



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 09:04 PM GMT

PDB ID : 3CF1
Title : Structure of P97/vcp in complex with ADP/ADP.alfx
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 4.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

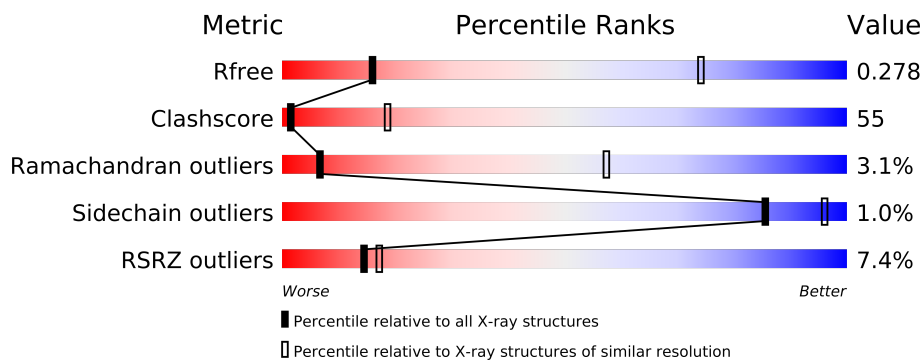
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1020 (5.30-3.50)
Clashscore	79885	1285 (5.30-3.50)
Ramachandran outliers	78287	1214 (5.26-3.50)
Sidechain outliers	78261	1195 (5.26-3.50)
RSRZ outliers	66119	1020 (5.30-3.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	806	
1	B	806	
1	C	806	

2 Entry composition i

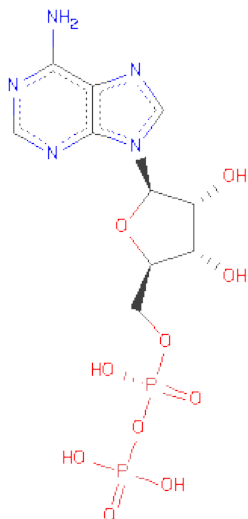
There are 3 unique types of molecules in this entry. The entry contains 17126 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5634	3547	990	1067	30			
1	B	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			
1	C	723	Total	C	N	O	S	0	0	0
			5659	3561	996	1072	30			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



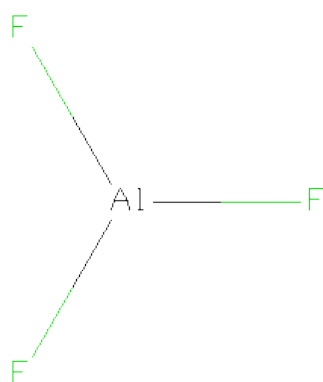
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).

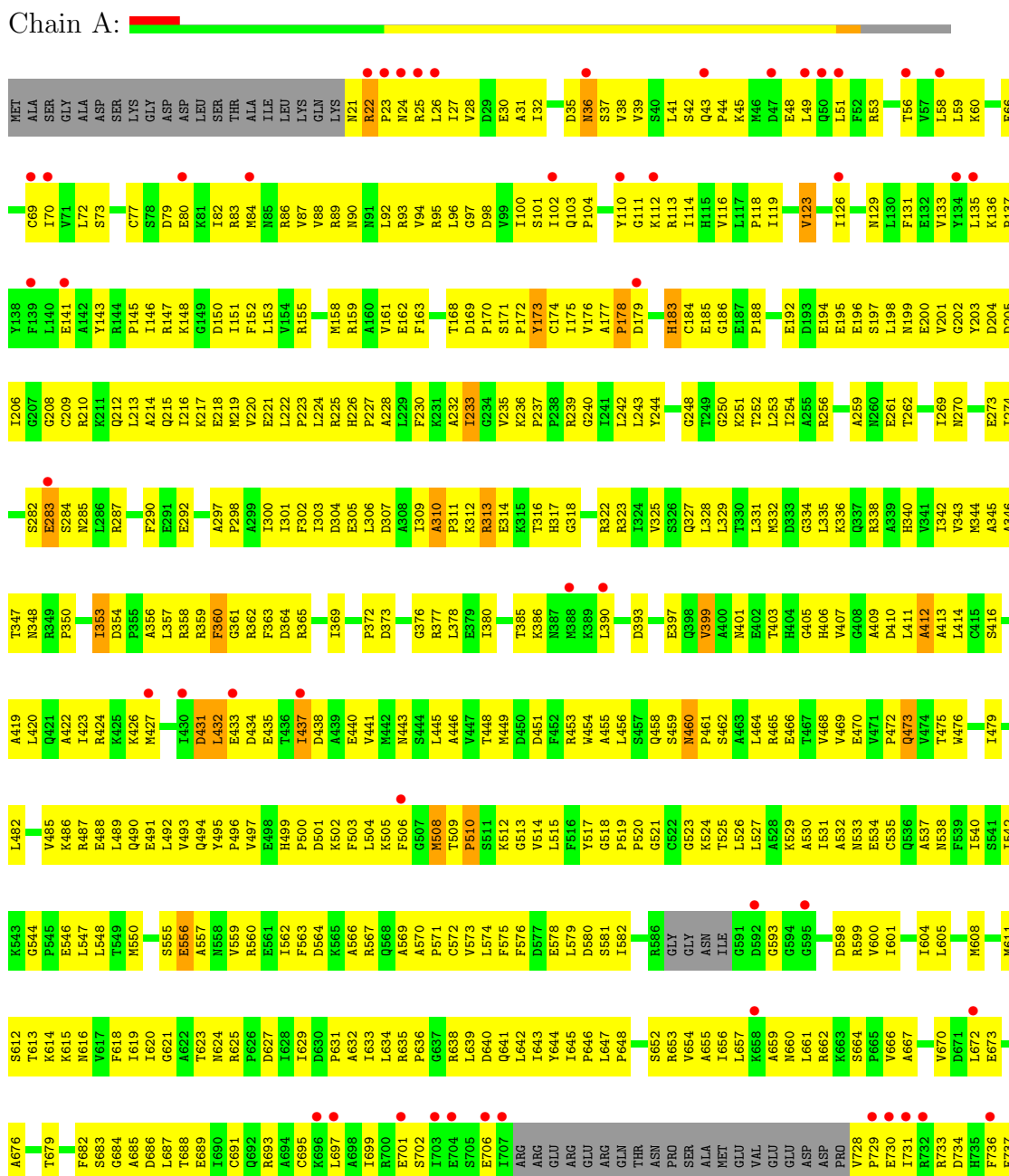


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			4	1	3		
3	B	1	Total	Al	F	0	0
			4	1	3		
3	C	1	Total	Al	F	0	0
			4	1	3		

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: Transitional endoplasmic reticulum ATPase





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.66Å 178.02Å 321.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 4.40 49.60 – 4.40	Depositor EDS
% Data completeness (in resolution range)	82.2 (29.87-4.40) 82.0 (49.60-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.229 , 0.286 0.237 , 0.278	Depositor DCC
R_{free} test set	1621 reflections (6.60%)	DCC
Wilson B-factor (Å ²)	176.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 181.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 28099 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17126	wwPDB-VP
Average B, all atoms (Å ²)	272.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, AF3

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	0.44	6/5724 (0.1%)	0.61	1/7727 (0.0%)
1	B	0.42	2/5751 (0.0%)	0.61	2/7767 (0.0%)
1	C	0.42	1/5751 (0.0%)	0.61	2/7767 (0.0%)
All	All	0.43	9/17226 (0.1%)	0.61	5/23261 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	755	TYR	CE1-CZ	7.97	1.49	1.38
1	A	755	TYR	CD2-CE2	-6.38	1.29	1.39
1	A	755	TYR	CG-CD1	6.23	1.47	1.39
1	A	755	TYR	CE2-CZ	6.20	1.46	1.38
1	B	625	ARG	CD-NE	-6.10	1.36	1.46
1	A	755	TYR	CD1-CE1	-5.63	1.30	1.39
1	A	755	TYR	CG-CD2	5.56	1.46	1.39
1	B	308	ALA	CA-CB	-5.54	1.40	1.52
1	C	755	TYR	CB-CG	-5.14	1.44	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ASP	N-CA-C	8.06	132.75	111.00
1	B	431	ASP	N-CA-C	6.58	128.76	111.00
1	B	706	GLU	N-CA-C	5.90	126.92	111.00
1	C	433	GLU	N-CA-C	5.25	125.16	111.00
1	C	625	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5634	0	5705	657	0
1	B	5659	0	5731	660	0
1	C	5659	0	5731	634	0
2	A	54	0	24	8	0
2	B	54	0	24	14	0
2	C	54	0	24	11	0
3	A	4	0	0	2	0
3	B	4	0	0	9	0
3	C	4	0	0	2	0
All	All	17126	0	17239	1892	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 55.

All (1892) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:427:MET:HG3	1:A:431:ASP:CB	1.69	1.22
1:A:464:LEU:HD11	1:A:466:GLU:HB2	1.22	1.17
1:A:203:TYR:O	1:A:206:ILE:HG12	1.49	1.13
1:A:427:MET:HG3	1:A:431:ASP:HB2	1.20	1.09
1:A:66:GLU:HB2	1:A:147:ARG:NH1	1.68	1.09
1:B:323:ARG:HH22	1:C:279:ALA:HB2	1.19	1.08
1:A:615:LYS:HG3	1:A:616:ASN:H	1.18	1.07
1:B:229:LEU:HD13	1:C:433:GLU:OE2	1.55	1.07
1:B:22:ARG:HG3	1:B:25:ARG:HH12	1.12	1.06
1:B:60:LYS:O	1:B:100:ILE:HG23	1.54	1.06
1:B:615:LYS:HG3	1:B:616:ASN:H	1.15	1.06
1:C:615:LYS:HG3	1:C:616:ASN:H	1.16	1.05
1:B:491:GLU:HA	1:B:495:TYR:CE2	1.91	1.05
1:A:427:MET:CG	1:A:431:ASP:HB2	1.86	1.04
1:C:89:ARG:NE	1:C:96:LEU:HD21	1.72	1.04
1:B:26:LEU:HD11	1:B:45:LYS:HE2	1.36	1.03
1:A:21:ASN:HB2	1:A:25:ARG:NH2	1.72	1.03
1:B:427:MET:HG3	1:B:432:LEU:HD13	1.41	1.03

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:232:ALA:HB2	1:C:125:GLY:HA3	1.41	1.02
1:C:464:LEU:HD11	1:C:466:GLU:HB3	1.40	1.01
1:A:169:ASP:HB3	1:A:170:PRO:HD3	1.42	1.01
1:B:169:ASP:HB3	1:B:170:PRO:HD3	1.44	1.00
1:A:397:GLU:HG2	1:A:401:ASN:HD21	1.24	1.00
1:B:397:GLU:HG2	1:B:401:ASN:HD21	1.23	0.99
1:B:93:ARG:HH21	1:B:194:GLU:HG3	1.25	0.98
1:A:526:LEU:HD11	2:A:900:ADP:H2'	1.45	0.98
1:C:524:LYS:HD3	1:C:622:ALA:HB1	1.44	0.98
1:C:397:GLU:HG2	1:C:401:ASN:HD21	1.22	0.98
1:C:93:ARG:HH21	1:C:194:GLU:HG3	1.24	0.97
1:C:169:ASP:HB3	1:C:170:PRO:HD3	1.45	0.97
1:A:472:PRO:HG2	1:A:532:ALA:HB3	1.44	0.97
1:A:206:ILE:CD1	1:A:213:LEU:HD21	1.95	0.96
1:A:93:ARG:HH21	1:A:194:GLU:HG3	1.25	0.96
1:C:111:GLY:HA2	1:C:170:PRO:HG2	1.47	0.96
1:A:111:GLY:HA2	1:A:170:PRO:HG2	1.48	0.95
1:C:206:ILE:CD1	1:C:213:LEU:HD21	1.97	0.95
1:A:100:ILE:HG22	1:A:101:SER:H	1.29	0.95
1:C:567:ARG:HG3	1:C:615:LYS:HE2	1.46	0.94
1:B:206:ILE:CD1	1:B:213:LEU:HD21	1.98	0.94
1:A:94:VAL:HG21	1:A:100:ILE:HD11	1.48	0.93
1:B:203:TYR:O	1:B:206:ILE:HG12	1.68	0.93
1:C:100:ILE:HG22	1:C:101:SER:H	1.31	0.93
1:B:111:GLY:HA2	1:B:170:PRO:HG2	1.50	0.93
1:C:491:GLU:HA	1:C:495:TYR:CD2	2.04	0.93
1:C:636:PRO:HA	1:C:640:ASP:HB3	1.51	0.93
1:C:94:VAL:HG21	1:C:100:ILE:HD11	1.50	0.93
1:A:224:LEU:HD21	1:A:300:ILE:HD11	1.51	0.92
1:B:464:LEU:HD11	1:B:466:GLU:HB2	1.49	0.92
1:A:627:ASP:HB3	1:A:758:PHE:CZ	2.05	0.92
1:B:636:PRO:HA	1:B:640:ASP:HB3	1.52	0.91
1:B:100:ILE:HG22	1:B:101:SER:H	1.32	0.91
1:C:206:ILE:HD11	1:C:213:LEU:HD11	1.52	0.91
1:A:445:LEU:HD23	1:A:446:ALA:N	1.86	0.91
1:A:636:PRO:HA	1:A:640:ASP:HB3	1.53	0.91
1:B:94:VAL:HG21	1:B:100:ILE:HD11	1.52	0.91
1:C:647:LEU:HB3	1:C:648:PRO:HD2	1.51	0.91
1:B:657:LEU:HD13	1:B:672:LEU:HD22	1.52	0.91
1:C:445:LEU:HD23	1:C:446:ALA:N	1.86	0.90
1:A:206:ILE:HD11	1:A:213:LEU:HD11	1.53	0.89
1:B:445:LEU:HD23	1:B:446:ALA:N	1.87	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:435:GLU:HG3	1:C:436:THR:H	1.36	0.89
1:A:464:LEU:HD11	1:A:466:GLU:CB	2.03	0.89
1:C:209:CYS:HB3	1:C:212:GLN:HB2	1.55	0.89
1:B:136:LYS:HB3	1:B:137:PRO:HD3	1.54	0.89
1:B:472:PRO:HG2	1:B:532:ALA:HB3	1.53	0.88
1:A:206:ILE:HD12	1:A:213:LEU:HD21	1.55	0.88
1:A:476:TRP:HA	1:A:479:ILE:HD13	1.55	0.88
1:A:209:CYS:HB3	1:A:212:GLN:HB2	1.54	0.88
1:C:464:LEU:HD11	1:C:466:GLU:CB	2.03	0.88
1:A:482:LEU:O	1:A:485:VAL:HG22	1.74	0.88
1:B:206:ILE:HD11	1:B:213:LEU:HD11	1.54	0.88
1:A:427:MET:HG3	1:A:431:ASP:HB3	1.56	0.88
1:B:615:LYS:HG3	1:B:616:ASN:N	1.88	0.87
1:B:206:ILE:HD12	1:B:213:LEU:HD21	1.56	0.87
1:C:89:ARG:HE	1:C:96:LEU:HD21	1.33	0.87
1:C:353:ILE:HG22	1:C:354:ASP:H	1.38	0.87
1:C:170:PRO:HB2	1:C:174:CYS:HB3	1.55	0.87
1:C:136:LYS:HB3	1:C:137:PRO:HD3	1.56	0.87
1:B:209:CYS:HB3	1:B:212:GLN:HB2	1.55	0.87
1:B:491:GLU:HA	1:B:495:TYR:CD2	2.10	0.87
1:A:353:ILE:HG22	1:A:354:ASP:H	1.38	0.87
1:B:482:LEU:O	1:B:485:VAL:HG22	1.75	0.87
1:A:433:GLU:HG2	1:A:437:ILE:HD11	1.55	0.87
1:B:170:PRO:HB2	1:B:174:CYS:HB3	1.56	0.87
1:C:491:GLU:HA	1:C:495:TYR:CE2	2.10	0.86
1:B:312:LYS:H	1:B:354:ASP:HB2	1.41	0.86
1:A:563:PHE:HZ	1:A:604:ILE:HG23	1.39	0.86
1:A:491:GLU:HA	1:A:495:TYR:HD2	1.40	0.86
1:A:136:LYS:HB3	1:A:137:PRO:HD3	1.57	0.86
1:C:472:PRO:HG2	1:C:532:ALA:HB3	1.58	0.86
1:C:748:SER:O	1:C:752:ILE:HG13	1.76	0.86
1:C:206:ILE:HD12	1:C:213:LEU:HD21	1.55	0.85
1:B:65:ARG:NH1	1:B:93:ARG:HH12	1.72	0.85
1:B:269:ILE:HB	1:B:303:ILE:HG22	1.57	0.85
1:C:615:LYS:HG3	1:C:616:ASN:N	1.90	0.85
1:A:489:LEU:HD22	1:A:531:ILE:HD13	1.57	0.85
1:B:748:SER:O	1:B:752:ILE:HG13	1.77	0.85
1:B:491:GLU:HA	1:B:495:TYR:HE2	1.38	0.85
1:A:170:PRO:HB2	1:A:174:CYS:HB3	1.57	0.85
1:C:427:MET:SD	1:C:433:GLU:HB2	2.17	0.84
1:A:615:LYS:HG3	1:A:616:ASN:N	1.91	0.84
1:A:475:THR:HG22	1:A:533:ASN:ND2	1.91	0.84

