Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:33 PM GMT

PDB ID	:	1KTV
Title	:	Crystal Structure of Elongation Factor G Dimer Without Nucleotide
Authors	:	Laurberg, M.; Kristensen, O.; Su, X.D.; Liljas, A.
Deposited on	:	2002-01-17
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

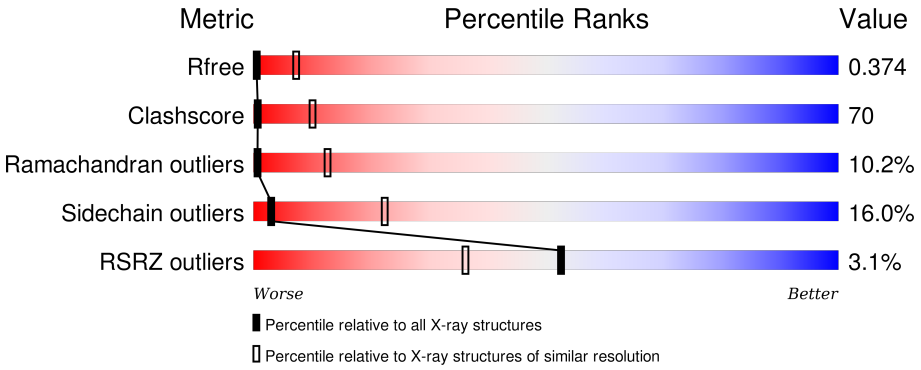
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	691	2% 21% 54% 14% • 9%
1	B	691	4% 20% 54% 16% • 9%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9914 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 ELONGATION FACTOR G.

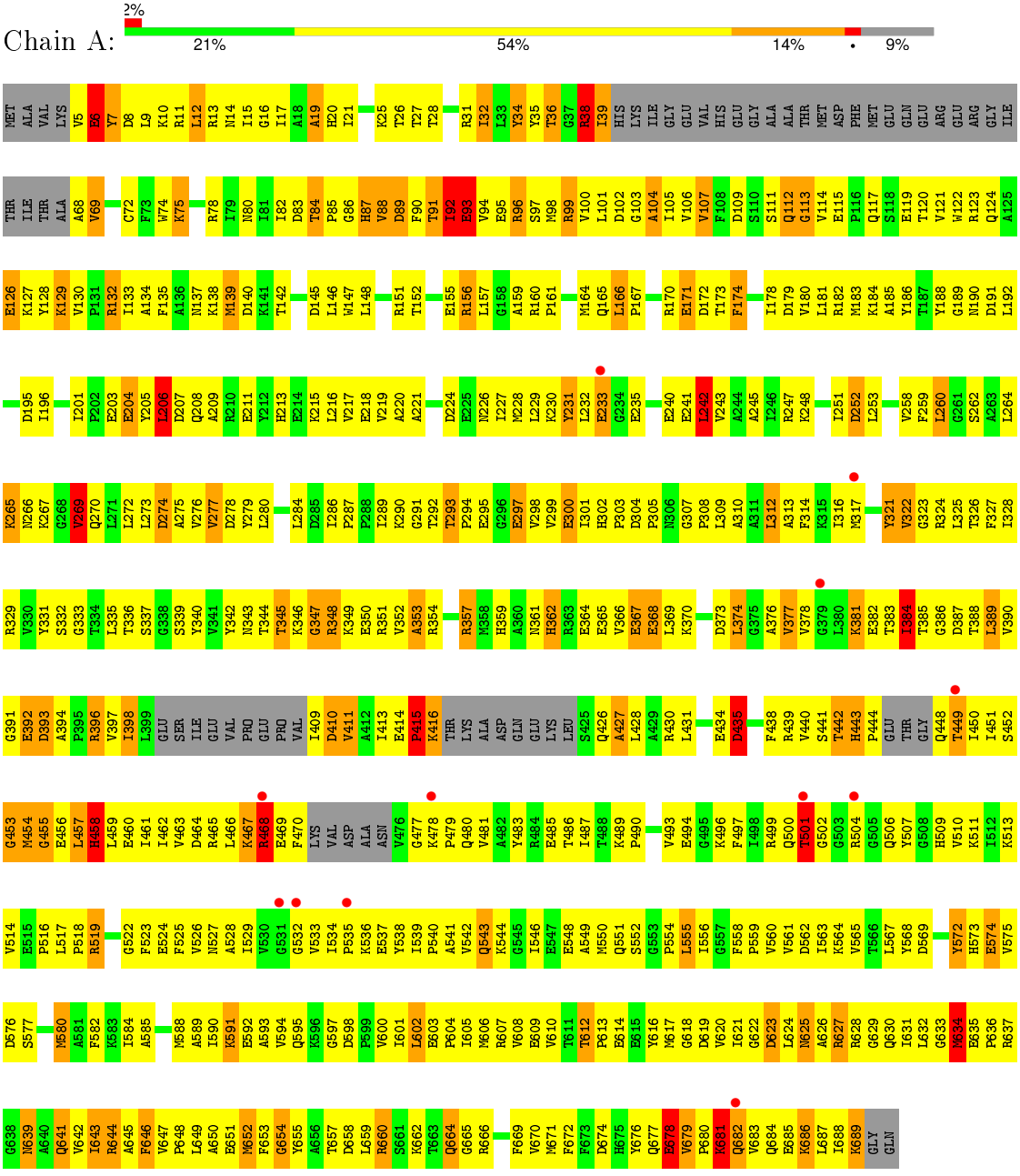
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	632	Total	C	N	O	S	0	0	0
			4957	3157	849	933	18			
1	B	632	Total	C	N	O	S	0	0	0
			4957	3157	849	933	18			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

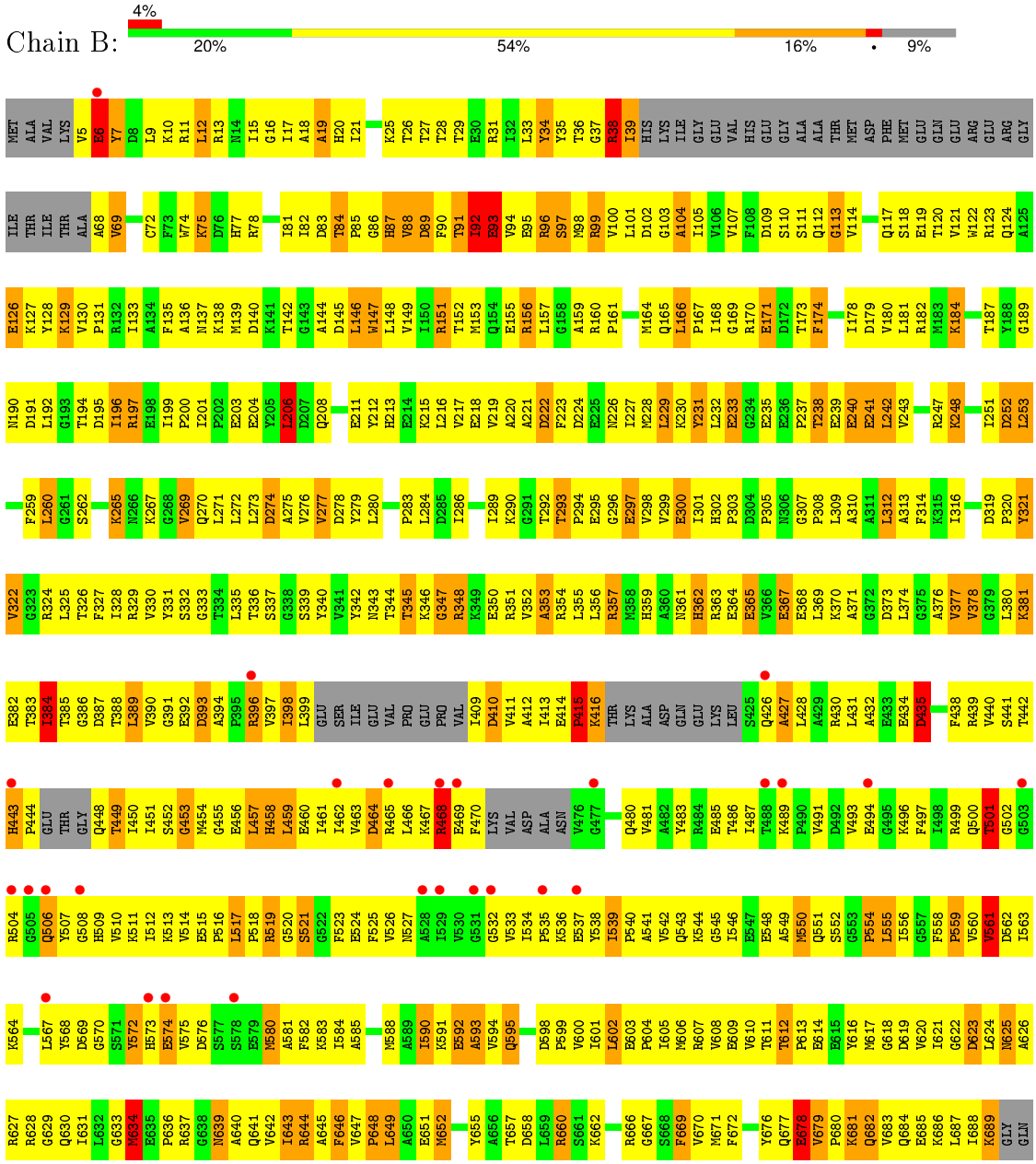
- Molecule 1: ELONGATION FACTOR G

Chain A:



• Molecule 1: ELONGATION FACTOR G

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.99Å 103.55Å 176.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.73 – 3.80 39.72 – 3.79	Depositor EDS
% Data completeness (in resolution range)	82.4 (39.73-3.80) 82.0 (39.72-3.79)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.76Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.287 , 0.374 0.278 , 0.374	Depositor DCC
R_{free} test set	674 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	1 of 14546 reflections (0.007%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	9914	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.38 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2024e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.61	0/5048	0.90	5/6829 (0.1%)
1	B	0.64	2/5048 (0.0%)	0.93	6/6829 (0.1%)
All	All	0.62	2/10096 (0.0%)	0.92	11/13658 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	TRP	NE1-CE2	-8.71	1.26	1.37
1	B	6	GLU	CD-OE2	-5.12	1.20	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	453	GLY	N-CA-C	7.52	131.90	113.10
1	B	147	TRP	CE2-CD2-CG	-7.29	101.47	107.30
1	B	147	TRP	CD2-CE2-CZ2	-6.81	114.13	122.30
1	B	453	GLY	N-CA-C	6.71	129.88	113.10
1	B	634	MET	CG-SD-CE	5.91	109.65	100.20
1	A	458	HIS	N-CA-C	-5.36	96.54	111.00
1	A	634	MET	CG-SD-CE	5.29	108.67	100.20
1	B	521	SER	N-CA-C	-5.29	96.71	111.00
1	A	93	GLU	N-CA-C	-5.27	96.78	111.00
1	A	533	VAL	N-CA-C	-5.21	96.95	111.00
1	B	533	VAL	N-CA-C	-5.18	97.03	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4957	0	5021	691	0
1	B	4957	0	5021	713	0
All	All	9914	0	10042	1392	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 70.

