Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:11 AM GMT

PDB ID	:	3DMQ
Title	:	Crystal structure of RapA, a Swi2/Snf2 protein that recycles RNA polymerase during transcription
Authors	:	Shaw, G.; Gan, J.; Zhou, Y.N.; Zhang, R.; Joachimiak, A.; Jin, D.J.; Ji, X.
Deposited on	:	2008-07-01
Resolution	:	3.20 Å(reported)

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

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

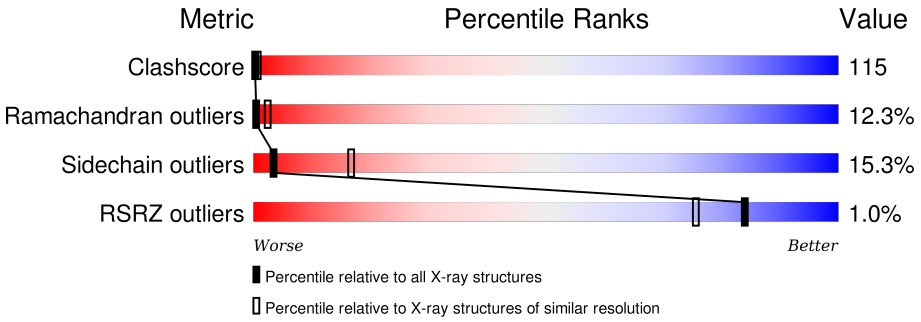
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	968	% 17% 62% 19%
1	B	968	% 16% 61% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1001	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15340 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

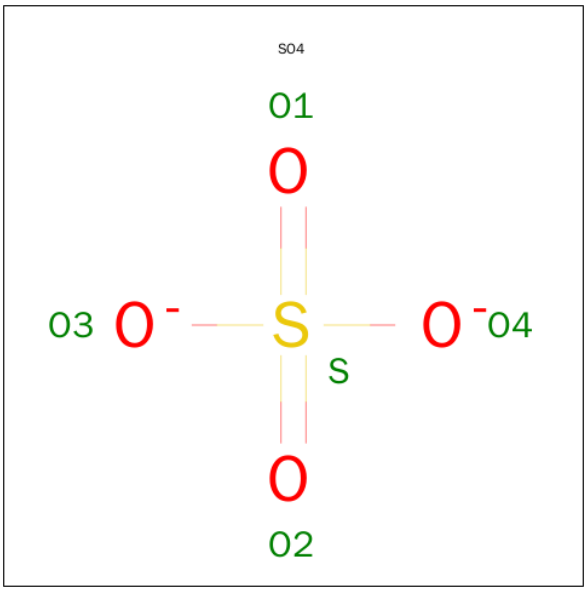
- Molecule 1 is a protein called RNA polymerase-associated protein rapA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	961	Total	C	N	O	S	Se	0	0	0
			7665	4797	1370	1468	7	23			
1	B	961	Total	C	N	O	S	Se	0	0	0
			7665	4797	1370	1468	7	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	350	CYS	ARG	ENGINEERED	UNP P60240
B	350	CYS	ARG	ENGINEERED	UNP P60240

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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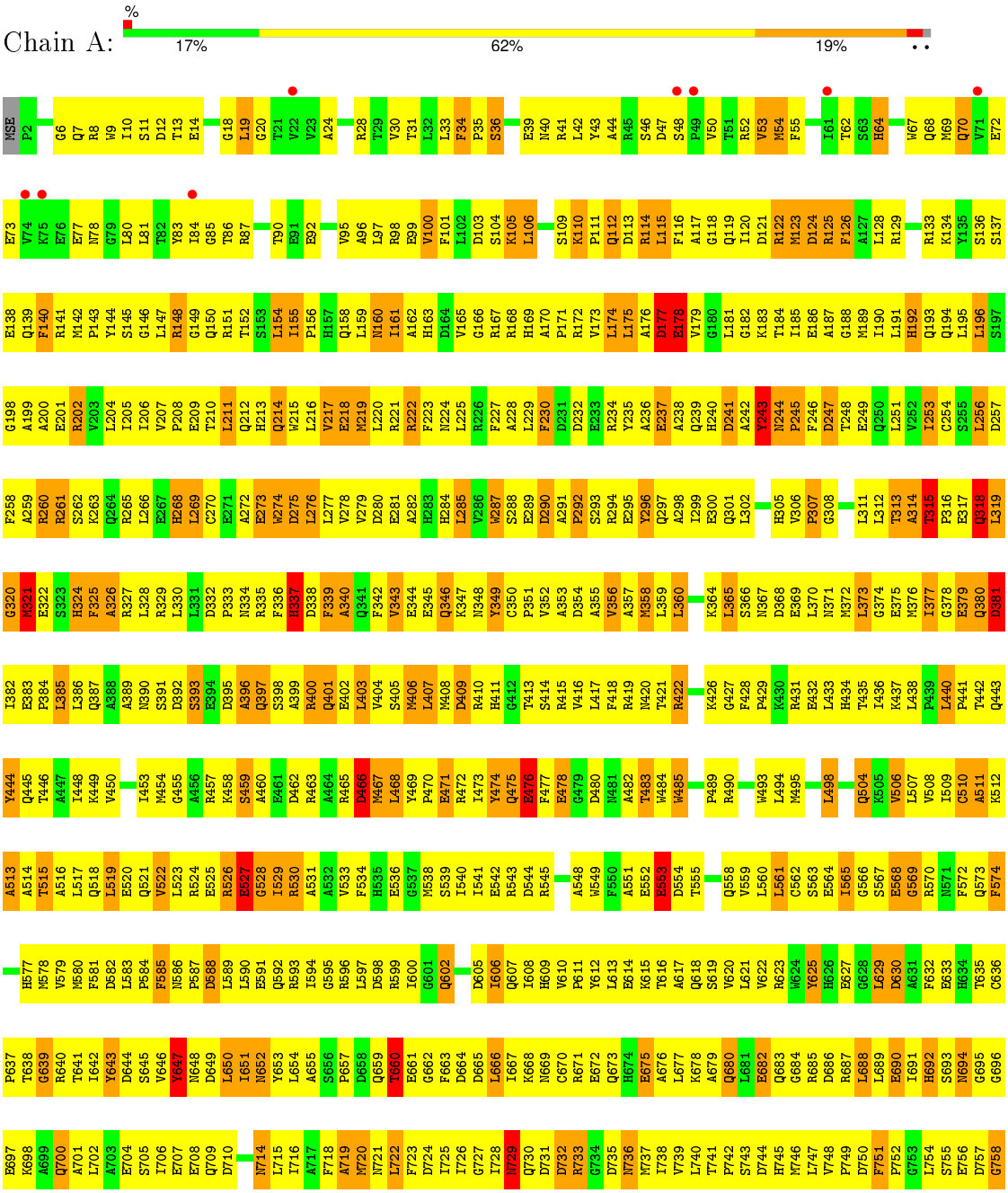
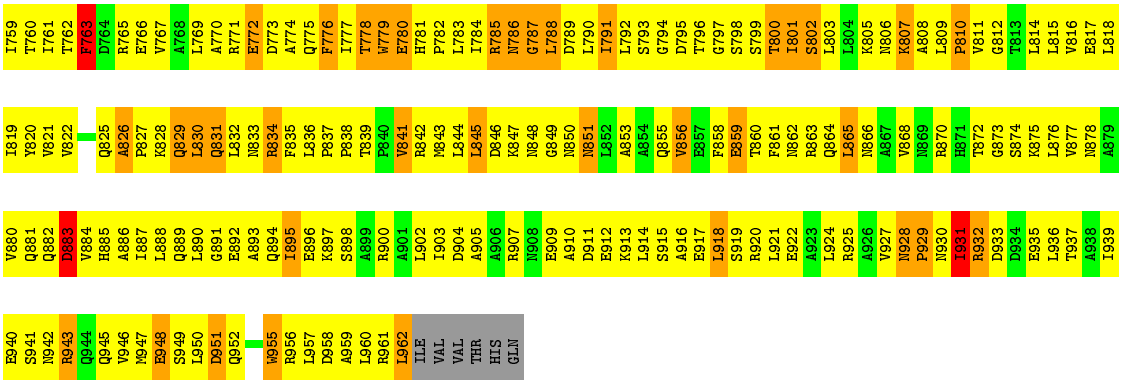
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0

