B:553:LEU:HD11	1.79	0.47
1:C:471:SER:HA	1:C:527:LEU:HA	1.97	0.47
1:C:593:GLN:O	1:C:594:LEU:C	2.54	0.47
1:C:158:THR:O	1:C:160:LYS:N	2.48	0.47
1:A:411:TYR:HE1	1:A:418:ASP:O	1.98	0.46
1:A:469:CYS:HA	1:A:528:ALA:O	2.16	0.46
2:B:164:SER:C	2:B:166:TRP:H	2.18	0.46
1:C:530:LEU:N	1:C:530:LEU:HD12	2.30	0.46
1:C:133:PRO:O	1:C:134:GLU:HB2	2.15	0.46
2:B:506:THR:HG23	2:B:507:LYS:HD2	1.97	0.46
2:B:571:MET:HB3	2:B:580:ILE:HD11	1.97	0.46
1:A:353:ARG:NE	1:A:422:ASP:HB2	2.27	0.46
1:C:242:PRO:HG2	1:C:288:VAL:HG21	1.98	0.46
1:C:289:ILE:N	1:C:289:ILE:HD12	2.30	0.46
1:C:552:VAL:HG12	1:C:553:LEU:H	1.80	0.46
2:B:448:LYS:HD2	2:B:537:GLU:HG3	1.97	0.46
1:C:598:ASN:C	1:C:598:ASN:ND2	2.69	0.46
2:B:377:ASN:C	2:B:379:GLU:H	2.19	0.46
1:A:278:LEU:H	1:A:278:LEU:CD2	2.16	0.46
1:A:384:SER:HA	1:A:418:ASP:HB2	1.97	0.46
2:B:398:LYS:HE3	2:B:403:LEU:HB2	1.97	0.46
2:B:373:HIS:CD2	2:B:585:SER:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:TRP:O	2:B:358:ILE:N	2.46	0.46
1:C:474:ARG:CB	1:C:523:SER:O	2.63	0.46
2:B:636:ILE:N	2:B:636:ILE:HD13	2.09	0.46
1:C:631:VAL:HG12	1:C:632:GLY:N	2.30	0.46
1:C:610:ARG:HD3	1:C:620:ASP:OD1	2.15	0.46
1:C:607:ALA:HA	1:C:649:GLY:O	2.14	0.46
1:C:178:TRP:CZ2	1:C:295:LEU:HB2	2.50	0.46
2:B:170:PHE:CE2	2:B:315:LYS:HB3	2.51	0.46
1:C:474:ARG:HB2	1:C:524:ASP:CA	2.46	0.46
1:A:391:ILE:HG23	1:A:411:TYR:OH	2.15	0.46
1:A:234:ILE:HG22	1:A:253:HIS:HB3	1.97	0.46
2:B:264:VAL:HG21	1:C:130:ILE:HG21	1.98	0.46
1:A:422:ASP:C	1:A:548:VAL:HG23	2.36	0.46
1:A:484:THR:OG1	1:A:511:PHE:O	2.32	0.46
1:A:287:LEU:C	1:A:287:LEU:HD23	2.36	0.46
1:C:416:ILE:HD12	1:C:503:ILE:CG1	2.34	0.46
1:C:471:SER:HB3	1:C:527:LEU:CB	2.42	0.46
1:C:621:ILE:CD1	1:C:631:VAL:HG22	2.46	0.46
1:C:404:GLY:HA3	1:C:509:ALA:HA	1.98	0.46
2:B:220:SER:HB2	2:B:311:THR:OG1	2.15	0.46
2:B:239:GLY:HA2	1:C:333:THR:CG2	2.45	0.46
1:A:199:PRO:HA	1:A:202:THR:HB	1.97	0.46
1:A:219:PHE:CD2	1:A:219:PHE:C	2.82	0.46
2:B:607:ALA:HA	2:B:650:ASN:HB3	1.97	0.46
1:A:221:ILE:CD1	1:A:223:GLY:H	2.28	0.46
1:A:196:LEU:H	1:A:196:LEU:HG	1.33	0.46
2:B:288:VAL:C	2:B:289:ILE:HD12	2.36	0.46
1:A:149:GLN:C	1:A:153:ALA:HB3	2.36	0.46
2:B:209:VAL:HB	2:B:324:LEU:HB2	1.97	0.46
1:A:376:PHE:CE2	1:A:601:LEU:HD22	2.51	0.46
1:C:377:ASN:O	1:C:378:GLN:HB2	2.15	0.46
1:C:453:SER:HB2	1:C:456:ILE:CG2	2.45	0.46
1:A:150:MET:O	1:A:151:SER:HB2	2.16	0.46
2:B:210:ALA:HB3	2:B:323:HIS:CB	2.37	0.46
1:C:631:VAL:CG1	1:C:632:GLY:N	2.79	0.46
1:C:326:LYS:HG2	1:C:327:PRO:N	2.31	0.46
1:A:173:HIS:CE1	1:A:197:LEU:HA	2.51	0.46
2:B:544:ARG:HH22	1:C:505:GLN:NE2	2.11	0.46
2:B:248:MET:O	2:B:250:GLN:N	2.48	0.46
1:C:348:LEU:O	1:C:348:LEU:CD1	2.64	0.46
1:C:343:PRO:HG3	1:C:589:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:GLN:O	2:B:446:GLN:HG2	2.16	0.46
2:B:521:GLN:C	2:B:523:SER:H	2.18	0.46
2:B:470:GLY:O	2:B:527:LEU:HA	2.15	0.46
1:A:149:GLN:HA	1:A:153:ALA:HB3	1.97	0.46
1:A:327:PRO:O	1:A:327:PRO:HG2	2.16	0.46
1:A:636:ILE:HD13	1:A:636:ILE:N	2.30	0.46
1:A:278:LEU:O	1:A:280:SER:N	2.49	0.45
1:A:392:THR:O	1:A:409:THR:CG2	2.63	0.45
1:C:192:SER:O	1:C:197:LEU:HD21	2.16	0.45
2:B:148:VAL:O	2:B:150:MET:N	2.49	0.45
1:C:611:ILE:CD1	1:C:611:ILE:N	2.74	0.45
1:A:428:GLU:HB3	1:A:498:ILE:HG22	1.96	0.45
1:C:386:PRO:O	1:C:588:LEU:HD21	2.17	0.45
1:A:176:VAL:HG11	1:A:188:LEU:HD22	1.98	0.45
1:A:623:ILE:HG13	1:A:623:ILE:H	1.50	0.45
2:B:374:PHE:CE2	2:B:380:THR:HG21	2.51	0.45
1:C:395:ILE:HD11	1:C:523:SER:HB3	1.98	0.45
1:C:469:CYS:CB	1:C:528:ALA:O	2.64	0.45
2:B:158:THR:O	2:B:158:THR:HG22	2.16	0.45
1:A:609:TYR:CD1	1:A:647:TYR:HB3	2.50	0.45
1:C:318:PRO:HG2	1:C:319:ASP:H	1.81	0.45
2:B:438:THR:HG23	2:B:457:ILE:HG23	1.97	0.45
1:A:405:ILE:HG23	1:A:510:ILE:CG1	2.45	0.45
1:C:503:ILE:HB	1:C:548:VAL:HG11	1.98	0.45
1:C:353:ARG:NH2	1:C:540:ILE:O	2.49	0.45
1:C:404:GLY:CA	1:C:509:ALA:HA	2.46	0.45
1:C:297:ASN:ND2	1:C:298:PRO:HD2	2.31	0.45
1:C:346:SER:CB	1:C:643:LEU:HB2	2.44	0.45
1:A:377:ASN:CB	1:C:559:ARG:HD3	2.47	0.45
1:A:398:LYS:C	1:A:400:GLY:H	2.19	0.45
2:B:484:THR:OG1	2:B:485:ALA:N	2.49	0.45
1:A:535:ILE:HD11	1:A:538:GLU:CB	2.43	0.45
1:A:230:LYS:HD2	1:A:293:ASN:ND2	2.31	0.45
1:C:243:ILE:N	1:C:243:ILE:HD13	2.32	0.45
1:A:375:ASP:O	1:A:594:LEU:HD22	2.17	0.45
1:A:221:ILE:CD1	1:A:221:ILE:O	2.62	0.45
2:B:633:VAL:CG1	2:B:634:SER:N	2.80	0.45
2:B:618:TRP:NE1	2:B:660:ASN:HB2	2.32	0.45
1:C:374:PHE:CE2	1:C:595:SER:HB3	2.51	0.45
2:B:230:LYS:H	2:B:293:ASN:HB2	1.82	0.45
1:A:478:ASN:HD22	1:A:478:ASN:N	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:HIS:HB3	2:B:281:ASP:OD2	2.16	0.45
1:A:130:ILE:HD13	1:C:260:GLN:HE22	1.80	0.45
2:B:162:VAL:O	2:B:163:ASP:C	2.55	0.45
1:A:359:THR:HG22	1:A:568:ARG:C	2.36	0.45
1:A:376:PHE:CD1	1:A:594:LEU:HD21	2.52	0.45
1:A:370:ALA:O	1:A:373:HIS:HB3	2.16	0.45
1:A:474:ARG:NH1	1:A:521:GLN:O	2.50	0.45
1:A:352:ASN:HD21	1:A:586:GLN:H	1.60	0.45
2:B:353:ARG:HB3	2:B:584:ASN:ND2	2.32	0.45
1:A:221:ILE:HD11	1:A:258:ALA:O	2.16	0.45
1:C:431:PRO:CD	1:C:495:ASN:O	2.65	0.45
1:A:217:VAL:HG12	1:A:218:ARG:N	2.31	0.45
2:B:606:PHE:CE1	2:B:625:SER:N	2.85	0.45
1:C:453:SER:HB2	1:C:456:ILE:HG23	1.98	0.45
1:C:368:PHE:HD1	1:C:547:VAL:HG21	1.82	0.45
1:A:631:VAL:HG12	1:A:633:VAL:HG23	1.98	0.45
2:B:439:ASN:ND2	2:B:456:ILE:CD1	2.79	0.45
1:A:423:THR:HG22	1:A:424:THR:N	2.31	0.45
1:A:473:GLN:O	1:A:524:ASP:HB3	2.17	0.45
1:C:479:LYS:HE3	1:C:516:VAL:HB	1.99	0.45
2:B:333:THR:HG23	2:B:334:HIS:H	1.82	0.45
1:C:405:ILE:HA	1:C:508:ILE:HG12	1.99	0.45
1:A:333:THR:HG22	1:C:239:GLY:C	2.36	0.45
2:B:179:SER:O	2:B:182:GLU:HG2	2.17	0.45
1:A:385:THR:CB	1:A:386:PRO:HD2	2.46	0.45
1:A:483:ASN:HB3	1:A:484:THR:H	1.38	0.45
2:B:349:TRP:HB2	2:B:358:ILE:HG12	1.97	0.45
2:B:358:ILE:O	2:B:359:THR:CB	2.65	0.45
2:B:393:VAL:O	2:B:393:VAL:HG13	2.17	0.45
1:A:223:GLY:CA	1:A:308:CYS:SG	3.05	0.45
1:A:186:LYS:HA	1:A:244:GLN:HG2	1.98	0.45
1:C:451:TYR:HA	1:C:458:SER:N	2.32	0.45
1:A:405:ILE:HG23	1:A:510:ILE:CG2	2.46	0.45
2:B:201:LEU:HD22	2:B:320:PHE:HE2	1.82	0.45
1:C:474:ARG:O	1:C:475:ALA:CB	2.63	0.45
1:C:403:LEU:HG	1:C:514:ASN:HD21	1.82	0.45
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.73	0.45
2:B:519:ASP:HB3	2:B:520:VAL:H	1.44	0.45
1:A:341:LEU:HB3	1:A:342:ILE:H	1.63	0.45
1:A:221:ILE:CD1	1:A:221:ILE:C	2.80	0.45
1:A:132:THR:O	1:A:133:PRO:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:ASN:HD22	1:C:429:LEU:HD21	1.82	0.45
1:C:171:SER:O	1:C:314:THR:N	2.43	0.45
1:C:451:TYR:HA	1:C:458:SER:HB2	1.98	0.44
2:B:342:ILE:HG23	2:B:587:ILE:HD12	1.99	0.44
2:B:344:LYS:CE	2:B:647:TYR:OH	2.65	0.44
2:B:137:THR:HG22	2:B:138:THR:H	1.81	0.44
2:B:439:ASN:HD21	2:B:456:ILE:CG1	2.30	0.44
1:A:459:ASN:O	1:A:460:ASN:ND2	2.49	0.44
1:C:176:VAL:CG1	1:C:177:ASN:N	2.80	0.44
2:B:500:SER:HB2	2:B:502:THR:CG2	2.47	0.44
1:A:210:ALA:HB2	1:A:278:LEU:HB3	1.99	0.44
1:A:369:GLN:O	1:A:554:PRO:HD2	2.17	0.44
1:A:393:VAL:N	1:A:525:ASP:HB2	2.32	0.44
1:A:408:ALA:CB	1:A:417:PRO:HG3	2.47	0.44
2:B:487:ILE:HG22	2:B:510:ILE:HA	1.98	0.44
1:C:552:VAL:HG12	1:C:553:LEU:N	2.33	0.44
2:B:151:SER:C	2:B:153:ALA:N	2.71	0.44
1:A:184:GLN:NE2	1:A:292:TYR:O	2.50	0.44
1:A:601:LEU:HD23	1:A:602:SER:O	2.17	0.44
1:A:250:GLN:O	2:B:328:PRO:CD	2.65	0.44
1:A:193:LEU:CG	1:A:194:GLY:N	2.81	0.44
2:B:573:LEU:HD23	2:B:573:LEU:HA	1.79	0.44
1:A:448:LYS:O	1:A:449:GLU:HB2	2.16	0.44
1:A:412:ILE:O	1:A:413:VAL:CG2	2.65	0.44
1:C:408:ALA:HB1	1:C:411:TYR:CE2	2.52	0.44
1:A:346:SER:O	1:A:348:LEU:N	2.51	0.44
1:A:367:VAL:O	1:A:555:GLU:HA	2.17	0.44
1:A:223:GLY:HA2	1:A:308:CYS:SG	2.58	0.44
1:C:300:ALA:O	1:C:301:ASN:CB	2.65	0.44
1:C:565:ILE:HG13	1:C:629:SER:HB2	1.99	0.44
1:A:145:GLU:N	1:A:146:PRO:CD	2.80	0.44
1:A:412:ILE:C	1:A:413:VAL:HG23	2.38	0.44