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:506:PHE:CD2	1:B:699:ILE:HG12	2.12	0.84
1:C:482:LEU:O	1:C:485:VAL:HG22	1.77	0.84
1:A:100:ILE:HG22	1:A:101:SER:N	1.93	0.84
1:A:66:GLU:CB	1:A:147:ARG:NH1	2.40	0.83
1:B:502:LYS:NZ	1:C:703:ILE:HG12	1.92	0.83
1:B:353:ILE:HG22	1:B:354:ASP:H	1.40	0.83
1:B:476:TRP:HA	1:B:479:ILE:HD13	1.60	0.83
1:A:653:ARG:HD2	1:A:676:ALA:HA	1.58	0.83
1:B:323:ARG:NH2	1:C:279:ALA:HB2	1.94	0.83
1:A:748:SER:O	1:A:752:ILE:HG13	1.77	0.83
1:B:221:GLU:O	1:B:225:ARG:HB2	1.79	0.82
1:A:240:GLY:HA3	1:A:362:ARG:O	1.80	0.82
1:B:100:ILE:HG22	1:B:101:SER:N	1.94	0.82
1:A:221:GLU:O	1:A:225:ARG:HB2	1.79	0.81
1:A:501:ASP:O	1:A:505:LYS:HG3	1.78	0.81
1:A:579:LEU:HD22	1:A:629:ILE:HD12	1.61	0.81
1:C:476:TRP:HA	1:C:479:ILE:HD13	1.59	0.81
1:C:221:GLU:O	1:C:225:ARG:HB2	1.79	0.81
1:B:240:GLY:HA3	1:B:362:ARG:O	1.81	0.81
1:C:203:TYR:O	1:C:206:ILE:HG12	1.80	0.81
1:A:563:PHE:CZ	1:A:604:ILE:HG23	2.16	0.81
1:C:464:LEU:HG	1:C:466:GLU:H	1.46	0.81
1:B:65:ARG:HH11	1:B:93:ARG:NH1	1.79	0.81
1:B:563:PHE:HZ	1:B:604:ILE:HG23	1.44	0.81
1:A:491:GLU:HA	1:A:495:TYR:CD2	2.17	0.80
1:A:155:ARG:NH2	1:A:386:LYS:HZ3	1.80	0.80
1:C:100:ILE:HG22	1:C:101:SER:N	1.94	0.80
1:C:475:THR:HG22	1:C:533:ASN:ND2	1.97	0.80
1:C:464:LEU:CD1	1:C:466:GLU:HB3	2.12	0.80
1:C:133:VAL:HG21	1:C:439:ALA:HB1	1.63	0.80
1:A:397:GLU:HG2	1:A:401:ASN:ND2	1.97	0.79
1:B:397:GLU:HG2	1:B:401:ASN:ND2	1.96	0.79
1:C:397:GLU:HG2	1:C:401:ASN:ND2	1.96	0.79
1:B:497:VAL:HG13	1:B:498:GLU:HG3	1.64	0.79
1:C:269:ILE:HB	1:C:303:ILE:HG22	1.64	0.79
1:B:540:ILE:HD12	1:B:566:ALA:HB2	1.64	0.79
1:B:282:SER:HA	1:B:285:ASN:HD22	1.47	0.79
1:A:66:GLU:HB2	1:A:147:ARG:HH12	1.41	0.79
1:B:26:LEU:HD21	1:B:45:LYS:NZ	1.98	0.79
1:C:523:GLY:HA2	2:C:900:ADP:O1A	1.83	0.79
1:A:758:PHE:HB3	1:A:762:LEU:HD11	1.62	0.79
1:A:66:GLU:CB	1:A:147:ARG:HH12	1.94	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:SER:HA	1:A:285:ASN:HD22	1.48	0.79
1:C:282:SER:HA	1:C:285:ASN:HD22	1.47	0.78
1:C:579:LEU:O	1:C:579:LEU:HD23	1.83	0.78
1:B:590:ILE:HG13	1:B:591:GLY:H	1.46	0.78
1:B:469:VAL:HG21	1:B:565:LYS:HE3	1.65	0.78
1:B:519:PRO:HG2	1:B:522:CYS:SG	2.22	0.78
1:C:240:GLY:HA3	1:C:362:ARG:O	1.84	0.78
1:B:427:MET:CE	1:B:432:LEU:HB2	2.12	0.78
1:A:21:ASN:HB2	1:A:25:ARG:HH21	1.43	0.78
1:C:60:LYS:HE3	1:C:103:GLN:HE22	1.47	0.78
1:B:22:ARG:CG	1:B:25:ARG:HH12	1.93	0.78
1:A:378:LEU:HD13	1:A:397:GLU:HA	1.66	0.78
1:C:224:LEU:HD21	1:C:300:ILE:HD11	1.65	0.78
1:B:523:GLY:HA2	2:B:900:ADP:O1A	1.83	0.78
1:B:495:TYR:CD1	1:C:703:ILE:HD13	2.19	0.78
1:B:378:LEU:HD13	1:B:397:GLU:HA	1.66	0.78
1:A:110:TYR:HD2	1:A:177:ALA:HB2	1.48	0.77
1:B:427:MET:HG3	1:B:432:LEU:CD1	2.12	0.77
1:A:364:ASP:OD1	1:A:365:ARG:HG2	1.84	0.77
1:C:659:ALA:HA	1:C:662:ARG:HG3	1.66	0.77
1:A:652:SER:O	1:A:656:ILE:HG13	1.85	0.77
1:C:155:ARG:NH2	1:C:386:LYS:HZ3	1.83	0.77
1:B:22:ARG:HG3	1:B:25:ARG:NH1	1.96	0.77
1:B:464:LEU:HG	1:B:466:GLU:H	1.49	0.77
1:C:548:LEU:HD21	1:C:581:SER:O	1.83	0.77
1:A:433:GLU:HG2	1:A:437:ILE:CD1	2.14	0.76
1:C:206:ILE:CD1	1:C:213:LEU:HD11	2.15	0.76
1:B:110:TYR:HD2	1:B:177:ALA:HB2	1.49	0.76
1:C:113:ARG:HH21	1:C:183:HIS:CE1	2.03	0.76
1:A:90:ASN:HD22	1:A:198:LEU:CD2	1.99	0.76
1:A:548:LEU:HD21	1:A:581:SER:O	1.85	0.76
1:C:634:LEU:HD22	1:C:642:LEU:HD11	1.68	0.76
1:B:521:GLY:HA3	1:B:685:ALA:HB2	1.66	0.76
1:C:378:LEU:HD13	1:C:397:GLU:HA	1.66	0.76
1:B:650:GLU:O	1:B:654:VAL:HG23	1.87	0.75
1:A:579:LEU:HD23	1:A:579:LEU:O	1.85	0.75
1:C:90:ASN:HD22	1:C:198:LEU:CD2	2.00	0.75
1:B:364:ASP:OD1	1:B:365:ARG:HG2	1.85	0.75
1:A:155:ARG:HH21	1:A:386:LYS:HZ3	1.34	0.75
1:B:206:ILE:CD1	1:B:213:LEU:HD11	2.16	0.75
1:A:489:LEU:HD22	1:A:531:ILE:CD1	2.17	0.75
1:A:113:ARG:HH21	1:A:183:HIS:CE1	2.05	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:113:ARG:HH21	1:B:183:HIS:CE1	2.05	0.75
1:C:515:LEU:HD13	1:C:634:LEU:HD21	1.69	0.75
1:C:499:HIS:N	1:C:500:PRO:HD3	2.00	0.75
1:C:143:TYR:HA	1:C:176:VAL:O	1.85	0.75
1:C:459:SER:C	1:C:461:PRO:HD2	2.07	0.74
1:B:464:LEU:HD11	1:B:466:GLU:CB	2.17	0.74
1:A:311:PRO:C	1:A:313:ARG:H	1.85	0.74
1:B:143:TYR:HA	1:B:176:VAL:O	1.86	0.74
1:C:364:ASP:OD1	1:C:365:ARG:HG2	1.87	0.74
1:C:665:PRO:O	1:C:731:ILE:HB	1.88	0.74
1:C:521:GLY:HA2	1:C:685:ALA:HB2	1.67	0.74
1:B:634:LEU:HD22	1:B:642:LEU:HD11	1.69	0.74
1:A:143:TYR:HA	1:A:176:VAL:O	1.87	0.74
1:B:90:ASN:HD22	1:B:198:LEU:CD2	2.00	0.74
1:B:658:LYS:O	1:B:662:ARG:HB2	1.87	0.74
1:B:615:LYS:CG	1:B:616:ASN:H	1.99	0.74
1:B:499:HIS:N	1:B:500:PRO:HD3	2.03	0.74
1:B:312:LYS:HB3	1:B:354:ASP:CG	2.08	0.74
1:A:206:ILE:CD1	1:A:213:LEU:HD11	2.17	0.74
1:B:647:LEU:HB3	1:B:648:PRO:HD2	1.69	0.74
1:C:110:TYR:HD2	1:C:177:ALA:HB2	1.53	0.74
1:C:435:GLU:HG3	1:C:436:THR:N	2.03	0.73
1:A:427:MET:SD	1:A:437:ILE:HD11	2.27	0.73
1:A:634:LEU:HD22	1:A:642:LEU:HD11	1.69	0.73
1:C:563:PHE:HZ	1:C:604:ILE:HG23	1.53	0.73
1:A:437:ILE:CG2	1:A:438:ASP:N	2.50	0.73
1:C:615:LYS:CG	1:C:616:ASN:H	2.00	0.73
1:A:647:LEU:HB3	1:A:648:PRO:HD2	1.69	0.73
1:C:270:ASN:HB2	1:C:273:GLU:HB2	1.70	0.73
1:C:89:ARG:CZ	1:C:96:LEU:HD21	2.18	0.73
1:A:758:PHE:O	1:A:762:LEU:HG	1.88	0.73
1:B:155:ARG:HH21	1:B:386:LYS:NZ	1.87	0.73
1:B:270:ASN:HB2	1:B:273:GLU:HB2	1.71	0.73
1:C:39:VAL:HG11	1:C:59:LEU:HD11	1.69	0.73
1:A:519:PRO:HD3	1:A:755:TYR:HD2	1.53	0.73
1:A:129:ASN:O	1:A:133:VAL:HG23	1.88	0.73
1:A:633:ILE:CG2	1:A:639:LEU:HD12	2.19	0.73
1:A:270:ASN:HB2	1:A:273:GLU:HB2	1.70	0.73
1:B:147:ARG:HG2	1:B:148:LYS:N	2.04	0.73
1:A:475:THR:HG22	1:A:533:ASN:HD21	1.54	0.72
1:A:317:HIS:CE1	1:B:317:HIS:NE2	2.57	0.72
1:A:313:ARG:HG2	1:A:314:GLU:H	1.53	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:ASN:O	1:B:133:VAL:HG23	1.89	0.72
1:C:32:ILE:HG12	1:C:83:ARG:HD3	1.70	0.72
1:A:506:PHE:HD2	1:B:699:ILE:HG12	1.52	0.72
1:C:633:ILE:CG2	1:C:639:LEU:HD12	2.19	0.72
1:C:599:ARG:HB3	1:C:599:ARG:NH1	2.04	0.72
1:B:627:ASP:HB3	1:B:758:PHE:CZ	2.24	0.72
1:B:563:PHE:CZ	1:B:604:ILE:HG23	2.25	0.72
1:C:309:ILE:C	1:C:311:PRO:HD2	2.10	0.72
1:A:437:ILE:HG23	1:A:438:ASP:N	2.02	0.72
1:B:582:ILE:HD12	1:B:601:ILE:HG12	1.72	0.72
1:C:155:ARG:HH21	1:C:386:LYS:HZ3	1.35	0.72
1:A:100:ILE:CG2	1:A:101:SER:H	2.02	0.72
1:C:129:ASN:O	1:C:133:VAL:HG23	1.90	0.72
1:A:32:ILE:HG12	1:A:83:ARG:HD3	1.71	0.72
1:C:90:ASN:ND2	1:C:198:LEU:HD23	2.04	0.72
1:B:427:MET:HE2	1:B:441:VAL:HG11	1.71	0.71
1:C:515:LEU:HD13	1:C:634:LEU:CD2	2.20	0.71
1:A:80:GLU:HG2	1:B:429:LEU:HD13	1.72	0.71
1:B:633:ILE:CG2	1:B:639:LEU:HD12	2.19	0.71
1:A:627:ASP:HB3	1:A:758:PHE:CE1	2.26	0.71
1:B:599:ARG:NH1	1:B:599:ARG:HB3	2.05	0.71
1:A:60:LYS:O	1:A:100:ILE:HG23	1.91	0.71
1:B:90:ASN:ND2	1:B:198:LEU:HD23	2.05	0.71
1:A:90:ASN:ND2	1:A:198:LEU:HD23	2.05	0.71
1:A:147:ARG:HG2	1:A:148:LYS:N	2.04	0.71
1:A:232:ALA:HB2	1:B:125:GLY:HA3	1.72	0.71
1:A:599:ARG:NH1	1:A:599:ARG:HB3	2.04	0.71
1:B:232:ALA:HB2	1:C:125:GLY:CA	2.19	0.71
1:A:582:ILE:HD13	1:A:600:VAL:HB	1.73	0.71
1:A:427:MET:CE	1:A:437:ILE:HD12	2.20	0.71
1:A:615:LYS:CG	1:A:616:ASN:H	2.01	0.71
1:A:612:SER:HB3	1:A:615:LYS:HB2	1.73	0.70
1:B:612:SER:HB3	1:B:615:LYS:HB2	1.73	0.70
1:B:100:ILE:CG2	1:B:101:SER:H	2.03	0.70
1:B:155:ARG:HE	1:B:386:LYS:HZ3	1.40	0.70
1:A:230:PHE:HA	1:A:233:ILE:HG22	1.72	0.70
1:C:427:MET:HG2	1:C:433:GLU:HB2	1.74	0.70
1:B:203:TYR:CE2	1:B:261:GLU:HG2	2.27	0.70
1:C:100:ILE:CG2	1:C:101:SER:H	2.04	0.70
1:C:92:LEU:HD13	1:C:100:ILE:HD13	1.73	0.70
1:B:749:ASP:HA	1:B:752:ILE:HD12	1.74	0.69
1:B:514:VAL:HG23	1:B:618:PHE:HZ	1.57	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:611:MET:HE3	1:A:619:ILE:HD11	1.72	0.69
1:C:460:ASN:N	1:C:461:PRO:CD	2.56	0.69
1:B:230:PHE:HA	1:B:233:ILE:HG22	1.73	0.69
1:B:230:PHE:HA	1:B:233:ILE:CG2	2.22	0.69
1:C:512:LYS:HZ1	1:C:611:MET:HB3	1.56	0.69
1:B:490:GLN:HB3	1:B:494:GLN:HG3	1.74	0.69
1:A:92:LEU:HD13	1:A:100:ILE:HD13	1.73	0.69
1:B:323:ARG:HH22	1:C:279:ALA:CB	2.02	0.69
1:C:612:SER:HB3	1:C:615:LYS:HB2	1.74	0.69
1:B:502:LYS:HZ2	1:C:703:ILE:HG12	1.57	0.69
1:B:32:ILE:HG12	1:B:83:ARG:HD3	1.72	0.69
1:B:155:ARG:NE	1:B:386:LYS:HZ3	1.91	0.69
1:C:427:MET:CG	1:C:433:GLU:HB2	2.23	0.69
1:C:63:LYS:O	1:C:65:ARG:HG3	1.93	0.69
1:C:62:LYS:NZ	1:C:98:ASP:HB3	2.07	0.69
1:B:514:VAL:HG11	1:B:643:ILE:HD12	1.74	0.69
1:B:92:LEU:HD13	1:B:100:ILE:HD13	1.74	0.69
1:B:65:ARG:NH1	1:B:93:ARG:NH1	2.38	0.69
1:A:93:ARG:HE	1:A:194:GLU:HB2	1.56	0.69
1:A:407:VAL:HG22	1:A:410:ASP:OD2	1.93	0.69
1:A:307:ASP:O	1:A:311:PRO:HD3	1.92	0.69
1:B:573:VAL:HG12	1:B:618:PHE:HB3	1.74	0.69
1:C:497:VAL:HG13	1:C:498:GLU:HG3	1.73	0.69
1:B:502:LYS:HB3	1:C:699:ILE:HG23	1.75	0.69
1:C:250:GLY:HA2	2:C:807:ADP:PA	2.33	0.69
1:A:749:ASP:HA	1:A:752:ILE:HD12	1.74	0.69
1:C:475:THR:HG22	1:C:533:ASN:HD21	1.57	0.69
1:A:110:TYR:CD2	1:A:177:ALA:HB2	2.28	0.69
1:B:110:TYR:CD2	1:B:177:ALA:HB2	2.28	0.69
1:A:26:LEU:HD21	1:A:45:LYS:NZ	2.07	0.69
1:C:403:THR:HB	1:C:406:HIS:CG	2.27	0.69
1:B:244:TYR:CE1	1:B:350:PRO:HG3	2.28	0.69
1:A:433:GLU:C	1:A:434:ASP:CA	2.61	0.69
1:A:230:PHE:HA	1:A:233:ILE:CG2	2.23	0.69
1:A:155:ARG:HH21	1:A:386:LYS:NZ	1.91	0.68
1:C:653:ARG:CD	1:C:679:THR:O	2.41	0.68
1:B:403:THR:HB	1:B:406:HIS:CG	2.28	0.68
1:A:44:PRO:HG2	1:A:79:ASP:OD1	1.93	0.68
1:B:224:LEU:HD21	1:B:300:ILE:HD11	1.75	0.68
1:B:65:ARG:HH11	1:B:93:ARG:HH12	1.40	0.68
1:C:512:LYS:NZ	1:C:611:MET:HB3	2.09	0.68
1:C:244:TYR:CE1	1:C:350:PRO:HG3	2.29	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:749:ASP:HA	1:C:752:ILE:HD12	1.74	0.68
1:C:733:ARG:HB2	1:C:733:ARG:NH1	2.09	0.68
1:A:303:ILE:HD11	1:A:345:ALA:HB2	1.76	0.68
1:C:312:LYS:HB3	1:C:354:ASP:CB	2.23	0.68
1:A:635:ARG:NH1	1:A:635:ARG:HB3	2.09	0.68
1:B:60:LYS:HB2	1:B:101:SER:OG	1.94	0.68
1:A:734:ASP:O	1:A:738:GLU:HB2	1.94	0.68
1:A:437:ILE:HG23	1:A:438:ASP:H	1.59	0.68
1:B:734:ASP:O	1:B:738:GLU:HB2	1.94	0.68
1:C:734:ASP:O	1:C:738:GLU:HB2	1.94	0.68
1:A:244:TYR:CE1	1:A:350:PRO:HG3	2.29	0.68
1:C:147:ARG:HG2	1:C:148:LYS:N	2.07	0.68
1:C:66:GLU:HB2	1:C:147:ARG:NH1	2.09	0.68
1:B:90:ASN:HD22	1:B:198:LEU:HD23	1.59	0.68
1:A:633:ILE:O	1:A:639:LEU:HB2	1.94	0.68
1:A:492:LEU:O	1:A:496:PRO:HG3	1.95	0.67
1:C:155:ARG:HH21	1:C:386:LYS:NZ	1.92	0.67
1:B:244:TYR:CZ	1:B:350:PRO:HG3	2.29	0.67
1:C:244:TYR:CZ	1:C:350:PRO:HG3	2.29	0.67
1:A:403:THR:HB	1:A:406:HIS:CG	2.28	0.67
1:C:407:VAL:HG22	1:C:410:ASP:OD2	1.93	0.67
1:B:70:ILE:HD11	1:B:145:PRO:HG3	1.76	0.67
1:A:633:ILE:HG22	1:A:639:LEU:HD12	1.75	0.67
1:B:407:VAL:HG22	1:B:410:ASP:OD2	1.94	0.67
1:C:230:PHE:HA	1:C:233:ILE:HG22	1.74	0.67
1:A:733:ARG:HB2	1:A:733:ARG:NH1	2.09	0.67
1:C:524:LYS:HB2	3:C:915:AF3:F2	1.84	0.67
1:A:514:VAL:HG23	1:A:618:PHE:HZ	1.60	0.67
1:A:758:PHE:HB3	1:A:762:LEU:CD1	2.24	0.67
1:A:357:LEU:HB3	1:A:363:PHE:HD2	1.59	0.67
1:C:635:ARG:NH1	1:C:635:ARG:HB3	2.10	0.67
1:C:63:LYS:HD2	1:C:93:ARG:HD2	1.77	0.67
1:A:503:PHE:HA	1:B:699:ILE:HD13	1.77	0.67
1:A:656:ILE:HG21	1:A:687:LEU:HD12	1.76	0.67
1:B:733:ARG:HB2	1:B:733:ARG:NH1	2.10	0.67
1:A:702:SER:O	1:A:706:GLU:HG3	1.94	0.67
1:C:230:PHE:HA	1:C:233:ILE:CG2	2.24	0.67
1:C:538:ASN:O	1:C:573:VAL:HG22	1.95	0.67
1:C:633:ILE:HG22	1:C:639:LEU:HD12	1.76	0.67
1:A:90:ASN:HD22	1:A:198:LEU:HD23	1.59	0.67
1:B:633:ILE:HG22	1:B:639:LEU:HD12	1.75	0.67
1:B:633:ILE:O	1:B:639:LEU:HB2	1.95	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:503:PHE:HD2	1:C:504:LEU:HD22	1.60	0.66
1:C:70:ILE:HD11	1:C:145:PRO:HG3	1.76	0.66
1:A:582:ILE:HD12	1:A:601:ILE:HG12	1.77	0.66
1:B:479:ILE:N	1:B:479:ILE:HD12	2.10	0.66
1:A:244:TYR:CZ	1:A:350:PRO:HG3	2.30	0.66
1:C:543:LYS:HA	1:C:577:ASP:HB3	1.78	0.66
1:B:201:VAL:HG21	1:B:256:ARG:HD2	1.77	0.66
1:A:427:MET:SD	1:A:437:ILE:CD1	2.82	0.66
1:C:93:ARG:HE	1:C:194:GLU:HB2	1.59	0.66
1:C:587:GLY:HA3	1:C:591:GLY:HA2	1.76	0.66
1:A:70:ILE:HD11	1:A:145:PRO:HG3	1.77	0.66
1:C:357:LEU:HB3	1:C:363:PHE:HD2	1.60	0.66
1:A:599:ARG:HH11	1:A:599:ARG:HB3	1.61	0.66
1:B:635:ARG:NH1	1:B:635:ARG:HB3	2.10	0.66
1:B:93:ARG:HE	1:B:194:GLU:HB2	1.60	0.66
1:C:641:GLN:C	1:C:642:LEU:HD22	2.16	0.66
1:B:653:ARG:CD	1:B:679:THR:O	2.44	0.66
1:C:633:ILE:O	1:C:639:LEU:HB2	1.94	0.66
1:C:647:LEU:HD12	1:C:647:LEU:H	1.60	0.66
1:B:329:LEU:HD13	1:C:272:PRO:HG2	1.78	0.66
1:C:563:PHE:CZ	1:C:604:ILE:HG23	2.29	0.66
1:C:599:ARG:HH11	1:C:599:ARG:HB3	1.61	0.66
1:A:306:LEU:HD22	1:A:345:ALA:HB1	1.78	0.66
1:A:169:ASP:CB	1:A:170:PRO:HD3	2.23	0.66
1:A:641:GLN:C	1:A:642:LEU:HD22	2.16	0.66
1:C:26:LEU:HD11	1:C:45:LYS:HE2	1.78	0.66
1:A:26:LEU:O	1:A:27:ILE:HD13	1.96	0.66
1:B:641:GLN:C	1:B:642:LEU:HD22	2.16	0.66
1:A:208:GLY:HA2	1:A:210:ARG:NH1	2.11	0.66
1:A:113:ARG:HG2	1:A:113:ARG:HH11	1.61	0.66
1:B:312:LYS:HB3	1:B:354:ASP:OD2	1.96	0.66
1:C:110:TYR:CD2	1:C:177:ALA:HB2	2.31	0.66
1:C:113:ARG:HH11	1:C:113:ARG:HG2	1.61	0.66
1:B:44:PRO:HG2	1:B:79:ASP:OD1	1.96	0.66
1:B:496:PRO:O	1:B:500:PRO:HG3	1.96	0.65
1:B:579:LEU:HD22	1:B:629:ILE:CD1	2.25	0.65
1:B:741:ARG:HE	1:B:741:ARG:HA	1.61	0.65
1:C:516:PHE:O	1:C:622:ALA:HA	1.97	0.65
1:A:500:PRO:O	1:A:504:LEU:HD13	1.96	0.65
1:C:741:ARG:HE	1:C:741:ARG:HA	1.61	0.65
1:A:741:ARG:HE	1:A:741:ARG:HA	1.62	0.65
1:B:495:TYR:HD1	1:C:703:ILE:HD13	1.61	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:169:ASP:CB	1:B:170:PRO:HD3	2.24	0.65
1:C:60:LYS:HB2	1:C:101:SER:OG	1.96	0.65
1:C:203:TYR:CE2	1:C:261:GLU:HG2	2.32	0.65
1:C:60:LYS:HE3	1:C:103:GLN:NE2	2.12	0.65
1:A:499:HIS:N	1:A:500:PRO:HD3	2.11	0.65
1:B:357:LEU:HB3	1:B:363:PHE:HD2	1.61	0.65
1:A:311:PRO:C	1:A:313:ARG:N	2.49	0.65
1:C:237:PRO:O	1:C:239:ARG:HG3	1.96	0.65
1:A:579:LEU:HD22	1:A:629:ILE:CD1	2.27	0.65
1:C:44:PRO:HG2	1:C:79:ASP:OD1	1.96	0.65
1:B:119:ILE:HD12	1:B:162:GLU:HB2	1.79	0.65
1:B:502:LYS:HA	1:B:505:LYS:HG3	1.77	0.65
1:B:520:PRO:HA	3:B:915:AF3:F2	1.86	0.65
1:A:216:ILE:HA	1:A:219:MET:HE3	1.77	0.65
1:B:113:ARG:HG2	1:B:113:ARG:HH11	1.62	0.65
1:C:667:ALA:HB2	1:C:731:ILE:O	1.97	0.65
1:A:435:GLU:HA	1:A:435:GLU:OE1	1.97	0.65
1:C:501:ASP:OD1	1:C:502:LYS:HD2	1.96	0.65
1:A:114:ILE:HD11	1:A:176:VAL:HG22	1.77	0.65
1:B:237:PRO:O	1:B:239:ARG:HG3	1.97	0.65
1:C:89:ARG:NE	1:C:96:LEU:CD2	2.54	0.65
1:C:491:GLU:HA	1:C:495:TYR:HD2	1.58	0.65
1:B:495:TYR:CD1	1:C:703:ILE:CD1	2.80	0.64
1:A:517:TYR:C	1:A:524:LYS:HE2	2.17	0.64
1:A:210:ARG:HD2	1:A:210:ARG:H	1.62	0.64
1:B:313:ARG:HG2	1:B:314:GLU:H	1.62	0.64
1:B:500:PRO:O	1:B:504:LEU:HD13	1.98	0.64
1:B:155:ARG:NH2	1:B:386:LYS:HZ3	1.94	0.64
1:B:427:MET:CG	1:B:432:LEU:HD13	2.25	0.64
1:B:208:GLY:HA2	1:B:210:ARG:NH1	2.12	0.64
1:A:654:VAL:HG22	1:A:676:ALA:HB2	1.78	0.64
1:A:512:LYS:HZ3	1:A:608:MET:CG	2.10	0.64
1:C:496:PRO:O	1:C:500:PRO:HG3	1.96	0.64
1:C:208:GLY:HA2	1:C:210:ARG:NH1	2.12	0.64
1:A:237:PRO:O	1:A:239:ARG:HG3	1.97	0.64
1:B:153:LEU:HD12	1:B:161:VAL:O	1.97	0.64
1:B:548:LEU:HD21	1:B:581:SER:O	1.98	0.64
1:B:664:SER:HB3	1:B:665:PRO:HD2	1.79	0.64
1:C:427:MET:CE	1:C:441:VAL:HG11	2.28	0.64
1:C:479:ILE:N	1:C:479:ILE:HD12	2.13	0.64
1:B:210:ARG:HD2	1:B:210:ARG:H	1.63	0.64
1:A:323:ARG:HH22	1:B:279:ALA:HB2	1.62	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:574:LEU:HG	1:A:576:PHE:HE1	1.63	0.64
1:B:155:ARG:HH21	1:B:386:LYS:HZ3	1.46	0.63
1:A:612:SER:CB	1:A:615:LYS:HB2	2.29	0.63
1:B:574:LEU:HG	1:B:576:PHE:CE1	2.33	0.63
1:C:373:ASP:HA	1:C:377:ARG:HH12	1.63	0.63
1:A:582:ILE:CD1	1:A:600:VAL:HB	2.27	0.63
1:B:599:ARG:HH11	1:B:599:ARG:HB3	1.61	0.63
1:B:580:ASP:OD2	1:B:584:LYS:NZ	2.31	0.63
1:C:119:ILE:HD12	1:C:162:GLU:HB2	1.81	0.63
1:C:503:PHE:HZ	1:C:510:PRO:N	1.97	0.63
1:B:472:PRO:HB2	1:B:533:ASN:HB2	1.80	0.63
1:A:119:ILE:HD12	1:A:162:GLU:HB2	1.81	0.63
1:C:259:ALA:HB2	1:C:300:ILE:HD12	1.81	0.63
1:C:114:ILE:HD11	1:C:176:VAL:HG22	1.79	0.63
1:C:270:ASN:O	1:C:273:GLU:HB3	1.99	0.63
1:B:373:ASP:HA	1:B:377:ARG:HH12	1.63	0.63
1:B:233:ILE:HD13	1:C:442:MET:CE	2.29	0.63
1:C:170:PRO:HB2	1:C:174:CYS:CB	2.29	0.63
1:B:251:LYS:HD3	1:B:346:ALA:HB1	1.80	0.63
1:A:222:LEU:HD12	1:B:420:LEU:HD22	1.81	0.63
1:C:758:PHE:HB3	1:C:762:LEU:CD1	2.27	0.63
1:A:49:LEU:HD12	1:A:49:LEU:N	2.14	0.63
1:C:155:ARG:HE	1:C:386:LYS:NZ	1.96	0.62
1:A:153:LEU:HD12	1:A:161:VAL:O	2.00	0.62
1:B:283:GLU:O	1:B:287:ARG:HB2	1.99	0.62
1:A:270:ASN:O	1:A:273:GLU:HB3	1.99	0.62
1:C:153:LEU:HD12	1:C:161:VAL:O	1.99	0.62
1:A:472:PRO:HG2	1:A:532:ALA:CB	2.24	0.62
1:B:645:ILE:HD12	1:B:645:ILE:N	2.15	0.62
1:A:373:ASP:HA	1:A:377:ARG:HH12	1.62	0.62
1:A:465:ARG:HB3	1:A:465:ARG:HH11	1.63	0.62
1:B:612:SER:CB	1:B:615:LYS:HB2	2.29	0.62
1:B:378:LEU:CD1	1:B:397:GLU:HA	2.29	0.62
1:C:169:ASP:CB	1:C:170:PRO:HD3	2.26	0.62
1:C:59:LEU:HD13	1:C:92:LEU:HD11	1.82	0.62
1:A:201:VAL:HG21	1:A:256:ARG:HD2	1.82	0.62
1:C:201:VAL:HG21	1:C:256:ARG:HD2	1.81	0.62
1:A:378:LEU:CD1	1:A:397:GLU:HA	2.29	0.62
1:C:210:ARG:H	1:C:210:ARG:HD2	1.65	0.62
1:A:250:GLY:HA2	2:A:807:ADP:PA	2.39	0.62
1:A:307:ASP:HA	1:A:310:ALA:HB3	1.81	0.62
1:B:49:LEU:HD12	1:B:49:LEU:N	2.14	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:LEU:HD21	1:C:45:LYS:NZ	2.15	0.62
1:B:524:LYS:HB2	1:B:524:LYS:NZ	2.15	0.62
1:A:479:ILE:N	1:A:479:ILE:HD12	2.13	0.62
1:C:251:LYS:HD3	1:C:346:ALA:HB1	1.81	0.62
1:A:251:LYS:HD3	1:A:346:ALA:HB1	1.80	0.62
1:B:114:ILE:HD11	1:B:176:VAL:HG22	1.80	0.62
1:C:242:LEU:C	1:C:243:LEU:HD12	2.20	0.62
1:C:49:LEU:N	1:C:49:LEU:HD12	2.15	0.62
1:A:242:LEU:C	1:A:243:LEU:HD12	2.20	0.62
1:A:283:GLU:O	1:A:287:ARG:HB2	2.00	0.62
1:C:90:ASN:HD22	1:C:198:LEU:HD23	1.58	0.62
1:A:427:MET:CE	1:A:441:VAL:HG11	2.30	0.61
1:C:612:SER:CB	1:C:615:LYS:HB2	2.29	0.61
1:C:312:LYS:HB3	1:C:354:ASP:CG	2.20	0.61
1:C:270:ASN:HB2	1:C:273:GLU:CB	2.30	0.61
1:B:242:LEU:C	1:B:243:LEU:HD12	2.20	0.61
1:B:501:ASP:OD1	1:B:502:LYS:HG3	2.01	0.61
1:B:582:ILE:HD11	1:B:600:VAL:HB	1.80	0.61
1:B:158:MET:HE1	1:B:419:ALA:HB1	1.82	0.61
1:B:230:PHE:HB2	1:B:340:HIS:NE2	2.15	0.61
1:B:466:GLU:HG2	1:B:467:THR:HG23	1.82	0.61
1:A:657:LEU:HD13	1:A:672:LEU:HD22	1.82	0.61
1:A:230:PHE:HB2	1:A:340:HIS:NE2	2.16	0.61
1:A:297:ALA:HA	1:A:298:PRO:C	2.20	0.61
1:C:297:ALA:HA	1:C:298:PRO:C	2.20	0.61
1:C:522:CYS:O	2:C:900:ADP:N7	2.33	0.61
1:B:579:LEU:O	1:B:579:LEU:HD23	2.00	0.61
1:C:206:ILE:HD11	1:C:213:LEU:CD1	2.28	0.61
1:A:578:GLU:HB3	1:A:581:SER:HB3	1.83	0.61
1:B:316:THR:OG1	1:B:322:ARG:HG2	2.00	0.61
1:A:90:ASN:ND2	1:A:198:LEU:CD2	2.63	0.61
1:B:270:ASN:O	1:B:273:GLU:HB3	2.00	0.61
1:A:567:ARG:NH1	1:A:567:ARG:HB2	2.16	0.60
1:C:647:LEU:HB3	1:C:648:PRO:CD	2.25	0.60
1:C:378:LEU:CD1	1:C:397:GLU:HA	2.29	0.60
1:A:177:ALA:C	1:A:179:ASP:H	2.04	0.60
1:A:153:LEU:HD13	1:A:162:GLU:HG2	1.83	0.60
1:B:758:PHE:HB3	1:B:762:LEU:HD11	1.82	0.60
1:C:230:PHE:HB2	1:C:340:HIS:NE2	2.15	0.60
1:B:297:ALA:HA	1:B:298:PRO:C	2.21	0.60
1:C:283:GLU:O	1:C:287:ARG:HB2	2.00	0.60
1:A:580:ASP:OD2	1:A:625:ARG:HB2	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:ILE:HA	1:B:219:MET:HE3	1.83	0.60
1:A:233:ILE:HD11	1:B:158:MET:SD	2.42	0.60
1:B:239:ARG:HH12	1:B:336:LYS:HB2	1.66	0.60
1:B:427:MET:CE	1:B:441:VAL:HG11	2.31	0.60
1:B:213:LEU:HB3	1:B:217:LYS:HE3	1.84	0.60
1:C:155:ARG:CZ	1:C:386:LYS:HZ3	2.14	0.60
1:A:313:ARG:HG2	1:A:314:GLU:N	2.16	0.60
1:C:503:PHE:CZ	1:C:510:PRO:N	2.70	0.60
1:A:155:ARG:CZ	1:A:386:LYS:HZ3	2.14	0.60
1:A:501:ASP:OD1	1:A:502:LYS:HG3	2.01	0.60
1:A:567:ARG:HD3	1:B:460:ASN:ND2	2.17	0.60
1:C:111:GLY:CA	1:C:170:PRO:HG2	2.29	0.60
1:A:493:VAL:HG21	1:A:531:ILE:HD11	1.84	0.60
1:B:270:ASN:HB2	1:B:273:GLU:CB	2.31	0.60
1:A:270:ASN:HB2	1:A:273:GLU:CB	2.30	0.60
1:C:656:ILE:HG23	2:C:900:ADP:C2	2.37	0.60
1:B:177:ALA:C	1:B:179:ASP:H	2.05	0.59
1:B:593:GLY:O	1:C:587:GLY:HA2	2.01	0.59
1:A:239:ARG:HH12	1:A:336:LYS:HB2	1.67	0.59
1:C:201:VAL:HG12	1:C:202:GLY:N	2.16	0.59
1:A:482:LEU:HD12	1:A:645:ILE:HG23	1.84	0.59
1:C:141:GLU:HG2	1:C:178:PRO:HB3	1.82	0.59
1:B:514:VAL:HG23	1:B:618:PHE:CZ	2.35	0.59
