



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:02 AM GMT

PDB ID : 3KLS
Title : Structure of complement C5 in complex with SSL7
Authors : Laursen, N.S.; Gordon, N.; Hermans, S.; Lorenz, N.; Jackson, N.; Wines, B.;
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Jensen, L.; Fraser, J.D.; Andersen, G.R.
Deposited on : 2009-11-09
Resolution : 3.60 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

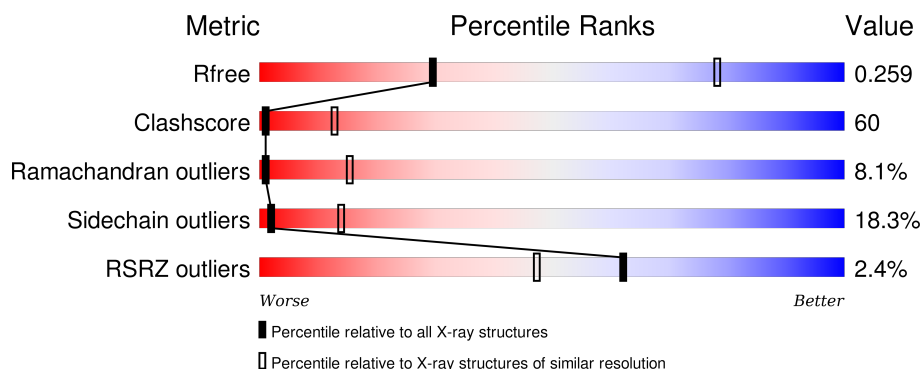
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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	1676	<div> <div>2%</div> <div>25% 53% 17% . .</div> </div>
1	B	1676	<div> <div>%</div> <div>23% 48% 16% • 12%</div> </div>
2	X	231	<div> <div>8%</div> <div>29% 42% 10% • 17%</div> </div>
2	Y	231	<div> <div>6%</div> <div>29% 42% 10% • 17%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 27683 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1622	Total	C	N	O	S	0	0	0
			12836	8224	2107	2452	53			
1	B	1478	Total	C	N	O	S	0	0	0
			11676	7478	1926	2226	46			

- Molecule 2 is a protein called Exotoxin 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			
2	Y	191	Total	C	N	O	S	0	0	0
			1539	965	267	306	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	35	GLY	GLU	ENGINEERED	UNP Q6GJP2
Y	35	GLY	GLU	ENGINEERED	UNP Q6GJP2

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Cd	0	0
			4	4		
3	A	5	Total	Cd	0	0
			5	5		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

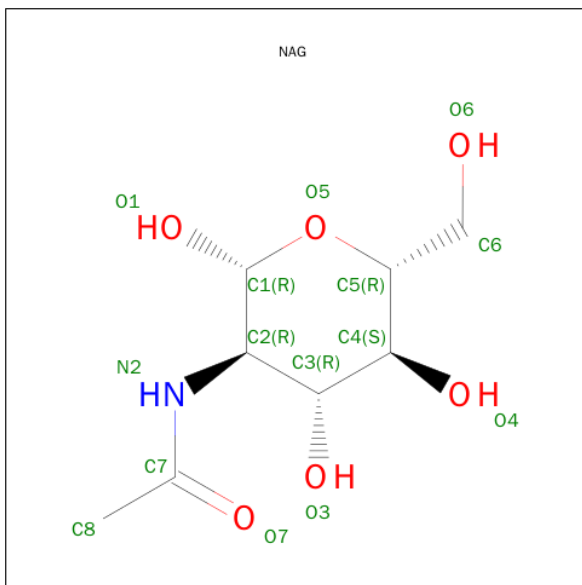
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

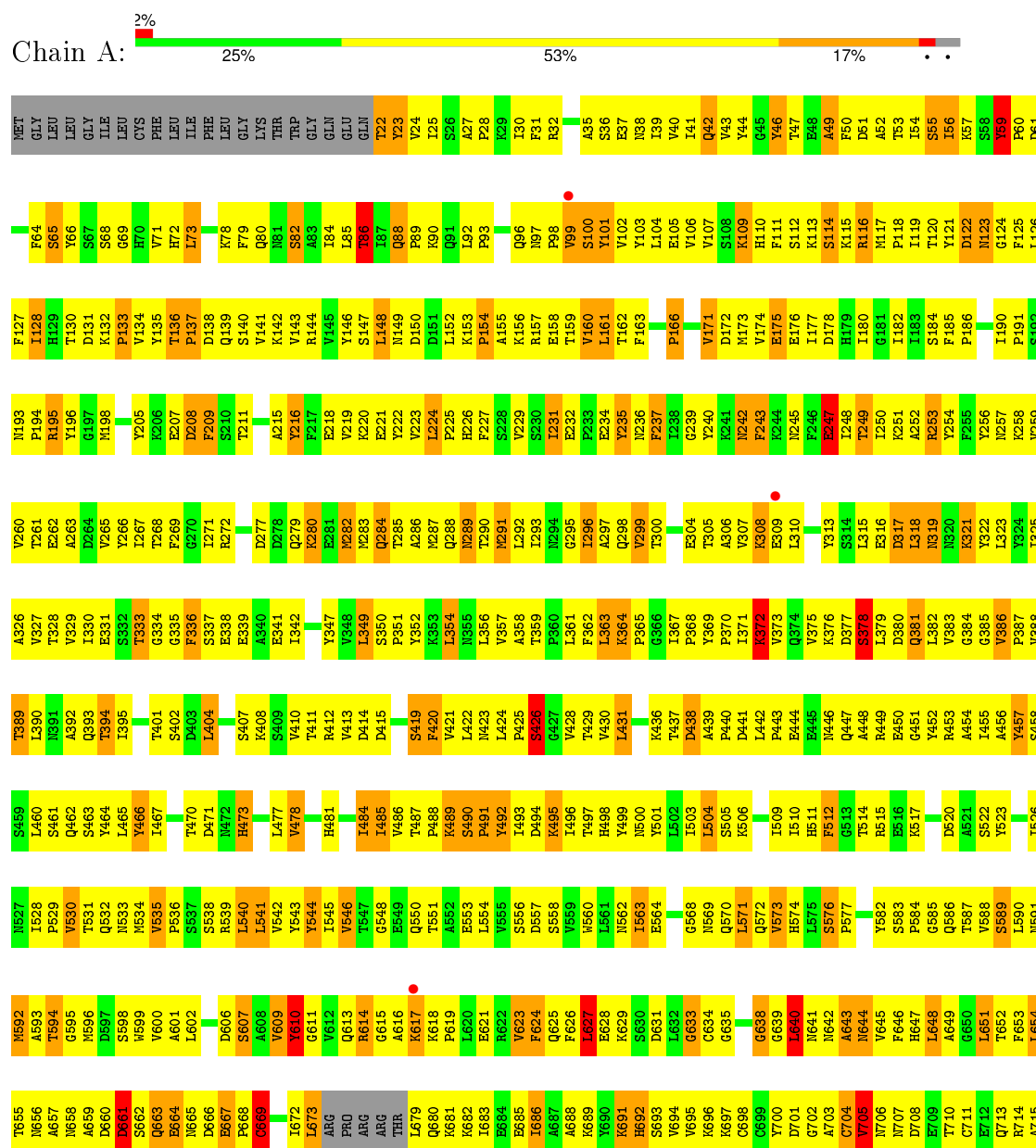


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

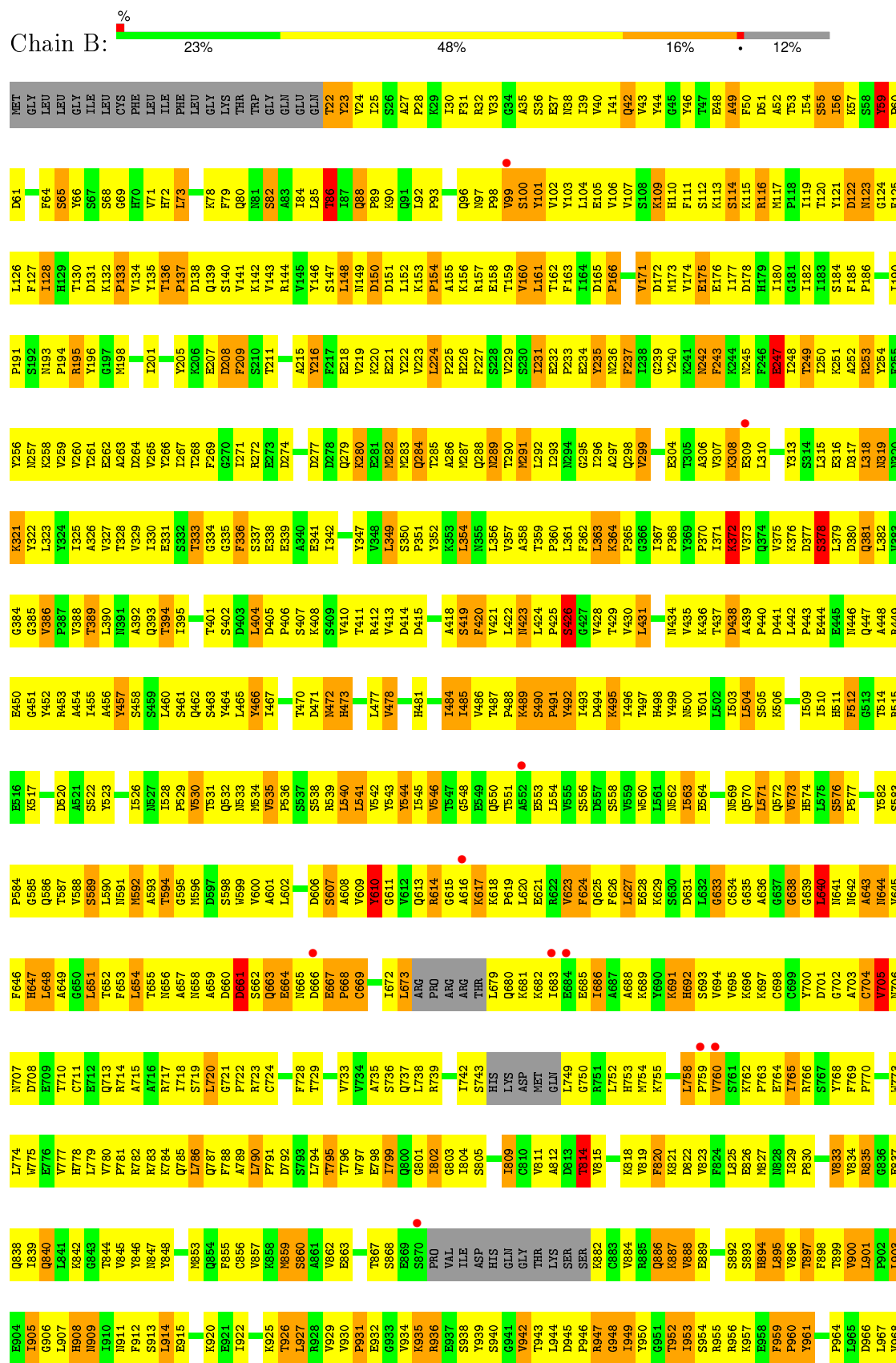
3 Residue-property plots

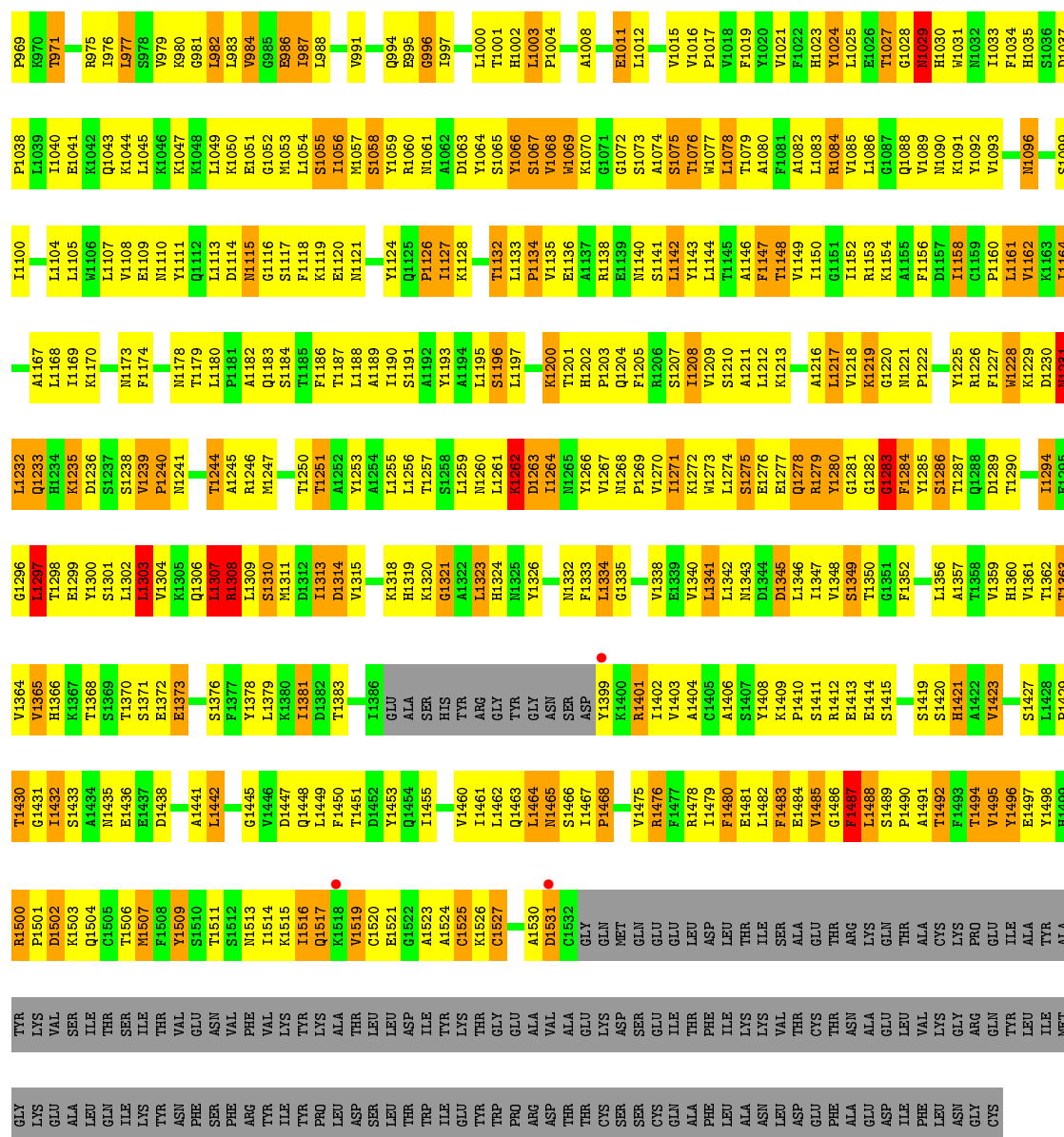
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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: Complement C5



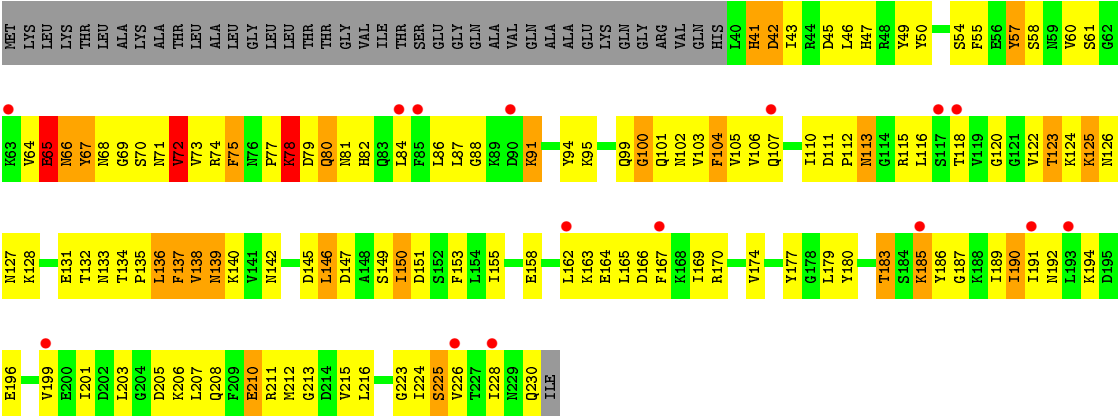
- Molecule 1: Complement C5







• Molecule 2: Exotoxin 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	143.88Å 143.88Å 241.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.05 – 3.60 29.31 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.05-3.60) 99.6 (29.31-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.198 , 0.263 0.192 , 0.259	Depositor DCC
R_{free} test set	3205 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	111.0	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 120.3	EDS
Estimated twinning fraction	0.025 for -h,-k,l 0.410 for h,-h-k,-l 0.028 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 64555 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27683	wwPDB-VP
Average B, all atoms (Å ²)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CD

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	0.59	1/13111 (0.0%)	0.82	7/17784 (0.0%)
1	B	0.60	2/11928 (0.0%)	0.83	6/16183 (0.0%)
2	X	0.33	0/1560	0.56	0/2096
2	Y	0.33	0/1560	0.57	1/2096 (0.0%)
All	All	0.57	3/28159 (0.0%)	0.80	14/38159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	GLU	CB-CG	5.75	1.63	1.52
1	B	247	GLU	CG-CD	5.70	1.60	1.51
1	A	247	GLU	CB-CG	5.40	1.62	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1487	PHE	N-CA-CB	7.79	124.62	110.60
1	A	1303	LEU	CA-CB-CG	6.25	129.68	115.30
1	B	1303	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	1283	GLY	N-CA-C	5.75	127.47	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1283	GLY	N-CA-C	5.71	127.37	113.10
1	A	942	VAL	CB-CA-C	-5.68	100.61	111.40
1	A	1297	LEU	CA-CB-CG	-5.46	102.73	115.30
1	B	942	VAL	CB-CA-C	-5.36	101.22	111.40
2	Y	65	GLU	CA-CB-CG	5.29	125.03	113.40
1	A	1307	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	1442	LEU	CA-CB-CG	-5.15	103.46	115.30
1	B	1442	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	1307	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	1226	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1179	THR	Peptide
1	A	1633	PHE	Peptide
1	A	1635	TYR	Peptide
1	A	651	LEU	Peptide
1	B	1179	THR	Peptide
1	B	651	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12836	0	12796	1596	1
1	B	11676	0	11649	1413	1
2	X	1539	0	1530	162	0
2	Y	1539	0	1530	163	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
4	A	28	0	25	3	0
4	B	28	0	25	2	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
All	All	27683	0	27581	3288	1

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 60.