2:B:503:ILE:HB	2:B:548:VAL:CG1	2.47	0.44
2:B:472:LEU:HB3	2:B:526:THR:O	2.16	0.44
2:B:525:ASP:O	2:B:527:LEU:HG	2.17	0.44
1:C:363:ILE:H	1:C:363:ILE:CD1	2.23	0.44
1:A:333:THR:N	1:C:239:GLY:O	2.48	0.44
2:B:391:ILE:CD1	2:B:391:ILE:N	2.80	0.44
1:C:166:TRP:C	1:C:168:ALA:N	2.71	0.44
1:A:210:ALA:HB2	1:A:278:LEU:CA	2.47	0.44
2:B:352:ASN:HD21	2:B:369:GLN:NE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:GLY:HA3	1:C:320:PHE:HA	2.00	0.44
2:B:602:SER:HB3	2:B:604:ASP:OD2	2.18	0.44
1:C:442:GLY:C	1:C:444:ASP:H	2.21	0.44
1:A:304:ASN:O	1:A:305:SER:C	2.55	0.44
2:B:383:TRP:HD1	2:B:384:SER:HG	1.57	0.44
2:B:287:LEU:C	2:B:288:VAL:HG23	2.38	0.44
1:A:376:PHE:HD1	1:A:594:LEU:HD21	1.83	0.44
1:A:231:LEU:HA	1:A:231:LEU:HD12	1.71	0.44
1:C:361:PHE:HE1	1:C:619:PHE:HZ	1.63	0.44
2:B:432:ALA:O	2:B:433:GLY:C	2.55	0.44
1:A:503:ILE:HB	1:A:548:VAL:CG1	2.48	0.44
1:A:458:SER:O	1:A:459:ASN:CB	2.66	0.44
1:C:344:LYS:O	1:C:345:SER:CB	2.64	0.44
2:B:168:ALA:HA	2:B:315:LYS:HZ3	1.83	0.44
2:B:139:VAL:HG12	2:B:140:GLY:N	2.32	0.44
1:C:438:THR:O	1:C:438:THR:HG23	2.18	0.44
2:B:437:ILE:C	2:B:439:ASN:H	2.21	0.44
1:A:371:ASN:HA	1:A:382:GLY:HA3	2.00	0.44
2:B:352:ASN:N	2:B:584:ASN:HD22	2.16	0.44
1:C:193:LEU:HD12	1:C:193:LEU:HA	1.78	0.44
1:C:367:VAL:HG23	1:C:564:PRO:HB2	2.00	0.44
2:B:158:THR:HB	2:B:160:LYS:HB3	1.99	0.44
1:A:624:ASP:HB2	1:A:630:PHE:CE1	2.52	0.44
1:C:652:LEU:O	1:C:655:ILE:HG13	2.17	0.44
1:A:170:PHE:CD2	1:A:315:LYS:HB2	2.53	0.44
2:B:604:ASP:OD2	2:B:604:ASP:N	2.50	0.44
1:C:179:SER:N	1:C:182:GLU:OE2	2.43	0.44
1:A:609:TYR:HA	1:A:647:TYR:HA	1.99	0.43
2:B:341:LEU:O	2:B:343:PRO:HD3	2.18	0.43
2:B:236:VAL:O	2:B:236:VAL:HG23	2.18	0.43
1:C:350:ILE:CA	1:C:357:ASP:HA	2.43	0.43
1:A:469:CYS:CB	1:A:527:LEU:HB2	2.48	0.43
1:A:624:ASP:C	1:A:626:ASP:H	2.20	0.43
2:B:505:GLN:HG3	2:B:506:THR:N	2.32	0.43
2:B:602:SER:O	2:B:604:ASP:N	2.49	0.43
1:C:251:TYR:CD1	1:C:252:PRO:HD2	2.52	0.43
1:A:214:SER:O	1:A:317:GLY:HA3	2.18	0.43
1:A:393:VAL:H	1:A:525:ASP:HB2	1.83	0.43
1:A:525:ASP:O	1:A:526:THR:O	2.36	0.43
1:A:219:PHE:HB2	1:A:311:THR:O	2.17	0.43
1:C:504:ASP:C	1:C:506:THR:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HG13	1:A:256:PHE:HE2	1.83	0.43
2:B:215:ILE:O	2:B:268:ILE:HG13	2.18	0.43
1:C:438:THR:C	1:C:457:ILE:HG13	2.38	0.43
1:A:391:ILE:CD1	1:A:391:ILE:N	2.81	0.43
2:B:474:ARG:HD3	2:B:525:ASP:OD1	2.19	0.43
1:C:518:ARG:HD3	1:C:520:VAL:HG13	2.01	0.43
2:B:147:SER:O	2:B:148:VAL:O	2.37	0.43
1:C:204:LEU:HD22	1:C:322:PHE:CZ	2.53	0.43
1:C:349:TRP:O	1:C:350:ILE:CG1	2.66	0.43
1:A:383:TRP:CZ3	1:A:550:ILE:HB	2.53	0.43
1:A:393:VAL:O	1:A:525:ASP:CB	2.59	0.43
1:C:288:VAL:HG12	1:C:289:ILE:H	1.80	0.43
2:B:188:LEU:O	2:B:188:LEU:CD2	2.63	0.43
2:B:189:PHE:HD2	2:B:289:ILE:HD13	1.82	0.43
1:A:433:GLY:HA3	1:A:462:ASN:OD1	2.18	0.43
2:B:414:PRO:O	2:B:416:ILE:HD12	2.19	0.43
2:B:470:GLY:N	2:B:528:ALA:O	2.51	0.43
1:C:576:VAL:HG12	1:C:577:ILE:HG12	2.01	0.43
1:A:150:MET:O	1:A:151:SER:CB	2.66	0.43
1:A:236:VAL:CG2	1:A:286:SER:HB2	2.48	0.43
1:A:166:TRP:NE1	1:A:200:TYR:HB3	2.34	0.43
1:A:208:TYR:HA	1:A:325:LEU:HA	1.99	0.43
2:B:297:ASN:C	2:B:297:ASN:OD1	2.57	0.43
1:A:484:THR:O	1:A:485:ALA:CB	2.65	0.43
1:A:513:ASP:N	1:A:513:ASP:OD2	2.50	0.43
1:A:528:ALA:O	1:A:530:LEU:HD13	2.19	0.43
2:B:383:TRP:HB2	2:B:413:VAL:HG21	2.01	0.43
2:B:358:ILE:O	2:B:359:THR:HB	2.18	0.43
1:C:527:LEU:HD23	1:C:527:LEU:N	2.34	0.43
1:C:582:VAL:HG12	1:C:583:PHE:N	2.33	0.43
1:C:392:THR:HG23	1:C:409:THR:CG2	2.48	0.43
1:A:533:THR:O	1:A:535:ILE:N	2.51	0.43
2:B:422:ASP:O	2:B:423:THR:C	2.56	0.43
2:B:623:ILE:CD1	2:B:623:ILE:N	2.56	0.43
2:B:474:ARG:O	2:B:475:ALA:HB2	2.19	0.43
2:B:153:ALA:O	2:B:154:ALA:C	2.56	0.43
1:C:190:LYS:HD3	1:C:651:GLN:NE2	2.33	0.43
2:B:608:VAL:CG1	2:B:609:TYR:N	2.82	0.43
1:C:652:LEU:HD12	1:C:652:LEU:H	1.84	0.43
1:C:652:LEU:HD12	1:C:652:LEU:N	2.34	0.43
2:B:639:LEU:CD2	2:B:639:LEU:N	2.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:THR:HG23	1:C:386:PRO:HD2	2.01	0.43
1:A:639:LEU:HD23	1:A:639:LEU:H	1.83	0.43
2:B:606:PHE:CE1	2:B:624:ASP:C	2.92	0.43
1:C:451:TYR:C	1:C:453:SER:H	2.22	0.43
1:A:439:ASN:CG	1:A:440:GLN:N	2.71	0.43
1:A:440:GLN:O	1:A:441:SER:HB2	2.19	0.43
2:B:486:PHE:CD2	2:B:486:PHE:N	2.85	0.43
1:C:398:LYS:O	1:C:399:GLU:CB	2.67	0.43
1:A:571:MET:CB	1:A:580:ILE:HD11	2.43	0.43
2:B:583:PHE:CD1	2:B:583:PHE:N	2.87	0.43
2:B:186:LYS:HE3	2:B:186:LYS:HB2	1.86	0.43
1:A:383:TRP:HD1	1:A:418:ASP:HA	1.84	0.43
2:B:353:ARG:CB	2:B:584:ASN:ND2	2.82	0.43
1:C:398:LYS:N	1:C:403:LEU:CD2	2.76	0.43
1:A:613:ASP:CG	1:A:614:SER:H	2.21	0.43
1:C:297:ASN:ND2	1:C:298:PRO:N	2.60	0.43
1:C:449:GLU:O	1:C:450:GLU:OE2	2.36	0.42
2:B:444:ASP:O	2:B:446:GLN:N	2.52	0.42
2:B:453:SER:C	2:B:456:ILE:HB	2.39	0.42
2:B:233:ALA:C	2:B:234:ILE:HG23	2.40	0.42
1:C:512:GLN:HB3	1:C:514:ASN:OD1	2.19	0.42
1:C:353:ARG:HB2	1:C:369:GLN:HE22	1.83	0.42
1:A:292:TYR:CD1	1:A:292:TYR:C	2.91	0.42
2:B:257:ASP:OD1	2:B:258:ALA:N	2.51	0.42
2:B:611:ILE:HD13	2:B:619:PHE:HD1	1.84	0.42
1:A:405:ILE:HG21	1:A:510:ILE:HG23	2.00	0.42
1:A:512:GLN:HB3	1:A:513:ASP:H	1.63	0.42
1:C:383:TRP:CZ3	1:C:503:ILE:HG21	2.54	0.42
1:A:151:SER:O	1:A:153:ALA:N	2.52	0.42
1:A:633:VAL:HG12	1:A:634:SER:N	2.34	0.42
2:B:389:ARG:HB3	2:B:390:PRO:HD2	2.00	0.42
1:C:280:SER:O	1:C:282:THR:HG23	2.19	0.42
1:A:411:TYR:CE2	1:A:417:PRO:HB3	2.54	0.42
1:A:525:ASP:HB2	1:A:526:THR:H	1.34	0.42
2:B:491:THR:HG22	2:B:492:VAL:H	1.84	0.42
2:B:352:ASN:HB3	2:B:586:GLN:O	2.20	0.42
2:B:198:ASN:OD1	2:B:200:TYR:N	2.51	0.42
1:C:175:SER:CB	1:C:311:THR:HA	2.47	0.42
1:A:564:PRO:HG3	1:A:630:PHE:CE2	2.54	0.42
2:B:621:ILE:CG2	2:B:629:SER:HB3	2.48	0.42
1:C:386:PRO:HG3	1:C:595:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:GLU:OE1	1:C:262:GLU:HA	2.19	0.42
1:C:451:TYR:O	1:C:453:SER:N	2.44	0.42
1:C:460:ASN:ND2	1:C:461:THR:H	2.17	0.42
2:B:395:ILE:HD11	2:B:510:ILE:CD1	2.49	0.42
1:A:457:ILE:HD11	1:A:460:ASN:HD21	1.85	0.42
1:A:463:PHE:O	1:A:463:PHE:CD1	2.72	0.42
1:A:350:ILE:HG13	1:A:350:ILE:O	2.18	0.42
1:C:210:ALA:HB3	1:C:324:LEU:N	2.24	0.42
1:A:197:LEU:CD1	1:A:215:ILE:HD12	2.45	0.42
2:B:630:PHE:CD1	2:B:630:PHE:N	2.88	0.42
2:B:193:LEU:HD11	2:B:215:ILE:HG12	2.01	0.42
2:B:318:PRO:HG2	2:B:319:ASP:H	1.84	0.42
2:B:219:PHE:CD2	2:B:312:VAL:HG22	2.54	0.42
2:B:463:PHE:O	2:B:465:SER:N	2.52	0.42
2:B:424:THR:O	2:B:465:SER:HB3	2.19	0.42
1:C:403:LEU:HD12	1:C:403:LEU:H	1.83	0.42
1:C:463:PHE:O	1:C:466:MET:HG2	2.19	0.42
1:C:607:ALA:HB3	1:C:623:ILE:CG1	2.49	0.42
2:B:178:TRP:HD1	2:B:182:GLU:HG3	1.83	0.42
1:C:374:PHE:CD2	1:C:380:THR:HB	2.54	0.42
1:C:162:VAL:C	1:C:164:SER:H	2.22	0.42
1:A:179:SER:C	1:A:181:SER:H	2.23	0.42
2:B:272:ARG:O	1:C:275:LEU:HD12	2.20	0.42
1:A:218:ARG:HB2	1:A:265:ILE:HG13	2.01	0.42
1:C:430:ILE:O	1:C:462:ASN:ND2	2.53	0.42
2:B:449:GLU:HA	2:B:449:GLU:OE2	2.20	0.42
2:B:463:PHE:HB3	2:B:466:MET:HE2	2.01	0.42
2:B:287:LEU:C	2:B:288:VAL:CG2	2.88	0.42
1:C:470:GLY:N	1:C:530:LEU:HD13	2.31	0.42
1:A:350:ILE:CD1	1:A:351:GLY:O	2.68	0.42
2:B:578:LYS:O	2:B:579:SER:CB	2.64	0.42
2:B:392:THR:HA	2:B:526:THR:H	1.83	0.42
2:B:187:ILE:HB	2:B:244:GLN:HE21	1.85	0.42
1:A:247:SER:C	1:A:249:LEU:N	2.70	0.42
2:B:535:ILE:HD11	2:B:538:GLU:O	2.19	0.42
2:B:237:PRO:HG2	2:B:240:ILE:HD11	2.01	0.42
1:C:507:LYS:N	1:C:508:ILE:HD13	2.34	0.42
1:A:341:LEU:CD1	1:A:590:THR:HG23	2.49	0.42
2:B:295:LEU:HD12	2:B:296:ILE:N	2.35	0.42
2:B:625:SER:O	2:B:627:GLY:N	2.53	0.42
1:A:469:CYS:O	1:A:485:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:THR:OG1	1:A:489:THR:N	2.51	0.42
2:B:395:ILE:HG21	2:B:523:SER:HB2	2.02	0.42
2:B:484:THR:OG1	2:B:511:PHE:O	2.21	0.42
2:B:370:ALA:HB1	2:B:381:ALA:HB3	2.02	0.42