1:C:613:THR:HG23	1:C:614:LYS:HG3	1.84	0.59
1:B:574:LEU:HG	1:B:576:PHE:HE1	1.67	0.59
1:C:90:ASN:ND2	1:C:198:LEU:CD2	2.63	0.59
1:B:320:VAL:O	1:B:324:ILE:HG13	2.00	0.59
1:A:613:THR:HG23	1:A:614:LYS:HG3	1.83	0.59
1:C:515:LEU:HB3	1:C:642:LEU:CD1	2.33	0.59
1:A:28:VAL:HG13	1:A:96:LEU:HA	1.85	0.59
1:C:433:GLU:O	1:C:433:GLU:HG2	2.03	0.59
1:A:90:ASN:HD22	1:A:198:LEU:HD21	1.68	0.59
1:B:155:ARG:CZ	1:B:386:LYS:HZ3	2.15	0.59
1:C:239:ARG:HH12	1:C:336:LYS:HB2	1.67	0.59
1:A:657:LEU:HB2	1:A:672:LEU:HD13	1.84	0.59
1:B:56:THR:HG22	1:B:70:ILE:CD1	2.32	0.59
1:B:220:VAL:HG12	1:B:342:ILE:HD13	1.85	0.59
1:B:28:VAL:HG13	1:B:96:LEU:HA	1.85	0.59
1:C:514:VAL:HG12	1:C:515:LEU:N	2.17	0.59
1:C:500:PRO:O	1:C:504:LEU:HD23	2.02	0.59
1:B:372:PRO:HD2	1:B:407:VAL:HA	1.84	0.59
1:B:613:THR:HG23	1:B:614:LYS:HG3	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:309:ILE:O	1:A:309:ILE:HG22	2.02	0.59
1:C:28:VAL:HG13	1:C:96:LEU:HA	1.85	0.59
1:B:208:GLY:C	1:B:209:CYS:SG	2.81	0.59
1:B:90:ASN:ND2	1:B:198:LEU:CD2	2.64	0.59
1:B:201:VAL:HG12	1:B:202:GLY:N	2.17	0.59
1:A:427:MET:HE1	1:A:437:ILE:HD12	1.83	0.59
1:C:208:GLY:C	1:C:209:CYS:SG	2.81	0.59
1:A:313:ARG:CG	1:A:314:GLU:H	2.16	0.59
1:A:632:ALA:HA	1:A:635:ARG:CD	2.33	0.59
1:A:206:ILE:HD11	1:A:213:LEU:CD1	2.28	0.58
1:C:642:LEU:HD22	1:C:642:LEU:N	2.18	0.58
1:C:177:ALA:C	1:C:179:ASP:H	2.06	0.58
1:B:513:GLY:HA3	1:B:619:ILE:O	2.03	0.58
1:C:427:MET:HE2	1:C:441:VAL:HG11	1.85	0.58
1:A:635:ARG:HH11	1:A:635:ARG:HB3	1.68	0.58
1:C:372:PRO:HD2	1:C:407:VAL:HA	1.84	0.58
1:A:290:PHE:CD1	1:A:301:ILE:CD1	2.86	0.58
1:B:235:VAL:HG11	1:C:420:LEU:HD21	1.86	0.58
1:C:656:ILE:HG21	1:C:687:LEU:HD12	1.86	0.58
1:C:611:MET:HE3	1:C:619:ILE:HD11	1.85	0.58
1:B:584:LYS:HZ2	1:B:625:ARG:HG3	1.68	0.58
1:C:574:LEU:HG	1:C:576:PHE:HE1	1.68	0.58
1:B:36:ASN:OD1	1:B:87:VAL:HG21	2.03	0.58
1:C:82:ILE:O	1:C:82:ILE:HG23	2.04	0.58
1:A:220:VAL:HG12	1:A:342:ILE:HD13	1.86	0.58
1:A:642:LEU:HD22	1:A:642:LEU:N	2.19	0.58
1:A:599:ARG:HG2	1:B:552:PHE:CD1	2.38	0.58
1:C:632:ALA:HA	1:C:635:ARG:CD	2.34	0.58
1:B:632:ALA:HA	1:B:635:ARG:CD	2.34	0.58
1:B:153:LEU:HD13	1:B:162:GLU:HG2	1.84	0.58
1:B:173:TYR:HD1	1:B:173:TYR:O	1.87	0.58
1:A:523:GLY:HA3	1:A:526:LEU:HD12	1.85	0.58
1:A:501:ASP:OD1	1:A:502:LYS:N	2.36	0.58
1:A:155:ARG:HE	1:A:386:LYS:NZ	2.02	0.58
1:C:220:VAL:HG12	1:C:342:ILE:HD13	1.85	0.58
1:A:314:GLU:CD	1:A:314:GLU:H	2.07	0.58
1:C:635:ARG:HH11	1:C:635:ARG:HB3	1.69	0.58
1:A:213:LEU:HB3	1:A:217:LYS:HE3	1.85	0.58
1:B:170:PRO:HB2	1:B:174:CYS:CB	2.30	0.58
1:C:213:LEU:HB3	1:C:217:LYS:HE3	1.86	0.58
1:B:158:MET:CE	1:B:419:ALA:HB1	2.34	0.58
1:A:547:LEU:HD23	1:A:550:MET:HE3	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:393:ASP:OD2	1:C:448:THR:HB	2.04	0.58
1:A:170:PRO:HB2	1:A:174:CYS:CB	2.32	0.58
1:A:524:LYS:HB2	3:A:915:AF3:F2	1.94	0.58
1:C:153:LEU:HD13	1:C:162:GLU:HG2	1.86	0.58
1:B:642:LEU:N	1:B:642:LEU:HD22	2.19	0.58
1:C:318:GLY:O	1:C:322:ARG:HG3	2.04	0.58
1:A:645:ILE:HD12	1:A:645:ILE:N	2.19	0.57
1:A:653:ARG:CZ	1:A:679:THR:O	2.51	0.57
1:B:147:ARG:CG	1:B:148:LYS:N	2.67	0.57
1:A:632:ALA:HA	1:A:635:ARG:HD2	1.85	0.57
1:A:56:THR:HG22	1:A:70:ILE:CD1	2.34	0.57
1:B:135:LEU:HD22	1:B:135:LEU:N	2.19	0.57
1:A:201:VAL:HG12	1:A:202:GLY:N	2.18	0.57
1:A:111:GLY:CA	1:A:170:PRO:HG2	2.30	0.57
1:B:206:ILE:HD11	1:B:213:LEU:CD1	2.29	0.57
1:B:141:GLU:HG2	1:B:178:PRO:HB3	1.84	0.57
1:B:512:LYS:HD3	1:B:637:GLY:O	2.04	0.57
1:A:82:ILE:O	1:A:82:ILE:HG23	2.05	0.57
1:C:60:LYS:HB2	1:C:101:SER:HG	1.69	0.57
1:C:482:LEU:HD13	1:C:646:PRO:HD2	1.86	0.57
1:B:393:ASP:OD2	1:B:448:THR:HB	2.05	0.57
1:C:36:ASN:OD1	1:C:87:VAL:HG21	2.04	0.57
1:C:158:MET:HE1	1:C:419:ALA:HB1	1.87	0.57
1:B:580:ASP:O	1:B:583:ALA:N	2.38	0.57
1:A:495:TYR:HD1	1:B:703:ILE:HD13	1.68	0.57
1:B:521:GLY:HA3	1:B:685:ALA:CB	2.34	0.57
1:A:508:MET:HE3	1:A:509:THR:O	2.05	0.57
1:A:427:MET:CB	1:A:431:ASP:HB2	2.34	0.57
1:A:372:PRO:HD2	1:A:407:VAL:HA	1.85	0.57
1:C:227:PRO:HG2	1:C:298:PRO:HG2	1.86	0.57
1:C:632:ALA:HA	1:C:635:ARG:HD2	1.85	0.57
1:A:147:ARG:CG	1:A:148:LYS:N	2.68	0.57
1:A:512:LYS:HZ3	1:A:608:MET:HG2	1.69	0.57
1:A:605:LEU:HD22	1:A:638:ARG:HH11	1.70	0.57
1:A:520:PRO:HG3	1:A:624:ASN:CB	2.34	0.57
1:A:465:ARG:CB	1:A:465:ARG:NH1	2.68	0.57
1:A:227:PRO:HG2	1:A:298:PRO:HG2	1.87	0.57
1:C:135:LEU:N	1:C:135:LEU:HD22	2.20	0.57
1:A:494:GLN:O	1:A:497:VAL:HG12	2.04	0.57
1:A:141:GLU:HG2	1:A:178:PRO:HB3	1.85	0.57
1:A:316:THR:OG1	1:A:322:ARG:HG2	2.05	0.57
1:B:632:ALA:HA	1:B:635:ARG:HD2	1.85	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:574:LEU:HG	1:A:576:PHE:CE1	2.40	0.57
1:A:695:CYS:C	1:A:697:LEU:H	2.08	0.57
1:B:491:GLU:HG2	1:B:495:TYR:HE2	1.69	0.57
1:C:556:GLU:N	1:C:556:GLU:OE1	2.38	0.57
1:B:579:LEU:C	1:B:579:LEU:HD23	2.25	0.57
1:A:393:ASP:OD2	1:A:448:THR:HB	2.05	0.57
1:B:465:ARG:HH11	1:B:465:ARG:HB3	1.69	0.57
1:C:112:LYS:H	1:C:170:PRO:CD	2.18	0.56
1:C:605:LEU:HD22	1:C:638:ARG:HH11	1.69	0.56
1:A:514:VAL:HG12	1:A:515:LEU:N	2.19	0.56
1:A:544:GLY:O	1:A:547:LEU:HB2	2.05	0.56
1:A:173:TYR:HD1	1:A:173:TYR:O	1.87	0.56
1:A:22:ARG:C	1:A:24:ASN:H	2.07	0.56
1:C:574:LEU:HG	1:C:576:PHE:CE1	2.39	0.56
1:C:650:GLU:HA	1:C:653:ARG:NH2	2.20	0.56
1:A:89:ARG:NH1	1:A:261:GLU:OE2	2.37	0.56
1:A:312:LYS:HB3	1:A:354:ASP:CG	2.26	0.56
1:B:306:LEU:HD22	1:B:345:ALA:HB1	1.87	0.56
1:C:155:ARG:NE	1:C:386:LYS:HZ3	2.03	0.56
1:A:158:MET:HE1	1:A:419:ALA:HB1	1.85	0.56
1:A:36:ASN:OD1	1:A:87:VAL:HG21	2.05	0.56
1:B:547:LEU:HD23	1:B:550:MET:HE3	1.87	0.56
1:C:654:VAL:HG22	1:C:676:ALA:CB	2.35	0.56
1:A:464:LEU:HG	1:A:466:GLU:H	1.69	0.56
1:B:65:ARG:HH11	1:B:93:ARG:CZ	2.19	0.56
1:B:90:ASN:HD22	1:B:198:LEU:HD21	1.70	0.56
1:C:544:GLY:O	1:C:547:LEU:HB2	2.06	0.56
1:B:460:ASN:N	1:B:461:PRO:CD	2.68	0.56
1:B:524:LYS:CB	1:B:524:LYS:HZ2	2.18	0.56
1:B:584:LYS:NZ	1:B:625:ARG:HG3	2.20	0.56
1:C:90:ASN:HD22	1:C:198:LEU:HD21	1.70	0.56
1:B:758:PHE:HB3	1:B:762:LEU:CD1	2.35	0.56
1:A:26:LEU:HD11	1:A:45:LYS:HE2	1.86	0.56
1:C:216:ILE:HA	1:C:219:MET:HE3	1.88	0.56
1:B:488:GLU:O	1:B:491:GLU:HB2	2.05	0.56
1:B:42:SER:OG	1:B:45:LYS:HB2	2.06	0.56
1:C:173:TYR:HD1	1:C:173:TYR:O	1.87	0.56
1:B:233:ILE:HD11	1:C:158:MET:SD	2.46	0.56
1:C:488:GLU:O	1:C:491:GLU:HB2	2.05	0.56
1:B:155:ARG:HD3	1:B:386:LYS:O	2.06	0.56
1:C:653:ARG:HD2	1:C:679:THR:O	2.05	0.56
1:B:58:LEU:HD23	1:B:103:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:28:VAL:HG13	1:C:97:GLY:H	1.70	0.56
1:A:682:PHE:CE1	1:A:745:ARG:HG2	2.41	0.56
1:B:635:ARG:HH11	1:B:635:ARG:HB3	1.69	0.56
1:B:544:GLY:O	1:B:547:LEU:HB2	2.06	0.56
1:A:208:GLY:C	1:A:209:CYS:SG	2.83	0.56
1:B:243:LEU:HB3	1:B:369:ILE:HD11	1.88	0.56
1:B:275:MET:SD	1:B:309:ILE:HG12	2.46	0.56
1:C:158:MET:CE	1:C:419:ALA:HB1	2.36	0.55
1:B:93:ARG:HG2	1:B:93:ARG:HH11	1.70	0.55
1:C:632:ALA:HA	1:C:635:ARG:HG3	1.88	0.55
1:A:427:MET:CG	1:A:431:ASP:CB	2.58	0.55
1:C:93:ARG:HG2	1:C:93:ARG:HH11	1.71	0.55
1:C:497:VAL:HG13	1:C:498:GLU:N	2.21	0.55
1:C:596:ALA:HB1	1:C:630:ASP:HA	1.88	0.55
1:A:405:GLY:HA3	1:A:465:ARG:HG2	1.88	0.55
1:C:203:TYR:C	1:C:205:ASP:H	2.10	0.55
1:A:488:GLU:O	1:A:491:GLU:HB2	2.06	0.55
1:C:62:LYS:HZ1	1:C:98:ASP:HB3	1.70	0.55
1:C:222:LEU:H	1:C:223:PRO:HD2	1.71	0.55
1:B:605:LEU:HD22	1:B:638:ARG:HH11	1.70	0.55
1:A:60:LYS:HG2	1:A:66:GLU:HG2	1.89	0.55
1:B:427:MET:HG3	1:B:432:LEU:HB2	1.88	0.55
1:C:42:SER:OG	1:C:45:LYS:HB2	2.06	0.55
1:A:42:SER:OG	1:A:45:LYS:HB2	2.05	0.55
1:A:632:ALA:HA	1:A:635:ARG:HG3	1.88	0.55
1:B:695:CYS:C	1:B:697:LEU:H	2.08	0.55
1:C:695:CYS:C	1:C:697:LEU:H	2.08	0.55
1:C:274:ILE:O	1:C:274:ILE:HG22	2.07	0.55
1:A:432:LEU:O	1:A:432:LEU:HD12	2.07	0.55
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.70	0.55
1:A:445:LEU:HD23	1:A:445:LEU:C	2.26	0.55
1:C:177:ALA:HB1	1:C:178:PRO:HD2	1.89	0.55
1:C:733:ARG:HB2	1:C:733:ARG:HH11	1.72	0.55
1:C:23:PRO:O	1:C:49:LEU:HD21	2.07	0.55
1:C:482:LEU:CD1	1:C:646:PRO:HD2	2.37	0.55
1:C:494:GLN:O	1:C:497:VAL:HG12	2.07	0.55
1:B:697:LEU:O	1:B:697:LEU:HD13	2.07	0.55
1:A:465:ARG:CB	1:A:465:ARG:HH11	2.19	0.55
1:B:26:LEU:HD21	1:B:45:LYS:HZ1	1.72	0.55
1:C:466:GLU:HG2	1:C:467:THR:HG23	1.87	0.55
1:C:151:ILE:HD11	1:C:195:GLU:OE2	2.07	0.55
1:A:224:LEU:CD2	1:A:300:ILE:HD11	2.31	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:536:GLN:O	1:C:536:GLN:HG2	2.06	0.55
1:B:445:LEU:HD23	1:B:445:LEU:C	2.27	0.55
1:B:82:ILE:HG23	1:B:82:ILE:O	2.06	0.55
1:C:94:VAL:O	1:C:94:VAL:HG23	2.07	0.55
1:A:353:ILE:HG22	1:A:354:ASP:N	2.18	0.55
1:B:590:ILE:HG13	1:B:591:GLY:N	2.17	0.55
1:C:599:ARG:HH11	1:C:599:ARG:CB	2.19	0.55
1:C:654:VAL:HG22	1:C:676:ALA:HB1	1.89	0.55
1:B:111:GLY:CA	1:B:170:PRO:HG2	2.32	0.55
1:A:684:GLY:HA3	2:A:900:ADP:C8	2.42	0.55
1:A:251:LYS:HG3	2:A:807:ADP:O2B	2.06	0.55
1:B:227:PRO:HG2	1:B:298:PRO:HG2	1.89	0.55
1:C:147:ARG:CG	1:C:148:LYS:N	2.70	0.55
1:A:427:MET:O	1:A:431:ASP:N	2.38	0.54
1:B:26:LEU:HD21	1:B:45:LYS:HZ3	1.71	0.54
1:C:492:LEU:O	1:C:496:PRO:HG3	2.07	0.54
1:C:353:ILE:HG22	1:C:354:ASP:N	2.17	0.54
1:B:733:ARG:HB2	1:B:733:ARG:HH11	1.72	0.54
1:C:25:ARG:HA	1:C:100:ILE:O	2.07	0.54
1:B:493:VAL:HG21	1:B:531:ILE:HD11	1.90	0.54
1:B:112:LYS:H	1:B:170:PRO:CD	2.20	0.54
1:B:493:VAL:HG23	1:B:494:GLN:N	2.21	0.54
1:A:502:LYS:HA	1:A:505:LYS:CD	2.37	0.54
1:A:438:ASP:OD2	1:A:440:GLU:HB2	2.07	0.54
1:C:521:GLY:HA3	1:C:683:SER:OG	2.07	0.54
1:B:600:VAL:O	1:B:604:ILE:HG13	2.07	0.54
1:C:243:LEU:HB3	1:C:369:ILE:HD11	1.89	0.54
1:B:222:LEU:H	1:B:223:PRO:HD2	1.71	0.54
1:B:427:MET:HE2	1:B:432:LEU:HB2	1.89	0.54
1:C:464:LEU:CD1	1:C:466:GLU:CB	2.79	0.54
1:B:66:GLU:HB2	1:B:147:ARG:NH1	2.23	0.54
1:A:222:LEU:H	1:A:223:PRO:HD2	1.72	0.54
1:A:135:LEU:HD22	1:A:135:LEU:N	2.22	0.54
1:A:427:MET:HE2	1:A:441:VAL:HG11	1.89	0.54
1:A:733:ARG:HB2	1:A:733:ARG:HH11	1.72	0.54
1:C:56:THR:HG22	1:C:70:ILE:CD1	2.38	0.54
1:A:697:LEU:O	1:A:697:LEU:HD13	2.08	0.54
1:B:274:ILE:O	1:B:274:ILE:HG22	2.08	0.54
1:A:112:LYS:H	1:A:170:PRO:CD	2.20	0.54
1:C:111:GLY:CA	1:C:174:CYS:HB2	2.37	0.54
1:C:605:LEU:HD22	1:C:638:ARG:NH1	2.23	0.54
1:B:524:LYS:CB	1:B:524:LYS:NZ	2.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:312:LYS:H	1:B:354:ASP:CB	2.16	0.54
1:B:582:ILE:CD1	1:B:600:VAL:HB	2.37	0.54
1:A:556:GLU:N	1:A:556:GLU:OE1	2.39	0.54
1:A:599:ARG:HH11	1:A:599:ARG:CB	2.19	0.54
1:A:306:LEU:HD22	1:A:345:ALA:CB	2.37	0.54
1:C:656:ILE:HG12	2:C:900:ADP:N1	2.22	0.54
1:B:203:TYR:C	1:B:205:ASP:H	2.11	0.54
1:A:210:ARG:N	1:A:210:ARG:HD2	2.22	0.54
1:B:155:ARG:HE	1:B:386:LYS:NZ	2.05	0.54
1:C:184:CYS:C	1:C:186:GLY:H	2.10	0.54
1:A:89:ARG:NH2	1:A:96:LEU:HD21	2.23	0.54
1:B:28:VAL:HG13	1:B:97:GLY:H	1.73	0.54
1:B:77:CYS:HB2	1:B:83:ARG:HE	1.72	0.54
1:C:313:ARG:HD2	1:C:351:ASN:O	2.08	0.54
1:B:409:ALA:O	1:B:412:ALA:HB3	2.08	0.54
1:C:586:ARG:HD2	1:C:598:ASP:OD2	2.07	0.54
1:B:599:ARG:HH11	1:B:599:ARG:CB	2.20	0.54
1:C:184:CYS:O	1:C:186:GLY:N	2.41	0.54
1:B:92:LEU:HB2	1:B:94:VAL:HG22	1.89	0.53
1:C:89:ARG:HE	1:C:96:LEU:CD2	2.12	0.53
1:B:432:LEU:N	1:B:432:LEU:HD12	2.22	0.53
1:C:113:ARG:NH2	1:C:183:HIS:CE1	2.75	0.53
1:B:582:ILE:CD1	1:B:601:ILE:HG12	2.36	0.53
1:B:661:LEU:HD21	1:B:691:CYS:SG	2.48	0.53
1:B:31:ALA:HB2	1:B:84:MET:C	2.29	0.53
1:C:60:LYS:CE	1:C:103:GLN:HE22	2.19	0.53
1:B:650:GLU:HA	1:B:653:ARG:NH2	2.23	0.53
1:A:409:ALA:O	1:A:412:ALA:HB3	2.09	0.53
1:A:114:ILE:HG22	1:A:116:VAL:HG13	1.90	0.53
1:B:317:HIS:NE2	1:C:317:HIS:CE1	2.76	0.53
1:C:26:LEU:HD21	1:C:45:LYS:HE2	1.91	0.53
1:B:632:ALA:HA	1:B:635:ARG:HG3	1.88	0.53
1:A:243:LEU:HB3	1:A:369:ILE:HD11	1.89	0.53
1:B:94:VAL:O	1:B:94:VAL:HG23	2.08	0.53
1:C:196:GLU:HB3	1:C:200:GLU:OE1	2.08	0.53
1:A:100:ILE:CG2	1:A:101:SER:N	2.63	0.53
1:B:224:LEU:CD2	1:B:300:ILE:HD11	2.38	0.53
1:B:358:ARG:HH11	1:B:358:ARG:HG3	1.74	0.53
1:A:113:ARG:HG2	1:A:113:ARG:NH1	2.24	0.53
1:C:114:ILE:HG22	1:C:116:VAL:HG13	1.90	0.53
1:B:736:PHE:O	1:B:739:ALA:HB3	2.09	0.53
1:A:358:ARG:HH11	1:A:358:ARG:HG3	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:TYR:CE2	1:A:261:GLU:HG2	2.43	0.53
1:C:472:PRO:HG2	1:C:532:ALA:CB	2.35	0.53
1:B:540:ILE:HG13	1:B:572:CYS:SG	2.49	0.53
1:A:233:ILE:HG13	1:A:235:VAL:HG23	1.91	0.53
1:B:556:GLU:N	1:B:556:GLU:OE1	2.39	0.53
1:A:95:ARG:CB	1:A:225:ARG:HH12	2.22	0.53
1:A:476:TRP:HE1	1:A:534:GLU:HB2	1.71	0.53
1:C:752:ILE:O	1:C:756:GLU:HG2	2.09	0.53
1:B:518:GLY:O	1:B:755:TYR:HE2	1.92	0.53
1:A:460:ASN:N	1:A:461:PRO:CD	2.72	0.53
1:A:206:ILE:HD13	1:A:213:LEU:HD21	1.87	0.53
1:C:58:LEU:HD23	1:C:103:GLN:NE2	2.23	0.53
1:A:654:VAL:HG22	1:A:676:ALA:CB	2.39	0.53
1:A:216:ILE:HA	1:A:219:MET:CE	2.39	0.53
1:A:605:LEU:HD22	1:A:638:ARG:NH1	2.24	0.53
1:C:697:LEU:O	1:C:697:LEU:HD13	2.09	0.53
1:A:736:PHE:O	1:A:739:ALA:HB3	2.09	0.53
1:A:66:GLU:HB2	1:A:147:ARG:CZ	2.36	0.53
1:A:92:LEU:HB2	1:A:94:VAL:HG22	1.90	0.53
1:B:506:PHE:CE2	1:C:699:ILE:HG12	2.43	0.53
1:B:63:LYS:HD2	1:B:93:ARG:HD2	1.90	0.53
1:A:259:ALA:HB2	1:A:300:ILE:HD12	1.90	0.53
1:B:210:ARG:HD2	1:B:210:ARG:N	2.23	0.53
1:A:317:HIS:CE1	1:B:317:HIS:CE1	2.97	0.53
1:B:69:CYS:O	1:B:70:ILE:HD13	2.09	0.53
2:B:900:ADP:O1B	3:B:915:AF3:F3	2.18	0.52
1:C:248:GLY:C	1:C:250:GLY:H	2.12	0.52
1:A:274:ILE:HG22	1:A:274:ILE:O	2.09	0.52
1:C:53:ARG:NH1	1:C:73:SER:OG	2.42	0.52
1:C:28:VAL:HG22	1:C:96:LEU:HD22	1.91	0.52
1:A:151:ILE:HD11	1:A:195:GLU:OE2	2.10	0.52
1:C:445:LEU:C	1:C:445:LEU:HD23	2.28	0.52
1:C:251:LYS:HG3	2:C:807:ADP:O2B	2.07	0.52
1:A:248:GLY:C	1:A:250:GLY:H	2.13	0.52
1:A:316:THR:O	1:A:316:THR:HG23	2.10	0.52
1:B:579:LEU:HD22	1:B:629:ILE:HD12	1.91	0.52
1:A:512:LYS:HZ3	1:A:608:MET:HG3	1.73	0.52
1:A:48:GLU:C	1:A:49:LEU:HD12	2.29	0.52
1:B:427:MET:HE1	1:B:432:LEU:HB2	1.90	0.52
1:C:312:LYS:HD3	1:C:354:ASP:OD2	2.09	0.52
1:A:290:PHE:CD1	1:A:301:ILE:HD13	2.44	0.52
1:C:316:THR:O	1:C:316:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:728:VAL:N	1:C:729:PRO:CD	2.72	0.52
1:A:465:ARG:HB2	1:A:465:ARG:NH1	2.25	0.52
1:A:177:ALA:O	1:A:179:ASP:N	2.42	0.52
1:C:69:CYS:O	1:C:70:ILE:HD13	2.09	0.52
1:B:605:LEU:HD22	1:B:638:ARG:NH1	2.25	0.52
1:A:427:MET:CA	1:A:431:ASP:HB2	2.39	0.52
1:A:31:ALA:HB2	1:A:84:MET:C	2.30	0.52
1:A:526:LEU:CD1	2:A:900:ADP:H2'	2.29	0.52
1:B:575:PHE:HA	1:B:620:ILE:O	2.10	0.52
1:A:519:PRO:HA	1:A:755:TYR:HE2	1.74	0.52
1:A:27:ILE:HG13	1:B:429:LEU:CD2	2.38	0.52
1:A:58:LEU:HD23	1:A:103:GLN:NE2	2.24	0.52
1:A:686:ASP:O	1:A:689:GLU:HB3	2.10	0.52
1:A:203:TYR:CE2	1:A:217:LYS:HE2	2.44	0.52
1:C:206:ILE:CD1	1:C:213:LEU:CD2	2.79	0.52
1:B:248:GLY:C	1:B:250:GLY:H	2.12	0.52
1:B:310:ALA:N	1:B:311:PRO:CD	2.73	0.52
1:C:155:ARG:HE	1:C:386:LYS:HZ3	1.58	0.52
1:C:26:LEU:HD21	1:C:45:LYS:CE	2.40	0.52
1:A:514:VAL:HG23	1:A:618:PHE:CZ	2.42	0.52
1:C:736:PHE:O	1:C:739:ALA:HB3	2.09	0.52
1:A:464:LEU:CD1	1:A:466:GLU:HB2	2.16	0.52
1:A:28:VAL:HG13	1:A:97:GLY:H	1.75	0.52
1:A:569:ALA:O	1:A:572:CYS:HB2	2.10	0.52
1:B:151:ILE:HD11	1:B:195:GLU:OE2	2.10	0.52
1:B:656:ILE:HG21	1:B:687:LEU:HD12	1.92	0.52
1:C:62:LYS:HZ3	1:C:98:ASP:HB3	1.74	0.52
1:C:283:GLU:HB3	1:C:327:GLN:NE2	2.25	0.52
1:C:316:THR:OG1	1:C:322:ARG:HG2	2.10	0.52
1:A:422:ALA:O	1:A:426:LYS:HG2	2.10	0.52
1:B:113:ARG:HG2	1:B:113:ARG:NH1	2.25	0.52
1:B:516:PHE:O	1:B:622:ALA:HA	2.10	0.52
1:A:283:GLU:HB3	1:A:327:GLN:NE2	2.25	0.52
1:C:177:ALA:O	1:C:179:ASP:N	2.42	0.52
1:C:409:ALA:O	1:C:412:ALA:HB3	2.09	0.52
1:B:686:ASP:O	1:B:689:GLU:HB3	2.09	0.52
1:A:252:THR:HG23	1:A:302:PHE:CE2	2.45	0.52
1:C:31:ALA:HB2	1:C:84:MET:C	2.31	0.52
1:A:111:GLY:CA	1:A:174:CYS:HB2	2.39	0.52
1:C:210:ARG:NH2	1:C:375:THR:HG22	2.25	0.52
1:A:155:ARG:HD3	1:A:386:LYS:O	2.09	0.52
1:B:521:GLY:CA	1:B:685:ALA:HB2	2.39	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:567:ARG:HH22	1:A:611:MET:HG2	1.75	0.52
1:C:513:GLY:HA3	1:C:619:ILE:O	2.10	0.52
1:B:640:ASP:OD1	1:B:641:GLN:HG2	2.10	0.52
1:A:502:LYS:HA	1:A:505:LYS:CG	2.40	0.52
1:C:686:ASP:O	1:C:689:GLU:HB3	2.10	0.52
1:A:171:SER:OG	1:A:172:PRO:HA	2.09	0.52
1:A:473:GLN:N	1:A:473:GLN:OE1	2.42	0.52
1:B:114:ILE:HG22	1:B:116:VAL:HG13	1.92	0.51
1:C:758:PHE:HB3	1:C:762:LEU:HD11	1.90	0.51
1:C:422:ALA:O	1:C:426:LYS:HG2	2.09	0.51
1:C:465:ARG:HH11	1:C:465:ARG:HB3	1.74	0.51
1:A:94:VAL:O	1:A:94:VAL:HG23	2.10	0.51
1:A:644:TYR:CE2	1:A:646:PRO:HB3	2.44	0.51
1:A:490:GLN:CD	1:A:494:GLN:NE2	2.62	0.51
1:C:313:ARG:HG2	1:C:314:GLU:HG2	1.92	0.51
1:A:269:ILE:HD12	1:A:303:ILE:HG22	1.93	0.51
1:C:689:GLU:O	1:C:693:ARG:HG3	2.11	0.51
1:C:290:PHE:CD1	1:C:301:ILE:CD1	2.94	0.51
1:C:24:ASN:CG	1:C:25:ARG:N	2.64	0.51
1:C:503:PHE:HZ	1:C:509:THR:C	2.13	0.51
1:B:752:ILE:O	1:B:756:GLU:HG2	2.10	0.51
1:A:502:LYS:HA	1:A:505:LYS:HG3	1.92	0.51
1:A:752:ILE:O	1:A:756:GLU:HG2	2.10	0.51
1:C:310:ALA:N	1:C:311:PRO:CD	2.73	0.51
1:B:56:THR:HG22	1:B:70:ILE:HD12	1.92	0.51
1:C:243:LEU:HD12	1:C:243:LEU:N	2.25	0.51
1:A:158:MET:CE	1:A:419:ALA:HB1	2.41	0.51
1:C:216:ILE:HA	1:C:219:MET:CE	2.41	0.51
1:C:290:PHE:CD1	1:C:301:ILE:HD13	2.46	0.51
1:A:203:TYR:C	1:A:205:ASP:H	2.14	0.51
1:C:438:ASP:HB3	1:C:441:VAL:HG23	1.93	0.51
1:C:325:VAL:HG12	1:C:329:LEU:CD1	2.41	0.51
1:C:42:SER:HB3	1:C:77:CYS:O	2.10	0.51
1:A:42:SER:HB3	1:A:77:CYS:O	2.10	0.51
1:B:283:GLU:HB3	1:B:327:GLN:NE2	2.26	0.51
1:C:210:ARG:N	1:C:210:ARG:HD2	2.25	0.51
1:C:250:GLY:HA2	2:C:807:ADP:O3A	2.10	0.51
1:A:600:VAL:O	1:A:604:ILE:HG13	2.11	0.51
1:B:307:ASP:O	1:B:311:PRO:HD3	2.11	0.51
1:B:43:GLN:N	1:B:44:PRO:HD2	2.26	0.51
1:B:613:THR:HG23	1:B:614:LYS:N	2.26	0.51
1:C:413:ALA:O	1:C:416:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:521:GLY:HA2	1:C:685:ALA:CB	2.37	0.51
1:C:63:LYS:HD2	1:C:93:ARG:CD	2.40	0.51
1:C:92:LEU:HB2	1:C:94:VAL:HG22	1.91	0.51
1:B:494:GLN:NE2	1:B:534:GLU:HG3	2.25	0.51
1:B:327:GLN:O	1:B:331:LEU:HG	2.09	0.51
1:B:689:GLU:O	1:B:693:ARG:HG3	2.11	0.51
1:B:422:ALA:O	1:B:426:LYS:HG2	2.10	0.51
1:A:21:ASN:CB	1:A:25:ARG:HH21	2.19	0.51
1:B:564:ASP:HA	1:B:567:ARG:HH12	1.76	0.51
1:C:522:CYS:HB2	3:C:915:AF3:F3	2.01	0.51
1:A:493:VAL:HG23	1:A:494:GLN:N	2.26	0.51
1:A:43:GLN:N	1:A:44:PRO:HD2	2.26	0.51
1:A:303:ILE:HG12	1:A:344:MET:O	2.11	0.51
1:C:587:GLY:HA3	1:C:591:GLY:CA	2.41	0.51
1:C:327:GLN:O	1:C:331:LEU:HG	2.11	0.51
1:B:216:ILE:HA	1:B:219:MET:CE	2.40	0.51
1:B:413:ALA:O	1:B:416:SER:HB2	2.11	0.51
1:B:319:GLU:OE2	1:C:320:VAL:HG11	2.11	0.51
1:A:113:ARG:NH2	1:A:183:HIS:CE1	2.77	0.51
1:A:53:ARG:NH1	1:A:73:SER:OG	2.43	0.51
1:A:147:ARG:HB3	1:A:150:ASP:OD2	2.11	0.51
1:B:232:ALA:O	1:B:233:ILE:HB	2.11	0.51
1:A:495:TYR:N	1:A:496:PRO:HD2	2.26	0.51
1:B:177:ALA:O	1:B:179:ASP:N	2.44	0.51
1:A:613:THR:HG23	1:A:614:LYS:N	2.26	0.51
1:B:196:GLU:HB3	1:B:200:GLU:OE1	2.10	0.51
1:B:86:ARG:O	1:B:89:ARG:HB3	2.11	0.51
1:B:491:GLU:HG2	1:B:495:TYR:CE2	2.45	0.51
1:B:499:HIS:N	1:B:500:PRO:CD	2.74	0.51
1:B:111:GLY:CA	1:B:174:CYS:HB2	2.40	0.51
1:C:93:ARG:NH2	1:C:195:GLU:HG2	2.26	0.51
1:C:491:GLU:HG2	1:C:495:TYR:CE2	2.46	0.51
1:B:682:PHE:CE1	1:B:745:ARG:HG2	2.46	0.51
1:A:519:PRO:CD	1:A:755:TYR:HD2	2.22	0.51
1:B:584:LYS:NZ	1:B:625:ARG:CG	2.74	0.51
1:C:77:CYS:HB2	1:C:83:ARG:HE	1.75	0.51
1:B:243:LEU:N	1:B:243:LEU:HD12	2.26	0.51
1:B:502:LYS:CD	1:C:703:ILE:HG12	2.41	0.50
1:B:93:ARG:HG2	1:B:93:ARG:NH1	2.26	0.50
1:B:654:VAL:HG22	1:B:676:ALA:CB	2.41	0.50
1:B:147:ARG:HB3	1:B:150:ASP:OD2	2.11	0.50
1:B:758:PHE:HB3	1:B:762:LEU:CG	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:473:GLN:CD	1:A:473:GLN:H	2.14	0.50
1:A:660:ASN:HD21	1:A:688:THR:HG23	1.75	0.50
1:C:408:GLY:HA3	2:C:807:ADP:N7	2.26	0.50
1:A:327:GLN:O	1:A:331:LEU:HG	2.11	0.50
1:C:147:ARG:HB3	1:C:150:ASP:OD2	2.11	0.50
1:C:413:ALA:HA	1:C:416:SER:OG	2.11	0.50
1:B:53:ARG:NH1	1:B:73:SER:OG	2.44	0.50
1:A:413:ALA:O	1:A:416:SER:HB2	2.11	0.50
1:A:438:ASP:HB3	1:A:441:VAL:HG23	1.93	0.50
1:A:567:ARG:C	1:A:569:ALA:H	2.15	0.50
1:C:659:ALA:HA	1:C:662:ARG:CG	2.40	0.50