All (3288) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:ARG:HG3	1:B:1284:PHE:CB	1.60	1.32
1:B:1488:LEU:O	1:B:1488:LEU:HD12	1.31	1.30
1:A:1279:ARG:HG3	1:A:1284:PHE:CB	1.60	1.29
1:A:1486:GLY:O	1:A:1487:PHE:CD2	1.86	1.27
1:B:1323:LEU:HD12	1:B:1324:HIS:H	1.04	1.15
1:B:886:GLN:HG2	1:B:894:HIS:CD2	1.82	1.14
1:A:886:GLN:HG2	1:A:894:HIS:CE1	1.82	1.13
1:A:617:LYS:HE3	1:A:625:GLN:HE22	1.14	1.11
1:A:386:VAL:H	1:A:411:THR:HG22	1.06	1.11
1:B:617:LYS:HE3	1:B:625:GLN:HE22	1.14	1.10
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.04	1.10
1:A:987:ILE:HD13	1:A:1294:ILE:HD13	1.27	1.09
1:B:987:ILE:HD13	1:B:1294:ILE:HD13	1.29	1.08
1:A:38:ASN:ND2	2:X:150:ILE:HG12	1.68	1.08
1:A:38:ASN:HD21	2:X:150:ILE:HG12	0.96	1.08
1:B:38:ASN:HD21	2:Y:150:ILE:HG12	1.00	1.08
1:B:1279:ARG:CG	1:B:1284:PHE:HB2	1.84	1.07
1:A:1279:ARG:CG	1:A:1284:PHE:HB2	1.84	1.07
1:A:25:ILE:HB	1:A:654:LEU:HB3	1.37	1.07
1:B:386:VAL:H	1:B:411:THR:HG22	1.09	1.07
1:A:1612:VAL:HB	1:A:1615:ARG:HD2	1.35	1.06
1:A:307:VAL:CG1	1:A:313:TYR:HB2	1.84	1.06
1:A:1229:LYS:HD2	1:A:1239:VAL:HG12	1.35	1.06
1:B:38:ASN:ND2	2:Y:150:ILE:HG12	1.70	1.05
1:A:922:ILE:HD12	4:A:2001:NAG:H82	1.33	1.05
1:A:1096:ASN:ND2	1:A:1099:SER:H	1.54	1.05
2:Y:43:ILE:HD12	2:Y:185:LYS:HE2	1.38	1.04
1:B:307:VAL:CG1	1:B:313:TYR:HB2	1.86	1.04
1:B:1423:VAL:HG22	1:B:1496:TYR:CE1	1.92	1.04
1:B:1096:ASN:ND2	1:B:1099:SER:H	1.53	1.04
1:A:439:ALA:HB3	1:A:447:GLN:HE22	1.21	1.04
1:A:1423:VAL:HG22	1:A:1496:TYR:CE1	1.94	1.03
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.22	1.03
1:B:115:LYS:HG2	1:B:117:MET:HE3	1.39	1.03
1:B:1229:LYS:HD2	1:B:1239:VAL:HG12	1.36	1.02
1:A:1675:GLY:O	1:A:1676:CYS:SG	2.17	1.02
1:B:1068:VAL:HG13	1:B:1069:TRP:H	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:HG2	1:A:835:ARG:HH11	1.25	1.02
1:B:25:ILE:HB	1:B:654:LEU:HB3	1.41	1.02
2:X:43:ILE:HD12	2:X:185:LYS:HE2	1.38	1.01
1:B:835:ARG:HG2	1:B:835:ARG:HH11	1.25	1.00
1:A:1488:LEU:HD12	1:A:1488:LEU:O	1.60	1.00
1:B:1202:HIS:CD2	1:B:1203:PRO:HD2	1.98	0.99
1:A:1565:ILE:HG12	1:A:1611:LEU:HD13	1.41	0.99
1:A:386:VAL:H	1:A:411:THR:CG2	1.75	0.99
1:B:855:PHE:HZ	1:B:894:HIS:CD2	1.82	0.98
1:B:617:LYS:O	1:B:618:LYS:HG2	1.62	0.98
1:A:617:LYS:O	1:A:618:LYS:HG2	1.62	0.98
1:B:535:VAL:HG23	1:B:536:PRO:HD3	1.43	0.98
1:A:1202:HIS:CD2	1:A:1203:PRO:HD2	1.98	0.97
1:A:886:GLN:HG2	1:A:894:HIS:ND1	1.77	0.97
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.44	0.97
1:A:1673:LEU:HB2	1:B:258:LYS:HG3	1.48	0.96
1:B:55:SER:HB3	1:B:68:SER:HB3	1.48	0.95
1:A:160:VAL:HG23	1:A:175:GLU:HB3	1.48	0.95
1:B:1084:ARG:O	1:B:1088:GLN:HG3	1.66	0.95
1:B:386:VAL:H	1:B:411:THR:CG2	1.78	0.95
1:A:1323:LEU:CD1	1:A:1324:HIS:H	1.80	0.95
1:A:439:ALA:HB3	1:A:442:LEU:HB2	1.46	0.94
1:A:55:SER:HB3	1:A:68:SER:HB3	1.49	0.94
1:A:895:LEU:HD13	1:A:1555:PRO:HB2	1.48	0.94
1:A:1636:ILE:HG13	1:A:1637:TYR:H	1.32	0.94
1:A:1084:ARG:O	1:A:1088:GLN:HG3	1.66	0.94
2:Y:142:ASN:HB3	2:Y:145:ASP:HB2	1.49	0.94
1:A:386:VAL:N	1:A:411:THR:HG22	1.82	0.94
1:B:1279:ARG:HG3	1:B:1284:PHE:HB2	0.94	0.94
1:A:115:LYS:HG2	1:A:117:MET:HE3	1.46	0.93
1:A:1279:ARG:HG3	1:A:1284:PHE:HB2	0.95	0.93
1:A:1323:LEU:HD12	1:A:1324:HIS:N	1.83	0.93
1:B:242:ASN:HD22	1:B:242:ASN:H	1.10	0.93
1:A:1423:VAL:HG22	1:A:1496:TYR:HE1	1.33	0.93
1:B:1423:VAL:HG22	1:B:1496:TYR:HE1	1.31	0.93
1:A:1633:PHE:HD1	1:A:1634:ARG:HG2	1.32	0.93
1:B:1023:HIS:HD2	1:B:1092:TYR:OH	1.51	0.93
1:A:389:THR:HG23	1:A:408:LYS:HE2	1.48	0.93
1:A:1023:HIS:HD2	1:A:1092:TYR:OH	1.50	0.93
1:B:1323:LEU:CD1	1:B:1324:HIS:H	1.82	0.93
1:A:467:ILE:HD12	1:A:484:ILE:HD11	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:ASN:HA	1:B:258:LYS:HZ2	1.33	0.92
1:B:439:ALA:HB3	1:B:447:GLN:HE22	1.31	0.92
2:X:142:ASN:HB3	2:X:145:ASP:HB2	1.49	0.91
1:B:160:VAL:HG23	1:B:175:GLU:HB3	1.50	0.91
1:B:467:ILE:HD12	1:B:484:ILE:HD11	1.50	0.91
1:B:439:ALA:HB3	1:B:442:LEU:HB2	1.51	0.91
1:B:1323:LEU:HD12	1:B:1324:HIS:N	1.84	0.91
1:A:242:ASN:HD22	1:A:242:ASN:H	1.09	0.91
1:B:271:ILE:HG22	1:B:272:ARG:H	1.35	0.90
1:B:1488:LEU:O	1:B:1488:LEU:CD1	2.18	0.90
1:B:1334:LEU:H	1:B:1334:LEU:HD22	1.37	0.90
1:B:386:VAL:N	1:B:411:THR:HG22	1.85	0.90
1:A:1577:TYR:O	1:A:1599:THR:HG23	1.72	0.90
1:A:1538:GLU:O	1:A:1539:LEU:HG	1.72	0.90
1:A:1603:LYS:HG3	1:A:1604:VAL:N	1.87	0.89
1:A:271:ILE:HG22	1:A:272:ARG:H	1.34	0.89
1:B:1233:GLN:HA	1:B:1235:LYS:NZ	1.86	0.89
1:A:1233:GLN:HA	1:A:1235:LYS:NZ	1.85	0.89
1:B:618:LYS:HG3	1:B:621:GLU:CD	1.93	0.89
1:B:1200:LYS:HE3	1:B:1261:LEU:HD23	1.53	0.89
1:A:1100:ILE:HG21	1:A:1158:ILE:HD12	1.54	0.89
1:A:1334:LEU:H	1:A:1334:LEU:HD22	1.38	0.89
1:A:571:LEU:HD12	1:A:572:GLN:N	1.87	0.89
1:A:85:LEU:O	1:A:86:THR:HB	1.73	0.89
1:A:59:TYR:HB3	1:A:60:PRO:HD3	1.54	0.89
1:B:59:TYR:CD1	1:B:103:TYR:HE1	1.91	0.88
1:A:1486:GLY:O	1:A:1487:PHE:HD2	1.49	0.88
1:B:85:LEU:O	1:B:86:THR:HB	1.72	0.88
1:B:412:ARG:HB3	1:B:415:ASP:HB3	1.55	0.88
1:B:571:LEU:HD12	1:B:572:GLN:N	1.89	0.88
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.09	0.88
1:A:59:TYR:HD1	1:A:103:TYR:HE1	1.22	0.88
1:A:1564:SER:HB2	1:A:1616:GLN:HG2	1.53	0.88
1:B:906:GLY:O	1:B:908:HIS:CE1	2.27	0.88
1:B:389:THR:HG23	1:B:408:LYS:HE2	1.54	0.88
1:B:609:VAL:HG23	1:B:610:TYR:H	1.39	0.88
1:A:855:PHE:HZ	1:A:894:HIS:ND1	1.70	0.88
1:A:242:ASN:ND2	1:A:242:ASN:H	1.72	0.87
1:B:59:TYR:HD1	1:B:103:TYR:HE1	1.20	0.87
1:A:609:VAL:HG23	1:A:610:TYR:H	1.40	0.87
1:B:560:TRP:CH2	1:B:562:ASN:HB2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LYS:HG3	1:A:621:GLU:CD	1.94	0.87
1:A:136:THR:HG21	1:A:222:TYR:HB2	1.56	0.87
1:A:1012:LEU:O	1:A:1015:VAL:HG12	1.75	0.87
1:B:367:ILE:HG21	1:B:466:TYR:CD2	2.08	0.87
1:A:1674:ASN:HA	1:B:258:LYS:NZ	1.89	0.87
1:A:412:ARG:HB3	1:A:415:ASP:HB3	1.55	0.87
1:A:232:GLU:OE2	1:A:251:LYS:HE2	1.74	0.87
1:B:123:ASN:C	1:B:123:ASN:HD22	1.78	0.87
1:B:136:THR:HG21	1:B:222:TYR:HB2	1.57	0.87
1:B:1012:LEU:O	1:B:1015:VAL:HG12	1.73	0.87
1:B:1488:LEU:HD12	1:B:1488:LEU:C	1.95	0.86
1:A:23:TYR:HA	1:A:43:VAL:HG23	1.55	0.86
1:A:59:TYR:CD1	1:A:103:TYR:HE1	1.92	0.86
1:B:59:TYR:HB3	1:B:60:PRO:HD3	1.54	0.86
1:B:242:ASN:ND2	1:B:242:ASN:H	1.73	0.86
1:B:1381:ILE:HD13	1:B:1509:TYR:CD1	2.10	0.86
1:A:977:LEU:HD12	1:A:1361:VAL:CG2	2.05	0.86
1:A:367:ILE:HG21	1:A:466:TYR:CD2	2.09	0.86
1:A:1200:LYS:HE3	1:A:1261:LEU:HD23	1.56	0.86
1:A:906:GLY:O	1:A:908:HIS:CE1	2.29	0.86
1:B:42:GLN:HG3	1:B:80:GLN:HE21	1.40	0.86
1:A:1381:ILE:HD13	1:A:1509:TYR:CD1	2.11	0.86
1:B:160:VAL:HG12	1:B:160:VAL:O	1.75	0.85
1:B:982:LEU:HD23	1:B:982:LEU:N	1.89	0.85
2:X:57:TYR:HD2	2:X:58:SER:H	1.25	0.85
1:B:886:GLN:HG2	1:B:894:HIS:HD2	1.39	0.85
1:B:23:TYR:HA	1:B:43:VAL:HG23	1.56	0.85
1:A:1427:SER:OG	1:A:1491:ALA:HB1	1.75	0.84
1:A:1657:CYS:O	1:A:1658:GLN:HB2	1.74	0.84
1:A:1585:TYR:HB3	1:A:1671:ILE:HG12	1.60	0.84
1:B:1115:ASN:ND2	1:B:1117:SER:H	1.76	0.84
1:B:1100:ILE:HG21	1:B:1158:ILE:HD12	1.58	0.84
1:B:99:VAL:HG13	1:B:119:ILE:HD11	1.59	0.84
2:Y:57:TYR:HD2	2:Y:58:SER:H	1.25	0.84
1:A:478:VAL:HA	1:A:530:VAL:CG1	2.08	0.84
1:A:1115:ASN:ND2	1:A:1117:SER:H	1.76	0.84
1:A:160:VAL:O	1:A:160:VAL:HG12	1.76	0.83
1:A:982:LEU:N	1:A:982:LEU:HD23	1.92	0.83
1:A:371:ILE:O	1:A:371:ILE:HG22	1.76	0.83
1:B:232:GLU:OE2	1:B:251:LYS:HE2	1.77	0.83
2:X:46:LEU:HD22	2:X:206:LYS:HE3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1624:ALA:HB1	1:A:1636:ILE:HA	1.60	0.83
1:A:1673:LEU:HB2	1:B:258:LYS:CG	2.09	0.83
1:B:618:LYS:CB	1:B:621:GLU:HB3	2.08	0.83
1:B:493:ILE:HG23	1:B:494:ASP:H	1.42	0.83
1:A:1096:ASN:HD21	1:A:1099:SER:H	1.24	0.83
1:A:99:VAL:HG13	1:A:119:ILE:HD11	1.59	0.82
1:A:38:ASN:HD21	2:X:150:ILE:CG1	1.88	0.82
1:B:371:ILE:O	1:B:371:ILE:HG22	1.76	0.82
1:B:1430:THR:O	1:B:1485:VAL:HG11	1.79	0.82
1:A:1578:LYS:HA	1:A:1599:THR:HA	1.61	0.82
1:A:493:ILE:HG23	1:A:494:ASP:H	1.45	0.82
1:A:42:GLN:HG3	1:A:80:GLN:HE21	1.43	0.82
1:A:59:TYR:CB	1:A:60:PRO:HD3	2.10	0.82
1:B:1127:ILE:HD12	1:B:1127:ILE:H	1.43	0.82
1:A:618:LYS:CB	1:A:621:GLU:HB3	2.10	0.82
1:B:156:LYS:O	1:B:157:ARG:HG3	1.78	0.82
1:A:497:THR:HG23	1:A:498:HIS:H	1.42	0.82
1:A:439:ALA:CB	1:A:442:LEU:HB2	2.10	0.82
1:B:497:THR:HG23	1:B:498:HIS:H	1.42	0.82
1:B:120:THR:HG22	1:B:121:TYR:H	1.44	0.82
1:A:478:VAL:HA	1:A:530:VAL:HG13	1.61	0.82
1:A:778:HIS:CE1	1:A:786:LEU:HD13	2.15	0.82
1:A:1614:GLY:HA3	1:B:1519:VAL:HG21	1.62	0.82
1:B:478:VAL:HA	1:B:530:VAL:CG1	2.10	0.82
1:B:1486:GLY:O	1:B:1487:PHE:C	2.18	0.81
1:B:1488:LEU:CD1	1:B:1488:LEU:C	2.48	0.81
2:Y:113:ASN:HD21	2:Y:115:ARG:HG2	1.44	0.81
1:A:123:ASN:C	1:A:123:ASN:HD22	1.79	0.81
1:A:1535:MET:HG2	1:A:1609:ALA:HA	1.61	0.81
1:A:1423:VAL:CG2	1:A:1496:TYR:HE1	1.94	0.81
1:B:1259:LEU:HD11	1:B:1300:TYR:HB2	1.63	0.81
1:B:1438:ASP:O	1:B:1441:ALA:HB3	1.81	0.81
1:B:66:TYR:CE1	1:B:90:LYS:HG3	2.15	0.81
2:X:113:ASN:HD21	2:X:115:ARG:HG2	1.44	0.81
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.15	0.81
1:B:1096:ASN:HD21	1:B:1099:SER:H	1.23	0.81
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.63	0.81
1:B:977:LEU:HD12	1:B:1361:VAL:CG2	2.09	0.81
1:A:1652:THR:O	1:A:1653:THR:HB	1.80	0.81
1:B:478:VAL:HA	1:B:530:VAL:HG13	1.62	0.81
1:A:1259:LEU:HD11	1:A:1300:TYR:HB2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:702:GLY:HA2	1:B:728:PHE:CE1	2.16	0.81
1:B:59:TYR:CB	1:B:60:PRO:HD3	2.09	0.81
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.62	0.81
1:B:96:GLN:O	1:B:98:PRO:HD3	1.81	0.81
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.63	0.81
1:B:820:PHE:CE2	1:B:848:TYR:HD2	1.97	0.81
1:B:253:ARG:HH21	1:B:257:ASN:HA	1.44	0.81
1:A:968:VAL:HG12	1:A:1368:THR:HG22	1.63	0.81
1:A:156:LYS:O	1:A:157:ARG:HG3	1.79	0.80
1:B:786:LEU:HD23	1:B:786:LEU:N	1.97	0.80
1:A:857:VAL:HG12	1:A:914:LEU:HB3	1.62	0.80
1:A:930:VAL:HG12	1:A:931:PRO:N	1.96	0.80
1:A:307:VAL:HG11	1:A:313:TYR:HB2	1.63	0.80
1:A:96:GLN:O	1:A:98:PRO:HD3	1.81	0.80
1:B:778:HIS:CE1	1:B:786:LEU:HD13	2.15	0.80
1:B:1132:THR:HB	1:B:1134:PRO:HD2	1.63	0.80
1:A:253:ARG:HH21	1:A:257:ASN:HA	1.44	0.80
1:A:120:THR:HG22	1:A:121:TYR:H	1.46	0.80
1:B:1429:PRO:HG2	1:B:1511:THR:HB	1.62	0.80
1:B:1068:VAL:HG13	1:B:1069:TRP:N	1.96	0.80
1:A:100:SER:O	1:A:101:TYR:HB2	1.80	0.80
1:B:38:ASN:HD21	2:Y:150:ILE:CG1	1.90	0.80
2:Y:46:LEU:HD22	2:Y:206:LYS:HE3	1.62	0.80
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.17	0.80
1:B:100:SER:O	1:B:101:TYR:HB2	1.81	0.80
1:A:1127:ILE:HD12	1:A:1127:ILE:H	1.46	0.80
1:B:1423:VAL:CG2	1:B:1496:TYR:HE1	1.94	0.80
1:A:820:PHE:CE2	1:A:848:TYR:HD2	1.99	0.80
1:A:1068:VAL:HG13	1:A:1069:TRP:N	1.94	0.80
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.62	0.80
1:B:1514:ILE:HG21	1:B:1516:ILE:HG12	1.64	0.80
1:A:542:VAL:O	1:A:556:SER:HB2	1.82	0.79
1:B:464:TYR:H	1:B:491:PRO:HD3	1.48	0.79
1:B:1378:TYR:CZ	1:B:1409:LYS:HE3	2.17	0.79
1:B:679:LEU:HD13	1:B:742:ILE:HG12	1.64	0.79
1:A:1671:ILE:HG23	1:A:1672:PHE:H	1.48	0.79
1:B:710:THR:HG23	1:B:713:GLN:CD	2.02	0.79
1:B:855:PHE:CZ	1:B:894:HIS:CD2	2.69	0.79
1:A:617:LYS:HE3	1:A:625:GLN:NE2	1.96	0.79
1:A:66:TYR:CE1	1:A:90:LYS:HG3	2.18	0.79
1:B:1431:GLY:HA3	1:B:1483:PHE:CE1	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:ILE:CG2	1:B:900:VAL:HG23	2.13	0.79
1:A:786:LEU:N	1:A:786:LEU:HD23	1.98	0.79
1:A:886:GLN:CG	1:A:894:HIS:CE1	2.64	0.79
1:A:1429:PRO:HG2	1:A:1511:THR:HB	1.63	0.79
1:B:59:TYR:CG	1:B:60:PRO:HD3	2.17	0.79
2:Y:128:LYS:HB2	2:Y:158:GLU:HB2	1.65	0.79
1:A:886:GLN:HE22	1:A:1623:GLU:HG2	1.46	0.79
1:B:1084:ARG:HD2	1:B:1154:LYS:HG3	1.65	0.78
1:A:545:ILE:HG23	1:A:554:LEU:HD23	1.65	0.78
1:B:617:LYS:HE3	1:B:625:GLN:NE2	1.96	0.78
2:Y:150:ILE:HD12	2:Y:151:ASP:N	1.98	0.78
1:A:443:PRO:HA	1:B:443:PRO:HA	1.65	0.78
1:A:464:TYR:H	1:A:491:PRO:HD3	1.47	0.78
1:A:1411:SER:O	1:A:1414:GLU:HB2	1.84	0.78
1:A:1438:ASP:O	1:A:1441:ALA:HB3	1.84	0.78
1:B:307:VAL:HG11	1:B:313:TYR:HB2	1.64	0.78
1:B:1334:LEU:N	1:B:1334:LEU:HD22	1.99	0.78
1:B:857:VAL:HG12	1:B:914:LEU:HB3	1.63	0.78
1:A:1216:ALA:HB2	1:A:1228:TRP:CE2	2.19	0.78
2:Y:102:ASN:HB2	2:Y:123:THR:HG23	1.66	0.78
1:A:1423:VAL:CG2	1:A:1496:TYR:CE1	2.67	0.78
1:B:859:MET:HB2	1:B:912:PHE:CE1	2.18	0.78
1:A:1517:GLN:O	1:A:1518:LYS:HG2	1.83	0.78
1:A:977:LEU:HD12	1:A:1361:VAL:HG21	1.65	0.77
1:B:66:TYR:HE1	1:B:90:LYS:HG3	1.47	0.77
2:X:150:ILE:HD12	2:X:151:ASP:N	1.99	0.77
1:A:1431:GLY:HA3	1:A:1483:PHE:CE1	2.19	0.77
1:B:1161:LEU:HB3	1:B:1164:ILE:HG23	1.66	0.77
1:B:543:TYR:HB3	1:B:556:SER:HB3	1.66	0.77
1:A:839:ILE:CG2	1:A:900:VAL:HG23	2.14	0.77
1:A:679:LEU:HD13	1:A:742:ILE:HG12	1.65	0.77
1:B:1427:SER:OG	1:B:1491:ALA:HB1	1.83	0.77
1:A:835:ARG:CG	1:A:835:ARG:HH11	1.96	0.77
1:B:440:PRO:HD2	1:B:441:ASP:OD2	1.83	0.77
1:B:930:VAL:HG12	1:B:931:PRO:N	1.99	0.77
1:A:440:PRO:HD2	1:A:441:ASP:OD2	1.85	0.77
1:A:1673:LEU:CB	1:B:258:LYS:HG3	2.15	0.77
1:B:542:VAL:O	1:B:556:SER:HB2	1.85	0.77
1:B:835:ARG:CG	1:B:835:ARG:HH11	1.96	0.77
1:A:710:THR:HG23	1:A:713:GLN:CD	2.04	0.77
2:X:102:ASN:HB2	2:X:123:THR:HG23	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:MET:HB2	1:A:912:PHE:CE1	2.19	0.77
1:A:697:LYS:HE3	1:A:701:ASP:OD2	1.83	0.77
1:B:1244:THR:HG22	1:B:1247:MET:H	1.49	0.77
1:B:833:VAL:HG21	1:B:927:LEU:HD21	1.67	0.76
1:A:66:TYR:HE1	1:A:90:LYS:HG3	1.50	0.76
1:B:1025:LEU:HD13	1:B:1031:TRP:CZ3	2.20	0.76
1:B:1423:VAL:CG2	1:B:1496:TYR:CE1	2.67	0.76
1:B:545:ILE:HG23	1:B:554:LEU:HD23	1.66	0.76
1:B:492:TYR:OH	1:B:548:GLY:HA2	1.85	0.76
1:A:639:GLY:H	1:A:645:VAL:HG22	1.50	0.76
2:X:128:LYS:HB2	2:X:158:GLU:HB2	1.66	0.76
1:A:1361:VAL:O	1:A:1361:VAL:HG12	1.83	0.76
1:A:1599:THR:O	1:A:1636:ILE:HG12	1.85	0.76
1:A:885:ARG:HG3	1:A:1626:GLN:HB2	1.67	0.76
1:A:1025:LEU:HD13	1:A:1031:TRP:CZ3	2.20	0.76
1:A:1563:VAL:HG12	1:A:1581:LEU:HG	1.67	0.76
1:B:384:GLY:HA2	1:B:411:THR:HG23	1.68	0.76
1:B:59:TYR:HD1	1:B:103:TYR:CE1	2.03	0.76
1:B:790:LEU:HD13	1:B:819:VAL:HG11	1.66	0.76
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.67	0.76
1:B:823:VAL:HG22	1:B:847:ASN:HA	1.68	0.76
1:A:489:LYS:O	1:A:491:PRO:HD2	1.86	0.76
1:B:318:LEU:O	1:B:319:ASN:HB2	1.84	0.76
1:A:1636:ILE:CG1	1:A:1637:TYR:H	1.99	0.76
1:B:439:ALA:CB	1:B:442:LEU:HB2	2.16	0.75
1:A:1334:LEU:CD2	1:A:1334:LEU:H	1.99	0.75
1:B:38:ASN:O	1:B:39:ILE:HD13	1.86	0.75
1:A:354:LEU:H	1:A:354:LEU:HD22	1.51	0.75
1:B:1485:VAL:CG2	1:B:1488:LEU:HB3	2.16	0.75
1:B:1334:LEU:H	1:B:1334:LEU:CD2	1.99	0.75
1:A:975:ARG:HB3	1:A:1363:THR:HB	1.69	0.75
1:A:1161:LEU:HB3	1:A:1164:ILE:HG23	1.69	0.75
1:B:354:LEU:HD22	1:B:354:LEU:H	1.51	0.75
1:B:1085:VAL:O	1:B:1089:VAL:HG23	1.86	0.75
1:A:1378:TYR:CZ	1:A:1409:LYS:HE3	2.21	0.75
2:X:42:ASP:O	2:X:46:LEU:HG	1.87	0.75
1:A:833:VAL:HG21	1:A:927:LEU:HD21	1.68	0.75
1:A:1603:LYS:HG3	1:A:1604:VAL:H	1.49	0.75
1:A:1334:LEU:N	1:A:1334:LEU:HD22	2.00	0.75
1:B:938:SER:OG	1:B:1279:ARG:NH1	2.20	0.75
1:A:1673:LEU:HB2	1:B:258:LYS:CD	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:VAL:HG21	1:A:896:VAL:HG11	1.69	0.75
1:B:968:VAL:HG12	1:B:1368:THR:HG22	1.69	0.75
1:A:855:PHE:CZ	1:A:894:HIS:ND1	2.55	0.75
1:B:492:TYR:CD2	1:B:493:ILE:N	2.55	0.75
1:A:823:VAL:HG22	1:A:847:ASN:HA	1.69	0.75
1:B:765:ILE:O	1:B:765:ILE:HG23	1.87	0.75
1:A:1318:LYS:HG2	1:A:1319:HIS:CE1	2.22	0.75
1:A:38:ASN:O	1:A:39:ILE:HD13	1.88	0.74
1:A:492:TYR:CD2	1:A:493:ILE:N	2.54	0.74
1:B:697:LYS:HE3	1:B:701:ASP:OD2	1.86	0.74
1:A:855:PHE:CE2	1:A:888:VAL:HG13	2.22	0.74
1:A:57:LYS:O	1:A:103:TYR:HB2	1.87	0.74
1:A:968:VAL:HG23	1:A:971:THR:HG21	1.68	0.74
1:A:318:LEU:O	1:A:319:ASN:HB2	1.86	0.74
1:B:1142:LEU:HD13	1:B:1187:THR:CG2	2.17	0.74
1:A:1244:THR:HG22	1:A:1247:MET:H	1.52	0.74
2:Y:42:ASP:O	2:Y:46:LEU:HG	1.87	0.74
1:B:66:TYR:HD1	1:B:90:LYS:HE3	1.53	0.74
1:A:412:ARG:HD2	1:A:415:ASP:HB2	1.67	0.74
1:A:492:TYR:OH	1:A:548:GLY:HA2	1.87	0.74
2:Y:139:ASN:HB3	2:Y:146:LEU:HD21	1.68	0.74
1:B:975:ARG:HB3	1:B:1363:THR:HB	1.68	0.74
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	1.69	0.74
1:B:1411:SER:O	1:B:1414:GLU:HB2	1.86	0.74
1:B:231:ILE:HD12	1:B:327:VAL:HG23	1.69	0.74
1:B:977:LEU:HD12	1:B:1361:VAL:HG21	1.68	0.74
1:A:384:GLY:HA2	1:A:411:THR:HG23	1.69	0.74
1:B:968:VAL:HG23	1:B:971:THR:HG21	1.70	0.74
1:A:707:ASN:HB3	1:A:739:ARG:HH22	1.52	0.74
1:B:268:THR:HA	1:B:286:ALA:HB1	1.69	0.74
2:Y:65:GLU:N	2:Y:65:GLU:OE1	2.20	0.74
1:B:639:GLY:H	1:B:645:VAL:HG22	1.50	0.74
1:A:492:TYR:HD2	1:A:493:ILE:H	1.34	0.74
1:A:351:PRO:HD2	1:A:442:LEU:HD11	1.69	0.74
2:Y:70:SER:HB3	2:Y:91:LYS:HE3	1.68	0.74
1:A:1229:LYS:HE3	1:A:1231:ASN:OD1	1.88	0.73
1:B:835:ARG:HG2	1:B:835:ARG:NH1	2.02	0.73
1:A:290:THR:O	1:A:290:THR:HG22	1.87	0.73
1:B:412:ARG:HD2	1:B:415:ASP:HB2	1.68	0.73
1:B:1318:LYS:HG2	1:B:1319:HIS:CE1	2.23	0.73
1:A:1515:LYS:O	1:A:1516:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1146:ALA:HB1	1:B:1190:ILE:HG22	1.70	0.73
1:B:829:ILE:HG22	1:B:830:PRO:HD2	1.69	0.73
2:X:139:ASN:HB3	2:X:146:LEU:HD21	1.68	0.73
1:A:886:GLN:HG3	1:A:887:LYS:H	1.54	0.73
1:B:351:PRO:HD2	1:B:442:LEU:HD11	1.69	0.73
1:A:1023:HIS:CD2	1:A:1092:TYR:OH	2.40	0.73
1:B:907:LEU:HD12	1:B:908:HIS:H	1.54	0.73
1:B:493:ILE:HG23	1:B:494:ASP:N	2.04	0.73
1:B:1427:SER:HB3	1:B:1492:THR:H	1.54	0.73
1:B:707:ASN:HB3	1:B:739:ARG:HH22	1.53	0.73
1:A:1233:GLN:HA	1:A:1235:LYS:HZ3	1.54	0.73
1:B:1229:LYS:HE3	1:B:1231:ASN:OD1	1.88	0.73
1:B:149:ASN:O	1:B:151:ASP:N	2.21	0.73
1:A:790:LEU:HD13	1:A:819:VAL:HG11	1.69	0.73
1:A:470:THR:HG22	1:A:471:ASP:N	2.04	0.73
1:A:307:VAL:HG12	1:A:313:TYR:HB2	1.70	0.73
1:B:1228:TRP:N	1:B:1228:TRP:CE3	2.56	0.73
1:A:59:TYR:HD1	1:A:103:TYR:CE1	2.04	0.73
1:A:92:LEU:N	1:A:93:PRO:HD3	2.04	0.73
1:A:829:ILE:HG22	1:A:830:PRO:HD2	1.70	0.73
1:A:59:TYR:HB3	1:A:60:PRO:CD	2.19	0.73
1:B:92:LEU:N	1:B:93:PRO:HD3	2.04	0.73
1:B:1061:ASN:HB2	1:B:1065:SER:O	1.89	0.73
2:X:190:ILE:HG12	2:X:190:ILE:O	1.89	0.73
1:B:307:VAL:HG12	1:B:313:TYR:HB2	1.70	0.73
1:B:290:THR:HG22	1:B:290:THR:O	1.87	0.73
1:B:470:THR:HG22	1:B:471:ASP:N	2.05	0.72
1:B:1361:VAL:HG12	1:B:1361:VAL:O	1.87	0.72
1:B:171:VAL:HG13	1:B:1057:MET:CE	2.19	0.72
1:B:242:ASN:N	1:B:242:ASN:HD22	1.86	0.72
1:B:961:TYR:OH	1:B:1343:ASN:CG	2.28	0.72
1:B:1076:THR:HG21	1:B:1144:LEU:HD21	1.71	0.72
1:B:886:GLN:HG3	1:B:887:LYS:H	1.54	0.72
1:A:1430:THR:O	1:A:1485:VAL:HG11	1.89	0.72
1:B:1233:GLN:HA	1:B:1235:LYS:HZ2	1.52	0.72
1:A:242:ASN:HD22	1:A:242:ASN:N	1.85	0.72
1:B:489:LYS:O	1:B:491:PRO:HD2	1.89	0.72
1:B:492:TYR:HD2	1:B:493:ILE:H	1.36	0.72
1:A:493:ILE:HG23	1:A:494:ASP:N	2.04	0.72
1:B:857:VAL:HG21	1:B:896:VAL:HG11	1.71	0.72
1:A:1142:LEU:HD13	1:A:1187:THR:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:VAL:HG11	1:A:809:ILE:HD13	1.70	0.72
2:Y:169:ILE:HG21	2:Y:189:ILE:HD13	1.70	0.72
1:A:765:ILE:HG23	1:A:765:ILE:O	1.89	0.72
1:A:1620:MET:O	1:A:1643:THR:HA	1.88	0.72
1:B:1228:TRP:N	1:B:1228:TRP:HE3	1.86	0.72
1:A:253:ARG:NH2	1:A:257:ASN:HA	2.05	0.72
1:A:268:THR:HA	1:A:286:ALA:HB1	1.70	0.72
1:A:160:VAL:CG2	1:A:175:GLU:HB3	2.20	0.72
2:Y:190:ILE:HG12	2:Y:190:ILE:O	1.89	0.72
1:A:1535:MET:HB3	1:A:1645:ILE:HD11	1.72	0.72
1:B:253:ARG:NH2	1:B:257:ASN:HA	2.05	0.72
1:B:855:PHE:CE2	1:B:888:VAL:HG13	2.24	0.71
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.25	0.71
1:A:231:ILE:HD12	1:A:327:VAL:HG23	1.71	0.71
1:B:1283:GLY:HA3	1:B:1290:THR:HG23	1.72	0.71
1:B:73:LEU:HB2	1:B:79:PHE:HA	1.72	0.71
1:A:833:VAL:CG2	1:A:927:LEU:HD21	2.20	0.71
1:A:1286:SER:OG	1:A:1287:THR:N	2.21	0.71
2:Y:82:HIS:HA	2:Y:115:ARG:HB2	1.72	0.71
1:B:1111:TYR:CE1	1:B:1121:ASN:HB2	2.25	0.71
1:B:1450:PHE:CZ	1:B:1475:VAL:HB	2.25	0.71
2:X:169:ILE:HG21	2:X:189:ILE:HD13	1.70	0.71
1:A:907:LEU:HD12	1:A:908:HIS:H	1.55	0.71
1:B:1030:HIS:CE1	1:B:1306:GLN:NE2	2.58	0.71
1:A:1076:THR:HG21	1:A:1144:LEU:HD21	1.71	0.71
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.28	0.71
1:B:1207:SER:O	1:B:1210:SER:HB3	1.91	0.71
1:B:1233:GLN:HA	1:B:1235:LYS:HZ3	1.55	0.71
1:B:57:LYS:O	1:B:103:TYR:HB2	1.88	0.71
2:X:125:LYS:HA	2:X:127:ASN:N	2.06	0.71
1:B:365:PRO:HD2	1:B:464:TYR:CD2	2.26	0.71
1:A:1279:ARG:HG3	1:A:1284:PHE:CG	2.26	0.71
1:A:386:VAL:HG23	1:A:411:THR:HG21	1.73	0.71
1:B:59:TYR:HB3	1:B:60:PRO:CD	2.19	0.71
1:A:243:PHE:CE1	1:A:316:GLU:HG3	2.25	0.71
1:A:598:SER:HA	1:A:805:SER:OG	1.90	0.71
1:A:1233:GLN:HA	1:A:1235:LYS:HZ2	1.52	0.71
1:A:1488:LEU:O	1:A:1488:LEU:CD1	2.36	0.71
1:A:968:VAL:O	1:A:971:THR:HG23	1.90	0.71
1:A:1438:ASP:OD2	1:A:1478:ARG:HG3	1.90	0.71
1:A:1283:GLY:HA3	1:A:1290:THR:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ARG:HD3	1:B:414:ASP:OD1	1.91	0.71
2:X:107:GLN:CD	2:X:110:ILE:HD11	2.10	0.71
1:A:1311:MET:HG2	1:A:1350:THR:OG1	1.91	0.71
2:X:65:GLU:N	2:X:65:GLU:OE1	2.23	0.71
1:B:1279:ARG:HG3	1:B:1284:PHE:CG	2.25	0.71
1:A:85:LEU:H	1:A:85:LEU:HD22	1.56	0.71
1:A:73:LEU:HB2	1:A:79:PHE:HA	1.73	0.71
1:A:1633:PHE:CD1	1:A:1634:ARG:HG2	2.21	0.71
1:B:1216:ALA:HB2	1:B:1228:TRP:CE2	2.26	0.71
2:Y:107:GLN:CD	2:Y:110:ILE:HD11	2.11	0.71
1:B:582:TYR:HB2	1:B:819:VAL:HG12	1.71	0.71
1:B:833:VAL:CG2	1:B:927:LEU:HD21	2.21	0.70
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.55	0.70
1:A:829:ILE:HG13	1:A:925:LYS:HG3	1.73	0.70
1:B:932:GLU:OE1	1:B:932:GLU:N	2.24	0.70
2:X:77:PRO:HG3	2:X:82:HIS:CD2	2.26	0.70
1:B:598:SER:HA	1:B:805:SER:OG	1.90	0.70
1:A:1207:SER:O	1:A:1210:SER:HB3	1.90	0.70
1:B:1485:VAL:HG23	1:B:1488:LEU:HB3	1.71	0.70
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.72	0.70
2:X:73:VAL:HG23	2:X:74:ARG:N	2.05	0.70
1:B:242:ASN:ND2	1:B:242:ASN:N	2.38	0.70
2:X:82:HIS:HA	2:X:115:ARG:HB2	1.71	0.70
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.73	0.70
1:A:1085:VAL:O	1:A:1089:VAL:HG23	1.89	0.70
1:A:1576:LYS:HG2	1:A:1602:LYS:H	1.56	0.70
2:X:77:PRO:O	2:X:78:LYS:HG3	1.91	0.70
2:Y:125:LYS:HA	2:Y:127:ASN:N	2.06	0.70
1:A:1651:ASP:HB3	1:A:1654:CYS:HB3	1.73	0.70
1:B:987:ILE:HD13	1:B:1294:ILE:CD1	2.16	0.70
2:Y:77:PRO:HG3	2:Y:82:HIS:CD2	2.25	0.70
1:A:1111:TYR:CE1	1:A:1121:ASN:HB2	2.26	0.70
1:B:623:VAL:HG11	1:B:809:ILE:HD13	1.73	0.70
1:A:73:LEU:H	1:A:73:LEU:HD23	1.57	0.70
1:A:1228:TRP:N	1:A:1228:TRP:CE3	2.60	0.70
2:Y:77:PRO:O	2:Y:78:LYS:HG3	1.91	0.70
1:A:1030:HIS:CE1	1:A:1306:GLN:NE2	2.60	0.70
2:X:70:SER:HB3	2:X:91:LYS:HE3	1.72	0.70
1:B:85:LEU:H	1:B:85:LEU:HD22	1.57	0.70
1:B:1063:ASP:O	1:B:1064:TYR:HB2	1.91	0.70
1:A:1652:THR:HB	1:B:868:SER:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1228:TRP:H	1:B:1251:THR:HG22	1.56	0.70
1:A:66:TYR:HD1	1:A:90:LYS:HE3	1.57	0.70
1:B:829:ILE:HG13	1:B:925:LYS:HG3	1.74	0.70
1:B:218:GLU:OE1	1:B:220:LYS:HE2	1.91	0.70
1:A:1557:ILE:HG22	1:A:1557:ILE:O	1.92	0.69
1:A:987:ILE:HD13	1:A:1294:ILE:CD1	2.14	0.69
1:A:1488:LEU:CD1	1:A:1488:LEU:C	2.60	0.69
1:B:160:VAL:CG2	1:B:175:GLU:HB3	2.22	0.69
1:B:679:LEU:HB3	1:B:738:LEU:HD21	1.74	0.69
1:B:73:LEU:HD23	1:B:73:LEU:H	1.58	0.69
1:A:412:ARG:HD3	1:A:414:ASP:OD1	1.91	0.69
1:B:1378:TYR:CE1	1:B:1409:LYS:HE3	2.27	0.69
1:A:218:GLU:OE1	1:A:220:LYS:HE2	1.91	0.69
1:A:1577:TYR:CD2	1:A:1611:LEU:HD11	2.27	0.69
1:A:1649:PRO:O	1:A:1661:LEU:HD11	1.91	0.69
1:B:506:LYS:HZ2	1:B:536:PRO:HD2	1.56	0.69
1:A:1063:ASP:O	1:A:1064:TYR:HB2	1.91	0.69
1:B:123:ASN:HD22	1:B:124:GLY:N	1.89	0.69
1:B:248:ILE:HD13	1:B:325:ILE:HD13	1.75	0.69
1:B:1023:HIS:CD2	1:B:1092:TYR:OH	2.40	0.69
1:A:123:ASN:HD22	1:A:124:GLY:N	1.89	0.69
1:A:157:ARG:O	1:A:178:ASP:HB2	1.92	0.69
1:A:829:ILE:HG13	1:A:925:LYS:CG	2.23	0.69
1:A:635:GLY:HA2	1:A:672:ILE:HG23	1.73	0.69
1:A:1637:TYR:CD2	1:A:1638:PRO:HD2	2.27	0.69
1:A:717:ARG:NH1	1:A:1447:ASP:O	2.25	0.69
1:B:171:VAL:HG13	1:B:1057:MET:HE2	1.74	0.69
1:B:1110:ASN:HB2	1:B:1111:TYR:CD2	2.27	0.69
1:A:1061:ASN:HB2	1:A:1065:SER:O	1.93	0.69
2:X:134:THR:HG22	2:X:153:PHE:O	1.92	0.69
1:A:932:GLU:OE1	1:A:932:GLU:N	2.26	0.69
1:B:367:ILE:HD13	1:B:466:TYR:CB	2.23	0.69
1:A:242:ASN:ND2	1:A:242:ASN:N	2.38	0.69
1:B:702:GLY:HA2	1:B:728:PHE:CD1	2.28	0.69
1:A:827:MET:HG3	1:A:912:PHE:CD2	2.28	0.69
1:A:99:VAL:CG1	1:A:119:ILE:HD11	2.22	0.69
1:A:142:LYS:HD3	1:A:775:TRP:CG	2.28	0.69
1:A:171:VAL:HG13	1:A:1057:MET:CE	2.23	0.69
1:A:1496:TYR:HB3	1:A:1504:GLN:HG3	1.75	0.69
1:B:242:ASN:HB2	1:B:245:ASN:O	1.93	0.69
1:B:99:VAL:CG1	1:B:119:ILE:HD11	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:TYR:HB2	1:A:819:VAL:HG12	1.75	0.69
1:A:679:LEU:HB3	1:A:738:LEU:HD21	1.73	0.69
1:B:635:GLY:HA2	1:B:672:ILE:HG23	1.75	0.69
1:A:1622:LYS:O	1:A:1637:TYR:CE2	2.46	0.68
1:A:532:GLN:O	1:A:535:VAL:HG22	1.93	0.68
1:B:1311:MET:HG2	1:B:1350:THR:OG1	1.93	0.68
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	1.76	0.68
1:A:702:GLY:HA2	1:A:728:PHE:CD1	2.27	0.68
1:B:1525:CYS:SG	1:B:1526:LYS:N	2.66	0.68
1:B:1496:TYR:HB3	1:B:1504:GLN:HG3	1.75	0.68
1:A:367:ILE:HD13	1:A:466:TYR:CB	2.23	0.68
1:A:56:ILE:HG13	1:A:66:TYR:HD2	1.59	0.68
1:A:855:PHE:HE2	1:A:888:VAL:HG13	1.58	0.68
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.28	0.68
1:B:968:VAL:O	1:B:971:THR:HG23	1.94	0.68
1:A:1348:VAL:HG11	1:A:1359:VAL:HG21	1.75	0.68
1:A:185:PHE:HB3	1:A:186:PRO:CD	2.23	0.68
1:B:599:TRP:CZ3	1:B:779:LEU:HB2	2.29	0.68
2:Y:134:THR:HG22	2:Y:153:PHE:O	1.93	0.68
1:B:243:PHE:CE1	1:B:316:GLU:HG3	2.28	0.68
1:A:248:ILE:HD13	1:A:325:ILE:HD13	1.75	0.68
1:A:1548:ARG:NH1	1:A:1646:GLU:OE1	2.27	0.68
1:B:157:ARG:O	1:B:178:ASP:HB2	1.93	0.68
1:A:1146:ALA:HB1	1:A:1190:ILE:HG22	1.74	0.68
1:A:1340:VAL:HG21	1:A:1346:LEU:HD22	1.76	0.68
1:B:56:ILE:HG13	1:B:66:TYR:HD2	1.59	0.68
1:B:98:PRO:HB2	1:B:99:VAL:HG23	1.76	0.68
1:A:243:PHE:CZ	1:A:316:GLU:HB2	2.28	0.68
1:B:101:TYR:HE1	1:B:116:ARG:CZ	2.07	0.68
1:A:98:PRO:HB2	1:A:99:VAL:HG23	1.76	0.68
1:B:1011:GLU:HG3	1:B:1055:SER:OG	1.94	0.68
1:A:242:ASN:HB2	1:A:245:ASN:O	1.94	0.67
1:A:571:LEU:HA	1:A:593:ALA:O	1.94	0.67
1:A:1110:ASN:HB2	1:A:1111:TYR:CD2	2.28	0.67
1:A:356:LEU:HG	1:A:452:TYR:CZ	2.29	0.67
1:B:539:ARG:NH1	1:B:631:ASP:OD1	2.27	0.67
1:B:356:LEU:HG	1:B:452:TYR:CZ	2.29	0.67
1:A:1228:TRP:N	1:A:1228:TRP:HE3	1.92	0.67
1:A:328:THR:HG23	1:A:339:GLU:HG3	1.76	0.67
1:A:494:ASP:C	1:A:496:ILE:HD12	2.15	0.67
1:B:473:HIS:N	1:B:473:HIS:CD2	2.62	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1612:VAL:CB	1:A:1615:ARG:HD2	2.19	0.67
1:B:1320:LYS:HG2	1:B:1342:LEU:HD12	1.74	0.67
1:A:377:ASP:O	1:A:379:LEU:N	2.27	0.67
1:B:855:PHE:CZ	1:B:894:HIS:HD2	2.09	0.67
1:A:1559:TYR:CE1	1:A:1622:LYS:O	2.47	0.67
1:A:54:ILE:HG23	1:A:105:GLU:O	1.94	0.67
1:A:1011:GLU:HG3	1:A:1055:SER:OG	1.94	0.67
1:B:1461:ILE:O	1:B:1461:ILE:HG22	1.95	0.67
1:A:1621:GLY:HA3	1:A:1637:TYR:OH	1.94	0.67
1:A:1649:PRO:C	1:A:1651:ASP:H	1.98	0.67
1:B:494:ASP:C	1:B:496:ILE:HD12	2.15	0.67
1:B:779:LEU:O	1:B:781:PRO:HD3	1.95	0.67
1:B:123:ASN:ND2	1:B:150:ASP:H	1.92	0.67
1:B:185:PHE:HB3	1:B:186:PRO:CD	2.25	0.67
1:A:589:SER:HA	1:A:787:GLN:HA	1.77	0.67
1:B:377:ASP:O	1:B:379:LEU:N	2.27	0.67
1:B:829:ILE:HG13	1:B:925:LYS:CG	2.24	0.67
1:B:271:ILE:HG22	1:B:272:ARG:N	2.10	0.67
1:B:44:TYR:CE1	1:B:497:THR:HG21	2.30	0.67
1:B:42:GLN:HG3	1:B:80:GLN:NE2	2.09	0.67
2:X:137:PHE:N	2:X:137:PHE:CD1	2.61	0.67
2:X:47:HIS:O	2:X:47:HIS:HD2	1.77	0.67
1:B:1027:THR:O	1:B:1027:THR:CG2	2.43	0.67
1:A:506:LYS:HZ2	1:A:536:PRO:HD2	1.58	0.67
1:B:54:ILE:HG23	1:B:105:GLU:O	1.95	0.67
1:B:571:LEU:HA	1:B:593:ALA:O	1.94	0.67
1:B:541:LEU:HD12	1:B:645:VAL:HG12	1.77	0.67
1:A:381:GLN:HE21	1:A:381:GLN:H	1.42	0.67
1:A:42:GLN:HG3	1:A:80:GLN:NE2	2.10	0.67
1:A:1084:ARG:NE	1:A:1088:GLN:OE1	2.27	0.67
1:A:488:PRO:O	1:A:491:PRO:HD2	1.94	0.67
2:Y:106:VAL:HG22	2:Y:163:LYS:HE3	1.77	0.67
1:A:71:VAL:HG23	1:A:71:VAL:O	1.94	0.67
1:B:589:SER:HA	1:B:787:GLN:HA	1.77	0.67
1:B:938:SER:O	1:B:940:SER:N	2.28	0.66
1:A:1232:LEU:HG	1:A:1233:GLN:HG2	1.76	0.66
1:B:24:VAL:HA	1:B:655:THR:OG1	1.95	0.66
1:A:1490:PRO:HB3	1:A:1509:TYR:O	1.95	0.66
1:A:101:TYR:HE1	1:A:116:ARG:CZ	2.09	0.66
1:A:163:PHE:HD1	1:A:163:PHE:H	1.41	0.66
1:A:1620:MET:O	1:A:1643:THR:HG23	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ILE:HD13	1:A:485:ILE:N	2.09	0.66
1:A:779:LEU:O	1:A:781:PRO:HD3	1.95	0.66
1:A:1538:GLU:HG3	1:A:1539:LEU:N	2.11	0.66
1:A:1427:SER:HB3	1:A:1492:THR:H	1.58	0.66
1:A:599:TRP:CZ3	1:A:779:LEU:HB2	2.30	0.66
1:B:142:LYS:HD3	1:B:775:TRP:CG	2.30	0.66
1:A:1520:CYS:SG	1:A:1526:LYS:HG3	2.35	0.66
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.31	0.66
1:A:976:ILE:HD12	1:A:1362:THR:HG23	1.77	0.66
1:B:243:PHE:CZ	1:B:316:GLU:HB2	2.31	0.66
2:Y:47:HIS:O	2:Y:47:HIS:HD2	1.79	0.66
1:A:284:GLN:NE2	1:A:310:LEU:HD22	2.10	0.66
1:A:1599:THR:HG22	1:A:1600:PHE:N	2.11	0.66
1:B:488:PRO:O	1:B:491:PRO:HD2	1.96	0.66
1:A:356:LEU:HD12	1:A:452:TYR:CD1	2.31	0.66
1:B:284:GLN:OE1	1:B:310:LEU:HB3	1.96	0.66
1:B:959:PHE:N	1:B:959:PHE:CD2	2.64	0.66
1:B:1232:LEU:HG	1:B:1233:GLN:HG2	1.78	0.66
1:A:24:VAL:HA	1:A:655:THR:OG1	1.95	0.66
1:B:160:VAL:O	1:B:160:VAL:CG1	2.43	0.66
1:B:328:THR:HG23	1:B:339:GLU:HG3	1.77	0.66
1:B:584:PRO:HG2	1:B:821:LYS:HB2	1.77	0.66
1:A:234:GLU:HG2	1:A:235:TYR:CE2	2.30	0.66
1:A:1577:TYR:C	1:A:1578:LYS:HG2	2.14	0.66
1:B:532:GLN:O	1:B:535:VAL:HG22	1.96	0.66
1:B:1361:VAL:CG1	1:B:1361:VAL:O	2.44	0.66
1:A:1361:VAL:CG1	1:A:1361:VAL:O	2.43	0.66
1:A:1577:TYR:O	1:A:1578:LYS:HG2	1.95	0.66
1:B:536:PRO:HG3	1:B:624:PHE:HE2	1.60	0.66
1:B:163:PHE:HD1	1:B:163:PHE:H	1.43	0.66
1:B:560:TRP:CZ3	1:B:562:ASN:HB2	2.31	0.66
2:X:106:VAL:HG22	2:X:163:LYS:HE3	1.76	0.66
1:B:71:VAL:HG23	1:B:71:VAL:O	1.95	0.66
1:B:1340:VAL:HG21	1:B:1346:LEU:HD22	1.78	0.65
1:B:855:PHE:HE2	1:B:888:VAL:HG13	1.61	0.65
1:B:618:LYS:HG3	1:B:621:GLU:OE1	1.96	0.65
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.11	0.65
1:B:367:ILE:HG21	1:B:466:TYR:HD2	1.56	0.65
1:B:485:ILE:N	1:B:485:ILE:HD13	2.10	0.65
1:B:1514:ILE:CG2	1:B:1516:ILE:HG12	2.26	0.65
1:A:707:ASN:HB3	1:A:739:ARG:NH2	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1144:LEU:O	1:B:1148:THR:HG22	1.96	0.65
1:B:492:TYR:HD2	1:B:493:ILE:N	1.92	0.65
1:B:531:THR:HG22	1:B:534:MET:HG3	1.79	0.65
1:B:1438:ASP:OD2	1:B:1478:ARG:HG3	1.97	0.65
1:A:1630:ASN:O	1:A:1631:PHE:HB2	1.96	0.65
1:B:1348:VAL:HG11	1:B:1359:VAL:HG21	1.79	0.65
1:A:1068:VAL:HA	1:A:1078:LEU:HD13	1.78	0.65
1:B:123:ASN:N	1:B:211:THR:HG23	2.11	0.65
2:Y:190:ILE:HG23	2:Y:225:SER:O	1.97	0.65
2:X:73:VAL:HG23	2:X:74:ARG:H	1.61	0.65
1:B:1274:LEU:O	1:B:1276:GLU:N	2.29	0.65
1:A:583:SER:OG	1:A:586:GLN:HB2	1.96	0.65
1:A:894:HIS:CD2	1:A:895:LEU:O	2.48	0.65
1:A:439:ALA:HB3	1:A:447:GLN:NE2	2.05	0.65
1:A:1427:SER:CB	1:A:1491:ALA:HB1	2.26	0.65
1:A:120:THR:HG22	1:A:121:TYR:N	2.12	0.65
1:B:284:GLN:NE2	1:B:310:LEU:HD22	2.11	0.65
1:A:1027:THR:O	1:A:1027:THR:CG2	2.44	0.65
1:B:827:MET:HG3	1:B:912:PHE:CD2	2.31	0.65
1:B:934:VAL:HG22	1:B:1366:HIS:CD2	2.31	0.65
2:X:140:LYS:O	2:X:146:LEU:HA	1.97	0.65
2:X:87:LEU:HA	2:X:91:LYS:HD3	1.78	0.65
1:A:1274:LEU:O	1:A:1276:GLU:N	2.29	0.65
1:A:1624:ALA:CB	1:A:1636:ILE:HA	2.26	0.65
1:A:541:LEU:HD12	1:A:645:VAL:HG12	1.78	0.65
2:Y:87:LEU:HA	2:Y:91:LYS:HD3	1.78	0.65
1:B:505:SER:HB3	1:B:510:ILE:HD11	1.79	0.65
1:A:1019:PHE:HE2	1:A:1088:GLN:HE21	1.44	0.65
1:B:1024:TYR:HB2	1:B:1298:THR:CG2	2.27	0.65
1:A:1024:TYR:HB2	1:A:1298:THR:CG2	2.26	0.65
1:B:493:ILE:CG2	1:B:494:ASP:N	2.59	0.65
1:A:157:ARG:H	1:A:178:ASP:HB3	1.61	0.65
2:Y:140:LYS:O	2:Y:146:LEU:HA	1.96	0.65
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.62	0.65
1:B:1236:ASP:HB2	1:B:1412:ARG:HH22	1.61	0.65
1:A:1548:ARG:HA	1:A:1548:ARG:HE	1.61	0.65
1:A:1673:LEU:CD1	1:B:258:LYS:HE3	2.27	0.65
1:A:253:ARG:HB2	1:A:253:ARG:CZ	2.27	0.65
1:A:1378:TYR:CE1	1:A:1409:LYS:HE3	2.31	0.65
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.31	0.65
1:B:237:PHE:N	1:B:237:PHE:CD2	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:976:ILE:HD12	1:B:1362:THR:HG23	1.78	0.65
1:A:271:ILE:HG22	1:A:272:ARG:N	2.09	0.65
1:B:23:TYR:O	1:B:655:THR:HG23	1.97	0.65
2:Y:165:LEU:O	2:Y:169:ILE:HG12	1.96	0.65
2:X:86:LEU:HG	2:X:91:LYS:HG3	1.79	0.65
1:B:208:ASP:O	1:B:209:PHE:HB2	1.96	0.65
1:A:385:GLY:N	1:A:411:THR:HG23	2.12	0.65
1:B:1490:PRO:HB3	1:B:1509:TYR:O	1.97	0.65
1:A:123:ASN:N	1:A:211:THR:HG23	2.10	0.65
1:A:938:SER:O	1:A:940:SER:N	2.30	0.64
1:A:1647:TYR:O	1:A:1649:PRO:HD3	1.98	0.64
1:A:886:GLN:HG2	1:A:894:HIS:HD1	1.56	0.64
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.32	0.64
1:A:885:ARG:NH1	1:A:1628:LYS:HD3	2.11	0.64
2:X:190:ILE:HG23	2:X:225:SER:O	1.97	0.64
1:B:717:ARG:NH1	1:B:1447:ASP:O	2.27	0.64
1:B:153:LYS:HB3	1:B:154:PRO:HD2	1.78	0.64
1:B:120:THR:HG22	1:B:121:TYR:N	2.12	0.64
1:A:584:PRO:HG2	1:A:821:LYS:HB2	1.79	0.64
1:B:1180:LEU:HD21	1:B:1208:ILE:HA	1.79	0.64
1:A:356:LEU:CD1	1:A:452:TYR:CD1	2.80	0.64
1:B:386:VAL:HG23	1:B:411:THR:HG21	1.79	0.64
1:A:835:ARG:HG2	1:A:835:ARG:NH1	2.02	0.64
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.31	0.64
1:A:493:ILE:CG2	1:A:494:ASP:N	2.59	0.64
1:B:707:ASN:HB3	1:B:739:ARG:NH2	2.12	0.64
1:A:1144:LEU:O	1:A:1148:THR:HG22	1.97	0.64
1:B:1180:LEU:HD11	1:B:1208:ILE:N	2.13	0.64
1:B:390:LEU:O	1:B:390:LEU:HG	1.97	0.64
2:X:165:LEU:O	2:X:169:ILE:HG12	1.97	0.64
1:B:618:LYS:HB3	1:B:621:GLU:HB3	1.79	0.64
2:Y:138:VAL:HG11	2:Y:177:TYR:CD2	2.32	0.64
1:B:1084:ARG:NE	1:B:1088:GLN:OE1	2.29	0.64
1:A:1563:VAL:HG22	1:A:1619:ILE:HD13	1.79	0.64
1:B:1053:MET:CE	1:B:1086:LEU:HD22	2.28	0.64
1:B:356:LEU:HD12	1:B:452:TYR:CD1	2.32	0.64
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.27	0.64
1:B:1156:PHE:CZ	1:B:1160:PRO:HA	2.32	0.64
1:A:653:PHE:CZ	1:A:660:ASP:HA	2.33	0.64
1:B:1280:TYR:HD2	1:B:1281:GLY:N	1.96	0.64
1:B:1056:ILE:HD11	1:B:1066:TYR:HE2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:NH1	1:A:631:ASP:OD1	2.31	0.64
1:A:618:LYS:HB2	1:A:621:GLU:HB3	1.79	0.64
2:Y:78:LYS:NZ	2:Y:79:ASP:HB2	2.13	0.64
1:B:253:ARG:CZ	1:B:253:ARG:HB2	2.26	0.64
1:B:1142:LEU:HD13	1:B:1187:THR:HG22	1.79	0.64
1:B:231:ILE:HD12	1:B:327:VAL:CG2	2.28	0.64
2:Y:86:LEU:HG	2:Y:91:LYS:HG3	1.80	0.64
1:B:782:ARG:O	1:B:783:ARG:HG3	1.98	0.64
1:B:1016:VAL:HB	1:B:1017:PRO:HD3	1.79	0.64
1:B:1280:TYR:C	1:B:1280:TYR:CD2	2.70	0.64
1:A:1639:LEU:HD11	1:A:1645:ILE:HG21	1.78	0.64
1:A:505:SER:HB3	1:A:510:ILE:HD11	1.79	0.64
1:B:610:TYR:HB2	1:B:614:ARG:HD2	1.79	0.64
2:Y:58:SER:HB3	2:Y:102:ASN:ND2	2.13	0.64
1:B:1056:ILE:HD11	1:B:1066:TYR:CE2	2.33	0.64
1:B:234:GLU:HG2	1:B:235:TYR:CE2	2.32	0.64
1:A:1629:TYR:CE1	1:A:1632:SER:HA	2.33	0.64
1:A:361:LEU:O	1:A:454:ALA:HA	1.98	0.64
1:B:466:TYR:C	1:B:466:TYR:CD1	2.70	0.64
1:A:531:THR:HG22	1:A:534:MET:HG3	1.80	0.64
1:B:377:ASP:C	1:B:379:LEU:H	2.02	0.64
1:A:952:THR:OG1	1:A:953:ILE:N	2.29	0.64
1:B:1244:THR:HG22	1:B:1246:ARG:N	2.13	0.64
2:X:103:VAL:HG22	2:X:122:VAL:HG22	1.79	0.64
2:Y:75:PHE:O	2:Y:77:PRO:HD3	1.98	0.64
1:A:1115:ASN:HD22	1:A:1116:GLY:N	1.96	0.64
1:A:968:VAL:HG23	1:A:971:THR:CG2	2.28	0.64
1:B:857:VAL:HG21	1:B:896:VAL:CG1	2.27	0.64
1:A:885:ARG:CG	1:A:1626:GLN:HB2	2.27	0.64
2:X:73:VAL:HG22	2:X:84:LEU:HB3	1.80	0.64
1:B:577:PRO:HD2	1:B:588:VAL:HG23	1.80	0.64
1:A:392:ALA:HB1	1:A:431:LEU:HD21	1.79	0.64
1:B:439:ALA:HB3	1:B:447:GLN:NE2	2.09	0.63
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.17	0.63
1:B:354:LEU:HD21	1:B:448:ALA:O	1.99	0.63
1:B:249:THR:HG23	1:B:298:GLN:CG	2.28	0.63
1:B:109:LYS:HD2	1:B:110:HIS:N	2.13	0.63
2:Y:137:PHE:CD1	2:Y:137:PHE:N	2.62	0.63
1:B:392:ALA:HB1	1:B:431:LEU:HD21	1.78	0.63
1:B:583:SER:OG	1:B:586:GLN:HB2	1.98	0.63
1:B:149:ASN:N	1:B:155:ALA:HB2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:LEU:HD13	1:B:819:VAL:CG1	2.29	0.63
1:A:284:GLN:OE1	1:A:310:LEU:HB3	1.97	0.63
1:A:128:ILE:HB	1:A:215:ALA:HB2	1.80	0.63
1:A:109:LYS:HD2	1:A:110:HIS:N	2.13	0.63
1:B:618:LYS:HB2	1:B:621:GLU:HB3	1.78	0.63
1:A:857:VAL:HG21	1:A:896:VAL:CG1	2.28	0.63
1:B:1427:SER:CB	1:B:1491:ALA:HB1	2.27	0.63
1:A:586:GLN:O	1:A:789:ALA:HA	1.98	0.63
1:A:1461:ILE:O	1:A:1461:ILE:HG22	1.98	0.63
1:A:600:VAL:HG12	1:A:601:ALA:H	1.63	0.63
1:A:959:PHE:CD2	1:A:959:PHE:N	2.65	0.63
2:Y:41:HIS:O	2:Y:42:ASP:HB2	1.98	0.63
1:B:1239:VAL:HG23	1:B:1239:VAL:O	1.98	0.63
1:B:1008:ALA:HB2	1:B:1059:TYR:CD2	2.33	0.63
1:A:609:VAL:HG23	1:A:610:TYR:CD2	2.33	0.63
1:B:586:GLN:O	1:B:789:ALA:HA	1.99	0.63
1:B:361:LEU:O	1:B:454:ALA:HA	1.98	0.63
1:B:1286:SER:OG	1:B:1287:THR:N	2.27	0.63
1:A:940:SER:HB2	1:A:959:PHE:HD1	1.63	0.63
1:B:41:ILE:O	1:B:80:GLN:HA	1.98	0.63
2:X:75:PHE:O	2:X:77:PRO:HD3	1.98	0.63
1:A:639:GLY:HA3	1:A:645:VAL:N	2.12	0.63
1:A:99:VAL:HB	1:A:121:TYR:OH	1.99	0.63
2:X:170:ARG:O	2:X:174:VAL:HG23	1.98	0.63
1:A:41:ILE:O	1:A:80:GLN:HA	1.99	0.63
1:B:1247:MET:O	1:B:1251:THR:HG23	1.99	0.63
2:X:41:HIS:O	2:X:42:ASP:HB2	1.99	0.63
1:B:1202:HIS:HD2	1:B:1204:GLN:H	1.47	0.63
1:B:157:ARG:H	1:B:178:ASP:HB3	1.62	0.63
1:B:182:ILE:HG13	1:B:804:ILE:HD11	1.81	0.63
1:A:1236:ASP:HB2	1:A:1412:ARG:HH22	1.64	0.63
1:A:1180:LEU:HD21	1:A:1208:ILE:HA	1.81	0.63
1:B:700:TYR:CE1	1:B:758:LEU:HB2	2.33	0.63
1:A:489:LYS:C	1:A:491:PRO:HD2	2.19	0.63
1:A:544:TYR:HD1	1:A:544:TYR:H	1.46	0.63
1:B:653:PHE:CZ	1:B:660:ASP:HA	2.33	0.63