2:B:416:ILE:HA	2:B:417:PRO:HD3	1.89	0.42
1:C:234:ILE:HD11	1:C:288:VAL:HB	2.02	0.42
1:C:234:ILE:CD1	1:C:288:VAL:HB	2.50	0.42
1:A:187:ILE:CD1	1:A:290:MET:HE3	2.50	0.42
1:C:599:TYR:N	1:C:599:TYR:CD1	2.87	0.42
1:C:340:ASP:O	1:C:340:ASP:CG	2.58	0.42
1:A:411:TYR:CE1	1:A:418:ASP:O	2.73	0.42
2:B:421:PRO:HB2	2:B:422:ASP:H	1.74	0.42
2:B:167:GLU:HA	2:B:316:PRO:HG2	2.01	0.42
1:C:368:PHE:CD1	1:C:547:VAL:HG21	2.55	0.42
2:B:155:ASP:O	2:B:156:MET:C	2.58	0.42
1:A:602:SER:HB2	1:A:605:SER:OG	2.19	0.42
1:A:496:LYS:O	1:A:497:LEU:HD23	2.20	0.42
2:B:612:ILE:HD11	2:B:644:THR:OG1	2.20	0.42
2:B:205:ALA:HA	2:B:322:PHE:HE2	1.84	0.42
1:A:280:SER:O	1:A:281:ASP:O	2.37	0.42
1:A:484:THR:HG21	1:A:512:GLN:HE22	1.85	0.42
2:B:201:LEU:HD22	2:B:320:PHE:CE2	2.55	0.42
1:C:255:LEU:N	1:C:255:LEU:HD12	2.34	0.42
1:C:473:GLN:HA	1:C:524:ASP:CG	2.40	0.42
1:C:425:ILE:HA	1:C:465:SER:OG	2.19	0.42
2:B:149:GLN:O	2:B:153:ALA:HB2	2.20	0.42
2:B:272:ARG:C	1:C:276:TYR:HE1	2.24	0.42
1:C:637:GLY:O	1:C:639:LEU:HD23	2.20	0.42
1:C:359:THR:O	1:C:360:ASP:HB2	2.21	0.41
1:A:476:TRP:CD1	1:A:520:VAL:CB	2.92	0.41
1:A:436:ALA:CB	1:A:461:THR:HA	2.49	0.41
2:B:428:GLU:HA	2:B:498:ILE:HA	2.01	0.41
1:C:393:VAL:HG11	1:C:406:GLY:O	2.19	0.41
1:C:519:ASP:O	1:C:519:ASP:CG	2.58	0.41
1:C:540:ILE:HB	1:C:582:VAL:HG22	2.02	0.41
2:B:192:SER:CA	2:B:286:SER:HB3	2.39	0.41
1:A:375:ASP:CG	1:A:376:PHE:H	2.23	0.41
2:B:613:ASP:HB2	2:B:640:GLU:O	2.20	0.41
2:B:264:VAL:CG1	2:B:265:ILE:N	2.83	0.41
1:A:251:TYR:CE1	2:B:325:LEU:O	2.72	0.41
1:A:344:LYS:HA	1:A:645:ALA:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:MET:HE2	2:B:512:GLN:N	2.34	0.41
2:B:373:HIS:ND1	2:B:586:GLN:NE2	2.68	0.41
2:B:466:MET:SD	2:B:486:PHE:HB3	2.59	0.41
2:B:187:ILE:HG23	2:B:288:VAL:CG1	2.50	0.41
1:A:233:ALA:HA	1:A:288:VAL:O	2.20	0.41
1:A:573:LEU:HA	1:A:573:LEU:HD23	1.61	0.41
1:C:641:PHE:N	1:C:642:PRO:CD	2.82	0.41
2:B:539:ALA:CB	2:B:583:PHE:HE1	2.33	0.41
2:B:448:LYS:HA	2:B:448:LYS:CE	2.47	0.41
2:B:191:GLN:HG2	2:B:197:LEU:CD2	2.50	0.41
1:C:458:SER:O	1:C:459:ASN:HB3	2.20	0.41
1:A:488:THR:O	1:A:509:ALA:HB3	2.20	0.41
1:A:405:ILE:HG21	1:A:509:ALA:CA	2.50	0.41
2:B:402:MET:CE	2:B:512:GLN:N	2.78	0.41
1:C:339:CYS:SG	1:C:649:GLY:CA	3.04	0.41
2:B:432:ALA:HB3	2:B:462:ASN:HB3	2.03	0.41
2:B:233:ALA:O	2:B:234:ILE:CG2	2.68	0.41
1:A:613:ASP:HB2	1:A:640:GLU:O	2.20	0.41
1:A:367:VAL:HG23	1:A:564:PRO:HB2	2.02	0.41
1:A:573:LEU:CG	1:A:580:ILE:HG23	2.47	0.41
2:B:338:PRO:HD3	2:B:599:TYR:HB3	2.01	0.41
1:C:130:ILE:N	1:C:130:ILE:HD13	2.29	0.41
1:C:185:GLY:HA2	1:C:290:MET:CG	2.50	0.41
2:B:530:LEU:HA	2:B:530:LEU:HD23	1.92	0.41
1:A:526:THR:C	1:A:527:LEU:HG	2.41	0.41
2:B:291:ILE:H	2:B:291:ILE:HG12	1.52	0.41
1:C:490:ALA:HB1	1:C:499:PRO:HA	2.02	0.41
1:C:212:SER:O	1:C:320:PHE:HA	2.20	0.41
2:B:618:TRP:CD1	2:B:660:ASN:HB2	2.54	0.41
2:B:605:SER:HB3	2:B:651:GLN:O	2.21	0.41
1:A:198:ASN:HB2	1:A:314:THR:OG1	2.21	0.41
2:B:497:LEU:O	2:B:498:ILE:O	2.38	0.41
1:A:399:GLU:HA	1:A:516:VAL:HB	2.02	0.41
1:A:234:ILE:CG2	1:A:253:HIS:HB3	2.51	0.41
1:A:253:HIS:N	1:A:253:HIS:HD1	2.19	0.41
1:C:484:THR:CG2	1:C:485:ALA:H	2.27	0.41
1:C:423:THR:HG22	1:C:546:LYS:O	2.21	0.41
1:C:583:PHE:HB3	1:C:584:ASN:H	1.65	0.41
1:A:565:ILE:CD1	1:A:566:PHE:N	2.79	0.41
1:A:190:LYS:CD	1:A:651:GLN:HE22	2.33	0.41
1:C:555:GLU:CD	1:C:555:GLU:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:ILE:HG12	2:B:440:GLN:N	2.36	0.41
1:A:415:GLY:O	1:A:416:ILE:C	2.59	0.41
2:B:483:ASN:O	2:B:484:THR:O	2.39	0.41
2:B:251:TYR:CD2	2:B:252:PRO:HD2	2.55	0.41
2:B:534:GLY:HA2	2:B:573:LEU:HD22	2.03	0.41
2:B:208:TYR:CD2	2:B:322:PHE:HB3	2.56	0.41
1:A:388:PHE:HE1	1:A:588:LEU:HD13	1.85	0.41
1:A:361:PHE:HE1	1:A:619:PHE:HZ	1.68	0.41
1:C:451:TYR:O	1:C:456:ILE:HG12	2.21	0.41
2:B:449:GLU:CB	2:B:452:GLU:CD	2.89	0.41
1:A:437:ILE:HD12	1:A:439:ASN:O	2.21	0.41
1:A:440:GLN:H	1:A:440:GLN:HG3	1.70	0.41
2:B:166:TRP:CD1	2:B:200:TYR:CD2	3.09	0.41
1:C:151:SER:HA	1:C:154:ALA:HB3	2.03	0.41
2:B:188:LEU:O	2:B:189:PHE:HB2	2.21	0.41
1:A:287:LEU:HD21	1:A:289:ILE:HD11	2.03	0.41
1:C:383:TRP:O	1:C:413:VAL:HG21	2.21	0.41
1:C:140:GLY:O	1:C:141:GLY:O	2.38	0.41
1:A:565:ILE:HG21	1:A:631:VAL:CG2	2.50	0.41
2:B:620:ASP:O	2:B:621:ILE:HD12	2.21	0.41
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.66	0.41
1:C:445:ILE:C	1:C:447:THR:H	2.06	0.41
1:A:394:THR:O	1:A:395:ILE:HG23	2.21	0.41
1:A:371:ASN:C	1:A:373:HIS:H	2.24	0.41
1:A:413:VAL:O	1:A:415:GLY:N	2.54	0.41
2:B:374:PHE:HA	2:B:380:THR:HB	2.02	0.41
1:C:408:ALA:CB	1:C:411:TYR:HD2	2.33	0.41
1:C:481:VAL:O	1:C:481:VAL:CG1	2.68	0.41
1:C:472:LEU:HD22	1:C:473:GLN:N	2.36	0.41
1:C:367:VAL:HG13	1:C:566:PHE:CZ	2.55	0.41
1:C:584:ASN:HA	1:C:584:ASN:HD22	1.69	0.41
1:A:331:MET:H	1:C:243:ILE:HD11	1.86	0.41
2:B:309:ILE:HG13	2:B:310:VAL:N	2.35	0.41
1:A:342:ILE:HG12	1:A:343:PRO:N	2.35	0.41
1:C:297:ASN:HA	1:C:298:PRO:HD3	1.95	0.41
1:A:275:LEU:HB2	1:A:276:TYR:CD2	2.56	0.41
2:B:353:ARG:HH21	2:B:422:ASP:HB3	1.85	0.41
1:A:131:THR:OG1	1:C:255:LEU:CB	2.66	0.41
2:B:287:LEU:CD1	2:B:288:VAL:N	2.82	0.41
1:C:516:VAL:CG1	1:C:520:VAL:HG21	2.51	0.41
1:A:173:HIS:O	1:A:173:HIS:CD2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ILE:HD12	1:C:296:ILE:C	2.40	0.41
1:C:249:LEU:C	1:C:251:TYR:N	2.74	0.41
1:C:245:SER:OG	1:C:246:THR:N	2.54	0.41
1:C:179:SER:HB3	1:C:182:GLU:CD	2.41	0.41
1:C:224:SER:O	1:C:226:VAL:N	2.54	0.41
1:C:437:ILE:HD12	1:C:438:THR:N	2.36	0.40
2:B:395:ILE:HD11	2:B:510:ILE:HD11	2.02	0.40
2:B:590:THR:O	2:B:591:SER:C	2.60	0.40
1:C:151:SER:O	1:C:152:ALA:C	2.60	0.40
2:B:190:LYS:HA	2:B:288:VAL:HG13	2.03	0.40
1:C:535:ILE:CD1	1:C:546:LYS:NZ	2.81	0.40
1:C:621:ILE:HA	1:C:621:ILE:HD13	1.87	0.40
1:A:339:CYS:SG	1:A:649:GLY:HA2	2.60	0.40
2:B:265:ILE:HG22	2:B:266:PHE:N	2.35	0.40
1:A:403:LEU:HD12	1:A:512:GLN:HG3	2.03	0.40
2:B:383:TRP:CD1	2:B:384:SER:OG	2.65	0.40
1:C:189:PHE:C	1:C:191:GLN:H	2.25	0.40
2:B:189:PHE:HB3	2:B:289:ILE:HD13	2.01	0.40
1:A:189:PHE:CE2	1:A:191:GLN:CB	3.02	0.40
2:B:151:SER:O	2:B:153:ALA:N	2.55	0.40
1:A:613:ASP:HA	1:A:643:LEU:HD23	2.03	0.40
1:C:350:ILE:HA	1:C:356:SER:O	2.22	0.40
1:A:473:GLN:CB	1:A:482:SER:HA	2.41	0.40
1:A:219:PHE:CD2	1:A:219:PHE:O	2.75	0.40
2:B:278:LEU:O	2:B:280:SER:N	2.55	0.40
1:A:236:VAL:HG22	1:A:286:SER:O	2.22	0.40
2:B:256:PHE:HD2	2:B:257:ASP:H	1.68	0.40
1:A:251:TYR:HE1	2:B:325:LEU:O	2.05	0.40
1:C:588:LEU:C	1:C:588:LEU:HD23	2.41	0.40
2:B:604:ASP:O	2:B:652:LEU:HG	2.21	0.40
2:B:272:ARG:C	1:C:276:TYR:CE1	2.94	0.40
1:A:198:ASN:HA	1:A:199:PRO:HD2	1.89	0.40
1:A:411:TYR:CD2	1:A:417:PRO:HA	2.56	0.40
2:B:399:GLU:OE1	2:B:399:GLU:HA	2.20	0.40
1:C:337:VAL:HG12	1:C:339:CYS:H	1.87	0.40
1:A:215:ILE:HG23	1:A:315:LYS:O	2.22	0.40
1:C:374:PHE:HZ	1:C:386:PRO:HD3	1.87	0.40
1:A:387:ARG:HB3	1:A:388:PHE:H	1.76	0.40
1:A:299:TYR:CD1	1:A:299:TYR:N	2.89	0.40
1:A:165:GLU:O	1:A:169:PHE:HE2	2.05	0.40
1:A:310:VAL:CG1	1:A:311:THR:N	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:SER:O	2:B:592:ARG:C	2.59	0.40
1:C:285:THR:CG2	1:C:286:SER:N	2.84	0.40
1:A:227:PHE:CE1	1:A:308:CYS:HB2	2.56	0.40
1:C:264:VAL:C	1:C:265:ILE:HG13	2.42	0.40
2:B:214:SER:N	2:B:319:ASP:OD2	2.55	0.40
2:B:248:MET:C	2:B:250:GLN:N	2.75	0.40
1:A:176:VAL:CG1	1:A:188:LEU:HD22	2.50	0.40
2:B:219:PHE:CE2	2:B:312:VAL:HG22	2.57	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:TYR:CE1	1:C:299:TYR:OH[2_555]	1.77	0.43
2:B:299:TYR:CD1	1:C:299:TYR:CZ[2_555]	1.97	0.23
2:B:229:GLY:N	1:C:222:SER:OG[2_555]	2.06	0.14
2:B:292:TYR:OH	1:C:313:GLU:OE1[2_555]	2.07	0.13
2:B:252:PRO:N	1:C:169:PHE:CE1[2_555]	2.10	0.10
1:C:480:LYS:CG	1:C:575:TYR:CD1[2_555]	2.17	0.03
2:B:299:TYR:CD1	1:C:299:TYR:OH[2_555]	2.18	0.02