All (1392) 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:411:VAL:HB	1:B:453:GLY:CA	1.63	1.28
1:A:411:VAL:HB	1:A:453:GLY:CA	1.69	1.19
1:A:411:VAL:HB	1:A:453:GLY:HA2	1.26	1.09
1:B:276:VAL:HG13	1:B:280:LEU:HD12	1.29	1.08
1:B:321:TYR:O	1:B:322:VAL:HG22	1.51	1.08
1:A:276:VAL:HG13	1:A:280:LEU:HD12	1.35	1.05
1:B:5:VAL:HG13	1:B:6:GLU:H	1.16	1.05
1:B:87:HIS:NE2	1:B:90:PHE:HB2	1.72	1.05
1:A:87:HIS:NE2	1:A:90:PHE:HB2	1.73	1.03
1:B:6:GLU:HG2	1:B:7:TYR:H	1.19	1.03
1:B:411:VAL:CB	1:B:453:GLY:HA3	1.89	1.02
1:B:329:ARG:HA	1:B:374:LEU:HB3	1.43	0.99
1:A:5:VAL:HG13	1:A:6:GLU:H	1.26	0.99
1:A:434:GLU:O	1:A:435:ASP:HB2	1.63	0.97
1:A:459:LEU:H	1:A:459:LEU:HD12	1.28	0.97
1:B:434:GLU:O	1:B:435:ASP:HB2	1.62	0.96
1:A:612:THR:HG21	1:A:620:VAL:HG21	1.44	0.96
1:B:411:VAL:HB	1:B:453:GLY:HA3	0.98	0.96
1:A:411:VAL:HB	1:A:453:GLY:HA3	1.48	0.95
1:A:329:ARG:HG3	1:A:374:LEU:HD23	1.48	0.95
1:B:457:LEU:HG	1:B:460:GLU:HB2	1.48	0.94
1:B:413:ILE:HD11	1:B:454:MET:O	1.67	0.94
1:A:224:ASP:HB3	1:A:227:ILE:HG13	1.49	0.94
1:B:346:LYS:HE3	1:B:382:GLU:O	1.68	0.94
1:B:688:ILE:HG13	1:B:689:LYS:NZ	1.83	0.94
1:A:6:GLU:HG2	1:A:7:TYR:H	1.31	0.93
1:A:213:HIS:O	1:A:217:VAL:HG23	1.69	0.92
1:A:203:GLU:HA	1:A:206:LEU:HD23	1.49	0.92
1:B:561:VAL:O	1:B:563:ILE:HG23	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:GLU:HA	1:B:206:LEU:HD23	1.51	0.92
1:A:633:GLY:O	1:A:634:MET:HB3	1.68	0.91
1:A:181:LEU:HD21	1:A:243:VAL:HG22	1.52	0.91
1:B:6:GLU:CG	1:B:7:TYR:H	1.83	0.90
1:A:99:ARG:O	1:A:99:ARG:HD3	1.72	0.90
1:B:181:LEU:HD21	1:B:243:VAL:HG22	1.52	0.90
1:A:427:ALA:HA	1:A:470:PHE:CE2	2.05	0.90
1:B:354:ARG:HG3	1:B:378:VAL:CG1	2.02	0.89
1:A:522:GLY:HA3	1:B:194:THR:O	1.73	0.89
1:A:11:ARG:HG3	1:A:11:ARG:HH11	1.37	0.88
1:B:99:ARG:HD3	1:B:99:ARG:O	1.73	0.88
1:A:426:GLN:HE21	1:A:430:ARG:NH2	1.70	0.88
1:A:657:THR:HA	1:A:660:ARG:HB2	1.56	0.87
1:B:123:ARG:NH2	1:B:639:ASN:HB3	1.89	0.87
1:B:5:VAL:HG13	1:B:6:GLU:N	1.90	0.87
1:B:11:ARG:HH11	1:B:11:ARG:HG3	1.40	0.86
1:A:550:MET:SD	1:A:563:ILE:HD11	2.15	0.86
1:A:454:MET:HG2	1:A:455:GLY:H	1.39	0.86
1:B:290:LYS:HB3	1:B:298:VAL:HG12	1.54	0.86
1:B:213:HIS:O	1:B:217:VAL:HG23	1.75	0.86
1:A:346:LYS:HZ1	1:A:383:THR:HA	1.41	0.86
1:B:329:ARG:HG3	1:B:374:LEU:HD23	1.57	0.86
1:B:224:ASP:HB3	1:B:227:ILE:HG13	1.58	0.86
1:A:321:TYR:O	1:A:322:VAL:HG22	1.74	0.86
1:B:164:MET:O	1:B:180:VAL:HG22	1.76	0.86
1:B:6:GLU:HG2	1:B:7:TYR:N	1.90	0.86
1:B:426:GLN:HE21	1:B:430:ARG:NH2	1.73	0.86
1:A:84:THR:HG22	1:A:85:PRO:HD2	1.58	0.85
1:A:329:ARG:HA	1:A:374:LEU:HB3	1.59	0.85
1:A:346:LYS:HE3	1:A:382:GLU:O	1.75	0.85
1:A:348:ARG:HH11	1:A:348:ARG:HB3	1.38	0.84
1:A:536:LYS:HA	1:A:539:ILE:HD12	1.58	0.84
1:B:339:SER:O	1:B:352:VAL:HG12	1.77	0.84
1:A:105:ILE:HG23	1:A:133:ILE:HG13	1.60	0.84
1:B:481:VAL:HB	1:B:483:TYR:CE2	2.13	0.84
1:A:427:ALA:HA	1:A:470:PHE:CD2	2.12	0.83
1:A:354:ARG:HG3	1:A:378:VAL:CG1	2.08	0.83
1:A:680:PRO:HB2	1:A:682:GLN:HE21	1.44	0.83
1:A:309:LEU:HA	1:A:332:SER:O	1.79	0.83
1:B:612:THR:HG21	1:B:620:VAL:HG21	1.61	0.83
1:A:6:GLU:CG	1:A:7:TYR:H	1.91	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HG23	1:B:301:ILE:HB	1.60	0.82
1:B:388:THR:HG21	1:B:397:VAL:O	1.78	0.82
1:A:411:VAL:CB	1:A:453:GLY:HA2	2.08	0.82
1:B:312:LEU:HD22	1:B:313:ALA:O	1.80	0.82
1:B:457:LEU:HG	1:B:460:GLU:CB	2.09	0.82
1:B:300:GLU:HB3	1:B:302:HIS:CE1	2.15	0.81
1:B:348:ARG:HH11	1:B:348:ARG:HB3	1.41	0.81
1:A:518:PRO:HG2	1:B:39:ILE:CG2	2.11	0.81
1:A:102:ASP:HB3	1:A:286:ILE:HD11	1.63	0.81
1:B:294:PRO:O	1:B:295:GLU:HB3	1.80	0.81
1:A:327:PHE:CE1	1:A:376:ALA:HB2	2.16	0.81
1:A:343:ASN:HD21	1:A:387:ASP:HB3	1.44	0.81
1:B:681:LYS:H	1:B:681:LYS:HD3	1.44	0.81
1:A:129:LYS:O	1:A:129:LYS:HG2	1.80	0.81
1:A:221:ALA:HB1	1:A:228:MET:HG3	1.63	0.80
1:A:157:LEU:O	1:A:639:ASN:HB2	1.81	0.80
1:A:500:GLN:C	1:A:502:GLY:H	1.82	0.80
1:A:290:LYS:HA	1:A:299:VAL:O	1.81	0.80
1:B:680:PRO:HB2	1:B:682:GLN:HE21	1.45	0.80
1:A:481:VAL:HG13	1:A:649:LEU:HD12	1.61	0.80
1:B:519:ARG:HA	1:B:562:ASP:OD2	1.81	0.80
1:B:354:ARG:HG3	1:B:378:VAL:HG12	1.64	0.79
1:A:201:ILE:HD12	1:A:201:ILE:H	1.45	0.79
1:A:457:LEU:HG	1:A:460:GLU:HB2	1.65	0.79
1:B:427:ALA:HA	1:B:470:PHE:CE2	2.18	0.79
1:B:683:VAL:O	1:B:687:LEU:HG	1.83	0.79
1:B:688:ILE:HG13	1:B:689:LYS:HZ2	1.45	0.79
1:B:91:THR:O	1:B:93:GLU:N	2.16	0.79
1:B:119:GLU:O	1:B:122:TRP:HB3	1.83	0.79
1:B:357:ARG:HG3	1:B:357:ARG:HH11	1.47	0.79
1:B:97:SER:O	1:B:101:LEU:HD22	1.83	0.79
1:A:165:GLN:HB2	1:A:178:ILE:O	1.82	0.79
1:A:166:LEU:HD21	1:A:208:GLN:HG2	1.63	0.79
1:B:411:VAL:HB	1:B:453:GLY:HA2	1.65	0.78
1:B:165:GLN:HG3	1:B:260:LEU:CD1	2.12	0.78
1:A:119:GLU:O	1:A:122:TRP:HB3	1.84	0.78
1:B:165:GLN:HB2	1:B:178:ILE:O	1.82	0.78
1:A:127:LYS:HB2	1:A:637:ARG:NH1	1.97	0.78
1:A:601:ILE:HD12	1:A:684:GLN:HG3	1.65	0.78
1:A:518:PRO:HG2	1:B:39:ILE:HG23	1.66	0.78
1:A:6:GLU:HG2	1:A:7:TYR:N	1.98	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ASP:HA	1:A:265:LYS:O	1.83	0.78
1:A:5:VAL:HG13	1:A:6:GLU:N	1.98	0.78
1:A:290:LYS:HB3	1:A:298:VAL:HG12	1.65	0.78
1:A:573:HIS:ND1	1:A:576:ASP:HB2	1.98	0.78
1:A:190:ASN:HD21	1:A:195:ASP:HB2	1.48	0.77
1:A:388:THR:HG21	1:A:397:VAL:O	1.84	0.77
1:A:506:GLN:HA	1:A:576:ASP:O	1.83	0.77
1:A:606:MET:HB2	1:A:647:VAL:O	1.84	0.77
1:A:132:ARG:NH1	1:A:132:ARG:HG2	1.99	0.77
1:A:459:LEU:N	1:A:459:LEU:HD12	1.99	0.77
1:B:276:VAL:CG1	1:B:280:LEU:HD12	2.12	0.77
1:B:38:ARG:CG	1:B:39:ILE:H	1.97	0.77
1:A:25:LYS:NZ	1:A:84:THR:OG1	2.18	0.76
1:B:290:LYS:HA	1:B:299:VAL:O	1.86	0.76
1:A:221:ALA:HB1	1:A:228:MET:CE	2.15	0.76
1:A:688:ILE:HG13	1:A:689:LYS:NZ	2.01	0.76
1:A:548:GLU:O	1:A:551:GLN:HB2	1.85	0.76
1:B:541:ALA:O	1:B:544:LYS:HB3	1.86	0.76
1:B:113:GLY:HA2	1:B:149:VAL:HG22	1.67	0.75
1:B:357:ARG:HB3	1:B:364:GLU:HB3	1.66	0.75
1:B:454:MET:HG2	1:B:455:GLY:H	1.51	0.75
1:A:340:TYR:HB2	1:A:392:GLU:OE2	1.86	0.75
1:B:517:LEU:HD22	1:B:521:SER:CB	2.15	0.75
1:B:455:GLY:O	1:B:458:HIS:HB3	1.86	0.75
1:B:345:THR:HG23	1:B:388:THR:H	1.51	0.75
1:A:346:LYS:NZ	1:A:383:THR:HA	2.01	0.75
1:B:119:GLU:OE1	1:B:666:ARG:NH1	2.19	0.75
1:A:294:PRO:O	1:A:295:GLU:HB3	1.84	0.75
1:B:454:MET:HB3	1:B:458:HIS:CD2	2.22	0.75
1:A:535:PRO:HG2	1:A:538:TYR:CD2	2.22	0.74
1:A:681:LYS:HE3	1:A:682:GLN:HE22	1.52	0.74
1:A:91:THR:O	1:A:93:GLU:N	2.20	0.74
1:B:91:THR:O	1:B:94:VAL:N	2.18	0.74
1:A:90:PHE:O	1:A:94:VAL:HG23	1.86	0.74
1:B:608:VAL:HG12	1:B:609:GLU:N	2.03	0.74
1:A:361:ASN:O	1:A:362:HIS:ND1	2.21	0.74
1:B:633:GLY:O	1:B:634:MET:HB3	1.87	0.74
1:B:319:ASP:HB2	1:B:325:LEU:HD12	1.67	0.74
1:A:605:ILE:HD11	1:A:677:GLN:HB3	1.69	0.74
1:B:276:VAL:HG13	1:B:280:LEU:CD1	2.14	0.73
1:A:91:THR:O	1:A:94:VAL:N	2.16	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:ILE:O	1:B:594:VAL:HG23	1.88	0.73
1:B:350:GLU:OE1	1:B:380:LEU:HD22	1.89	0.73
1:A:631:ILE:N	1:A:631:ILE:HD12	2.04	0.73
1:A:348:ARG:NH2	1:A:382:GLU:HG3	2.04	0.73
1:B:602:LEU:HD12	1:B:678:GLU:HA	1.69	0.73
1:A:680:PRO:HG2	1:A:683:VAL:HG23	1.71	0.73
1:A:500:GLN:O	1:A:502:GLY:N	2.21	0.73
1:B:11:ARG:NH1	1:B:11:ARG:HG3	2.03	0.73
1:A:293:THR:HG23	1:A:297:GLU:O	1.88	0.73
1:B:468:ARG:HA	1:B:468:ARG:NE	2.04	0.73
1:A:303:PRO:HA	1:A:331:TYR:O	1.87	0.73
1:B:443:HIS:ND1	1:B:450:ILE:HD11	2.04	0.73
1:B:229:LEU:H	1:B:229:LEU:CD1	2.02	0.73
1:B:201:ILE:H	1:B:201:ILE:HD12	1.54	0.73
1:B:459:LEU:HD12	1:B:459:LEU:H	1.53	0.72
1:A:190:ASN:ND2	1:A:195:ASP:HB2	2.02	0.72
1:B:500:GLN:C	1:B:502:GLY:H	1.92	0.72
1:B:605:ILE:CD1	1:B:677:GLN:HB3	2.19	0.72
1:A:680:PRO:HG2	1:A:683:VAL:CG2	2.20	0.72
1:B:606:MET:HB2	1:B:647:VAL:O	1.88	0.72
1:B:5:VAL:CG1	1:B:6:GLU:H	1.93	0.72
1:A:165:GLN:HG3	1:A:260:LEU:HD13	1.71	0.72
1:A:357:ARG:HG3	1:A:357:ARG:HH11	1.54	0.71
1:A:166:LEU:CD2	1:A:208:GLN:HG2	2.20	0.71
1:B:634:MET:C	1:B:634:MET:SD	2.69	0.71
1:B:361:ASN:O	1:B:362:HIS:ND1	2.23	0.71
1:A:413:ILE:HD11	1:A:454:MET:O	1.91	0.71
1:A:114:VAL:HG11	1:A:157:LEU:HD11	1.72	0.71
1:B:359:HIS:ND1	1:B:362:HIS:NE2	2.38	0.71
1:B:38:ARG:HG3	1:B:39:ILE:H	1.56	0.71
1:B:517:LEU:HD22	1:B:521:SER:HB3	1.71	0.71
1:A:605:ILE:CD1	1:A:677:GLN:HB3	2.20	0.70
1:A:157:LEU:C	1:A:639:ASN:HD22	1.94	0.70
1:A:500:GLN:O	1:A:501:THR:HG22	1.91	0.70
1:A:631:ILE:H	1:A:631:ILE:HD12	1.56	0.70
1:B:480:GLN:HE22	1:B:558:PHE:HZ	1.38	0.70
1:A:276:VAL:CG1	1:A:280:LEU:HD12	2.18	0.70
1:B:427:ALA:O	1:B:431:LEU:HG	1.92	0.70
1:B:554:PRO:HG2	1:B:594:VAL:HB	1.72	0.70
1:B:127:LYS:HB2	1:B:637:ARG:NH1	2.07	0.70
1:B:409:ILE:O	1:B:411:VAL:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HH22	1:A:373:ASP:CG	1.95	0.70
1:B:688:ILE:HG13	1:B:689:LYS:HZ1	1.57	0.70
1:A:524:GLU:OE1	1:A:564:LYS:HE3	1.91	0.70
1:B:191:ASP:HA	1:B:265:LYS:O	1.92	0.70
1:A:34:TYR:CD1	1:A:34:TYR:C	2.64	0.70
1:B:300:GLU:HB3	1:B:302:HIS:HE1	1.55	0.70
1:B:109:ASP:OD1	1:B:111:SER:HB2	1.92	0.70
1:A:295:GLU:HA	1:B:26:THR:OG1	1.91	0.69
1:A:459:LEU:CD1	1:A:459:LEU:H	2.03	0.69
1:A:426:GLN:HE21	1:A:430:ARG:HH21	1.38	0.69
1:A:289:ILE:HG23	1:A:301:ILE:HB	1.74	0.69
1:B:416:LYS:HA	1:B:449:THR:O	1.91	0.69
1:B:129:LYS:HG2	1:B:253:LEU:HD11	1.74	0.69
1:B:414:GLU:HB3	1:B:452:SER:HB2	1.74	0.69
1:B:354:ARG:HG3	1:B:378:VAL:HG11	1.74	0.69
1:B:120:THR:HA	1:B:123:ARG:HG3	1.74	0.69
1:A:427:ALA:HA	1:A:470:PHE:HE2	1.57	0.69
1:A:11:ARG:NH1	1:A:11:ARG:HG3	2.04	0.69
1:A:132:ARG:HH11	1:A:132:ARG:HG2	1.57	0.69
1:B:152:THR:O	1:B:155:GLU:N	2.25	0.69
1:B:84:THR:HG22	1:B:85:PRO:HD2	1.73	0.69
1:B:414:GLU:HB3	1:B:452:SER:CB	2.22	0.69
1:A:8:ASP:HB3	1:A:11:ARG:CG	2.23	0.69
1:A:191:ASP:O	1:A:192:LEU:HD23	1.93	0.69
1:A:359:HIS:ND1	1:A:362:HIS:NE2	2.40	0.69
1:A:486:THR:O	1:A:600:VAL:HG22	1.92	0.68
1:A:416:LYS:HA	1:A:449:THR:O	1.92	0.68
1:A:170:ARG:H	1:A:173:THR:HB	1.56	0.68
1:B:535:PRO:HG2	1:B:538:TYR:CD2	2.28	0.68
1:B:329:ARG:HA	1:B:374:LEU:CB	2.23	0.68
1:B:681:LYS:N	1:B:681:LYS:HD3	2.08	0.68
1:A:628:ARG:HD2	1:A:648:PRO:HG2	1.75	0.68
1:B:293:THR:HG23	1:B:297:GLU:O	1.93	0.68
1:B:96:ARG:NH2	1:B:386:GLY:HA3	2.09	0.68
1:B:427:ALA:HA	1:B:470:PHE:CD2	2.29	0.68
1:B:552:SER:O	1:B:591:LYS:HE3	1.94	0.68
1:A:184:LYS:HE2	1:A:186:TYR:OH	1.94	0.68
1:A:467:LYS:O	1:A:467:LYS:HG2	1.94	0.68
1:A:357:ARG:NH2	1:A:373:ASP:OD2	2.26	0.68
1:A:554:PRO:HG2	1:A:594:VAL:HB	1.75	0.68
1:B:26:THR:HG22	1:B:27:THR:N	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:GLU:HB2	1:B:128:TYR:OH	1.93	0.68
1:B:328:ILE:O	1:B:374:LEU:HB2	1.94	0.67
1:A:606:MET:HE3	1:A:671:MET:HG3	1.75	0.67
1:B:114:VAL:HG11	1:B:157:LEU:HD11	1.74	0.67
1:B:367:GLU:O	1:B:368:GLU:HB3	1.95	0.67
1:B:573:HIS:ND1	1:B:576:ASP:HB2	2.08	0.67
1:A:339:SER:O	1:A:352:VAL:HG12	1.94	0.67
1:B:348:ARG:CZ	1:B:382:GLU:HG3	2.25	0.67
1:A:683:VAL:O	1:A:687:LEU:HG	1.94	0.67
1:A:270:GLN:O	1:A:273:LEU:HB2	1.94	0.67
1:B:324:ARG:NH2	1:B:383:THR:O	2.28	0.67
1:A:631:ILE:CD1	1:A:631:ILE:H	2.07	0.67
1:A:415:PRO:HD2	1:A:451:ILE:O	1.94	0.67
1:B:321:TYR:O	1:B:322:VAL:CG2	2.36	0.67
1:A:322:VAL:HB	1:A:378:VAL:HG21	1.77	0.67
1:B:345:THR:CG2	1:B:388:THR:H	2.08	0.67
1:A:229:LEU:HD12	1:A:229:LEU:H	1.60	0.67
1:B:78:ARG:NH2	1:B:357:ARG:HE	1.93	0.67
1:B:549:ALA:HA	1:B:591:LYS:NZ	2.09	0.67
1:B:327:PHE:CE1	1:B:376:ALA:HB2	2.29	0.66
1:A:326:THR:O	1:A:377:VAL:HG12	1.95	0.66
1:A:608:VAL:HG22	1:A:671:MET:HB3	1.77	0.66
1:B:348:ARG:NH2	1:B:382:GLU:HG3	2.09	0.66
1:B:500:GLN:O	1:B:502:GLY:N	2.29	0.66
1:B:103:GLY:O	1:B:104:ALA:HB2	1.96	0.66
1:B:85:PRO:HG3	1:B:94:VAL:HA	1.76	0.66
1:B:680:PRO:O	1:B:683:VAL:HG23	1.94	0.66
1:A:8:ASP:HB3	1:A:11:ARG:HG2	1.78	0.66
1:A:561:VAL:O	1:A:563:ILE:HG23	1.95	0.66
1:B:165:GLN:HG3	1:B:260:LEU:HD13	1.75	0.66
1:A:609:GLU:O	1:A:669:PHE:HA	1.95	0.66
1:B:102:ASP:HB3	1:B:286:ILE:HD11	1.76	0.66
1:A:98:MET:O	1:A:101:LEU:HD23	1.96	0.66
1:B:680:PRO:HG2	1:B:683:VAL:CG2	2.25	0.66
1:B:628:ARG:HD2	1:B:648:PRO:HG2	1.77	0.66
1:A:348:ARG:NH1	1:A:348:ARG:HB3	2.09	0.66
1:A:468:ARG:HA	1:A:468:ARG:NE	2.11	0.66
1:B:616:TYR:O	1:B:618:GLY:N	2.28	0.66
1:B:657:THR:HA	1:B:660:ARG:HB2	1.77	0.66
1:B:146:LEU:O	1:B:146:LEU:HD23	1.96	0.66
1:A:669:PHE:O	1:A:670:VAL:CG2	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:LEU:HG	1:B:460:GLU:CG	2.26	0.65
1:B:485:GLU:HA	1:B:600:VAL:O	1.96	0.65
1:B:292:THR:O	1:B:398:ILE:HD12	1.96	0.65
1:B:259:PHE:CE2	1:B:275:ALA:HB1	2.31	0.65
1:A:78:ARG:NH2	1:A:357:ARG:HE	1.94	0.65
1:B:38:ARG:O	1:B:39:ILE:HG22	1.97	0.65
1:B:546:ILE:HG23	1:B:590:ILE:HG13	1.79	0.65
1:B:247:ARG:HD2	1:B:278:ASP:O	1.97	0.65
1:B:309:LEU:HG	1:B:310:ALA:N	2.10	0.65
1:A:139:MET:HE2	1:A:260:LEU:HB2	1.77	0.65
1:B:69:VAL:O	1:B:69:VAL:HG12	1.97	0.65
1:B:230:LYS:O	1:B:235:GLU:N	2.30	0.65
1:B:221:ALA:HB1	1:B:228:MET:CE	2.27	0.65
1:A:342:TYR:O	1:A:390:VAL:HG22	1.96	0.65
1:B:15:ILE:HG22	1:B:103:GLY:HA3	1.79	0.65
1:B:548:GLU:O	1:B:551:GLN:HB2	1.96	0.65
1:A:290:LYS:HB3	1:A:298:VAL:CG1	2.27	0.65
1:B:605:ILE:HD13	1:B:677:GLN:HB3	1.78	0.64
1:B:519:ARG:HG2	1:B:676:TYR:O	1.96	0.64
1:B:337:SER:OG	1:B:354:ARG:HA	1.97	0.64
1:B:137:ASN:OD1	1:B:138:LYS:N	2.28	0.64
1:A:410:ASP:O	1:A:411:VAL:HG22	1.97	0.64
1:B:603:GLU:OE2	1:B:679:VAL:HG23	1.97	0.64
1:A:354:ARG:HG3	1:A:378:VAL:HG11	1.78	0.64
1:A:201:ILE:HD12	1:A:201:ILE:N	2.13	0.64
1:A:573:HIS:O	1:A:575:VAL:N	2.31	0.64
1:A:16:GLY:N	1:A:101:LEU:HD12	2.12	0.64
1:B:426:GLN:O	1:B:427:ALA:CB	2.44	0.64
1:A:499:ARG:HG3	1:A:500:GLN:H	1.61	0.64
1:A:602:LEU:HB3	1:A:676:TYR:HD2	1.63	0.64
1:B:585:ALA:HA	1:B:588:MET:SD	2.37	0.64
1:B:105:ILE:HG12	1:B:133:ILE:HD11	1.80	0.64
1:A:19:ALA:HB3	1:A:25:LYS:HB2	1.80	0.64
1:A:157:LEU:HD12	1:A:157:LEU:N	2.12	0.64
1:B:523:PHE:CD1	1:B:524:GLU:N	2.66	0.64
1:B:348:ARG:NH1	1:B:348:ARG:HB3	2.12	0.63
1:A:367:GLU:O	1:A:368:GLU:HB3	1.98	0.63
1:A:606:MET:O	1:A:646:PHE:HA	1.97	0.63
1:B:580:MET:O	1:B:584:ILE:HD13	1.97	0.63
1:B:148:LEU:O	1:B:148:LEU:HD12	1.99	0.63
1:B:218:GLU:O	1:B:221:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:CD1	1:A:335:LEU:HB2	2.29	0.63
1:A:165:GLN:HG3	1:A:260:LEU:CD1	2.27	0.63
1:B:309:LEU:HA	1:B:332:SER:O	1.98	0.63
1:B:218:GLU:O	1:B:221:ALA:N	2.31	0.63
1:B:415:PRO:HD2	1:B:451:ILE:O	1.99	0.63
1:A:549:ALA:HA	1:A:591:LYS:NZ	2.14	0.63
1:B:342:TYR:O	1:B:390:VAL:HG22	1.98	0.63
1:A:384:ILE:C	1:A:387:ASP:OD2	2.37	0.63
1:A:604:PRO:HG2	1:A:649:LEU:HB3	1.78	0.63
1:A:164:MET:HB2	1:A:258:VAL:O	1.97	0.63
1:B:92:ILE:HD13	1:B:92:ILE:N	2.13	0.63
1:A:461:ILE:O	1:A:465:ARG:HG3	1.99	0.63
1:B:426:GLN:HE21	1:B:430:ARG:HH21	1.44	0.63
1:B:78:ARG:CZ	1:B:357:ARG:HH21	2.12	0.63
1:A:230:LYS:O	1:A:235:GLU:N	2.31	0.63
1:A:426:GLN:O	1:A:427:ALA:CB	2.47	0.62
1:A:426:GLN:O	1:A:427:ALA:HB3	1.99	0.62
1:B:221:ALA:HB1	1:B:228:MET:HG3	1.82	0.62
1:A:681:LYS:HD3	1:A:681:LYS:N	2.14	0.62
1:A:68:ALA:HB3	1:A:327:PHE:CE2	2.34	0.62
1:A:688:ILE:HG13	1:A:689:LYS:HZ2	1.63	0.62
1:B:110:SER:OG	1:B:136:ALA:HB1	1.99	0.62
1:A:526:VAL:CG1	1:A:527:ASN:N	2.62	0.62
1:A:17:ILE:HD13	1:A:28:THR:HG22	1.80	0.62
1:A:35:TYR:CE1	1:A:269:VAL:HG21	2.34	0.62
1:B:681:LYS:HE3	1:B:682:GLN:HE22	1.63	0.62
1:B:229:LEU:H	1:B:229:LEU:HD12	1.63	0.62
1:A:74:TRP:CE3	1:A:273:LEU:HD13	2.35	0.62
1:B:616:TYR:O	1:B:620:VAL:HG23	1.98	0.62
1:A:19:ALA:HB2	1:A:107:VAL:HG13	1.81	0.62
1:B:458:HIS:O	1:B:461:ILE:HB	1.98	0.62