1:A:208:ASP:O	1:A:209:PHE:HB2	1.97	0.63
2:X:131:GLU:O	2:X:131:GLU:HG2	1.98	0.63
2:X:78:LYS:HD2	2:X:78:LYS:O	1.99	0.62
1:A:546:VAL:HG12	1:A:546:VAL:O	1.98	0.62
1:A:377:ASP:C	1:A:379:LEU:H	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HB	1:B:215:ALA:HB2	1.81	0.62
1:A:1238:SER:C	1:A:1240:PRO:HD3	2.20	0.62
2:Y:131:GLU:HG2	2:Y:131:GLU:O	1.97	0.62
1:A:895:LEU:HD13	1:A:1555:PRO:CB	2.26	0.62
1:B:1229:LYS:HD2	1:B:1239:VAL:CG1	2.23	0.62
1:B:1244:THR:HB	1:B:1247:MET:HB2	1.81	0.62
1:A:610:TYR:CB	1:A:614:ARG:HD2	2.29	0.62
1:A:492:TYR:HD2	1:A:493:ILE:N	1.90	0.62
1:A:790:LEU:HD13	1:A:819:VAL:CG1	2.29	0.62
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.80	0.62
1:A:909:ASN:N	1:A:926:THR:HG22	2.14	0.62
1:A:31:PHE:HA	1:A:37:GLU:OE2	1.99	0.62
1:A:1566:THR:HG21	1:A:1580:THR:OG1	1.99	0.62
1:B:1332:ASN:CG	1:B:1332:ASN:O	2.37	0.62
1:A:1671:ILE:HG23	1:A:1672:PHE:N	2.14	0.62
1:A:23:TYR:CA	1:A:43:VAL:HG23	2.29	0.62
1:A:442:LEU:HB2	1:A:447:GLN:HE22	1.64	0.62
1:B:1019:PHE:HE2	1:B:1088:GLN:HE21	1.47	0.62
2:Y:103:VAL:HG22	2:Y:122:VAL:HG22	1.81	0.62
2:X:140:LYS:O	2:X:146:LEU:HD23	1.99	0.62
1:A:195:ARG:NH2	1:A:1060:ARG:O	2.32	0.62
1:A:171:VAL:HG13	1:A:1057:MET:HE2	1.80	0.62
1:A:261:THR:HG22	1:A:262:GLU:N	2.12	0.62
1:B:395:ILE:HG22	1:B:401:THR:HG22	1.81	0.62
1:A:618:LYS:HG3	1:A:621:GLU:OE1	1.97	0.62
1:A:1239:VAL:HG23	1:A:1239:VAL:O	1.98	0.62
1:B:610:TYR:CB	1:B:614:ARG:HD2	2.30	0.62
2:X:58:SER:HB3	2:X:102:ASN:ND2	2.14	0.62
1:A:1156:PHE:CZ	1:A:1160:PRO:HA	2.33	0.62
2:Y:140:LYS:O	2:Y:146:LEU:HD23	1.98	0.62
1:B:599:TRP:CH2	1:B:779:LEU:HD13	2.34	0.62
1:B:30:ILE:HG22	1:B:31:PHE:O	1.99	0.62
1:A:1599:THR:CG2	1:A:1600:PHE:N	2.63	0.62
1:A:1594:LYS:O	1:A:1595:ASP:HB2	1.98	0.62
1:B:356:LEU:CD1	1:B:452:TYR:CD1	2.82	0.62
1:A:782:ARG:O	1:A:783:ARG:HG3	1.99	0.62
1:A:390:LEU:HG	1:A:390:LEU:O	1.99	0.62
1:A:330:ILE:HG22	1:A:337:SER:CB	2.30	0.62
1:B:84:ILE:HD11	2:Y:135:PRO:HG3	1.81	0.62
1:A:395:ILE:HG22	1:A:401:THR:HG22	1.81	0.62
1:A:1332:ASN:O	1:A:1332:ASN:CG	2.37	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1280:TYR:CD2	1:B:1281:GLY:N	2.67	0.62
1:B:838:GLN:HB3	1:B:1486:GLY:HA3	1.81	0.62
1:B:987:ILE:CD1	1:B:1294:ILE:HD13	2.17	0.62
1:A:536:PRO:HG3	1:A:624:PHE:HE2	1.63	0.62
1:B:600:VAL:HG12	1:B:601:ALA:H	1.63	0.62
2:X:47:HIS:O	2:X:47:HIS:CD2	2.53	0.62
1:B:952:THR:OG1	1:B:953:ILE:N	2.30	0.62
1:A:700:TYR:CE1	1:A:758:LEU:HB2	2.34	0.62
1:B:1238:SER:C	1:B:1240:PRO:HD3	2.20	0.62
1:B:261:THR:HG22	1:B:262:GLU:N	2.13	0.62
1:A:367:ILE:HG21	1:A:466:TYR:HD2	1.59	0.62
1:A:1180:LEU:HD11	1:A:1208:ILE:N	2.14	0.62
1:B:285:THR:HG23	1:B:681:LYS:HD3	1.82	0.62
1:A:1372:GLU:HG3	1:A:1373:GLU:H	1.65	0.62
1:B:894:HIS:CE1	1:B:895:LEU:O	2.52	0.62
2:X:138:VAL:HG11	2:X:177:TYR:CD2	2.33	0.62
1:B:1096:ASN:ND2	1:B:1099:SER:N	2.38	0.62
1:A:1518:LYS:HE2	1:A:1529:GLU:OE2	2.00	0.62
1:A:247:GLU:HG2	1:A:298:GLN:OE1	1.99	0.62
1:A:1262:LYS:O	1:A:1264:ILE:HG13	2.00	0.62
1:A:940:SER:OG	1:A:1361:VAL:HG12	2.00	0.62
1:A:618:LYS:HB3	1:A:621:GLU:HB3	1.80	0.62
1:A:497:THR:HG23	1:A:498:HIS:N	2.14	0.62
2:Y:189:ILE:HG23	2:Y:226:VAL:HG22	1.82	0.62
1:A:249:THR:HG23	1:A:298:GLN:CG	2.29	0.62
1:A:1202:HIS:HD2	1:A:1204:GLN:H	1.47	0.62
1:A:610:TYR:HB2	1:A:614:ARG:HD2	1.82	0.62
1:A:222:TYR:CD2	1:A:222:TYR:C	2.73	0.62
2:Y:78:LYS:C	2:Y:78:LYS:HD2	2.21	0.62
1:A:984:VAL:HG11	1:A:1024:TYR:CE1	2.34	0.62
1:B:31:PHE:HA	1:B:37:GLU:OE2	1.99	0.62
1:A:23:TYR:O	1:A:655:THR:HG23	1.99	0.61
2:X:78:LYS:HD2	2:X:78:LYS:C	2.20	0.61
1:B:99:VAL:HB	1:B:121:TYR:OH	1.99	0.61
2:X:68:ASN:OD1	2:X:69:GLY:N	2.30	0.61
1:B:909:ASN:N	1:B:926:THR:HG22	2.15	0.61
2:Y:208:GLN:O	2:Y:212:MET:HG3	2.00	0.61
1:A:895:LEU:CD1	1:A:1555:PRO:HB2	2.28	0.61
2:X:78:LYS:NZ	2:X:79:ASP:HB2	2.15	0.61
1:B:1132:THR:H	1:B:1135:VAL:HB	1.65	0.61
1:B:968:VAL:HG23	1:B:971:THR:CG2	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:189:ILE:HG23	2:X:226:VAL:HG22	1.83	0.61
1:B:1303:LEU:HD13	1:B:1303:LEU:C	2.20	0.61
2:X:208:GLN:O	2:X:212:MET:HG3	2.00	0.61
2:Y:73:VAL:HG12	2:Y:74:ARG:N	2.14	0.61
1:B:1115:ASN:HD22	1:B:1116:GLY:N	1.98	0.61
1:A:473:HIS:CD2	1:A:473:HIS:N	2.67	0.61
1:B:385:GLY:N	1:B:411:THR:HG23	2.16	0.61
1:A:442:LEU:CB	1:A:447:GLN:NE2	2.63	0.61
1:A:1202:HIS:CD2	1:A:1203:PRO:CD	2.81	0.61
2:Y:78:LYS:HD2	2:Y:78:LYS:O	2.00	0.61
1:A:1303:LEU:C	1:A:1303:LEU:HD13	2.21	0.61
1:A:237:PHE:CD2	1:A:237:PHE:N	2.66	0.61
1:B:940:SER:HB2	1:B:959:PHE:HD1	1.64	0.61
1:A:1565:ILE:HD12	1:A:1565:ILE:H	1.66	0.61
1:A:1576:LYS:N	1:A:1576:LYS:HD2	2.15	0.61
1:B:544:TYR:HD1	1:B:544:TYR:H	1.47	0.61
1:B:702:GLY:HA2	1:B:728:PHE:HE1	1.65	0.61
1:A:599:TRP:CH2	1:A:779:LEU:HD13	2.34	0.61
1:A:182:ILE:HG13	1:A:804:ILE:HD11	1.82	0.61
1:B:770:PRO:HG2	1:B:795:THR:HG21	1.82	0.61
1:B:796:THR:HA	1:B:818:LYS:HA	1.82	0.61
1:B:1433:SER:HB2	1:B:1480:PHE:CD1	2.35	0.61
1:B:1464:LEU:N	1:B:1464:LEU:HD12	2.15	0.61
1:A:1577:TYR:CE2	1:A:1611:LEU:HD11	2.35	0.61
1:B:101:TYR:CE1	1:B:116:ARG:CZ	2.83	0.61
1:A:984:VAL:HG13	1:A:984:VAL:O	2.00	0.61
1:A:490:SER:O	1:A:491:PRO:C	2.39	0.61
1:B:1372:GLU:HG3	1:B:1373:GLU:H	1.64	0.61
1:B:1486:GLY:O	1:B:1488:LEU:N	2.33	0.61
1:A:367:ILE:HD13	1:A:466:TYR:HB2	1.81	0.61
1:B:609:VAL:HG23	1:B:610:TYR:CD2	2.35	0.61
1:A:1132:THR:H	1:A:1135:VAL:HB	1.65	0.61
1:A:1520:CYS:HA	1:A:1525:CYS:CB	2.30	0.61
1:A:1557:ILE:HG23	1:A:1559:TYR:O	2.00	0.61
1:A:350:SER:HB2	1:A:446:ASN:O	1.99	0.61
1:A:571:LEU:C	1:A:571:LEU:HD12	2.21	0.61
1:B:1024:TYR:CD2	1:B:1024:TYR:C	2.74	0.61
1:A:149:ASN:N	1:A:155:ALA:HB2	2.16	0.61
1:A:153:LYS:HB3	1:A:154:PRO:HD2	1.82	0.61
1:A:1516:ILE:HD12	1:A:1516:ILE:O	2.01	0.61
2:Y:47:HIS:CD2	2:Y:47:HIS:O	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:ILE:HD12	1:B:528:ILE:H	1.65	0.61
1:A:1016:VAL:HB	1:A:1017:PRO:HD3	1.83	0.61
1:A:884:VAL:HG12	1:A:1625:LEU:HB3	1.83	0.61
1:A:1247:MET:O	1:A:1251:THR:HG23	2.00	0.61
1:B:251:LYS:HG2	1:B:296:ILE:HD13	1.82	0.61
1:B:707:ASN:HB3	1:B:739:ARG:HH12	1.66	0.61
1:B:1274:LEU:C	1:B:1276:GLU:H	2.04	0.61
1:B:323:LEU:HD13	1:B:323:LEU:C	2.22	0.61
1:B:950:TYR:CE2	1:B:1356:LEU:HD11	2.35	0.61
1:A:1636:ILE:CG1	1:A:1637:TYR:N	2.64	0.60
1:A:1244:THR:HB	1:A:1247:MET:HB2	1.82	0.60
1:B:489:LYS:C	1:B:491:PRO:HD2	2.20	0.60
2:Y:170:ARG:O	2:Y:174:VAL:HG23	2.00	0.60
1:A:307:VAL:HG12	1:A:313:TYR:O	2.01	0.60
1:B:1174:PHE:O	1:B:1178:ASN:HB2	2.01	0.60
1:A:1183:GLN:OE1	1:A:1183:GLN:HA	2.01	0.60
1:B:639:GLY:HA3	1:B:645:VAL:N	2.15	0.60
1:B:700:TYR:HE1	1:B:758:LEU:HB2	1.66	0.60
1:A:796:THR:HA	1:A:818:LYS:HA	1.83	0.60
2:Y:68:ASN:OD1	2:Y:69:GLY:N	2.30	0.60
1:A:1558:ALA:O	1:A:1559:TYR:HB3	2.00	0.60
1:B:272:ARG:HB3	1:B:322:TYR:HB2	1.84	0.60
1:A:982:LEU:CD2	1:A:982:LEU:N	2.64	0.60
1:B:381:GLN:H	1:B:381:GLN:HE21	1.47	0.60
1:B:237:PHE:N	1:B:237:PHE:HD2	1.99	0.60
1:B:330:ILE:HG22	1:B:337:SER:CB	2.31	0.60
1:A:272:ARG:HB3	1:A:322:TYR:HB2	1.83	0.60
1:B:1244:THR:CG2	1:B:1247:MET:H	2.15	0.60
2:X:205:ASP:OD2	2:X:207:LEU:HB2	2.02	0.60
1:B:367:ILE:HD13	1:B:466:TYR:HB2	1.84	0.60
1:B:546:VAL:HG12	1:B:546:VAL:O	2.01	0.60
1:B:829:ILE:HG22	1:B:830:PRO:CD	2.32	0.60
1:B:988:LEU:HD23	1:B:1021:VAL:HG22	1.83	0.60
1:B:1267:VAL:O	1:B:1270:VAL:HB	2.02	0.60
1:A:839:ILE:HG22	1:A:900:VAL:HG23	1.84	0.60
1:B:984:VAL:HG11	1:B:1024:TYR:CE1	2.37	0.60
1:B:982:LEU:N	1:B:982:LEU:CD2	2.62	0.60
1:B:491:PRO:O	1:B:493:ILE:N	2.35	0.60
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.36	0.60
1:B:195:ARG:NH2	1:B:1060:ARG:O	2.34	0.60
1:A:88:GLN:HB3	1:A:89:PRO:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ILE:HG22	1:A:830:PRO:CD	2.32	0.60
1:B:673:LEU:O	1:B:673:LEU:HG	2.02	0.60
1:B:392:ALA:HB3	1:B:404:LEU:HD12	1.84	0.60
1:A:770:PRO:HG2	1:A:795:THR:HG21	1.82	0.60
1:A:1650:ARG:O	1:A:1652:THR:HG23	2.02	0.60
1:A:1229:LYS:HD2	1:A:1239:VAL:CG1	2.22	0.60
1:B:23:TYR:CA	1:B:43:VAL:HG23	2.30	0.60
1:B:497:THR:HG23	1:B:498:HIS:N	2.15	0.60
1:B:1202:HIS:CD2	1:B:1203:PRO:CD	2.80	0.60
1:B:490:SER:O	1:B:491:PRO:C	2.39	0.60
1:A:494:ASP:O	1:A:496:ILE:HD12	2.00	0.60
1:A:231:ILE:HD12	1:A:327:VAL:CG2	2.31	0.60
1:A:285:THR:HG23	1:A:681:LYS:HD3	1.83	0.60
1:A:208:ASP:O	1:A:209:PHE:CB	2.50	0.60
1:A:30:ILE:HG22	1:A:31:PHE:O	2.01	0.60
1:A:198:MET:HA	1:A:198:MET:HE2	1.84	0.60
1:B:1429:PRO:HB2	1:B:1432:ILE:HG13	1.83	0.60
1:A:739:ARG:HD3	1:A:754:MET:SD	2.42	0.60
1:B:1016:VAL:CB	1:B:1017:PRO:HD3	2.32	0.60
1:B:22:THR:O	1:B:43:VAL:HG23	2.02	0.60
1:B:984:VAL:HG13	1:B:984:VAL:O	2.01	0.60
1:B:739:ARG:HD3	1:B:754:MET:SD	2.42	0.60
1:A:749:LEU:HG	1:A:750:GLY:H	1.66	0.60
2:X:132:THR:HG22	2:X:155:ILE:HB	1.83	0.60
1:A:1433:SER:HB2	1:A:1480:PHE:CD1	2.37	0.60
1:A:1673:LEU:HD13	1:B:258:LYS:HE3	1.84	0.59
1:A:1008:ALA:HB2	1:A:1059:TYR:CD2	2.36	0.59
1:B:571:LEU:C	1:B:571:LEU:HD12	2.21	0.59
1:A:101:TYR:CE1	1:A:116:ARG:CZ	2.85	0.59
1:B:1341:LEU:HB3	1:B:1342:LEU:HD23	1.84	0.59
1:B:1156:PHE:CE1	1:B:1160:PRO:HA	2.37	0.59
1:B:749:LEU:HG	1:B:750:GLY:H	1.67	0.59
1:B:695:VAL:HA	1:B:698:CYS:HB2	1.84	0.59
1:B:428:VAL:HG22	1:B:429:THR:H	1.67	0.59
1:A:528:ILE:H	1:A:528:ILE:HD12	1.67	0.59
1:A:617:LYS:O	1:A:618:LYS:CG	2.46	0.59
1:B:236:ASN:C	1:B:237:PHE:CD2	2.75	0.59
1:B:884:VAL:O	1:B:884:VAL:HG23	2.02	0.59
2:Y:132:THR:HG22	2:Y:155:ILE:HB	1.84	0.59
1:B:1423:VAL:HG12	1:B:1463:GLN:HG2	1.83	0.59
1:A:354:LEU:HD21	1:A:448:ALA:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:987:ILE:CD1	1:A:1294:ILE:HD13	2.17	0.59
1:A:1142:LEU:HD13	1:A:1187:THR:HG22	1.82	0.59
1:B:1445:GLY:O	1:B:1448:GLN:N	2.36	0.59
1:A:1320:LYS:HG2	1:A:1342:LEU:CD1	2.32	0.59
1:B:1053:MET:O	1:B:1056:ILE:HG23	2.02	0.59
1:A:1274:LEU:C	1:A:1276:GLU:H	2.05	0.59
1:A:1536:GLN:CD	1:A:1644:TRP:CH2	2.76	0.59
1:B:1496:TYR:O	1:B:1496:TYR:HD1	1.86	0.59
1:A:466:TYR:CD1	1:A:466:TYR:C	2.71	0.59
1:A:1255:LEU:HB2	1:A:1270:VAL:HG11	1.84	0.59
1:A:1267:VAL:O	1:A:1270:VAL:HB	2.02	0.59
1:A:123:ASN:C	1:A:123:ASN:ND2	2.52	0.59
1:A:1118:PHE:O	1:A:1144:LEU:HD23	2.02	0.59
1:B:1320:LYS:HG2	1:B:1342:LEU:CD1	2.31	0.59
1:A:284:GLN:OE1	1:A:284:GLN:N	2.35	0.59
1:A:428:VAL:HG22	1:A:429:THR:H	1.67	0.59
1:A:1280:TYR:CD2	1:A:1280:TYR:C	2.73	0.59
1:A:930:VAL:CG1	1:A:931:PRO:N	2.65	0.59
1:B:92:LEU:N	1:B:93:PRO:CD	2.66	0.59
1:B:215:ALA:C	1:B:216:TYR:CD2	2.76	0.59
1:A:700:TYR:HE1	1:A:758:LEU:HB2	1.67	0.59
1:A:357:VAL:O	1:A:359:THR:HG23	2.03	0.59
1:A:1608:ASN:O	1:A:1609:ALA:HB2	2.02	0.59
1:A:22:THR:O	1:A:43:VAL:HG23	2.03	0.59
1:A:982:LEU:HD23	1:A:1309:LEU:HD11	1.83	0.59
1:A:92:LEU:N	1:A:93:PRO:CD	2.65	0.59
1:B:470:THR:CG2	1:B:471:ASP:N	2.66	0.59
1:B:1262:LYS:O	1:B:1264:ILE:HG13	2.01	0.59
1:A:364:LYS:H	1:A:364:LYS:HD2	1.67	0.59
1:B:940:SER:OG	1:B:1361:VAL:HG12	2.03	0.59
1:A:1623:GLU:HG3	1:A:1624:ALA:N	2.18	0.59
1:A:1668:ALA:O	1:A:1671:ILE:HG22	2.03	0.59
1:A:258:LYS:NZ	1:A:1676:CYS:OXT	2.35	0.59
1:B:222:TYR:C	1:B:222:TYR:CD2	2.76	0.59
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.75	0.59
1:B:1118:PHE:O	1:B:1144:LEU:HD23	2.02	0.59
1:B:182:ILE:CG1	1:B:804:ILE:HD11	2.32	0.59
1:A:84:ILE:HD11	2:X:135:PRO:HG3	1.85	0.59
1:B:50:PHE:CB	1:B:109:LYS:HE2	2.33	0.59
1:A:1174:PHE:O	1:A:1178:ASN:HB2	2.03	0.59
2:X:150:ILE:HD12	2:X:150:ILE:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:150:ILE:HD12	2:Y:150:ILE:C	2.23	0.59
1:B:1019:PHE:CE2	1:B:1088:GLN:HB3	2.38	0.59
1:A:1019:PHE:CE2	1:A:1088:GLN:HB3	2.38	0.59
1:B:494:ASP:O	1:B:496:ILE:HD12	2.03	0.59
1:A:470:THR:CG2	1:A:471:ASP:N	2.65	0.59
1:A:1445:GLY:O	1:A:1448:GLN:N	2.35	0.59
1:B:1255:LEU:HB2	1:B:1270:VAL:HG11	1.85	0.59
1:A:695:VAL:HA	1:A:698:CYS:HB2	1.85	0.59
1:A:1654:CYS:O	1:A:1656:SER:N	2.35	0.59
1:A:1096:ASN:ND2	1:A:1099:SER:N	2.38	0.59
1:B:123:ASN:C	1:B:123:ASN:ND2	2.51	0.59
1:B:1127:ILE:HD12	1:B:1127:ILE:N	2.17	0.59
1:B:350:SER:HB2	1:B:446:ASN:O	2.03	0.59
1:A:707:ASN:HB3	1:A:739:ARG:HH12	1.66	0.59
1:A:1016:VAL:CB	1:A:1017:PRO:HD3	2.33	0.59
1:B:691:LYS:O	1:B:692:HIS:HB2	2.03	0.59
1:A:1589:GLU:HB2	1:A:1623:GLU:OE1	2.02	0.58
1:A:884:VAL:O	1:A:884:VAL:HG23	2.02	0.58
1:A:1244:THR:CG2	1:A:1247:MET:H	2.15	0.58
1:A:1228:TRP:H	1:A:1251:THR:CG2	2.16	0.58
1:B:1143:TYR:CD1	1:B:1186:PHE:HE2	2.21	0.58
1:B:823:VAL:HA	1:B:846:TYR:O	2.03	0.58
1:B:356:LEU:HG	1:B:452:TYR:CE1	2.38	0.58
1:A:934:VAL:HG12	1:A:934:VAL:O	2.03	0.58
1:B:208:ASP:O	1:B:209:PHE:CB	2.50	0.58
2:Y:136:LEU:HG	2:Y:136:LEU:O	2.02	0.58
2:X:67:TYR:CG	2:X:68:ASN:N	2.71	0.58
1:A:695:VAL:O	1:A:698:CYS:HB2	2.03	0.58
1:B:1028:GLY:O	1:B:1029:ASN:C	2.41	0.58
1:A:1535:MET:HB3	1:A:1645:ILE:CD1	2.32	0.58
1:B:491:PRO:C	1:B:493:ILE:N	2.54	0.58
1:A:491:PRO:O	1:A:493:ILE:N	2.36	0.58
2:X:170:ARG:HH21	2:X:201:ILE:CG2	2.15	0.58
1:B:82:SER:O	2:Y:137:PHE:HE2	1.86	0.58
1:B:359:THR:HG21	1:B:372:LYS:N	2.18	0.58
1:B:839:ILE:HG22	1:B:900:VAL:HG23	1.85	0.58
1:A:571:LEU:HG	1:A:812:ALA:HB2	1.85	0.58
1:A:840:GLN:HE22	1:A:842:LYS:HE2	1.68	0.58
1:A:1341:LEU:HB3	1:A:1342:LEU:HD23	1.83	0.58
1:A:1561:TYR:O	1:A:1561:TYR:HD2	1.87	0.58
1:A:440:PRO:HD2	1:A:441:ASP:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1525:CYS:O	1:B:1526:LYS:HG2	2.02	0.58
1:A:1053:MET:O	1:A:1056:ILE:HG23	2.04	0.58
1:B:284:GLN:N	1:B:284:GLN:OE1	2.36	0.58
2:Y:137:PHE:HD1	2:Y:137:PHE:N	2.01	0.58
1:A:1548:ARG:NH2	1:A:1644:TRP:CD1	2.72	0.58
1:A:545:ILE:HG23	1:A:554:LEU:CD2	2.33	0.58
1:A:1143:TYR:CD1	1:A:1186:PHE:HE2	2.21	0.58
1:B:96:GLN:O	1:B:98:PRO:CD	2.52	0.58
2:Y:170:ARG:HH21	2:Y:201:ILE:CG2	2.16	0.58
1:A:1280:TYR:CD2	1:A:1281:GLY:N	2.72	0.58
1:A:1663:ASN:HA	1:A:1666:GLU:HB3	1.86	0.58
2:X:46:LEU:HA	2:X:206:LYS:HZ1	1.68	0.58
1:A:536:PRO:HG3	1:A:624:PHE:CE2	2.39	0.58
1:A:1024:TYR:OH	1:A:1306:GLN:NE2	2.37	0.58
1:A:702:GLY:HA2	1:A:728:PHE:HE1	1.64	0.58
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.33	0.58
1:A:1308:ARG:HG2	1:A:1308:ARG:HH11	1.68	0.58
1:B:961:TYR:CE2	1:B:1343:ASN:HA	2.38	0.58
1:B:364:LYS:N	1:B:364:LYS:HD2	2.18	0.58
2:Y:205:ASP:OD2	2:Y:207:LEU:HB2	2.03	0.58
1:B:536:PRO:HG3	1:B:624:PHE:CE2	2.38	0.58
1:B:571:LEU:HG	1:B:812:ALA:HB2	1.85	0.58
1:A:823:VAL:HA	1:A:846:TYR:O	2.04	0.58
1:B:586:GLN:HG2	1:B:587:THR:O	2.03	0.58
1:B:815:VAL:O	1:B:815:VAL:HG12	2.04	0.58
1:B:1465:ASN:H	1:B:1465:ASN:ND2	2.02	0.58
1:A:1202:HIS:CD2	1:A:1204:GLN:HB3	2.39	0.58
1:A:1616:GLN:NE2	1:B:1521:GLU:OE1	2.37	0.58
1:A:1142:LEU:HD13	1:A:1187:THR:HG21	1.86	0.58
1:A:50:PHE:CB	1:A:109:LYS:HE2	2.33	0.58
1:B:429:THR:OG1	1:B:430:VAL:N	2.33	0.58
1:A:942:VAL:HG21	1:A:957:LYS:HB3	1.86	0.58
1:A:485:ILE:CD1	1:A:485:ILE:N	2.67	0.58
1:A:257:ASN:OD1	1:A:893:SER:O	2.22	0.58
1:B:1142:LEU:HD13	1:B:1187:THR:HG21	1.85	0.58
1:A:218:GLU:CD	1:A:220:LYS:HE2	2.23	0.58
1:A:696:LYS:HZ1	1:A:700:TYR:HD2	1.51	0.58
1:B:1205:PHE:HA	1:B:1208:ILE:HG13	1.86	0.57
1:A:356:LEU:HG	1:A:452:TYR:CE1	2.38	0.57
2:Y:132:THR:CG2	2:Y:155:ILE:HB	2.34	0.57
1:B:682:LYS:HD2	1:B:685:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLN:HB3	1:B:89:PRO:HD2	1.85	0.57
1:A:682:LYS:HD2	1:A:685:GLU:OE2	2.04	0.57
2:X:45:ASP:O	2:X:49:TYR:HD2	1.87	0.57
1:B:609:VAL:HG23	1:B:610:TYR:N	2.15	0.57
1:A:1449:LEU:HG	1:A:1450:PHE:CE1	2.39	0.57
2:Y:67:TYR:CG	2:Y:68:ASN:N	2.72	0.57
1:B:307:VAL:HG12	1:B:313:TYR:O	2.04	0.57
1:B:54:ILE:HG22	1:B:55:SER:N	2.19	0.57
2:X:137:PHE:N	2:X:137:PHE:HD1	2.00	0.57
1:B:1053:MET:HE2	1:B:1086:LEU:HD13	1.86	0.57
1:A:215:ALA:C	1:A:216:TYR:CD2	2.78	0.57
1:A:1585:TYR:CD1	1:A:1671:ILE:HG21	2.38	0.57
1:B:1213:LYS:NZ	1:B:1263:ASP:OD2	2.38	0.57
1:B:412:ARG:HB3	1:B:415:ASP:CB	2.33	0.57
1:A:1515:LYS:O	1:A:1516:ILE:HG23	2.04	0.57
1:B:961:TYR:HH	1:B:1343:ASN:CG	2.07	0.57
2:Y:73:VAL:CG1	2:Y:74:ARG:N	2.66	0.57
1:B:372:LYS:HA	1:B:419:SER:HA	1.86	0.57
2:X:107:GLN:HB3	2:X:116:LEU:HD22	1.86	0.57
1:A:488:PRO:O	1:A:489:LYS:O	2.22	0.57
1:A:1205:PHE:HA	1:A:1208:ILE:HG13	1.86	0.57
1:B:577:PRO:CD	1:B:588:VAL:HG23	2.33	0.57
1:B:758:LEU:C	1:B:760:VAL:H	2.08	0.57
1:A:236:ASN:C	1:A:237:PHE:CD2	2.77	0.57
1:B:1308:ARG:HG2	1:B:1308:ARG:HH11	1.70	0.57
1:B:1003:LEU:N	1:B:1003:LEU:HD23	2.18	0.57
1:A:1654:CYS:SG	1:A:1654:CYS:O	2.63	0.57
1:A:1216:ALA:HB2	1:A:1228:TRP:NE1	2.18	0.57
1:A:950:TYR:CE2	1:A:1356:LEU:HD11	2.39	0.57
1:B:1264:ILE:HG12	1:B:1303:LEU:HD11	1.86	0.57
1:B:1193:TYR:CD1	1:B:1256:LEU:HB3	2.40	0.57
1:A:123:ASN:C	1:A:211:THR:HG21	2.25	0.57
1:B:290:THR:O	1:B:291:MET:C	2.42	0.57
2:Y:166:ASP:CG	2:Y:201:ILE:HD13	2.25	0.57
1:A:961:TYR:CZ	1:A:1343:ASN:HA	2.39	0.57
1:A:600:VAL:HG12	1:A:601:ALA:N	2.19	0.57
1:A:691:LYS:O	1:A:692:HIS:HB2	2.03	0.57
1:A:1585:TYR:CG	1:A:1671:ILE:HG21	2.39	0.57
1:A:251:LYS:HG2	1:A:296:ILE:HD13	1.87	0.57
1:B:1030:HIS:O	1:B:1033:ILE:HG13	2.05	0.57
1:B:1024:TYR:OH	1:B:1306:GLN:NE2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:107:GLN:HB3	2:Y:116:LEU:HD22	1.87	0.57
1:A:491:PRO:C	1:A:493:ILE:N	2.55	0.57
1:B:266:TYR:CE2	1:B:755:LYS:HB2	2.39	0.57
1:A:758:LEU:C	1:A:760:VAL:H	2.08	0.57
1:B:359:THR:HG21	1:B:372:LYS:H	1.70	0.57
1:A:349:LEU:HD22	1:A:446:ASN:HD22	1.69	0.57
1:B:1228:TRP:HE3	1:B:1228:TRP:H	1.53	0.57
1:A:777:VAL:CG1	1:A:778:HIS:N	2.68	0.57
1:B:531:THR:CG2	1:B:534:MET:HG3	2.34	0.57
1:B:754:MET:O	1:B:755:LYS:HG2	2.05	0.57
1:A:142:LYS:HD3	1:A:775:TRP:CD1	2.40	0.57
2:X:132:THR:CG2	2:X:155:ILE:HB	2.34	0.57
1:A:1000:LEU:HD13	1:A:1282:GLY:HA3	1.87	0.57
2:Y:88:GLY:HA2	2:Y:210:GLU:O	2.05	0.57
1:B:123:ASN:HD21	1:B:150:ASP:H	1.51	0.57
1:B:934:VAL:O	1:B:934:VAL:HG12	2.04	0.57
2:X:106:VAL:HG22	2:X:163:LYS:CE	2.34	0.57
1:B:420:PHE:O	1:B:421:VAL:HG23	2.05	0.57
1:A:412:ARG:CD	1:A:415:ASP:HB2	2.34	0.56
2:X:102:ASN:CB	2:X:123:THR:HG23	2.35	0.56
1:B:511:HIS:HE2	1:B:531:THR:CG2	2.18	0.56
1:A:290:THR:O	1:A:291:MET:C	2.42	0.56
1:A:1066:TYR:N	1:A:1066:TYR:CD1	2.72	0.56
1:A:237:PHE:HD2	1:A:237:PHE:N	2.01	0.56
1:B:695:VAL:O	1:B:698:CYS:HB2	2.04	0.56
1:B:1195:LEU:O	1:B:1197:LEU:N	2.38	0.56
1:A:1465:ASN:H	1:A:1465:ASN:ND2	2.03	0.56
1:A:938:SER:HB3	1:A:1279:ARG:CZ	2.35	0.56
1:A:1334:LEU:CD2	1:A:1334:LEU:N	2.65	0.56
1:A:292:LEU:HD13	1:A:293:ILE:N	2.20	0.56
1:A:123:ASN:HD21	1:A:150:ASP:H	1.52	0.56
1:B:820:PHE:HZ	1:B:848:TYR:CB	2.18	0.56
1:B:823:VAL:HG13	1:B:846:TYR:O	2.05	0.56
1:B:362:PHE:CD1	1:B:639:GLY:O	2.58	0.56
1:A:961:TYR:OH	1:A:1343:ASN:HA	2.05	0.56
2:Y:55:PHE:HD2	2:Y:105:VAL:CG1	2.19	0.56
1:A:1280:TYR:HD2	1:A:1281:GLY:N	2.02	0.56
2:Y:45:ASP:O	2:Y:49:TYR:HD2	1.88	0.56
1:A:442:LEU:HB2	1:A:447:GLN:NE2	2.20	0.56
1:A:1496:TYR:O	1:A:1496:TYR:HD1	1.87	0.56
1:B:23:TYR:HE2	1:B:111:PHE:HB3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:LEU:HD22	1:B:225:PRO:HD3	1.87	0.56
1:B:1161:LEU:O	1:B:1162:VAL:C	2.44	0.56
1:A:1156:PHE:CE1	1:A:1160:PRO:HA	2.39	0.56
1:A:266:TYR:CE2	1:A:755:LYS:HB2	2.41	0.56
1:B:142:LYS:HD3	1:B:775:TRP:CD1	2.40	0.56
1:A:392:ALA:HB3	1:A:404:LEU:HD12	1.86	0.56
1:A:359:THR:HG21	1:A:372:LYS:N	2.20	0.56
1:A:1003:LEU:HD13	1:A:1498:TYR:CE1	2.41	0.56
1:A:1195:LEU:O	1:A:1197:LEU:N	2.38	0.56
1:A:703:ALA:O	1:A:704:CYS:C	2.43	0.56
1:A:136:THR:CG2	1:A:222:TYR:HB2	2.33	0.56
2:Y:106:VAL:HG22	2:Y:163:LYS:CE	2.35	0.56
1:A:1016:VAL:HG12	1:A:1017:PRO:CD	2.36	0.56
1:B:569:ASN:OD1	1:B:596:MET:HB2	2.04	0.56
1:B:1431:GLY:HA3	1:B:1483:PHE:HE1	1.70	0.56
1:B:617:LYS:O	1:B:618:LYS:CG	2.46	0.56
1:A:1658:GLN:C	1:A:1660:PHE:H	2.09	0.56
1:A:1024:TYR:HB2	1:A:1298:THR:HG22	1.86	0.56
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.35	0.56
2:X:73:VAL:CG2	2:X:74:ARG:N	2.67	0.56
1:A:586:GLN:HG2	1:A:587:THR:O	2.04	0.56
1:A:1465:ASN:H	1:A:1465:ASN:HD22	1.54	0.56
1:B:683:ILE:HD13	1:B:735:ALA:HB2	1.87	0.56
1:A:938:SER:OG	1:A:1279:ARG:HD2	2.06	0.56
1:A:23:TYR:HE1	1:A:656:ASN:HB2	1.71	0.56
1:B:710:THR:HG23	1:B:713:GLN:OE1	2.05	0.56
1:A:364:LYS:N	1:A:364:LYS:HD2	2.20	0.56
1:B:1003:LEU:HD13	1:B:1498:TYR:CE1	2.41	0.56
2:X:55:PHE:HD2	2:X:105:VAL:CG1	2.18	0.56
1:A:32:ARG:HB2	1:A:35:ALA:CB	2.35	0.56
2:X:110:ILE:HG22	2:X:111:ASP:N	2.21	0.56
1:A:511:HIS:HE2	1:A:531:THR:CG2	2.18	0.56
1:B:420:PHE:N	1:B:420:PHE:CD2	2.73	0.56
1:A:392:ALA:O	1:A:404:LEU:HB2	2.05	0.56
1:B:82:SER:O	2:Y:137:PHE:CE2	2.59	0.56
1:A:420:PHE:CD2	1:A:420:PHE:N	2.72	0.56
1:B:364:LYS:H	1:B:364:LYS:HD2	1.70	0.56
1:B:1080:ALA:O	1:B:1083:LEU:HB2	2.05	0.56
2:Y:104:PHE:CE1	2:Y:164:GLU:HG3	2.41	0.56
1:A:259:VAL:HG23	1:A:260:VAL:O	2.05	0.56
1:B:600:VAL:HG12	1:B:601:ALA:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PHE:O	1:A:421:VAL:HG23	2.06	0.56
1:A:198:MET:CE	1:A:198:MET:HA	2.36	0.56
1:B:1465:ASN:H	1:B:1465:ASN:HD22	1.53	0.56
1:B:979:VAL:HB	1:B:1326:TYR:OH	2.05	0.56
1:A:815:VAL:HG12	1:A:815:VAL:O	2.06	0.56
1:A:156:LYS:C	1:A:157:ARG:HG3	2.26	0.56
1:A:820:PHE:HZ	1:A:848:TYR:CB	2.19	0.56
1:A:822:ASP:O	1:A:848:TYR:HB2	2.06	0.56
1:A:859:MET:HB2	1:A:912:PHE:HE1	1.69	0.56
1:B:961:TYR:CZ	1:B:1343:ASN:HA	2.41	0.56
1:B:592:MET:HG2	1:B:600:VAL:HG21	1.88	0.56
1:A:429:THR:OG1	1:A:430:VAL:N	2.35	0.56
1:A:1264:ILE:HG12	1:A:1303:LEU:HD11	1.88	0.56
2:X:104:PHE:CE1	2:X:164:GLU:HG3	2.41	0.56
1:B:1000:LEU:HD13	1:B:1282:GLY:HA3	1.88	0.56
1:A:1028:GLY:O	1:A:1029:ASN:C	2.42	0.56
1:A:1419:SER:OG	1:A:1420:SER:N	2.39	0.56
1:A:1535:MET:CG	1:A:1609:ALA:HA	2.35	0.56
1:A:1618:LEU:HD12	1:A:1618:LEU:C	2.27	0.56
1:B:1228:TRP:H	1:B:1251:THR:CG2	2.19	0.56
1:A:1604:VAL:HG12	1:A:1605:THR:N	2.21	0.56
1:B:412:ARG:CD	1:B:415:ASP:HB2	2.35	0.56
2:Y:102:ASN:CB	2:Y:123:THR:HG23	2.35	0.56
1:B:349:LEU:HD22	1:B:446:ASN:HD22	1.71	0.56
1:A:754:MET:O	1:A:755:LYS:HG2	2.06	0.56
1:A:180:ILE:HD12	1:A:599:TRP:CD2	2.41	0.56
1:B:599:TRP:HB2	1:B:804:ILE:O	2.06	0.56
1:A:585:GLY:O	1:A:789:ALA:HB1	2.06	0.56
1:A:733:VAL:O	1:A:737:GLN:HG2	2.06	0.56
1:B:1183:GLN:OE1	1:B:1183:GLN:HA	2.05	0.56
1:A:410:VAL:HG12	1:A:411:THR:N	2.21	0.55
1:B:123:ASN:C	1:B:211:THR:HG21	2.26	0.55
1:A:1030:HIS:O	1:A:1033:ILE:HG13	2.05	0.55
1:B:491:PRO:O	1:B:492:TYR:C	2.44	0.55
1:B:440:PRO:HD2	1:B:441:ASP:H	1.71	0.55
1:A:362:PHE:CD1	1:A:638:GLY:O	2.58	0.55
1:B:362:PHE:CD1	1:B:638:GLY:O	2.59	0.55
2:X:136:LEU:HG	2:X:136:LEU:O	2.05	0.55
2:X:88:GLY:HA2	2:X:210:GLU:O	2.06	0.55
1:A:569:ASN:OD1	1:A:596:MET:HB2	2.04	0.55
1:A:986:GLU:HA	1:A:986:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1534:GLN:O	1:A:1645:ILE:HG13	2.05	0.55
1:B:439:ALA:CB	1:B:447:GLN:HE22	2.14	0.55
1:A:1255:LEU:HD12	1:A:1267:VAL:HG22	1.88	0.55
1:A:1208:ILE:O	1:A:1211:ALA:HB3	2.06	0.55
1:B:585:GLY:O	1:B:789:ALA:HB1	2.07	0.55
1:A:1467:ILE:O	1:A:1468:PRO:O	2.24	0.55
1:B:634:CYS:HB3	1:B:648:LEU:HD23	1.88	0.55
1:B:352:TYR:HB3	1:B:375:VAL:HG13	1.88	0.55
1:B:942:VAL:HG21	1:B:957:LYS:HB3	1.87	0.55
1:B:259:VAL:HG23	1:B:260:VAL:O	2.06	0.55
1:B:820:PHE:CZ	1:B:848:TYR:HD2	2.23	0.55
1:B:1190:ILE:HG12	1:B:1253:TYR:CZ	2.41	0.55
1:B:247:GLU:HG2	1:B:298:GLN:OE1	2.06	0.55
1:A:1003:LEU:HD23	1:A:1003:LEU:N	2.22	0.55
1:A:1535:MET:HG2	1:A:1609:ALA:CA	2.33	0.55
1:A:23:TYR:HE2	1:A:111:PHE:HB3	1.72	0.55
1:B:42:GLN:HA	1:B:79:PHE:O	2.07	0.55
1:B:136:THR:CG2	1:B:222:TYR:HB2	2.33	0.55
2:Y:77:PRO:O	2:Y:78:LYS:CG	2.55	0.55
2:X:166:ASP:CG	2:X:201:ILE:HD13	2.26	0.55
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.21	0.55
1:A:1348:VAL:HG11	1:A:1359:VAL:CG2	2.35	0.55
1:A:54:ILE:HG22	1:A:55:SER:N	2.21	0.55
1:A:823:VAL:HG13	1:A:846:TYR:O	2.05	0.55
1:B:961:TYR:OH	1:B:1343:ASN:HA	2.07	0.55
1:B:180:ILE:HD12	1:B:599:TRP:CD2	2.41	0.55
1:B:563:ILE:HG13	1:B:564:GLU:N	2.22	0.55
1:B:23:TYR:HE1	1:B:656:ASN:HB2	1.71	0.55
2:X:46:LEU:CD2	2:X:206:LYS:HE3	2.36	0.55
1:A:136:THR:O	1:A:139:GLN:HG3	2.06	0.55
2:X:113:ASN:HD21	2:X:115:ARG:CG	2.18	0.55
1:A:205:TYR:HD1	1:A:211:THR:HG1	1.52	0.55
1:B:1188:LEU:CD2	1:B:1212:LEU:HA	2.37	0.55
1:A:1522:GLY:O	1:A:1523:ALA:HB3	2.07	0.55
1:B:357:VAL:O	1:B:359:THR:HG23	2.07	0.55
1:A:32:ARG:O	1:A:35:ALA:HB3	2.07	0.55
1:A:127:PHE:HB2	1:A:146:TYR:O	2.06	0.55
1:B:930:VAL:CG1	1:B:931:PRO:N	2.68	0.55
1:B:703:ALA:O	1:B:704:CYS:C	2.44	0.55
1:B:1419:SER:OG	1:B:1420:SER:N	2.40	0.55
1:B:194:PRO:O	1:B:1070:LYS:NZ	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:986:GLU:HA	1:B:986:GLU:OE2	2.06	0.55
1:A:777:VAL:HG12	1:A:778:HIS:N	2.22	0.55
1:B:253:ARG:HG3	1:B:253:ARG:O	2.07	0.55
1:A:1161:LEU:O	1:A:1162:VAL:C	2.44	0.55
1:B:350:SER:OG	1:B:448:ALA:HB2	2.06	0.55
1:A:707:ASN:HB3	1:A:739:ARG:NH1	2.22	0.55
1:B:1146:ALA:CB	1:B:1190:ILE:HG22	2.37	0.55
1:B:707:ASN:HB3	1:B:739:ARG:NH1	2.21	0.55
1:A:673:LEU:O	1:A:673:LEU:HG	2.05	0.55
1:A:450:GLU:HB3	1:A:452:TYR:HE2	1.72	0.55
1:A:163:PHE:N	1:A:163:PHE:CD1	2.74	0.55
1:B:528:ILE:HG22	1:B:529:PRO:O	2.07	0.55
1:B:936:ARG:NH1	1:B:1002:HIS:CE1	2.75	0.55
1:B:886:GLN:HG2	1:B:894:HIS:NE2	2.20	0.55
1:A:385:GLY:N	1:A:411:THR:CG2	2.69	0.55
1:A:1423:VAL:HG12	1:A:1463:GLN:HG2	1.88	0.55
1:A:224:LEU:HD22	1:A:225:PRO:HD3	1.88	0.55
1:B:1024:TYR:HB2	1:B:1298:THR:HG22	1.87	0.55
2:Y:110:ILE:HG22	2:Y:111:ASP:N	2.22	0.55
1:A:491:PRO:O	1:A:492:TYR:C	2.44	0.55
1:A:122:ASP:HA	1:A:211:THR:HG23	1.89	0.55
1:B:777:VAL:CG1	1:B:778:HIS:N	2.70	0.55
1:A:359:THR:HG21	1:A:372:LYS:H	1.71	0.55
1:A:683:ILE:HD13	1:A:735:ALA:HB2	1.88	0.55
1:A:1464:LEU:HD22	1:A:1466:SER:O	2.07	0.55
1:A:113:LYS:HG3	1:A:114:SER:N	2.21	0.55
2:X:77:PRO:O	2:X:78:LYS:CG	2.55	0.55
2:Y:79:ASP:HB3	2:Y:80:GLN:NE2	2.22	0.55
1:A:123:ASN:H	1:A:211:THR:HG23	1.72	0.55
1:B:1283:GLY:HA3	1:B:1290:THR:CG2	2.35	0.55
1:B:1066:TYR:N	1:B:1066:TYR:CD1	2.74	0.55
1:B:602:LEU:HB2	1:B:774:LEU:O	2.07	0.55
1:B:909:ASN:H	1:B:926:THR:HG22	1.72	0.55
1:B:1299:GLU:O	1:B:1302:LEU:HB2	2.07	0.55
1:B:733:VAL:O	1:B:737:GLN:HG2	2.07	0.55
1:A:976:ILE:O	1:A:1361:VAL:HA	2.07	0.54
1:A:1548:ARG:HH12	1:A:1618:LEU:HD21	1.72	0.54
1:A:1625:LEU:HD12	1:A:1625:LEU:O	2.08	0.54
2:Y:45:ASP:HB3	2:Y:49:TYR:HE2	1.72	0.54
1:B:271:ILE:O	1:B:280:LYS:HB2	2.07	0.54
1:B:1202:HIS:CD2	1:B:1204:GLN:HB3	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1213:LYS:NZ	1:A:1263:ASP:OD2	2.39	0.54
1:B:365:PRO:HD2	1:B:464:TYR:CE2	2.42	0.54
1:A:909:ASN:H	1:A:926:THR:HG22	1.72	0.54
1:A:1193:TYR:CD1	1:A:1256:LEU:HB3	2.42	0.54
1:A:1047:LYS:O	1:A:1050:LYS:N	2.39	0.54
1:B:85:LEU:O	1:B:86:THR:CB	2.49	0.54
1:B:1259:LEU:CD1	1:B:1300:TYR:HB2	2.36	0.54
1:A:820:PHE:CZ	1:A:848:TYR:HD2	2.24	0.54
1:B:1076:THR:HG22	1:B:1077:TRP:N	2.22	0.54
1:B:1208:ILE:O	1:B:1211:ALA:HB3	2.06	0.54
1:B:218:GLU:CD	1:B:220:LYS:HE2	2.28	0.54
1:A:814:THR:OG1	1:A:815:VAL:N	2.40	0.54
2:Y:61:SER:N	2:Y:75:PHE:HZ	2.05	0.54
1:A:982:LEU:CD2	1:A:1309:LEU:HD11	2.38	0.54
1:A:123:ASN:N	1:A:211:THR:CG2	2.70	0.54
1:A:1517:GLN:C	1:A:1518:LYS:HG2	2.28	0.54
1:A:243:PHE:CE1	1:A:316:GLU:CG	2.90	0.54
1:B:1047:LYS:O	1:B:1050:LYS:N	2.40	0.54
1:B:32:ARG:HB2	1:B:35:ALA:CB	2.37	0.54
1:A:936:ARG:NH1	1:A:1002:HIS:CE1	2.76	0.54
1:B:837:GLU:CG	1:B:1488:LEU:HA	2.37	0.54
1:A:1636:ILE:HG13	1:A:1637:TYR:N	2.13	0.54
1:A:386:VAL:O	1:A:410:VAL:HG13	2.07	0.54
1:B:410:VAL:HG12	1:B:411:THR:N	2.22	0.54
1:B:282:MET:HA	1:B:282:MET:HE2	1.90	0.54
1:B:54:ILE:HG12	1:B:106:VAL:HG22	1.89	0.54
1:A:609:VAL:HG23	1:A:610:TYR:N	2.16	0.54
1:A:98:PRO:O	1:A:100:SER:N	2.40	0.54
1:B:156:LYS:C	1:B:157:ARG:HG3	2.26	0.54
1:B:822:ASP:O	1:B:848:TYR:HB2	2.08	0.54
1:B:778:HIS:CE1	1:B:786:LEU:CD1	2.89	0.54
1:A:362:PHE:CD1	1:A:639:GLY:O	2.60	0.54
1:A:470:THR:CG2	1:A:471:ASP:H	2.20	0.54
1:A:721:GLY:C	1:A:723:ARG:H	2.10	0.54
1:A:1080:ALA:O	1:A:1083:LEU:HB2	2.06	0.54
1:A:543:TYR:HB3	1:A:556:SER:CB	2.37	0.54
2:Y:46:LEU:HA	2:Y:206:LYS:HZ1	1.72	0.54
1:B:113:LYS:HG3	1:B:114:SER:N	2.22	0.54
1:A:368:PRO:O	1:A:370:PRO:HD3	2.07	0.54
1:A:907:LEU:HD12	1:A:908:HIS:N	2.22	0.54
1:B:292:LEU:HD13	1:B:293:ILE:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:OD1	1:B:893:SER:O	2.25	0.54
1:B:1514:ILE:CG2	1:B:1515:LYS:N	2.71	0.54
1:B:470:THR:CG2	1:B:471:ASP:H	2.21	0.54
1:B:131:ASP:HB3	1:B:142:LYS:HB2	1.89	0.54
1:A:592:MET:HG2	1:A:600:VAL:HG21	1.89	0.54
1:B:1271:ILE:HD12	1:B:1271:ILE:C	2.28	0.54
1:B:814:THR:OG1	1:B:815:VAL:N	2.39	0.54
1:B:193:ASN:OD1	1:B:1070:LYS:CE	2.56	0.54
1:B:721:GLY:C	1:B:723:ARG:H	2.10	0.54
1:A:1591:VAL:O	1:A:1592:ALA:HB2	2.08	0.54
1:A:24:VAL:HG22	1:A:655:THR:OG1	2.08	0.54
1:A:1244:THR:HG22	1:A:1246:ARG:H	1.72	0.54
1:B:98:PRO:O	1:B:100:SER:N	2.39	0.54
1:A:531:THR:CG2	1:A:534:MET:HG3	2.37	0.54
1:B:1182:ALA:HB2	1:B:1188:LEU:HD13	1.90	0.54
1:A:451:GLY:C	1:A:452:TYR:CD2	2.81	0.54
1:B:237:PHE:CE1	1:B:378:SER:O	2.61	0.54
1:B:388:VAL:O	1:B:388:VAL:HG12	2.08	0.54
1:B:704:CYS:O	1:B:705:VAL:HG13	2.07	0.54
1:A:504:LEU:CD1	1:A:509:ILE:HG12	2.38	0.54
1:B:385:GLY:N	1:B:411:THR:CG2	2.71	0.54
1:B:545:ILE:HG23	1:B:554:LEU:CD2	2.35	0.54
1:A:96:GLN:O	1:A:98:PRO:CD	2.52	0.54
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.43	0.54
1:A:1464:LEU:N	1:A:1464:LEU:HD12	2.23	0.54
1:A:901:LEU:O	1:A:901:LEU:HD23	2.08	0.54
1:A:1673:LEU:HD22	1:B:258:LYS:HG3	1.90	0.54
1:A:384:GLY:CA	1:A:411:THR:HG23	2.36	0.54
1:A:350:SER:OG	1:A:448:ALA:HB2	2.08	0.54
1:B:153:LYS:HE2	2:Y:133:ASN:OD1	2.08	0.54
1:B:136:THR:O	1:B:139:GLN:HG3	2.07	0.54
2:X:61:SER:N	2:X:75:PHE:HZ	2.05	0.54
1:A:1515:LYS:O	1:A:1516:ILE:CG1	2.54	0.54
1:A:470:THR:HG22	1:A:471:ASP:H	1.73	0.54
2:X:79:ASP:HB3	2:X:80:GLN:NE2	2.22	0.54
1:A:544:TYR:CE2	1:A:546:VAL:HG23	2.43	0.54
1:A:602:LEU:HB2	1:A:774:LEU:O	2.07	0.54
1:B:991:VAL:HG21	1:B:1017:PRO:O	2.08	0.54
1:A:1453:TYR:HA	1:A:1462:LEU:HD23	1.90	0.54
1:A:1182:ALA:HB2	1:A:1188:LEU:HD13	1.90	0.54
1:A:1521:GLU:CD	1:A:1522:GLY:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:CYS:O	1:A:705:VAL:HG13	2.08	0.54
1:B:1153:ARG:NH1	1:B:1168:LEU:HD13	2.23	0.54
1:B:847:ASN:ND2	1:B:853:MET:HG2	2.23	0.53
1:B:1514:ILE:HG22	1:B:1515:LYS:N	2.22	0.53
1:A:267:ILE:HG12	1:A:327:VAL:HG13	1.90	0.53
1:B:392:ALA:O	1:B:404:LEU:HB2	2.09	0.53
1:B:646:PHE:O	1:B:649:ALA:HB3	2.08	0.53
1:A:350:SER:CB	1:A:446:ASN:O	2.56	0.53
1:A:242:ASN:CB	1:A:245:ASN:O	2.56	0.53
1:B:488:PRO:O	1:B:489:LYS:O	2.26	0.53
1:A:1133:LEU:N	1:A:1134:PRO:CD	2.71	0.53
1:B:1133:LEU:N	1:B:1134:PRO:CD	2.70	0.53
1:B:171:VAL:HG13	1:B:1057:MET:HE3	1.89	0.53
1:B:1449:LEU:HG	1:B:1450:PHE:CE1	2.43	0.53
1:A:1076:THR:HG22	1:A:1077:TRP:N	2.24	0.53
1:A:1283:GLY:HA3	1:A:1290:THR:CG2	2.39	0.53
1:B:451:GLY:C	1:B:452:TYR:CD2	2.81	0.53
1:B:193:ASN:OD1	1:B:1070:LYS:HE2	2.08	0.53
1:A:1624:ALA:HB2	1:A:1636:ILE:HD12	1.90	0.53
1:A:1654:CYS:O	1:A:1655:SER:C	2.46	0.53
1:A:1673:LEU:HD13	1:B:258:LYS:CE	2.39	0.53
1:A:922:ILE:HD12	4:A:2001:NAG:C8	2.23	0.53
2:Y:57:TYR:HD2	2:Y:58:SER:N	2.02	0.53
1:A:1245:ALA:HA	1:A:1285:TYR:HB3	1.89	0.53
1:B:131:ASP:OD1	1:B:135:TYR:OH	2.22	0.53
1:B:696:LYS:NZ	1:B:700:TYR:CD2	2.76	0.53
1:A:1188:LEU:CD2	1:A:1212:LEU:HA	2.38	0.53
1:A:988:LEU:HD23	1:A:1021:VAL:HG22	1.91	0.53
1:A:563:ILE:HG13	1:A:564:GLU:N	2.21	0.53
1:B:55:SER:HB3	1:B:68:SER:CB	2.32	0.53
1:A:59:TYR:HA	1:A:103:TYR:CD1	2.44	0.53
1:B:857:VAL:HA	1:B:913:SER:O	2.09	0.53
1:B:528:ILE:HD12	1:B:528:ILE:N	2.24	0.53
1:B:384:GLY:CA	1:B:411:THR:HG23	2.37	0.53
1:A:354:LEU:CD2	1:A:354:LEU:H	2.18	0.53
1:B:1091:LYS:HE2	1:B:1092:TYR:CE1	2.44	0.53
1:B:205:TYR:HD1	1:B:211:THR:HG1	1.55	0.53
2:Y:113:ASN:HD21	2:Y:115:ARG:CG	2.18	0.53
1:A:1104:LEU:HD13	1:A:1164:ILE:CD1	2.38	0.53
1:A:1045:LEU:O	1:A:1049:LEU:HB2	2.09	0.53
1:B:1320:LYS:HD2	1:B:1321:GLY:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASP:C	1:A:379:LEU:N	2.62	0.53
1:A:372:LYS:HA	1:A:419:SER:HA	1.89	0.53
1:B:936:ARG:HB3	1:B:1364:VAL:HG22	1.89	0.53
1:B:1310:SER:O	1:B:1310:SER:OG	2.25	0.53
1:B:1485:VAL:HG21	1:B:1488:LEU:HB3	1.89	0.53
1:A:1648:TRP:CZ3	1:A:1664:LEU:HD22	2.44	0.53
2:X:45:ASP:HB3	2:X:49:TYR:HE2	1.72	0.53
1:A:1431:GLY:C	1:A:1432:ILE:HG12	2.28	0.53
1:A:506:LYS:NZ	1:A:536:PRO:HD2	2.22	0.53
1:B:242:ASN:CB	1:B:245:ASN:O	2.56	0.53
1:B:59:TYR:HA	1:B:103:TYR:CD1	2.43	0.53
1:B:120:THR:CG2	1:B:121:TYR:H	2.17	0.53
1:A:847:ASN:ND2	1:A:853:MET:HG2	2.23	0.53
1:B:195:ARG:HD3	1:B:1058:SER:HA	1.91	0.53
1:B:131:ASP:OD1	1:B:132:LYS:N	2.41	0.53
1:B:1016:VAL:HG12	1:B:1017:PRO:CD	2.38	0.53
1:B:1028:GLY:O	1:B:1029:ASN:O	2.26	0.53
2:Y:55:PHE:HD2	2:Y:105:VAL:HG13	1.73	0.53
1:B:640:LEU:HB3	1:B:644:ASN:OD1	2.08	0.53
1:A:1279:ARG:CG	1:A:1284:PHE:CB	2.56	0.53
1:A:1535:MET:CB	1:A:1645:ILE:HD11	2.39	0.53
1:B:466:TYR:HD1	1:B:467:ILE:N	2.07	0.53
1:A:599:TRP:HB2	1:A:804:ILE:O	2.08	0.53
1:A:961:TYR:HH	1:A:1343:ASN:CG	2.12	0.53
1:A:979:VAL:HB	1:A:1326:TYR:OH	2.08	0.53
1:B:1453:TYR:HA	1:B:1462:LEU:HD23	1.90	0.53
1:B:1239:VAL:O	1:B:1241:ASN:N	2.42	0.53
1:B:1008:ALA:N	1:B:1068:VAL:O	2.38	0.53
1:B:59:TYR:CD2	1:B:60:PRO:HD3	2.44	0.53
1:B:123:ASN:N	1:B:211:THR:CG2	2.72	0.53
1:B:1030:HIS:CE1	1:B:1306:GLN:HE21	2.27	0.53
1:B:492:TYR:O	1:B:493:ILE:HG13	2.09	0.53
1:B:544:TYR:CE2	1:B:546:VAL:HG23	2.43	0.53
1:B:371:ILE:CG2	1:B:371:ILE:O	2.46	0.53
1:A:1259:LEU:CD1	1:A:1300:TYR:HB2	2.37	0.53
1:B:696:LYS:HE3	1:B:700:TYR:CD2	2.44	0.53
1:A:388:VAL:O	1:A:388:VAL:HG12	2.07	0.53
1:A:352:TYR:HB3	1:A:375:VAL:HG13	1.90	0.53
1:B:976:ILE:O	1:B:1361:VAL:HA	2.09	0.53
1:A:1585:TYR:HB3	1:A:1671:ILE:CG1	2.35	0.53
1:A:42:GLN:HA	1:A:79:PHE:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ILE:HG12	1:A:106:VAL:HG22	1.90	0.53
1:B:149:ASN:O	1:B:152:LEU:N	2.37	0.53
1:A:778:HIS:CE1	1:A:786:LEU:CD1	2.90	0.53
1:A:820:PHE:CE2	1:A:821:LYS:O	2.62	0.53
1:A:646:PHE:O	1:A:649:ALA:HB3	2.09	0.53
1:B:350:SER:CB	1:B:446:ASN:O	2.57	0.53
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.39	0.53
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.74	0.53
1:A:195:ARG:HD3	1:A:1058:SER:HA	1.90	0.53
1:B:1016:VAL:HG12	1:B:1017:PRO:N	2.24	0.53
1:A:359:THR:CG2	1:A:372:LYS:HG3	2.39	0.53
1:A:323:LEU:C	1:A:323:LEU:HD13	2.30	0.53
1:B:1279:ARG:CG	1:B:1284:PHE:CB	2.57	0.53
1:B:901:LEU:HD23	1:B:901:LEU:O	2.09	0.53
1:A:1231:ASN:HD22	1:A:1232:LEU:N	2.07	0.53
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.90	0.53
2:Y:78:LYS:HZ2	2:Y:79:ASP:HB2	1.74	0.53
1:B:354:LEU:N	1:B:354:LEU:HD22	2.21	0.53
1:A:131:ASP:OD1	1:A:132:LYS:N	2.42	0.53
1:B:1348:VAL:HG11	1:B:1359:VAL:CG2	2.39	0.53
1:A:1016:VAL:HG12	1:A:1017:PRO:N	2.23	0.53
1:A:935:LYS:O	1:A:1365:VAL:O	2.27	0.53
1:A:354:LEU:HD22	1:A:354:LEU:N	2.20	0.52
1:B:122:ASP:HA	1:B:211:THR:HG23	1.90	0.52
1:A:120:THR:CG2	1:A:121:TYR:H	2.18	0.52
1:A:857:VAL:HA	1:A:913:SER:O	2.09	0.52
1:B:1245:ALA:HA	1:B:1285:TYR:HB3	1.91	0.52
1:A:1189:ALA:HB1	1:A:1253:TYR:CB	2.38	0.52
1:A:576:SER:CB	1:A:577:PRO:HD3	2.39	0.52
1:B:576:SER:CB	1:B:577:PRO:HD3	2.39	0.52
1:A:528:ILE:HG22	1:A:529:PRO:O	2.09	0.52
1:A:113:LYS:HD3	1:A:656:ASN:OD1	2.08	0.52
1:B:271:ILE:HD11	1:B:283:MET:SD	2.48	0.52
1:A:466:TYR:HD1	1:A:467:ILE:N	2.07	0.52
1:A:59:TYR:CD2	1:A:60:PRO:HD3	2.43	0.52
1:A:1271:ILE:C	1:A:1271:ILE:HD12	2.30	0.52
1:B:1045:LEU:O	1:B:1049:LEU:HB2	2.09	0.52
1:A:82:SER:O	2:X:137:PHE:HE2	1.91	0.52
1:B:804:ILE:HG22	1:B:809:ILE:HA	1.90	0.52
1:A:379:LEU:HB3	1:A:381:GLN:NE2	2.25	0.52
1:A:1153:ARG:NH1	1:A:1168:LEU:HD13	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:935:LYS:O	1:B:1365:VAL:O	2.27	0.52
2:X:215:VAL:O	2:X:216:LEU:HD13	2.09	0.52
1:A:1228:TRP:N	1:A:1251:THR:HG22	2.24	0.52
2:X:110:ILE:HG22	2:X:111:ASP:O	2.08	0.52
1:A:491:PRO:HG3	1:A:544:TYR:OH	2.09	0.52
1:B:777:VAL:HG12	1:B:778:HIS:N	2.23	0.52
1:A:736:SER:O	1:A:739:ARG:HG2	2.09	0.52
1:A:235:TYR:CD2	1:A:235:TYR:N	2.77	0.52
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.91	0.52
1:B:1511:THR:HG23	1:B:1511:THR:O	2.09	0.52
1:A:1602:LYS:N	1:A:1602:LYS:HD3	2.24	0.52
1:B:907:LEU:HD12	1:B:908:HIS:N	2.21	0.52
2:Y:110:ILE:HG22	2:Y:111:ASP:O	2.09	0.52
1:B:511:HIS:HE2	1:B:531:THR:HG21	1.73	0.52
1:A:147:SER:O	1:A:148:LEU:HD12	2.10	0.52
1:A:290:THR:O	1:A:290:THR:CG2	2.57	0.52
1:B:592:MET:HB3	1:B:780:VAL:HG11	1.91	0.52
1:B:1326:TYR:N	1:B:1326:TYR:CD2	2.78	0.52
2:Y:215:VAL:O	2:Y:216:LEU:HD13	2.09	0.52
1:B:1279:ARG:HD3	1:B:1284:PHE:CD2	2.44	0.52
1:B:1431:GLY:C	1:B:1432:ILE:HG12	2.29	0.52
1:B:27:ALA:CB	1:B:39:ILE:HD12	2.40	0.52
1:B:506:LYS:NZ	1:B:536:PRO:HD2	2.24	0.52
1:B:367:ILE:CD1	1:B:466:TYR:HB2	2.40	0.52
1:B:205:TYR:HD1	1:B:211:THR:OG1	1.93	0.52
2:X:111:ASP:HB3	2:X:115:ARG:HG2	1.92	0.52
1:A:1027:THR:O	1:A:1027:THR:HG23	2.09	0.52
1:A:226:HIS:CD2	1:A:336:PHE:CE2	2.97	0.52
1:A:936:ARG:CB	1:A:1364:VAL:HG22	2.40	0.52
1:B:590:LEU:HD22	1:B:799:ILE:HD11	1.92	0.52
1:B:625:GLN:O	1:B:629:LYS:HE2	2.09	0.52
1:A:1239:VAL:O	1:A:1241:ASN:N	2.42	0.52
1:B:1216:ALA:HB2	1:B:1228:TRP:NE1	2.24	0.52
1:A:837:GLU:CG	1:A:1488:LEU:HA	2.40	0.52
1:A:295:GLY:C	1:A:296:ILE:HG12	2.28	0.52
1:B:123:ASN:H	1:B:211:THR:HG23	1.73	0.52
1:A:1658:GLN:HG3	1:A:1659:ALA:H	1.74	0.52
1:A:492:TYR:O	1:A:493:ILE:HG13	2.09	0.52
1:A:710:THR:HG23	1:A:713:GLN:OE1	2.07	0.52
1:A:1189:ALA:HB1	1:A:1253:TYR:HB2	1.90	0.52
1:B:450:GLU:HB3	1:B:452:TYR:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HB3	1:B:381:GLN:NE2	2.24	0.52
1:B:32:ARG:O	1:B:35:ALA:HB3	2.09	0.52