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	532/534 (100%)	310 (58%)	147 (28%)	75 (14%)	0 3
1	C	532/534 (100%)	332 (62%)	126 (24%)	74 (14%)	0 3
2	B	528/530 (100%)	321 (61%)	132 (25%)	75 (14%)	0 3
All	All	1592/1598 (100%)	963 (60%)	405 (25%)	224 (14%)	0 3

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	145	GLU
1	A	146	PRO
1	A	151	SER
1	A	279	MET
1	A	280	SER
1	A	281	ASP
1	A	300	ALA
1	A	303	SER
1	A	305	SER
1	A	340	ASP
1	A	341	LEU
1	A	347	SER
1	A	350	ILE
1	A	457	ILE
1	A	461	THR
1	A	473	GLN
1	A	475	ALA
1	A	479	LYS
1	A	481	VAL
1	A	482	SER
1	A	484	THR
1	A	513	ASP
1	A	525	ASP
1	A	526	THR
1	A	534	GLY
1	A	580	ILE
2	B	142	VAL
2	B	147	SER
2	B	148	VAL
2	B	149	GLN
2	B	274	THR
2	B	298	PRO
2	B	302	ASP
2	B	340	ASP
2	B	399	GLU
2	B	401	GLU
2	B	402	MET
2	B	407	VAL
2	B	421	PRO
2	B	429	LEU
2	B	440	GLN
2	B	450	GLU