1:B:524:LYS:HE3	3:B:915:AF3:F2	2.01	0.50
1:B:479:ILE:N	1:B:479:ILE:CD1	2.74	0.50
1:A:155:ARG:NE	1:A:386:LYS:HZ3	2.09	0.50
1:C:579:LEU:C	1:C:579:LEU:HD23	2.32	0.50
1:B:110:TYR:H	1:B:110:TYR:HD1	1.58	0.50
1:A:411:LEU:O	1:A:414:LEU:HB3	2.12	0.50
1:B:206:ILE:CD1	1:B:213:LEU:CD2	2.81	0.50
1:B:206:ILE:HD13	1:B:213:LEU:HD21	1.89	0.50
1:C:514:VAL:HG11	1:C:643:ILE:HD12	1.93	0.50
1:C:131:PHE:O	1:C:136:LYS:HB2	2.12	0.50
1:A:77:CYS:HB2	1:A:83:ARG:HE	1.76	0.50
1:B:145:PRO:HB3	1:B:175:ILE:HG12	1.92	0.50
1:A:41:LEU:HD23	1:A:82:ILE:HA	1.93	0.50
1:C:547:LEU:HA	1:C:550:MET:HE3	1.94	0.50
1:B:413:ALA:HA	1:B:416:SER:OG	2.12	0.50
1:B:171:SER:OG	1:B:172:PRO:HA	2.11	0.50
1:A:523:GLY:O	1:A:526:LEU:HB2	2.11	0.50
1:C:640:ASP:OD1	1:C:641:GLN:HG2	2.12	0.50
1:A:502:LYS:HA	1:A:505:LYS:HD2	1.93	0.50
1:B:758:PHE:O	1:B:762:LEU:HG	2.10	0.50
1:B:113:ARG:NH2	1:B:183:HIS:CE1	2.77	0.50
1:A:209:CYS:HB3	1:A:212:GLN:CB	2.36	0.50
1:C:347:THR:HG21	1:C:353:ILE:HD11	1.93	0.50
1:C:600:VAL:O	1:C:604:ILE:HG13	2.11	0.50
1:C:233:ILE:HG13	1:C:235:VAL:HG23	1.93	0.50
1:C:613:THR:HG23	1:C:614:LYS:N	2.26	0.50
1:A:614:LYS:HD3	1:B:402:GLU:HB2	1.91	0.50
1:B:542:ILE:HG23	1:B:546:GLU:OE1	2.11	0.50
1:A:93:ARG:NH1	1:A:93:ARG:HG2	2.27	0.50
1:C:512:LYS:NZ	1:C:608:MET:O	2.44	0.50
1:B:325:VAL:HG12	1:B:329:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:502:LYS:HA	1:B:505:LYS:CG	2.42	0.50
1:B:651:LYS:O	1:B:654:VAL:HB	2.12	0.50
2:B:900:ADP:O3B	3:B:915:AF3:F1	2.20	0.50
1:A:640:ASP:OD1	1:A:641:GLN:HG2	2.11	0.50
1:B:688:THR:O	1:B:691:CYS:HB2	2.12	0.50
1:A:728:VAL:HG12	1:A:728:VAL:O	2.12	0.50
1:A:468:VAL:HG12	1:A:470:GLU:H	1.77	0.50
1:C:358:ARG:HH11	1:C:358:ARG:HG3	1.76	0.50
1:A:196:GLU:HB3	1:A:200:GLU:OE1	2.11	0.50
1:A:69:CYS:O	1:A:70:ILE:HD13	2.12	0.50
1:B:411:LEU:O	1:B:414:LEU:HB3	2.12	0.50
1:B:233:ILE:HD13	1:C:442:MET:HE1	1.93	0.49
1:C:206:ILE:HD13	1:C:213:LEU:HD21	1.88	0.49
1:B:206:ILE:O	1:B:206:ILE:HG13	2.11	0.49
1:C:306:LEU:HD22	1:C:345:ALA:HB1	1.94	0.49
1:C:43:GLN:N	1:C:44:PRO:HD2	2.27	0.49
1:A:527:LEU:O	1:A:531:ILE:HG22	2.12	0.49
1:A:502:LYS:O	1:A:505:LYS:HB2	2.13	0.49
1:C:627:ASP:HB3	1:C:758:PHE:CZ	2.47	0.49
1:B:284:SER:HA	1:B:287:ARG:HB2	1.94	0.49
1:C:728:VAL:N	1:C:729:PRO:HD3	2.27	0.49
1:B:332:MET:C	1:B:334:GLY:H	2.15	0.49
1:A:184:CYS:C	1:A:186:GLY:H	2.14	0.49
1:B:427:MET:HE2	1:B:432:LEU:HD22	1.94	0.49
1:B:438:ASP:HB3	1:B:441:VAL:HG23	1.94	0.49
1:C:113:ARG:H	1:C:169:ASP:HB3	1.77	0.49
1:C:491:GLU:HA	1:C:495:TYR:HE2	1.73	0.49
1:A:251:LYS:H	2:A:807:ADP:PB	2.35	0.49
1:B:347:THR:OG1	1:B:348:ASN:N	2.45	0.49
1:B:269:ILE:HD12	1:B:303:ILE:CG2	2.43	0.49
1:C:682:PHE:CE1	1:C:745:ARG:HG2	2.47	0.49
1:B:48:GLU:C	1:B:49:LEU:HD12	2.31	0.49
1:B:728:VAL:N	1:B:729:PRO:HD3	2.27	0.49
1:B:113:ARG:H	1:B:169:ASP:HB3	1.77	0.49
1:C:206:ILE:HG13	1:C:206:ILE:O	2.12	0.49
1:A:582:ILE:HG21	1:A:598:ASP:CG	2.32	0.49
1:B:584:LYS:HZ1	1:B:625:ARG:HG2	1.77	0.49
1:C:145:PRO:HB3	1:C:175:ILE:HG12	1.93	0.49
1:B:556:GLU:O	1:B:559:VAL:HB	2.12	0.49
1:A:688:THR:O	1:A:691:CYS:HB2	2.12	0.49
1:A:666:VAL:HG23	1:A:666:VAL:O	2.13	0.49
1:B:464:LEU:CD1	1:B:466:GLU:HB2	2.32	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:347:THR:OG1	1:C:348:ASN:N	2.45	0.49
1:A:359:ARG:C	1:A:361:GLY:H	2.16	0.49
1:B:250:GLY:HA2	2:B:807:ADP:O3A	2.13	0.49
1:A:284:SER:HA	1:A:287:ARG:HB2	1.95	0.49
1:A:313:ARG:CG	1:A:314:GLU:N	2.76	0.49
1:A:413:ALA:HA	1:A:416:SER:OG	2.12	0.49
1:C:93:ARG:HG2	1:C:93:ARG:NH1	2.27	0.49
1:A:347:THR:OG1	1:A:348:ASN:N	2.46	0.49
1:A:312:LYS:HB3	1:A:354:ASP:OD2	2.12	0.49
1:B:114:ILE:HA	1:B:168:THR:HG22	1.94	0.49
1:C:733:ARG:HH11	1:C:733:ARG:CB	2.26	0.49
1:A:635:ARG:HH11	1:A:635:ARG:CB	2.25	0.49
1:A:243:LEU:HD12	1:A:243:LEU:N	2.27	0.49
1:B:465:ARG:NH1	1:B:465:ARG:HB3	2.28	0.49
1:C:332:MET:C	1:C:334:GLY:H	2.15	0.49
1:B:184:CYS:O	1:B:186:GLY:N	2.46	0.49
1:C:520:PRO:HD3	1:C:624:ASN:HB2	1.93	0.49
1:C:542:ILE:HG23	1:C:546:GLU:OE1	2.11	0.49
1:B:564:ASP:HA	1:B:567:ARG:NH1	2.27	0.49
1:A:399:VAL:C	1:A:401:ASN:H	2.16	0.49
1:A:325:VAL:HG12	1:A:329:LEU:CD1	2.43	0.49
1:A:114:ILE:HA	1:A:168:THR:HG22	1.95	0.49
1:B:177:ALA:HB1	1:B:178:PRO:HD2	1.95	0.49
1:C:48:GLU:C	1:C:49:LEU:HD12	2.32	0.49
1:C:284:SER:HA	1:C:287:ARG:HB2	1.95	0.49
1:C:359:ARG:C	1:C:361:GLY:H	2.15	0.49
1:B:89:ARG:NH2	1:B:96:LEU:HD21	2.27	0.49
1:C:700:ARG:O	1:C:704:GLU:HG3	2.13	0.49
1:B:397:GLU:O	1:B:401:ASN:ND2	2.45	0.49
2:A:900:ADP:O3B	3:A:915:AF3:F1	2.20	0.49
1:B:699:ILE:O	1:B:702:SER:HB3	2.13	0.49
1:A:648:PRO:CD	1:A:683:SER:HA	2.42	0.49
1:C:325:VAL:HG12	1:C:329:LEU:HD11	1.95	0.49
1:B:48:GLU:HB3	1:B:49:LEU:HD12	1.95	0.49
1:A:184:CYS:O	1:A:186:GLY:N	2.46	0.49
1:A:542:ILE:HG23	1:A:546:GLU:OE1	2.13	0.49
1:C:171:SER:OG	1:C:172:PRO:HA	2.12	0.49
1:A:206:ILE:CD1	1:A:213:LEU:CD2	2.79	0.49
1:A:28:VAL:HG23	1:A:84:MET:HG2	1.95	0.49
1:C:460:ASN:N	1:C:461:PRO:HD2	2.24	0.49
1:A:113:ARG:H	1:A:169:ASP:HB3	1.77	0.49
1:C:661:LEU:HD21	1:C:691:CYS:SG	2.53	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:519:PRO:HG3	1:B:647:LEU:HD12	1.95	0.49
1:B:648:PRO:CD	1:B:683:SER:HA	2.42	0.49
1:A:499:HIS:N	1:A:500:PRO:CD	2.76	0.49
1:B:706:GLU:HG2	1:B:707:ILE:N	2.28	0.49
1:C:303:ILE:HD12	1:C:306:LEU:HD13	1.94	0.49
1:C:579:LEU:HD22	1:C:629:ILE:CD1	2.42	0.49
1:B:184:CYS:C	1:B:186:GLY:H	2.15	0.49
1:B:28:VAL:HG23	1:B:84:MET:HG2	1.95	0.49
1:B:233:ILE:HG13	1:B:235:VAL:HG23	1.95	0.49
1:C:499:HIS:ND1	1:C:502:LYS:HD3	2.27	0.49
1:B:515:LEU:HD23	1:B:515:LEU:C	2.34	0.49
1:B:359:ARG:O	1:B:361:GLY:N	2.46	0.49
1:A:647:LEU:N	1:A:647:LEU:HD12	2.28	0.49
1:B:313:ARG:CG	1:B:314:GLU:H	2.26	0.49
1:A:323:ARG:NH2	1:B:279:ALA:HB2	2.26	0.49
1:C:359:ARG:O	1:C:361:GLY:N	2.46	0.49
1:A:206:ILE:O	1:A:206:ILE:HG13	2.12	0.48
1:A:86:ARG:O	1:A:89:ARG:HB3	2.13	0.48
1:B:650:GLU:H	1:B:650:GLU:CD	2.16	0.48
1:A:519:PRO:HD3	1:A:755:TYR:CD2	2.42	0.48
1:B:666:VAL:O	1:B:666:VAL:HG23	2.13	0.48
1:C:666:VAL:HG23	1:C:666:VAL:O	2.13	0.48
1:C:657:LEU:HB2	1:C:672:LEU:HD13	1.95	0.48
1:C:399:VAL:C	1:C:401:ASN:H	2.16	0.48
1:C:397:GLU:O	1:C:401:ASN:ND2	2.45	0.48
1:C:113:ARG:NH1	1:C:113:ARG:HG2	2.24	0.48
1:B:225:ARG:C	1:B:227:PRO:HD3	2.34	0.48
1:A:177:ALA:HB1	1:A:178:PRO:HD2	1.95	0.48
1:C:309:ILE:C	1:C:311:PRO:CD	2.79	0.48
1:A:145:PRO:HB3	1:A:175:ILE:HG12	1.94	0.48
1:B:635:ARG:HH11	1:B:635:ARG:CB	2.25	0.48
1:A:689:GLU:O	1:A:693:ARG:HG3	2.13	0.48
1:A:332:MET:C	1:A:334:GLY:H	2.16	0.48
1:C:612:SER:OG	1:C:615:LYS:HB2	2.13	0.48
1:B:427:MET:O	1:B:431:ASP:HA	2.13	0.48
1:B:399:VAL:C	1:B:401:ASN:H	2.17	0.48
1:B:515:LEU:HD13	1:B:634:LEU:HD21	1.94	0.48
1:B:359:ARG:C	1:B:361:GLY:H	2.16	0.48
1:A:359:ARG:O	1:A:361:GLY:N	2.46	0.48
1:B:353:ILE:HG22	1:B:354:ASP:N	2.20	0.48
1:B:312:LYS:N	1:B:354:ASP:HB2	2.19	0.48
1:A:499:HIS:CD2	1:B:703:ILE:HD13	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:503:PHE:CE2	1:A:510:PRO:HG3	2.48	0.48
1:A:56:THR:HG22	1:A:70:ILE:HD12	1.94	0.48
1:B:283:GLU:OE1	1:B:283:GLU:N	2.47	0.48
1:B:455:ALA:O	1:B:458:GLN:HB3	2.13	0.48
1:C:468:VAL:HG12	1:C:470:GLU:H	1.79	0.48
1:A:540:ILE:CD1	1:A:566:ALA:HA	2.43	0.48
1:C:411:LEU:O	1:C:414:LEU:HB3	2.13	0.48
1:A:24:ASN:O	1:A:101:SER:HA	2.13	0.48
1:B:250:GLY:HA2	2:B:807:ADP:PA	2.54	0.48
1:A:653:ARG:HH11	1:A:653:ARG:HG3	1.78	0.48
1:A:427:MET:CE	1:A:437:ILE:CD1	2.91	0.48
1:C:86:ARG:O	1:C:89:ARG:HB3	2.13	0.48
1:C:688:THR:O	1:C:691:CYS:HB2	2.13	0.48
1:B:524:LYS:HZ2	1:B:622:ALA:HB1	1.78	0.48
1:B:620:ILE:HG22	1:B:621:GLY:N	2.29	0.48
1:B:653:ARG:NE	1:B:679:THR:O	2.47	0.48
1:B:347:THR:HG21	1:B:353:ILE:HD11	1.95	0.48
1:A:490:GLN:HA	1:A:493:VAL:HG22	1.95	0.48
1:C:493:VAL:HG23	1:C:494:GLN:N	2.27	0.48
1:C:635:ARG:CB	1:C:635:ARG:HH11	2.26	0.48
1:C:41:LEU:HD23	1:C:82:ILE:HA	1.96	0.48
1:A:697:LEU:O	1:A:701:GLU:HG2	2.13	0.48
1:B:508:MET:SD	1:C:695:CYS:HB3	2.53	0.48
1:C:455:ALA:O	1:C:458:GLN:HB3	2.13	0.48
1:A:126:ILE:HG23	1:A:159:ARG:CZ	2.44	0.48
1:A:567:ARG:CZ	1:A:567:ARG:HB2	2.43	0.48
1:B:60:LYS:HD2	1:B:101:SER:OG	2.14	0.48
1:C:571:PRO:HA	1:C:616:ASN:OD1	2.14	0.48
1:A:397:GLU:O	1:A:401:ASN:ND2	2.46	0.48
2:B:900:ADP:O2B	3:B:915:AF3:F1	2.21	0.48
1:A:110:TYR:H	1:A:110:TYR:HD1	1.57	0.48
1:A:316:THR:C	1:A:318:GLY:H	2.17	0.48
1:A:94:VAL:HG21	1:A:100:ILE:CD1	2.34	0.48
1:B:325:VAL:HG12	1:B:329:LEU:HD11	1.96	0.48
1:C:556:GLU:O	1:C:559:VAL:HB	2.14	0.48
1:B:508:MET:SD	1:C:695:CYS:CB	3.02	0.48
1:B:728:VAL:N	1:B:729:PRO:CD	2.77	0.48
1:A:612:SER:OG	1:A:615:LYS:HB2	2.13	0.48
1:A:131:PHE:O	1:A:136:LYS:HB2	2.14	0.48
1:B:143:TYR:HE1	1:B:178:PRO:HD2	1.79	0.48
1:B:599:ARG:HG2	1:C:552:PHE:CD1	2.48	0.48
1:B:173:TYR:CD1	1:B:173:TYR:O	2.67	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:573:VAL:HG23	1:A:573:VAL:O	2.14	0.48
1:A:570:ALA:HA	1:A:571:PRO:C	2.33	0.48
1:B:473:GLN:OE1	1:B:473:GLN:N	2.44	0.48
1:C:515:LEU:HB3	1:C:642:LEU:HD13	1.96	0.48
1:A:253:LEU:HD23	1:A:253:LEU:C	2.35	0.48
1:A:225:ARG:C	1:A:227:PRO:HD3	2.34	0.48
1:B:482:LEU:HD12	1:B:645:ILE:HG23	1.96	0.48
1:B:758:PHE:HB3	1:B:762:LEU:HG	1.96	0.48
1:C:697:LEU:O	1:C:701:GLU:HG2	2.14	0.48
1:B:222:LEU:N	1:B:223:PRO:HD2	2.28	0.48
1:B:473:GLN:H	1:B:473:GLN:CD	2.17	0.48
1:B:93:ARG:NH2	1:B:195:GLU:HG2	2.29	0.47
1:A:627:ASP:CB	1:A:758:PHE:CZ	2.89	0.47
1:B:650:GLU:CD	1:B:650:GLU:N	2.68	0.47
1:A:683:SER:O	1:A:687:LEU:HG	2.14	0.47
1:A:26:LEU:HD21	1:A:45:LYS:HZ1	1.77	0.47
1:C:232:ALA:O	1:C:233:ILE:HB	2.14	0.47
1:A:487:ARG:NH1	1:A:487:ARG:CB	2.77	0.47
1:C:501:ASP:CG	1:C:502:LYS:HD2	2.34	0.47
1:B:758:PHE:C	1:B:762:LEU:HG	2.34	0.47
1:A:222:LEU:N	1:A:223:PRO:HD2	2.29	0.47
1:C:239:ARG:NH1	1:C:336:LYS:HB2	2.30	0.47
1:B:465:ARG:CB	1:B:465:ARG:NH1	2.77	0.47
1:A:538:ASN:O	1:A:573:VAL:HG22	2.14	0.47
1:A:39:VAL:HG11	1:A:59:LEU:HD11	1.96	0.47
1:C:518:GLY:C	1:C:755:TYR:HE2	2.17	0.47
1:A:427:MET:HE1	1:A:437:ILE:CD1	2.43	0.47
1:B:495:TYR:N	1:B:496:PRO:HD2	2.28	0.47
1:C:114:ILE:HA	1:C:168:THR:HG22	1.96	0.47
1:A:232:ALA:O	1:A:233:ILE:HB	2.14	0.47
1:A:512:LYS:NZ	1:A:608:MET:O	2.43	0.47
1:C:222:LEU:N	1:C:223:PRO:HD2	2.28	0.47
1:A:487:ARG:HB3	1:A:487:ARG:NH1	2.29	0.47
1:B:468:VAL:HG12	1:B:470:GLU:H	1.80	0.47
1:C:320:VAL:O	1:C:324:ILE:HG13	2.13	0.47
1:B:42:SER:HB3	1:B:77:CYS:O	2.13	0.47
1:C:659:ALA:C	1:C:661:LEU:H	2.18	0.47
1:A:733:ARG:CB	1:A:733:ARG:HH11	2.26	0.47
1:A:537:ALA:CB	1:A:571:PRO:HB2	2.45	0.47
1:B:304:ASP:O	1:B:305:GLU:HB2	2.14	0.47
1:C:427:MET:SD	1:C:433:GLU:CB	2.97	0.47
1:B:233:ILE:HD13	1:C:442:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:464:LEU:CG	1:C:466:GLU:HB3	2.45	0.47
1:C:94:VAL:HG21	1:C:100:ILE:CD1	2.34	0.47
1:B:210:ARG:NH2	1:B:375:THR:HG22	2.29	0.47
1:A:284:SER:HA	1:A:287:ARG:CB	2.44	0.47
1:C:143:TYR:HE1	1:C:178:PRO:HD2	1.79	0.47
1:C:620:ILE:HG22	1:C:621:GLY:N	2.29	0.47
1:B:567:ARG:HG2	1:C:460:ASN:HD21	1.80	0.47
1:C:502:LYS:HD2	1:C:502:LYS:H	1.79	0.47
1:B:253:LEU:HD23	1:B:253:LEU:C	2.35	0.47
1:A:325:VAL:HG12	1:A:329:LEU:HD11	1.96	0.47
1:C:479:ILE:N	1:C:479:ILE:CD1	2.77	0.47
1:C:579:LEU:HD11	1:C:633:ILE:HD13	1.97	0.47
1:C:407:VAL:HG23	1:C:409:ALA:H	1.80	0.47
1:B:733:ARG:CB	1:B:733:ARG:HH11	2.27	0.47
1:C:283:GLU:N	1:C:283:GLU:OE1	2.47	0.47
1:C:173:TYR:CD1	1:C:173:TYR:O	2.67	0.47
1:A:451:ASP:O	1:A:454:TRP:HB3	2.13	0.47
1:B:491:GLU:OE1	1:C:700:ARG:HD2	2.15	0.47
1:C:28:VAL:HG11	1:C:95:ARG:O	2.14	0.47
1:B:359:ARG:NH1	2:C:807:ADP:O3B	2.47	0.47
1:A:407:VAL:HG23	1:A:409:ALA:H	1.80	0.47
1:A:251:LYS:HE2	1:A:347:THR:O	2.15	0.47
1:C:225:ARG:C	1:C:227:PRO:HD3	2.34	0.47
1:A:283:GLU:OE1	1:A:283:GLU:N	2.47	0.47
1:A:310:ALA:N	1:A:311:PRO:CD	2.78	0.47
1:A:556:GLU:O	1:A:559:VAL:HB	2.13	0.47
1:B:41:LEU:HD23	1:B:82:ILE:HA	1.96	0.47
1:A:455:ALA:O	1:A:458:GLN:HB3	2.14	0.47
1:A:620:ILE:HG22	1:A:621:GLY:N	2.30	0.47
1:A:35:ASP:C	1:A:37:SER:H	2.18	0.47
1:A:517:TYR:CZ	1:A:644:TYR:HB2	2.50	0.47
1:A:479:ILE:HG21	1:A:486:LYS:HE2	1.97	0.47
1:A:519:PRO:CA	1:A:755:TYR:HE2	2.28	0.47
1:A:102:ILE:HG12	1:A:103:GLN:N	2.30	0.47
1:C:252:THR:HG23	1:C:302:PHE:CE2	2.50	0.47
1:C:28:VAL:HG23	1:C:84:MET:HG2	1.97	0.47
1:A:93:ARG:NH2	1:A:195:GLU:HG2	2.29	0.47
1:A:173:TYR:O	1:A:173:TYR:CD1	2.67	0.47
1:C:547:LEU:HD23	1:C:550:MET:HE3	1.97	0.47
1:A:525:THR:HG23	1:A:575:PHE:CE2	2.50	0.47
1:C:437:ILE:HG23	1:C:442:MET:SD	2.55	0.47
1:C:513:GLY:HA2	1:C:618:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:490:GLN:HA	1:B:493:VAL:HG22	1.97	0.47
1:C:253:LEU:HD12	2:C:807:ADP:H3'	1.98	0.47
1:C:110:TYR:HD1	1:C:110:TYR:H	1.61	0.47
1:B:313:ARG:HG2	1:B:314:GLU:N	2.27	0.47
1:B:284:SER:HA	1:B:287:ARG:CB	2.44	0.47
1:A:575:PHE:HA	1:A:620:ILE:O	2.14	0.47
1:B:451:ASP:O	1:B:454:TRP:HB3	2.14	0.47
1:C:376:GLY:O	1:C:380:ILE:HG13	2.16	0.47
1:B:515:LEU:HB3	1:B:642:LEU:CD1	2.45	0.46
1:C:253:LEU:HD23	1:C:253:LEU:C	2.35	0.46
1:B:251:LYS:HE2	1:B:347:THR:O	2.15	0.46
1:A:495:TYR:HD1	1:B:703:ILE:CD1	2.28	0.46
1:B:469:VAL:HG21	1:B:565:LYS:CE	2.41	0.46
1:A:514:VAL:HG11	1:A:643:ILE:HD12	1.97	0.46
1:C:451:ASP:O	1:C:454:TRP:HB3	2.13	0.46
1:C:555:SER:C	1:C:557:ALA:H	2.18	0.46
1:A:89:ARG:HH21	1:A:96:LEU:HD21	1.80	0.46
1:B:28:VAL:HG11	1:B:95:ARG:O	2.15	0.46
1:B:490:GLN:HB3	1:B:494:GLN:CG	2.43	0.46
1:A:657:LEU:CD1	1:A:672:LEU:HD22	2.44	0.46
1:A:579:LEU:HD23	1:A:579:LEU:C	2.36	0.46
1:C:633:ILE:HG21	1:C:639:LEU:HD12	1.96	0.46
1:A:239:ARG:NH1	1:A:336:LYS:HB2	2.30	0.46
1:B:729:PRO:C	1:B:730:GLU:CD	2.74	0.46
1:A:644:TYR:C	1:A:645:ILE:HD12	2.36	0.46
1:B:683:SER:O	1:B:687:LEU:HG	2.14	0.46
1:A:479:ILE:N	1:A:479:ILE:CD1	2.78	0.46
1:C:283:GLU:HB3	1:C:327:GLN:HE21	1.81	0.46
1:C:184:CYS:C	1:C:186:GLY:N	2.68	0.46
1:C:473:GLN:CD	1:C:473:GLN:H	2.18	0.46
1:C:753:ARG:O	1:C:757:MET:HG2	2.16	0.46
1:B:22:ARG:CG	1:B:25:ARG:NH1	2.69	0.46
1:C:662:ARG:HH11	1:C:662:ARG:HB2	1.79	0.46
1:C:683:SER:O	1:C:687:LEU:HG	2.14	0.46
1:C:93:ARG:NH2	1:C:194:GLU:HG3	2.08	0.46
1:C:495:TYR:N	1:C:496:PRO:HD2	2.31	0.46
1:B:580:ASP:O	1:B:581:SER:C	2.53	0.46
1:B:147:ARG:HG2	1:B:148:LYS:H	1.77	0.46
1:A:303:ILE:HG13	1:A:345:ALA:HA	1.97	0.46
1:C:284:SER:HA	1:C:287:ARG:CB	2.45	0.46
1:B:697:LEU:O	1:B:701:GLU:HG2	2.14	0.46
1:C:473:GLN:OE1	1:C:473:GLN:N	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:487:ARG:NH1	1:C:487:ARG:HB3	2.31	0.46
1:A:427:MET:SD	1:A:437:ILE:HD12	2.54	0.46
1:C:660:ASN:HD21	1:C:688:THR:HG23	1.81	0.46
1:B:679:THR:HB	1:B:682:PHE:CD1	2.51	0.46
1:B:147:ARG:CG	1:B:148:LYS:H	2.28	0.46
1:A:23:PRO:O	1:A:49:LEU:HD21	2.15	0.46
1:A:292:GLU:O	1:A:292:GLU:HG2	2.16	0.46
1:B:118:PRO:HB3	1:B:163:PHE:CE1	2.51	0.46
1:A:28:VAL:HG11	1:A:95:ARG:O	2.15	0.46
1:B:22:ARG:HB2	1:B:25:ARG:NH1	2.31	0.46
1:A:641:GLN:NE2	1:B:696:LYS:NZ	2.64	0.46
1:A:329:LEU:HD22	1:A:362:ARG:NH1	2.31	0.46
1:B:627:ASP:HB3	1:B:758:PHE:CE1	2.50	0.46
1:C:490:GLN:HA	1:C:493:VAL:HG22	1.98	0.46
1:C:80:GLU:O	1:C:80:GLU:HG3	2.16	0.46
1:A:89:ARG:NE	1:A:96:LEU:HD21	2.31	0.46
1:B:501:ASP:O	1:B:505:LYS:N	2.49	0.46
1:A:192:GLU:HB2	1:A:195:GLU:OE1	2.15	0.46
1:B:131:PHE:O	1:B:136:LYS:HB2	2.16	0.46
1:A:250:GLY:HA2	2:A:807:ADP:O3A	2.15	0.46
1:B:329:LEU:HD22	1:B:362:ARG:NH1	2.31	0.46
1:A:114:ILE:CD1	1:A:176:VAL:HG22	2.45	0.46
1:C:307:ASP:O	1:C:311:PRO:HD3	2.15	0.46
1:A:49:LEU:CD1	1:A:49:LEU:N	2.79	0.46
1:B:695:CYS:C	1:B:697:LEU:N	2.69	0.46
1:A:252:THR:HA	1:A:302:PHE:CZ	2.51	0.46
1:A:753:ARG:O	1:A:757:MET:HG2	2.16	0.46
1:B:214:ALA:O	1:B:218:GLU:HG2	2.16	0.46
1:C:460:ASN:O	1:C:462:SER:N	2.46	0.46
1:B:502:LYS:HG2	1:B:505:LYS:HE3	1.98	0.46
1:B:647:LEU:HB3	1:B:648:PRO:CD	2.42	0.46
1:B:251:LYS:HG3	2:B:807:ADP:O2B	2.15	0.46
1:B:540:ILE:CG2	1:B:574:LEU:HD12	2.46	0.46
1:A:235:VAL:HG11	1:B:420:LEU:HD21	1.98	0.46
1:B:407:VAL:HG23	1:B:409:ALA:H	1.80	0.46
1:A:376:GLY:O	1:A:380:ILE:HG13	2.16	0.46
1:C:201:VAL:CG2	1:C:256:ARG:HD2	2.45	0.46
1:C:112:LYS:H	1:C:170:PRO:CG	2.29	0.46
1:A:93:ARG:NH2	1:A:194:GLU:HG3	2.10	0.46
1:A:647:LEU:HD12	1:A:647:LEU:H	1.81	0.46
1:B:631:PRO:O	1:B:635:ARG:HG3	2.16	0.46
1:B:512:LYS:NZ	1:B:608:MET:O	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:695:CYS:C	1:C:697:LEU:N	2.70	0.46
1:B:459:SER:C	1:B:461:PRO:HD2	2.35	0.46
1:B:93:ARG:NH2	1:B:194:GLU:HG3	2.10	0.46
1:A:653:ARG:HA	1:A:656:ILE:HD12	1.97	0.46
1:B:114:ILE:HD13	1:B:146:ILE:HD11	1.98	0.46
1:A:520:PRO:HG3	1:A:624:ASN:HB3	1.98	0.46
1:B:555:SER:C	1:B:557:ALA:H	2.18	0.46
1:A:730:GLU:CD	1:A:730:GLU:N	2.69	0.46
1:A:513:GLY:HA3	1:A:619:ILE:O	2.16	0.45
1:C:24:ASN:CG	1:C:25:ARG:H	2.19	0.45
1:C:269:ILE:HD12	1:C:303:ILE:CG2	2.45	0.45
1:A:48:GLU:HB3	1:A:49:LEU:HD12	1.98	0.45
1:A:667:ALA:HB2	1:A:731:ILE:O	2.16	0.45
1:A:615:LYS:HZ2	1:B:460:ASN:CG	2.19	0.45
1:C:28:VAL:CG1	1:C:97:GLY:H	2.28	0.45
1:B:209:CYS:HB3	1:B:212:GLN:CB	2.36	0.45
1:A:347:THR:HG21	1:A:353:ILE:HD11	1.97	0.45
1:B:625:ARG:HA	1:B:625:ARG:HD3	1.79	0.45
1:B:753:ARG:O	1:B:757:MET:HG2	2.16	0.45
1:B:449:MET:CE	1:B:453:ARG:HH21	2.28	0.45
1:C:35:ASP:C	1:C:37:SER:H	2.20	0.45
1:B:560:ARG:HH11	1:B:560:ARG:HG3	1.81	0.45
1:A:464:LEU:HG	1:A:465:ARG:N	2.32	0.45
1:B:22:ARG:CB	1:B:25:ARG:NH1	2.79	0.45
1:B:501:ASP:O	1:B:505:LYS:HG3	2.16	0.45
1:A:476:TRP:HE1	1:A:534:GLU:CG	2.29	0.45
1:B:306:LEU:HG	1:B:310:ALA:HB3	1.98	0.45
1:B:155:ARG:HH21	1:B:386:LYS:HZ1	1.62	0.45
1:B:66:GLU:O	1:B:67:ALA:HB2	2.17	0.45
1:C:631:PRO:O	1:C:635:ARG:HG3	2.17	0.45
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.81	0.45
1:A:580:ASP:CG	1:A:625:ARG:HB2	2.36	0.45
1:B:376:GLY:O	1:B:380:ILE:HG13	2.17	0.45
1:B:28:VAL:CG1	1:B:97:GLY:H	2.29	0.45
1:C:126:ILE:HG23	1:C:159:ARG:CZ	2.46	0.45
1:B:540:ILE:HD12	1:B:566:ALA:CB	2.42	0.45
1:C:679:THR:HB	1:C:682:PHE:CD1	2.51	0.45
1:C:48:GLU:HB3	1:C:49:LEU:HD12	1.98	0.45
1:C:528:ALA:HB1	1:C:539:PHE:HE1	1.81	0.45
1:A:22:ARG:HH21	1:A:25:ARG:HD3	1.81	0.45
1:A:95:ARG:HB2	1:A:225:ARG:HH12	1.80	0.45
1:C:84:MET:HB2	1:C:88:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:420:LEU:HB3	1:A:424:ARG:NH1	2.31	0.45
1:A:304:ASP:O	1:A:305:GLU:HB2	2.16	0.45
1:A:197:SER:C	1:A:199:ASN:H	2.19	0.45
1:B:35:ASP:C	1:B:37:SER:H	2.19	0.45
1:C:645:ILE:HD12	1:C:645:ILE:N	2.31	0.45
1:C:292:GLU:O	1:C:292:GLU:HG2	2.16	0.45
1:C:360:PHE:H	1:C:360:PHE:HD1	1.64	0.45
1:B:612:SER:OG	1:B:615:LYS:HB2	2.16	0.45
1:C:499:HIS:N	1:C:500:PRO:CD	2.76	0.45
1:C:514:VAL:HG23	1:C:618:PHE:HZ	1.81	0.45
1:B:523:GLY:O	1:B:527:LEU:HG	2.16	0.45
2:B:900:ADP:PB	3:B:915:AF3:F3	2.65	0.45
1:C:251:LYS:HE2	1:C:347:THR:O	2.16	0.45
1:C:749:ASP:HA	1:C:752:ILE:CD1	2.44	0.45
1:A:749:ASP:HA	1:A:752:ILE:CD1	2.44	0.45
1:C:329:LEU:HD22	1:C:362:ARG:NH1	2.32	0.45
1:C:582:ILE:CD1	1:C:600:VAL:HB	2.47	0.45
1:B:573:VAL:HA	1:B:618:PHE:O	2.17	0.45
1:B:48:GLU:CB	1:B:49:LEU:HD12	2.47	0.45
1:A:487:ARG:CZ	1:A:487:ARG:HB3	2.46	0.45
1:C:487:ARG:CB	1:C:487:ARG:NH1	2.80	0.45
1:B:290:PHE:CD1	1:B:301:ILE:HD12	2.51	0.45
1:C:63:LYS:HD2	1:C:93:ARG:CG	2.47	0.45
1:C:102:ILE:HG12	1:C:103:GLN:N	2.32	0.45
1:B:749:ASP:HA	1:B:752:ILE:CD1	2.44	0.45
1:C:311:PRO:C	1:C:313:ARG:H	2.19	0.45
1:A:80:GLU:HG3	1:A:80:GLU:O	2.17	0.45
1:C:490:GLN:HB3	1:C:494:GLN:HG3	1.98	0.45
1:A:403:THR:HB	1:A:406:HIS:ND1	2.32	0.45
1:C:573:VAL:O	1:C:573:VAL:HG23	2.17	0.45
1:C:49:LEU:N	1:C:49:LEU:CD1	2.80	0.45
1:A:695:CYS:C	1:A:697:LEU:N	2.69	0.45
1:A:469:VAL:O	1:A:469:VAL:HG12	2.17	0.45
1:A:431:ASP:HB3	1:A:432:LEU:H	1.51	0.45
1:B:232:ALA:HA	1:C:159:ARG:NH2	2.32	0.45
1:B:112:LYS:H	1:B:170:PRO:CG	2.30	0.45
1:C:209:CYS:HB3	1:C:212:GLN:CB	2.36	0.45
1:B:580:ASP:O	1:B:582:ILE:N	2.50	0.45
1:B:360:PHE:H	1:B:360:PHE:HD1	1.63	0.45
1:B:518:GLY:O	1:B:755:TYR:CE2	2.70	0.45
1:B:487:ARG:HB3	1:B:487:ARG:NH1	2.31	0.45
1:A:407:VAL:HG23	1:A:410:ASP:H	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:403:THR:HB	1:C:406:HIS:ND1	2.31	0.45
1:A:269:ILE:HB	1:A:303:ILE:HG22	1.98	0.45