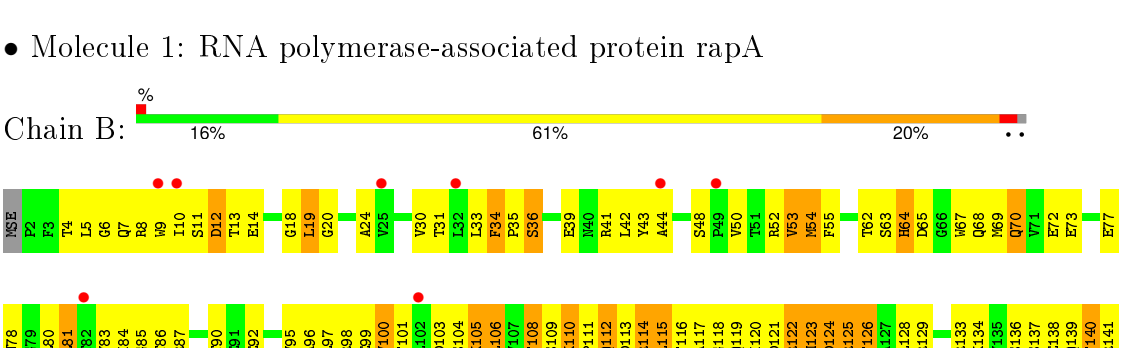
3 Residue-property plots (i)

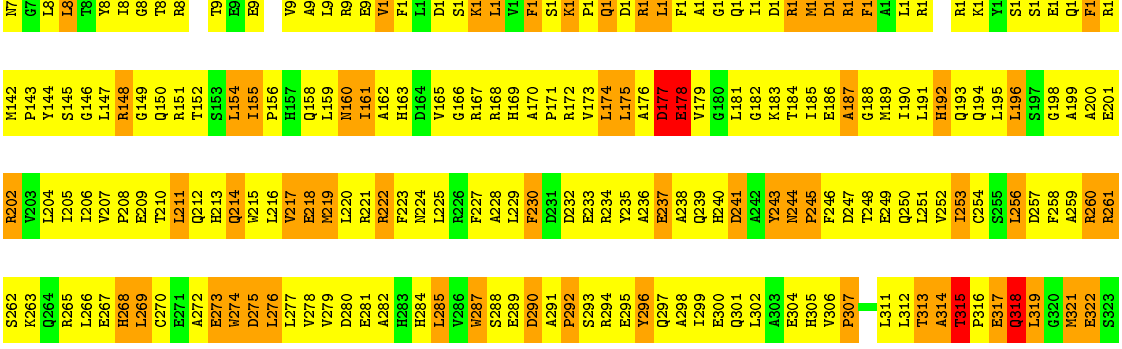
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

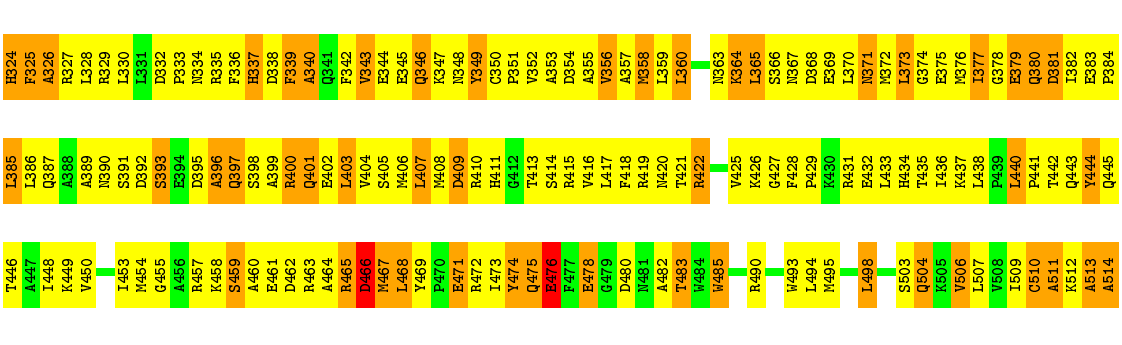
- Molecule 1: RNA polymerase-associated protein rapA