1:B:198:MET:CE	1:B:198:MET:HA	2.40	0.52
1:B:43:VAL:HG22	1:B:44:TYR:N	2.24	0.52
1:A:367:ILE:CD1	1:A:466:TYR:HB2	2.40	0.52
2:X:101:GLN:HA	2:X:125:LYS:HB3	1.91	0.52
1:A:804:ILE:HG22	1:A:809:ILE:HA	1.91	0.52
2:X:67:TYR:HB3	2:X:72:VAL:HG21	1.92	0.52
1:A:1408:TYR:O	1:A:1410:PRO:HD3	2.10	0.52
1:A:193:ASN:OD1	1:A:1070:LYS:HE2	2.10	0.52
1:A:663:GLN:O	1:A:664:GLU:O	2.28	0.52
1:A:1652:THR:CB	1:B:868:SER:HB3	2.39	0.52
1:B:1246:ARG:O	1:B:1250:THR:HG23	2.10	0.52
1:A:1538:GLU:C	1:A:1539:LEU:HG	2.29	0.52
2:Y:101:GLN:HA	2:Y:125:LYS:HB3	1.91	0.52
1:A:786:LEU:CD2	1:A:786:LEU:N	2.69	0.52
1:A:541:LEU:CD1	1:A:645:VAL:HG12	2.40	0.52
1:B:936:ARG:CB	1:B:1364:VAL:HG22	2.39	0.52
1:A:1578:LYS:HD2	1:A:1599:THR:OG1	2.10	0.52
1:A:1669:GLU:HA	1:A:1672:PHE:HE2	1.74	0.52
1:A:1244:THR:CG2	1:A:1246:ARG:H	2.23	0.52
1:B:272:ARG:O	1:B:321:LYS:HB2	2.09	0.52
1:B:1231:ASN:HD22	1:B:1232:LEU:N	2.07	0.52
1:B:24:VAL:HG22	1:B:655:THR:OG1	2.10	0.52
1:B:1213:LYS:HG3	1:B:1266:TYR:CZ	2.44	0.52
1:B:736:SER:O	1:B:739:ARG:HG2	2.09	0.52
2:X:169:ILE:CG2	2:X:189:ILE:HD13	2.38	0.52
1:A:171:VAL:HG13	1:A:1057:MET:HE3	1.90	0.52
1:A:653:PHE:CE2	1:A:660:ASP:HA	2.45	0.52
1:A:592:MET:HB3	1:A:780:VAL:HG11	1.91	0.52
1:B:326:ALA:HA	1:B:341:GLU:HA	1.92	0.52
1:A:487:THR:HG22	1:A:523:TYR:HB3	1.92	0.52
1:A:634:CYS:HB3	1:A:648:LEU:HD23	1.92	0.52
1:B:628:GLU:O	1:B:628:GLU:HG3	2.10	0.52
1:A:1535:MET:CA	1:A:1645:ILE:HD11	2.40	0.52
1:A:412:ARG:HB3	1:A:415:ASP:CB	2.32	0.52
2:X:60:VAL:HB	2:X:75:PHE:CZ	2.45	0.52
1:B:786:LEU:HD23	1:B:786:LEU:H	1.73	0.52
2:X:139:ASN:CB	2:X:146:LEU:HD21	2.39	0.52
1:A:991:VAL:HG21	1:A:1017:PRO:O	2.10	0.52
1:A:193:ASN:OD1	1:A:1070:LYS:CE	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:ASN:N	1:B:258:LYS:HE3	2.25	0.51
1:A:1096:ASN:HD22	1:A:1099:SER:H	1.52	0.51
1:B:367:ILE:HD13	1:B:466:TYR:CD2	2.45	0.51
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.45	0.51
2:Y:111:ASP:HB3	2:Y:115:ARG:HG2	1.92	0.51
1:A:968:VAL:CG2	1:A:971:THR:HG21	2.36	0.51
1:A:640:LEU:O	1:A:640:LEU:HD12	2.10	0.51
1:B:1189:ALA:HB1	1:B:1253:TYR:CB	2.41	0.51
1:A:1077:TRP:NE1	1:A:1147:PHE:CE1	2.78	0.51
1:A:1120:GLU:OE2	1:A:1121:ASN:N	2.43	0.51
2:Y:67:TYR:HB3	2:Y:72:VAL:HG21	1.92	0.51
1:A:1028:GLY:O	1:A:1029:ASN:O	2.27	0.51
1:A:936:ARG:HB3	1:A:1364:VAL:HG22	1.91	0.51
1:A:721:GLY:O	1:A:723:ARG:N	2.43	0.51
1:B:663:GLN:O	1:B:664:GLU:O	2.28	0.51
1:A:73:LEU:N	1:A:73:LEU:HD23	2.24	0.51
1:B:1213:LYS:HG3	1:B:1266:TYR:OH	2.10	0.51
1:B:908:HIS:N	1:B:908:HIS:ND1	2.57	0.51
1:B:295:GLY:C	1:B:296:ILE:HG12	2.30	0.51
1:B:1435:ASN:O	1:B:1436:GLU:C	2.49	0.51
2:Y:139:ASN:CB	2:Y:146:LEU:HD21	2.39	0.51
1:A:450:GLU:HB3	1:A:452:TYR:CE2	2.45	0.51
1:A:942:VAL:HG12	1:A:943:THR:N	2.24	0.51
2:X:55:PHE:HD2	2:X:105:VAL:HG13	1.73	0.51
1:A:1220:GLY:O	1:A:1222:PRO:O	2.27	0.51
1:A:271:ILE:O	1:A:280:LYS:HB2	2.10	0.51
1:A:1091:LYS:HE2	1:A:1092:TYR:CE1	2.44	0.51
1:A:137:PRO:O	1:A:138:ASP:HB2	2.10	0.51
1:B:339:GLU:HB2	1:B:766:ARG:HH21	1.75	0.51
1:A:1190:ILE:HG12	1:A:1253:TYR:CZ	2.45	0.51
1:A:1467:ILE:O	1:A:1467:ILE:HG22	2.10	0.51
1:A:936:ARG:CZ	1:A:1002:HIS:HE1	2.24	0.51
1:A:1326:TYR:CD2	1:A:1326:TYR:N	2.77	0.51
1:B:987:ILE:HD13	1:B:1294:ILE:HG23	1.92	0.51
1:B:485:ILE:N	1:B:485:ILE:CD1	2.69	0.51
1:A:908:HIS:ND1	1:A:908:HIS:N	2.58	0.51
1:A:1594:LYS:O	1:A:1595:ASP:CB	2.58	0.51
1:B:840:GLN:HE22	1:B:842:LYS:HE2	1.75	0.51
1:B:290:THR:O	1:B:290:THR:CG2	2.57	0.51
1:A:599:TRP:CZ2	1:A:779:LEU:HD13	2.46	0.51
1:A:1060:ARG:NH2	1:A:1064:TYR:CE1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.91	0.51
1:B:377:ASP:C	1:B:379:LEU:N	2.63	0.51
1:A:1299:GLU:O	1:A:1302:LEU:HB2	2.10	0.51
1:A:1653:THR:HG23	1:A:1653:THR:O	2.11	0.51
1:A:23:TYR:CE1	1:A:656:ASN:HB2	2.45	0.51
1:B:23:TYR:CE1	1:B:656:ASN:HB2	2.46	0.51
1:A:1431:GLY:HA3	1:A:1483:PHE:HE1	1.72	0.51
1:A:1538:GLU:O	1:A:1539:LEU:CG	2.54	0.51
1:A:511:HIS:HE2	1:A:531:THR:HG21	1.74	0.51
1:A:156:LYS:O	1:A:157:ARG:CG	2.55	0.51
1:A:827:MET:HE3	1:A:842:LYS:O	2.11	0.51
1:B:968:VAL:CG2	1:B:971:THR:HG21	2.38	0.51
1:B:829:ILE:CG1	1:B:925:LYS:HG2	2.40	0.51
1:B:739:ARG:HB2	1:B:752:LEU:HD21	1.93	0.51
1:B:1027:THR:HG23	1:B:1027:THR:O	2.10	0.51
1:B:226:HIS:CD2	1:B:336:PHE:CE2	2.98	0.51
1:A:633:GLY:O	1:A:634:CYS:HB2	2.10	0.51
1:B:1315:VAL:HG11	1:B:1324:HIS:NE2	2.25	0.51
1:A:282:MET:HA	1:A:282:MET:HE2	1.91	0.51
1:A:438:ASP:O	1:A:439:ALA:C	2.47	0.51
1:A:982:LEU:HD11	1:A:1306:GLN:OE1	2.10	0.51
1:B:1379:LEU:HD21	1:B:1495:VAL:HG11	1.92	0.51
1:B:1188:LEU:HD21	1:B:1212:LEU:HA	1.93	0.51
1:A:235:TYR:HD2	1:A:235:TYR:N	2.09	0.51
1:B:653:PHE:CE2	1:B:660:ASP:HA	2.45	0.51
1:B:719:SER:O	1:B:721:GLY:N	2.43	0.51
1:A:590:LEU:HD22	1:A:799:ILE:HD11	1.93	0.51
1:A:1651:ASP:HB3	1:A:1654:CYS:CB	2.41	0.51
1:A:253:ARG:HG3	1:A:253:ARG:O	2.09	0.51
1:B:268:THR:HA	1:B:286:ALA:CB	2.40	0.51
2:X:136:LEU:C	2:X:137:PHE:HD1	2.13	0.51
1:A:249:THR:HG23	1:A:298:GLN:HG2	1.93	0.51
1:B:163:PHE:CD1	1:B:163:PHE:N	2.75	0.51
1:B:249:THR:HG23	1:B:298:GLN:HG2	1.92	0.51
1:B:653:PHE:O	1:B:660:ASP:HB2	2.11	0.51
1:A:696:LYS:NZ	1:A:700:TYR:CD2	2.78	0.51
1:B:1193:TYR:CE1	1:B:1256:LEU:HB3	2.45	0.51
1:A:326:ALA:HA	1:A:341:GLU:HA	1.93	0.51
1:A:43:VAL:HG22	1:A:44:TYR:N	2.26	0.51
1:A:1432:ILE:HG22	1:A:1479:ILE:HB	1.92	0.51
1:B:137:PRO:O	1:B:138:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:LEU:N	1:B:786:LEU:CD2	2.68	0.51
1:A:243:PHE:CD1	1:A:316:GLU:HG3	2.45	0.51
1:B:1077:TRP:NE1	1:B:1147:PHE:CE1	2.79	0.51
1:A:1245:ALA:HA	1:A:1285:TYR:CB	2.41	0.51
1:B:1403:VAL:HG22	1:B:1476:ARG:HB3	1.91	0.51
1:B:1467:ILE:O	1:B:1468:PRO:O	2.28	0.51
1:A:1624:ALA:HB1	1:A:1635:TYR:HB3	1.92	0.51
1:A:1673:LEU:HD12	1:A:1674:ASN:H	1.75	0.51
1:A:505:SER:HB3	1:A:510:ILE:CD1	2.41	0.51
1:A:1563:VAL:CG2	1:A:1619:ILE:HD13	2.41	0.51
1:B:1082:ALA:O	1:B:1086:LEU:HD23	2.11	0.51
1:A:234:GLU:C	1:A:235:TYR:HD2	2.14	0.51
1:B:721:GLY:O	1:B:723:ARG:N	2.44	0.51
1:B:1408:TYR:O	1:B:1410:PRO:HD3	2.10	0.51
1:A:453:ARG:HD3	1:A:455:ILE:HD11	1.93	0.51
1:B:423:ASN:N	1:B:423:ASN:ND2	2.58	0.51
1:B:543:TYR:HB3	1:B:556:SER:CB	2.38	0.51
2:X:41:HIS:CD2	2:X:205:ASP:HB2	2.46	0.51
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.46	0.51
1:A:339:GLU:HB2	1:A:766:ARG:HH21	1.76	0.51
1:B:1135:VAL:HG12	1:B:1136:GLU:N	2.26	0.51
1:B:859:MET:HB2	1:B:912:PHE:HE1	1.68	0.51
1:B:717:ARG:HD3	1:B:1449:LEU:HA	1.93	0.51
2:X:170:ARG:NH2	2:X:201:ILE:HG22	2.26	0.51
1:B:599:TRP:CZ2	1:B:779:LEU:HD13	2.45	0.51
1:A:220:LYS:HG2	1:A:763:PRO:HB3	1.93	0.51
1:B:450:GLU:HB3	1:B:452:TYR:CE2	2.46	0.51
1:A:1435:ASN:O	1:A:1436:GLU:C	2.49	0.51
1:B:1231:ASN:ND2	1:B:1232:LEU:N	2.60	0.50
1:A:496:ILE:HD13	1:A:517:LYS:NZ	2.26	0.50
1:A:362:PHE:CE1	1:A:638:GLY:O	2.64	0.50
1:B:1190:ILE:HG12	1:B:1253:TYR:CE2	2.46	0.50
1:B:1210:SER:O	1:B:1211:ALA:C	2.49	0.50
1:B:504:LEU:CD1	1:B:509:ILE:HG12	2.41	0.50
1:B:288:GLN:NE2	1:B:680:GLN:OE1	2.44	0.50
1:B:1230:ASP:OD2	1:B:1246:ARG:HD2	2.10	0.50
1:B:113:LYS:HD3	1:B:656:ASN:OD1	2.11	0.50
1:B:56:ILE:HG13	1:B:66:TYR:CD2	2.44	0.50
1:B:412:ARG:HG2	1:B:413:VAL:N	2.26	0.50
1:A:223:VAL:HB	1:A:766:ARG:HD3	1.93	0.50
1:A:743:SER:OG	1:A:752:LEU:HD13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:70:SER:CB	2:Y:91:LYS:HE3	2.41	0.50
2:Y:166:ASP:OD2	2:Y:201:ILE:HG21	2.11	0.50
1:B:243:PHE:CE1	1:B:316:GLU:CG	2.93	0.50
1:A:269:PHE:CE2	1:A:325:ILE:HG23	2.46	0.50
1:A:1146:ALA:CB	1:A:1190:ILE:HG22	2.41	0.50
1:A:1190:ILE:O	1:A:1191:SER:C	2.50	0.50
1:B:1054:LEU:O	1:B:1056:ILE:N	2.44	0.50
1:A:50:PHE:HB2	1:A:109:LYS:HG3	1.92	0.50
1:B:1480:PHE:O	1:B:1482:LEU:N	2.44	0.50
1:B:486:VAL:CG2	1:B:526:ILE:HG13	2.41	0.50
1:A:977:LEU:HD13	1:A:1346:LEU:HD21	1.93	0.50
1:B:1496:TYR:C	1:B:1496:TYR:HD1	2.15	0.50
1:A:1496:TYR:C	1:A:1496:TYR:HD1	2.14	0.50
1:B:1228:TRP:N	1:B:1251:THR:HG22	2.24	0.50
1:A:59:TYR:CB	1:A:60:PRO:CD	2.80	0.50
1:B:236:ASN:C	1:B:237:PHE:HD2	2.13	0.50
1:B:50:PHE:HB2	1:B:109:LYS:HG3	1.92	0.50
1:B:695:VAL:HG22	1:B:724:CYS:HB3	1.94	0.50
1:B:127:PHE:HB2	1:B:146:TYR:O	2.11	0.50
1:B:825:LEU:HG	1:B:826:GLU:N	2.26	0.50
1:A:1135:VAL:HG12	1:A:1136:GLU:N	2.25	0.50
2:Y:136:LEU:C	2:Y:137:PHE:HD1	2.14	0.50
1:B:696:LYS:NZ	1:B:700:TYR:HD2	2.08	0.50
1:B:1464:LEU:HD22	1:B:1466:SER:O	2.12	0.50
1:A:194:PRO:O	1:A:1070:LYS:NZ	2.45	0.50
1:B:1467:ILE:O	1:B:1467:ILE:HG22	2.11	0.50
1:A:1067:SER:OG	1:A:1072:GLY:O	2.29	0.50
1:A:825:LEU:HD12	1:A:844:THR:O	2.12	0.50
1:A:288:GLN:NE2	1:A:680:GLN:OE1	2.44	0.50
1:A:39:ILE:HG13	1:A:85:LEU:HD23	1.94	0.50
2:Y:45:ASP:HB3	2:Y:49:TYR:CE2	2.47	0.50
1:A:442:LEU:CD2	1:A:443:PRO:HD3	2.41	0.50
1:B:982:LEU:HD23	1:B:1309:LEU:HD11	1.92	0.50
1:B:982:LEU:HD11	1:B:1306:GLN:OE1	2.12	0.50
1:A:489:LYS:O	1:A:491:PRO:CD	2.59	0.50
1:A:829:ILE:HG13	1:A:925:LYS:HG2	1.93	0.50
1:B:717:ARG:CD	1:B:1449:LEU:HA	2.42	0.50
1:A:717:ARG:HD3	1:A:1449:LEU:HA	1.94	0.50
1:A:330:ILE:HG22	1:A:337:SER:HB2	1.93	0.50
1:A:1370:THR:O	1:A:1371:SER:C	2.50	0.50
1:B:936:ARG:CZ	1:B:1002:HIS:HE1	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:456:ALA:HA	2.12	0.50
1:A:53:THR:HA	1:A:69:GLY:O	2.12	0.50
1:B:1280:TYR:HD1	1:B:1362:THR:CG2	2.25	0.50
1:B:1432:ILE:HG22	1:B:1479:ILE:HB	1.93	0.50
1:A:1565:ILE:N	1:A:1565:ILE:HD12	2.26	0.50
1:B:554:LEU:HB3	1:B:642:ASN:OD1	2.11	0.50
1:B:505:SER:HB3	1:B:510:ILE:CD1	2.41	0.50
1:B:223:VAL:HB	1:B:766:ARG:HD3	1.93	0.50
2:Y:60:VAL:HB	2:Y:75:PHE:CZ	2.46	0.50
1:B:491:PRO:HG3	1:B:544:TYR:OH	2.11	0.50
1:B:1245:ALA:HA	1:B:1285:TYR:CB	2.41	0.50
1:A:1180:LEU:HD11	1:A:1208:ILE:CA	2.42	0.50
1:A:1523:ALA:C	1:A:1525:CYS:H	2.14	0.50
1:A:696:LYS:HE3	1:A:700:TYR:CD2	2.46	0.50
1:A:331:GLU:OE1	1:A:336:PHE:HD1	1.95	0.50
1:A:113:LYS:HG3	1:A:114:SER:H	1.77	0.50
1:A:272:ARG:O	1:A:321:LYS:HB2	2.11	0.50
1:B:73:LEU:CD2	1:B:73:LEU:H	2.20	0.50
2:X:45:ASP:HB3	2:X:49:TYR:CE2	2.46	0.50
1:B:981:GLY:HA3	1:B:1309:LEU:HD11	1.94	0.50
2:X:78:LYS:HZ2	2:X:79:ASP:HB2	1.76	0.50
1:A:205:TYR:HD1	1:A:211:THR:OG1	1.94	0.50
1:A:640:LEU:HB3	1:A:644:ASN:OD1	2.11	0.50
2:Y:170:ARG:NH2	2:Y:201:ILE:HG22	2.27	0.50
2:Y:50:TYR:CE2	2:Y:170:ARG:HD2	2.47	0.50
1:A:696:LYS:NZ	1:A:700:TYR:HD2	2.10	0.50
1:A:323:LEU:HB2	1:A:347:TYR:CE2	2.46	0.50
1:A:86:THR:O	1:A:86:THR:HG23	2.12	0.50
1:A:271:ILE:HD11	1:A:283:MET:SD	2.52	0.50
2:Y:41:HIS:CD2	2:Y:205:ASP:HB2	2.46	0.50
1:A:739:ARG:HB2	1:A:752:LEU:HD21	1.93	0.50
1:B:541:LEU:CD1	1:B:645:VAL:HG12	2.40	0.50
1:B:707:ASN:OD1	1:B:707:ASN:N	2.45	0.50
2:Y:170:ARG:HH21	2:Y:201:ILE:HG22	1.76	0.50
1:B:1442:LEU:HD22	1:B:1449:LEU:HD23	1.94	0.50
1:A:1049:LEU:HD21	1:A:1089:VAL:HG13	1.93	0.50
1:B:220:LYS:HG2	1:B:763:PRO:HB3	1.94	0.50
1:B:1262:LYS:C	1:B:1264:ILE:H	2.15	0.50
1:A:628:GLU:O	1:A:628:GLU:HG3	2.11	0.50
1:A:860:SER:HB3	1:A:911:ASN:HB2	1.93	0.50
1:B:1244:THR:HG22	1:B:1246:ARG:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:HD3	1:A:903:LEU:O	2.12	0.50
1:B:765:ILE:CG2	1:B:765:ILE:O	2.58	0.50
1:A:707:ASN:N	1:A:707:ASN:OD1	2.45	0.50
1:A:1190:ILE:HG12	1:A:1253:TYR:CE2	2.47	0.50
1:A:886:GLN:CG	1:A:894:HIS:HE1	2.21	0.49
1:B:835:ARG:HD3	1:B:903:LEU:O	2.12	0.49
1:A:56:ILE:HG13	1:A:66:TYR:CD2	2.44	0.49
1:B:56:ILE:CD1	1:B:66:TYR:HB2	2.42	0.49
1:A:1213:LYS:HG3	1:A:1266:TYR:CZ	2.47	0.49
2:X:57:TYR:HD2	2:X:58:SER:N	2.02	0.49
2:X:166:ASP:OD2	2:X:201:ILE:HG21	2.11	0.49
1:B:1180:LEU:HD11	1:B:1208:ILE:CA	2.42	0.49
1:B:330:ILE:HG22	1:B:337:SER:HB2	1.94	0.49
1:A:528:ILE:N	1:A:528:ILE:HD12	2.26	0.49
1:B:1488:LEU:HD21	1:B:1511:THR:HG22	1.93	0.49
1:A:915:GLU:OE2	1:A:920:LYS:HE3	2.13	0.49
1:A:498:HIS:HB3	1:A:514:THR:HG23	1.94	0.49
1:A:1511:THR:HG23	1:A:1511:THR:O	2.10	0.49
1:A:530:VAL:HA	1:A:534:MET:SD	2.53	0.49
1:B:511:HIS:ND1	2:Y:149:SER:HB3	2.26	0.49
1:B:1515:LYS:O	1:B:1515:LYS:HG3	2.12	0.49
1:B:354:LEU:HD21	1:B:448:ALA:C	2.33	0.49
2:Y:86:LEU:CG	2:Y:91:LYS:HG3	2.42	0.49
1:A:82:SER:O	2:X:137:PHE:CE2	2.65	0.49
1:B:1120:GLU:OE2	1:B:1121:ASN:N	2.42	0.49
2:X:50:TYR:CE2	2:X:170:ARG:HD2	2.47	0.49
1:B:802:ILE:HG13	1:B:803:GLY:N	2.25	0.49
2:X:86:LEU:O	2:X:91:LYS:HD2	2.12	0.49
2:X:134:THR:HG23	2:X:153:PHE:HB3	1.94	0.49
1:B:235:TYR:CD2	1:B:235:TYR:N	2.81	0.49
1:A:719:SER:O	1:A:721:GLY:N	2.44	0.49
1:B:838:GLN:HA	1:B:901:LEU:HB2	1.95	0.49
2:X:111:ASP:CG	2:X:112:PRO:HD2	2.33	0.49
1:B:531:THR:HG22	1:B:534:MET:CG	2.42	0.49
1:A:1442:LEU:HD22	1:A:1449:LEU:HD23	1.94	0.49
1:A:780:VAL:HG22	1:A:784:LYS:HB3	1.93	0.49
1:A:237:PHE:CE1	1:A:378:SER:O	2.65	0.49
1:B:1255:LEU:HD12	1:B:1267:VAL:HG22	1.93	0.49
1:A:967:LEU:HD13	1:A:1365:VAL:HG22	1.94	0.49
1:A:889:GLU:HG2	1:A:892:SER:HB2	1.94	0.49
1:A:1079:THR:HG22	1:A:1107:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1536:GLN:HG3	1:A:1644:TRP:CZ2	2.47	0.49
1:A:1577:TYR:CE1	1:A:1602:LYS:HD2	2.48	0.49
1:A:1624:ALA:CB	1:A:1635:TYR:HB3	2.42	0.49
1:A:616:ALA:O	1:A:617:LYS:C	2.51	0.49
1:A:1496:TYR:CD1	1:A:1496:TYR:C	2.86	0.49
1:B:498:HIS:HB3	1:B:514:THR:HG23	1.94	0.49
2:Y:86:LEU:O	2:Y:91:LYS:HD2	2.12	0.49
1:B:829:ILE:HG13	1:B:925:LYS:HG2	1.94	0.49
2:X:170:ARG:HH21	2:X:201:ILE:HG22	1.76	0.49
2:Y:134:THR:HG23	2:Y:153:PHE:HB3	1.95	0.49
1:B:144:ARG:NH2	1:B:602:LEU:O	2.45	0.49
1:B:825:LEU:HD12	1:B:844:THR:O	2.12	0.49
1:B:147:SER:O	1:B:148:LEU:HD12	2.13	0.49
1:A:1542:THR:O	1:A:1543:ILE:HB	2.12	0.49
1:A:1315:VAL:HG11	1:A:1324:HIS:NE2	2.27	0.49
1:A:354:LEU:HD11	1:A:437:THR:HG23	1.94	0.49
1:A:59:TYR:CD1	1:A:103:TYR:CE1	2.84	0.49
2:Y:125:LYS:HA	2:Y:126:ASN:C	2.32	0.49
1:A:494:ASP:HA	1:A:496:ILE:CD1	2.42	0.49
1:B:156:LYS:O	1:B:157:ARG:CG	2.55	0.49
1:B:1378:TYR:CE2	1:B:1409:LYS:HG2	2.48	0.49
1:A:639:GLY:N	1:A:645:VAL:HG22	2.23	0.49
1:B:362:PHE:CE1	1:B:638:GLY:O	2.65	0.49
1:A:109:LYS:CD	1:A:110:HIS:N	2.76	0.49
1:B:706:ASN:HB3	1:B:714:ARG:HD2	1.95	0.49
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.45	0.49
1:B:860:SER:HB3	1:B:911:ASN:HB2	1.94	0.49
1:A:977:LEU:HD13	1:A:1346:LEU:CD2	2.43	0.49
1:A:625:GLN:O	1:A:629:LYS:HE2	2.13	0.49
1:A:27:ALA:CB	1:A:39:ILE:HD12	2.42	0.49
1:B:1496:TYR:C	1:B:1496:TYR:CD1	2.85	0.49
1:B:73:LEU:HD23	1:B:73:LEU:N	2.24	0.49
1:B:494:ASP:HA	1:B:496:ILE:CD1	2.42	0.49
1:A:1379:LEU:HD21	1:A:1495:VAL:HG11	1.95	0.49
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.13	0.49
1:A:234:GLU:C	1:A:235:TYR:CD2	2.86	0.49
1:B:1412:ARG:O	1:B:1413:GLU:HB2	2.13	0.49
1:B:216:TYR:N	1:B:216:TYR:CD2	2.80	0.49
1:A:390:LEU:HB3	1:A:420:PHE:CE1	2.48	0.49
1:A:1016:VAL:HG12	1:A:1017:PRO:HD3	1.95	0.49
1:B:721:GLY:C	1:B:723:ARG:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:643:ALA:O	1:B:644:ASN:C	2.50	0.49
1:A:1627:ILE:HD13	1:A:1627:ILE:H	1.78	0.49
1:A:838:GLN:O	1:A:1486:GLY:N	2.45	0.49
1:A:1578:LYS:HE3	1:A:1597:GLU:OE2	2.13	0.49
1:A:385:GLY:H	1:A:411:THR:HG23	1.78	0.49
1:A:1230:ASP:O	1:A:1231:ASN:O	2.31	0.49
1:A:1231:ASN:ND2	1:A:1232:LEU:N	2.60	0.49
1:A:1268:ASN:HB2	1:A:1269:PRO:HD3	1.93	0.49
1:B:743:SER:OG	1:B:752:LEU:HD13	2.11	0.49
1:A:653:PHE:O	1:A:660:ASP:HB2	2.12	0.49
1:B:109:LYS:CD	1:B:110:HIS:N	2.76	0.49
2:X:64:VAL:HG23	2:X:71:ASN:OD1	2.13	0.49
1:A:942:VAL:HG21	1:A:957:LYS:CB	2.42	0.49
1:A:814:THR:O	1:A:815:VAL:HG23	2.12	0.49
1:B:198:MET:HE2	1:B:198:MET:HA	1.94	0.49
1:A:1547:THR:O	1:A:1551:THR:HG23	2.12	0.49
1:A:1648:TRP:O	1:A:1650:ARG:N	2.45	0.49
2:X:49:TYR:HB2	2:X:206:LYS:HZ2	1.78	0.49
1:A:55:SER:HB3	1:A:68:SER:CB	2.33	0.49
1:B:368:PRO:O	1:B:370:PRO:HD3	2.13	0.49
1:B:614:ARG:HH22	1:B:798:GLU:CD	2.16	0.49
1:A:222:TYR:CD2	1:A:223:VAL:N	2.81	0.49
1:A:263:ALA:HB3	1:A:292:LEU:CB	2.39	0.49
1:A:1540:ASP:HB2	1:A:1660:PHE:CD1	2.48	0.49
1:A:153:LYS:HE2	2:X:133:ASN:OD1	2.12	0.49
1:B:820:PHE:CE2	1:B:821:LYS:O	2.65	0.49
1:A:639:GLY:HA3	1:A:645:VAL:CA	2.42	0.49
2:Y:169:ILE:CG2	2:Y:189:ILE:HD13	2.38	0.49
1:B:1110:ASN:HB2	1:B:1111:TYR:HD2	1.73	0.49
1:B:780:VAL:HG22	1:B:784:LYS:HB3	1.93	0.49
1:A:239:GLY:O	1:A:240:TYR:C	2.50	0.49
1:B:915:GLU:OE2	1:B:920:LYS:HE3	2.13	0.49
1:A:307:VAL:O	1:A:308:LYS:O	2.31	0.49
1:A:1143:TYR:HD1	1:A:1186:PHE:HE2	1.61	0.49
1:A:160:VAL:HG23	1:A:175:GLU:CB	2.33	0.49
1:B:57:LYS:HE2	1:B:65:SER:HB2	1.95	0.49
1:B:571:LEU:HD11	1:B:573:VAL:HG13	1.95	0.49
1:B:494:ASP:HA	1:B:496:ILE:HD11	1.95	0.49
1:A:679:LEU:HD22	1:A:738:LEU:HD11	1.95	0.49
1:A:541:LEU:HB2	1:A:558:SER:HB3	1.95	0.49
1:B:470:THR:HG22	1:B:471:ASP:H	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:86:LEU:CG	2:X:91:LYS:HG3	2.42	0.49
1:B:243:PHE:CD1	1:B:316:GLU:HG3	2.47	0.49
1:A:695:VAL:HG22	1:A:724:CYS:HB3	1.94	0.49
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.48	0.49
1:A:595:GLY:O	1:A:596:MET:HG2	2.13	0.49
1:B:942:VAL:HG21	1:B:957:LYS:CB	2.43	0.49
1:A:1651:ASP:O	1:A:1653:THR:N	2.46	0.49
1:A:1653:THR:CG2	1:A:1653:THR:O	2.61	0.49
1:A:855:PHE:HA	1:A:915:GLU:O	2.13	0.49
1:A:1323:LEU:CG	1:A:1324:HIS:H	2.24	0.49
1:A:1246:ARG:O	1:A:1250:THR:HG23	2.13	0.49
1:B:438:ASP:O	1:B:439:ALA:C	2.51	0.49
1:B:1204:GLN:HA	1:B:1204:GLN:OE1	2.13	0.49
1:A:57:LYS:HE2	1:A:65:SER:HB2	1.94	0.49
2:X:125:LYS:HA	2:X:126:ASN:C	2.32	0.49
1:B:354:LEU:CD2	1:B:354:LEU:H	2.20	0.49
2:Y:224:ILE:HG22	2:Y:225:SER:N	2.28	0.49
1:A:1245:ALA:CA	1:A:1285:TYR:HB3	2.42	0.49
1:A:717:ARG:CD	1:A:1449:LEU:HA	2.43	0.49
1:A:248:ILE:CD1	1:A:325:ILE:HD13	2.43	0.49
1:A:49:ALA:O	1:A:50:PHE:HB3	2.13	0.49
1:A:1262:LYS:C	1:A:1264:ILE:H	2.16	0.49
1:B:1220:GLY:O	1:B:1222:PRO:O	2.29	0.49
1:B:922:ILE:HD12	4:B:2001:NAG:H82	1.94	0.49
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.93	0.48
1:A:1559:TYR:HB3	1:A:1588:GLY:HA2	1.94	0.48
1:A:442:LEU:HB3	1:A:447:GLN:NE2	2.28	0.48
1:B:1227:PHE:C	1:B:1228:TRP:CE3	2.86	0.48
1:B:1104:LEU:HD13	1:B:1164:ILE:CD1	2.42	0.48
1:B:1190:ILE:O	1:B:1191:SER:C	2.51	0.48
1:A:144:ARG:NH2	1:A:602:LEU:O	2.46	0.48
1:A:1520:CYS:CB	1:A:1526:LYS:HZ2	2.25	0.48
1:B:1433:SER:HB2	1:B:1480:PHE:HD1	1.78	0.48
1:A:1480:PHE:O	1:A:1482:LEU:N	2.46	0.48
1:B:640:LEU:O	1:B:640:LEU:HD12	2.13	0.48
1:A:177:ILE:C	1:A:177:ILE:HD12	2.33	0.48
1:B:53:THR:HA	1:B:69:GLY:O	2.13	0.48
1:B:1323:LEU:HD11	1:B:1324:HIS:HD2	1.78	0.48
1:B:1143:TYR:HD1	1:B:1186:PHE:HE2	1.60	0.48
2:Y:111:ASP:CG	2:Y:112:PRO:HD2	2.33	0.48
1:A:268:THR:HA	1:A:286:ALA:CB	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1110:ASN:HB2	1:A:1111:TYR:HD2	1.74	0.48
1:A:364:LYS:CD	1:A:364:LYS:H	2.26	0.48
1:A:486:VAL:CG2	1:A:526:ILE:HG13	2.42	0.48
1:B:889:GLU:HG2	1:B:892:SER:HB2	1.95	0.48
1:B:158:GLU:HG2	1:B:177:ILE:HA	1.96	0.48
1:A:940:SER:HB2	1:A:959:PHE:CD1	2.47	0.48
1:A:614:ARG:HH22	1:A:798:GLU:CD	2.16	0.48
1:B:354:LEU:HD11	1:B:437:THR:HG23	1.95	0.48
1:B:267:ILE:HG12	1:B:327:VAL:HG13	1.94	0.48
1:A:250:ILE:HD12	1:A:327:VAL:HG11	1.95	0.48
1:A:1049:LEU:HD23	1:A:1093:VAL:CG2	2.43	0.48
1:B:359:THR:CG2	1:B:372:LYS:HG3	2.44	0.48
1:A:1193:TYR:O	1:A:1196:SER:HB3	2.13	0.48
1:A:227:PHE:HB3	1:A:254:TYR:HD2	1.78	0.48
2:Y:183:THR:HB	2:Y:230:GLN:HB3	1.95	0.48
1:A:1279:ARG:HD3	1:A:1284:PHE:CD2	2.48	0.48
1:A:1548:ARG:NH2	1:A:1620:MET:HE1	2.27	0.48
1:A:1649:PRO:C	1:A:1651:ASP:N	2.65	0.48
1:A:835:ARG:NH1	1:A:835:ARG:CG	2.66	0.48
2:X:49:TYR:HB2	2:X:206:LYS:NZ	2.29	0.48
1:A:160:VAL:O	1:A:160:VAL:CG1	2.44	0.48
1:B:906:GLY:O	1:B:908:HIS:NE2	2.46	0.48
1:A:1594:LYS:HE3	1:B:1399:TYR:HE1	1.77	0.48
1:A:1518:LYS:NZ	1:A:1518:LYS:HB3	2.26	0.48
1:A:1378:TYR:CE2	1:A:1409:LYS:HG2	2.47	0.48
1:B:390:LEU:HB3	1:B:420:PHE:CE1	2.47	0.48
1:B:234:GLU:C	1:B:235:TYR:HD2	2.17	0.48
2:X:68:ASN:CG	2:X:69:GLY:H	2.15	0.48
1:A:1433:SER:HB2	1:A:1480:PHE:CE1	2.48	0.48
1:A:424:LEU:HA	1:A:425:PRO:HD3	1.82	0.48
1:B:227:PHE:HB3	1:B:254:TYR:HD2	1.79	0.48
1:B:453:ARG:HD3	1:B:455:ILE:HD11	1.95	0.48
2:Y:211:ARG:C	2:Y:213:GLY:H	2.17	0.48
1:A:442:LEU:HD22	1:A:443:PRO:CD	2.43	0.48
1:A:1564:SER:HB2	1:A:1616:GLN:CG	2.36	0.48
1:A:1030:HIS:CE1	1:A:1306:GLN:HE21	2.29	0.48
1:A:710:THR:N	1:A:713:GLN:OE1	2.40	0.48
1:A:1412:ARG:O	1:A:1413:GLU:HB2	2.14	0.48
2:Y:64:VAL:HG23	2:Y:71:ASN:OD1	2.12	0.48
1:A:721:GLY:C	1:A:723:ARG:N	2.66	0.48
1:A:501:TYR:OH	2:X:147:ASP:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1530:ALA:O	1:B:1531:ASP:OD2	2.31	0.48
1:A:1310:SER:OG	1:A:1310:SER:O	2.26	0.48
1:B:386:VAL:O	1:B:410:VAL:HG13	2.14	0.48
1:B:307:VAL:O	1:B:308:LYS:O	2.31	0.48
2:X:79:ASP:C	2:X:80:GLN:HE21	2.16	0.48
2:Y:79:ASP:C	2:Y:80:GLN:HE21	2.17	0.48
1:A:531:THR:HG23	1:A:533:ASN:H	1.78	0.48
2:X:224:ILE:HG22	2:X:225:SER:N	2.28	0.48
1:A:635:GLY:C	1:A:673:LEU:HA	2.34	0.48
1:B:49:ALA:O	1:B:50:PHE:HB3	2.13	0.48
1:A:216:TYR:N	1:A:216:TYR:CD2	2.82	0.48
1:A:592:MET:HB2	1:A:592:MET:HE3	1.68	0.48
1:B:1238:SER:C	1:B:1240:PRO:CD	2.82	0.48
2:X:67:TYR:HB3	2:X:72:VAL:CG2	2.44	0.48
1:B:1433:SER:HB2	1:B:1480:PHE:CE1	2.48	0.48
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.39	0.48
1:B:942:VAL:HG12	1:B:943:THR:N	2.29	0.48
1:B:133:PRO:O	1:B:134:VAL:HG23	2.14	0.48
1:A:708:ASP:OD2	1:A:1401:ARG:NH2	2.45	0.48
1:B:27:ALA:HB2	1:B:39:ILE:HD12	1.96	0.48
1:A:465:LEU:HD21	1:A:542:VAL:HG12	1.95	0.48
1:A:839:ILE:HD11	1:A:1483:PHE:CZ	2.48	0.48
1:A:786:LEU:H	1:A:786:LEU:HD23	1.76	0.48
1:B:478:VAL:CG1	1:B:478:VAL:O	2.60	0.48
1:B:511:HIS:ND1	2:Y:149:SER:CB	2.77	0.48
1:A:1582:LEU:O	1:A:1583:ASP:CG	2.52	0.48
1:B:1189:ALA:HB1	1:B:1253:TYR:HB2	1.96	0.48
1:A:1445:GLY:O	1:A:1448:GLN:HB3	2.14	0.48
1:A:88:GLN:HB3	1:A:88:GLN:HE21	1.52	0.48
1:A:335:GLY:O	1:A:336:PHE:O	2.32	0.48
1:B:694:VAL:CG1	1:B:720:LEU:HD13	2.44	0.48
1:A:647:HIS:CE1	1:A:667:GLU:HG3	2.49	0.48
1:B:1273:TRP:O	1:B:1277:GLU:HB2	2.13	0.48
1:B:855:PHE:HA	1:B:915:GLU:O	2.12	0.48
1:A:1534:GLN:O	1:A:1534:GLN:HG2	2.13	0.48
1:A:922:ILE:CD1	4:A:2001:NAG:H82	2.25	0.48
1:B:903:LEU:N	1:B:903:LEU:HD22	2.29	0.48
1:A:412:ARG:HG2	1:A:413:VAL:N	2.27	0.48
2:Y:79:ASP:HB3	2:Y:80:GLN:HE22	1.79	0.48
1:B:92:LEU:H	1:B:93:PRO:HD3	1.79	0.48
1:B:1144:LEU:O	1:B:1148:THR:CG2	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1144:LEU:O	1:A:1148:THR:CG2	2.62	0.48
1:A:381:GLN:N	1:A:381:GLN:HE21	2.10	0.48
1:A:394:THR:HG22	1:A:402:SER:OG	2.14	0.48
1:B:942:VAL:CG2	1:B:957:LYS:CB	2.92	0.48
1:B:193:ASN:OD1	1:B:1070:LYS:NZ	2.46	0.48
1:A:352:TYR:HA	1:A:376:LYS:O	2.13	0.48
1:B:839:ILE:HG23	1:B:900:VAL:HG23	1.92	0.48
1:B:442:LEU:HD23	1:B:442:LEU:HA	1.44	0.48
1:A:466:TYR:CD1	1:A:467:ILE:N	2.82	0.48
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.49	0.48
1:B:153:LYS:CB	1:B:154:PRO:HD2	2.43	0.48
2:Y:82:HIS:ND1	2:Y:116:LEU:HG	2.28	0.48
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.97	0.48
1:A:1180:LEU:HG	1:A:1208:ILE:HG23	1.94	0.48
1:A:195:ARG:CD	1:A:1058:SER:HA	2.43	0.48
1:B:758:LEU:O	1:B:760:VAL:N	2.46	0.48
1:B:683:ILE:CD1	1:B:735:ALA:HB2	2.44	0.48
1:A:1591:VAL:O	1:A:1592:ALA:CB	2.62	0.48
1:A:1188:LEU:HD21	1:A:1212:LEU:HA	1.96	0.48
1:A:590:LEU:HD12	1:A:591:ASN:H	1.78	0.48
1:A:706:ASN:HB3	1:A:714:ARG:HD2	1.95	0.48
1:A:1169:ILE:HG22	1:A:1170:LYS:N	2.28	0.48
1:B:647:HIS:CE1	1:B:667:GLU:HG3	2.48	0.48
1:B:667:GLU:O	1:B:669:CYS:N	2.44	0.48
1:B:1067:SER:OG	1:B:1072:GLY:O	2.29	0.48
1:B:39:ILE:HG13	1:B:85:LEU:HD23	1.96	0.48
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.49	0.48
1:A:367:ILE:HG23	1:A:368:PRO:CD	2.44	0.48
1:A:1209:VAL:O	1:A:1213:LYS:HB2	2.13	0.48
1:B:1113:LEU:C	1:B:1115:ASN:H	2.17	0.48
1:B:440:PRO:CD	1:B:441:ASP:H	2.26	0.48
1:A:1066:TYR:H	1:A:1066:TYR:HD1	1.62	0.48
1:A:607:SER:HB3	1:A:796:THR:O	2.14	0.48
1:B:814:THR:O	1:B:815:VAL:HG23	2.13	0.48
1:B:254:TYR:HB3	1:B:256:TYR:CE2	2.49	0.48
1:B:1067:SER:OG	1:B:1074:ALA:HA	2.13	0.48
2:X:162:LEU:HD23	2:X:211:ARG:HG2	1.95	0.48
1:B:466:TYR:CD1	1:B:467:ILE:N	2.82	0.47
1:A:859:MET:HB3	1:A:898:PHE:CE1	2.48	0.47
1:A:942:VAL:CG2	1:A:957:LYS:CB	2.92	0.47
1:B:595:GLY:O	1:B:596:MET:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:837:GLU:HG2	1:B:1488:LEU:HA	1.94	0.47
1:A:855:PHE:HD2	1:A:888:VAL:HG22	1.79	0.47
1:A:354:LEU:HD21	1:A:448:ALA:C	2.35	0.47
1:B:219:VAL:HG12	1:B:219:VAL:O	2.14	0.47
2:X:107:GLN:OE1	2:X:110:ILE:HD11	2.13	0.47
1:B:235:TYR:HD2	1:B:235:TYR:N	2.12	0.47
1:B:590:LEU:HD12	1:B:591:ASN:N	2.29	0.47
1:A:590:LEU:HD12	1:A:591:ASN:N	2.29	0.47
2:Y:191:ILE:HG13	2:Y:199:VAL:O	2.14	0.47
2:X:183:THR:HB	2:X:230:GLN:HB3	1.95	0.47
1:A:423:ASN:N	1:A:423:ASN:ND2	2.62	0.47
1:B:977:LEU:HD13	1:B:1346:LEU:HD21	1.95	0.47
1:A:1637:TYR:CG	1:A:1638:PRO:HD2	2.49	0.47
1:B:616:ALA:O	1:B:617:LYS:C	2.51	0.47
1:A:572:GLN:HE21	1:A:574:HIS:CE1	2.31	0.47
1:B:679:LEU:HD22	1:B:738:LEU:HD11	1.96	0.47
1:B:639:GLY:N	1:B:645:VAL:HG22	2.24	0.47
1:B:1283:GLY:O	1:B:1285:TYR:N	2.47	0.47
1:A:234:GLU:HG2	1:A:235:TYR:CD2	2.49	0.47
1:A:953:ILE:HD12	1:A:955:ARG:CZ	2.44	0.47
2:X:211:ARG:C	2:X:213:GLY:H	2.16	0.47
1:A:1524:ALA:O	1:A:1528:VAL:HG23	2.14	0.47
1:A:1569:THR:OG1	1:A:1574:PHE:HB3	2.13	0.47
1:A:1280:TYR:HD1	1:A:1362:THR:CG2	2.28	0.47
1:A:1624:ALA:HB1	1:A:1636:ILE:CA	2.39	0.47
1:A:1622:LYS:C	1:A:1637:TYR:HE2	2.18	0.47
1:A:1670:ASP:HA	1:A:1673:LEU:HD11	1.96	0.47
1:B:1096:ASN:HD22	1:B:1099:SER:H	1.51	0.47
1:A:56:ILE:CD1	1:A:66:TYR:HB2	2.43	0.47
1:B:102:VAL:HG23	1:B:103:TYR:N	2.30	0.47
1:B:136:THR:O	1:B:137:PRO:C	2.53	0.47
1:B:710:THR:N	1:B:713:GLN:OE1	2.39	0.47
2:X:146:LEU:C	2:X:146:LEU:HD22	2.35	0.47
1:B:420:PHE:N	1:B:420:PHE:HD2	2.13	0.47
1:B:234:GLU:HG2	1:B:235:TYR:CD2	2.49	0.47
2:Y:67:TYR:HB3	2:Y:72:VAL:CG2	2.44	0.47
1:A:357:VAL:O	1:A:358:ALA:C	2.52	0.47
1:A:683:ILE:CD1	1:A:735:ALA:HB2	2.45	0.47
1:A:193:ASN:OD1	1:A:1070:LYS:NZ	2.47	0.47
1:B:363:LEU:O	1:B:456:ALA:HA	2.15	0.47
1:B:239:GLY:O	1:B:240:TYR:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1169:ILE:HG22	1:B:1170:LYS:N	2.28	0.47
1:A:554:LEU:HB3	1:A:642:ASN:OD1	2.13	0.47
1:B:1186:PHE:CD1	1:B:1250:THR:HG22	2.49	0.47
1:B:54:ILE:HG22	1:B:55:SER:H	1.79	0.47
1:B:159:THR:HG22	1:B:160:VAL:N	2.29	0.47
1:B:1381:ILE:HG13	1:B:1404:ALA:HB2	1.96	0.47
1:A:494:ASP:HA	1:A:496:ILE:HD11	1.95	0.47
1:B:777:VAL:O	1:B:778:HIS:CD2	2.68	0.47
1:B:1049:LEU:HD21	1:B:1089:VAL:HG13	1.96	0.47
1:B:1180:LEU:HG	1:B:1208:ILE:HG23	1.95	0.47
1:B:237:PHE:HE1	1:B:378:SER:O	1.98	0.47
1:A:1238:SER:C	1:A:1240:PRO:CD	2.82	0.47
1:B:953:ILE:HD12	1:B:955:ARG:CZ	2.44	0.47
1:A:758:LEU:HD22	1:A:760:VAL:H	1.78	0.47
1:B:1196:SER:HB2	1:B:1257:THR:HG23	1.96	0.47
1:B:177:ILE:C	1:B:177:ILE:HD12	2.34	0.47
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	1.95	0.47
1:A:1663:ASN:O	1:A:1667:PHE:N	2.45	0.47
2:Y:46:LEU:CD2	2:Y:206:LYS:HE3	2.37	0.47
1:B:1244:THR:CG2	1:B:1246:ARG:H	2.28	0.47
1:A:1564:SER:O	1:A:1579:ALA:HB1	2.14	0.47
1:B:100:SER:O	1:B:101:TYR:CB	2.56	0.47
1:B:101:TYR:HE1	1:B:116:ARG:NE	2.11	0.47
1:A:122:ASP:OD2	1:A:211:THR:HG22	2.14	0.47
1:B:541:LEU:HB2	1:B:558:SER:HB3	1.97	0.47
1:B:639:GLY:HA3	1:B:645:VAL:CA	2.44	0.47
1:A:802:ILE:HG13	1:A:803:GLY:N	2.24	0.47
1:B:1445:GLY:O	1:B:1448:GLN:HB3	2.14	0.47
1:B:364:LYS:H	1:B:364:LYS:CD	2.26	0.47
1:A:1168:LEU:HD23	1:A:1168:LEU:HA	1.59	0.47
1:B:663:GLN:OE1	1:B:663:GLN:HA	2.14	0.47
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.95	0.47
1:A:460:LEU:C	1:A:462:GLN:H	2.18	0.47
1:A:1623:GLU:O	1:A:1637:TYR:HD2	1.98	0.47
1:A:886:GLN:HG3	1:A:887:LYS:N	2.27	0.47
1:A:543:TYR:CB	1:A:556:SER:HB3	2.40	0.47
2:Y:49:TYR:HB2	2:Y:206:LYS:NZ	2.30	0.47
1:A:440:PRO:CD	1:A:441:ASP:H	2.26	0.47
1:A:1068:VAL:CG1	1:A:1069:TRP:N	2.69	0.47
1:A:833:VAL:HA	1:A:1430:THR:HG21	1.95	0.47
1:B:1381:ILE:HD13	1:B:1509:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:HIS:ND1	2:X:149:SER:HB3	2.30	0.47
1:B:499:TYR:CE2	1:B:517:LYS:CG	2.97	0.47
1:A:496:ILE:HG23	1:A:544:TYR:HB2	1.96	0.47
1:A:1127:ILE:N	1:A:1127:ILE:HD12	2.19	0.47
1:B:859:MET:HB3	1:B:898:PHE:CE1	2.50	0.47
2:Y:146:LEU:HD22	2:Y:146:LEU:C	2.35	0.47
1:B:1245:ALA:CA	1:B:1285:TYR:HB3	2.43	0.47
1:A:1342:LEU:HD23	1:A:1342:LEU:N	2.30	0.47
1:A:780:VAL:HG13	1:A:783:ARG:C	2.35	0.47
2:Y:120:GLY:HA3	2:Y:212:MET:O	2.14	0.47
1:A:768:TYR:HE2	1:A:770:PRO:HA	1.80	0.47
1:B:394:THR:HG23	1:B:428:VAL:HG23	1.96	0.47
1:B:394:THR:HG22	1:B:402:SER:OG	2.14	0.47
1:B:501:TYR:OH	2:Y:147:ASP:HA	2.14	0.47
1:B:1484:GLU:OE1	1:B:1484:GLU:N	2.37	0.47
1:B:1494:THR:HB	1:B:1506:THR:HG23	1.97	0.47
1:B:855:PHE:CZ	1:B:886:GLN:HB3	2.50	0.47
2:X:79:ASP:HB3	2:X:80:GLN:HE22	1.80	0.47
1:A:531:THR:HG22	1:A:534:MET:CG	2.45	0.47
1:A:1136:GLU:OE1	1:A:1415:SER:CB	2.63	0.47
1:A:643:ALA:O	1:A:644:ASN:C	2.52	0.47
2:X:120:GLY:HA3	2:X:212:MET:O	2.15	0.47
2:Y:68:ASN:CG	2:Y:69:GLY:H	2.16	0.47
1:B:88:GLN:HE21	1:B:88:GLN:HB3	1.53	0.47
1:A:1401:ARG:HG2	1:A:1402:ILE:N	2.28	0.47
1:B:959:PHE:HD2	1:B:959:PHE:H	1.60	0.47
1:A:1644:TRP:O	1:A:1645:ILE:C	2.53	0.47
1:A:1228:TRP:H	1:A:1228:TRP:HE3	1.60	0.47
1:A:1008:ALA:N	1:A:1068:VAL:O	2.38	0.47
1:B:367:ILE:HG23	1:B:368:PRO:CD	2.45	0.47
1:A:1300:TYR:C	1:A:1300:TYR:CD2	2.88	0.47
1:B:820:PHE:HE2	1:B:848:TYR:HD2	1.55	0.47
1:A:693:SER:O	1:A:696:LYS:HB3	2.15	0.47
1:B:331:GLU:OE1	1:B:336:PHE:HD1	1.97	0.47
1:A:32:ARG:HB2	1:A:35:ALA:HB2	1.97	0.47
2:X:104:PHE:CZ	2:X:164:GLU:HG3	2.50	0.47
1:A:1420:SER:HB3	1:A:1497:GLU:OE2	2.15	0.47
1:A:288:GLN:O	1:A:289:ASN:O	2.33	0.47
1:A:1367:LYS:HE2	1:A:1367:LYS:HB3	1.56	0.47
1:A:1568:ILE:HD13	1:A:1577:TYR:CD2	2.50	0.47
1:A:1611:LEU:O	1:A:1611:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1674:ASN:CG	1:B:258:LYS:HZ1	2.18	0.47
1:A:442:LEU:HD23	1:A:443:PRO:HD3	1.95	0.47
1:B:153:LYS:O	1:B:155:ALA:N	2.48	0.47
1:A:1270:VAL:HG12	1:A:1271:ILE:N	2.30	0.47
1:A:1132:THR:N	1:A:1135:VAL:HB	2.30	0.47
1:A:1210:SER:O	1:A:1211:ALA:C	2.53	0.47
1:B:323:LEU:HB2	1:B:347:TYR:CE2	2.50	0.47
2:Y:104:PHE:CZ	2:Y:164:GLU:HG3	2.50	0.47
2:Y:162:LEU:HD23	2:Y:211:ARG:HG2	1.96	0.47
1:A:1486:GLY:O	1:A:1487:PHE:CE2	2.57	0.46
1:A:322:TYR:CD2	1:A:322:TYR:N	2.84	0.46
1:B:1075:SER:HG	1:B:1078:LEU:H	1.59	0.46
2:X:82:HIS:ND1	2:X:116:LEU:HG	2.30	0.46
1:B:592:MET:HE3	1:B:592:MET:HB2	1.67	0.46
1:B:166:PRO:HG2	1:B:195:ARG:O	2.15	0.46
1:B:1066:TYR:H	1:B:1066:TYR:HD1	1.64	0.46
1:B:335:GLY:O	1:B:336:PHE:O	2.33	0.46
1:B:1003:LEU:HA	1:B:1004:PRO:HD2	1.41	0.46
1:A:1067:SER:OG	1:A:1074:ALA:HA	2.14	0.46
1:B:227:PHE:CZ	1:B:338:GLU:HB2	2.50	0.46
1:B:944:LEU:HD23	1:B:944:LEU:HA	1.55	0.46
1:A:959:PHE:HD2	1:A:959:PHE:H	1.63	0.46
1:A:1562:LYS:NZ	1:A:1648:TRP:CE2	2.83	0.46
1:B:982:LEU:CD2	1:B:1309:LEU:HD11	2.46	0.46
2:Y:57:TYR:CD2	2:Y:58:SER:N	2.79	0.46
1:B:1378:TYR:O	1:B:1406:ALA:HA	2.14	0.46
1:A:92:LEU:H	1:A:93:PRO:HD3	1.79	0.46
1:A:1049:LEU:HD23	1:A:1093:VAL:HG23	1.96	0.46
1:A:310:LEU:N	1:A:310:LEU:HD23	2.31	0.46
1:A:758:LEU:O	1:A:760:VAL:N	2.48	0.46
1:B:945:ASP:OD2	1:B:950:TYR:HB2	2.15	0.46
1:A:1592:ALA:HB1	1:A:1596:SER:OG	2.16	0.46
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.97	0.46
1:B:967:LEU:HD13	1:B:1365:VAL:HG22	1.97	0.46
1:A:825:LEU:HG	1:A:826:GLU:N	2.28	0.46
2:Y:192:ASN:ND2	2:Y:223:GLY:O	2.49	0.46
1:B:606:ASP:C	1:B:606:ASP:OD1	2.52	0.46
1:B:1323:LEU:CG	1:B:1324:HIS:H	2.26	0.46
1:A:25:ILE:HD13	1:A:41:ILE:HB	1.96	0.46
1:A:1230:ASP:OD2	1:A:1246:ARG:HD2	2.16	0.46
1:B:122:ASP:OD2	1:B:211:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:LEU:C	1:A:1115:ASN:H	2.18	0.46
1:B:263:ALA:HB3	1:B:292:LEU:CB	2.39	0.46
1:B:269:PHE:CE2	1:B:325:ILE:HG23	2.50	0.46
1:A:774:LEU:HD23	1:A:774:LEU:HA	1.70	0.46
1:A:234:GLU:HG2	1:A:235:TYR:HE2	1.78	0.46
1:B:234:GLU:C	1:B:235:TYR:CD2	2.89	0.46
1:A:1303:LEU:C	1:A:1303:LEU:CD1	2.84	0.46
1:B:1303:LEU:C	1:B:1303:LEU:CD1	2.84	0.46
1:B:1502:ASP:C	1:B:1503:LYS:HD2	2.35	0.46
1:A:158:GLU:HG2	1:A:177:ILE:HA	1.97	0.46
1:B:570:GLN:O	1:B:594:THR:HA	2.15	0.46
1:A:570:GLN:O	1:A:594:THR:HA	2.15	0.46
1:B:839:ILE:HD11	1:B:1483:PHE:CZ	2.50	0.46
1:B:322:TYR:CD2	1:B:322:TYR:N	2.83	0.46
1:B:1227:PHE:HB2	1:B:1251:THR:HG21	1.97	0.46
1:B:1230:ASP:O	1:B:1231:ASN:O	2.33	0.46
1:A:572:GLN:HG3	1:A:574:HIS:NE2	2.30	0.46
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.97	0.46
1:B:530:VAL:HA	1:B:534:MET:SD	2.55	0.46
1:A:1617:TYR:O	1:A:1619:ILE:HD12	2.16	0.46
1:B:780:VAL:HG13	1:B:783:ARG:C	2.35	0.46
1:B:1060:ARG:NH2	1:B:1064:TYR:CE1	2.83	0.46
1:B:635:GLY:C	1:B:673:LEU:HA	2.36	0.46
1:A:948:GLY:HA2	1:A:952:THR:O	2.15	0.46
1:A:420:PHE:HD2	1:A:420:PHE:N	2.13	0.46
1:B:357:VAL:O	1:B:358:ALA:C	2.53	0.46
1:A:1050:LYS:O	1:A:1051:GLU:C	2.53	0.46
1:B:590:LEU:HD12	1:B:591:ASN:H	1.79	0.46
1:A:1323:LEU:HD11	1:A:1324:HIS:HD2	1.80	0.46
1:A:1227:PHE:C	1:A:1228:TRP:CE3	2.89	0.46
1:A:833:VAL:HG23	1:A:927:LEU:HD21	1.98	0.46
1:B:1334:LEU:N	1:B:1334:LEU:CD2	2.65	0.46
1:B:125:PHE:CE1	1:B:152:LEU:HD11	2.51	0.46
2:X:57:TYR:CD2	2:X:58:SER:N	2.79	0.46
1:B:544:TYR:CD2	1:B:546:VAL:HG23	2.50	0.46
1:A:829:ILE:CG2	1:A:830:PRO:CD	2.94	0.46
1:A:1082:ALA:O	1:A:1086:LEU:HD23	2.15	0.46
2:X:192:ASN:ND2	2:X:223:GLY:O	2.48	0.46
1:B:1279:ARG:CG	1:B:1284:PHE:CG	2.98	0.46
1:A:1673:LEU:HB2	1:B:258:LYS:HD2	1.97	0.46
1:B:86:THR:O	1:B:86:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:VAL:HG11	1:B:543:TYR:OH	2.16	0.46
1:A:506:LYS:HE2	1:A:506:LYS:HB2	1.56	0.46
1:A:531:THR:N	1:A:534:MET:SD	2.80	0.46
1:B:1104:LEU:O	1:B:1108:VAL:HG12	2.15	0.46
1:B:1108:VAL:HG21	1:B:1167:ALA:HB2	1.98	0.46
1:A:1273:TRP:O	1:A:1277:GLU:HB2	2.16	0.46
1:B:955:ARG:O	1:B:956:ARG:HG3	2.16	0.46
1:A:236:ASN:C	1:A:237:PHE:HD2	2.18	0.46
1:A:1622:LYS:HE2	1:A:1637:TYR:OH	2.15	0.46
1:A:1674:ASN:O	1:A:1675:GLY:C	2.54	0.46
1:B:1268:ASN:HB2	1:B:1269:PRO:HD3	1.97	0.46
1:A:906:GLY:O	1:A:908:HIS:NE2	2.49	0.46
1:A:1381:ILE:HD13	1:A:1509:TYR:CE1	2.51	0.46
1:B:292:LEU:HA	1:B:297:ALA:HB2	1.98	0.46
1:B:511:HIS:NE2	1:B:531:THR:HG21	2.30	0.46
1:A:1595:ASP:OD2	1:B:1514:ILE:HD11	2.16	0.46
1:B:829:ILE:CG2	1:B:830:PRO:CD	2.94	0.46
1:A:774:LEU:HD11	1:A:788:PHE:CZ	2.51	0.46
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.51	0.46
1:B:1342:LEU:HD23	1:B:1342:LEU:N	2.31	0.46
1:B:381:GLN:N	1:B:381:GLN:HE21	2.14	0.46
1:B:247:GLU:CG	1:B:298:GLN:OE1	2.64	0.46
1:B:1464:LEU:N	1:B:1464:LEU:CD1	2.79	0.46
1:B:1197:LEU:CD2	1:B:1260:ASN:HD21	2.29	0.46
1:A:1221:ASN:ND2	1:A:1222:PRO:HA	2.31	0.46
1:B:288:GLN:O	1:B:289:ASN:O	2.33	0.46
2:X:191:ILE:HG13	2:X:199:VAL:O	2.16	0.46
2:X:194:LYS:HZ2	2:X:197:ASN:HB2	1.81	0.46
2:X:66:ASN:N	2:X:66:ASN:OD1	2.48	0.46
1:B:855:PHE:HD2	1:B:888:VAL:HG22	1.81	0.46
1:A:1244:THR:HG22	1:A:1247:MET:N	2.26	0.46
1:B:442:LEU:HD23	1:B:443:PRO:HD3	1.97	0.46
1:A:1429:PRO:HB3	1:A:1488:LEU:HD22	1.97	0.46
1:A:252:ALA:HB1	1:A:260:VAL:HG21	1.96	0.46
1:B:141:VAL:CG2	1:B:190:ILE:HD11	2.46	0.46
1:B:225:PRO:HG3	1:B:766:ARG:O	2.14	0.46
1:A:101:TYR:HE1	1:A:116:ARG:NE	2.13	0.46
1:B:840:GLN:CG	1:B:899:THR:HG22	2.45	0.46
1:A:1146:ALA:O	1:A:1150:ILE:HG13	2.16	0.46
1:A:377:ASP:O	1:A:380:ASP:N	2.42	0.46
1:B:284:GLN:CD	1:B:310:LEU:HD22	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:THR:HA	1:A:789:ALA:HA	1.98	0.46
1:A:394:THR:HG23	1:A:428:VAL:HG23	1.97	0.46
1:A:606:ASP:C	1:A:606:ASP:OD1	2.53	0.46
1:B:977:LEU:HD13	1:B:1346:LEU:CD2	2.45	0.46
1:B:894:HIS:ND1	1:B:895:LEU:O	2.49	0.46
1:A:1664:LEU:HD23	1:A:1664:LEU:HA	1.59	0.46
1:B:25:ILE:HD13	1:B:41:ILE:HB	1.96	0.46
1:A:225:PRO:HG3	1:A:766:ARG:O	2.16	0.46
1:B:496:ILE:HD13	1:B:517:LYS:NZ	2.30	0.46
1:A:777:VAL:O	1:A:778:HIS:CD2	2.69	0.46
1:B:827:MET:HE3	1:B:842:LYS:O	2.16	0.46
1:B:930:VAL:CG1	1:B:931:PRO:CD	2.94	0.46
1:A:945:ASP:OD2	1:A:950:TYR:HB2	2.16	0.46
1:B:171:VAL:HG12	1:B:171:VAL:O	2.16	0.46
1:A:802:ILE:CD1	1:A:809:ILE:HG13	2.46	0.46
1:B:377:ASP:O	1:B:380:ASP:N	2.41	0.46
1:A:1629:TYR:CZ	1:A:1632:SER:HA	2.51	0.46
1:A:663:GLN:HA	1:A:663:GLN:OE1	2.15	0.46
1:A:694:VAL:CG1	1:A:720:LEU:HD13	2.46	0.46
1:A:1638:PRO:O	1:A:1639:LEU:HB3	2.15	0.46
1:A:1096:ASN:C	1:A:1096:ASN:ND2	2.69	0.46
1:A:54:ILE:HG22	1:A:55:SER:H	1.80	0.46
1:A:136:THR:O	1:A:137:PRO:C	2.54	0.46
1:B:969:PRO:O	1:B:971:THR:HG23	2.16	0.46
1:B:1274:LEU:HB3	1:B:1297:LEU:HD11	1.98	0.46
1:A:693:SER:O	1:A:696:LYS:N	2.48	0.46
1:B:1050:LYS:O	1:B:1051:GLU:C	2.53	0.46
1:A:1346:LEU:HG	1:A:1347:ILE:N	2.32	0.45
1:A:1618:LEU:HD12	1:A:1618:LEU:O	2.16	0.45
1:A:1651:ASP:HB3	1:A:1654:CYS:SG	2.56	0.45
1:B:304:GLU:O	1:B:308:LYS:HG3	2.16	0.45
1:B:1096:ASN:C	1:B:1096:ASN:ND2	2.69	0.45
1:A:903:LEU:N	1:A:903:LEU:HD22	2.31	0.45
1:B:222:TYR:CD2	1:B:223:VAL:N	2.85	0.45
2:Y:101:GLN:HB3	2:Y:123:THR:O	2.17	0.45
2:Y:107:GLN:OE1	2:Y:110:ILE:HD11	2.14	0.45
2:Y:77:PRO:O	2:Y:78:LYS:CB	2.64	0.45
1:A:488:PRO:O	1:A:489:LYS:C	2.54	0.45
1:A:930:VAL:CG1	1:A:931:PRO:CD	2.93	0.45
1:B:1136:GLU:OE1	1:B:1415:SER:CB	2.64	0.45
1:B:1016:VAL:HG12	1:B:1017:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:693:SER:O	1:B:696:LYS:HB3	2.16	0.45
1:B:1500:ARG:C	1:B:1502:ASP:H	2.20	0.45
1:B:1370:THR:O	1:B:1371:SER:C	2.54	0.45
1:A:410:VAL:CG1	1:A:411:THR:N	2.79	0.45
1:B:38:ASN:C	1:B:39:ILE:HD13	2.37	0.45
1:B:385:GLY:H	1:B:411:THR:HG23	1.80	0.45
1:A:389:THR:CG2	1:A:408:LYS:HE2	2.32	0.45
1:A:511:HIS:ND1	2:X:149:SER:CB	2.80	0.45
1:A:820:PHE:HE2	1:A:848:TYR:HD2	1.57	0.45