1:B:239:ARG:NH1	1:B:336:LYS:HB2	2.29	0.45
1:A:38:VAL:HG21	1:A:72:LEU:HD12	1.99	0.45
1:B:292:GLU:HG2	1:B:292:GLU:O	2.17	0.45
1:A:86:ARG:NH2	1:A:202:GLY:HA3	2.32	0.45
1:B:491:GLU:OE2	1:C:700:ARG:CZ	2.65	0.45
1:A:169:ASP:HB3	1:A:170:PRO:CD	2.30	0.45
1:C:647:LEU:HD12	1:C:647:LEU:N	2.29	0.45
1:A:679:THR:HB	1:A:682:PHE:CD1	2.52	0.45
1:A:631:PRO:O	1:A:635:ARG:HG3	2.17	0.45
1:B:49:LEU:N	1:B:49:LEU:CD1	2.79	0.45
1:C:487:ARG:HB3	1:C:487:ARG:CZ	2.47	0.45
1:A:360:PHE:HD1	1:A:360:PHE:H	1.63	0.45
1:C:368:ASP:HB2	1:C:568:GLN:CD	2.37	0.45
1:C:399:VAL:C	1:C:401:ASN:N	2.70	0.44
1:A:495:TYR:O	1:A:499:HIS:HB2	2.17	0.44
1:A:578:GLU:O	1:A:581:SER:N	2.33	0.44
1:A:313:ARG:CZ	1:A:314:GLU:OE1	2.65	0.44
1:A:537:ALA:HB2	1:A:571:PRO:HB2	1.99	0.44
1:A:147:ARG:HG2	1:A:148:LYS:H	1.79	0.44
1:A:92:LEU:O	1:A:94:VAL:HG13	2.17	0.44
1:A:399:VAL:C	1:A:401:ASN:N	2.70	0.44
1:C:519:PRO:HG3	1:C:647:LEU:HD11	2.00	0.44
1:A:240:GLY:HA3	1:A:363:PHE:HA	2.00	0.44
1:A:435:GLU:CA	1:A:435:GLU:OE1	2.62	0.44
1:A:686:ASP:OD2	1:A:746:SER:OG	2.28	0.44
1:B:729:PRO:O	1:B:730:GLU:OE2	2.35	0.44
1:C:133:VAL:HG21	1:C:439:ALA:CB	2.40	0.44
1:B:571:PRO:O	1:B:572:CYS:HB2	2.18	0.44
1:B:469:VAL:O	1:B:469:VAL:HG12	2.17	0.44
1:C:632:ALA:HA	1:C:635:ARG:CG	2.47	0.44
1:C:56:THR:HG22	1:C:70:ILE:HD12	1.97	0.44
1:A:184:CYS:C	1:A:186:GLY:N	2.71	0.44
1:C:560:ARG:HG3	1:C:560:ARG:HH11	1.82	0.44
1:B:95:ARG:HH22	1:B:196:GLU:CD	2.20	0.44
1:B:501:ASP:OD1	1:B:502:LYS:N	2.51	0.44
1:B:523:GLY:CA	2:B:900:ADP:O1A	2.62	0.44
1:C:667:ALA:HB3	1:C:670:VAL:HG23	1.99	0.44
1:A:26:LEU:HD21	1:A:45:LYS:CE	2.47	0.44
1:B:579:LEU:C	1:B:579:LEU:CD2	2.86	0.44
1:A:459:SER:C	1:A:461:PRO:HD2	2.37	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:449:MET:CE	1:A:453:ARG:HH21	2.30	0.44
1:C:459:SER:C	1:C:461:PRO:CD	2.81	0.44
1:C:437:ILE:CG2	1:C:442:MET:SD	3.05	0.44
1:B:399:VAL:C	1:B:401:ASN:N	2.71	0.44
1:A:506:PHE:HE2	1:B:699:ILE:HA	1.83	0.44
1:A:283:GLU:HB3	1:A:327:GLN:HE21	1.82	0.44
1:B:420:LEU:HB3	1:B:424:ARG:NH1	2.32	0.44
1:A:123:VAL:O	1:A:126:ILE:HG12	2.18	0.44
1:B:80:GLU:O	1:B:80:GLU:HG3	2.17	0.44
1:B:525:THR:HG23	1:B:575:PHE:CE2	2.53	0.44
1:B:531:ILE:HG23	1:B:532:ALA:N	2.31	0.44
1:B:356:ALA:O	1:B:362:ARG:NH1	2.51	0.44
1:A:114:ILE:HD13	1:A:146:ILE:HD11	2.00	0.44
1:B:632:ALA:HA	1:B:635:ARG:CG	2.48	0.44
1:C:243:LEU:HD23	1:C:369:ILE:HD11	1.98	0.44
1:C:586:ARG:NH1	1:C:598:ASP:HA	2.33	0.44
1:A:254:ILE:HG13	1:A:254:ILE:H	1.51	0.44
1:A:593:GLY:O	1:B:586:ARG:O	2.35	0.44
1:B:89:ARG:NE	1:B:96:LEU:HD21	2.33	0.44
1:C:89:ARG:NH2	1:C:96:LEU:HD21	2.33	0.44
1:C:420:LEU:HB3	1:C:424:ARG:NH1	2.32	0.44
1:A:460:ASN:O	1:A:462:SER:N	2.49	0.44
1:B:487:ARG:CB	1:B:487:ARG:NH1	2.80	0.44
1:A:464:LEU:HD21	1:A:466:GLU:HB3	2.00	0.44
1:A:89:ARG:HG3	1:A:94:VAL:O	2.18	0.44
1:C:647:LEU:CB	1:C:648:PRO:HD2	2.36	0.44
1:C:39:VAL:CG1	1:C:59:LEU:HD11	2.42	0.44
1:C:751:ASP:O	1:C:752:ILE:C	2.56	0.44
1:A:653:ARG:HD2	1:A:676:ALA:CA	2.39	0.44
1:B:419:ALA:O	1:B:423:ILE:HG13	2.18	0.44
1:C:66:GLU:HB2	1:C:147:ARG:HH12	1.83	0.44
1:A:118:PRO:HB3	1:A:163:PHE:CE1	2.53	0.44
1:C:164:LYS:HB3	1:C:189:ILE:CD1	2.48	0.44
1:A:147:ARG:CG	1:A:148:LYS:H	2.29	0.44
1:B:94:VAL:HG21	1:B:100:ILE:CD1	2.36	0.44
1:C:169:ASP:HB3	1:C:170:PRO:CD	2.32	0.44
1:B:528:ALA:O	1:B:531:ILE:HG22	2.18	0.44
1:A:492:LEU:C	1:A:496:PRO:HG3	2.37	0.44
1:A:503:PHE:CD1	1:B:699:ILE:CD1	3.01	0.44
1:C:259:ALA:CB	1:C:300:ILE:HD12	2.47	0.44
1:B:114:ILE:HD13	1:B:146:ILE:CD1	2.48	0.44
1:B:102:ILE:HG12	1:B:103:GLN:N	2.33	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:290:PHE:HA	1:B:301:ILE:HD11	2.00	0.44
1:C:197:SER:C	1:C:199:ASN:H	2.20	0.44
1:C:469:VAL:HG12	1:C:469:VAL:O	2.18	0.44
1:C:562:ILE:C	1:C:564:ASP:H	2.20	0.44
1:C:569:ALA:O	1:C:572:CYS:HB2	2.18	0.44
1:A:112:LYS:H	1:A:170:PRO:CG	2.30	0.43
2:B:900:ADP:O2B	3:B:915:AF3:F3	2.26	0.43
1:A:647:LEU:HB3	1:A:648:PRO:CD	2.44	0.43
1:A:329:LEU:HD13	1:B:272:PRO:HG2	2.00	0.43
1:B:403:THR:HB	1:B:406:HIS:ND1	2.32	0.43
1:A:119:ILE:HG13	1:A:162:GLU:O	2.18	0.43
1:A:48:GLU:CB	1:A:49:LEU:HD12	2.47	0.43
1:A:667:ALA:HB3	1:A:670:VAL:HG23	1.99	0.43
1:A:555:SER:C	1:A:557:ALA:H	2.18	0.43
1:C:449:MET:CE	1:C:453:ARG:HH21	2.31	0.43
1:A:560:ARG:HG3	1:A:560:ARG:HH11	1.82	0.43
1:A:28:VAL:CG1	1:A:97:GLY:H	2.31	0.43
1:A:567:ARG:CB	1:A:567:ARG:NH1	2.81	0.43
1:B:92:LEU:O	1:B:94:VAL:HG13	2.18	0.43
1:C:657:LEU:HD21	1:C:687:LEU:HB3	2.00	0.43
1:A:582:ILE:HG22	1:A:598:ASP:OD2	2.18	0.43
1:A:155:ARG:HE	1:A:386:LYS:HZ2	1.66	0.43
1:B:465:ARG:CZ	1:B:465:ARG:HB2	2.49	0.43
1:B:309:ILE:HG22	1:B:309:ILE:O	2.18	0.43
1:A:728:VAL:N	1:A:729:PRO:CD	2.81	0.43
1:A:214:ALA:O	1:A:218:GLU:HG2	2.18	0.43
1:B:562:ILE:C	1:B:564:ASP:N	2.71	0.43
1:B:192:GLU:HB2	1:B:195:GLU:OE1	2.18	0.43
1:B:251:LYS:H	2:B:807:ADP:PB	2.40	0.43
1:A:502:LYS:HD3	1:B:702:SER:OG	2.19	0.43
1:B:177:ALA:C	1:B:179:ASP:N	2.71	0.43
1:A:252:THR:HA	1:A:302:PHE:CE2	2.53	0.43
1:A:562:ILE:C	1:A:564:ASP:N	2.71	0.43
1:C:580:ASP:O	1:C:583:ALA:N	2.46	0.43
1:A:256:ARG:HG3	1:A:256:ARG:HH11	1.83	0.43
1:A:615:LYS:NZ	1:B:460:ASN:ND2	2.66	0.43
1:B:438:ASP:OD2	1:B:440:GLU:HB2	2.18	0.43
1:A:519:PRO:HG3	1:A:647:LEU:CD1	2.48	0.43
1:A:328:LEU:O	1:A:329:LEU:C	2.57	0.43
1:B:240:GLY:HA3	1:B:363:PHE:HA	1.99	0.43
1:B:329:LEU:HD23	1:B:357:LEU:CD2	2.49	0.43
1:B:582:ILE:HD12	1:B:601:ILE:CG1	2.44	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:563:PHE:CE1	1:C:574:LEU:CD2	3.01	0.43
1:C:586:ARG:HH12	1:C:598:ASP:HA	1.82	0.43
1:C:38:VAL:HG21	1:C:72:LEU:HD12	2.01	0.43
1:B:62:LYS:NZ	1:B:98:ASP:HB3	2.32	0.43
1:A:433:GLU:HG2	1:A:437:ILE:HD13	2.00	0.43
1:A:233:ILE:CG1	1:A:235:VAL:HG23	2.48	0.43
1:C:147:ARG:HG2	1:C:148:LYS:H	1.81	0.43
1:A:95:ARG:HH22	1:A:196:GLU:CD	2.21	0.43
1:A:529:LYS:O	1:A:532:ALA:HB3	2.19	0.43
1:C:512:LYS:HB2	1:C:638:ARG:O	2.19	0.43
1:B:524:LYS:NZ	1:B:622:ALA:HB1	2.33	0.43
1:A:533:ASN:C	1:A:535:CYS:N	2.70	0.43
1:A:648:PRO:HG3	1:A:683:SER:HA	2.00	0.43
1:A:356:ALA:O	1:A:362:ARG:NH1	2.52	0.43
1:B:329:LEU:HD23	1:B:357:LEU:HD23	2.01	0.43
1:A:373:ASP:HA	1:A:377:ARG:NH1	2.33	0.43
1:A:515:LEU:HD21	1:A:623:THR:HG22	1.99	0.43
1:A:625:ARG:HD3	1:A:625:ARG:HA	1.74	0.43
1:C:518:GLY:C	1:C:755:TYR:CE2	2.91	0.43
1:C:562:ILE:C	1:C:564:ASP:N	2.70	0.43
1:C:118:PRO:HB3	1:C:163:PHE:CE1	2.54	0.43
1:C:214:ALA:O	1:C:218:GLU:HG2	2.18	0.43
1:C:63:LYS:O	1:C:64:ARG:C	2.56	0.43
1:B:653:ARG:HG2	1:B:687:LEU:HD11	2.00	0.43
1:A:110:TYR:CD1	1:A:110:TYR:N	2.81	0.43
1:A:143:TYR:HE1	1:A:178:PRO:HD2	1.84	0.43
1:C:582:ILE:HD13	1:C:600:VAL:HB	2.01	0.43
1:B:573:VAL:HG23	1:B:573:VAL:O	2.19	0.43
1:C:407:VAL:HG23	1:C:410:ASP:H	1.83	0.43
1:A:215:GLN:O	1:A:219:MET:HG3	2.19	0.43
1:B:197:SER:C	1:B:199:ASN:H	2.21	0.43
1:A:89:ARG:CZ	1:A:96:LEU:HD21	2.48	0.43
1:C:648:PRO:CD	1:C:683:SER:HA	2.49	0.43
1:B:582:ILE:HG21	1:B:598:ASP:CG	2.39	0.43
1:C:155:ARG:HE	1:C:386:LYS:HZ2	1.67	0.43
1:B:407:VAL:HG23	1:B:410:ASP:H	1.84	0.43
1:C:95:ARG:HH22	1:C:196:GLU:CD	2.21	0.43
1:C:405:GLY:O	1:C:464:LEU:O	2.37	0.43
1:C:523:GLY:O	1:C:526:LEU:N	2.51	0.43
1:A:445:LEU:C	1:A:445:LEU:CD2	2.88	0.43
1:A:519:PRO:N	1:A:755:TYR:CE2	2.86	0.43
1:B:110:TYR:CD1	1:B:110:TYR:N	2.81	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:728:VAL:HG12	1:B:728:VAL:O	2.19	0.43
1:C:542:ILE:N	1:C:542:ILE:HD12	2.34	0.43
1:A:562:ILE:C	1:A:564:ASP:H	2.22	0.43
1:B:649:ASP:N	1:B:652:SER:HB2	2.34	0.43
1:B:491:GLU:CA	1:B:495:TYR:HE2	2.21	0.43
1:B:206:ILE:CD1	1:B:213:LEU:CD1	2.94	0.43
1:C:356:ALA:O	1:C:362:ARG:NH1	2.51	0.43
1:C:377:ARG:HD2	1:C:403:THR:OG1	2.19	0.43
1:B:373:ASP:HA	1:B:377:ARG:NH1	2.33	0.43
1:A:512:LYS:HE2	1:A:512:LYS:HB3	1.83	0.43
1:C:673:GLU:O	1:C:676:ALA:HB3	2.18	0.43
1:A:655:ALA:O	1:A:659:ALA:N	2.52	0.43
1:C:93:ARG:HH22	1:C:195:GLU:HG2	1.83	0.42
1:A:758:PHE:C	1:A:762:LEU:HG	2.38	0.42
1:A:506:PHE:CZ	1:B:698:ALA:HB1	2.54	0.42
1:A:177:ALA:C	1:A:179:ASP:N	2.71	0.42
1:C:309:ILE:O	1:C:311:PRO:HD2	2.18	0.42
1:B:244:TYR:CD1	1:B:350:PRO:HG3	2.54	0.42
1:B:220:VAL:CG1	1:B:342:ILE:HD13	2.49	0.42
1:B:135:LEU:N	1:B:135:LEU:CD2	2.81	0.42
1:C:625:ARG:HA	1:C:625:ARG:HD3	1.64	0.42
1:B:138:TYR:CZ	1:B:144:ARG:HD3	2.55	0.42
1:C:567:ARG:HG3	1:C:615:LYS:CE	2.32	0.42
1:C:353:ILE:CG2	1:C:354:ASP:H	2.18	0.42
1:B:248:GLY:C	1:B:250:GLY:N	2.72	0.42
1:B:328:LEU:O	1:B:329:LEU:C	2.57	0.42
1:C:328:LEU:O	1:C:329:LEU:C	2.56	0.42
1:C:596:ALA:CB	1:C:630:ASP:HA	2.48	0.42
1:B:737:GLU:C	1:B:739:ALA:H	2.22	0.42
1:B:487:ARG:CZ	1:B:487:ARG:HB3	2.49	0.42
1:C:164:LYS:HB3	1:C:189:ILE:HD11	2.01	0.42
1:C:657:LEU:C	1:C:659:ALA:N	2.70	0.42
2:B:900:ADP:PB	3:B:915:AF3:F1	2.68	0.42
1:A:673:GLU:O	1:A:676:ALA:HB3	2.19	0.42
1:A:357:LEU:HB3	1:A:363:PHE:CD2	2.47	0.42
1:C:303:ILE:HD11	1:C:345:ALA:HB2	2.01	0.42
1:C:579:LEU:C	1:C:579:LEU:CD2	2.88	0.42
1:C:177:ALA:C	1:C:179:ASP:N	2.71	0.42
1:B:669:ASP:HB2	1:B:733:ARG:HH12	1.84	0.42
1:B:275:MET:HG2	1:B:309:ILE:HD11	2.01	0.42
1:B:508:MET:SD	1:C:695:CYS:HB2	2.60	0.42
1:B:184:CYS:C	1:B:186:GLY:N	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:414:LEU:HD12	1:C:455:ALA:HB1	2.01	0.42
1:B:667:ALA:HB3	1:B:670:VAL:HG23	2.00	0.42
1:B:504:LEU:N	1:B:504:LEU:HD12	2.35	0.42
1:A:155:ARG:NE	1:A:386:LYS:NZ	2.66	0.42
1:A:737:GLU:C	1:A:739:ALA:H	2.23	0.42
1:C:483:GLU:OE1	1:C:486:LYS:HD2	2.20	0.42
1:B:169:ASP:HB3	1:B:170:PRO:CD	2.31	0.42
1:A:526:LEU:O	1:A:530:ALA:HB2	2.19	0.42
1:B:303:ILE:HD11	1:B:345:ALA:HB2	2.01	0.42
1:A:518:GLY:C	1:A:755:TYR:CE2	2.93	0.42
1:A:329:LEU:HD23	1:A:357:LEU:CD2	2.50	0.42
1:A:632:ALA:HA	1:A:635:ARG:CG	2.47	0.42
1:C:215:GLN:O	1:C:219:MET:HG3	2.19	0.42
1:C:123:VAL:O	1:C:126:ILE:HG12	2.20	0.42
1:C:503:PHE:CZ	1:C:510:PRO:HG3	2.55	0.42
1:B:673:GLU:O	1:B:676:ALA:HB3	2.18	0.42
1:A:243:LEU:HD23	1:A:369:ILE:HD11	2.01	0.42
1:C:649:ASP:OD2	1:C:651:LYS:HB2	2.20	0.42
1:B:123:VAL:O	1:B:126:ILE:HG12	2.19	0.42
1:A:206:ILE:CD1	1:A:213:LEU:CD1	2.94	0.42
1:C:256:ARG:HG3	1:C:256:ARG:HH11	1.84	0.42
1:C:436:THR:OG1	1:C:437:ILE:N	2.52	0.42
1:C:464:LEU:HD11	1:C:466:GLU:HB2	1.93	0.42
1:A:136:LYS:HB3	1:A:137:PRO:CD	2.40	0.42
1:C:240:GLY:HA3	1:C:363:PHE:HA	2.01	0.42
1:C:114:ILE:CD1	1:C:176:VAL:HG22	2.48	0.42
1:B:256:ARG:HH11	1:B:256:ARG:HG3	1.85	0.42
1:C:135:LEU:N	1:C:135:LEU:CD2	2.82	0.42
1:A:661:LEU:O	1:A:664:SER:HB2	2.19	0.42
1:B:38:VAL:HG21	1:B:72:LEU:HD12	2.01	0.42
1:A:360:PHE:CD1	1:A:360:PHE:N	2.87	0.42
1:B:562:ILE:C	1:B:564:ASP:H	2.21	0.42
1:C:86:ARG:NH2	1:C:202:GLY:HA3	2.35	0.42
1:C:210:ARG:HH22	1:C:375:THR:HG22	1.85	0.42
1:B:377:ARG:HD2	1:B:403:THR:OG1	2.19	0.42
1:B:665:PRO:HG2	1:B:731:ILE:HD12	2.01	0.42
1:B:318:GLY:O	1:B:322:ARG:HG3	2.20	0.42
1:B:542:ILE:HD12	1:B:542:ILE:N	2.35	0.42
1:B:414:LEU:HD12	1:B:455:ALA:HB1	2.00	0.42
1:B:35:ASP:HB3	1:B:38:VAL:CG1	2.49	0.42
1:C:438:ASP:OD2	1:C:440:GLU:HB2	2.20	0.42
1:C:419:ALA:O	1:C:423:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:524:LYS:HB2	3:B:915:AF3:F3	2.10	0.42
1:B:497:VAL:HG13	1:B:498:GLU:N	2.35	0.42
1:A:520:PRO:HG3	1:A:624:ASN:HB2	2.01	0.42
1:C:580:ASP:OD2	1:C:625:ARG:HB2	2.20	0.42
1:C:254:ILE:H	1:C:254:ILE:HG13	1.52	0.42
1:C:427:MET:HG3	1:C:432:LEU:HB2	2.02	0.42
1:B:519:PRO:HA	1:B:520:PRO:HD3	1.93	0.42
1:C:248:GLY:C	1:C:250:GLY:N	2.72	0.42
1:A:751:ASP:O	1:A:752:ILE:C	2.56	0.42
1:A:311:PRO:O	1:A:313:ARG:N	2.53	0.42
1:C:493:VAL:HG21	1:C:531:ILE:HD11	2.01	0.42
1:B:737:GLU:C	1:B:739:ALA:N	2.74	0.42
1:C:360:PHE:N	1:C:360:PHE:CD1	2.88	0.42
1:C:138:TYR:CZ	1:C:144:ARG:HD3	2.55	0.42
1:A:152:PHE:HD1	1:A:152:PHE:H	1.66	0.42
1:B:612:SER:HB3	1:B:615:LYS:CB	2.46	0.41
1:B:445:LEU:CD2	1:B:445:LEU:C	2.88	0.41
1:B:253:LEU:HD12	2:B:807:ADP:H2'	2.02	0.41
1:C:664:SER:HA	1:C:665:PRO:HD3	1.79	0.41
1:C:32:ILE:HG12	1:C:83:ARG:CD	2.45	0.41
1:C:147:ARG:CG	1:C:148:LYS:H	2.32	0.41
1:C:48:GLU:CB	1:C:49:LEU:HD12	2.50	0.41
1:B:243:LEU:HD23	1:B:369:ILE:HD11	2.00	0.41
1:A:419:ALA:O	1:A:423:ILE:HG13	2.20	0.41
1:B:226:HIS:C	1:B:228:ALA:N	2.73	0.41
1:C:335:LEU:HD11	1:C:343:VAL:HG21	2.02	0.41
1:B:751:ASP:O	1:B:752:ILE:C	2.57	0.41
1:A:329:LEU:HD23	1:A:357:LEU:HD23	2.02	0.41
1:B:114:ILE:CD1	1:B:176:VAL:HG22	2.49	0.41
1:A:235:VAL:HG12	1:A:236:LYS:N	2.35	0.41
1:A:303:ILE:HD12	1:A:306:LEU:HD13	2.02	0.41
1:A:741:ARG:HA	1:A:741:ARG:NE	2.31	0.41
1:A:697:LEU:C	1:A:697:LEU:HD13	2.41	0.41
1:C:252:THR:HA	1:C:302:PHE:CE2	2.55	0.41
1:B:35:ASP:HB3	1:B:38:VAL:HG12	2.02	0.41
1:B:152:PHE:HD1	1:B:152:PHE:H	1.67	0.41
1:C:430:ILE:O	1:C:430:ILE:HG22	2.19	0.41
1:A:427:MET:HE3	1:A:441:VAL:HG11	2.01	0.41
1:C:612:SER:HB3	1:C:615:LYS:CB	2.46	0.41
1:C:113:ARG:HG3	1:C:169:ASP:HB2	2.02	0.41
1:B:209:CYS:HA	1:B:212:GLN:HG2	2.02	0.41
1:A:248:GLY:C	1:A:250:GLY:N	2.73	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:359:ARG:NH1	2:B:807:ADP:O3B	2.53	0.41
1:A:653:ARG:O	1:A:657:LEU:HG	2.19	0.41
1:A:633:ILE:HG21	1:A:639:LEU:HD12	1.96	0.41
1:C:737:GLU:C	1:C:739:ALA:H	2.22	0.41
1:A:35:ASP:HB3	1:A:38:VAL:CG1	2.49	0.41
1:A:659:ALA:HA	1:A:662:ARG:HG3	2.02	0.41
1:C:192:GLU:HB2	1:C:195:GLU:OE1	2.20	0.41
1:A:506:PHE:CD2	1:B:699:ILE:CG1	2.95	0.41
1:A:502:LYS:NZ	1:B:706:GLU:OE1	2.53	0.41
1:C:489:LEU:HD22	1:C:531:ILE:HG12	2.01	0.41
1:A:244:TYR:CD1	1:A:350:PRO:HG3	2.55	0.41
1:B:665:PRO:HG2	1:B:731:ILE:CD1	2.51	0.41
1:B:215:GLN:O	1:B:219:MET:HG3	2.20	0.41
1:C:220:VAL:CG1	1:C:342:ILE:HD13	2.50	0.41
1:B:697:LEU:HD13	1:B:697:LEU:C	2.40	0.41
1:B:567:ARG:HG3	1:B:615:LYS:HE2	2.02	0.41
1:B:113:ARG:HG3	1:B:169:ASP:HB2	2.03	0.41
1:C:329:LEU:HD23	1:C:357:LEU:HD23	2.02	0.41
1:C:32:ILE:HG22	1:C:32:ILE:O	2.20	0.41
1:B:360:PHE:N	1:B:360:PHE:CD1	2.87	0.41
1:B:360:PHE:HE2	1:C:410:ASP:OD1	2.03	0.41
1:A:514:VAL:CG1	1:A:515:LEU:N	2.83	0.41
1:A:414:LEU:HD11	1:A:456:LEU:HD23	2.02	0.41
1:A:335:LEU:HD11	1:A:343:VAL:HG21	2.02	0.41
1:C:648:PRO:HD3	1:C:683:SER:HA	2.02	0.41
1:C:92:LEU:O	1:C:94:VAL:HG13	2.20	0.41
1:A:489:LEU:CD2	1:A:531:ILE:HD13	2.40	0.41
1:B:580:ASP:C	1:B:582:ILE:N	2.73	0.41
1:B:741:ARG:HA	1:B:741:ARG:NE	2.30	0.41
1:C:586:ARG:HH11	1:C:598:ASP:HB2	1.84	0.41
1:A:414:LEU:HD12	1:A:455:ALA:HB1	2.01	0.41
1:B:197:SER:C	1:B:199:ASN:N	2.74	0.41
1:A:427:MET:HA	1:A:431:ASP:HB2	2.02	0.41
1:B:319:GLU:OE2	1:B:323:ARG:NH2	2.54	0.41
1:C:427:MET:SD	1:C:433:GLU:CG	3.09	0.41
1:B:515:LEU:HD23	1:B:516:PHE:O	2.20	0.41
1:C:209:CYS:HA	1:C:212:GLN:HG2	2.03	0.41
1:A:209:CYS:HA	1:A:212:GLN:HG2	2.02	0.41
1:C:408:GLY:HA3	2:C:807:ADP:C8	2.56	0.41
1:B:566:ALA:O	1:B:569:ALA:C	2.59	0.41
1:C:233:ILE:CG1	1:C:235:VAL:HG23	2.50	0.41
1:B:243:LEU:HB3	1:B:369:ILE:CD1	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:564:ASP:C	1:C:566:ALA:H	2.22	0.41
1:C:730:GLU:N	1:C:730:GLU:CD	2.74	0.41
1:A:226:HIS:C	1:A:228:ALA:N	2.73	0.41
1:B:89:ARG:HH21	1:B:96:LEU:HD21	1.85	0.41
1:B:506:PHE:HE2	1:C:699:ILE:HG12	1.83	0.41
1:B:515:LEU:HA	1:B:621:GLY:O	2.21	0.41
1:B:479:ILE:HG21	1:B:486:LYS:HE2	2.03	0.41
1:A:114:ILE:HD13	1:A:146:ILE:CD1	2.51	0.41
1:A:699:ILE:O	1:A:702:SER:HB3	2.21	0.41
1:C:741:ARG:NE	1:C:741:ARG:HA	2.30	0.41
1:C:613:THR:HG23	1:C:614:LYS:H	1.86	0.41
1:C:596:ALA:HB1	1:C:630:ASP:CA	2.50	0.41
1:A:542:ILE:HD12	1:A:542:ILE:N	2.36	0.41
1:A:84:MET:HB2	1:A:88:VAL:HB	2.02	0.41
1:B:22:ARG:HG3	1:B:22:ARG:HH11	1.85	0.41
1:B:89:ARG:CZ	1:B:96:LEU:HD21	2.51	0.41
1:B:32:ILE:O	1:B:32:ILE:HG22	2.21	0.41
1:B:235:VAL:HG12	1:B:236:LYS:N	2.35	0.41
1:C:65:ARG:NH1	1:C:93:ARG:NH1	2.69	0.41
1:A:642:LEU:N	1:A:642:LEU:CD2	2.84	0.41
1:A:503:PHE:CD1	1:B:699:ILE:HD13	2.55	0.41
1:A:682:PHE:CE2	1:A:744:ARG:O	2.74	0.41
1:B:540:ILE:CD1	1:B:566:ALA:HB2	2.43	0.41
1:C:559:VAL:HG13	1:C:563:PHE:HE2	1.86	0.41
1:B:244:TYR:CE2	1:B:350:PRO:HG3	2.56	0.41
1:C:244:TYR:CD1	1:C:350:PRO:HG3	2.54	0.41
1:B:201:VAL:CG1	1:B:202:GLY:N	2.82	0.41
1:C:43:GLN:HB3	1:C:44:PRO:CD	2.51	0.41
1:B:153:LEU:HD13	1:B:162:GLU:CG	2.51	0.41
1:B:23:PRO:O	1:B:49:LEU:HD21	2.20	0.41
1:A:737:GLU:C	1:A:739:ALA:N	2.74	0.41
1:A:521:GLY:CA	1:A:685:ALA:HB2	2.50	0.41
1:A:51:LEU:CD2	1:A:104:PRO:HB3	2.50	0.41
1:C:312:LYS:HG2	1:C:312:LYS:O	2.21	0.41
1:A:287:ARG:HA	1:A:287:ARG:HD2	1.88	0.41
1:B:143:TYR:CE1	1:B:178:PRO:HD2	2.55	0.41
1:C:244:TYR:CE2	1:C:350:PRO:HG3	2.56	0.41
1:C:693:ARG:NE	1:C:742:PHE:HB2	2.36	0.41
1:A:440:GLU:O	1:A:441:VAL:C	2.60	0.40
1:B:89:ARG:HG3	1:B:94:VAL:O	2.21	0.40
1:B:92:LEU:CB	1:B:94:VAL:HG22	2.49	0.40
1:C:514:VAL:CG1	1:C:515:LEU:N	2.84	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:225:ARG:HD3	1:B:262:THR:HG22	2.03	0.40
1:C:329:LEU:HD23	1:C:357:LEU:CD2	2.50	0.40
1:C:119:ILE:HG13	1:C:162:GLU:O	2.21	0.40
1:A:135:LEU:CD2	1:A:135:LEU:N	2.84	0.40
1:C:737:GLU:C	1:C:739:ALA:N	2.74	0.40
1:A:197:SER:C	1:A:199:ASN:N	2.74	0.40
1:C:197:SER:C	1:C:199:ASN:N	2.74	0.40
1:B:649:ASP:OD1	1:B:652:SER:OG	2.38	0.40
1:C:651:LYS:O	1:C:652:SER:C	2.59	0.40
1:A:95:ARG:HG3	1:A:225:ARG:HH12	1.86	0.40
1:B:517:TYR:C	1:B:524:LYS:HD3	2.42	0.40
1:B:653:ARG:O	1:B:657:LEU:HG	2.20	0.40
1:A:348:ASN:HD22	1:A:348:ASN:N	2.18	0.40
1:A:283:GLU:O	1:A:327:GLN:NE2	2.51	0.40
1:A:32:ILE:HG12	1:A:83:ARG:CD	2.47	0.40
1:A:556:GLU:OE2	1:A:599:ARG:NH1	2.53	0.40
1:C:653:ARG:NE	1:C:679:THR:O	2.54	0.40
1:C:243:LEU:HB3	1:C:369:ILE:CD1	2.51	0.40
1:A:290:PHE:CD1	1:A:301:ILE:HD12	2.55	0.40
1:B:660:ASN:ND2	1:B:688:THR:OG1	2.54	0.40
1:A:487:ARG:HH11	1:A:487:ARG:HB2	1.86	0.40
1:B:38:VAL:HG22	1:B:39:VAL:N	2.37	0.40
1:C:152:PHE:H	1:C:152:PHE:HD1	1.68	0.40
1:A:221:GLU:O	1:A:225:ARG:CB	2.62	0.40
1:B:502:LYS:HZ3	1:C:703:ILE:HG12	1.75	0.40
1:C:201:VAL:CG1	1:C:202:GLY:N	2.82	0.40
1:C:423:ILE:O	1:C:425:LYS:N	2.55	0.40
1:A:645:ILE:HA	1:A:646:PRO:HD2	1.88	0.40
1:C:659:ALA:O	1:C:662:ARG:HG3	2.21	0.40
1:C:92:LEU:CB	1:C:94:VAL:HG22	2.51	0.40
1:C:608:MET:SD	1:C:638:ARG:HB3	2.61	0.40
1:C:445:LEU:C	1:C:445:LEU:CD2	2.89	0.40
1:A:476:TRP:NE1	1:A:534:GLU:HB2	2.35	0.40
1:C:579:LEU:HD22	1:C:629:ILE:HD12	2.03	0.40
1:B:43:GLN:HB3	1:B:44:PRO:CD	2.51	0.40
1:B:119:ILE:HG13	1:B:162:GLU:O	2.21	0.40
1:B:335:LEU:HD11	1:B:343:VAL:HG21	2.03	0.40
1:B:518:GLY:C	1:B:755:TYR:CE2	2.95	0.40
1:B:126:ILE:HG23	1:B:159:ARG:CZ	2.51	0.40
1:A:385:THR:HB	1:A:390:LEU:HD11	2.04	0.40
1:A:225:ARG:HD3	1:A:262:THR:HG22	2.04	0.40
1:C:256:ARG:HH22	1:C:268:LEU:HD22	1.87	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:259:ALA:CB	1:A:300:ILE:HD12	2.52	0.40
1:B:642:LEU:CD2	1:B:642:LEU:N	2.84	0.40
1:B:657:LEU:HB2	1:B:672:LEU:HD13	2.03	0.40
1:B:136:LYS:HB3	1:B:137:PRO:CD	2.37	0.40
1:B:239:ARG:HD2	1:B:335:LEU:CB	2.51	0.40
1:C:702:SER:O	1:C:706:GLU:HG3	2.20	0.40
1:B:502:LYS:HD3	1:C:703:ILE:HG12	2.02	0.40
1:B:32:ILE:HG12	1:B:83:ARG:CD	2.48	0.40
1:C:523:GLY:O	1:C:524:LYS:C	2.59	0.40
1:A:476:TRP:HE1	1:A:534:GLU:CB	2.34	0.40
1:A:248:GLY:O	1:A:409:ALA:HB2	2.21	0.40
1:B:348:ASN:HD22	1:B:348:ASN:N	2.19	0.40
1:B:357:LEU:HB3	1:B:363:PHE:CD2	2.49	0.40
1:B:584:LYS:HZ1	1:B:625:ARG:CG	2.34	0.40
1:A:282:SER:HB2	1:A:283:GLU:OE1	2.22	0.40
1:C:114:ILE:HD13	1:C:146:ILE:HD11	2.03	0.40
1:A:313:ARG:O	1:A:316:THR:HG22	2.22	0.40
1:C:582:ILE:O	1:C:582:ILE:HG22	2.21	0.40
1:A:133:VAL:HG13	1:A:443:ASN:HD22	1.86	0.40
1:A:244:TYR:CE2	1:A:350:PRO:HG3	2.57	0.40
1:A:377:ARG:HD2	1:A:403:THR:OG1	2.21	0.40
1:B:372:PRO:CD	1:B:407:VAL:HA	2.52	0.40
1:A:145:PRO:HA	1:A:175:ILE:HA	2.02	0.40
1:A:661:LEU:HD21	1:A:691:CYS:SG	2.62	0.40
1:C:226:HIS:C	1:C:228:ALA:N	2.73	0.40
1:C:187:GLU:OE2	1:C:188:PRO:HD2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	711/806 (88%)	536 (75%)	155 (22%)	20 (3%)	8	59
1	B	719/806 (89%)	548 (76%)	148 (21%)	23 (3%)	6	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	719/806 (89%)	533 (74%)	163 (23%)	23 (3%)	6	56
All	All	2149/2418 (89%)	1617 (75%)	466 (22%)	66 (3%)	7	57