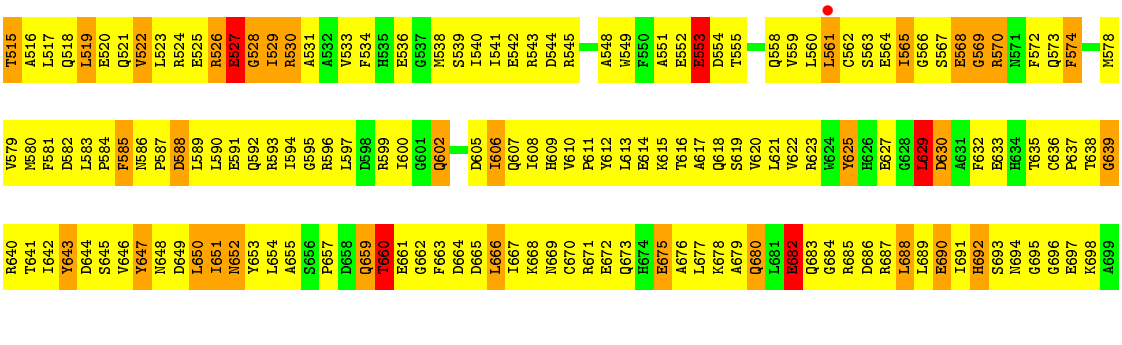






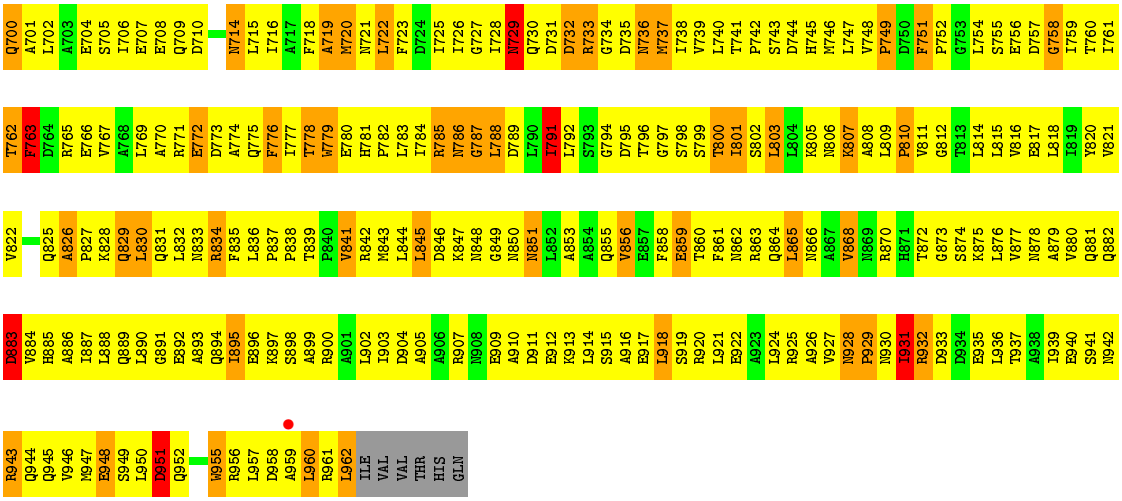






- Molecule 1: RNA polymerase-associated protein rapA

Chain B:


Q700 A701 L702 A703 E704 S705 I706 E707 E708 Q709 D710 N714 L715 I716 A717 F718 A719 M720 N721 L722 F723 D724 I725 I726 G727 I728 N729 Q730 D731 D732 R733 G734 D735 N736 M737 I738 V739 L740 T741 P742 S743 D744 H745 M746 L747 V748 P749 D750 F751 P752 G753 L754 S755 E756 D757 G758 I759 T760 I761
T762 F763 D764 R765 E766 V767 A768 L769 A770 R771 E772 D773 A774 Q775 F776 I777 T778 W779 E780 H781 F782 L783 I784 R785 N786 G787 L788 D789 L790 I791 L792 S793 G794 D795 T796 G797 S798 S799 T800 I801 S802 L803 L804 K805 N806 K807 A808 L809 P810 V811 G812 T813 L814 L815 V816 E817 L818 I819 Y820 V821
V822 Q825 A826 P827 K828 Q829 L830 Q831 L832 N833 R834 F835 L836 P837 P838 T839 P840 V841 R842 M843 L844 L845 D846 K847 N848 G849 N850 N851 L852 A853 A854 Q855 V856 E857 F858 E859 T860 F861 N862 R863 Q864 L865 N866 A867 V868 N869 R870 H871 T872 G873 S874 K875 L876 V877 N878 A879 V880 Q881 Q882
D883 V884 H885 A886 I887 L888 Q889 L890 G891 E892 A893 Q894 I895 E896 K897 S898 A899 R900 A901 L902 I903 D904 A905 A906 R907 N908 E909 A910 D911 E912 N913 L914 S915 A916 E917 L918 S919 R920 L921 E922 A923 L924 R925 A926 V927 N928 P929 N930 I931 R932 D933 D934 E935 L936 T937 A938 I939 E940 S941 N942
R943 Q944 Q945 V946 M947 E948 S949 L950 D951 Q952 W955 R956 L957 D958 A959 L960 R961 L962 ILE VAL VAL THR HIS GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	123.86Å 123.86Å 187.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.79 – 3.20 43.79 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (43.79-3.20) 97.3 (43.79-3.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.250 , 0.300 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	85.3	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 96.8	EDS
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 45546 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	15340	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.69	2/7785 (0.0%)	0.73	3/10507 (0.0%)
1	B	0.56	0/7785	0.71	1/10507 (0.0%)
All	All	0.63	2/15570 (0.0%)	0.72	4/21014 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	MSE	CG-SE	34.50	3.12	1.95
1	A	321	MSE	SE-CE	11.35	2.62	1.95

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	321	MSE	CB-CG-SE	-17.74	59.49	112.70
1	A	321	MSE	CG-SE-CE	-7.84	81.65	98.90
1	B	791	ILE	CB-CA-C	-5.61	100.38	111.60
1	A	406	MSE	CB-CG-SE	-5.11	97.39	112.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	GLY	Peptide
1	A	807	LYS	Peptide
1	B	807	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7665	0	7524	1736	0
1	B	7665	0	7524	1758	0
2	A	5	0	0	0	0
2	B	5	0	0	2	0
All	All	15340	0	15048	3479	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 115.