1:B:318:LEU:O	1:B:319:ASN:CB	2.58	0.45
1:B:195:ARG:CD	1:B:1058:SER:HA	2.46	0.45
1:B:693:SER:O	1:B:696:LYS:N	2.48	0.45
1:A:862:VAL:HG21	1:A:909:ASN:O	2.16	0.45
1:A:737:GLN:HG2	1:A:737:GLN:H	1.61	0.45
1:A:227:PHE:CZ	1:A:338:GLU:HB2	2.52	0.45
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.51	0.45
1:B:460:LEU:C	1:B:462:GLN:H	2.20	0.45
1:B:946:PRO:HD2	1:B:947:ARG:H	1.81	0.45
1:A:1651:ASP:CB	1:A:1654:CYS:SG	3.05	0.45
2:X:138:VAL:HG12	2:X:138:VAL:O	2.16	0.45
1:A:544:TYR:CD2	1:A:546:VAL:HG23	2.51	0.45
1:A:949:ILE:HB	1:A:950:TYR:HD2	1.81	0.45
1:B:754:MET:O	1:B:755:LYS:CG	2.65	0.45
1:A:428:VAL:HG22	1:A:429:THR:N	2.30	0.45
1:B:504:LEU:N	1:B:504:LEU:CD1	2.79	0.45
1:B:1401:ARG:HG2	1:B:1402:ILE:N	2.28	0.45
1:A:1673:LEU:HB2	1:B:258:LYS:CE	2.46	0.45
1:A:27:ALA:HB2	1:A:39:ILE:HD12	1.98	0.45
1:A:73:LEU:H	1:A:73:LEU:CD2	2.20	0.45
1:B:465:LEU:HD21	1:B:542:VAL:HG12	1.98	0.45
1:B:1201:THR:O	1:B:1202:HIS:C	2.55	0.45
1:A:159:THR:HG22	1:A:160:VAL:N	2.31	0.45
2:X:77:PRO:O	2:X:78:LYS:CB	2.64	0.45
1:A:511:HIS:NE2	1:A:531:THR:HG21	2.31	0.45
1:B:310:LEU:HD23	1:B:310:LEU:N	2.30	0.45
1:B:758:LEU:HD22	1:B:760:VAL:H	1.82	0.45
1:B:1421:HIS:C	1:B:1421:HIS:CD2	2.88	0.45
1:A:1196:SER:HB2	1:A:1257:THR:HG23	1.99	0.45
1:B:1420:SER:HB3	1:B:1497:GLU:OE2	2.16	0.45
1:B:1168:LEU:HA	1:B:1168:LEU:HD23	1.57	0.45
1:A:425:PRO:O	1:A:426:SER:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLU:O	1:A:669:CYS:N	2.44	0.45
2:Y:66:ASN:OD1	2:Y:66:ASN:N	2.48	0.45
1:A:1568:ILE:O	1:A:1568:ILE:HG23	2.16	0.45
2:Y:138:VAL:O	2:Y:138:VAL:HG12	2.16	0.45
1:B:113:LYS:HG3	1:B:114:SER:H	1.80	0.45
1:B:572:GLN:HG3	1:B:574:HIS:NE2	2.32	0.45
1:A:1012:LEU:HA	1:A:1012:LEU:HD23	1.79	0.45
1:B:981:GLY:H	1:B:1333:PHE:HB2	1.81	0.45
1:B:101:TYR:CE1	1:B:116:ARG:NE	2.84	0.45
1:B:496:ILE:HG23	1:B:544:TYR:HB2	1.97	0.45
1:A:969:PRO:O	1:A:971:THR:HG23	2.17	0.45
1:A:639:GLY:HA3	1:A:645:VAL:HA	1.98	0.45
1:A:1379:LEU:HD23	1:A:1406:ALA:HA	1.98	0.45
1:A:707:ASN:HB3	1:A:739:ARG:CZ	2.46	0.45
1:B:755:LYS:HD2	1:B:755:LYS:HA	1.82	0.45
1:A:379:LEU:CB	1:A:381:GLN:HE22	2.29	0.45
1:A:247:GLU:HG3	1:A:300:THR:HG23	1.97	0.45
1:A:373:VAL:HG21	1:A:388:VAL:HG11	1.98	0.45
1:A:127:PHE:HE1	1:A:626:PHE:CD2	2.34	0.45
1:A:895:LEU:CD1	1:A:1555:PRO:CB	2.93	0.45
1:A:1670:ASP:O	1:A:1670:ASP:OD2	2.34	0.45
1:A:987:ILE:HD13	1:A:1294:ILE:HG23	1.97	0.45
1:A:79:PHE:O	1:A:80:GLN:HG2	2.16	0.45
1:B:444:GLU:O	1:B:447:GLN:HB2	2.17	0.45
1:A:833:VAL:HG13	1:A:839:ILE:HD13	1.99	0.45
1:B:572:GLN:HE21	1:B:574:HIS:CE1	2.33	0.45
1:B:489:LYS:O	1:B:491:PRO:CD	2.61	0.45
1:B:379:LEU:CB	1:B:381:GLN:HE22	2.30	0.45
1:B:774:LEU:HD23	1:B:774:LEU:HA	1.69	0.45
1:A:583:SER:O	1:A:585:GLY:N	2.49	0.45
1:A:592:MET:HE3	1:A:780:VAL:HG21	1.99	0.45
1:A:1016:VAL:CG1	1:A:1017:PRO:HD3	2.47	0.45
1:A:481:HIS:CE1	1:A:529:PRO:HG3	2.52	0.45
1:B:375:VAL:HG12	1:B:376:LYS:N	2.31	0.45
1:A:626:PHE:O	1:A:628:GLU:N	2.49	0.45
1:A:935:LYS:HD2	1:A:935:LYS:HA	1.65	0.45
1:B:1090:ASN:OD1	1:B:1090:ASN:O	2.34	0.45
1:A:1637:TYR:CZ	1:A:1638:PRO:HG2	2.51	0.45
1:A:837:GLU:HG3	1:A:1488:LEU:HA	1.99	0.45
1:A:260:VAL:HG11	1:A:263:ALA:HB2	1.99	0.45
1:A:1213:LYS:HG3	1:A:1266:TYR:OH	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ARG:H	1:A:178:ASP:CB	2.28	0.45
1:B:1300:TYR:CZ	1:B:1304:VAL:HG21	2.52	0.45
1:A:1563:VAL:HA	1:A:1582:LEU:HD13	1.98	0.45
2:Y:73:VAL:CG1	2:Y:74:ARG:H	2.29	0.45
1:B:1270:VAL:HG12	1:B:1271:ILE:N	2.31	0.45
1:A:769:PHE:HA	1:A:770:PRO:HD3	1.78	0.45
1:B:503:ILE:HG12	1:B:540:LEU:HB3	1.97	0.45
1:B:512:PHE:N	1:B:512:PHE:CD2	2.85	0.45
1:B:1279:ARG:CB	1:B:1284:PHE:HB2	2.45	0.45
1:A:977:LEU:HD12	1:A:1361:VAL:HG23	1.92	0.45
1:B:654:LEU:HA	1:B:654:LEU:HD12	1.57	0.45
1:A:292:LEU:HD13	1:A:293:ILE:H	1.81	0.45
2:X:81:ASN:O	2:X:115:ARG:HB2	2.17	0.45
1:B:531:THR:N	1:B:534:MET:SD	2.80	0.45
1:A:156:LYS:HG2	1:A:178:ASP:O	2.17	0.45
1:B:1132:THR:N	1:B:1135:VAL:HB	2.29	0.45
1:B:1049:LEU:HD23	1:B:1093:VAL:HG23	1.99	0.45
2:X:146:LEU:C	2:X:146:LEU:CD2	2.86	0.45
1:A:1052:GLY:O	1:A:1055:SER:HB3	2.17	0.45
1:B:1451:THR:HG23	1:B:1464:LEU:HA	1.98	0.45
1:B:1307:LEU:O	1:B:1308:ARG:C	2.54	0.45
1:B:1037:ASP:HA	1:B:1038:PRO:HD3	1.73	0.45
1:A:1035:HIS:CD2	1:A:1035:HIS:H	2.35	0.45
1:A:1599:THR:CG2	1:A:1600:PHE:H	2.30	0.45
1:A:1666:GLU:O	1:A:1667:PHE:C	2.55	0.45
1:B:444:GLU:OE1	1:B:449:ARG:NH2	2.49	0.45
1:B:702:GLY:CA	1:B:728:PHE:CD1	2.98	0.45
1:A:885:ARG:HG2	1:A:1626:GLN:O	2.17	0.45
1:B:707:ASN:HB3	1:B:739:ARG:CZ	2.46	0.45
1:A:180:ILE:HD12	1:A:599:TRP:CG	2.52	0.45
1:B:587:THR:HA	1:B:789:ALA:HA	1.99	0.45
1:A:942:VAL:HG22	1:A:957:LYS:HD3	1.99	0.45
1:B:1037:ASP:C	1:B:1037:ASP:OD1	2.55	0.45
1:B:665:ASN:CG	1:B:666:ASP:H	2.20	0.45
1:A:686:ILE:C	1:A:688:ALA:H	2.21	0.45
1:A:133:PRO:O	1:A:134:VAL:HG23	2.17	0.45
1:A:1280:TYR:HD1	1:A:1362:THR:HG21	1.81	0.45
1:A:1279:ARG:CG	1:A:1284:PHE:CG	2.99	0.45
1:A:1096:ASN:C	1:A:1096:ASN:HD22	2.19	0.45
1:B:1230:ASP:CG	1:B:1246:ARG:HD2	2.38	0.45
1:B:153:LYS:O	1:B:154:PRO:C	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLN:O	1:A:299:VAL:HG13	2.17	0.45
1:B:71:VAL:CG2	1:B:71:VAL:O	2.64	0.45
1:A:1277:GLU:OE2	1:A:1277:GLU:HA	2.17	0.45
1:A:208:ASP:O	1:A:209:PHE:CG	2.70	0.45
2:X:104:PHE:CD2	2:X:164:GLU:HB2	2.52	0.45
1:B:626:PHE:O	1:B:628:GLU:N	2.49	0.45
1:A:667:GLU:C	1:A:669:CYS:H	2.20	0.45
1:A:1531:ASP:OD1	1:A:1531:ASP:O	2.34	0.45
1:B:1429:PRO:HB3	1:B:1488:LEU:HD22	1.99	0.44
1:A:1279:ARG:CB	1:A:1284:PHE:HB2	2.42	0.44
2:Y:150:ILE:CD1	2:Y:150:ILE:C	2.82	0.44
1:A:304:GLU:O	1:A:308:LYS:HG3	2.17	0.44
1:B:59:TYR:HA	1:B:59:TYR:HD1	1.63	0.44
2:X:61:SER:N	2:X:75:PHE:CZ	2.84	0.44
1:A:981:GLY:HA3	1:A:1309:LEU:HD11	1.98	0.44
1:B:265:VAL:HG23	1:B:292:LEU:H	1.82	0.44
1:A:499:TYR:CE2	1:A:517:LYS:CG	3.00	0.44
1:B:819:VAL:O	1:B:820:PHE:CB	2.66	0.44
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	2.35	0.44
1:A:758:LEU:C	1:A:760:VAL:N	2.71	0.44
1:B:768:TYR:HE2	1:B:770:PRO:HA	1.82	0.44
1:B:1255:LEU:HD13	1:B:1270:VAL:HG11	2.00	0.44
1:B:1195:LEU:C	1:B:1197:LEU:N	2.70	0.44
1:A:254:TYR:HB3	1:A:256:TYR:CE2	2.52	0.44
1:A:503:ILE:HG12	1:A:540:LEU:HB3	1.98	0.44
1:A:986:GLU:CG	1:A:1281:GLY:H	2.30	0.44
1:B:845:VAL:HG12	1:B:894:HIS:O	2.16	0.44
1:A:886:GLN:CD	1:A:894:HIS:HE1	2.20	0.44
1:A:367:ILE:HG23	1:A:368:PRO:HD2	1.99	0.44
1:A:1604:VAL:CG1	1:A:1605:THR:N	2.79	0.44
1:A:610:TYR:HB3	1:A:614:ARG:HD2	2.00	0.44
2:Y:61:SER:N	2:Y:75:PHE:CZ	2.85	0.44
1:B:252:ALA:HB1	1:B:260:VAL:HG21	1.99	0.44
1:B:156:LYS:HG2	1:B:178:ASP:O	2.17	0.44
1:B:531:THR:HG23	1:B:533:ASN:H	1.81	0.44
1:B:931:PRO:HB2	1:B:1366:HIS:CD2	2.52	0.44
1:B:639:GLY:HA3	1:B:645:VAL:HA	1.98	0.44
1:B:180:ILE:HD12	1:B:599:TRP:CG	2.51	0.44
1:A:234:GLU:HB2	1:A:247:GLU:N	2.32	0.44
1:B:428:VAL:HG22	1:B:429:THR:N	2.32	0.44
1:A:444:GLU:OE1	1:A:449:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:855:PHE:CZ	1:A:886:GLN:HB3	2.53	0.44
1:A:845:VAL:HG12	1:A:894:HIS:O	2.16	0.44
1:A:24:VAL:HG11	1:A:543:TYR:OH	2.17	0.44
1:B:1143:TYR:CD1	1:B:1186:PHE:CE2	3.05	0.44
1:B:367:ILE:HD13	1:B:466:TYR:HD2	1.82	0.44
1:B:571:LEU:C	1:B:571:LEU:CD1	2.85	0.44
1:B:1012:LEU:HD23	1:B:1012:LEU:HA	1.81	0.44
1:A:1381:ILE:HG13	1:A:1404:ALA:HB2	1.99	0.44
2:Y:190:ILE:CG1	2:Y:190:ILE:O	2.63	0.44
1:B:1054:LEU:O	1:B:1055:SER:C	2.54	0.44
1:B:1027:THR:O	1:B:1027:THR:HG22	2.16	0.44
1:A:1274:LEU:HB3	1:A:1297:LEU:HD11	2.00	0.44
1:B:50:PHE:HB3	1:B:109:LYS:HE2	1.99	0.44
1:B:127:PHE:HE1	1:B:626:PHE:CD2	2.35	0.44
1:A:665:ASN:CG	1:A:666:ASP:H	2.20	0.44
1:B:833:VAL:HA	1:B:1430:THR:HG21	1.98	0.44
1:A:1535:MET:HA	1:A:1645:ILE:HD11	1.99	0.44
1:A:38:ASN:C	1:A:39:ILE:HD13	2.37	0.44
1:B:280:LYS:HG2	1:B:282:MET:HE3	1.99	0.44
1:A:153:LYS:O	1:A:155:ALA:N	2.51	0.44
1:B:820:PHE:CZ	1:B:848:TYR:CD2	3.05	0.44
1:A:847:ASN:HD21	1:A:853:MET:HG2	1.82	0.44
1:B:1108:VAL:CG2	1:B:1167:ALA:HB2	2.46	0.44
1:A:1484:GLU:N	1:A:1484:GLU:OE1	2.41	0.44
1:A:284:GLN:CD	1:A:310:LEU:HD22	2.37	0.44
2:Y:104:PHE:CD2	2:Y:164:GLU:HB2	2.53	0.44
1:A:1182:ALA:CB	1:A:1188:LEU:HD13	2.47	0.44
1:B:643:ALA:O	1:B:646:PHE:N	2.50	0.44
1:A:375:VAL:HG12	1:A:376:LYS:N	2.32	0.44
1:B:504:LEU:HD21	1:B:651:LEU:HG	1.99	0.44
2:Y:211:ARG:C	2:Y:213:GLY:N	2.71	0.44
1:A:1278:GLN:O	1:A:1360:HIS:NE2	2.49	0.44
1:A:1558:ALA:HB3	1:A:1623:GLU:N	2.33	0.44
1:A:1548:ARG:O	1:A:1667:PHE:HE1	2.01	0.44
1:B:442:LEU:CD2	1:B:443:PRO:HD3	2.47	0.44
1:A:1204:GLN:OE1	1:A:1204:GLN:HA	2.18	0.44
1:B:367:ILE:CD1	1:B:466:TYR:CB	2.94	0.44
1:B:56:ILE:HG12	1:B:56:ILE:H	1.62	0.44
1:A:1328:MET:O	1:A:1329:THR:HG23	2.18	0.44
2:Y:128:LYS:HD3	2:Y:158:GLU:HG2	1.99	0.44
2:Y:71:ASN:O	2:Y:72:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:LEU:HA	1:A:1000:LEU:HD23	1.73	0.44
1:B:352:TYR:HA	1:B:376:LYS:O	2.16	0.44
1:B:32:ARG:HB2	1:B:35:ALA:HB2	1.99	0.44
1:A:1569:THR:HG21	1:A:1574:PHE:HD2	1.82	0.44
1:A:995:GLU:O	1:A:996:GLY:O	2.36	0.44
1:B:995:GLU:O	1:B:996:GLY:O	2.36	0.44
1:A:1673:LEU:HB2	1:B:258:LYS:HE3	1.99	0.44
2:X:43:ILE:HB	2:X:185:LYS:HZ3	1.83	0.44
2:Y:57:TYR:HE1	2:Y:77:PRO:HA	1.83	0.44
1:B:315:LEU:O	1:B:318:LEU:HB2	2.16	0.44
1:A:946:PRO:HD2	1:A:947:ARG:H	1.82	0.44
1:A:754:MET:O	1:A:755:LYS:CG	2.65	0.44
1:A:1522:GLY:O	1:A:1523:ALA:CB	2.65	0.44
1:B:862:VAL:HG21	1:B:909:ASN:O	2.17	0.44
1:A:1421:HIS:CD2	1:A:1421:HIS:C	2.91	0.44
1:A:1502:ASP:C	1:A:1503:LYS:HD2	2.38	0.44
1:A:141:VAL:CG2	1:A:190:ILE:HD11	2.46	0.44
1:B:1105:LEU:HD22	1:B:1109:GLU:OE1	2.18	0.44
1:A:1345:ASP:OD2	1:A:1345:ASP:N	2.51	0.44
1:B:1279:ARG:HG3	1:B:1284:PHE:HB3	1.82	0.44
1:A:1638:PRO:O	1:A:1639:LEU:CB	2.65	0.44
1:A:894:HIS:C	1:A:894:HIS:CD2	2.91	0.44
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	1.99	0.44
1:B:42:GLN:CD	1:B:543:TYR:HH	2.21	0.44
1:A:369:TYR:HA	1:A:370:PRO:HD3	1.73	0.44
1:A:484:ILE:C	1:A:485:ILE:HD13	2.38	0.44
1:A:102:VAL:HG23	1:A:103:TYR:N	2.31	0.44
1:A:1261:LEU:O	1:A:1263:ASP:N	2.51	0.44
2:X:101:GLN:HB3	2:X:123:THR:O	2.17	0.44
1:B:930:VAL:HG12	1:B:931:PRO:CD	2.47	0.44
1:A:859:MET:HE2	1:A:910:ILE:HG21	1.99	0.44
1:A:185:PHE:HB3	1:A:186:PRO:HD3	1.99	0.44
1:A:1520:CYS:HB3	1:A:1526:LYS:NZ	2.33	0.44
1:B:1236:ASP:HB2	1:B:1412:ARG:NH2	2.32	0.44
1:B:696:LYS:HZ1	1:B:700:TYR:HD2	1.57	0.44
2:X:71:ASN:O	2:X:72:VAL:HG23	2.18	0.44
1:A:1307:LEU:O	1:A:1308:ARG:C	2.56	0.44
1:B:633:GLY:O	1:B:634:CYS:HB2	2.18	0.44
1:B:486:VAL:HG21	1:B:526:ILE:HG13	2.00	0.44
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.51	0.44
1:A:1090:ASN:O	1:A:1090:ASN:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1568:ILE:CG2	1:A:1613:LYS:HB2	2.48	0.44
1:A:1647:TYR:C	1:A:1649:PRO:HD3	2.38	0.44
1:A:1201:THR:O	1:A:1202:HIS:C	2.56	0.44
1:B:66:TYR:CD1	1:B:90:LYS:HG3	2.53	0.44
1:A:101:TYR:CE1	1:A:116:ARG:NE	2.86	0.44
1:A:496:ILE:HD12	1:A:496:ILE:H	1.82	0.44
1:A:155:ALA:O	1:A:157:ARG:HG3	2.17	0.44
1:A:388:VAL:O	1:A:420:PHE:HZ	2.01	0.44
1:B:550:GLN:HG2	1:B:551:THR:N	2.33	0.44
1:A:1105:LEU:HD22	1:A:1109:GLU:OE1	2.18	0.44
1:B:410:VAL:CG1	1:B:411:THR:N	2.80	0.44
1:B:1209:VAL:O	1:B:1213:LYS:HB2	2.17	0.44
1:A:946:PRO:CD	1:A:947:ARG:H	2.31	0.44
1:A:829:ILE:HD11	1:A:925:LYS:HG2	1.99	0.44
1:A:1283:GLY:O	1:A:1285:TYR:N	2.50	0.44
1:B:577:PRO:HD2	1:B:588:VAL:CG2	2.45	0.44
1:A:955:ARG:O	1:A:956:ARG:HG3	2.17	0.44
1:B:607:SER:HB3	1:B:796:THR:O	2.18	0.44
1:B:703:ALA:HB1	1:B:735:ALA:HB3	2.00	0.44
1:B:423:ASN:N	1:B:423:ASN:HD22	2.15	0.44
2:X:211:ARG:C	2:X:213:GLY:N	2.70	0.44
1:A:550:GLN:HG2	1:A:551:THR:N	2.32	0.44
1:A:265:VAL:HG23	1:A:292:LEU:H	1.83	0.43
1:A:1200:LYS:HG2	1:A:1200:LYS:H	1.59	0.43
1:A:315:LEU:O	1:A:318:LEU:HB2	2.18	0.43
1:A:947:ARG:O	1:A:949:ILE:N	2.51	0.43
2:Y:189:ILE:HD12	2:Y:201:ILE:HD12	1.99	0.43
1:B:248:ILE:CD1	1:B:325:ILE:HD13	2.44	0.43
1:A:1274:LEU:HA	1:A:1274:LEU:HD23	1.81	0.43
1:A:1257:THR:O	1:A:1260:ASN:HB2	2.17	0.43
1:A:686:ILE:O	1:A:686:ILE:HG22	2.18	0.43
1:B:1035:HIS:CD2	1:B:1035:HIS:H	2.35	0.43
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.82	0.43
1:B:1096:ASN:HD22	1:B:1096:ASN:C	2.21	0.43
1:B:1186:PHE:HD1	1:B:1250:THR:HG22	1.83	0.43
1:B:79:PHE:O	1:B:80:GLN:HG2	2.18	0.43
1:B:505:SER:O	1:B:506:LYS:HB2	2.18	0.43
1:A:106:VAL:HG12	1:A:107:VAL:N	2.33	0.43
1:B:1200:LYS:HE3	1:B:1261:LEU:CD2	2.37	0.43
1:A:56:ILE:HG12	1:A:56:ILE:H	1.61	0.43
1:B:59:TYR:CD1	1:B:103:TYR:CE1	2.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:81:ASN:O	2:Y:115:ARG:HB2	2.17	0.43
1:B:260:VAL:HG11	1:B:263:ALA:HB2	2.00	0.43
1:B:292:LEU:HD13	1:B:293:ILE:H	1.83	0.43
1:B:544:TYR:CE2	1:B:546:VAL:CG2	3.01	0.43
1:B:847:ASN:HD21	1:B:853:MET:HG2	1.82	0.43
1:A:1104:LEU:O	1:A:1108:VAL:HG12	2.18	0.43
1:A:949:ILE:HG12	1:A:949:ILE:H	1.59	0.43
1:B:717:ARG:HD2	1:B:1448:GLN:O	2.17	0.43
1:A:356:LEU:CD1	1:A:452:TYR:CE1	3.01	0.43
1:B:773:TRP:HZ3	1:B:788:PHE:CE1	2.36	0.43
1:B:653:PHE:CD2	1:B:653:PHE:N	2.86	0.43
1:B:944:LEU:HB2	1:B:1357:ALA:O	2.19	0.43
1:A:886:GLN:CD	1:A:894:HIS:CE1	2.91	0.43
1:B:271:ILE:CG2	1:B:272:ARG:H	2.19	0.43
1:A:968:VAL:CG1	1:A:1368:THR:HG22	2.41	0.43
1:A:975:ARG:CB	1:A:1363:THR:HB	2.45	0.43
2:Y:146:LEU:CD2	2:Y:146:LEU:C	2.86	0.43
1:A:703:ALA:HB1	1:A:735:ALA:HB3	2.00	0.43
2:X:104:PHE:CG	2:X:164:GLU:HB2	2.54	0.43
1:B:686:ILE:O	1:B:686:ILE:HG22	2.18	0.43
1:A:512:PHE:N	1:A:512:PHE:CD2	2.86	0.43
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.73	0.43
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.65	0.43
1:B:1279:ARG:CD	1:B:1284:PHE:CG	3.02	0.43
2:X:151:ASP:OD2	2:X:177:TYR:OH	2.27	0.43
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.45	0.43
1:B:442:LEU:HD22	1:B:443:PRO:CD	2.48	0.43
1:A:154:PRO:O	1:A:155:ALA:HB3	2.19	0.43
1:B:1300:TYR:CD2	1:B:1300:TYR:C	2.91	0.43
1:B:1515:LYS:O	1:B:1517:GLN:NE2	2.51	0.43
1:B:1379:LEU:HD23	1:B:1406:ALA:HA	2.01	0.43
2:X:70:SER:CB	2:X:91:LYS:HE3	2.45	0.43
1:B:1052:GLY:O	1:B:1055:SER:HB3	2.19	0.43
1:B:161:LEU:HD11	1:B:185:PHE:CD1	2.54	0.43
1:A:1451:THR:HG23	1:A:1464:LEU:HA	2.01	0.43
1:B:667:GLU:C	1:B:669:CYS:H	2.21	0.43
1:B:1507:MET:HB3	1:B:1507:MET:HE3	1.41	0.43
1:A:1667:PHE:O	1:A:1670:ASP:HB3	2.18	0.43
1:A:104:LEU:O	1:A:114:SER:CB	2.67	0.43
1:B:554:LEU:HD11	1:B:655:THR:HG21	2.00	0.43
1:B:367:ILE:HG23	1:B:368:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:ASN:H	1:B:155:ALA:HB2	1.82	0.43
1:A:1255:LEU:CD1	1:A:1267:VAL:HG22	2.49	0.43
2:X:57:TYR:HE1	2:X:77:PRO:HA	1.83	0.43
1:B:1115:ASN:C	1:B:1115:ASN:HD22	2.21	0.43
1:A:1108:VAL:CG2	1:A:1167:ALA:HB2	2.49	0.43
2:Y:86:LEU:HG	2:Y:91:LYS:HB2	2.00	0.43
1:A:144:ARG:HG2	1:A:775:TRP:CZ2	2.53	0.43
1:B:364:LYS:N	1:B:364:LYS:CD	2.81	0.43
1:B:1277:GLU:OE2	1:B:1277:GLU:HA	2.17	0.43
1:B:425:PRO:O	1:B:426:SER:C	2.56	0.43
1:A:172:ASP:OD2	1:A:173:MET:N	2.42	0.43
1:A:495:LYS:HA	1:A:495:LYS:CE	2.48	0.43
1:A:1654:CYS:C	1:A:1656:SER:N	2.71	0.43
1:A:1266:TYR:O	1:A:1269:PRO:HD2	2.19	0.43
1:A:981:GLY:H	1:A:1333:PHE:HB2	1.84	0.43
1:B:182:ILE:HD11	1:B:599:TRP:HB3	2.01	0.43
1:A:774:LEU:HD11	1:A:788:PHE:CE2	2.54	0.43
1:B:388:VAL:O	1:B:420:PHE:HZ	2.02	0.43
1:A:1044:LYS:O	1:A:1047:LYS:HB3	2.17	0.43
1:B:764:GLU:H	1:B:764:GLU:HG2	1.68	0.43
1:B:495:LYS:CE	1:B:495:LYS:HA	2.48	0.43
1:A:85:LEU:O	1:A:86:THR:CB	2.50	0.43
1:A:271:ILE:CG2	1:A:272:ARG:H	2.19	0.43
1:B:485:ILE:HA	1:B:485:ILE:HD12	1.75	0.43
1:A:1135:VAL:O	1:A:1138:ARG:HB3	2.19	0.43
1:B:250:ILE:HD12	1:B:327:VAL:HG11	1.99	0.43
1:A:1053:MET:HE1	1:A:1086:LEU:HD22	1.99	0.43
1:B:769:PHE:HA	1:B:770:PRO:HD3	1.78	0.43
1:B:193:ASN:C	1:B:193:ASN:OD1	2.57	0.43
1:A:504:LEU:HA	1:A:509:ILE:HA	2.00	0.43
1:B:591:ASN:OD1	1:B:785:GLN:HB2	2.19	0.43
1:B:938:SER:OG	1:B:1279:ARG:CZ	2.66	0.43
1:A:1560:ALA:CB	1:A:1620:MET:HG2	2.49	0.43
1:A:554:LEU:HD11	1:A:655:THR:HG21	2.01	0.43
1:A:307:VAL:O	1:A:308:LYS:C	2.55	0.43
1:A:571:LEU:HD11	1:A:573:VAL:HG13	1.99	0.43
1:B:149:ASN:C	1:B:151:ASP:N	2.72	0.43
1:B:137:PRO:HG3	1:B:196:TYR:OH	2.18	0.43
1:A:1255:LEU:HD13	1:A:1270:VAL:HG11	2.01	0.43
1:A:819:VAL:O	1:A:820:PHE:HB2	2.19	0.43
1:B:144:ARG:NH1	1:B:775:TRP:CE2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:CE1	1:B:378:SER:HB2	2.54	0.43
1:B:208:ASP:O	1:B:209:PHE:CG	2.72	0.43
1:A:191:PRO:O	1:A:194:PRO:HG3	2.19	0.43
1:B:1221:ASN:ND2	1:B:1222:PRO:HA	2.33	0.43
1:B:472:ASN:OD1	1:B:472:ASN:N	2.46	0.43
1:A:387:PRO:HA	1:A:410:VAL:HG22	2.01	0.43
2:Y:151:ASP:OD2	2:Y:177:TYR:OH	2.29	0.43
1:A:350:SER:HA	1:A:351:PRO:HD3	1.90	0.43
1:A:1432:ILE:HG22	1:A:1432:ILE:O	2.18	0.43
1:B:1158:ILE:H	1:B:1158:ILE:HG13	1.52	0.43
1:A:544:TYR:CD1	1:A:544:TYR:N	2.85	0.43
1:A:930:VAL:HG12	1:A:931:PRO:CD	2.47	0.43
1:A:1289:ASP:CG	1:A:1290:THR:N	2.73	0.43
2:X:134:THR:HA	2:X:135:PRO:HD2	1.92	0.43
1:A:956:ARG:CG	1:A:1349:SER:HB3	2.49	0.43
1:B:84:ILE:CD1	2:Y:135:PRO:HG3	2.48	0.43
1:B:948:GLY:HA2	1:B:952:THR:O	2.19	0.43
1:B:1257:THR:O	1:B:1260:ASN:HB2	2.19	0.43
1:B:1000:LEU:HD23	1:B:1000:LEU:HA	1.72	0.43
1:B:1149:VAL:HG13	1:B:1153:ARG:HG2	1.99	0.43
1:B:662:SER:O	1:B:663:GLN:C	2.56	0.43
1:B:424:LEU:HA	1:B:425:PRO:HD3	1.82	0.43
1:B:1346:LEU:HG	1:B:1347:ILE:N	2.33	0.43
1:A:1622:LYS:O	1:A:1637:TYR:HE2	2.00	0.43
1:B:307:VAL:O	1:B:308:LYS:C	2.55	0.43
1:B:497:THR:CG2	1:B:498:HIS:H	2.23	0.43
1:B:52:ALA:CB	1:B:73:LEU:HD21	2.49	0.43
1:B:389:THR:CG2	1:B:408:LYS:HE2	2.38	0.43
1:A:1267:VAL:O	1:A:1268:ASN:C	2.58	0.43
1:A:1115:ASN:C	1:A:1115:ASN:HD22	2.19	0.43
1:B:477:LEU:O	1:B:530:VAL:HG11	2.18	0.43
1:B:847:ASN:O	1:B:848:TYR:HD1	2.02	0.43
1:B:899:THR:OG1	1:B:1523:ALA:HB1	2.18	0.43
1:B:975:ARG:CB	1:B:1363:THR:HB	2.45	0.43
1:A:182:ILE:HD11	1:A:599:TRP:HB3	2.01	0.43
1:B:1188:LEU:HD21	1:B:1212:LEU:CA	2.49	0.43
1:A:1180:LEU:CD1	1:A:1207:SER:HB3	2.49	0.43
1:B:1016:VAL:CG1	1:B:1017:PRO:HD3	2.48	0.43
1:A:1500:ARG:C	1:A:1502:ASP:H	2.21	0.43
1:B:1079:THR:HG22	1:B:1107:LEU:HD11	2.01	0.43
1:B:27:ALA:HB1	1:B:28:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:HG12	1:B:42:GLN:N	2.34	0.42
1:B:981:GLY:HA3	1:B:1309:LEU:CD1	2.48	0.42
1:B:461:SER:C	1:B:463:SER:N	2.72	0.42
1:A:166:PRO:HG2	1:A:195:ARG:O	2.18	0.42
1:A:717:ARG:HD2	1:A:1448:GLN:O	2.18	0.42
1:B:774:LEU:HD11	1:B:788:PHE:CZ	2.54	0.42
1:A:395:ILE:HG13	1:A:395:ILE:O	2.18	0.42
1:B:1465:ASN:N	1:B:1465:ASN:ND2	2.67	0.42
1:B:946:PRO:CD	1:B:947:ARG:H	2.31	0.42
1:A:229:VAL:HG21	1:A:329:VAL:HB	2.01	0.42
1:B:1345:ASP:N	1:B:1345:ASP:OD2	2.52	0.42
1:B:1485:VAL:HG21	1:B:1488:LEU:CB	2.49	0.42
1:A:1535:MET:HA	1:A:1645:ILE:CD1	2.48	0.42
1:A:833:VAL:O	1:A:929:VAL:HA	2.19	0.42
1:A:544:TYR:CE2	1:A:546:VAL:CG2	3.02	0.42
1:A:820:PHE:CZ	1:A:848:TYR:CD2	3.06	0.42
2:X:128:LYS:HD3	2:X:158:GLU:HG2	2.00	0.42
1:B:968:VAL:CG1	1:B:1368:THR:HG22	2.46	0.42
1:B:707:ASN:CB	1:B:739:ARG:HH22	2.28	0.42
1:B:1182:ALA:CB	1:B:1188:LEU:HD13	2.48	0.42
1:A:356:LEU:HD12	1:A:452:TYR:CE1	2.54	0.42
1:A:1523:ALA:C	1:A:1525:CYS:N	2.73	0.42
1:B:1372:GLU:HG3	1:B:1373:GLU:N	2.33	0.42
1:A:504:LEU:CD1	1:A:504:LEU:N	2.81	0.42
1:A:659:ALA:C	1:A:661:ASP:H	2.22	0.42
1:B:1455:ILE:HG13	1:B:1460:VAL:HG22	2.01	0.42
1:B:51:ASP:OD1	1:B:72:HIS:ND1	2.52	0.42
1:A:505:SER:O	1:A:506:LYS:HB2	2.19	0.42
1:B:484:ILE:C	1:B:485:ILE:HD13	2.40	0.42
2:X:110:ILE:CG2	2:X:111:ASP:N	2.82	0.42
1:B:488:PRO:O	1:B:489:LYS:C	2.57	0.42
1:B:840:GLN:HG2	1:B:899:THR:HG22	2.01	0.42
1:B:1108:VAL:CG2	1:B:1167:ALA:CB	2.97	0.42
1:A:1108:VAL:HG21	1:A:1167:ALA:HB2	2.00	0.42
1:A:316:GLU:O	1:A:317:ASP:C	2.57	0.42
1:A:1225:TYR:HE1	1:A:1272:LYS:HG3	1.84	0.42
1:A:587:THR:HA	1:A:789:ALA:CA	2.49	0.42
1:B:249:THR:HG23	1:B:298:GLN:HE21	1.84	0.42
1:B:1255:LEU:HD13	1:B:1270:VAL:CG1	2.50	0.42
1:B:1193:TYR:O	1:B:1196:SER:HB3	2.19	0.42
1:A:1037:ASP:C	1:A:1037:ASP:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:99:GLN:O	2:Y:100:GLY:C	2.58	0.42
1:A:1279:ARG:HG3	1:A:1284:PHE:HB3	1.81	0.42
1:A:1669:GLU:O	1:A:1673:LEU:HD21	2.18	0.42
1:A:27:ALA:HB1	1:A:28:PRO:HD2	2.01	0.42
1:A:447:GLN:HA	1:A:447:GLN:OE1	2.17	0.42
1:B:154:PRO:O	1:B:155:ALA:HB3	2.19	0.42
1:B:224:LEU:HD22	1:B:224:LEU:HA	1.72	0.42
1:B:534:MET:HB3	1:B:538:SER:OG	2.18	0.42
1:A:1132:THR:CB	1:A:1134:PRO:HD2	2.43	0.42
1:A:819:VAL:O	1:A:820:PHE:CB	2.66	0.42
1:B:1053:MET:CE	1:B:1086:LEU:HD13	2.49	0.42
1:B:1053:MET:HE1	1:B:1086:LEU:HD22	2.01	0.42
1:B:388:VAL:HG12	1:B:420:PHE:CZ	2.54	0.42
1:A:1370:THR:O	1:A:1372:GLU:N	2.52	0.42
1:A:1149:VAL:HG13	1:A:1153:ARG:HG2	2.02	0.42
1:A:662:SER:O	1:A:663:GLN:C	2.57	0.42
2:X:99:GLN:O	2:X:100:GLY:C	2.58	0.42
1:A:219:VAL:HG12	1:A:219:VAL:O	2.18	0.42
1:B:977:LEU:HD12	1:B:1361:VAL:HG23	1.94	0.42
1:B:1008:ALA:CB	1:B:1068:VAL:O	2.68	0.42
1:B:104:LEU:O	1:B:114:SER:CB	2.67	0.42
1:A:1616:GLN:NE2	1:B:1521:GLU:CD	2.72	0.42
1:B:232:GLU:HA	1:B:233:PRO:HD3	1.75	0.42
1:B:820:PHE:HZ	1:B:848:TYR:HB2	1.83	0.42
1:B:599:TRP:CH2	1:B:779:LEU:HB2	2.54	0.42
1:A:144:ARG:NH1	1:A:775:TRP:CE2	2.87	0.42
1:A:1521:GLU:C	1:A:1523:ALA:H	2.22	0.42
1:B:388:VAL:HG12	1:B:420:PHE:HZ	1.84	0.42
1:B:956:ARG:CG	1:B:1349:SER:HB3	2.50	0.42
1:B:950:TYR:HB3	1:B:1272:LYS:HD3	2.00	0.42
1:A:336:PHE:CE2	1:A:1480:PHE:CZ	3.08	0.42
1:A:1195:LEU:C	1:A:1197:LEU:N	2.71	0.42
1:B:229:VAL:HG21	1:B:329:VAL:HB	2.01	0.42
1:A:515:ARG:HG3	1:A:515:ARG:HH11	1.84	0.42
1:A:1674:ASN:CA	1:B:258:LYS:HZ2	2.18	0.42
1:A:1323:LEU:CD1	1:A:1324:HIS:N	2.62	0.42
1:B:85:LEU:N	1:B:85:LEU:HD22	2.29	0.42
1:A:113:LYS:NZ	1:A:656:ASN:HD21	2.18	0.42
1:B:23:TYR:HE1	1:B:656:ASN:H	1.67	0.42
1:B:614:ARG:O	1:B:615:GLY:C	2.58	0.42
1:A:1509:TYR:CD2	1:A:1509:TYR:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:LEU:O	1:A:530:VAL:HG11	2.19	0.42
1:A:153:LYS:O	1:A:154:PRO:C	2.57	0.42
1:A:1159:CYS:O	1:A:1160:PRO:C	2.58	0.42
2:X:86:LEU:HG	2:X:91:LYS:HB2	2.00	0.42
1:A:171:VAL:HG12	1:A:171:VAL:O	2.19	0.42
1:A:577:PRO:HD2	1:A:588:VAL:CG2	2.45	0.42
1:A:653:PHE:N	1:A:653:PHE:CD2	2.87	0.42
1:B:336:PHE:CE2	1:B:1480:PHE:CZ	3.08	0.42
1:A:51:ASP:OD1	1:A:72:HIS:HB2	2.20	0.42
1:A:1494:THR:HB	1:A:1506:THR:HG23	2.00	0.42
1:A:689:LYS:HE2	1:A:689:LYS:HB3	1.66	0.42
1:B:689:LYS:HB3	1:B:689:LYS:HE2	1.66	0.42
1:B:833:VAL:HG13	1:B:839:ILE:HD13	2.02	0.42
1:A:1558:ALA:HB3	1:A:1622:LYS:C	2.40	0.42
1:A:884:VAL:HG12	1:A:1625:LEU:CB	2.48	0.42
1:A:839:ILE:HD12	1:A:1485:VAL:HG12	2.01	0.42
1:A:137:PRO:HG3	1:A:196:TYR:OH	2.19	0.42
1:B:33:VAL:HG23	1:B:120:THR:O	2.20	0.42
1:A:847:ASN:O	1:A:848:TYR:HD1	2.03	0.42
1:B:897:THR:C	1:B:898:PHE:CD2	2.93	0.42
1:B:1049:LEU:HD23	1:B:1093:VAL:CG2	2.49	0.42
2:Y:179:LEU:HD13	2:Y:228:ILE:HD11	2.02	0.42
1:B:1412:ARG:O	1:B:1413:GLU:CB	2.68	0.42
1:B:234:GLU:HB2	1:B:247:GLU:N	2.35	0.42
1:B:1044:LYS:O	1:B:1047:LYS:HB3	2.19	0.42
1:B:405:ASP:HA	1:B:406:PRO:HD3	1.74	0.42
1:B:964:PRO:C	1:B:966:ASP:H	2.23	0.42
2:Y:49:TYR:HB2	2:Y:206:LYS:HZ2	1.85	0.42
1:B:1216:ALA:C	1:B:1217:LEU:HG	2.39	0.42
2:X:42:ASP:OD1	2:X:43:ILE:N	2.53	0.42
1:B:506:LYS:HB2	1:B:506:LYS:HE2	1.56	0.42
1:A:408:LYS:HE2	1:A:408:LYS:HB2	1.85	0.42
1:A:339:GLU:HB2	1:A:766:ARG:NH2	2.34	0.42
1:A:292:LEU:HD11	1:A:295:GLY:CA	2.49	0.42
2:X:61:SER:C	2:X:75:PHE:HZ	2.22	0.42
1:B:292:LEU:HD11	1:B:295:GLY:CA	2.50	0.42
1:B:489:LYS:O	1:B:490:SER:CB	2.67	0.42
1:B:496:ILE:HD12	1:B:496:ILE:H	1.83	0.42
1:B:499:TYR:HE2	1:B:517:LYS:HG2	1.84	0.42
1:B:1289:ASP:CG	1:B:1290:THR:N	2.73	0.42
2:X:169:ILE:HA	2:X:169:ILE:HD13	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1054:LEU:O	1:A:1055:SER:C	2.58	0.42
1:B:758:LEU:C	1:B:760:VAL:N	2.71	0.42
1:B:481:HIS:CE1	1:B:529:PRO:HG3	2.55	0.42
1:A:1433:SER:HB2	1:A:1480:PHE:HD1	1.80	0.42
1:B:659:ALA:C	1:B:661:ASP:H	2.23	0.42
1:B:940:SER:HB2	1:B:959:PHE:CD1	2.49	0.42
1:A:1608:ASN:O	1:A:1609:ALA:CB	2.67	0.42
1:A:1674:ASN:CA	1:B:258:LYS:NZ	2.72	0.42
1:A:1230:ASP:CG	1:A:1246:ARG:HD2	2.40	0.42
1:B:106:VAL:HG12	1:B:107:VAL:N	2.35	0.42
1:A:1255:LEU:HD13	1:A:1270:VAL:CG1	2.50	0.42
1:A:1658:GLN:C	1:A:1660:PHE:N	2.73	0.42
1:B:157:ARG:O	1:B:178:ASP:CB	2.67	0.42
1:B:819:VAL:O	1:B:820:PHE:HB2	2.19	0.42
1:B:1104:LEU:HD22	1:B:1152:ILE:HG23	2.02	0.42
1:B:905:ILE:HD12	1:B:931:PRO:HG3	2.02	0.42
1:A:641:ASN:O	1:A:645:VAL:HG23	2.19	0.42
2:Y:169:ILE:HD13	2:Y:169:ILE:HA	1.89	0.42
2:X:84:LEU:HD13	2:X:118:THR:HG23	2.01	0.42
1:A:377:ASP:N	1:A:377:ASP:OD1	2.43	0.42
1:B:333:THR:OG1	1:B:334:GLY:N	2.53	0.42
1:A:715:ALA:O	1:A:718:ILE:HB	2.19	0.42
1:A:461:SER:C	1:A:463:SER:N	2.73	0.42
2:Y:150:ILE:O	2:Y:150:ILE:HG13	2.19	0.42
1:A:52:ALA:CB	1:A:73:LEU:HD21	2.50	0.42
1:A:1143:TYR:CD1	1:A:1186:PHE:CE2	3.06	0.42
1:B:160:VAL:CG2	1:B:175:GLU:CB	2.96	0.42
1:A:614:ARG:O	1:A:615:GLY:C	2.57	0.42
1:A:296:ILE:HG22	1:A:297:ALA:N	2.34	0.42
1:B:463:SER:OG	1:B:491:PRO:HG3	2.20	0.42
1:B:157:ARG:H	1:B:178:ASP:CB	2.30	0.42
1:A:840:GLN:CG	1:A:899:THR:HG22	2.50	0.42
1:A:1159:CYS:O	1:A:1161:LEU:HB2	2.20	0.42
1:B:802:ILE:CD1	1:B:809:ILE:HG13	2.49	0.42
2:Y:47:HIS:HB2	2:Y:180:TYR:HB3	2.02	0.42
1:B:284:GLN:O	1:B:285:THR:C	2.58	0.42
1:B:390:LEU:CB	1:B:420:PHE:CE1	3.03	0.42
2:X:187:GLY:HA3	2:X:203:LEU:HD12	2.02	0.42
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.64	0.42
1:A:964:PRO:C	1:A:966:ASP:H	2.22	0.42
1:A:1346:LEU:HA	1:A:1346:LEU:HD12	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:886:GLN:HG3	1:B:887:LYS:N	2.27	0.41
1:B:485:ILE:O	1:B:485:ILE:HG22	2.16	0.41
1:A:224:LEU:HA	1:A:225:PRO:HD3	1.77	0.41
1:B:371:ILE:HD13	1:B:371:ILE:HG21	1.81	0.41
1:A:1411:SER:N	1:A:1414:GLU:OE1	2.39	0.41
1:A:71:VAL:CG2	1:A:71:VAL:O	2.64	0.41
1:A:404:LEU:HD23	1:A:404:LEU:HA	1.71	0.41
1:B:942:VAL:HG22	1:B:957:LYS:HD3	2.02	0.41
1:B:922:ILE:HB	4:B:2001:NAG:H82	2.02	0.41
2:Y:54:SER:HB2	2:Y:167:PHE:CE1	2.55	0.41
2:X:54:SER:HB2	2:X:167:PHE:CE1	2.55	0.41
1:A:1664:LEU:O	1:A:1668:ALA:HB2	2.20	0.41
1:A:41:ILE:HG12	1:A:42:GLN:N	2.35	0.41
1:B:175:GLU:H	1:B:175:GLU:HG2	1.60	0.41
2:X:77:PRO:HG3	2:X:82:HIS:HD2	1.83	0.41
2:Y:61:SER:C	2:Y:75:PHE:HZ	2.22	0.41
1:A:534:MET:HB3	1:A:538:SER:OG	2.20	0.41
1:B:1135:VAL:O	1:B:1138:ARG:HB3	2.20	0.41
1:B:1108:VAL:HG21	1:B:1167:ALA:CB	2.50	0.41
2:Y:174:VAL:HA	2:Y:179:LEU:HB3	2.02	0.41
1:B:592:MET:HE3	1:B:780:VAL:HG21	2.00	0.41
1:B:762:LYS:HA	1:B:763:PRO:HD3	1.95	0.41
1:A:356:LEU:HD11	1:A:452:TYR:CD1	2.54	0.41
1:B:587:THR:HA	1:B:789:ALA:CA	2.49	0.41
1:A:1332:ASN:O	1:A:1332:ASN:OD1	2.38	0.41
2:Y:84:LEU:HD13	2:Y:118:THR:HG23	2.01	0.41
1:B:1280:TYR:HD1	1:B:1362:THR:HG21	1.84	0.41
2:X:150:ILE:O	2:X:150:ILE:HG13	2.20	0.41
1:A:307:VAL:HG11	1:A:313:TYR:CB	2.43	0.41
1:B:1261:LEU:O	1:B:1263:ASP:N	2.53	0.41
1:B:641:ASN:O	1:B:645:VAL:HG23	2.19	0.41
1:B:1189:ALA:HB1	1:B:1253:TYR:HB3	2.02	0.41
2:X:174:VAL:HA	2:X:179:LEU:HB3	2.01	0.41
2:X:134:THR:CG2	2:X:153:PHE:HB3	2.50	0.41
1:B:144:ARG:HG2	1:B:775:TRP:CZ2	2.55	0.41
1:A:1027:THR:O	1:A:1027:THR:HG22	2.21	0.41
1:A:1197:LEU:CD2	1:A:1260:ASN:HD21	2.32	0.41
1:B:515:ARG:HG3	1:B:515:ARG:HH11	1.85	0.41
1:A:627:LEU:HG	1:A:627:LEU:O	2.20	0.41
2:X:228:ILE:O	2:X:228:ILE:HG22	2.19	0.41
1:A:61:ASP:CG	1:A:61:ASP:O	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1559:TYR:CD2	1:A:1559:TYR:C	2.93	0.41
1:A:1216:ALA:C	1:A:1217:LEU:HG	2.39	0.41
1:B:113:LYS:NZ	1:B:656:ASN:HD21	2.18	0.41
1:A:505:SER:CB	1:A:510:ILE:HD11	2.48	0.41
1:A:117:MET:HA	1:A:118:PRO:HD3	1.90	0.41
1:B:224:LEU:HA	1:B:225:PRO:HD3	1.78	0.41
2:X:107:GLN:NE2	2:X:110:ILE:HD11	2.36	0.41
2:Y:110:ILE:CG2	2:Y:111:ASP:N	2.83	0.41
1:B:296:ILE:HG22	1:B:297:ALA:N	2.36	0.41
1:B:1126:PRO:HD2	1:B:1127:ILE:H	1.84	0.41
1:A:643:ALA:O	1:A:646:PHE:N	2.53	0.41
1:B:109:LYS:CD	1:B:110:HIS:HB2	2.51	0.41
1:A:330:ILE:HG22	1:A:337:SER:OG	2.20	0.41
1:A:395:ILE:HG13	1:A:429:THR:OG1	2.21	0.41
1:A:486:VAL:HG21	1:A:526:ILE:HG13	2.00	0.41
1:B:606:ASP:O	1:B:608:ALA:N	2.53	0.41
1:B:960:PRO:HA	1:B:1345:ASP:HA	2.03	0.41
1:A:1455:ILE:HG13	1:A:1460:VAL:HG22	2.01	0.41
1:B:61:ASP:O	1:B:61:ASP:CG	2.58	0.41
1:A:1323:LEU:CG	1:A:1324:HIS:N	2.83	0.41
1:A:86:THR:O	1:A:86:THR:CG2	2.68	0.41
1:B:1229:LYS:HB3	1:B:1231:ASN:OD1	2.21	0.41
1:A:485:ILE:HA	1:A:485:ILE:HD12	1.74	0.41
1:B:196:TYR:HD1	1:B:219:VAL:HG12	1.85	0.41
1:B:1509:TYR:CD2	1:B:1509:TYR:C	2.92	0.41
2:X:58:SER:HA	2:X:101:GLN:O	2.20	0.41
1:A:153:LYS:CB	1:A:154:PRO:HD2	2.48	0.41
1:A:1108:VAL:CG2	1:A:1167:ALA:CB	2.99	0.41
1:A:602:LEU:HD23	1:A:602:LEU:N	2.36	0.41
1:B:356:LEU:CD1	1:B:452:TYR:CE1	3.04	0.41
1:B:949:ILE:HB	1:B:950:TYR:HD2	1.85	0.41
1:B:1124:TYR:HA	1:B:1465:ASN:OD1	2.20	0.41
1:A:656:ASN:HD22	1:A:656:ASN:HA	1.60	0.41
1:A:1488:LEU:HD13	1:A:1488:LEU:C	2.39	0.41
1:B:1266:TYR:O	1:B:1269:PRO:HD2	2.20	0.41
1:A:492:TYR:C	1:A:492:TYR:CD2	2.94	0.41
1:B:1435:ASN:HB2	1:B:1478:ARG:O	2.21	0.41
2:X:136:LEU:HA	2:X:224:ILE:O	2.21	0.41
1:A:1147:PHE:CD2	1:A:1147:PHE:C	2.94	0.41
2:Y:134:THR:CG2	2:Y:153:PHE:HB3	2.50	0.41
1:A:1054:LEU:O	1:A:1056:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:VAL:HG12	1:A:420:PHE:HZ	1.86	0.41
1:A:1188:LEU:HD23	1:A:1212:LEU:HA	2.01	0.41
1:B:227:PHE:O	1:B:338:GLU:HG2	2.20	0.41
1:A:40:VAL:HB	1:A:512:PHE:CD1	2.55	0.41
1:B:51:ASP:OD1	1:B:72:HIS:HB2	2.20	0.41
1:B:791:PRO:HD2	1:B:797:TRP:HE1	1.84	0.41
1:A:1034:PHE:CE1	1:A:1041:GLU:HG2	2.56	0.41
1:A:1425:ASP:C	1:A:1425:ASP:OD2	2.59	0.41
1:B:165:ASP:OD1	1:B:165:ASP:C	2.59	0.41
1:B:837:GLU:OE1	1:B:1430:THR:OG1	2.39	0.41
1:A:1217:LEU:O	1:A:1226:ARG:HA	2.20	0.41
1:A:442:LEU:HD22	1:A:443:PRO:HD2	2.02	0.41
2:Y:102:ASN:O	2:Y:122:VAL:HA	2.21	0.41
1:A:371:ILE:CG2	1:A:371:ILE:O	2.46	0.41
1:B:163:PHE:CE2	1:B:201:ILE:HD11	2.55	0.41
1:A:109:LYS:CD	1:A:110:HIS:HB2	2.51	0.41
1:A:37:GLU:OE1	1:A:37:GLU:HA	2.20	0.41
1:A:390:LEU:CB	1:A:420:PHE:CE1	3.04	0.41
1:B:88:GLN:HB3	1:B:89:PRO:CD	2.50	0.41
1:B:1034:PHE:CE1	1:B:1041:GLU:HG2	2.55	0.41
1:B:715:ALA:O	1:B:718:ILE:HB	2.20	0.41
1:A:42:GLN:CD	1:A:543:TYR:HH	2.23	0.41
1:A:305:THR:O	1:A:307:VAL:N	2.53	0.41
1:B:442:LEU:HD22	1:B:443:PRO:HD2	2.03	0.41
1:B:447:GLN:OE1	1:B:447:GLN:HA	2.20	0.41
1:A:839:ILE:HG23	1:A:900:VAL:HG23	1.97	0.41
1:B:56:ILE:O	1:B:65:SER:HA	2.20	0.41
1:B:190:ILE:HG12	1:B:190:ILE:H	1.58	0.41
2:Y:58:SER:HA	2:Y:101:GLN:O	2.21	0.41
1:A:820:PHE:HZ	1:A:848:TYR:HB2	1.85	0.41
1:A:541:LEU:HD21	1:A:646:PHE:CZ	2.56	0.41
1:A:317:ASP:HB3	1:A:318:LEU:H	1.69	0.41
1:B:1180:LEU:O	1:B:1182:ALA:N	2.53	0.41
1:A:379:LEU:HB3	1:A:381:GLN:HE22	1.84	0.41
1:B:249:THR:HG23	1:B:298:GLN:HG3	2.01	0.41
1:B:587:THR:HA	1:B:789:ALA:HB2	2.01	0.41
1:B:30:ILE:HG22	1:B:31:PHE:N	2.36	0.41
1:B:37:GLU:HA	1:B:37:GLU:OE1	2.21	0.41
2:Y:104:PHE:CG	2:Y:164:GLU:HB2	2.55	0.41
1:B:504:LEU:HA	1:B:509:ILE:HA	2.02	0.41
1:B:833:VAL:O	1:B:929:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1625:LEU:O	1:A:1635:TYR:O	2.38	0.41
1:A:280:LYS:HG2	1:A:282:MET:HE3	2.02	0.41
2:Y:185:LYS:HD2	2:Y:186:TYR:CZ	2.56	0.41
2:Y:42:ASP:OD1	2:Y:43:ILE:N	2.53	0.41
1:B:313:TYR:HE2	1:B:321:LYS:HZ2	1.67	0.41
1:A:1202:HIS:HA	1:A:1203:PRO:HD3	1.87	0.41
1:A:485:ILE:HG22	1:A:485:ILE:O	2.18	0.41
1:B:160:VAL:HG23	1:B:175:GLU:CB	2.34	0.41
1:A:56:ILE:HD11	1:A:66:TYR:HB2	2.02	0.41
1:B:412:ARG:HG2	1:B:413:VAL:H	1.86	0.41
1:A:981:GLY:HA3	1:A:1309:LEU:CD1	2.51	0.41
1:A:371:ILE:HD13	1:A:371:ILE:HG21	1.86	0.41
1:B:1132:THR:CB	1:B:1134:PRO:HD2	2.43	0.41
1:A:885:ARG:HH12	1:A:1628:LYS:HD3	1.83	0.41
1:A:707:ASN:CB	1:A:739:ARG:HH22	2.27	0.41
1:A:599:TRP:CH2	1:A:779:LEU:HB2	2.56	0.41
1:A:1180:LEU:HD23	1:A:1180:LEU:HA	1.69	0.41
1:B:182:ILE:HG12	1:B:804:ILE:HD11	2.01	0.41
2:X:47:HIS:HB2	2:X:180:TYR:HB3	2.01	0.41
1:B:576:SER:HB2	1:B:577:PRO:HD3	2.03	0.41
1:A:284:GLN:O	1:A:285:THR:C	2.58	0.41
1:A:249:THR:HG23	1:A:298:GLN:HG3	2.03	0.41
1:A:587:THR:HA	1:A:789:ALA:HB2	2.03	0.41
1:A:1273:TRP:CZ3	1:A:1274:LEU:HD23	2.56	0.41
1:B:298:GLN:O	1:B:299:VAL:HG13	2.20	0.41
1:B:583:SER:O	1:B:585:GLY:N	2.51	0.41
1:B:949:ILE:HG12	1:B:949:ILE:H	1.58	0.41
1:B:1271:ILE:HD12	1:B:1271:ILE:O	2.20	0.41
1:A:1561:TYR:O	1:A:1561:TYR:CD2	2.72	0.41
1:A:936:ARG:CZ	1:A:1002:HIS:CE1	3.04	0.41
1:A:193:ASN:OD1	1:A:193:ASN:C	2.58	0.41
1:A:1531:ASP:O	1:A:1532:CYS:O	2.39	0.41
1:A:960:PRO:HA	1:A:1345:ASP:HA	2.03	0.41
1:A:963:ILE:HA	1:A:964:PRO:HD3	1.76	0.41
1:A:333:THR:OG1	1:A:334:GLY:N	2.53	0.41
1:B:172:ASP:OD2	1:B:173:MET:N	2.42	0.41
2:Y:187:GLY:HA3	2:Y:203:LEU:HD12	2.02	0.41
1:A:125:PHE:CE1	1:A:152:LEU:HD11	2.56	0.41
1:A:46:TYR:HB2	1:A:47:THR:H	1.77	0.41
1:A:309:GLU:HG3	1:A:309:GLU:O	2.21	0.41
1:A:384:GLY:C	1:A:411:THR:HG23	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD22	1:A:296:ILE:C	2.41	0.41
1:B:98:PRO:C	1:B:100:SER:H	2.24	0.41
1:A:100:SER:O	1:A:101:TYR:CB	2.56	0.41
1:B:250:ILE:HD13	1:B:250:ILE:HG21	1.81	0.41
1:A:250:ILE:HG21	1:A:250:ILE:HD13	1.81	0.41
1:A:231:ILE:HG12	1:A:342:ILE:HD11	2.02	0.41
2:Y:64:VAL:HG11	2:Y:95:LYS:O	2.21	0.41
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	2.21	0.41
1:B:191:PRO:O	1:B:194:PRO:HG3	2.20	0.41
1:B:360:PRO:HA	1:B:636:ALA:HB3	2.03	0.41
1:B:272:ARG:HG2	1:B:274:ASP:O	2.20	0.40
1:A:439:ALA:HA	1:A:440:PRO:HD3	1.80	0.40
1:A:56:ILE:O	1:A:65:SER:HA	2.21	0.40
1:B:149:ASN:O	1:B:150:ASP:C	2.59	0.40
1:B:138:ASP:HA	1:B:190:ILE:O	2.21	0.40
2:X:102:ASN:O	2:X:122:VAL:HA	2.21	0.40
1:A:489:LYS:O	1:A:490:SER:CB	2.68	0.40
1:A:157:ARG:HD2	1:A:205:TYR:CE2	2.55	0.40
1:A:1218:VAL:HA	1:A:1225:TYR:O	2.20	0.40
1:B:231:ILE:HG12	1:B:342:ILE:HD11	2.04	0.40
1:A:802:ILE:HD11	1:A:804:ILE:HG23	2.03	0.40
1:B:781:PRO:C	1:B:783:ARG:H	2.25	0.40
1:A:226:HIS:CD2	1:A:336:PHE:CD2	3.08	0.40
1:A:733:VAL:HG13	1:A:737:GLN:NE2	2.36	0.40
1:A:127:PHE:HB2	1:A:146:TYR:HB2	2.03	0.40
1:A:227:PHE:O	1:A:338:GLU:HG2	2.21	0.40
1:B:455:ILE:CG2	1:B:456:ALA:N	2.84	0.40
1:A:51:ASP:OD1	1:A:72:HIS:ND1	2.54	0.40
1:B:1432:ILE:HG22	1:B:1432:ILE:O	2.21	0.40
1:B:505:SER:CB	1:B:510:ILE:HD11	2.49	0.40
1:A:981:GLY:H	1:A:1328:MET:HE2	1.85	0.40
1:B:251:LYS:CG	1:B:296:ILE:HD13	2.50	0.40
1:A:1104:LEU:HD22	1:A:1152:ILE:HG23	2.02	0.40
2:Y:139:ASN:CA	2:Y:146:LEU:HD21	2.52	0.40
1:B:592:MET:CB	1:B:780:VAL:HG21	2.51	0.40
1:B:576:SER:OG	1:B:589:SER:HB2	2.20	0.40
1:A:237:PHE:HE1	1:A:378:SER:O	2.03	0.40
1:B:942:VAL:CG2	1:B:957:LYS:HB3	2.50	0.40
1:B:935:LYS:HD2	1:B:935:LYS:HA	1.63	0.40
1:A:661:ASP:OD2	1:A:663:GLN:NE2	2.54	0.40
1:A:1543:ILE:O	1:A:1543:ILE:HG22	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:HB	1:B:512:PHE:CD1	2.56	0.40
1:B:620:LEU:HD13	1:B:811:VAL:HB	2.03	0.40
1:B:1278:GLN:O	1:B:1360:HIS:NE2	2.54	0.40
1:B:309:GLU:O	1:B:309:GLU:HG3	2.22	0.40
1:A:944:LEU:HA	1:A:944:LEU:HD23	1.56	0.40
1:A:1557:ILE:C	1:A:1559:TYR:H	2.24	0.40
1:A:66:TYR:CD1	1:A:90:LYS:HG3	2.54	0.40
1:A:950:TYR:HB3	1:A:1272:LYS:HD3	2.02	0.40
2:Y:228:ILE:HG22	2:Y:228:ILE:O	2.21	0.40
1:B:681:LYS:HG3	1:B:681:LYS:H	1.70	0.40
1:A:357:VAL:HG12	1:A:357:VAL:O	2.20	0.40
1:B:1421:HIS:CE1	1:B:1498:TYR:CD2	3.10	0.40
1:B:1497:GLU:OE1	1:B:1500:ARG:HD2	2.21	0.40
2:X:194:LYS:O	2:X:196:GLU:N	2.54	0.40
1:B:686:ILE:C	1:B:688:ALA:H	2.22	0.40
2:Y:194:LYS:O	2:Y:196:GLU:N	2.54	0.40
1:A:313:TYR:HE2	1:A:321:LYS:HZ2	1.68	0.40
1:A:441:ASP:OD2	1:A:441:ASP:N	2.43	0.40
1:B:834:VAL:CG1	1:B:835:ARG:N	2.85	0.40
1:B:339:GLU:HB2	1:B:766:ARG:NH2	2.36	0.40
1:A:124:GLY:HA3	1:A:148:LEU:O	2.22	0.40
1:A:123:ASN:CG	1:A:157:ARG:HH22	2.25	0.40
1:B:1136:GLU:OE1	1:B:1415:SER:HB3	2.22	0.40
1:B:1188:LEU:HD23	1:B:1212:LEU:HA	2.03	0.40
1:B:185:PHE:HB3	1:B:186:PRO:HD3	1.99	0.40
1:A:576:SER:OG	1:A:589:SER:HB2	2.21	0.40
1:B:379:LEU:HB3	1:B:381:GLN:HE22	1.85	0.40
1:B:774:LEU:HD11	1:B:788:PHE:CE2	2.56	0.40
1:B:48:GLU:C	1:B:49:ALA:O	2.59	0.40
1:A:50:PHE:HB3	1:A:109:LYS:HE2	2.00	0.40
1:B:264:ASP:HB3	1:B:330:ILE:CG1	2.51	0.40
1:B:882:LYS:HG3	1:B:884:VAL:HG13	2.04	0.40
1:A:1420:SER:O	1:A:1421:HIS:C	2.58	0.40
1:B:1503:LYS:HD2	1:B:1503:LYS:N	2.37	0.40
1:B:668:PRO:O	1:B:669:CYS:O	2.40	0.40
1:A:277:ASP:OD2	1:A:279:GLN:O	2.40	0.40
1:B:277:ASP:CG	1:B:279:GLN:O	2.60	0.40
1:A:568:GLY:HA3	1:A:807:THR:HB	2.02	0.40
1:B:54:ILE:CG2	1:B:55:SER:N	2.84	0.40
1:A:614:ARG:NH1	1:A:798:GLU:OE1	2.55	0.40
1:B:149:ASN:C	1:B:151:ASP:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:75:PHE:O	2:Y:77:PRO:CD	2.69	0.40
1:A:478:VAL:CG1	1:A:478:VAL:O	2.62	0.40
1:B:1126:PRO:HD2	1:B:1127:ILE:HD12	2.03	0.40
1:A:846:TYR:HD2	1:A:893:SER:HB2	1.87	0.40
1:A:840:GLN:NE2	1:A:1484:GLU:OE1	2.54	0.40
1:A:557:ASP:CG	1:A:558:SER:N	2.75	0.40
1:B:1141:SER:O	1:B:1142:LEU:C	2.60	0.40
2:X:189:ILE:HD12	2:X:201:ILE:HD12	2.03	0.40
1:A:220:LYS:HG2	1:A:763:PRO:CB	2.51	0.40
1:B:284:GLN:HG2	1:B:310:LEU:HD13	2.04	0.40
1:A:1372:GLU:HG3	1:A:1373:GLU:N	2.34	0.40
1:B:1313:ILE:HG22	1:B:1314:ASP:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:ARG:NH2	1:B:434:ASN:OD1[3_454]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1612/1676 (96%)	1199 (74%)	273 (17%)	140 (9%)	1	14
1	B	1468/1676 (88%)	1126 (77%)	224 (15%)	118 (8%)	1	16
2	X	189/231 (82%)	150 (79%)	28 (15%)	11 (6%)	2	25
2	Y	189/231 (82%)	150 (79%)	29 (15%)	10 (5%)	2	27
All	All	3458/3814 (91%)	2625 (76%)	554 (16%)	279 (8%)	1	15