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	PHE
1	B	360	PHE
1	C	360	PHE
1	A	185	GLU
1	A	353	ILE
1	B	185	GLU
1	B	353	ILE
1	C	185	GLU
1	C	353	ILE
1	A	30	GLU
1	A	98	ASP
1	A	313	ARG
1	A	508	MET
1	B	30	GLU
1	B	98	ASP
1	B	204	ASP
1	B	315	LYS
1	B	588	GLY
1	C	30	GLU
1	C	204	ASP
1	A	22	ARG
1	A	36	ASN
1	A	178	PRO
1	A	204	ASP
1	A	233	ILE
1	A	412	ALA
1	B	36	ASN
1	B	233	ILE
1	B	311	PRO
1	B	412	ALA
1	C	22	ARG
1	C	36	ASN
1	C	98	ASP
1	C	178	PRO
1	C	233	ILE
1	C	412	ALA

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Mol	Chain	Res	Type
1	C	431	ASP
1	C	522	CYS
1	C	597	ALA
1	C	647	LEU
1	A	338	ARG
1	B	178	PRO
1	B	338	ARG
1	B	462	SER
1	B	500	PRO
1	C	310	ALA
1	C	338	ARG
1	C	660	ASN
1	C	702	SER
1	A	510	PRO
1	B	22	ARG
1	B	310	ALA
1	C	123	VAL
1	A	123	VAL
1	B	123	VAL
1	B	188	PRO
1	B	729	PRO
1	C	460	ASN
1	A	188	PRO
1	A	399	VAL
1	A	460	ASN
1	B	460	ASN
1	C	399	VAL
1	B	399	VAL
1	C	188	PRO
1	A	310	ALA