1:A:542:VAL:HG22	1:A:582:PHE:HB3	1.80	0.62
1:A:326:THR:HB	1:A:377:VAL:HG13	1.81	0.62
1:A:96:ARG:O	1:A:100:VAL:HG22	1.99	0.62
1:A:339:SER:H	1:A:352:VAL:HG13	1.65	0.62
1:A:526:VAL:HG12	1:A:527:ASN:N	2.14	0.62
1:B:610:VAL:HG22	1:B:669:PHE:CB	2.30	0.62
1:B:550:MET:SD	1:B:563:ILE:HD11	2.40	0.62
1:B:689:LYS:NZ	1:B:689:LYS:HB2	2.15	0.62
1:A:99:ARG:NE	1:A:289:ILE:HD12	2.14	0.62
1:B:157:LEU:O	1:B:639:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:GLN:HA	1:B:576:ASP:O	2.00	0.62
1:B:218:GLU:O	1:B:221:ALA:CB	2.48	0.62
1:B:457:LEU:CG	1:B:460:GLU:HB2	2.25	0.61
1:B:681:LYS:CD	1:B:681:LYS:H	2.13	0.61
1:A:590:ILE:O	1:A:592:GLU:N	2.33	0.61
1:A:103:GLY:O	1:A:104:ALA:HB2	1.99	0.61
1:B:319:ASP:HB2	1:B:325:LEU:CD1	2.29	0.61
1:B:685:GLU:O	1:B:688:ILE:HG12	2.00	0.61
1:B:689:LYS:HB2	1:B:689:LYS:HZ3	1.65	0.61
1:B:441:SER:HB3	1:B:450:ILE:HG13	1.82	0.61
1:A:229:LEU:CD1	1:A:229:LEU:H	2.13	0.61
1:B:467:LYS:O	1:B:467:LYS:HG2	2.00	0.61
1:A:215:LYS:O	1:A:219:VAL:HG23	2.00	0.61
1:A:120:THR:HA	1:A:123:ARG:HG3	1.83	0.61
1:B:262:SER:OG	1:B:265:LYS:HB2	2.01	0.61
1:A:247:ARG:HG2	1:A:251:ILE:HD11	1.82	0.61
1:A:454:MET:HG2	1:A:455:GLY:N	2.11	0.61
1:B:427:ALA:HA	1:B:470:PHE:HE2	1.64	0.61
1:B:521:SER:O	1:B:562:ASP:OD1	2.18	0.61
1:B:439:ARG:HB2	1:B:439:ARG:HH11	1.65	0.61
1:B:98:MET:O	1:B:101:LEU:HD23	2.00	0.61
1:A:220:ALA:O	1:A:221:ALA:C	2.35	0.61
1:B:481:VAL:HG13	1:B:649:LEU:HD12	1.81	0.61
1:A:123:ARG:NH2	1:A:639:ASN:HB3	2.15	0.61
1:A:140:ASP:HA	1:A:171:GLU:O	2.01	0.61
1:A:409:ILE:O	1:A:411:VAL:N	2.32	0.61
1:A:634:MET:O	1:A:634:MET:HE3	2.00	0.61
1:B:538:TYR:O	1:B:541:ALA:N	2.30	0.61
1:B:129:LYS:O	1:B:129:LYS:HG2	2.00	0.61
1:A:552:SER:O	1:A:591:LYS:HE3	2.00	0.61
1:A:159:ALA:O	1:A:161:PRO:HD3	2.00	0.61
1:B:303:PRO:HA	1:B:331:TYR:O	1.99	0.61
1:B:457:LEU:HA	1:B:460:GLU:HB2	1.82	0.61
1:A:68:ALA:HB2	1:A:317:MET:SD	2.40	0.61
1:A:500:GLN:C	1:A:502:GLY:N	2.52	0.61
1:A:653:PHE:O	1:A:655:TYR:N	2.33	0.61
1:A:671:MET:C	1:A:672:PHE:HD1	2.04	0.61
1:A:247:ARG:HD2	1:A:278:ASP:O	2.01	0.61
1:A:632:LEU:HG	1:A:644:ARG:O	2.00	0.61
1:B:411:VAL:CB	1:B:453:GLY:CA	2.57	0.61
1:A:457:LEU:HG	1:A:460:GLU:CB	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLU:C	1:A:470:PHE:HD1	2.04	0.61
1:A:354:ARG:HG3	1:A:378:VAL:HG12	1.83	0.61
1:A:129:LYS:HG2	1:A:253:LEU:HD11	1.83	0.61
1:A:572:TYR:HD1	1:A:572:TYR:N	1.97	0.61
1:A:411:VAL:O	1:A:411:VAL:HG23	1.99	0.61
1:A:218:GLU:O	1:A:221:ALA:HB3	2.01	0.61
1:B:346:LYS:HZ1	1:B:383:THR:HA	1.66	0.61
1:A:669:PHE:O	1:A:670:VAL:HG22	1.99	0.61
1:A:343:ASN:ND2	1:A:387:ASP:HB3	2.15	0.60
1:A:122:TRP:CD2	1:A:157:LEU:HD23	2.35	0.60
1:B:558:PHE:O	1:B:559:PRO:C	2.39	0.60
1:B:156:ARG:HB3	1:B:666:ARG:HH12	1.66	0.60
1:B:35:TYR:CZ	1:B:269:VAL:HG21	2.36	0.60
1:A:219:VAL:O	1:A:220:ALA:C	2.39	0.60
1:A:221:ALA:HB1	1:A:228:MET:HE3	1.83	0.60
1:A:262:SER:OG	1:A:265:LYS:HB2	2.02	0.60
1:B:496:LYS:CG	1:B:509:HIS:ND1	2.64	0.60
1:B:608:VAL:CG1	1:B:609:GLU:N	2.65	0.60
1:B:501:THR:HG22	1:B:504:ARG:O	2.02	0.60
1:A:443:HIS:ND1	1:A:450:ILE:HD11	2.17	0.60
1:A:17:ILE:HD13	1:A:28:THR:CG2	2.31	0.60
1:B:69:VAL:HG21	1:B:314:PHE:HZ	1.66	0.60
1:B:87:HIS:CE1	1:B:90:PHE:HB2	2.36	0.60
1:A:348:ARG:CZ	1:A:382:GLU:HG3	2.30	0.60
1:A:85:PRO:HG3	1:A:94:VAL:HA	1.83	0.60
1:A:601:ILE:CD1	1:A:684:GLN:HG3	2.32	0.60
1:B:121:VAL:O	1:B:124:GLN:HB2	2.02	0.60
1:A:215:LYS:O	1:A:218:GLU:HB3	2.01	0.60
1:A:132:ARG:HH11	1:A:132:ARG:CG	2.11	0.60
1:A:340:TYR:CE1	1:A:351:ARG:HB2	2.37	0.60
1:A:38:ARG:CG	1:A:39:ILE:H	2.15	0.60
1:A:286:ILE:H	1:A:286:ILE:HD12	1.65	0.60
1:A:602:LEU:HD12	1:A:678:GLU:HA	1.84	0.60
1:B:456:GLU:C	1:B:458:HIS:H	2.05	0.60
1:B:679:VAL:O	1:B:679:VAL:CG1	2.49	0.60
1:A:295:GLU:HA	1:B:26:THR:CB	2.31	0.60
1:A:603:GLU:OE2	1:A:648:PRO:HB3	2.01	0.60
1:A:89:ASP:N	1:A:89:ASP:OD1	2.31	0.60
1:B:604:PRO:HG2	1:B:649:LEU:HB3	1.83	0.60
1:A:518:PRO:HG2	1:B:39:ILE:HG21	1.84	0.59
1:B:309:LEU:HD23	1:B:309:LEU:C	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HG12	1:B:92:ILE:O	2.01	0.59
1:A:631:ILE:HA	1:A:645:ALA:HB2	1.84	0.59
1:B:325:LEU:HD23	1:B:378:VAL:HG23	1.84	0.59
1:B:90:PHE:O	1:B:94:VAL:HG23	2.01	0.59
1:A:538:TYR:O	1:A:541:ALA:N	2.35	0.59
1:B:13:ARG:HH11	1:B:13:ARG:HG2	1.67	0.59
1:A:204:GLU:OE1	1:A:204:GLU:N	2.35	0.59
1:A:121:VAL:O	1:A:124:GLN:HB2	2.02	0.59
1:A:634:MET:HB2	1:A:642:VAL:O	2.02	0.59
1:A:572:TYR:CD1	1:A:572:TYR:N	2.69	0.59
1:A:171:GLU:HG3	1:A:172:ASP:H	1.66	0.59
1:B:247:ARG:HG2	1:B:251:ILE:HD11	1.85	0.59
1:B:260:LEU:C	1:B:260:LEU:HD22	2.23	0.59
1:B:613:PRO:HG3	1:B:666:ARG:HE	1.67	0.59
1:A:101:LEU:HD23	1:A:101:LEU:H	1.66	0.59
1:A:31:ARG:O	1:A:32:ILE:C	2.38	0.59
1:A:327:PHE:CD1	1:A:376:ALA:HB2	2.37	0.59
1:A:165:GLN:CB	1:A:178:ILE:O	2.50	0.59
1:B:78:ARG:CZ	1:B:357:ARG:HE	2.16	0.59
1:A:497:PHE:CG	1:A:584:ILE:HG21	2.37	0.59
1:A:357:ARG:HB3	1:A:364:GLU:HB3	1.83	0.59
1:B:122:TRP:CD2	1:B:157:LEU:HD23	2.38	0.59
1:B:499:ARG:HG3	1:B:500:GLN:H	1.66	0.59
1:B:340:TYR:CE1	1:B:351:ARG:HB2	2.37	0.59
1:B:340:TYR:HB2	1:B:392:GLU:OE2	2.03	0.59
1:B:229:LEU:N	1:B:229:LEU:HD12	2.17	0.59
1:A:122:TRP:CE2	1:A:157:LEU:HD23	2.38	0.59
1:B:443:HIS:O	1:B:448:GLN:N	2.35	0.58
1:B:290:LYS:HB3	1:B:298:VAL:CG1	2.30	0.58
1:B:627:ARG:NH2	1:B:658:ASP:OD2	2.36	0.58
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.67	0.58
1:B:563:ILE:HG13	1:B:563:ILE:O	2.04	0.58
1:B:350:GLU:OE1	1:B:380:LEU:CD2	2.51	0.58
1:A:487:ILE:HD12	1:A:489:LYS:O	2.02	0.58
1:B:439:ARG:HB2	1:B:439:ARG:NH1	2.17	0.58
1:A:90:PHE:O	1:A:91:THR:O	2.21	0.58
1:A:455:GLY:O	1:A:459:LEU:CD1	2.51	0.58
1:A:181:LEU:HD21	1:A:243:VAL:CG2	2.29	0.58
1:A:345:THR:HG22	1:A:398:ILE:HG22	1.85	0.58
1:B:457:LEU:HG	1:B:460:GLU:HG2	1.85	0.58
1:B:534:ILE:HD12	1:B:582:PHE:HE2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:CD1	1:A:157:LEU:N	2.66	0.58
1:B:322:VAL:HB	1:B:378:VAL:HG21	1.84	0.58
1:B:468:ARG:HH11	1:B:468:ARG:HG2	1.68	0.58
1:B:681:LYS:HA	1:B:684:GLN:HB3	1.86	0.58
1:B:494:GLU:HG3	1:B:509:HIS:CE1	2.39	0.58
1:A:573:HIS:ND1	1:A:576:ASP:OD2	2.37	0.58
1:A:305:PRO:O	1:A:333:GLY:HA2	2.02	0.58
1:B:6:GLU:CG	1:B:7:TYR:N	2.53	0.58
1:A:69:VAL:HG21	1:A:314:PHE:HZ	1.68	0.58
1:B:259:PHE:CE2	1:B:275:ALA:CB	2.86	0.57
1:A:189:GLY:HA3	1:A:195:ASP:CG	2.23	0.57
1:A:616:TYR:O	1:A:618:GLY:N	2.38	0.57
1:A:26:THR:HG22	1:A:27:THR:N	2.18	0.57
1:A:443:HIS:O	1:A:448:GLN:N	2.36	0.57
1:A:580:MET:O	1:A:584:ILE:HD13	2.03	0.57
1:B:339:SER:H	1:B:352:VAL:HG13	1.68	0.57
1:A:277:VAL:HG22	1:A:278:ASP:N	2.19	0.57
1:A:481:VAL:HB	1:A:483:TYR:CE2	2.39	0.57
1:B:434:GLU:HG2	1:B:434:GLU:O	2.05	0.57
1:A:519:ARG:HA	1:A:562:ASP:OD2	2.05	0.57
1:A:681:LYS:CE	1:A:682:GLN:HE22	2.18	0.57
1:A:201:ILE:H	1:A:201:ILE:CD1	2.16	0.57
1:A:631:ILE:HA	1:A:645:ALA:CB	2.33	0.57
1:B:331:TYR:O	1:B:371:ALA:HB1	2.04	0.57
1:A:324:ARG:NH2	1:A:383:THR:O	2.35	0.57
1:B:235:GLU:O	1:B:237:PRO:HD3	2.04	0.57
1:B:560:VAL:O	1:B:561:VAL:HG13	2.04	0.57
1:B:658:ASP:O	1:B:662:LYS:HG2	2.05	0.57
1:A:273:LEU:O	1:A:276:VAL:N	2.38	0.57
1:B:432:ALA:HA	1:B:438:PHE:HZ	1.69	0.57
1:A:228:MET:O	1:A:231:TYR:HB3	2.04	0.57
1:B:416:LYS:HD3	1:B:416:LYS:C	2.25	0.57
1:A:523:PHE:HE1	1:A:565:VAL:HG23	1.69	0.57
1:A:681:LYS:H	1:A:681:LYS:HD3	1.68	0.57
1:A:542:VAL:CG2	1:A:582:PHE:HB3	2.35	0.57
1:B:636:PRO:HB3	1:B:641:GLN:OE1	2.05	0.57
1:A:240:GLU:CD	1:A:240:GLU:H	2.08	0.57
1:A:152:THR:O	1:A:155:GLU:N	2.38	0.57
1:B:426:GLN:O	1:B:427:ALA:HB3	2.04	0.57
1:B:606:MET:O	1:B:646:PHE:HA	2.03	0.57
1:A:443:HIS:HB2	1:A:450:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASP:O	1:A:662:LYS:HG2	2.05	0.57
1:A:613:PRO:HG3	1:A:666:ARG:HE	1.69	0.57
1:A:416:LYS:O	1:A:449:THR:HG22	2.05	0.57
1:A:439:ARG:HH11	1:A:439:ARG:HB2	1.70	0.57
1:B:549:ALA:O	1:B:551:GLN:N	2.38	0.56
1:A:139:MET:CE	1:A:260:LEU:HB2	2.35	0.56
1:A:631:ILE:N	1:A:631:ILE:CD1	2.67	0.56
1:A:416:LYS:HD3	1:A:416:LYS:C	2.25	0.56
1:A:95:GLU:HB2	1:A:128:TYR:OH	2.04	0.56
1:B:85:PRO:HG3	1:B:94:VAL:HG22	1.87	0.56
1:A:634:MET:C	1:A:634:MET:SD	2.84	0.56
1:B:289:ILE:CG2	1:B:301:ILE:HB	2.33	0.56
1:A:456:GLU:O	1:A:458:HIS:N	2.38	0.56
1:A:458:HIS:CE1	1:A:462:ILE:HD11	2.40	0.56
1:A:458:HIS:HA	1:A:461:ILE:CD1	2.35	0.56
1:B:602:LEU:HB3	1:B:676:TYR:HD2	1.70	0.56
1:B:592:GLU:O	1:B:595:GLN:HG2	2.05	0.56
1:B:523:PHE:CZ	1:B:525:PHE:HB2	2.40	0.56
1:B:123:ARG:HH22	1:B:639:ASN:HB3	1.67	0.56
1:B:608:VAL:HG21	1:B:647:VAL:CG1	2.35	0.56
1:A:309:LEU:HD23	1:A:309:LEU:C	2.26	0.56
1:B:500:GLN:O	1:B:501:THR:HG22	2.05	0.56
1:B:118:SER:O	1:B:121:VAL:HB	2.04	0.56
1:A:517:LEU:HB2	1:A:562:ASP:C	2.26	0.56
1:B:526:VAL:CG1	1:B:527:ASN:N	2.68	0.56
1:B:17:ILE:HG22	1:B:17:ILE:O	2.05	0.56
1:B:524:GLU:OE1	1:B:564:LYS:HE3	2.05	0.56
1:A:672:PHE:CD1	1:A:672:PHE:N	2.74	0.56
1:A:448:GLN:O	1:A:449:THR:CB	2.53	0.56
1:B:457:LEU:CA	1:B:460:GLU:HB2	2.35	0.56
1:B:468:ARG:HG2	1:B:468:ARG:NH1	2.21	0.56
1:A:439:ARG:NH1	1:A:439:ARG:HB2	2.20	0.56
1:B:411:VAL:HG23	1:B:411:VAL:O	2.06	0.56
1:B:517:LEU:HD23	1:B:518:PRO:HD2	1.87	0.56
1:B:601:ILE:HD12	1:B:684:GLN:HG3	1.88	0.56
1:A:300:GLU:HB3	1:A:302:HIS:CE1	2.41	0.56
1:A:457:LEU:C	1:A:460:GLU:H	2.09	0.56
1:A:292:THR:HB	1:A:398:ILE:HD12	1.87	0.56
1:A:431:LEU:CD1	1:A:466:LEU:HD12	2.36	0.56
1:A:220:ALA:HB1	1:A:227:ILE:HD12	1.87	0.56
1:B:220:ALA:O	1:B:221:ALA:C	2.43	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:O	1:A:377:VAL:HG22	2.06	0.56
1:A:114:VAL:HG11	1:A:157:LEU:CD1	2.36	0.55
1:B:101:LEU:HD23	1:B:101:LEU:H	1.71	0.55
1:B:228:MET:O	1:B:231:TYR:N	2.39	0.55
1:B:526:VAL:HG12	1:B:527:ASN:N	2.20	0.55
1:A:247:ARG:NH1	1:A:251:ILE:HD11	2.22	0.55
1:A:129:LYS:O	1:A:129:LYS:CG	2.53	0.55
1:A:38:ARG:O	1:A:39:ILE:HG22	2.06	0.55
1:B:98:MET:HA	1:B:101:LEU:CD2	2.36	0.55
1:A:6:GLU:CG	1:A:7:TYR:N	2.59	0.55
1:A:5:VAL:HG22	1:A:6:GLU:N	2.22	0.55
1:A:114:VAL:CG1	1:A:157:LEU:HD11	2.36	0.55
1:A:688:ILE:HG13	1:A:689:LYS:HZ1	1.70	0.55
1:B:36:THR:HG22	1:B:74:TRP:HB2	1.89	0.55
1:B:431:LEU:HD11	1:B:466:LEU:HD12	1.89	0.55
1:B:549:ALA:O	1:B:550:MET:C	2.43	0.55
1:A:164:MET:O	1:A:180:VAL:HG22	2.06	0.55
1:B:432:ALA:HA	1:B:438:PHE:CZ	2.41	0.55
1:A:15:ILE:HG22	1:A:103:GLY:HA3	1.89	0.55
1:B:486:THR:OG1	1:B:561:VAL:O	2.23	0.55
1:B:496:LYS:HG2	1:B:509:HIS:ND1	2.21	0.55
1:B:636:PRO:HA	1:B:641:GLN:HG2	1.89	0.55
1:A:9:LEU:HD12	1:A:12:LEU:HD13	1.88	0.55
1:A:343:ASN:HD22	1:A:389:LEU:HD11	1.71	0.55
1:A:634:MET:HB2	1:A:643:ILE:HA	1.89	0.55
1:A:677:GLN:O	1:A:678:GLU:O	2.24	0.55
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.72	0.55
1:B:85:PRO:CG	1:B:94:VAL:HG22	2.37	0.54
1:B:616:TYR:C	1:B:618:GLY:H	2.09	0.54
1:B:410:ASP:O	1:B:411:VAL:HG22	2.07	0.54
1:B:295:GLU:O	1:B:295:GLU:HG3	2.07	0.54
1:A:84:THR:CG2	1:A:85:PRO:HD2	2.34	0.54
1:B:605:ILE:HD11	1:B:677:GLN:HB3	1.89	0.54
1:B:608:VAL:HG21	1:B:647:VAL:HG11	1.89	0.54
1:B:610:VAL:HG22	1:B:669:PHE:HB3	1.89	0.54
1:B:38:ARG:CG	1:B:39:ILE:N	2.69	0.54
1:A:133:ILE:HG23	1:A:280:LEU:HD21	1.90	0.54
1:A:431:LEU:HD11	1:A:466:LEU:HD12	1.90	0.54
1:A:322:VAL:HG21	1:A:325:LEU:HD21	1.89	0.54
1:A:309:LEU:HG	1:A:310:ALA:N	2.22	0.54
1:B:357:ARG:CB	1:B:364:GLU:HB3	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:C	1:A:267:LYS:HG2	2.28	0.54
1:B:277:VAL:HG22	1:B:278:ASP:N	2.22	0.54
1:A:276:VAL:HG13	1:A:280:LEU:CD1	2.25	0.54
1:A:608:VAL:HG22	1:A:671:MET:CB	2.37	0.54
1:B:637:ARG:HG3	1:B:637:ARG:O	2.06	0.54
1:B:204:GLU:N	1:B:204:GLU:OE1	2.41	0.54
1:A:92:ILE:O	1:A:92:ILE:HG12	2.07	0.54
1:B:486:THR:O	1:B:600:VAL:HG22	2.08	0.54
1:A:35:TYR:CZ	1:A:269:VAL:HG21	2.43	0.54
1:A:343:ASN:HB2	1:A:389:LEU:HD12	1.90	0.54
1:A:434:GLU:O	1:A:435:ASP:CB	2.48	0.54
1:B:585:ALA:O	1:B:588:MET:HB2	2.08	0.54
1:B:356:LEU:HD23	1:B:365:GLU:HA	1.90	0.54
1:A:312:LEU:HD22	1:A:313:ALA:O	2.07	0.54
1:A:224:ASP:HB3	1:A:227:ILE:CG1	2.32	0.54
1:A:523:PHE:HE1	1:A:565:VAL:CG2	2.21	0.54
1:B:159:ALA:O	1:B:161:PRO:HD3	2.08	0.54
1:A:156:ARG:HB3	1:A:666:ARG:HH12	1.73	0.54
1:B:535:PRO:HB2	1:B:537:GLU:OE1	2.08	0.54
1:B:536:LYS:HA	1:B:539:ILE:HD12	1.90	0.54
1:B:534:ILE:HG23	1:B:582:PHE:CE2	2.43	0.54
1:B:17:ILE:HD13	1:B:28:THR:HG22	1.87	0.54
1:B:631:ILE:HD12	1:B:631:ILE:H	1.73	0.54
1:B:342:TYR:OH	1:B:347:GLY:HA2	2.07	0.54
1:A:272:LEU:O	1:A:276:VAL:HG23	2.08	0.54
1:A:357:ARG:CB	1:A:364:GLU:HB3	2.38	0.54
1:B:680:PRO:CB	1:B:682:GLN:HE21	2.16	0.54
1:A:679:VAL:CG1	1:A:679:VAL:O	2.54	0.54
1:B:247:ARG:HD2	1:B:279:TYR:HA	1.90	0.53
1:B:19:ALA:HB2	1:B:107:VAL:CG1	2.38	0.53
1:B:11:ARG:HA	1:B:77:HIS:HD2	1.73	0.53
1:B:634:MET:HB2	1:B:642:VAL:O	2.08	0.53
1:A:78:ARG:CZ	1:A:357:ARG:HE	2.21	0.53
1:B:443:HIS:ND1	1:B:450:ILE:CD1	2.71	0.53
1:A:504:ARG:HH11	1:A:504:ARG:HG2	1.72	0.53
1:A:507:TYR:N	1:A:576:ASP:O	2.41	0.53
1:A:584:ILE:HG22	1:A:585:ALA:N	2.23	0.53
1:B:99:ARG:C	1:B:99:ARG:HD3	2.27	0.53
1:A:127:LYS:HE2	1:A:637:ARG:NH2	2.22	0.53
1:A:610:VAL:HA	1:A:669:PHE:HA	1.90	0.53
1:A:361:ASN:O	1:A:362:HIS:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:636:PRO:HB3	1:A:641:GLN:OE1	2.08	0.53
1:A:494:GLU:HB2	1:A:511:LYS:HG2	1.90	0.53
1:B:147:TRP:O	1:B:151:ARG:HB2	2.08	0.53
1:B:5:VAL:HG22	1:B:6:GLU:N	2.23	0.53
1:B:549:ALA:HA	1:B:591:LYS:HZ3	1.74	0.53
1:B:220:ALA:HB1	1:B:227:ILE:HD12	1.90	0.53
1:A:391:GLY:O	1:A:393:ASP:N	2.40	0.53
1:A:381:LYS:O	1:A:382:GLU:HB2	2.08	0.53
1:B:679:VAL:HG13	1:B:683:VAL:HB	1.90	0.53
1:A:652:MET:O	1:A:652:MET:HG3	2.09	0.53
1:B:542:VAL:HG22	1:B:582:PHE:HB3	1.91	0.53
1:A:229:LEU:N	1:A:229:LEU:HD12	2.21	0.53
1:B:271:LEU:O	1:B:274:ASP:N	2.40	0.53
1:B:38:ARG:HG3	1:B:39:ILE:N	2.23	0.53
1:B:346:LYS:NZ	1:B:383:THR:HA	2.23	0.53
1:B:114:VAL:O	1:B:114:VAL:HG12	2.08	0.53
1:B:221:ALA:HB1	1:B:228:MET:HE3	1.91	0.53
1:A:119:GLU:OE1	1:A:666:ARG:NH1	2.41	0.53
1:A:170:ARG:N	1:A:173:THR:HB	2.23	0.53
1:B:610:VAL:HG22	1:B:669:PHE:HB2	1.90	0.53
1:A:343:ASN:OD1	1:A:346:LYS:HB2	2.08	0.53
1:A:525:PHE:CE1	1:A:543:GLN:NE2	2.76	0.53
1:A:679:VAL:HG22	1:A:683:VAL:HG21	1.91	0.53
1:B:168:ILE:HD11	1:B:178:ILE:HD11	1.90	0.53
1:B:392:GLU:O	1:B:392:GLU:HG3	2.08	0.53
1:B:384:ILE:C	1:B:387:ASP:OD2	2.48	0.53
1:A:525:PHE:HB3	1:B:197:ARG:HB3	1.90	0.53
1:B:504:ARG:HH11	1:B:504:ARG:HG2	1.73	0.53
1:B:34:TYR:CD1	1:B:34:TYR:C	2.77	0.53
1:B:684:GLN:O	1:B:688:ILE:HG23	2.09	0.53
1:B:357:ARG:HG3	1:B:357:ARG:NH1	2.19	0.53
1:A:608:VAL:HG12	1:A:609:GLU:N	2.23	0.53
1:A:410:ASP:O	1:A:411:VAL:CG2	2.57	0.53
1:A:657:THR:CA	1:A:660:ARG:HB2	2.33	0.53
1:A:106:VAL:O	1:A:134:ALA:HA	2.09	0.53
1:A:301:ILE:HG22	1:A:301:ILE:O	2.08	0.52
1:A:636:PRO:HA	1:A:641:GLN:HG2	1.91	0.52
1:A:13:ARG:HH11	1:A:13:ARG:HG2	1.73	0.52
1:B:182:ARG:HH11	1:B:239:GLU:CD	2.11	0.52
1:B:182:ARG:NH1	1:B:239:GLU:OE2	2.43	0.52
1:B:374:LEU:O	1:B:374:LEU:HD12	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:HD12	1:B:242:LEU:HD23	1.92	0.52
1:A:252:ASP:O	1:A:253:LEU:HB2	2.09	0.52
1:B:355:LEU:HD23	1:B:377:VAL:HA	1.89	0.52
1:B:434:GLU:O	1:B:435:ASP:CB	2.46	0.52
1:B:469:GLU:C	1:B:470:PHE:HD1	2.13	0.52
1:B:454:MET:HG2	1:B:455:GLY:N	2.23	0.52
1:A:458:HIS:HA	1:A:461:ILE:HG13	1.92	0.52
1:B:519:ARG:CA	1:B:562:ASP:OD2	2.56	0.52
1:B:681:LYS:O	1:B:685:GLU:HB2	2.10	0.52