All (279) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	TYR
1	A	59	TYR
1	A	97	ASN
1	A	209	PHE
1	A	243	PHE
1	A	282	MET
1	A	289	ASN
1	A	308	LYS
1	A	318	LEU
1	A	319	ASN
1	A	336	PHE
1	A	378	SER
1	A	426	SER
1	A	489	LYS
1	A	490	SER
1	A	520	ASP
1	A	657	ALA
1	A	664	GLU
1	A	669	CYS
1	A	704	CYS
1	A	705	VAL
1	A	931	PRO
1	A	1196	SER
1	A	1231	ASN
1	A	1262	LYS
1	A	1275	SER
1	A	1284	PHE
1	A	1352	PHE
1	A	1373	GLU
1	A	1468	PRO
1	A	1481	GLU
1	A	1487	PHE
1	A	1516	ILE
1	A	1531	ASP
1	A	1532	CYS
1	A	1573	VAL
1	A	1592	ALA
1	A	1604	VAL
1	A	1631	PHE
1	A	1636	ILE
1	A	1653	THR
1	A	1655	SER
1	A	1658	GLN

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Mol	Chain	Res	Type
2	X	41	HIS
2	X	78	LYS
2	X	100	GLY
1	B	46	TYR
1	B	59	TYR
1	B	97	ASN
1	B	150	ASP
1	B	209	PHE
1	B	243	PHE
1	B	282	MET
1	B	289	ASN
1	B	308	LYS
1	B	318	LEU
1	B	319	ASN
1	B	336	PHE
1	B	378	SER
1	B	404	LEU
1	B	426	SER
1	B	489	LYS
1	B	490	SER
1	B	520	ASP
1	B	657	ALA
1	B	664	GLU
1	B	669	CYS
1	B	704	CYS
1	B	705	VAL
1	B	931	PRO
1	B	1196	SER
1	B	1231	ASN
1	B	1262	LYS
1	B	1284	PHE
1	B	1352	PHE
1	B	1373	GLU
1	B	1468	PRO
1	B	1481	GLU
2	Y	41	HIS
2	Y	78	LYS
2	Y	100	GLY
1	A	49	ALA
1	A	86	THR
1	A	99	VAL
1	A	207	GLU