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	612/678 (90%)	605 (99%)	7 (1%)	84	95
1	B	615/678 (91%)	610 (99%)	5 (1%)	89	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	615/678 (91%)	609 (99%)	6 (1%)	85	96
All	All	1842/2034 (91%)	1824 (99%)	18 (1%)	85	96

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	TYR
1	A	183	HIS
1	A	283	GLU
1	A	432	LEU
1	A	437	ILE
1	A	473	GLN
1	A	556	GLU
1	B	173	TYR
1	B	183	HIS
1	B	283	GLU
1	B	473	GLN
1	B	556	GLU
1	C	173	TYR
1	C	283	GLU
1	C	434	ASP
1	C	473	GLN
1	C	556	GLU
1	C	649	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	103	GLN
1	A	260	ASN
1	A	285	ASN
1	A	317	HIS
1	A	327	GLN
1	A	348	ASN
1	A	401	ASN
1	A	443	ASN
1	A	458	GLN
1	A	490	GLN
1	A	494	GLN
1	A	499	HIS

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Mol	Chain	Res	Type
1	A	533	ASN
1	A	641	GLN
1	A	660	ASN
1	B	90	ASN
1	B	103	GLN
1	B	260	ASN
1	B	285	ASN
1	B	327	GLN
1	B	348	ASN
1	B	401	ASN
1	B	458	GLN
1	B	460	ASN
1	B	490	GLN
1	B	533	ASN
1	B	641	GLN
1	B	660	ASN
1	C	90	ASN
1	C	103	GLN
1	C	260	ASN
1	C	285	ASN
1	C	317	HIS
1	C	327	GLN
1	C	348	ASN
1	C	401	ASN
1	C	458	GLN
1	C	490	GLN
1	C	533	ASN
1	C	660	ASN
1	C	763	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 ligands 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$
2	ADP	A	807	-	29,29,29	1.70	7 (24%)	45,45,45	2.21	5 (11%)
2	ADP	A	900	-	29,29,29	1.89	4 (13%)	45,45,45	2.20	7 (15%)
3	AF3	A	915	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ADP	B	807	-	29,29,29	1.76	8 (27%)	45,45,45	2.21	6 (13%)
2	ADP	B	900	-	29,29,29	1.61	5 (17%)	45,45,45	2.30	5 (11%)
3	AF3	B	915	-	0,3,3	0.00	-	0,3,3	0.00	-
2	ADP	C	807	-	29,29,29	1.87	7 (24%)	45,45,45	2.30	5 (11%)
2	ADP	C	900	-	29,29,29	1.66	3 (10%)	45,45,45	2.31	7 (15%)
3	AF3	C	915	-	0,3,3	0.00	-	0,3,3	0.00	-