All (3479) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:MSE:SE	1:A:321:MSE:HB3	1.84	1.25
1:A:141:ARG:NE	1:A:837:PRO:HD2	1.55	1.20
1:B:125:ARG:HH11	1:B:125:ARG:HB3	1.05	1.16
1:B:506:VAL:HG12	1:B:507:LEU:H	1.08	1.14
1:B:141:ARG:NE	1:B:837:PRO:HD2	1.60	1.14
1:A:586:ASN:HB3	1:A:589:LEU:HD12	1.25	1.14
1:A:506:VAL:HG12	1:A:507:LEU:H	1.03	1.12
1:A:380:GLN:HE21	1:A:382:ILE:HB	1.06	1.12
1:B:123:MSE:HE2	1:B:961:ARG:HH22	1.14	1.11
1:A:586:ASN:HD22	1:A:589:LEU:HG	0.99	1.11
1:B:18:GLY:HA2	1:B:106:LEU:HD21	1.12	1.11
1:A:125:ARG:HH11	1:A:125:ARG:HB3	1.06	1.11
1:A:145:SER:HA	1:A:148:ARG:NE	1.67	1.09
1:B:769:LEU:HD22	1:B:771:ARG:HH21	1.17	1.09
1:B:141:ARG:HE	1:B:837:PRO:HD2	0.93	1.09
1:A:897:LYS:HD2	1:A:897:LYS:H	1.01	1.08
1:B:586:ASN:HD22	1:B:589:LEU:HG	1.09	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ASN:HB3	1:B:589:LEU:HD12	1.31	1.08
1:B:897:LYS:HD2	1:B:897:LYS:H	1.02	1.08
1:A:779:TRP:O	1:A:782:PRO:HD2	1.54	1.07
1:B:380:GLN:HE21	1:B:382:ILE:HB	1.03	1.07
1:B:313:THR:HB	1:B:316:PRO:HD2	1.34	1.07
1:A:188:GLY:HA3	1:A:223:PHE:CE2	1.90	1.06
1:A:507:LEU:HA	1:A:558:GLN:HE22	1.20	1.06
1:A:123:MSE:HE2	1:A:961:ARG:HH22	1.21	1.06
1:A:383:GLU:HB2	1:A:387:GLN:HG2	1.37	1.05
1:B:285:LEU:HB2	1:B:314:ALA:HB1	1.35	1.05
1:A:962:LEU:HD13	1:A:962:LEU:H	1.21	1.05
1:B:962:LEU:H	1:B:962:LEU:HD13	1.21	1.04
1:A:287:TRP:CZ2	1:A:289:GLU:HA	1.91	1.04
1:B:287:TRP:CZ2	1:B:289:GLU:HA	1.92	1.04
1:A:285:LEU:HB2	1:A:314:ALA:HB1	1.38	1.04
1:B:837:PRO:HB2	1:B:838:PRO:HD2	1.37	1.04
1:A:780:GLU:OE1	1:A:780:GLU:HA	1.56	1.03
1:A:586:ASN:ND2	1:A:589:LEU:HG	1.72	1.03
1:B:859:GLU:HB3	1:B:863:ARG:HH22	1.15	1.03
1:B:553:GLU:HG2	1:B:554:ASP:H	1.18	1.03
1:A:521:GLN:HE22	1:A:525:GLU:HB2	1.19	1.03
1:A:28:ARG:HH12	1:A:240:HIS:CE1	1.76	1.03
1:B:380:GLN:NE2	1:B:382:ILE:HB	1.72	1.03
1:A:141:ARG:HE	1:A:837:PRO:HD2	0.91	1.03
1:A:553:GLU:HG2	1:A:554:ASP:H	1.21	1.03
1:A:769:LEU:HD22	1:A:771:ARG:HH21	1.24	1.02
1:A:859:GLU:HB3	1:A:863:ARG:HH22	1.13	1.02
1:B:779:TRP:O	1:B:782:PRO:HD2	1.58	1.02
1:B:507:LEU:HA	1:B:558:GLN:HE22	1.21	1.02
1:B:383:GLU:HB2	1:B:387:GLN:HG2	1.36	1.02
1:B:521:GLN:HE22	1:B:525:GLU:HB2	1.17	1.02
1:A:380:GLN:NE2	1:A:382:ILE:HB	1.72	1.02
1:A:188:GLY:HA3	1:A:223:PHE:HE2	1.21	1.02
1:A:685:ARG:HB2	1:A:687:ARG:NE	1.74	1.01
1:B:685:ARG:HB2	1:B:687:ARG:NE	1.75	1.01
1:B:220:LEU:O	1:B:224:ASN:HA	1.58	1.01
1:B:586:ASN:HD21	1:B:588:ASP:HB2	1.22	1.01
1:A:859:GLU:HB3	1:A:863:ARG:NH2	1.75	1.01
1:A:885:HIS:HA	1:A:888:LEU:HD23	1.43	1.01
1:A:837:PRO:HB2	1:A:838:PRO:HD2	1.39	1.00
1:A:122:ARG:HE	1:A:122:ARG:H	1.04	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:THR:HB	1:A:316:PRO:HD2	1.40	1.00
1:A:399:ALA:HB3	1:A:400:ARG:NH2	1.77	1.00
1:A:175:LEU:HD22	1:A:312:LEU:HG	1.39	1.00
1:B:151:ARG:NH2	1:B:771:ARG:H	1.60	1.00
1:B:188:GLY:HA3	1:B:223:PHE:CE2	1.96	0.99
1:A:141:ARG:HE	1:A:837:PRO:CD	1.74	0.99
1:B:145:SER:HA	1:B:148:ARG:NE	1.75	0.99
1:B:259:ALA:HA	1:B:265:ARG:HG2	1.41	0.99
1:A:428:PHE:HE1	1:A:599:ARG:HA	1.27	0.99
1:A:173:VAL:HA	1:A:416:VAL:HG13	1.45	0.99
1:B:428:PHE:HE1	1:B:599:ARG:HA	1.26	0.99
1:B:885:HIS:HA	1:B:888:LEU:HD23	1.44	0.98
1:B:122:ARG:H	1:B:122:ARG:HE	1.08	0.98
1:A:207:VAL:HG13	1:A:212:GLN:HG2	1.43	0.98
1:B:578:MSE:HE2	1:B:608:ILE:HD11	1.44	0.98
1:B:175:LEU:HD22	1:B:312:LEU:HG	1.44	0.98
1:A:229:LEU:HA	1:A:253:ILE:HG12	1.44	0.98