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Mol	Chain	Res	Type
2	B	453	SER
2	B	475	ALA
2	B	481	VAL
2	B	484	THR
2	B	517	ASN
2	B	518	ARG
2	B	520	VAL
2	B	523	SER
2	B	580	ILE
2	B	625	SER
2	B	658	ALA
1	C	134	GLU
1	C	146	PRO
1	C	149	GLN
1	C	294	ASP
1	C	300	ALA
1	C	301	ASN
1	C	303	SER
1	C	305	SER
1	C	340	ASP
1	C	345	SER
1	C	347	SER
1	C	350	ILE
1	C	421	PRO
1	C	434	ASP
1	C	438	THR
1	C	439	ASN
1	C	449	GLU
1	C	474	ARG
1	C	481	VAL
1	C	482	SER
1	C	505	GLN
1	C	523	SER
1	C	524	ASP
1	C	534	GLY
1	C	576	VAL
1	C	580	ILE
1	C	583	PHE
1	A	148	VAL
1	A	149	GLN
1	A	162	VAL
1	A	168	ALA

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Mol	Chain	Res	Type
1	A	244	GLN
1	A	346	SER
1	A	371	ASN
1	A	437	ILE
1	A	447	THR
1	A	455	MET
1	A	460	ASN
1	A	462	ASN
1	A	485	ALA
1	A	515	HIS
1	A	522	THR
1	A	558	ALA
1	A	592	ARG
1	A	637	GLY
2	B	150	MET
2	B	259	ARG
2	B	261	VAL
2	B	338	PRO
2	B	341	LEU
2	B	355	TRP
2	B	360	ASP
2	B	394	THR
2	B	408	ALA
2	B	433	GLY
2	B	445	ILE
2	B	457	ILE
2	B	460	ASN
2	B	464	LYS
2	B	485	ALA
2	B	498	ILE
2	B	524	ASP
2	B	526	THR
2	B	575	TYR
2	B	577	ILE
2	B	589	HIS
1	C	141	GLY
1	C	159	GLY
1	C	185	GLY
1	C	227	PHE
1	C	247	SER
1	C	322	PHE
1	C	323	HIS