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Mol	Chain	Res	Type
1	A	291	MET
1	A	306	ALA
1	A	317	ASP
1	A	404	LEU
1	A	457	TYR
1	A	522	SER
1	A	611	GLY
1	A	613	GLN
1	A	619	PRO
1	A	633	GLY
1	A	638	GLY
1	A	691	LYS
1	A	692	HIS
1	A	720	LEU
1	A	856	CYS
1	A	939	TYR
1	A	948	GLY
1	A	949	ILE
1	A	996	GLY
1	A	1029	ASN
1	A	1233	GLN
1	A	1240	PRO
1	A	1264	ILE
1	A	1283	GLY
1	A	1335	GLY
1	A	1432	ILE
1	A	1595	ASP
1	A	1609	ALA
1	A	1633	PHE
1	A	1639	LEU
1	A	1652	THR
2	X	42	ASP
2	X	72	VAL
2	X	136	LEU
2	X	185	LYS
1	B	49	ALA
1	B	86	THR
1	B	99	VAL
1	B	207	GLU
1	B	291	MET
1	B	306	ALA
1	B	317	ASP

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Mol	Chain	Res	Type
1	B	457	TYR
1	B	522	SER
1	B	611	GLY
1	B	613	GLN
1	B	619	PRO
1	B	633	GLY
1	B	638	GLY
1	B	691	LYS
1	B	692	HIS
1	B	720	LEU
1	B	856	CYS
1	B	939	TYR
1	B	948	GLY
1	B	949	ILE
1	B	996	GLY
1	B	1029	ASN
1	B	1233	GLN
1	B	1240	PRO
1	B	1264	ILE
1	B	1275	SER
1	B	1283	GLY
1	B	1335	GLY
1	B	1432	ILE
1	B	1487	PHE
1	B	1527	CYS
2	Y	42	ASP
2	Y	72	VAL
2	Y	136	LEU
2	Y	185	LYS
1	A	372	LYS
1	A	491	PRO
1	A	607	SER
1	A	617	LYS
1	A	627	LEU
1	A	643	ALA
1	A	661	ASP
1	A	663	GLN
1	A	722	PRO
1	A	792	ASP
1	A	814	THR
1	A	1055	SER
1	A	1263	ASP