1:A:422:ARG:N	1:A:422:ARG:HD3	1.75	0.98
1:A:775:GLN:NE2	1:A:776:PHE:H	1.61	0.98
1:B:859:GLU:HB3	1:B:863:ARG:NH2	1.78	0.98
1:A:151:ARG:NH2	1:A:771:ARG:H	1.62	0.97
1:A:472:ARG:HA	1:A:475:GLN:HE22	1.27	0.97
1:B:207:VAL:HG13	1:B:212:GLN:HG2	1.44	0.97
1:A:321:MSE:SE	1:A:321:MSE:CE	2.62	0.97
1:A:258:PHE:HA	1:A:261:ARG:NE	1.79	0.97
1:B:465:ARG:HA	1:B:468:LEU:HD12	1.44	0.97
1:A:586:ASN:HD21	1:A:588:ASP:HB2	1.27	0.97
1:A:344:GLU:HA	1:A:347:LYS:HD3	1.47	0.97
1:B:141:ARG:HE	1:B:837:PRO:CD	1.78	0.97
1:A:259:ALA:HA	1:A:265:ARG:HG2	1.42	0.97
1:A:792:LEU:HA	1:A:795:ASP:HB2	1.46	0.96
1:A:952:GLN:NE2	1:B:948:GLU:HG2	1.78	0.96
1:A:204:LEU:HD12	1:A:205:ILE:H	1.31	0.96
1:B:716:ILE:H	1:B:716:ILE:HD12	1.27	0.96
1:A:775:GLN:HE22	1:A:776:PHE:HB2	1.30	0.96
1:B:204:LEU:HD12	1:B:205:ILE:H	1.30	0.95
1:B:229:LEU:HA	1:B:253:ILE:HG12	1.45	0.95
1:B:779:TRP:O	1:B:783:LEU:HG	1.64	0.95
1:B:586:ASN:ND2	1:B:589:LEU:HG	1.81	0.95
1:A:716:ILE:HD12	1:A:716:ILE:H	1.29	0.95
1:A:8:ARG:HB3	1:A:19:LEU:HD21	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ARG:HA	1:A:468:LEU:HD12	1.46	0.95
1:B:775:GLN:NE2	1:B:776:PHE:H	1.65	0.95
1:B:399:ALA:HB3	1:B:400:ARG:NH2	1.82	0.94
1:B:258:PHE:HA	1:B:261:ARG:NE	1.82	0.94
1:A:281:GLU:CG	1:A:314:ALA:HA	1.98	0.94
1:B:151:ARG:HH21	1:B:771:ARG:H	1.09	0.94
1:A:578:MSE:HE2	1:A:608:ILE:HD11	1.47	0.94
1:B:364:LYS:H	1:B:364:LYS:HD2	1.29	0.94
1:B:188:GLY:HA3	1:B:223:PHE:HE2	1.29	0.94
1:B:472:ARG:HA	1:B:475:GLN:HE22	1.32	0.93
1:B:173:VAL:HA	1:B:416:VAL:HG13	1.51	0.93
1:A:507:LEU:HD23	1:A:559:VAL:HG13	1.50	0.93
1:B:507:LEU:HD23	1:B:559:VAL:HG13	1.49	0.93
1:B:299:ILE:HA	1:B:302:LEU:HD12	1.49	0.93
1:B:19:LEU:N	1:B:106:LEU:HD11	1.84	0.93
1:A:281:GLU:CD	1:A:314:ALA:HA	1.88	0.93
1:B:897:LYS:N	1:B:897:LYS:HD2	1.84	0.92
1:B:8:ARG:HB3	1:B:19:LEU:HD21	1.52	0.92
1:B:781:HIS:HB2	1:B:782:PRO:HD3	1.50	0.92
1:B:7:GLN:HA	1:B:99:GLU:OE1	1.69	0.92
1:A:779:TRP:O	1:A:783:LEU:HG	1.69	0.92
1:B:751:PHE:HD1	1:B:752:PRO:HD3	1.34	0.92
1:A:751:PHE:HD1	1:A:752:PRO:HD3	1.33	0.92
1:A:597:LEU:HA	1:A:602:GLN:NE2	1.85	0.92
1:B:775:GLN:HE22	1:B:776:PHE:HB2	1.35	0.91
1:A:155:ILE:HD13	1:A:158:GLN:HB2	1.51	0.91
1:B:792:LEU:HA	1:B:795:ASP:HB2	1.50	0.91
1:A:321:MSE:CB	1:A:321:MSE:SE	2.69	0.91
1:A:204:LEU:HD12	1:A:205:ILE:N	1.85	0.91
1:B:886:ALA:HA	1:B:889:GLN:NE2	1.83	0.91
1:B:422:ARG:N	1:B:422:ARG:HD3	1.85	0.91
1:A:284:HIS:HA	1:A:314:ALA:O	1.71	0.90
1:A:211:LEU:HD11	1:A:282:ALA:HB2	1.50	0.90
1:A:364:LYS:H	1:A:364:LYS:HD2	1.34	0.90
1:A:151:ARG:HH21	1:A:771:ARG:H	1.14	0.90
1:B:284:HIS:HA	1:B:314:ALA:O	1.72	0.90
1:B:433:LEU:HD21	1:B:435:THR:HG23	1.54	0.90
1:A:506:VAL:HG12	1:A:507:LEU:N	1.86	0.90
1:B:7:GLN:HA	1:B:99:GLU:CD	1.92	0.90
1:B:410:ARG:HD3	1:B:927:VAL:HG13	1.54	0.90
1:B:204:LEU:HD12	1:B:205:ILE:N	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ARG:NH1	1:B:125:ARG:HB3	1.87	0.90
1:B:24:ALA:HB3	1:B:31:THR:HB	1.54	0.90
1:A:178:GLU:N	1:A:181:LEU:HD12	1.86	0.90
1:B:202:ARG:HB3	1:B:274:TRP:CZ3	2.06	0.90
1:A:897:LYS:HD2	1:A:897:LYS:N	1.83	0.89
1:B:722:LEU:HD13	1:B:723:PHE:N	1.88	0.89
1:B:781:HIS:HA	1:B:784:ILE:HD12	1.54	0.89
1:A:751:PHE:CD1	1:A:752:PRO:HD3	2.06	0.89
1:B:281:GLU:CG	1:B:314:ALA:HA	2.00	0.89
1:B:584:PRO:HD3	1:B:593:ARG:CZ	2.02	0.89
1:A:220:LEU:O	1:A:224:ASN:HA	1.72	0.89
1:B:445:GLN:O	1:B:449:LYS:HG3	1.72	0.89
1:A:114:ARG:CZ	1:A:117:ALA:HB3	2.01	0.89