1:A:486:THR:HG22	1:A:487:ILE:O	2.10	0.52
1:A:450:ILE:O	1:A:450:ILE:HG13	2.09	0.52
1:B:431:LEU:CD1	1:B:466:LEU:HD12	2.40	0.52
1:B:517:LEU:CD2	1:B:518:PRO:HD2	2.39	0.52
1:A:178:ILE:HD13	1:A:185:ALA:HB2	1.91	0.52
1:A:17:ILE:CD1	1:A:28:THR:HG22	2.40	0.52
1:B:319:ASP:CG	1:B:320:PRO:HD2	2.30	0.52
1:A:203:GLU:HA	1:A:206:LEU:CD2	2.31	0.52
1:B:629:GLY:HA2	1:B:646:PHE:O	2.09	0.52
1:A:221:ALA:CB	1:A:228:MET:HG3	2.37	0.52
1:A:326:THR:O	1:A:377:VAL:CG1	2.58	0.52
1:B:321:TYR:C	1:B:322:VAL:HG13	2.29	0.52
1:A:82:ILE:HD12	1:A:101:LEU:HB3	1.91	0.52
1:A:373:ASP:C	1:A:374:LEU:HG	2.30	0.52
1:A:646:PHE:CZ	1:A:674:ASP:OD2	2.63	0.52
1:B:78:ARG:NH2	1:B:357:ARG:HH21	2.08	0.52
1:B:361:ASN:O	1:B:362:HIS:CB	2.57	0.52
1:A:148:LEU:HD12	1:A:148:LEU:O	2.10	0.52
1:B:312:LEU:CD2	1:B:313:ALA:O	2.54	0.51
1:B:96:ARG:O	1:B:100:VAL:HG22	2.10	0.51
1:B:335:LEU:HG	1:B:335:LEU:O	2.05	0.51
1:B:114:VAL:HG11	1:B:157:LEU:CD1	2.40	0.51
1:B:219:VAL:HG12	1:B:223:PHE:HE2	1.75	0.51
1:B:672:PHE:N	1:B:672:PHE:CD1	2.78	0.51
1:A:597:GLY:O	1:A:598:ASP:C	2.48	0.51
1:A:410:ASP:C	1:A:411:VAL:HG22	2.31	0.51
1:A:344:THR:C	1:A:346:LYS:H	2.13	0.51
1:B:391:GLY:O	1:B:393:ASP:N	2.43	0.51
1:B:428:LEU:O	1:B:432:ALA:HB2	2.11	0.51
1:A:99:ARG:HD3	1:A:99:ARG:C	2.28	0.51
1:A:325:LEU:HD23	1:A:378:VAL:HG23	1.92	0.51
1:A:69:VAL:HG12	1:A:69:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:O	1:A:114:VAL:HG12	2.09	0.51
1:B:129:LYS:CG	1:B:129:LYS:O	2.59	0.51
1:A:626:ALA:C	1:A:628:ARG:H	2.13	0.51
1:A:590:ILE:O	1:A:591:LYS:C	2.49	0.51
1:A:411:VAL:CB	1:A:453:GLY:HA3	2.33	0.51
1:B:274:ASP:O	1:B:278:ASP:HB2	2.11	0.51
1:B:7:TYR:C	1:B:7:TYR:CD1	2.83	0.51
1:A:97:SER:O	1:A:101:LEU:HD22	2.10	0.51
1:B:211:GLU:OE2	1:B:215:LYS:HE3	2.10	0.51
1:B:481:VAL:HB	1:B:483:TYR:CZ	2.45	0.51
1:B:20:HIS:CG	1:B:21:ILE:H	2.28	0.51
1:A:91:THR:O	1:A:92:ILE:C	2.49	0.51
1:A:669:PHE:C	1:A:670:VAL:HG23	2.31	0.51
1:A:411:VAL:CB	1:A:453:GLY:CA	2.63	0.51
1:B:352:VAL:HG23	1:B:377:VAL:HG23	1.93	0.51
1:A:272:LEU:O	1:A:275:ALA:HB3	2.11	0.51
1:B:608:VAL:O	1:B:644:ARG:HA	2.10	0.51
1:A:291:GLY:H	1:A:299:VAL:H	1.57	0.51
1:B:138:LYS:O	1:B:140:ASP:N	2.43	0.51
1:B:13:ARG:HG2	1:B:13:ARG:NH1	2.25	0.51
1:B:322:VAL:HG21	1:B:325:LEU:HD21	1.92	0.51
1:B:170:ARG:H	1:B:173:THR:HB	1.75	0.51
1:A:182:ARG:HB2	1:A:184:LYS:HD3	1.93	0.51
1:A:427:ALA:O	1:A:431:LEU:HG	2.11	0.51
1:B:485:GLU:OE2	1:B:556:ILE:CG1	2.59	0.51
1:A:501:THR:HG22	1:A:504:ARG:O	2.11	0.51
1:A:558:PHE:O	1:A:559:PRO:C	2.47	0.51
1:B:19:ALA:HB3	1:B:25:LYS:HB2	1.93	0.51
1:B:457:LEU:C	1:B:460:GLU:H	2.13	0.51
1:A:541:ALA:O	1:A:544:LYS:HB3	2.11	0.51
1:B:534:ILE:HD12	1:B:582:PHE:CE2	2.45	0.51
1:A:539:ILE:HB	1:A:540:PRO:HD3	1.93	0.50
1:B:649:LEU:O	1:B:652:MET:HB3	2.11	0.50
1:B:428:LEU:HA	1:B:431:LEU:HB2	1.93	0.50
1:B:286:ILE:HD12	1:B:286:ILE:N	2.26	0.50
1:A:493:VAL:HG21	1:A:593:ALA:HB2	1.92	0.50
1:B:189:GLY:HA3	1:B:195:ASP:CG	2.32	0.50
1:A:295:GLU:HA	1:B:26:THR:HB	1.93	0.50
1:B:190:ASN:ND2	1:B:195:ASP:HB2	2.26	0.50
1:B:94:VAL:HG11	1:B:124:GLN:OE1	2.11	0.50
1:B:680:PRO:HG2	1:B:683:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LYS:HG2	1:B:449:THR:HB	1.94	0.50
1:B:590:ILE:HG22	1:B:591:LYS:N	2.26	0.50
1:A:590:ILE:C	1:A:592:GLU:N	2.64	0.50
1:A:135:PHE:HE2	1:A:137:ASN:ND2	2.10	0.50
1:B:330:VAL:CG1	1:B:371:ALA:HA	2.41	0.50
1:B:630:GLN:HB2	1:B:646:PHE:HB2	1.93	0.50
1:A:157:LEU:O	1:A:639:ASN:CB	2.55	0.50
1:A:336:THR:HG22	1:A:368:GLU:HB3	1.94	0.50
1:B:621:ILE:O	1:B:625:ASN:HB2	2.12	0.50
1:B:608:VAL:CG2	1:B:647:VAL:CG1	2.89	0.50
1:A:137:ASN:OD1	1:A:138:LYS:N	2.42	0.50
1:B:82:ILE:HD12	1:B:101:LEU:HB3	1.93	0.50
1:A:312:LEU:CD2	1:A:313:ALA:N	2.75	0.50
1:B:485:GLU:OE2	1:B:556:ILE:HG13	2.12	0.50
1:A:109:ASP:OD1	1:A:111:SER:HB2	2.10	0.50
1:A:274:ASP:O	1:A:278:ASP:HB2	2.12	0.50
1:A:543:GLN:HE22	1:B:199:ILE:HG22	1.76	0.50
1:B:508:GLY:O	1:B:585:ALA:HB2	2.12	0.50
1:A:85:PRO:HG3	1:A:94:VAL:HG22	1.93	0.49
1:A:468:ARG:HH11	1:A:468:ARG:HG2	1.77	0.49
1:A:123:ARG:O	1:A:126:GLU:HB3	2.12	0.49
1:B:112:GLN:O	1:B:113:GLY:C	2.51	0.49
1:B:573:HIS:ND1	1:B:576:ASP:OD2	2.45	0.49
1:A:145:ASP:O	1:A:148:LEU:HB3	2.12	0.49
1:B:270:GLN:O	1:B:273:LEU:N	2.41	0.49
1:B:34:TYR:OH	1:B:38:ARG:NH2	2.45	0.49
1:A:312:LEU:HD23	1:A:387:ASP:O	2.12	0.49
1:A:458:HIS:O	1:A:461:ILE:HB	2.12	0.49
1:A:616:TYR:OH	1:A:664:GLN:NE2	2.45	0.49
1:B:613:PRO:HA	1:B:640:ALA:CB	2.42	0.49
1:B:652:MET:CE	1:B:655:TYR:CD2	2.95	0.49
1:A:295:GLU:O	1:A:295:GLU:HG3	2.11	0.49
1:A:361:ASN:O	1:A:362:HIS:HB3	2.12	0.49
1:A:34:TYR:CD1	1:A:34:TYR:O	2.65	0.49
1:B:631:ILE:HA	1:B:645:ALA:CB	2.41	0.49
1:A:10:LYS:HG2	1:A:284:LEU:HD21	1.93	0.49
1:B:270:GLN:O	1:B:273:LEU:HB2	2.12	0.49
1:B:312:LEU:O	1:B:328:ILE:HA	2.12	0.49
1:B:88:VAL:HG12	1:B:89:ASP:N	2.27	0.49
1:B:448:GLN:O	1:B:449:THR:CB	2.60	0.49
1:B:491:VAL:CG2	1:B:593:ALA:HB1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PRO:O	1:A:682:GLN:N	2.45	0.49
1:A:506:GLN:CA	1:A:576:ASP:O	2.58	0.49
1:B:182:ARG:HB2	1:B:184:LYS:HD3	1.94	0.49
1:A:19:ALA:HB2	1:A:107:VAL:CG1	2.43	0.49
1:A:514:VAL:HA	1:A:564:LYS:O	2.12	0.49
1:B:169:GLY:C	1:B:174:PHE:HA	2.33	0.49
1:A:443:HIS:HB2	1:A:450:ILE:HD13	1.93	0.49
1:B:196:ILE:O	1:B:196:ILE:HG23	2.13	0.49
1:B:16:GLY:N	1:B:101:LEU:HD12	2.27	0.49
1:A:87:HIS:CE1	1:A:90:PHE:HB2	2.45	0.49
1:A:190:ASN:ND2	1:A:195:ASP:CB	2.74	0.49
1:B:572:TYR:N	1:B:572:TYR:CD1	2.80	0.49
1:A:102:ASP:HB3	1:A:286:ILE:CD1	2.40	0.49
1:A:608:VAL:HG13	1:A:670:VAL:O	2.12	0.49
1:B:26:THR:O	1:B:29:THR:N	2.45	0.49
1:A:352:VAL:O	1:A:353:ALA:O	2.31	0.49
1:B:330:VAL:HG12	1:B:371:ALA:HA	1.95	0.49
1:A:20:HIS:CE1	1:A:117:GLN:HE22	2.31	0.49
1:A:385:THR:HG22	1:A:386:GLY:N	2.28	0.49
1:A:468:ARG:NH1	1:A:468:ARG:HG2	2.28	0.49
1:B:679:VAL:O	1:B:679:VAL:HG12	2.12	0.49
1:B:606:MET:HE3	1:B:671:MET:HG3	1.95	0.49
1:B:628:ARG:HH12	1:B:651:GLU:HB2	1.76	0.49
1:A:292:THR:O	1:A:398:ILE:HD12	2.12	0.49
1:B:539:ILE:O	1:B:542:VAL:HB	2.12	0.49
1:B:68:ALA:HB3	1:B:327:PHE:CE2	2.48	0.49
1:A:8:ASP:HB3	1:A:11:ARG:HG3	1.92	0.49
1:B:211:GLU:O	1:B:215:LYS:HG3	2.13	0.49
1:B:538:TYR:O	1:B:539:ILE:C	2.51	0.49
1:A:414:GLU:HB3	1:A:452:SER:CB	2.43	0.49
1:B:89:ASP:OD1	1:B:89:ASP:N	2.39	0.49
1:A:535:PRO:CG	1:A:538:TYR:CD2	2.94	0.49
1:A:680:PRO:O	1:A:683:VAL:HG23	2.12	0.49
1:A:82:ILE:HD12	1:A:101:LEU:CB	2.43	0.49
1:A:221:ALA:HB1	1:A:228:MET:HE2	1.92	0.49
1:B:572:TYR:N	1:B:572:TYR:HD1	2.10	0.49
1:B:634:MET:HB2	1:B:643:ILE:HA	1.94	0.49
1:B:409:ILE:C	1:B:411:VAL:H	2.13	0.48
1:A:653:PHE:C	1:A:655:TYR:N	2.66	0.48
1:B:343:ASN:O	1:B:343:ASN:OD1	2.30	0.48
1:A:92:ILE:N	1:A:92:ILE:HD13	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:O	1:B:465:ARG:HG3	2.14	0.48
1:A:181:LEU:CD2	1:A:243:VAL:HG22	2.33	0.48
1:B:122:TRP:CE3	1:B:157:LEU:HD23	2.48	0.48
1:A:499:ARG:HG3	1:A:500:GLN:N	2.27	0.48
1:B:385:THR:HG22	1:B:386:GLY:N	2.28	0.48
1:B:325:LEU:CD2	1:B:378:VAL:HG23	2.42	0.48
1:A:462:ILE:O	1:A:466:LEU:HB2	2.14	0.48
1:A:657:THR:HA	1:A:660:ARG:CB	2.36	0.48
1:B:173:THR:O	1:B:174:PHE:C	2.51	0.48
1:A:608:VAL:HG13	1:A:669:PHE:HD2	1.78	0.48
1:B:138:LYS:C	1:B:140:ASP:H	2.15	0.48
1:B:584:ILE:HG22	1:B:585:ALA:N	2.29	0.48
1:A:535:PRO:HB2	1:A:537:GLU:OE1	2.13	0.48
1:A:669:PHE:CD2	1:A:670:VAL:N	2.81	0.48
1:B:631:ILE:HA	1:B:645:ALA:HB2	1.95	0.48
1:A:146:LEU:HD12	1:A:167:PRO:HD3	1.96	0.48
1:B:68:ALA:O	1:B:69:VAL:HG23	2.14	0.48
1:A:607:ARG:NH1	1:A:672:PHE:CG	2.81	0.48
1:A:669:PHE:C	1:A:670:VAL:CG2	2.81	0.48
1:A:38:ARG:CD	1:A:39:ILE:H	2.26	0.48
1:B:20:HIS:CE1	1:B:117:GLN:HE22	2.30	0.48
1:B:456:GLU:O	1:B:458:HIS:N	2.47	0.48
1:A:485:GLU:OE1	1:A:555:LEU:HB2	2.12	0.48
1:B:212:TYR:CD1	1:B:215:LYS:HD2	2.48	0.48
1:B:191:ASP:O	1:B:192:LEU:HD23	2.12	0.48
1:A:628:ARG:HH12	1:A:651:GLU:HB2	1.79	0.48
1:B:166:LEU:CD2	1:B:208:GLN:HG2	2.43	0.48
1:B:74:TRP:CE3	1:B:273:LEU:HD13	2.47	0.48
1:A:312:LEU:HD23	1:A:313:ALA:H	1.77	0.48
1:A:457:LEU:HA	1:A:460:GLU:HB2	1.95	0.48
1:A:203:GLU:CA	1:A:206:LEU:HD23	2.32	0.48
1:B:170:ARG:N	1:B:173:THR:HB	2.28	0.48
1:A:466:LEU:O	1:A:470:PHE:N	2.35	0.48
1:B:344:THR:O	1:B:346:LYS:N	2.47	0.48
1:B:517:LEU:HD23	1:B:518:PRO:CD	2.43	0.48
1:B:520:GLY:N	1:B:562:ASP:OD2	2.46	0.48
1:B:491:VAL:HG21	1:B:593:ALA:HB1	1.96	0.48
1:A:510:VAL:HB	1:A:567:LEU:HD11	1.95	0.48
1:A:241:GLU:O	1:A:245:ALA:HB2	2.14	0.48
1:A:105:ILE:HG23	1:A:133:ILE:CG1	2.37	0.48
1:A:616:TYR:C	1:A:618:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:THR:CG2	1:B:397:VAL:O	2.57	0.48
1:B:151:ARG:HG2	1:B:151:ARG:HH11	1.79	0.48
1:A:151:ARG:HG2	1:A:151:ARG:HH11	1.78	0.48
1:B:240:GLU:O	1:B:241:GLU:C	2.50	0.48
1:A:455:GLY:O	1:A:459:LEU:HD11	2.14	0.48
1:A:192:LEU:HA	1:A:266:ASN:HD22	1.78	0.48
1:A:345:THR:CG2	1:A:388:THR:H	2.27	0.48
1:A:361:ASN:O	1:A:362:HIS:CG	2.67	0.48
1:A:549:ALA:HA	1:A:591:LYS:HZ3	1.77	0.48
1:B:509:HIS:CD2	1:B:570:GLY:HA2	2.49	0.48
1:B:343:ASN:OD1	1:B:343:ASN:C	2.52	0.47
1:B:35:TYR:C	1:B:37:GLY:N	2.66	0.47
1:B:38:ARG:C	1:B:39:ILE:HG22	2.34	0.47
1:A:457:LEU:CG	1:A:460:GLU:HB2	2.42	0.47
1:A:523:PHE:N	1:B:194:THR:O	2.42	0.47
1:B:464:ASP:O	1:B:468:ARG:HB2	2.14	0.47
1:A:428:LEU:H	1:A:428:LEU:HD12	1.79	0.47
1:B:19:ALA:HB2	1:B:107:VAL:HG13	1.96	0.47
1:B:590:ILE:O	1:B:591:LYS:C	2.50	0.47
1:B:634:MET:CE	1:B:634:MET:O	2.61	0.47
1:A:88:VAL:HG12	1:A:89:ASP:N	2.29	0.47
1:B:329:ARG:CG	1:B:374:LEU:HD23	2.36	0.47
1:A:672:PHE:HD1	1:A:672:PHE:N	2.11	0.47
1:A:19:ALA:CB	1:A:107:VAL:HG13	2.43	0.47
1:A:7:TYR:C	1:A:7:TYR:CD1	2.87	0.47
1:A:466:LEU:O	1:A:468:ARG:N	2.44	0.47
1:B:647:VAL:HG21	1:B:652:MET:SD	2.55	0.47
1:B:361:ASN:O	1:B:362:HIS:CG	2.67	0.47
1:B:343:ASN:HD21	1:B:387:ASP:HB3	1.80	0.47
1:B:624:LEU:HD13	1:B:655:TYR:OH	2.15	0.47
1:A:573:HIS:HB3	1:A:576:ASP:HB2	1.96	0.47
1:B:494:GLU:HG3	1:B:509:HIS:HE1	1.80	0.47
1:B:342:TYR:HE1	1:B:347:GLY:O	1.97	0.47
1:B:680:PRO:HG2	1:B:683:VAL:HG23	1.95	0.47
1:B:181:LEU:CD1	1:B:242:LEU:HD23	2.44	0.47
1:B:165:GLN:CB	1:B:178:ILE:O	2.58	0.47
1:B:35:TYR:CE1	1:B:269:VAL:HG21	2.50	0.47
1:B:309:LEU:CD1	1:B:335:LEU:HB2	2.45	0.47
1:A:312:LEU:HD23	1:A:313:ALA:N	2.30	0.47
1:B:123:ARG:HH21	1:B:639:ASN:HB3	1.78	0.47
1:B:164:MET:HG3	1:B:259:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:LYS:HD3	1:B:583:LYS:HD3	1.95	0.47
1:B:584:ILE:O	1:B:588:MET:HG3	2.15	0.47
1:B:308:PRO:HB2	1:B:394:ALA:HB1	1.95	0.47
1:A:689:LYS:NZ	1:A:689:LYS:HB2	2.30	0.47
1:B:538:TYR:O	1:B:540:PRO:N	2.48	0.47
1:B:131:PRO:HG3	1:B:253:LEU:HD21	1.96	0.47
1:B:336:THR:HG22	1:B:368:GLU:HB3	1.97	0.47
1:B:396:ARG:HG2	1:B:396:ARG:O	2.15	0.47
1:B:319:ASP:CG	1:B:363:ARG:HH12	2.18	0.47
1:B:500:GLN:C	1:B:502:GLY:N	2.61	0.47
1:A:546:ILE:HG23	1:A:590:ILE:HG13	1.96	0.47
1:A:38:ARG:HD2	1:A:39:ILE:H	1.78	0.47
1:B:316:ILE:HD11	1:B:384:ILE:C	2.35	0.47
1:B:82:ILE:HD12	1:B:101:LEU:CB	2.46	0.47
1:A:438:PHE:O	1:A:439:ARG:HG3	2.15	0.47
1:B:187:THR:O	1:B:187:THR:HG23	2.15	0.47
1:A:105:ILE:HG12	1:A:133:ILE:HD11	1.96	0.46
1:A:329:ARG:HG2	1:A:329:ARG:HH11	1.80	0.46
1:B:462:ILE:O	1:B:466:LEU:HB2	2.15	0.46
1:B:688:ILE:O	1:B:689:LYS:HD3	2.14	0.46
1:B:443:HIS:HB2	1:B:450:ILE:CD1	2.45	0.46
1:B:549:ALA:HB3	1:B:590:ILE:HG21	1.97	0.46
1:A:643:ILE:N	1:A:643:ILE:HD13	2.30	0.46
1:B:114:VAL:CG1	1:B:157:LEU:HD11	2.42	0.46
1:B:218:GLU:O	1:B:219:VAL:C	2.52	0.46
1:A:322:VAL:HG12	1:A:354:ARG:NH2	2.31	0.46
1:A:629:GLY:HA2	1:A:646:PHE:O	2.15	0.46
1:B:286:ILE:HD12	1:B:286:ILE:H	1.78	0.46
1:A:36:THR:HG22	1:A:74:TRP:HB2	1.97	0.46
1:B:91:THR:O	1:B:92:ILE:C	2.52	0.46
1:B:677:GLN:NE2	1:B:678:GLU:H	2.14	0.46
1:B:485:GLU:OE1	1:B:555:LEU:HB2	2.15	0.46
1:B:78:ARG:CZ	1:B:357:ARG:NH2	2.78	0.46
1:A:409:ILE:C	1:A:411:VAL:H	2.19	0.46
1:A:312:LEU:HD21	1:A:386:GLY:HA2	1.96	0.46
1:A:660:ARG:O	1:A:665:GLY:N	2.48	0.46
1:B:648:PRO:O	1:B:649:LEU:C	2.53	0.46
1:A:573:HIS:CE1	1:A:576:ASP:OD2	2.68	0.46
1:A:610:VAL:HG22	1:A:669:PHE:HB2	1.97	0.46
1:B:361:ASN:O	1:B:362:HIS:HB3	2.15	0.46
1:B:313:ALA:HA	1:B:327:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:PRO:HD3	1:A:97:SER:OG	2.16	0.46
1:A:38:ARG:HD2	1:A:39:ILE:O	2.16	0.46
1:A:513:LYS:HG3	1:A:568:TYR:CE1	2.51	0.46
1:A:343:ASN:HD22	1:A:389:LEU:CD1	2.28	0.46
1:B:26:THR:O	1:B:27:THR:C	2.54	0.46
1:A:359:HIS:HD1	1:A:362:HIS:CE1	2.33	0.46
1:A:103:GLY:O	1:A:104:ALA:CB	2.64	0.46
1:B:353:ALA:HB3	1:B:378:VAL:O	2.16	0.46
1:A:328:ILE:O	1:A:374:LEU:HB2	2.14	0.46
1:B:590:ILE:O	1:B:592:GLU:N	2.49	0.46
1:B:229:LEU:N	1:B:229:LEU:CD1	2.69	0.46
1:B:652:MET:HE3	1:B:655:TYR:CD2	2.51	0.46
1:B:535:PRO:HD3	1:B:572:TYR:CD2	2.50	0.46
1:B:621:ILE:HG23	1:B:631:ILE:HG12	1.97	0.46
1:A:232:LEU:O	1:A:233:GLU:HB2	2.15	0.46
1:B:38:ARG:CD	1:B:39:ILE:H	2.28	0.46
1:B:623:ASP:O	1:B:626:ALA:HB3	2.16	0.46
1:A:434:GLU:O	1:A:434:GLU:HG2	2.14	0.46
1:B:443:HIS:HA	1:B:444:PRO:HD3	1.78	0.46
1:A:260:LEU:HD22	1:A:260:LEU:C	2.36	0.46
1:A:572:TYR:HD1	1:A:572:TYR:H	1.61	0.46
1:A:443:HIS:HA	1:A:444:PRO:HD3	1.78	0.46
1:B:145:ASP:O	1:B:148:LEU:HB3	2.16	0.46
1:B:352:VAL:O	1:B:352:VAL:HG13	2.16	0.46
1:A:312:LEU:O	1:A:328:ILE:HA	2.15	0.46
1:A:344:THR:O	1:A:346:LYS:N	2.48	0.46
1:B:456:GLU:C	1:B:458:HIS:N	2.69	0.46
1:B:685:GLU:O	1:B:688:ILE:CG1	2.62	0.46
1:A:157:LEU:C	1:A:639:ASN:ND2	2.65	0.46
1:A:610:VAL:HG22	1:A:669:PHE:CB	2.46	0.46
1:B:410:ASP:C	1:B:411:VAL:HG22	2.37	0.46
1:B:309:LEU:CG	1:B:310:ALA:N	2.77	0.46
1:B:546:ILE:O	1:B:550:MET:HG2	2.15	0.46
1:B:178:ILE:HG22	1:B:179:ASP:N	2.31	0.46
1:A:339:SER:H	1:A:352:VAL:CG1	2.28	0.46
1:B:232:LEU:O	1:B:233:GLU:HB2	2.15	0.46
1:B:466:LEU:HB3	1:B:467:LYS:H	1.60	0.45
1:B:381:LYS:C	1:B:383:THR:H	2.19	0.45
1:B:602:LEU:CD1	1:B:678:GLU:HA	2.42	0.45
1:A:216:LEU:O	1:A:217:VAL:C	2.54	0.45
1:B:157:LEU:N	1:B:157:LEU:HD12	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ARG:O	1:B:173:THR:N	2.42	0.45
1:A:264:LEU:O	1:A:265:LYS:HD3	2.15	0.45
1:B:439:ARG:NH1	1:B:439:ARG:CB	2.79	0.45
1:B:10:LYS:HG2	1:B:284:LEU:HD21	1.97	0.45
1:B:103:GLY:O	1:B:104:ALA:CB	2.61	0.45
1:B:74:TRP:O	1:B:75:LYS:C	2.55	0.45
1:A:523:PHE:CD1	1:A:524:GLU:N	2.84	0.45
1:A:192:LEU:HA	1:A:266:ASN:ND2	2.31	0.45
1:A:455:GLY:O	1:A:459:LEU:HD12	2.16	0.45
1:A:68:ALA:O	1:A:69:VAL:HG23	2.17	0.45
1:B:539:ILE:HB	1:B:540:PRO:HD3	1.97	0.45
1:A:349:LYS:C	1:A:350:GLU:HG2	2.36	0.45
1:A:621:ILE:O	1:A:625:ASN:HB2	2.16	0.45
1:B:611:THR:O	1:B:667:GLY:HA2	2.17	0.45
1:B:428:LEU:O	1:B:432:ALA:CB	2.65	0.45
1:B:554:PRO:O	1:B:555:LEU:O	2.35	0.45
1:B:199:ILE:HB	1:B:200:PRO:HD2	1.98	0.45
1:B:221:ALA:HB1	1:B:228:MET:HE2	1.96	0.45
1:A:481:VAL:HG21	1:A:650:ALA:HB2	1.98	0.45
1:A:345:THR:HG23	1:A:388:THR:H	1.82	0.45
1:B:359:HIS:HD1	1:B:362:HIS:CE1	2.34	0.45
1:A:344:THR:CG2	1:A:396:ARG:HB2	2.46	0.45
1:A:364:GLU:HG2	1:A:366:VAL:HG13	1.99	0.45
1:A:96:ARG:C	1:A:98:MET:N	2.70	0.45
1:A:99:ARG:HD2	1:A:289:ILE:HD12	1.99	0.45
1:B:215:LYS:O	1:B:219:VAL:HG23	2.16	0.45
1:A:653:PHE:O	1:A:654:GLY:C	2.55	0.45
1:A:188:TYR:CB	1:A:267:LYS:HD3	2.47	0.45
1:A:688:ILE:O	1:A:689:LYS:HD3	2.17	0.45
1:A:340:TYR:CB	1:A:392:GLU:OE2	2.61	0.45
1:B:201:ILE:H	1:B:201:ILE:CD1	2.27	0.45
1:B:252:ASP:O	1:B:253:LEU:HB2	2.16	0.45
1:A:344:THR:HG22	1:A:396:ARG:HB2	1.99	0.45