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
2	ADP	A	807	-	-	0/16/32/32	0/1/3/3
2	ADP	A	900	-	-	0/16/32/32	0/1/3/3
3	AF3	A	915	-	-	0/0/0/0	0/0/0/0
2	ADP	B	807	-	-	0/16/32/32	0/1/3/3
2	ADP	B	900	-	-	0/16/32/32	0/1/3/3
3	AF3	B	915	-	-	0/0/0/0	0/0/0/0
2	ADP	C	807	-	-	0/16/32/32	0/1/3/3
2	ADP	C	900	-	-	0/16/32/32	0/1/3/3
3	AF3	C	915	-	-	0/0/0/0	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	ADP	C4-N9	-6.92	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C4-N9	-6.02	1.29	1.37
2	C	900	ADP	C4-N9	-5.65	1.29	1.37
2	B	900	ADP	C4-N9	-4.89	1.30	1.37
2	A	807	ADP	C4-N9	-4.72	1.30	1.37
2	B	807	ADP	C4-N9	-4.47	1.31	1.37
2	B	807	ADP	PB-O3A	-3.26	1.54	1.60
2	B	807	ADP	PA-O3A	-3.23	1.54	1.59
2	C	807	ADP	C5-N7	-3.18	1.28	1.40
2	C	900	ADP	C5-N7	-3.15	1.28	1.40
2	A	900	ADP	C5-N7	-3.09	1.28	1.40
2	B	807	ADP	C5-N7	-3.02	1.28	1.40
2	A	900	ADP	C8-N9	-2.99	1.32	1.36
2	A	807	ADP	C5-N7	-2.92	1.29	1.40
2	B	900	ADP	C5-N7	-2.83	1.29	1.40
2	C	807	ADP	PA-O3A	-2.79	1.54	1.59
2	B	900	ADP	PB-O3A	-2.61	1.55	1.60
2	C	807	ADP	PB-O3A	-2.59	1.55	1.60
2	A	807	ADP	C2'-C1'	-2.52	1.49	1.53
2	A	807	ADP	C2-N3	2.44	1.37	1.32
2	A	807	ADP	PA-O3A	-2.42	1.55	1.59
2	A	807	ADP	PB-O3A	-2.40	1.56	1.60
2	C	807	ADP	C8-N9	-2.33	1.33	1.36
2	B	807	ADP	C2-N3	2.30	1.36	1.32
2	B	900	ADP	C2-N3	2.26	1.36	1.32
2	C	900	ADP	PA-O2A	-2.24	1.45	1.55
2	A	807	ADP	PA-O2A	-2.19	1.45	1.55
2	B	807	ADP	PA-O2A	-2.17	1.45	1.55
2	B	807	ADP	C2'-C1'	-2.17	1.50	1.53
2	C	807	ADP	PA-O2A	-2.13	1.45	1.55
2	B	900	ADP	PA-O2A	-2.09	1.45	1.55
2	A	900	ADP	PA-O2A	-2.03	1.46	1.55
2	B	807	ADP	PB-O3B	-2.02	1.47	1.54
2	C	807	ADP	C8-N7	-2.01	1.30	1.34

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	807	ADP	N3-C2-N1	-13.31	117.58	128.71
2	B	900	ADP	N3-C2-N1	-12.65	118.13	128.71
2	C	900	ADP	N3-C2-N1	-12.50	118.26	128.71
2	A	807	ADP	N3-C2-N1	-12.31	118.41	128.71
2	B	807	ADP	N3-C2-N1	-12.05	118.64	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	ADP	N3-C2-N1	-11.76	118.87	128.71
2	B	900	ADP	N3-C4-N9	4.67	133.86	125.43
2	A	807	ADP	N3-C4-N9	4.52	133.60	125.43
2	B	807	ADP	N3-C4-N9	4.46	133.48	125.43
2	C	900	ADP	N3-C4-N9	4.42	133.41	125.43
2	C	807	ADP	N3-C4-N9	3.97	132.60	125.43
2	A	900	ADP	N3-C4-N9	3.92	132.51	125.43
2	A	900	ADP	O4'-C1'-N9	-3.37	105.30	108.44
2	A	900	ADP	C2-N3-C4	3.19	123.10	114.01
2	C	807	ADP	C2-N3-C4	3.07	122.74	114.01
2	B	900	ADP	C2-N3-C4	3.04	122.67	114.01
2	B	807	ADP	C2-N3-C4	2.98	122.49	114.01
2	C	900	ADP	C2-N3-C4	2.97	122.47	114.01
2	A	807	ADP	C2-N3-C4	2.91	122.31	114.01
2	B	807	ADP	C5-C4-N3	-2.82	119.57	125.70
2	A	807	ADP	C5-C4-N3	-2.72	119.78	125.70
2	B	807	ADP	C4-C5-N7	-2.68	107.23	109.52
2	B	900	ADP	C5-C4-N3	-2.64	119.94	125.70
2	C	900	ADP	C5-C4-N3	-2.63	119.98	125.70
2	A	900	ADP	O4'-C4'-C5'	-2.61	100.05	109.36
2	A	900	ADP	C5-C4-N3	-2.55	120.14	125.70
2	C	900	ADP	O4'-C1'-N9	-2.53	106.08	108.44
2	A	807	ADP	C4-C5-N7	-2.51	107.38	109.52
2	C	900	ADP	C4-C5-N7	-2.38	107.48	109.52
2	C	807	ADP	C5-C4-N3	-2.34	120.60	125.70
2	A	900	ADP	C4'-O4'-C1'	2.31	112.26	109.75
2	C	900	ADP	C4'-O4'-C1'	2.28	112.23	109.75
2	B	900	ADP	C4'-O4'-C1'	2.11	112.04	109.75
2	B	807	ADP	C4'-O4'-C1'	2.08	112.01	109.75
2	C	807	ADP	C4'-O4'-C1'	2.08	112.00	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	719/806 (89%)	0.62	51 (7%) 16 18	50, 267, 356, 574	0
1	B	723/806 (89%)	0.61	57 (7%) 13 16	49, 264, 348, 571	0
1	C	723/806 (89%)	0.62	52 (7%) 15 18	51, 266, 367, 616	0
All	All	2165/2418 (89%)	0.62	160 (7%) 14 17	49, 266, 360, 616	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	429	LEU	6.0
1	A	25	ARG	5.9
1	A	23	PRO	5.6
1	C	729	PRO	5.3
1	A	26	LEU	4.7
1	B	731	ILE	4.7
1	C	731	ILE	4.6
1	B	134	TYR	3.8
1	A	102	ILE	3.8
1	B	665	PRO	3.6
1	A	112	LYS	3.6
1	C	75	ASP	3.6
1	B	102	ILE	3.6
1	B	110	TYR	3.6
1	C	105	CYS	3.5
1	A	729	PRO	3.4
1	C	658	LYS	3.4
1	A	80	GLU	3.4
1	C	80	GLU	3.4
1	B	338	ARG	3.4
1	C	736	PHE	3.3
1	C	106	PRO	3.3
1	C	597	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	731	ILE	3.3
1	B	588	GLY	3.2
1	C	173	TYR	3.2
1	A	110	TYR	3.2
1	A	50	GLN	3.2
1	C	81	LYS	3.2
1	B	597	ALA	3.2
1	A	69	CYS	3.2
1	A	135	LEU	3.1
1	B	173	TYR	3.1
1	A	141	GLU	3.1
1	A	139	PHE	3.1
1	A	84	MET	3.0
1	C	134	TYR	3.0
1	C	187	GLU	3.0
1	B	707	ILE	3.0
1	C	427	MET	3.0
1	C	594	GLY	2.9
1	C	189	ILE	2.9
1	C	102	ILE	2.9
1	A	730	GLU	2.9
1	C	335	LEU	2.9
1	A	430	ILE	2.9
1	A	732	ARG	2.8
1	C	287	ARG	2.8
1	B	139	PHE	2.8
1	C	188	PRO	2.8
1	B	146	ILE	2.8
1	C	145	PRO	2.8
1	A	703	ILE	2.8
1	B	94	VAL	2.8
1	B	84	MET	2.8
1	A	696	LYS	2.7
1	C	739	ALA	2.7
1	A	707	ILE	2.7
1	A	427	MET	2.7
1	B	732	ARG	2.7
1	A	36	ASN	2.7
1	B	589	ASN	2.7
1	B	693	ARG	2.7
1	A	437	ILE	2.7
1	A	672	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	735	HIS	2.7
1	C	672	LEU	2.7
1	B	591	GLY	2.7
1	A	736	PHE	2.6
1	C	703	ILE	2.6
1	B	736	PHE	2.6
1	B	498	GLU	2.6
1	A	24	ASN	2.6
1	A	51	LEU	2.6
1	A	704	GLU	2.6
1	B	95	ARG	2.6
1	A	388	MET	2.6
1	A	592	ASP	2.6
1	B	590	ILE	2.6
1	B	71	VAL	2.6
1	C	666	VAL	2.5
1	C	657	LEU	2.5
1	A	134	TYR	2.5
1	A	595	GLY	2.5
1	C	591	GLY	2.5
1	B	56	THR	2.5
1	B	497	VAL	2.5
1	C	433	GLU	2.5
1	C	588	GLY	2.5
1	B	763	GLN	2.5
1	B	666	VAL	2.5
1	A	126	ILE	2.4
1	C	53	ARG	2.4
1	A	701	GLU	2.4
1	A	43	GLN	2.4
1	A	706	GLU	2.4
1	B	140	LEU	2.4
1	C	23	PRO	2.4
1	B	594	GLY	2.4
1	C	706	GLU	2.4
1	B	141	GLU	2.4
1	A	49	LEU	2.4
1	C	593	GLY	2.4
1	C	592	ASP	2.4
1	B	502	LYS	2.4
1	B	21	ASN	2.4
1	C	590	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	43	GLN	2.3
1	B	729	PRO	2.3
1	C	665	PRO	2.3
1	A	390	LEU	2.3
1	A	22	ARG	2.3
1	B	135	LEU	2.3
1	A	47	ASP	2.3
1	B	198	LEU	2.3
1	B	430	ILE	2.3
1	B	174	CYS	2.3
1	B	670	VAL	2.3
1	C	707	ILE	2.3
1	B	312	LYS	2.2
1	B	98	ASP	2.2
1	C	388	MET	2.2
1	B	108	VAL	2.2
1	C	175	ILE	2.2
1	B	696	LYS	2.2
1	B	39	VAL	2.2
1	C	670	VAL	2.2
1	C	479	ILE	2.2
1	A	179	ASP	2.2
1	A	763	GLN	2.2
1	B	595	GLY	2.2
1	A	283	GLU	2.2
1	A	56	THR	2.1
1	C	110	TYR	2.1
1	C	139	PHE	2.1
1	C	763	GLN	2.1
1	B	33	ASN	2.1
1	C	174	CYS	2.1
1	C	176	VAL	2.1
1	C	146	ILE	2.1
1	C	732	ARG	2.1
1	A	58	LEU	2.1
1	B	109	LYS	2.1
1	A	433	GLU	2.1
1	A	506	PHE	2.1
1	B	175	ILE	2.1
1	A	658	LYS	2.1
1	C	73	SER	2.1
1	B	69	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	70	ILE	2.1
1	A	697	LEU	2.0
1	B	730	GLU	2.0
1	C	730	GLU	2.0
1	B	633	ILE	2.0
1	B	706	GLU	2.0
1	B	587	GLY	2.0
1	B	658	LYS	2.0
1	B	592	ASP	2.0
1	C	79	ASP	2.0
1	B	390	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	ADP	B	807	27/27	0.40	1.96	306,306,306,306	0
2	ADP	C	807	27/27	0.38	1.79	306,306,306,306	0
2	ADP	A	807	27/27	0.34	1.50	306,306,306,306	0
3	AF3	C	915	4/4	0.29	1.45	306,306,306,306	0
3	AF3	A	915	4/4	0.23	0.38	306,306,306,306	0
3	AF3	B	915	4/4	0.21	0.36	306,306,306,306	0
2	ADP	C	900	27/27	0.32	0.35	306,306,306,306	0
2	ADP	B	900	27/27	0.24	0.31	306,306,306,306	0
2	ADP	A	900	27/27	0.24	-0.07	306,306,306,306	0

6.5 Other polymers ⓘ

There are no such residues in this entry.