1:A:24:ALA:HB3	1:A:31:THR:HB	1.53	0.89
1:A:584:PRO:HD3	1:A:593:ARG:CZ	2.03	0.89
1:A:728:ILE:HA	1:A:743:SER:H	1.38	0.89
1:B:822:VAL:O	1:B:822:VAL:HG23	1.71	0.89
1:B:72:GLU:HG3	1:B:85:GLY:HA2	1.55	0.89
1:A:781:HIS:HB2	1:A:782:PRO:HD3	1.53	0.88
1:B:151:ARG:NH2	1:B:771:ARG:N	2.21	0.88
1:A:650:LEU:HD13	1:A:651:ILE:N	1.87	0.88
1:B:274:TRP:CE3	1:B:274:TRP:HA	2.07	0.88
1:A:727:GLY:C	1:A:743:SER:HB3	1.94	0.88
1:A:816:VAL:HG23	1:A:818:LEU:HD11	1.53	0.88
1:A:42:LEU:HD13	1:A:43:TYR:N	1.88	0.88
1:B:328:LEU:HB3	1:B:336:PHE:CE2	2.08	0.88
1:A:125:ARG:NH1	1:A:125:ARG:HB3	1.88	0.88
1:A:597:LEU:HA	1:A:602:GLN:HE21	1.37	0.88
1:B:751:PHE:CD1	1:B:752:PRO:HD3	2.07	0.88
1:B:246:PHE:CE2	1:B:268:HIS:HB2	2.09	0.88
1:A:299:ILE:HA	1:A:302:LEU:HD12	1.53	0.88
1:B:178:GLU:OE1	1:B:317:GLU:HB3	1.74	0.88
1:B:344:GLU:HA	1:B:347:LYS:HD3	1.53	0.88
1:B:114:ARG:CZ	1:B:117:ALA:HB3	2.03	0.88
1:A:246:PHE:CE2	1:A:268:HIS:HB2	2.09	0.88
1:A:886:ALA:HA	1:A:889:GLN:NE2	1.88	0.88
1:B:833:ASN:OD1	1:B:837:PRO:HB3	1.72	0.88
1:B:920:ARG:O	1:B:924:LEU:HD13	1.73	0.88
1:B:817:GLU:HB2	1:B:961:ARG:H	1.39	0.87
1:B:597:LEU:HA	1:B:602:GLN:NE2	1.89	0.87
1:A:325:PHE:HA	1:A:328:LEU:HD23	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:ARG:O	1:B:404:VAL:HG13	1.72	0.87
1:A:174:LEU:HD22	1:A:175:LEU:N	1.88	0.87
1:A:722:LEU:HD13	1:A:723:PHE:N	1.89	0.87
1:B:662:GLY:O	1:B:666:LEU:HD22	1.74	0.87
1:A:785:ARG:HA	1:A:789:ASP:OD2	1.74	0.87
1:B:728:ILE:HA	1:B:743:SER:H	1.40	0.87
1:A:445:GLN:O	1:A:449:LYS:HG3	1.75	0.87
1:B:925:ARG:HA	1:B:931:ILE:HD12	1.55	0.87
1:A:431:ARG:HB2	1:A:633:GLU:HA	1.55	0.87
1:A:859:GLU:CB	1:A:863:ARG:HH22	1.87	0.87
1:B:266:LEU:H	1:B:266:LEU:HD12	1.40	0.87
1:B:281:GLU:CD	1:B:314:ALA:HA	1.95	0.87
1:A:662:GLY:O	1:A:666:LEU:HD22	1.74	0.87
1:A:775:GLN:CD	1:A:776:PHE:H	1.78	0.87
1:B:431:ARG:HB2	1:B:633:GLU:HA	1.56	0.87
1:B:597:LEU:HA	1:B:602:GLN:HE21	1.40	0.86
1:B:174:LEU:HD22	1:B:175:LEU:N	1.89	0.86
1:B:675:GLU:O	1:B:678:LYS:HG2	1.75	0.86
1:A:151:ARG:NH2	1:A:771:ARG:N	2.23	0.86
1:B:780:GLU:HA	1:B:780:GLU:OE1	1.75	0.86
1:B:274:TRP:HE3	1:B:274:TRP:HA	1.40	0.86
1:B:816:VAL:HG23	1:B:818:LEU:HD11	1.56	0.86
1:A:780:GLU:OE1	1:A:783:LEU:HD12	1.75	0.86
1:B:178:GLU:N	1:B:181:LEU:HD12	1.91	0.86
1:B:506:VAL:HG12	1:B:507:LEU:N	1.91	0.86
1:A:675:GLU:O	1:A:678:LYS:HG2	1.76	0.86
1:B:370:LEU:C	1:B:371:ASN:HD22	1.79	0.85
1:B:236:ALA:HA	1:B:239:GLN:NE2	1.91	0.85
1:A:568:GLU:HG3	1:A:596:ARG:HH21	1.39	0.85
1:A:178:GLU:OE1	1:A:317:GLU:HB3	1.76	0.85
1:A:202:ARG:HB3	1:A:274:TRP:CZ3	2.10	0.85
1:A:115:LEU:HD13	1:A:116:PHE:H	1.40	0.85
1:B:211:LEU:HD11	1:B:282:ALA:HB2	1.56	0.85
1:A:586:ASN:HD22	1:A:589:LEU:CG	1.88	0.85
1:A:688:LEU:H	1:A:688:LEU:HD23	1.38	0.85
1:A:627:GLU:HA	1:A:671:ARG:HH12	1.42	0.85
1:A:219:MSE:HB3	1:A:225:LEU:HB2	1.56	0.85
1:B:261:ARG:HB2	1:B:265:ARG:HH21	1.42	0.85
1:A:311:LEU:HD23	1:A:311:LEU:H	1.39	0.85
1:B:627:GLU:HA	1:B:671:ARG:HH12	1.42	0.85
1:A:586:ASN:HB3	1:A:589:LEU:CD1	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLN:O	1:B:382:ILE:HG13	1.77	0.85
1:B:155:ILE:HD13	1:B:158:GLN:HB2	1.58	0.85
1:A:759:ILE:HD12	1:A:772:GLU:O	1.77	0.84
1:B:188:GLY:HA2	1:B:191:LEU:HD22	1.59	0.84
1:A:400:ARG:O	1:A:404:VAL:HG13	1.74	0.84
1:B:403:LEU:O	1:B:407:LEU:HD22	1.77	0.84
1:B:115:LEU:HD13	1:B:116:PHE:H	1.42	0.84
1:B:650:LEU:HD13	1:B:651:ILE:N	1.92	0.84