1:A:316:ILE:HD11	1:A:384:ILE:C	2.36	0.45
1:B:466:LEU:O	1:B:470:PHE:O	2.35	0.45
1:B:203:GLU:HA	1:B:206:LEU:CD2	2.36	0.45
1:A:635:GLU:O	1:A:642:VAL:HG22	2.17	0.45
1:A:289:ILE:CG2	1:A:301:ILE:HB	2.45	0.45
1:B:345:THR:HG22	1:B:398:ILE:HG22	1.98	0.45
1:B:336:THR:HG22	1:B:368:GLU:CB	2.46	0.45
1:B:507:TYR:O	1:B:581:ALA:HB1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:GLN:O	1:B:271:LEU:C	2.55	0.45
1:B:352:VAL:O	1:B:353:ALA:O	2.35	0.45
1:A:573:HIS:CG	1:A:576:ASP:HB2	2.52	0.45
1:B:542:VAL:HA	1:B:582:PHE:O	2.16	0.45
1:B:497:PHE:CG	1:B:584:ILE:HG21	2.51	0.45
1:A:526:VAL:CG1	1:A:527:ASN:H	2.29	0.45
1:A:38:ARG:C	1:A:39:ILE:HG22	2.37	0.45
1:A:440:VAL:O	1:A:440:VAL:HG13	2.17	0.45
1:A:259:PHE:CE2	1:A:275:ALA:HB1	2.52	0.45
1:B:450:ILE:O	1:B:450:ILE:HG13	2.16	0.45
1:A:649:LEU:O	1:A:652:MET:HB3	2.16	0.45
1:A:34:TYR:HD1	1:A:34:TYR:O	1.98	0.45
1:A:381:LYS:HB2	1:A:381:LYS:NZ	2.31	0.45
1:A:99:ARG:CD	1:A:289:ILE:HD12	2.47	0.45
1:B:628:ARG:NH1	1:B:648:PRO:HB2	2.32	0.45
1:A:681:LYS:H	1:A:681:LYS:CD	2.30	0.45
1:B:388:THR:C	1:B:389:LEU:HD13	2.38	0.45
1:A:301:ILE:HD13	1:A:301:ILE:HA	1.84	0.45
1:B:120:THR:O	1:B:123:ARG:HB2	2.17	0.45
1:A:292:THR:CB	1:A:398:ILE:HD12	2.47	0.45
1:A:443:HIS:ND1	1:A:450:ILE:CD1	2.80	0.45
1:A:623:ASP:O	1:A:626:ALA:HB3	2.17	0.45
1:B:496:LYS:CE	1:B:509:HIS:ND1	2.80	0.45
1:A:183:MET:CE	1:A:209:ALA:HB1	2.47	0.45
1:B:69:VAL:CG2	1:B:314:PHE:HZ	2.30	0.44
1:B:19:ALA:CB	1:B:107:VAL:HG13	2.46	0.44
1:A:456:GLU:C	1:A:458:HIS:H	2.21	0.44
1:A:469:GLU:O	1:A:470:PHE:HD1	1.98	0.44
1:A:620:VAL:C	1:A:622:GLY:N	2.69	0.44
1:B:441:SER:HG	1:B:450:ILE:HD11	1.82	0.44
1:B:156:ARG:HB3	1:B:666:ARG:NH1	2.30	0.44
1:B:647:VAL:CG2	1:B:652:MET:SD	3.05	0.44
1:B:78:ARG:NE	1:B:357:ARG:HH21	2.14	0.44
1:A:138:LYS:C	1:A:140:ASP:H	2.21	0.44
1:B:631:ILE:N	1:B:631:ILE:HD12	2.31	0.44
1:B:247:ARG:O	1:B:248:LYS:C	2.56	0.44
1:B:18:ALA:HB1	1:B:121:VAL:CG1	2.47	0.44
1:A:384:ILE:HB	1:A:385:THR:H	1.39	0.44
1:B:413:ILE:HA	1:B:480:GLN:O	2.17	0.44
1:B:678:GLU:HB3	1:B:679:VAL:H	1.49	0.44
1:B:123:ARG:O	1:B:126:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ILE:O	1:A:542:VAL:HB	2.16	0.44
1:B:168:ILE:O	1:B:174:PHE:HA	2.16	0.44
1:A:507:TYR:C	1:A:507:TYR:CD1	2.91	0.44
1:B:494:GLU:HB2	1:B:511:LYS:HG2	1.99	0.44
1:A:614:GLU:OE1	1:A:641:GLN:HG3	2.16	0.44
1:A:78:ARG:CZ	1:A:357:ARG:HH21	2.31	0.44
1:A:203:GLU:HA	1:A:206:LEU:HB2	1.98	0.44
1:A:242:LEU:HD12	1:A:242:LEU:HA	1.81	0.44
1:B:305:PRO:C	1:B:307:GLY:H	2.21	0.44
1:B:410:ASP:O	1:B:411:VAL:CG2	2.65	0.44
1:A:411:VAL:CA	1:A:453:GLY:HA2	2.47	0.44
1:A:458:HIS:CA	1:A:461:ILE:HG13	2.47	0.44
1:A:460:GLU:HA	1:A:463:VAL:HB	1.99	0.44
1:B:558:PHE:O	1:B:559:PRO:O	2.36	0.44
1:A:228:MET:O	1:A:231:TYR:N	2.50	0.44
1:B:612:THR:HG21	1:B:620:VAL:CG2	2.41	0.44
1:B:109:ASP:OD1	1:B:111:SER:CB	2.63	0.44
1:B:414:GLU:CB	1:B:452:SER:HB2	2.47	0.44
1:B:140:ASP:HA	1:B:171:GLU:O	2.17	0.44
1:A:147:TRP:O	1:A:151:ARG:N	2.40	0.44
1:A:624:LEU:O	1:A:627:ARG:HB2	2.17	0.44
1:B:525:PHE:HE2	1:B:546:ILE:HD12	1.83	0.44
1:B:444:PRO:HD3	1:B:551:GLN:OE1	2.18	0.44
1:A:517:LEU:HD12	1:A:563:ILE:O	2.17	0.44
1:A:208:GLN:O	1:A:211:GLU:HB3	2.18	0.44
1:A:391:GLY:O	1:A:394:ALA:N	2.51	0.44
1:B:301:ILE:HA	1:B:301:ILE:HD13	1.84	0.44
1:B:504:ARG:NH1	1:B:504:ARG:HG2	2.32	0.44
1:A:554:PRO:HG2	1:A:594:VAL:CG1	2.48	0.44
1:B:20:HIS:CG	1:B:21:ILE:N	2.85	0.44
1:A:625:ASN:HA	1:A:625:ASN:HD22	1.60	0.44
1:B:16:GLY:O	1:B:104:ALA:HA	2.18	0.44
1:B:342:TYR:HE1	1:B:347:GLY:C	2.20	0.44
1:A:85:PRO:CG	1:A:94:VAL:HG22	2.48	0.44
1:A:427:ALA:HA	1:A:470:PHE:HD2	1.71	0.44
1:B:435:ASP:O	1:B:438:PHE:CE2	2.70	0.44
1:B:203:GLU:HA	1:B:206:LEU:HB2	2.00	0.44
1:B:616:TYR:HE2	1:B:666:ARG:HD3	1.83	0.44
1:B:333:GLY:O	1:B:371:ALA:HB2	2.17	0.44
1:A:595:GLN:HE21	1:A:595:GLN:HB3	1.51	0.44
1:B:118:SER:HA	1:B:121:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LYS:HZ3	1:B:84:THR:CB	2.31	0.44
1:B:487:ILE:HD12	1:B:489:LYS:O	2.17	0.44
1:B:590:ILE:C	1:B:592:GLU:N	2.70	0.44
1:A:525:PHE:HB3	1:B:197:ARG:CB	2.48	0.44
1:B:649:LEU:O	1:B:652:MET:CB	2.66	0.44
1:A:604:PRO:HG2	1:A:649:LEU:CB	2.47	0.44
1:B:152:THR:O	1:B:153:MET:C	2.55	0.44
1:B:511:LYS:HD2	1:B:569:ASP:HB3	1.98	0.44
1:A:493:VAL:HG21	1:A:589:ALA:O	2.18	0.44
1:A:308:PRO:HB2	1:A:394:ALA:HB1	1.99	0.44
1:A:247:ARG:HG3	1:A:279:TYR:O	2.18	0.44
1:A:74:TRP:CD2	1:A:273:LEU:HD13	2.52	0.44
1:B:85:PRO:O	1:B:87:HIS:N	2.51	0.44
1:B:592:GLU:O	1:B:594:VAL:N	2.51	0.44
1:B:181:LEU:HD21	1:B:243:VAL:CG2	2.36	0.44
1:A:652:MET:O	1:A:655:TYR:HB2	2.17	0.44
1:A:605:ILE:HD13	1:A:677:GLN:HB3	1.98	0.44
1:A:632:LEU:HD23	1:A:645:ALA:HA	1.99	0.44
1:B:166:LEU:HD21	1:B:208:GLN:HG2	2.00	0.44
1:B:510:VAL:HB	1:B:567:LEU:HD11	1.99	0.44
1:A:357:ARG:HG3	1:A:357:ARG:NH1	2.27	0.43
1:B:220:ALA:O	1:B:221:ALA:O	2.36	0.43
1:B:644:ARG:H	1:B:644:ARG:HG3	1.68	0.43
1:A:290:LYS:HE2	1:A:298:VAL:HG11	2.00	0.43
1:A:441:SER:HB3	1:A:450:ILE:HG13	2.00	0.43
1:A:241:GLU:O	1:A:245:ALA:CB	2.65	0.43
1:B:96:ARG:C	1:B:98:MET:N	2.72	0.43
1:B:218:GLU:HG3	1:B:231:TYR:CE2	2.53	0.43
1:A:573:HIS:C	1:A:575:VAL:N	2.72	0.43
1:A:20:HIS:CG	1:A:21:ILE:H	2.36	0.43
1:A:274:ASP:O	1:A:277:VAL:HG13	2.19	0.43
1:A:96:ARG:C	1:A:98:MET:H	2.20	0.43
1:B:485:GLU:O	1:B:560:VAL:HA	2.19	0.43
1:B:626:ALA:C	1:B:628:ARG:H	2.20	0.43
1:A:336:THR:HG22	1:A:368:GLU:CB	2.48	0.43
1:A:20:HIS:CG	1:A:21:ILE:N	2.86	0.43
1:B:9:LEU:HD12	1:B:12:LEU:HD13	2.01	0.43
1:B:33:LEU:HD21	1:B:81:ILE:HD12	2.01	0.43
1:A:490:PRO:HG3	1:A:516:PRO:HD3	2.00	0.43
1:B:271:LEU:O	1:B:272:LEU:C	2.56	0.43
1:A:523:PHE:CZ	1:A:525:PHE:HB2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:HE2	1:B:137:ASN:ND2	2.16	0.43
1:B:312:LEU:HD21	1:B:386:GLY:HA2	2.00	0.43
1:A:218:GLU:O	1:A:219:VAL:C	2.57	0.43
1:A:534:ILE:HG23	1:A:582:PHE:CE2	2.54	0.43
1:A:573:HIS:CB	1:A:576:ASP:HB2	2.48	0.43
1:A:669:PHE:O	1:A:670:VAL:HG23	2.17	0.43
1:A:173:THR:O	1:A:174:PHE:C	2.56	0.43
1:B:575:VAL:HG23	1:B:576:ASP:N	2.32	0.43
1:B:92:ILE:N	1:B:92:ILE:CD1	2.81	0.43
1:A:309:LEU:CG	1:A:310:ALA:N	2.81	0.43
1:A:345:THR:HG23	1:A:388:THR:HB	1.99	0.43
1:A:554:PRO:HG2	1:A:594:VAL:CB	2.45	0.43
1:A:273:LEU:O	1:A:274:ASP:C	2.56	0.43
1:A:94:VAL:HG11	1:A:124:GLN:OE1	2.18	0.43
1:B:459:LEU:CD1	1:B:459:LEU:H	2.27	0.43
1:B:448:GLN:O	1:B:449:THR:OG1	2.31	0.43
1:B:592:GLU:HG3	1:B:593:ALA:N	2.33	0.43
1:B:228:MET:O	1:B:231:TYR:HB3	2.19	0.43
1:B:329:ARG:HG2	1:B:329:ARG:HH11	1.84	0.43
1:B:384:ILE:HB	1:B:385:THR:H	1.42	0.43
1:A:616:TYR:O	1:A:620:VAL:HG23	2.19	0.43
1:A:218:GLU:O	1:A:221:ALA:CB	2.66	0.43
1:B:441:SER:HB3	1:B:450:ILE:CD1	2.49	0.43
1:A:485:GLU:O	1:A:560:VAL:HG13	2.19	0.43
1:B:608:VAL:HG23	1:B:647:VAL:HG12	2.00	0.43
1:A:655:TYR:CE1	1:A:659:LEU:HB2	2.54	0.43
1:B:260:LEU:C	1:B:260:LEU:CD2	2.87	0.43
1:B:542:VAL:CG2	1:B:582:PHE:HB3	2.49	0.43
1:A:14:ASN:OD1	1:A:80:ASN:HB2	2.18	0.43
1:B:384:ILE:HG13	1:B:384:ILE:H	1.64	0.43
1:B:11:ARG:CG	1:B:11:ARG:NH1	2.73	0.43
1:A:178:ILE:HG22	1:A:179:ASP:N	2.33	0.43
1:B:165:GLN:HE21	1:B:165:GLN:HB3	1.55	0.43
1:B:494:GLU:CD	1:B:509:HIS:HE1	2.22	0.43
1:B:38:ARG:C	1:B:39:ILE:CG2	2.86	0.43
1:B:96:ARG:C	1:B:98:MET:H	2.20	0.43
1:B:118:SER:HA	1:B:121:VAL:HG23	2.01	0.43
1:A:96:ARG:NH2	1:A:386:GLY:HA3	2.33	0.43
1:A:224:ASP:O	1:A:227:ILE:HB	2.19	0.43
1:A:220:ALA:HB1	1:A:227:ILE:CD1	2.49	0.43
1:B:681:LYS:CD	1:B:681:LYS:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:HD22	1:A:649:LEU:O	2.19	0.43
1:B:326:THR:HB	1:B:377:VAL:HG13	2.01	0.42
1:A:457:LEU:CA	1:A:460:GLU:HB2	2.49	0.42
1:B:441:SER:HB3	1:B:450:ILE:CG1	2.48	0.42
1:B:525:PHE:CZ	1:B:543:GLN:HG3	2.55	0.42
1:B:646:PHE:HD1	1:B:646:PHE:HA	1.72	0.42
1:A:302:HIS:O	1:A:332:SER:HB2	2.18	0.42
1:B:191:ASP:HA	1:B:267:LYS:NZ	2.34	0.42
1:A:304:ASP:HA	1:A:305:PRO:HD3	1.82	0.42
1:B:493:VAL:HG21	1:B:593:ALA:HB2	2.01	0.42
1:B:181:LEU:HD11	1:B:242:LEU:HB3	2.00	0.42
1:B:616:TYR:C	1:B:618:GLY:N	2.71	0.42
1:A:292:THR:CG2	1:A:398:ILE:HD12	2.49	0.42
1:A:342:TYR:HE1	1:A:347:GLY:O	2.02	0.42
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.28	0.42
1:A:461:ILE:O	1:A:465:ARG:CG	2.66	0.42
1:B:228:MET:O	1:B:229:LEU:C	2.56	0.42
1:A:679:VAL:HG22	1:A:683:VAL:CG2	2.49	0.42
1:A:286:ILE:CG2	1:A:287:PRO:N	2.82	0.42
1:A:69:VAL:CG2	1:A:314:PHE:HZ	2.32	0.42
1:A:504:ARG:HG2	1:A:504:ARG:NH1	2.33	0.42
1:B:169:GLY:O	1:B:174:PHE:HA	2.19	0.42
1:B:319:ASP:HB3	1:B:322:VAL:HG22	2.01	0.42
1:B:458:HIS:O	1:B:461:ILE:CB	2.66	0.42
1:B:677:GLN:O	1:B:678:GLU:O	2.37	0.42
1:A:286:ILE:HG22	1:A:287:PRO:N	2.33	0.42
1:A:127:LYS:HB2	1:A:637:ARG:CZ	2.48	0.42
1:A:496:LYS:HG2	1:A:509:HIS:ND1	2.35	0.42
1:A:25:LYS:NZ	1:A:84:THR:CB	2.82	0.42
1:A:321:TYR:C	1:A:323:GLY:H	2.22	0.42
1:A:681:LYS:N	1:A:681:LYS:CD	2.82	0.42
1:B:496:LYS:HE3	1:B:509:HIS:CE1	2.54	0.42
1:A:477:GLY:C	1:A:479:PRO:HD3	2.40	0.42
1:B:513:LYS:HG3	1:B:568:TYR:CE1	2.54	0.42
1:B:15:ILE:HD13	1:B:276:VAL:HG11	2.02	0.42
1:B:319:ASP:OD1	1:B:320:PRO:HD2	2.20	0.42
1:B:89:ASP:HB2	1:B:90:PHE:H	1.53	0.42
1:B:467:LYS:HE3	1:B:467:LYS:HB3	1.69	0.42
1:B:457:LEU:CB	1:B:460:GLU:HB2	2.50	0.42
1:B:413:ILE:CD1	1:B:454:MET:O	2.54	0.42
1:B:607:ARG:O	1:B:671:MET:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:PHE:CG	1:A:670:VAL:N	2.87	0.42
1:A:632:LEU:CD2	1:A:645:ALA:HA	2.50	0.42
1:B:399:LEU:HA	1:B:399:LEU:HD23	1.87	0.42
1:B:515:GLU:HB3	1:B:516:PRO:CD	2.49	0.42
1:B:459:LEU:O	1:B:463:VAL:N	2.49	0.42
1:B:518:PRO:O	1:B:519:ARG:C	2.57	0.42
1:B:157:LEU:N	1:B:157:LEU:CD1	2.83	0.42
1:B:620:VAL:C	1:B:622:GLY:N	2.72	0.42
1:B:499:ARG:HG3	1:B:500:GLN:N	2.34	0.42
1:B:128:TYR:O	1:B:129:LYS:HB3	2.20	0.42
1:A:480:GLN:HE22	1:A:558:PHE:HZ	1.66	0.42
1:B:272:LEU:O	1:B:276:VAL:HG23	2.20	0.42
1:A:357:ARG:HD3	1:A:364:GLU:OE2	2.20	0.42
1:A:427:ALA:CB	1:A:470:PHE:HD2	2.32	0.42
1:B:444:PRO:HA	1:B:448:GLN:HG3	2.01	0.42
1:B:416:LYS:HG2	1:B:449:THR:CG2	2.50	0.42
1:B:231:TYR:CD1	1:B:231:TYR:C	2.93	0.42
1:A:31:ARG:NH2	1:A:34:TYR:CD2	2.88	0.42
1:A:626:ALA:C	1:A:628:ARG:N	2.73	0.42
1:A:247:ARG:NH1	1:A:251:ILE:CD1	2.83	0.42
1:B:165:GLN:HG3	1:B:260:LEU:HD11	2.00	0.42
1:B:545:GLY:N	1:B:583:LYS:HG3	2.35	0.42
1:B:293:THR:O	1:B:296:GLY:O	2.38	0.42
1:B:240:GLU:CD	1:B:240:GLU:H	2.23	0.42
1:A:275:ALA:O	1:A:276:VAL:C	2.56	0.41
1:A:5:VAL:CG1	1:A:6:GLU:H	2.01	0.41
1:A:499:ARG:HG3	1:A:501:THR:H	1.85	0.41
1:A:166:LEU:HD23	1:A:208:GLN:HG2	2.02	0.41
1:A:608:VAL:CG1	1:A:609:GLU:N	2.83	0.41
1:A:448:GLN:O	1:A:449:THR:HB	2.20	0.41
1:A:448:GLN:O	1:A:449:THR:OG1	2.38	0.41
1:A:493:VAL:CG2	1:A:593:ALA:HB2	2.50	0.41
1:B:272:LEU:HD23	1:B:272:LEU:O	2.20	0.41
1:B:31:ARG:O	1:B:35:TYR:HD1	2.03	0.41
1:A:292:THR:HG22	1:A:398:ILE:CD1	2.50	0.41
1:A:27:THR:O	1:A:31:ARG:HG2	2.20	0.41
1:A:585:ALA:HA	1:A:588:MET:SD	2.61	0.41
1:A:493:VAL:HB	1:A:494:GLU:H	1.55	0.41
1:A:528:ALA:HB3	1:A:568:TYR:HA	2.02	0.41
1:B:35:TYR:O	1:B:38:ARG:HG3	2.20	0.41
1:B:554:PRO:HG2	1:B:594:VAL:CB	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:LYS:HG3	1:A:687:LEU:N	2.34	0.41
1:A:188:TYR:HB2	1:A:267:LYS:HD3	2.00	0.41
1:A:507:TYR:O	1:A:577:SER:HA	2.20	0.41
1:B:309:LEU:HD23	1:B:390:VAL:HA	2.02	0.41
1:B:346:LYS:C	1:B:348:ARG:H	2.24	0.41
1:B:486:THR:HG22	1:B:487:ILE:N	2.35	0.41
1:B:119:GLU:O	1:B:123:ARG:HG2	2.19	0.41
1:B:221:ALA:O	1:B:223:PHE:N	2.53	0.41
1:A:295:GLU:HA	1:B:26:THR:HG1	1.84	0.41
1:A:31:ARG:O	1:A:34:TYR:N	2.53	0.41
1:B:573:HIS:HB3	1:B:576:ASP:HB2	2.02	0.41
1:B:631:ILE:CD1	1:B:631:ILE:H	2.34	0.41
1:A:74:TRP:CZ2	1:A:75:LYS:HE3	2.54	0.41
1:A:457:LEU:HG	1:A:460:GLU:CG	2.50	0.41
1:B:680:PRO:HB2	1:B:682:GLN:NE2	2.25	0.41
1:A:286:ILE:N	1:A:286:ILE:HD12	2.35	0.41
1:A:178:ILE:HD12	1:A:201:ILE:HG13	2.02	0.41
1:A:178:ILE:CD1	1:A:185:ALA:HB2	2.51	0.41
1:A:442:THR:OG1	1:A:443:HIS:N	2.45	0.41
1:A:511:LYS:HD2	1:A:569:ASP:HB3	2.03	0.41
1:B:344:THR:C	1:B:346:LYS:H	2.23	0.41
1:B:346:LYS:O	1:B:348:ARG:N	2.52	0.41
1:A:560:VAL:O	1:A:561:VAL:HG13	2.20	0.41
1:A:337:SER:OG	1:A:354:ARG:HA	2.20	0.41
1:B:652:MET:HE3	1:B:655:TYR:CG	2.56	0.41
1:B:127:LYS:HE2	1:B:637:ARG:NH2	2.36	0.41
1:A:416:LYS:C	1:A:416:LYS:CD	2.88	0.41
1:A:556:ILE:HG13	1:A:558:PHE:CD1	2.55	0.41
1:A:454:MET:HB3	1:A:458:HIS:CD2	2.55	0.41
1:A:325:LEU:CD2	1:A:378:VAL:HG23	2.51	0.41
1:B:606:MET:CE	1:B:671:MET:HG3	2.51	0.41
1:B:238:THR:OG1	1:B:241:GLU:HB2	2.21	0.41
1:A:205:TYR:O	1:A:207:ASP:N	2.53	0.41
1:A:112:GLN:O	1:A:113:GLY:C	2.59	0.41
1:B:598:ASP:N	1:B:599:PRO:CD	2.84	0.41
1:A:181:LEU:HD11	1:A:242:LEU:HB3	2.02	0.41
1:B:242:LEU:HA	1:B:242:LEU:HD12	1.76	0.41
1:A:538:TYR:O	1:A:539:ILE:C	2.58	0.41
1:A:680:PRO:C	1:A:682:GLN:N	2.74	0.41
1:B:634:MET:O	1:B:634:MET:HE2	2.21	0.41
1:A:352:VAL:HG13	1:A:352:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:HE2	1:B:509:HIS:ND1	2.36	0.41
1:B:335:LEU:HD21	1:B:355:LEU:HD21	2.03	0.41
1:B:517:LEU:HB2	1:B:562:ASP:C	2.41	0.41
1:B:220:ALA:HB1	1:B:227:ILE:CD1	2.51	0.41
1:A:322:VAL:HB	1:A:378:VAL:CG2	2.50	0.41
1:B:648:PRO:O	1:B:651:GLU:N	2.48	0.41
1:A:639:ASN:C	1:A:639:ASN:OD1	2.59	0.41
1:A:659:LEU:HA	1:A:659:LEU:HD12	1.83	0.41
1:A:685:GLU:O	1:A:689:LYS:NZ	2.53	0.41
1:A:340:TYR:CZ	1:A:351:ARG:HB2	2.55	0.41
1:A:527:ASN:OD1	1:A:529:ILE:HB	2.20	0.41
1:B:330:VAL:HB	1:B:371:ALA:HA	2.03	0.41
1:B:190:ASN:HD21	1:B:195:ASP:HB2	1.86	0.41
1:B:327:PHE:CD1	1:B:376:ALA:HB2	2.55	0.41
1:A:221:ALA:HB1	1:A:228:MET:CG	2.41	0.41
1:A:119:GLU:OE2	1:A:123:ARG:NH1	2.54	0.41
1:A:290:LYS:HE2	1:A:298:VAL:CG1	2.51	0.41
1:B:27:THR:O	1:B:28:THR:C	2.60	0.41
1:A:630:GLN:O	1:A:631:ILE:C	2.60	0.41
1:B:269:VAL:HG23	1:B:270:GLN:OE1	2.21	0.40
1:B:609:GLU:N	1:B:670:VAL:O	2.52	0.40
1:A:178:ILE:CG2	1:A:179:ASP:N	2.83	0.40
1:A:573:HIS:ND1	1:A:576:ASP:CB	2.77	0.40
1:B:496:LYS:HG3	1:B:509:HIS:ND1	2.35	0.40
1:B:216:LEU:HD12	1:B:216:LEU:O	2.21	0.40
1:A:277:VAL:CG2	1:A:278:ASP:N	2.84	0.40
1:A:101:LEU:H	1:A:101:LEU:CD2	2.33	0.40
1:A:25:LYS:HZ1	1:A:84:THR:CB	2.34	0.40
1:A:309:LEU:HD11	1:A:335:LEU:HB2	2.03	0.40
1:A:305:PRO:C	1:A:307:GLY:H	2.24	0.40
1:B:512:ILE:HD12	1:B:514:VAL:HG22	2.02	0.40
1:B:411:VAL:CB	1:B:453:GLY:HA2	2.43	0.40
1:A:457:LEU:C	1:A:459:LEU:N	2.73	0.40
1:B:602:LEU:HD12	1:B:678:GLU:CA	2.44	0.40
1:B:443:HIS:HB2	1:B:450:ILE:HD13	2.03	0.40
1:B:549:ALA:HA	1:B:591:LYS:HZ2	1.86	0.40
1:A:653:PHE:C	1:A:655:TYR:H	2.25	0.40
1:A:507:TYR:CE1	1:A:572:TYR:HA	2.56	0.40
1:A:385:THR:O	1:A:387:ASP:N	2.54	0.40
1:A:385:THR:HG22	1:A:386:GLY:H	1.86	0.40
1:B:459:LEU:O	1:B:462:ILE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:ILE:CD1	1:B:582:PHE:HE2	2.34	0.40
1:A:449:THR:O	1:A:449:THR:HG22	2.21	0.40
1:A:590:ILE:HG22	1:A:591:LYS:N	2.35	0.40
1:A:101:LEU:HD23	1:A:101:LEU:N	2.33	0.40
1:B:454:MET:HB3	1:B:458:HIS:NE2	2.36	0.40
1:B:485:GLU:OE2	1:B:556:ILE:HG12	2.21	0.40
1:B:122:TRP:CZ2	1:B:159:ALA:HB2	2.56	0.40
1:A:649:LEU:HD22	1:A:649:LEU:C	2.42	0.40
1:B:362:HIS:O	1:B:362:HIS:CD2	2.75	0.40
1:A:38:ARG:C	1:A:39:ILE:CG2	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/691 (90%)	446 (72%)	114 (18%)	60 (10%)	1	14
1	B	620/691 (90%)	437 (70%)	117 (19%)	66 (11%)	0	11
All	All	1240/1382 (90%)	883 (71%)	231 (19%)	126 (10%)	1	13