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Mol	Chain	Res	Type
1	C	355	TRP
1	C	400	GLY
1	C	405	ILE
1	C	433	GLY
1	C	460	ASN
1	C	463	PHE
1	C	475	ALA
1	C	479	LYS
1	C	483	ASN
1	C	516	VAL
1	C	577	ILE
1	A	137	THR
1	A	158	THR
1	A	184	GLN
1	A	301	ASN
1	A	328	PRO
1	A	414	PRO
1	A	449	GLU
1	A	494	GLU
1	A	498	ILE
1	A	505	GLN
1	A	510	ILE
1	A	527	LEU
1	A	535	ILE
1	A	551	GLY
2	B	152	ALA
2	B	285	THR
2	B	328	PRO
2	B	359	THR
2	B	369	GLN
2	B	409	THR
2	B	414	PRO
2	B	449	GLU
2	B	452	GLU
2	B	461	THR
2	B	494	GLU
2	B	616	GLY
1	C	281	ASP
1	C	408	ALA
1	C	432	ALA
1	C	540	ILE
1	C	584	ASN

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Mol	Chain	Res	Type
1	C	606	PHE
1	C	641	PHE
1	A	166	TRP
1	A	349	TRP
1	A	370	ALA
1	A	478	ASN
1	A	480	LYS
2	B	249	LEU
2	B	276	TYR
2	B	410	ASP
1	C	151	SER
1	C	167	GLU
1	C	197	LEU
1	C	260	GLN
1	C	448	LYS
1	C	462	ASN
1	C	558	ALA
1	A	409	THR
1	A	435	TYR
1	A	448	LYS
1	A	476	TRP
1	A	537	GLU
2	B	165	GLU
2	B	305	SER
2	B	321	LYS
2	B	339	CYS
2	B	358	ILE
2	B	424	THR
2	B	487	ILE
2	B	519	ASP
1	C	386	PRO
1	C	412	ILE
1	C	428	GLU
1	C	437	ILE
1	C	488	THR
1	C	603	PRO
1	C	616	GLY
2	B	189	PHE
2	B	378	GLN
1	C	445	ILE
1	C	510	ILE
1	A	298	PRO

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Mol	Chain	Res	Type
1	A	577	ILE
2	B	603	PRO
1	C	535	ILE
1	A	130	ILE
1	A	139	VAL
1	A	335	GLY
2	B	162	VAL
1	C	130	ILE
1	C	551	GLY
1	C	225	GLY
1	C	431	PRO
1	A	603	PRO
1	C	661	ILE

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	461/461 (100%)	370 (80%)	91 (20%)	1	8
1	C	461/461 (100%)	377 (82%)	84 (18%)	2	11
2	B	457/457 (100%)	354 (78%)	103 (22%)	1	5
All	All	1379/1379 (100%)	1101 (80%)	278 (20%)	1	7

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	PRO
1	A	134	GLU
1	A	135	GLN
1	A	137	THR
1	A	142	VAL
1	A	145	GLU
1	A	155	ASP
1	A	158	THR
1	A	162	VAL