1:A:822:VAL:HG23	1:A:822:VAL:O	1.77	0.84
1:B:328:LEU:H	1:B:328:LEU:HD22	1.43	0.84
1:B:769:LEU:HD22	1:B:771:ARG:NH2	1.91	0.84
1:B:202:ARG:HB3	1:B:274:TRP:HZ3	1.40	0.84
1:B:123:MSE:HE2	1:B:961:ARG:NH2	1.92	0.84
1:B:558:GLN:NE2	1:B:559:VAL:H	1.75	0.84
1:A:380:GLN:O	1:A:382:ILE:HG13	1.78	0.84
1:A:453:ILE:H	1:A:453:ILE:HD12	1.43	0.84
1:A:729:ASN:H	1:A:743:SER:HB2	1.41	0.84
1:B:884:VAL:HG13	1:B:887:ILE:HD12	1.60	0.84
1:A:507:LEU:HD23	1:A:559:VAL:CG1	2.07	0.84
1:A:952:GLN:HE22	1:B:948:GLU:CB	1.91	0.84
1:B:325:PHE:HA	1:B:328:LEU:HD23	1.58	0.84
1:A:370:LEU:C	1:A:371:ASN:HD22	1.80	0.84
1:B:42:LEU:HD13	1:B:43:TYR:N	1.92	0.84
1:A:775:GLN:CD	1:A:776:PHE:N	2.32	0.84
1:B:727:GLY:C	1:B:743:SER:HB3	1.98	0.84
1:A:274:TRP:HA	1:A:274:TRP:HE3	1.43	0.84
1:A:960:LEU:HD23	1:A:961:ARG:N	1.93	0.83
1:B:281:GLU:HG3	1:B:314:ALA:HA	1.57	0.83
1:B:507:LEU:HD23	1:B:559:VAL:CG1	2.08	0.83
1:A:495:MSE:SE	1:A:498:LEU:HD12	2.28	0.83
1:A:599:ARG:HB3	1:A:599:ARG:HH11	1.43	0.83
1:A:274:TRP:HA	1:A:274:TRP:CE3	2.10	0.83
1:A:236:ALA:HA	1:A:239:GLN:NE2	1.93	0.83
1:A:833:ASN:OD1	1:A:837:PRO:HB3	1.78	0.83
1:A:433:LEU:HD21	1:A:435:THR:HG23	1.59	0.83
1:A:72:GLU:HG3	1:A:85:GLY:HA2	1.58	0.83
1:A:281:GLU:HG3	1:A:314:ALA:HA	1.60	0.83
1:A:174:LEU:HD13	1:A:174:LEU:O	1.78	0.83
1:B:166:GLY:HA3	1:B:193:GLN:NE2	1.94	0.83
1:A:920:ARG:O	1:A:924:LEU:HD13	1.77	0.83
1:A:166:GLY:HA3	1:A:193:GLN:NE2	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:760:THR:HG21	1:B:766:GLU:HG2	1.60	0.83
1:B:507:LEU:HA	1:B:558:GLN:NE2	1.92	0.83
1:A:507:LEU:HA	1:A:558:GLN:NE2	1.93	0.83
1:B:523:LEU:HB3	1:B:529:ILE:HD13	1.57	0.83
1:B:780:GLU:HA	1:B:783:LEU:HD12	1.61	0.83
1:A:428:PHE:CE1	1:A:599:ARG:HA	2.13	0.83
1:A:403:LEU:O	1:A:407:LEU:HD22	1.79	0.83
1:A:925:ARG:HA	1:A:931:ILE:HD12	1.59	0.83
1:A:188:GLY:HA2	1:A:191:LEU:HD22	1.61	0.83
1:A:410:ARG:HD3	1:A:927:VAL:HG13	1.60	0.83
1:B:785:ARG:HA	1:B:789:ASP:OD2	1.78	0.83
1:B:616:THR:O	1:B:619:SER:HB3	1.78	0.83
1:A:582:ASP:HA	1:A:618:GLN:NE2	1.94	0.83
1:B:777:ILE:HG13	1:B:778:THR:H	1.43	0.83
1:B:688:LEU:HD23	1:B:688:LEU:H	1.42	0.83
1:A:952:GLN:HE22	1:B:948:GLU:HG2	1.43	0.83
1:A:52:ARG:NH1	1:A:54:MSE:HG3	1.93	0.83
1:A:669:ASN:HA	1:A:672:GLU:OE1	1.78	0.83
1:A:190:ILE:H	1:A:190:ILE:HD12	1.43	0.82
1:A:403:LEU:O	1:A:406:MSE:HB2	1.79	0.82
1:B:219:MSE:HB3	1:B:225:LEU:HB2	1.58	0.82
1:B:105:LYS:HD3	1:B:105:LYS:H	1.43	0.82
1:A:884:VAL:HG13	1:A:887:ILE:HD12	1.62	0.82
1:B:540:ILE:H	1:B:540:ILE:HD12	1.44	0.82
1:B:759:ILE:HD12	1:B:772:GLU:O	1.78	0.82
1:A:261:ARG:HB2	1:A:265:ARG:HH21	1.45	0.82
1:B:428:PHE:CE1	1:B:599:ARG:HA	2.12	0.82
1:B:599:ARG:HH11	1:B:599:ARG:HB3	1.42	0.82
1:A:328:LEU:H	1:A:328:LEU:HD22	1.45	0.82
1:B:184:THR:HB	1:B:222:ARG:HH22	1.43	0.82
1:B:568:GLU:HG3	1:B:596:ARG:HH21	1.43	0.82
1:A:396:ALA:O	1:A:400:ARG:HD2	1.78	0.82
1:B:612:TYR:HD2	1:B:619:SER:HA	1.45	0.82
1:B:859:GLU:CB	1:B:863:ARG:HH12	1.93	0.82
1:A:493:TRP:CD1	1:A:494:LEU:HD12	2.15	0.82
1:B:403:LEU:HD12	1:B:404:VAL:H	1.45	0.82
1:A:781:HIS:HA	1:A:784:ILE:HD12	1.60	0.82
1:B:194:GLN:NE2	1:B:199:ALA:HB3	1.95	0.82
1:B:468:LEU:HD22	1:B:469:TYR:CZ	2.15	0.82
1:A:145:SER:HA	1:A:148:ARG:HE	1.41	0.82
1:B:859:GLU:CB	1:B:863:ARG:HH22	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:HH21	1:A:19:LEU:HB3	1.42	0.82
1:A:784:ILE:HG22	1:A:788:LEU:HD11	1.60	0.82