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	91	THR
1	A	92	ILE
1	A	93	GLU
1	A	104	ALA
1	A	196	ILE
1	A	206	LEU
1	A	233	GLU

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Mol	Chain	Res	Type
1	A	353	ALA
1	A	362	HIS
1	A	410	ASP
1	A	427	ALA
1	A	435	ASP
1	A	442	THR
1	A	443	HIS
1	A	449	THR
1	A	457	LEU
1	A	555	LEU
1	A	574	GLU
1	A	617	MET
1	A	678	GLU
1	B	38	ARG
1	B	69	VAL
1	B	91	THR
1	B	92	ILE
1	B	93	GLU
1	B	104	ALA
1	B	139	MET
1	B	196	ILE
1	B	233	GLU
1	B	353	ALA
1	B	362	HIS
1	B	410	ASP
1	B	427	ALA
1	B	435	ASP
1	B	443	HIS
1	B	449	THR
1	B	457	LEU
1	B	555	LEU
1	B	592	GLU
1	B	617	MET
1	B	678	GLU
1	A	6	GLU
1	A	69	VAL
1	A	113	GLY
1	A	142	THR
1	A	174	PHE
1	A	297	GLU
1	A	345	THR
1	A	393	ASP

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Mol	Chain	Res	Type
1	A	455	GLY
1	A	467	LYS
1	A	468	ARG
1	A	501	THR
1	A	532	GLY
1	A	591	LYS
1	A	639	ASN
1	A	654	GLY
1	A	681	LYS
1	B	6	GLU
1	B	86	GLY
1	B	88	VAL
1	B	113	GLY
1	B	174	PHE
1	B	222	ASP
1	B	297	GLU
1	B	345	THR
1	B	393	ASP
1	B	415	PRO
1	B	442	THR
1	B	468	ARG
1	B	501	THR
1	B	532	GLY
1	B	574	GLU
1	B	593	ALA
1	A	88	VAL
1	A	112	GLN
1	A	139	MET
1	A	322	VAL
1	A	347	GLY
1	A	415	PRO
1	A	634	MET
1	B	171	GLU
1	B	206	LEU
1	B	412	ALA
1	B	550	MET
1	B	559	PRO
1	B	634	MET
1	B	652	MET
1	A	75	LYS
1	A	171	GLU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	392	GLU
1	A	454	MET
1	A	652	MET
1	B	240	GLU
1	B	347	GLY
1	B	373	ASP
1	B	639	ASN
1	B	649	LEU
1	A	19	ALA
1	A	368	GLU
1	A	478	LYS
1	A	627	ARG
1	B	19	ALA
1	B	75	LYS
1	B	142	THR
1	B	144	ALA
1	B	151	ARG
1	B	238	THR
1	B	241	GLU
1	B	539	ILE
1	A	384	ILE
1	B	126	GLU
1	B	253	LEU
1	B	322	VAL
1	B	554	PRO
1	A	411	VAL
1	B	384	ILE
1	A	86	GLY
1	A	32	ILE
1	A	269	VAL
1	B	283	PRO
1	B	561	VAL
1	B	648	PRO
1	B	590	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	534/582 (92%)	451 (84%)	83 (16%)	3 24
1	B	534/582 (92%)	446 (84%)	88 (16%)	3 20
All	All	1068/1164 (92%)	897 (84%)	171 (16%)	3 22