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Mol	Chain	Res	Type
1	A	167	GLU
1	A	170	PHE
1	A	172	PHE
1	A	175	SER
1	A	196	LEU
1	A	202	THR
1	A	203	HIS
1	A	219	PHE
1	A	231	LEU
1	A	234	ILE
1	A	235	VAL
1	A	245	SER
1	A	262	GLU
1	A	267	THR
1	A	277	HIS
1	A	278	LEU
1	A	287	LEU
1	A	288	VAL
1	A	291	ILE
1	A	292	TYR
1	A	325	LEU
1	A	328	PRO
1	A	340	ASP
1	A	341	LEU
1	A	342	ILE
1	A	350	ILE
1	A	357	ASP
1	A	363	ILE
1	A	368	PHE
1	A	369	GLN
1	A	371	ASN
1	A	380	THR
1	A	385	THR
1	A	392	THR
1	A	395	ILE
1	A	397	GLN
1	A	405	ILE
1	A	409	THR
1	A	418	ASP
1	A	420	TRP
1	A	422	ASP
1	A	444	ASP

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Mol	Chain	Res	Type
1	A	446	GLN
1	A	447	THR
1	A	453	SER
1	A	459	ASN
1	A	462	ASN
1	A	474	ARG
1	A	480	LYS
1	A	489	THR
1	A	498	ILE
1	A	504	ASP
1	A	506	THR
1	A	511	PHE
1	A	519	ASP
1	A	520	VAL
1	A	524	ASP
1	A	525	ASP
1	A	527	LEU
1	A	529	LEU
1	A	537	GLU
1	A	543	ASP
1	A	545	GLU
1	A	550	ILE
1	A	552	VAL
1	A	566	PHE
1	A	571	MET
1	A	573	LEU
1	A	579	SER
1	A	580	ILE
1	A	594	LEU
1	A	598	ASN
1	A	599	TYR
1	A	602	SER
1	A	604	ASP
1	A	614	SER
1	A	620	ASP
1	A	626	ASP
1	A	636	ILE
1	A	641	PHE
1	A	647	TYR
1	A	661	ILE
2	B	137	THR
2	B	143	ILE

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Mol	Chain	Res	Type
2	B	148	VAL
2	B	149	GLN
2	B	155	ASP
2	B	165	GLU
2	B	180	THR
2	B	181	SER
2	B	221	ILE
2	B	222	SER
2	B	241	GLU
2	B	246	THR
2	B	254	VAL
2	B	256	PHE
2	B	265	ILE
2	B	266	PHE
2	B	277	HIS
2	B	279	MET
2	B	280	SER
2	B	286	SER
2	B	291	ILE
2	B	299	TYR
2	B	314	THR
2	B	331	MET
2	B	332	LEU
2	B	339	CYS
2	B	348	LEU
2	B	354	PHE
2	B	357	ASP
2	B	360	ASP
2	B	361	PHE
2	B	363	ILE
2	B	366	PHE
2	B	368	PHE
2	B	369	GLN
2	B	371	ASN
2	B	378	GLN
2	B	380	THR
2	B	384	SER
2	B	385	THR
2	B	388	PHE
2	B	392	THR
2	B	397	GLN
2	B	398	LYS

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Mol	Chain	Res	Type
2	B	401	GLU
2	B	402	MET
2	B	405	ILE
2	B	407	VAL
2	B	412	ILE
2	B	425	ILE
2	B	435	TYR
2	B	438	THR
2	B	444	ASP
2	B	446	GLN
2	B	447	THR
2	B	448	LYS
2	B	449	GLU
2	B	453	SER
2	B	456	ILE
2	B	458	SER
2	B	460	ASN
2	B	463	PHE
2	B	471	SER
2	B	481	VAL
2	B	487	ILE
2	B	489	THR
2	B	494	GLU
2	B	498	ILE
2	B	501	ASN
2	B	502	THR
2	B	508	ILE
2	B	511	PHE
2	B	512	GLN
2	B	513	ASP
2	B	519	ASP
2	B	523	SER
2	B	527	LEU
2	B	543	ASP
2	B	550	ILE
2	B	566	PHE
2	B	569	ASN
2	B	571	MET
2	B	575	TYR
2	B	586	GLN
2	B	589	HIS
2	B	591	SER

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Mol	Chain	Res	Type
2	B	598	ASN
2	B	602	SER
2	B	604	ASP
2	B	611	ILE
2	B	617	SER
2	B	619	PHE
2	B	623	ILE
2	B	624	ASP
2	B	626	ASP
2	B	636	ILE
2	B	638	LYS
2	B	639	LEU
2	B	644	THR
2	B	647	TYR
2	B	652	LEU
2	B	660	ASN
2	B	661	ILE
1	C	129	SER
1	C	130	ILE
1	C	138	THR
1	C	143	ILE
1	C	146	PRO
1	C	150	MET
1	C	163	ASP
1	C	165	GLU
1	C	169	PHE
1	C	180	THR
1	C	183	THR
1	C	192	SER
1	C	202	THR
1	C	207	LEU
1	C	209	VAL
1	C	212	SER
1	C	219	PHE
1	C	221	ILE
1	C	243	ILE
1	C	246	THR
1	C	256	PHE
1	C	265	ILE
1	C	266	PHE
1	C	270	ASP
1	C	274	THR

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	297	ASN
1	C	299	TYR
1	C	302	ASP
1	C	323	HIS
1	C	336	SER
1	C	344	LYS
1	C	348	LEU
1	C	357	ASP
1	C	358	ILE
1	C	363	ILE
1	C	364	ARG
1	C	369	GLN
1	C	376	PHE
1	C	384	SER
1	C	391	ILE
1	C	394	THR
1	C	399	GLU
1	C	401	GLU
1	C	402	MET
1	C	403	LEU
1	C	410	ASP
1	C	413	VAL
1	C	418	ASP
1	C	438	THR
1	C	450	GLU
1	C	453	SER
1	C	455	MET
1	C	456	ILE
1	C	458	SER
1	C	473	GLN
1	C	478	ASN
1	C	489	THR
1	C	508	ILE
1	C	516	VAL
1	C	520	VAL
1	C	521	GLN
1	C	523	SER
1	C	524	ASP
1	C	526	THR
1	C	527	LEU
1	C	537	GLU

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Mol	Chain	Res	Type
1	C	543	ASP
1	C	549	ARG
1	C	550	ILE
1	C	555	GLU
1	C	569	ASN
1	C	572	LYS
1	C	580	ILE
1	C	584	ASN
1	C	591	SER
1	C	598	ASN
1	C	624	ASP
1	C	636	ILE
1	C	639	LEU
1	C	641	PHE
1	C	647	TYR
1	C	650	ASN
1	C	661	ILE

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

Mol	Chain	Res	Type
1	A	173	HIS
1	A	184	GLN
1	A	191	GLN
1	A	203	HIS
1	A	260	GLN
1	A	277	HIS
1	A	293	ASN
1	A	297	ASN
1	A	304	ASN
1	A	323	HIS
1	A	352	ASN
1	A	371	ASN
1	A	377	ASN
1	A	397	GLN
1	A	440	GLN
1	A	443	ASN
1	A	459	ASN
1	A	460	ASN
1	A	478	ASN
1	A	514	ASN
1	A	521	GLN