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Mol	Chain	Res	Type
1	A	1286	SER
1	A	1297	LEU
1	A	1308	ARG
1	A	1520	CYS
1	A	1523	ALA
1	A	1543	ILE
1	A	1650	ARG
2	X	125	LYS
1	B	78	LYS
1	B	491	PRO
1	B	607	SER
1	B	617	LYS
1	B	627	LEU
1	B	663	GLN
1	B	792	ASP
1	B	814	THR
1	B	1055	SER
1	B	1126	PRO
1	B	1235	LYS
1	B	1263	ASP
1	B	1286	SER
1	B	1308	ARG
1	B	1531	ASP
2	Y	125	LYS
1	A	78	LYS
1	A	287	MET
1	A	610	TYR
1	A	759	PRO
1	A	794	LEU
1	A	1126	PRO
1	A	1235	LYS
1	A	1622	LYS
2	X	104	PHE
1	B	287	MET
1	B	610	TYR
1	B	643	ALA
1	B	647	HIS
1	B	648	LEU
1	B	661	ASP
1	B	722	PRO
1	B	759	PRO
1	B	794	LEU

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Mol	Chain	Res	Type
1	B	820	PHE
1	B	1297	LEU
1	B	1349	SER
1	B	1525	CYS
2	Y	104	PHE
1	A	101	TYR
1	A	154	PRO
1	A	284	GLN
1	A	640	LEU
1	A	648	LEU
1	A	760	VAL
1	A	820	PHE
1	A	863	GLU
1	A	909	ASN
1	A	960	PRO
1	A	1114	ASP
1	A	1239	VAL
1	A	1321	GLY
1	A	1349	SER
1	A	1501	PRO
1	A	1526	LYS
1	A	1632	SER
1	A	1656	SER
1	A	1667	PHE
2	X	67	TYR
2	X	124	LYS
1	B	101	TYR
1	B	154	PRO
1	B	372	LYS
1	B	640	LEU
1	B	760	VAL
1	B	765	ILE
1	B	909	ASN
1	B	960	PRO
1	B	1114	ASP
1	B	1239	VAL
1	B	1524	ALA
2	Y	124	LYS
1	A	730	GLU
1	A	765	ILE
1	A	1310	SER
1	B	137	PRO

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Mol	Chain	Res	Type
1	B	284	GLN
1	B	1310	SER
1	B	1501	PRO
1	A	137	PRO
1	A	686	ILE
1	B	171	VAL
1	B	686	ILE
1	B	1321	GLY
1	A	133	PRO
1	A	171	VAL
1	A	668	PRO
1	A	1134	PRO
1	A	1519	VAL
1	B	133	PRO
1	B	668	PRO
1	B	1134	PRO
1	A	1638	PRO
1	B	166	PRO
1	B	1068	VAL
1	A	166	PRO
1	A	609	VAL
1	B	1519	VAL
1	A	801	GLY
1	A	1675	GLY
1	B	801	GLY
1	B	1296	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1438/1484 (97%)	1168 (81%)	270 (19%)	2	13
1	B	1311/1484 (88%)	1055 (80%)	256 (20%)	2	12
2	X	175/205 (85%)	155 (89%)	20 (11%)	7	36
2	Y	175/205 (85%)	154 (88%)	21 (12%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3099/3378 (92%)	2532 (82%)	567 (18%)	2 14

All (567) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	THR
1	A	23	TYR
1	A	36	SER
1	A	42	GLN
1	A	55	SER
1	A	56	ILE
1	A	59	TYR
1	A	64	PHE
1	A	65	SER
1	A	73	LEU
1	A	82	SER
1	A	86	THR
1	A	88	GLN
1	A	100	SER
1	A	109	LYS
1	A	112	SER
1	A	114	SER
1	A	116	ARG
1	A	122	ASP
1	A	123	ASN
1	A	126	LEU
1	A	128	ILE
1	A	130	THR
1	A	136	THR
1	A	140	SER
1	A	143	VAL
1	A	148	LEU
1	A	160	VAL
1	A	161	LEU
1	A	162	THR
1	A	174	VAL
1	A	175	GLU
1	A	176	GLU
1	A	184	SER
1	A	195	ARG
1	A	208	ASP
1	A	216	TYR

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Mol	Chain	Res	Type
1	A	224	LEU
1	A	231	ILE
1	A	235	TYR
1	A	237	PHE
1	A	242	ASN
1	A	247	GLU
1	A	249	THR
1	A	253	ARG
1	A	280	LYS
1	A	296	ILE
1	A	299	VAL
1	A	321	LYS
1	A	333	THR
1	A	349	LEU
1	A	354	LEU
1	A	363	LEU
1	A	364	LYS
1	A	372	LYS
1	A	378	SER
1	A	381	GLN
1	A	383	VAL
1	A	386	VAL
1	A	389	THR
1	A	393	GLN
1	A	394	THR
1	A	407	SER
1	A	419	SER
1	A	420	PHE
1	A	422	LEU
1	A	426	SER
1	A	431	LEU
1	A	436	LYS
1	A	438	ASP
1	A	457	TYR
1	A	458	SER
1	A	466	TYR
1	A	473	HIS
1	A	478	VAL
1	A	484	ILE
1	A	485	ILE
1	A	492	TYR
1	A	495	LYS

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Mol	Chain	Res	Type
1	A	500	ASN
1	A	504	LEU
1	A	512	PHE
1	A	530	VAL
1	A	535	VAL
1	A	540	LEU
1	A	541	LEU
1	A	544	TYR
1	A	546	VAL
1	A	553	GLU
1	A	563	ILE
1	A	571	LEU
1	A	573	VAL
1	A	576	SER
1	A	589	SER
1	A	592	MET
1	A	594	THR
1	A	610	TYR
1	A	614	ARG
1	A	623	VAL
1	A	624	PHE
1	A	627	LEU
1	A	640	LEU
1	A	644	ASN
1	A	652	THR
1	A	654	LEU
1	A	658	ASN
1	A	661	ASP
1	A	667	GLU
1	A	669	CYS
1	A	673	LEU
1	A	705	VAL
1	A	711	CYS
1	A	729	THR
1	A	753	HIS
1	A	758	LEU
1	A	786	LEU
1	A	790	LEU
1	A	795	THR
1	A	799	ILE
1	A	802	ILE
1	A	809	ILE

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Mol	Chain	Res	Type
1	A	814	THR
1	A	833	VAL
1	A	835	ARG
1	A	840	GLN
1	A	859	MET
1	A	860	SER
1	A	863	GLU
1	A	867	THR
1	A	886	GLN
1	A	887	LYS
1	A	888	VAL
1	A	895	LEU
1	A	897	THR
1	A	900	VAL
1	A	901	LEU
1	A	903	LEU
1	A	905	ILE
1	A	908	HIS
1	A	914	LEU
1	A	926	THR
1	A	927	LEU
1	A	935	LYS
1	A	936	ARG
1	A	947	ARG
1	A	952	THR
1	A	953	ILE
1	A	954	SER
1	A	959	PHE
1	A	961	TYR
1	A	971	THR
1	A	977	LEU
1	A	980	LYS
1	A	982	LEU
1	A	983	LEU
1	A	984	VAL
1	A	986	GLU
1	A	987	ILE
1	A	994	GLN
1	A	997	ILE
1	A	1001	THR
1	A	1003	LEU
1	A	1011	GLU

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Mol	Chain	Res	Type
1	A	1027	THR
1	A	1029	ASN
1	A	1040	ILE
1	A	1043	GLN
1	A	1056	ILE
1	A	1058	SER
1	A	1067	SER
1	A	1069	TRP
1	A	1073	SER
1	A	1075	SER
1	A	1076	THR
1	A	1078	LEU
1	A	1084	ARG
1	A	1096	ASN
1	A	1115	ASN
1	A	1119	LYS
1	A	1127	ILE
1	A	1128	LYS
1	A	1132	THR
1	A	1140	ASN
1	A	1142	LEU
1	A	1147	PHE
1	A	1148	THR
1	A	1150	ILE
1	A	1158	ILE
1	A	1161	LEU
1	A	1162	VAL
1	A	1164	ILE
1	A	1173	ASN
1	A	1184	SER
1	A	1200	LYS
1	A	1208	ILE
1	A	1217	LEU
1	A	1218	VAL
1	A	1219	LYS
1	A	1228	TRP
1	A	1231	ASN
1	A	1232	LEU
1	A	1244	THR
1	A	1251	THR
1	A	1262	LYS
1	A	1271	ILE

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Mol	Chain	Res	Type
1	A	1275	SER
1	A	1278	GLN
1	A	1279	ARG
1	A	1280	TYR
1	A	1294	ILE
1	A	1297	LEU
1	A	1301	SER
1	A	1303	LEU
1	A	1307	LEU
1	A	1308	ARG
1	A	1313	ILE
1	A	1314	ASP
1	A	1323	LEU
1	A	1334	LEU
1	A	1338	VAL
1	A	1341	LEU
1	A	1345	ASP
1	A	1363	THR
1	A	1365	VAL
1	A	1376	SER
1	A	1381	ILE
1	A	1383	THR
1	A	1401	ARG
1	A	1421	HIS
1	A	1423	VAL
1	A	1430	THR
1	A	1464	LEU
1	A	1465	ASN
1	A	1476	ARG
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1489	SER
1	A	1492	THR
1	A	1494	THR
1	A	1495	VAL
1	A	1496	TYR
1	A	1500	ARG
1	A	1502	ASP
1	A	1507	MET
1	A	1509	TYR

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Mol	Chain	Res	Type
1	A	1513	ASN
1	A	1518	LYS
1	A	1521	GLU
1	A	1535	MET
1	A	1540	ASP
1	A	1544	SER
1	A	1548	ARG
1	A	1553	CYS
1	A	1559	TYR
1	A	1561	TYR
1	A	1569	THR
1	A	1581	LEU
1	A	1602	LYS
1	A	1607	THR
1	A	1619	ILE
1	A	1622	LYS
1	A	1627	ILE
1	A	1629	TYR
1	A	1633	PHE
1	A	1636	ILE
1	A	1642	LEU
1	A	1650	ARG
1	A	1653	THR
2	X	57	TYR
2	X	65	GLU
2	X	66	ASN
2	X	67	TYR
2	X	72	VAL
2	X	75	PHE
2	X	78	LYS
2	X	80	GLN
2	X	91	LYS
2	X	94	TYR
2	X	113	ASN
2	X	123	THR
2	X	137	PHE
2	X	138	VAL
2	X	139	ASN
2	X	146	LEU
2	X	150	ILE
2	X	190	ILE
2	X	210	GLU

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Mol	Chain	Res	Type
2	X	225	SER
1	B	22	THR
1	B	23	TYR
1	B	36	SER
1	B	42	GLN
1	B	55	SER
1	B	56	ILE
1	B	59	TYR
1	B	64	PHE
1	B	65	SER
1	B	73	LEU
1	B	82	SER
1	B	86	THR
1	B	88	GLN
1	B	100	SER
1	B	109	LYS
1	B	112	SER
1	B	114	SER
1	B	116	ARG
1	B	122	ASP
1	B	123	ASN
1	B	126	LEU
1	B	128	ILE
1	B	130	THR
1	B	136	THR
1	B	140	SER
1	B	143	VAL
1	B	148	LEU
1	B	160	VAL
1	B	161	LEU
1	B	162	THR
1	B	174	VAL
1	B	175	GLU
1	B	176	GLU
1	B	184	SER
1	B	195	ARG
1	B	208	ASP
1	B	216	TYR
1	B	224	LEU
1	B	231	ILE
1	B	235	TYR
1	B	237	PHE

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Mol	Chain	Res	Type
1	B	242	ASN
1	B	247	GLU
1	B	249	THR
1	B	253	ARG
1	B	280	LYS
1	B	299	VAL
1	B	321	LYS
1	B	333	THR
1	B	349	LEU
1	B	354	LEU
1	B	363	LEU
1	B	364	LYS
1	B	372	LYS
1	B	378	SER
1	B	381	GLN
1	B	386	VAL
1	B	389	THR
1	B	393	GLN
1	B	394	THR
1	B	407	SER
1	B	419	SER
1	B	420	PHE
1	B	422	LEU
1	B	423	ASN
1	B	426	SER
1	B	431	LEU
1	B	435	VAL
1	B	436	LYS
1	B	438	ASP
1	B	457	TYR
1	B	458	SER
1	B	466	TYR
1	B	472	ASN
1	B	473	HIS
1	B	478	VAL
1	B	484	ILE
1	B	485	ILE
1	B	492	TYR
1	B	495	LYS
1	B	500	ASN
1	B	504	LEU
1	B	512	PHE

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Mol	Chain	Res	Type
1	B	530	VAL
1	B	535	VAL
1	B	540	LEU
1	B	541	LEU
1	B	544	TYR
1	B	546	VAL
1	B	553	GLU
1	B	563	ILE
1	B	571	LEU
1	B	573	VAL
1	B	576	SER
1	B	589	SER
1	B	592	MET
1	B	594	THR
1	B	610	TYR
1	B	614	ARG
1	B	623	VAL
1	B	624	PHE
1	B	627	LEU
1	B	640	LEU
1	B	644	ASN
1	B	652	THR
1	B	654	LEU
1	B	658	ASN
1	B	661	ASP
1	B	667	GLU
1	B	673	LEU
1	B	705	VAL
1	B	711	CYS
1	B	729	THR
1	B	753	HIS
1	B	758	LEU
1	B	786	LEU
1	B	790	LEU
1	B	795	THR
1	B	799	ILE
1	B	802	ILE
1	B	809	ILE
1	B	814	THR
1	B	833	VAL
1	B	835	ARG
1	B	840	GLN

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Mol	Chain	Res	Type
1	B	859	MET
1	B	860	SER
1	B	863	GLU
1	B	867	THR
1	B	886	GLN
1	B	887	LYS
1	B	888	VAL
1	B	894	HIS
1	B	895	LEU
1	B	897	THR
1	B	900	VAL
1	B	901	LEU
1	B	903	LEU
1	B	905	ILE
1	B	908	HIS
1	B	914	LEU
1	B	926	THR
1	B	927	LEU
1	B	935	LYS
1	B	936	ARG
1	B	947	ARG
1	B	952	THR
1	B	953	ILE
1	B	954	SER
1	B	959	PHE
1	B	961	TYR
1	B	971	THR
1	B	977	LEU
1	B	980	LYS
1	B	982	LEU
1	B	983	LEU
1	B	984	VAL
1	B	986	GLU
1	B	987	ILE
1	B	994	GLN
1	B	997	ILE
1	B	1001	THR
1	B	1003	LEU
1	B	1011	GLU
1	B	1024	TYR
1	B	1027	THR
1	B	1029	ASN

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Mol	Chain	Res	Type
1	B	1040	ILE
1	B	1043	GLN
1	B	1056	ILE
1	B	1058	SER
1	B	1066	TYR
1	B	1067	SER
1	B	1069	TRP
1	B	1073	SER
1	B	1075	SER
1	B	1076	THR
1	B	1078	LEU
1	B	1084	ARG
1	B	1096	ASN
1	B	1115	ASN
1	B	1119	LYS
1	B	1127	ILE
1	B	1128	LYS
1	B	1132	THR
1	B	1140	ASN
1	B	1142	LEU
1	B	1147	PHE
1	B	1148	THR
1	B	1150	ILE
1	B	1158	ILE
1	B	1161	LEU
1	B	1162	VAL
1	B	1164	ILE
1	B	1173	ASN
1	B	1184	SER
1	B	1200	LYS
1	B	1208	ILE
1	B	1217	LEU
1	B	1218	VAL
1	B	1219	LYS
1	B	1228	TRP
1	B	1231	ASN
1	B	1232	LEU
1	B	1244	THR
1	B	1251	THR
1	B	1262	LYS
1	B	1271	ILE
1	B	1275	SER

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Mol	Chain	Res	Type
1	B	1278	GLN
1	B	1279	ARG
1	B	1280	TYR
1	B	1294	ILE
1	B	1297	LEU
1	B	1301	SER
1	B	1303	LEU
1	B	1307	LEU
1	B	1308	ARG
1	B	1313	ILE
1	B	1314	ASP
1	B	1323	LEU
1	B	1334	LEU
1	B	1338	VAL
1	B	1341	LEU
1	B	1345	ASP
1	B	1363	THR
1	B	1365	VAL
1	B	1376	SER
1	B	1381	ILE
1	B	1383	THR
1	B	1401	ARG
1	B	1421	HIS
1	B	1423	VAL
1	B	1430	THR
1	B	1464	LEU
1	B	1465	ASN
1	B	1476	ARG
1	B	1480	PHE
1	B	1483	PHE
1	B	1485	VAL
1	B	1487	PHE
1	B	1488	LEU
1	B	1489	SER
1	B	1492	THR
1	B	1494	THR
1	B	1495	VAL
1	B	1496	TYR
1	B	1500	ARG
1	B	1502	ASP
1	B	1507	MET
1	B	1509	TYR

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Mol	Chain	Res	Type
1	B	1513	ASN
1	B	1516	ILE
1	B	1517	GLN
1	B	1520	CYS
1	B	1527	CYS
2	Y	57	TYR
2	Y	65	GLU
2	Y	66	ASN
2	Y	67	TYR
2	Y	72	VAL
2	Y	75	PHE
2	Y	78	LYS
2	Y	80	GLN
2	Y	91	LYS
2	Y	94	TYR
2	Y	113	ASN
2	Y	123	THR
2	Y	137	PHE
2	Y	138	VAL
2	Y	139	ASN
2	Y	146	LEU
2	Y	150	ILE
2	Y	183	THR
2	Y	190	ILE
2	Y	210	GLU
2	Y	225	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	80	GLN
1	A	88	GLN
1	A	110	HIS
1	A	123	ASN
1	A	242	ASN
1	A	288	GLN
1	A	381	GLN
1	A	393	GLN
1	A	399	GLN
1	A	423	ASN

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Mol	Chain	Res	Type
1	A	446	ASN
1	A	447	GLN
1	A	473	HIS
1	A	481	HIS
1	A	572	GLN
1	A	625	GLN
1	A	656	ASN
1	A	658	ASN
1	A	737	GLN
1	A	787	GLN
1	A	840	GLN
1	A	909	ASN
1	A	1002	HIS
1	A	1023	HIS
1	A	1029	ASN
1	A	1030	HIS
1	A	1090	ASN
1	A	1096	ASN
1	A	1115	ASN
1	A	1123	GLN
1	A	1140	ASN
1	A	1202	HIS
1	A	1221	ASN
1	A	1260	ASN
1	A	1278	GLN
1	A	1306	GLN
1	A	1324	HIS
1	A	1459	HIS
1	A	1463	GLN
1	A	1504	GLN
1	A	1616	GLN
2	X	59	ASN
2	X	76	ASN
2	X	80	GLN
2	X	81	ASN
2	X	113	ASN
2	X	139	ASN
2	X	175	ASN
2	X	176	ASN
1	B	38	ASN
1	B	42	GLN
1	B	88	GLN

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Mol	Chain	Res	Type
1	B	110	HIS
1	B	123	ASN
1	B	242	ASN
1	B	288	GLN
1	B	381	GLN
1	B	393	GLN
1	B	399	GLN
1	B	423	ASN
1	B	446	ASN
1	B	473	HIS
1	B	481	HIS
1	B	572	GLN
1	B	625	GLN
1	B	656	ASN
1	B	658	ASN
1	B	737	GLN
1	B	787	GLN
1	B	840	GLN
1	B	894	HIS
1	B	909	ASN
1	B	1002	HIS
1	B	1023	HIS
1	B	1029	ASN
1	B	1030	HIS
1	B	1090	ASN
1	B	1096	ASN
1	B	1115	ASN
1	B	1123	GLN
1	B	1140	ASN
1	B	1202	HIS
1	B	1221	ASN
1	B	1231	ASN
1	B	1260	ASN
1	B	1278	GLN
1	B	1306	GLN
1	B	1324	HIS
1	B	1463	GLN
1	B	1504	GLN
2	Y	59	ASN
2	Y	76	ASN
2	Y	80	GLN
2	Y	81	ASN

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Mol	Chain	Res	Type
2	Y	113	ASN
2	Y	139	ASN
2	Y	175	ASN
2	Y	176	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	2001	1,4	14,14,15	0.55	0	15,19,21	1.63	2 (13%)
4	NAG	A	2002	4	14,14,15	0.42	0	15,19,21	1.18	1 (6%)
4	NAG	B	2001	1,4	14,14,15	0.54	0	15,19,21	1.17	1 (6%)
4	NAG	B	2002	4	14,14,15	0.38	0	15,19,21	1.09	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2002	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	NAG	C2-N2-C7	-3.86	118.08	123.04
4	B	2001	NAG	C3-C4-C5	-2.73	105.44	110.20
4	B	2002	NAG	C1-O5-C5	3.53	116.73	112.25
4	A	2002	NAG	C1-O5-C5	3.69	116.93	112.25
4	A	2001	NAG	C1-O5-C5	3.95	117.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	NAG	3	0
4	B	2001	NAG	2	0

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 9 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	1682	1	14,14,15	0.66	0	15,19,21	0.97	0
5	NAG	B	1681	1	14,14,15	0.72	0	15,19,21	1.08	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	1682	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1681	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	B	1681	NAG	C1-O5-C5	2.32	115.19	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	1622/1676 (96%)	-0.08	37 (2%) 64 48	60, 136, 275, 372	0
1	B	1478/1676 (88%)	-0.16	13 (0%) 85 75	61, 129, 232, 340	0
2	X	191/231 (82%)	0.31	19 (9%) 9 7	150, 242, 308, 342	0
2	Y	191/231 (82%)	0.31	15 (7%) 15 10	149, 242, 308, 342	0
All	All	3482/3814 (91%)	-0.07	84 (2%) 62 47	60, 140, 279, 372	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1594	LYS	9.5
1	A	1593	GLU	8.7
1	A	1542	THR	6.7
1	A	1630	ASN	5.5
1	A	1522	GLY	5.4
2	X	118	THR	5.1
2	Y	63	LYS	5.0
1	A	1534	GLN	5.0
1	A	1595	ASP	5.0
2	X	193	LEU	4.6
2	Y	162	LEU	4.5
2	X	63	LYS	4.4
1	B	309	GLU	4.4
2	Y	118	THR	4.2
2	X	84	LEU	4.2
1	A	1523	ALA	4.1
2	X	117	SER	4.0
1	A	760	VAL	4.0
1	A	759	PRO	3.8
2	X	85	PHE	3.8
2	X	162	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	1607	THR	3.7
1	A	1521	GLU	3.7
1	B	760	VAL	3.7
1	A	1574	PHE	3.7
2	X	189	ILE	3.6
2	Y	84	LEU	3.5
1	A	1619	ILE	3.4
1	A	1647	TYR	3.4
1	B	1518	LYS	3.4
1	A	1627	ILE	3.4
1	B	759	PRO	3.4
2	X	221	ILE	3.4
1	A	1608	ASN	3.3
1	B	1399	TYR	3.3
1	A	1646	GLU	3.2
2	X	228	ILE	3.1
1	B	683	ILE	3.1
1	A	1625	LEU	3.1
1	A	1583	ASP	3.0
1	A	1591	VAL	3.0
1	A	1617	TYR	2.9
2	Y	107	GLN	2.9
1	A	1543	ILE	2.9
1	B	684	GLU	2.9
2	Y	199	VAL	2.8
1	B	870	SER	2.8
1	B	616	ALA	2.8
1	A	1572	ASN	2.8
1	A	309	GLU	2.7
1	A	617	LYS	2.7
1	A	1547	THR	2.7
2	Y	193	LEU	2.7
2	Y	228	ILE	2.6
1	B	666	ASP	2.6
2	Y	185	LYS	2.6
2	Y	85	PHE	2.6
1	A	1592	ALA	2.6
2	Y	167	PHE	2.6
2	Y	191	ILE	2.6
2	Y	117	SER	2.5
2	Y	90	ASP	2.5
2	X	192	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1546	GLU	2.5
1	B	99	VAL	2.5
1	A	1541	LEU	2.5
2	X	105	VAL	2.5
1	A	1638	PRO	2.4
2	X	185	LYS	2.4
2	X	199	VAL	2.4
1	B	1531	ASP	2.4
2	Y	226	VAL	2.3
1	B	552	ALA	2.2
2	X	107	GLN	2.2
1	A	99	VAL	2.2
1	A	1626	GLN	2.2
2	X	226	VAL	2.1
1	A	749	LEU	2.1
2	X	62	GLY	2.1
2	X	224	ILE	2.1
1	A	1524	ALA	2.1
1	A	761	SER	2.0
1	A	1575	VAL	2.0
2	X	116	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	2002	14/15	0.84	0.28	-	309,312,314,314	0
4	NAG	A	2001	14/15	0.82	0.46	-	304,306,310,312	0
4	NAG	B	2001	14/15	0.84	0.49	-	315,318,321,323	0
4	NAG	A	2002	14/15	0.81	0.35	-	302,303,305,305	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CD	A	1678	1/1	0.93	0.07	-2.60	261,261,261,261	0
3	CD	B	1678	1/1	0.39	0.09	-	271,271,271,271	0
5	NAG	A	1682	14/15	0.65	0.58	-	285,301,311,313	0
3	CD	A	1677	1/1	0.96	0.42	-	137,137,137,137	1
3	CD	A	1681	1/1	0.64	0.15	-	263,263,263,263	0
5	NAG	B	1681	14/15	0.81	0.36	-	268,294,323,333	0
3	CD	B	1677	1/1	0.93	0.06	-	255,255,255,255	0
3	CD	B	1680	1/1	0.67	0.13	-	252,252,252,252	0
3	CD	A	1680	1/1	0.81	0.10	-	241,241,241,241	0
3	CD	B	1679	1/1	0.95	0.12	-	240,240,240,240	0
3	CD	A	1679	1/1	0.91	0.08	-	270,270,270,270	0

6.5 Other polymers

There are no such residues in this entry.