All (171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	7	TYR
1	A	12	LEU
1	A	34	TYR
1	A	36	THR
1	A	38	ARG
1	A	39	ILE
1	A	72	CYS
1	A	83	ASP
1	A	84	THR
1	A	87	HIS
1	A	89	ASP
1	A	92	ILE
1	A	93	GLU
1	A	96	ARG
1	A	99	ARG
1	A	107	VAL
1	A	115	GLU
1	A	126	GLU
1	A	129	LYS
1	A	130	VAL
1	A	132	ARG
1	A	156	ARG
1	A	166	LEU
1	A	204	GLU
1	A	206	LEU
1	A	226	ASN
1	A	231	TYR
1	A	242	LEU
1	A	248	LYS
1	A	252	ASP
1	A	260	LEU
1	A	265	LYS
1	A	269	VAL
1	A	274	ASP

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Mol	Chain	Res	Type
1	A	277	VAL
1	A	293	THR
1	A	300	GLU
1	A	312	LEU
1	A	321	TYR
1	A	348	ARG
1	A	357	ARG
1	A	365	GLU
1	A	367	GLU
1	A	369	LEU
1	A	370	LYS
1	A	374	LEU
1	A	377	VAL
1	A	381	LYS
1	A	384	ILE
1	A	389	LEU
1	A	396	ARG
1	A	398	ILE
1	A	415	PRO
1	A	416	LYS
1	A	435	ASP
1	A	458	HIS
1	A	464	ASP
1	A	468	ARG
1	A	501	THR
1	A	519	ARG
1	A	543	GLN
1	A	572	TYR
1	A	574	GLU
1	A	580	MET
1	A	602	LEU
1	A	612	THR
1	A	619	ASP
1	A	623	ASP
1	A	625	ASN
1	A	634	MET
1	A	641	GLN
1	A	643	ILE
1	A	644	ARG
1	A	646	PHE
1	A	660	ARG
1	A	664	GLN