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Mol	Chain	Res	Type
1	A	569	ASN
1	A	584	ASN
1	A	593	GLN
1	A	598	ASN
2	B	135	GLN
2	B	149	GLN
2	B	191	GLN
2	B	277	HIS
2	B	293	ASN
2	B	304	ASN
2	B	369	GLN
2	B	378	GLN
2	B	397	GLN
2	B	443	ASN
2	B	473	GLN
2	B	514	ASN
2	B	569	ASN
2	B	584	ASN
2	B	586	GLN
2	B	598	ASN
1	C	135	GLN
1	C	173	HIS
1	C	191	GLN
1	C	244	GLN
1	C	297	ASN
1	C	334	HIS
1	C	352	ASN
1	C	371	ASN
1	C	397	GLN
1	C	427	ASN
1	C	439	ASN
1	C	443	ASN
1	C	462	ASN
1	C	505	GLN
1	C	514	ASN
1	C	521	GLN
1	C	569	ASN
1	C	584	ASN
1	C	589	HIS
1	C	598	ASN
1	C	650	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	534/534 (100%)	0.89	67 (12%) 5 5	48, 97, 120, 143	0
1	C	534/534 (100%)	1.07	88 (16%) 2 2	49, 95, 113, 123	0
2	B	530/530 (100%)	1.03	93 (17%) 2 2	48, 97, 112, 129	0
All	All	1598/1598 (100%)	1.00	248 (15%) 3 3	48, 96, 115, 143	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	522	THR	8.2
1	C	146	PRO	7.4
1	A	447	THR	7.0
1	A	450	GLU	6.4
2	B	451	TYR	6.4
2	B	412	ILE	6.2
1	C	450	GLU	6.0
2	B	475	ALA	6.0
1	A	452	GLU	5.9
1	A	386	PRO	5.9
1	A	451	TYR	5.8
1	C	514	ASN	5.6
1	A	308	CYS	5.6
2	B	522	THR	5.6
1	C	482	SER	5.5
1	A	435	TYR	5.4
2	B	439	ASN	5.4
2	B	450	GLU	5.4
2	B	503	ILE	5.3
1	C	447	THR	5.3
2	B	409	THR	5.2
2	B	449	GLU	5.2
1	C	345	SER	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	339	CYS	5.2
1	C	426	PRO	5.2
1	A	438	THR	5.0
1	C	344	LYS	5.0
2	B	410	ASP	5.0
1	A	441	SER	4.8
1	C	449	GLU	4.8
2	B	514	ASN	4.7
2	B	445	ILE	4.6
1	A	163	ASP	4.5
2	B	448	LYS	4.5
2	B	348	LEU	4.5
1	A	449	GLU	4.5
2	B	133	PRO	4.4
1	A	445	ILE	4.4
2	B	500	SER	4.3
1	A	303	SER	4.3
1	C	647	TYR	4.3
2	B	581	ASP	4.3
2	B	301	ASN	4.2
2	B	593	GLN	4.2
1	C	431	PRO	4.2
1	C	476	TRP	4.1
1	C	522	THR	4.1
1	A	448	LYS	4.1
1	C	161	SER	4.1
1	C	520	VAL	4.1
2	B	519	ASP	4.0
1	A	305	SER	4.0
2	B	552	VAL	4.0
1	A	517	ASN	4.0
1	C	305	SER	4.0
1	A	397	GLN	4.0
1	A	521	GLN	4.0
2	B	458	SER	3.9
1	A	307	GLY	3.9
1	C	441	SER	3.9
1	C	304	ASN	3.8
1	C	459	ASN	3.8
1	C	445	ILE	3.7
1	C	145	GLU	3.7
2	B	378	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	644	THR	3.7
1	C	534	GLY	3.7
1	A	476	TRP	3.6
2	B	644	THR	3.6
2	B	479	LYS	3.6
1	C	458	SER	3.6
1	A	409	THR	3.6
2	B	604	ASP	3.5
1	C	156	MET	3.5
1	C	519	ASP	3.5
1	A	396	SER	3.5
1	C	159	GLY	3.5
1	C	552	VAL	3.4
2	B	386	PRO	3.4
1	C	349	TRP	3.4
1	C	640	GLU	3.4
2	B	440	GLN	3.4
1	A	593	GLN	3.4
1	C	637	GLY	3.4
1	A	428	GLU	3.4
2	B	510	ILE	3.3
1	A	399	GLU	3.3
2	B	560	GLY	3.3
2	B	476	TRP	3.3
1	C	410	ASP	3.2
1	A	635	SER	3.2
1	C	615	ASN	3.2
1	A	437	ILE	3.2
1	A	638	LYS	3.2
2	B	542	ALA	3.1
1	C	216	GLU	3.1
1	A	597	ASN	3.1
1	C	600	LEU	3.1
1	A	304	ASN	3.1
2	B	437	ILE	3.1
2	B	526	THR	3.0
2	B	541	GLY	3.0
1	C	634	SER	3.0
1	C	343	PRO	3.0
2	B	614	SER	3.0
1	A	514	ASN	3.0
1	C	502	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	533	THR	3.0
1	A	410	ASP	2.9
1	A	516	VAL	2.9
1	A	552	VAL	2.9
2	B	478	ASN	2.9
1	C	537	GLU	2.9
2	B	447	THR	2.9
1	C	614	SER	2.9
2	B	142	VAL	2.9
2	B	260	GLN	2.9
1	A	398	LYS	2.9
2	B	340	ASP	2.9
1	C	405	ILE	2.9
1	C	638	LYS	2.8
1	A	575	TYR	2.8
1	A	453	SER	2.8
1	C	518	ARG	2.8
1	C	578	LYS	2.8
2	B	577	ILE	2.8
2	B	415	GLY	2.8
1	C	596	LEU	2.8
1	C	435	TYR	2.7
1	A	471	SER	2.7
1	C	512	GLN	2.7
1	A	499	PRO	2.7
2	B	385	THR	2.7
2	B	418	ASP	2.7
1	A	440	GLN	2.7
1	C	483	ASN	2.7
2	B	624	ASP	2.6
1	C	416	ILE	2.6
1	C	650	ASN	2.6
1	C	639	LEU	2.6
1	A	299	TYR	2.6
1	A	637	GLY	2.6
1	C	503	ILE	2.6
2	B	454	ALA	2.6
2	B	550	ILE	2.6
1	A	525	ASP	2.6
2	B	602	SER	2.6
2	B	408	ALA	2.6
1	C	403	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	459	ASN	2.5
2	B	192	SER	2.5
2	B	642	PRO	2.5
1	C	438	THR	2.5
2	B	474	ARG	2.5
1	C	444	ASP	2.5
2	B	629	SER	2.5
1	A	408	ALA	2.4
1	A	647	TYR	2.4
1	C	629	SER	2.4
1	A	455	MET	2.4
1	C	306	SER	2.4
1	C	517	ASN	2.4
2	B	517	ASN	2.4
1	C	499	PRO	2.4
2	B	551	GLY	2.4
1	C	532	TYR	2.4
2	B	435	TYR	2.4
2	B	369	GLN	2.4
1	A	578	LYS	2.4
1	A	662	ARG	2.4
2	B	349	TRP	2.4
1	C	408	ALA	2.4
2	B	403	LEU	2.4
2	B	360	ASP	2.3
1	C	342	ILE	2.3
1	A	640	GLU	2.3
2	B	428	GLU	2.3
1	C	498	ILE	2.3
1	C	434	ASP	2.3
1	A	489	THR	2.3
1	C	412	ILE	2.3
1	A	323	HIS	2.3
1	C	589	HIS	2.3
2	B	444	ASP	2.3
1	A	532	TYR	2.3
1	C	451	TYR	2.3
1	A	658	ALA	2.3
1	C	400	GLY	2.3
1	C	570	SER	2.3
2	B	294	ASP	2.3
2	B	141	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	654	LYS	2.3
2	B	496	LYS	2.3
1	C	521	GLN	2.2
2	B	345	SER	2.2
2	B	605	SER	2.2
1	A	434	ASP	2.2
1	A	406	GLY	2.2
1	A	331	MET	2.2
2	B	157	ALA	2.2
2	B	434	ASP	2.2
2	B	361	PHE	2.2
2	B	303	SER	2.2
1	A	642	PRO	2.2
2	B	242	PRO	2.2
2	B	531	GLY	2.2
2	B	350	ILE	2.2
1	C	544	ARG	2.2
1	C	275	LEU	2.2
2	B	362	VAL	2.2
1	A	537	GLU	2.2
2	B	377	ASN	2.2
2	B	305	SER	2.2
1	A	242	PRO	2.2
1	C	332	LEU	2.2
2	B	561	GLY	2.2
1	C	130	ILE	2.2
1	C	286	SER	2.1
1	A	620	ASP	2.1
2	B	515	HIS	2.1
2	B	459	ASN	2.1
1	C	616	GLY	2.1
1	C	139	VAL	2.1
1	C	478	ASN	2.1
1	A	529	LEU	2.1
1	C	369	GLN	2.1
1	A	547	VAL	2.1
1	C	437	ILE	2.1
2	B	637	GLY	2.1
1	C	662	ARG	2.1
1	C	541	GLY	2.1
2	B	363	ILE	2.0
1	A	439	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	643	LEU	2.0
2	B	374	PHE	2.0
2	B	598	ASN	2.0
2	B	534	GLY	2.0
2	B	421	PRO	2.0
2	B	396	SER	2.0
1	C	467	TYR	2.0
1	C	358	ILE	2.0
2	B	464	LYS	2.0
2	B	597	ASN	2.0
1	C	393	VAL	2.0
2	B	585	SER	2.0
2	B	468	ILE	2.0
1	C	325	LEU	2.0
2	B	606	PHE	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.