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Mol	Chain	Res	Type
1	A	678	GLU
1	A	679	VAL
1	A	681	LYS
1	A	682	GLN
1	A	686	LYS
1	A	689	LYS
1	B	7	TYR
1	B	12	LEU
1	B	34	TYR
1	B	38	ARG
1	B	39	ILE
1	B	72	CYS
1	B	83	ASP
1	B	84	THR
1	B	87	HIS
1	B	89	ASP
1	B	92	ILE
1	B	93	GLU
1	B	96	ARG
1	B	97	SER
1	B	99	ARG
1	B	129	LYS
1	B	130	VAL
1	B	146	LEU
1	B	156	ARG
1	B	166	LEU
1	B	167	PRO
1	B	184	LYS
1	B	197	ARG
1	B	206	LEU
1	B	222	ASP
1	B	226	ASN
1	B	229	LEU
1	B	231	TYR
1	B	242	LEU
1	B	248	LYS
1	B	252	ASP
1	B	260	LEU
1	B	265	LYS
1	B	269	VAL
1	B	274	ASP
1	B	277	VAL

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Mol	Chain	Res	Type
1	B	293	THR
1	B	300	GLU
1	B	312	LEU
1	B	321	TYR
1	B	348	ARG
1	B	357	ARG
1	B	365	GLU
1	B	367	GLU
1	B	369	LEU
1	B	370	LYS
1	B	377	VAL
1	B	378	VAL
1	B	381	LYS
1	B	384	ILE
1	B	389	LEU
1	B	396	ARG
1	B	398	ILE
1	B	415	PRO
1	B	416	LYS
1	B	435	ASP
1	B	440	VAL
1	B	458	HIS
1	B	459	LEU
1	B	464	ASP
1	B	468	ARG
1	B	501	THR
1	B	506	GLN
1	B	517	LEU
1	B	519	ARG
1	B	561	VAL
1	B	572	TYR
1	B	574	GLU
1	B	580	MET
1	B	595	GLN
1	B	602	LEU
1	B	612	THR
1	B	614	GLU
1	B	619	ASP
1	B	623	ASP
1	B	625	ASN
1	B	634	MET
1	B	643	ILE

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Mol	Chain	Res	Type
1	B	644	ARG
1	B	646	PHE
1	B	660	ARG
1	B	669	PHE
1	B	678	GLU
1	B	679	VAL
1	B	681	LYS
1	B	682	GLN
1	B	686	LYS
1	B	689	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	190	ASN
1	A	208	GLN
1	A	266	ASN
1	A	343	ASN
1	A	426	GLN
1	A	448	GLN
1	A	480	GLN
1	A	543	GLN
1	A	595	GLN
1	A	625	ASN
1	A	664	GLN
1	A	682	GLN
1	B	77	HIS
1	B	117	GLN
1	B	208	GLN
1	B	426	GLN
1	B	448	GLN
1	B	480	GLN
1	B	595	GLN
1	B	625	ASN
1	B	664	GLN
1	B	677	GLN
1	B	682	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	632/691 (91%)	-0.17	12 (1%)	70	54	0, 11, 91, 189	0
1	B	632/691 (91%)	-0.03	27 (4%)	39	25	0, 13, 95, 192	0
All	All	1264/1382 (91%)	-0.10	39 (3%)	52	36	0, 12, 94, 192	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	GLY	6.1
1	B	504	ARG	5.5
1	B	578	SER	5.1
1	A	532	GLY	4.6
1	B	532	GLY	3.7
1	B	426	GLN	3.7
1	B	531	GLY	3.6
1	B	468	ARG	3.3
1	B	508	GLY	3.0
1	B	488	THR	2.9
1	B	503	GLY	2.9
1	B	489	LYS	2.8
1	B	506	GLN	2.8
1	B	465	ARG	2.7
1	A	531	GLY	2.7
1	B	535	PRO	2.7
1	B	528	ALA	2.7
1	B	6	GLU	2.6
1	B	494	GLU	2.6
1	B	443	HIS	2.5
1	B	529	ILE	2.5
1	A	468	ARG	2.5
1	A	379	GLY	2.5
1	A	535	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	449	THR	2.4
1	A	504	ARG	2.4
1	B	462	ILE	2.4
1	A	233	GLU	2.3
1	B	537	GLU	2.3
1	B	477	GLY	2.3
1	B	574	GLU	2.2
1	A	317	MET	2.2
1	B	396	ARG	2.2
1	B	469	GLU	2.2
1	B	573	HIS	2.1
1	A	682	GLN	2.1
1	A	501	THR	2.1
1	B	567	LEU	2.1
1	A	478	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.