1:B:18:GLY:CA	1:B:106:LEU:HD21	2.03	0.82
1:A:328:LEU:HB3	1:A:336:PHE:CE2	2.15	0.81
1:A:817:GLU:HB2	1:A:961:ARG:H	1.43	0.81
1:B:775:GLN:CD	1:B:776:PHE:H	1.82	0.81
1:B:5:LEU:O	1:B:80:LEU:HD21	1.80	0.81
1:B:314:ALA:HB3	1:B:327:ARG:NE	1.95	0.81
1:B:905:ALA:O	1:B:909:GLU:HG2	1.79	0.81
1:B:784:ILE:HG22	1:B:788:LEU:HD11	1.60	0.81
1:A:558:GLN:NE2	1:A:559:VAL:H	1.78	0.81
1:B:950:LEU:HD12	1:B:951:ASP:OD1	1.78	0.81
1:A:115:LEU:HD13	1:A:116:PHE:N	1.93	0.81
1:A:877:VAL:HG13	1:A:878:ASN:H	1.44	0.81
1:A:266:LEU:HD12	1:A:266:LEU:H	1.44	0.81
1:A:314:ALA:HB3	1:A:327:ARG:NE	1.96	0.81
1:A:515:THR:HG23	1:A:562:CYS:SG	2.20	0.81
1:A:542:GLU:HA	1:A:545:ARG:HH21	1.45	0.81
1:A:785:ARG:O	1:A:789:ASP:HB2	1.79	0.81
1:A:523:LEU:HB3	1:A:529:ILE:HD13	1.60	0.81
1:A:516:ALA:HB2	1:A:562:CYS:HB2	1.62	0.81
1:B:115:LEU:HD13	1:B:116:PHE:N	1.95	0.81
1:B:702:LEU:O	1:B:706:ILE:HD13	1.79	0.81
1:B:123:MSE:HG2	1:B:865:LEU:HB2	1.62	0.81
1:B:176:ALA:CB	1:B:419:ARG:HB2	2.11	0.81
1:B:8:ARG:HE	1:B:19:LEU:HD22	1.45	0.81
1:B:287:TRP:CE3	1:B:292:PRO:HA	2.16	0.81
1:B:110:LYS:HB3	1:B:112:GLN:HE22	1.45	0.81
1:A:145:SER:HA	1:A:148:ARG:CZ	2.10	0.81
1:A:123:MSE:HG2	1:A:865:LEU:HB2	1.63	0.81
1:B:403:LEU:O	1:B:406:MSE:HB2	1.81	0.81
1:B:311:LEU:HD23	1:B:311:LEU:H	1.44	0.81
1:A:8:ARG:HE	1:A:19:LEU:HD22	1.45	0.81
1:A:125:ARG:CB	1:A:125:ARG:HH11	1.92	0.81
1:A:400:ARG:O	1:A:403:LEU:HD12	1.80	0.81
1:A:186:GLU:HA	1:A:189:MSE:SE	2.30	0.80
1:A:314:ALA:HB3	1:A:327:ARG:HE	1.45	0.80
1:B:775:GLN:CD	1:B:776:PHE:N	2.35	0.80
1:B:350:CYS:HB2	1:B:351:PRO:HD3	1.62	0.80
1:B:515:THR:HG23	1:B:562:CYS:SG	2.20	0.80
1:B:145:SER:HA	1:B:148:ARG:HE	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:851:ASN:N	1:B:851:ASN:HD22	1.77	0.80
1:B:842:ARG:HH11	1:B:856:VAL:HG23	1.43	0.80
1:A:18:GLY:HA2	1:A:106:LEU:HD21	1.63	0.80
1:A:763:PHE:O	1:A:767:VAL:HG23	1.81	0.80
1:B:179:VAL:HG22	1:B:317:GLU:OE1	1.82	0.80
1:B:960:LEU:HD23	1:B:961:ARG:N	1.96	0.80
1:A:859:GLU:O	1:A:862:ASN:HB3	1.81	0.80
1:B:244:ASN:HB3	1:B:245:PRO:CD	2.10	0.80
1:B:112:GLN:HE21	1:B:112:GLN:C	1.85	0.80
1:B:542:GLU:HA	1:B:545:ARG:HH21	1.45	0.80
1:A:769:LEU:HD22	1:A:771:ARG:NH2	1.96	0.80
1:A:816:VAL:O	1:A:844:LEU:HD23	1.82	0.80
1:B:859:GLU:O	1:B:862:ASN:HB3	1.80	0.80
1:B:403:LEU:HD12	1:B:404:VAL:N	1.96	0.80
1:B:516:ALA:HB2	1:B:562:CYS:HB2	1.64	0.80
1:B:400:ARG:O	1:B:403:LEU:HD12	1.82	0.80
1:A:256:LEU:HD22	1:A:257:ASP:N	1.97	0.80
1:A:760:THR:HG21	1:A:766:GLU:HG2	1.63	0.80
1:B:194:GLN:HE21	1:B:199:ALA:HB3	1.47	0.80
1:B:669:ASN:HA	1:B:672:GLU:OE1	1.82	0.80
1:A:176:ALA:CB	1:A:419:ARG:HB2	2.12	0.80
1:B:8:ARG:HH21	1:B:19:LEU:HB3	1.44	0.80
1:B:453:ILE:H	1:B:453:ILE:HD12	1.46	0.80
1:A:952:GLN:HE22	1:B:948:GLU:CG	1.95	0.80
1:A:714:ASN:ND2	1:A:714:ASN:H	1.80	0.80
1:B:578:MSE:HE3	1:B:580:MSE:SE	2.32	0.79
1:B:256:LEU:HD22	1:B:257:ASP:N	1.98	0.79
1:A:369:GLU:OE1	1:A:372:MSE:HG3	1.82	0.79
1:A:182:GLY:CA	1:A:185:ILE:HD13	2.12	0.79
1:B:582:ASP:HA	1:B:618:GLN:NE2	1.96	0.79
1:B:553:GLU:HG2	1:B:554:ASP:N	1.97	0.79
1:A:515:THR:O	1:A:519:LEU:HG	1.83	0.79
1:B:174:LEU:O	1:B:174:LEU:HD13	1.83	0.79
1:A:540:ILE:HD12	1:A:540:ILE:H	1.48	0.79
1:A:287:TRP:CE3	1:A:292:PRO:HA	2.18	0.79
1:B:962:LEU:CD1	1:B:962:LEU:H	1.96	0.79
1:B:763:PHE:O	1:B:767:VAL:HG23	1.83	0.79
1:B:822:VAL:HG22	1:B:839:THR:H	1.46	0.79
1:B:52:ARG:HG3	1:B:54:MSE:HG3	1.64	0.79
1:A:385:LEU:H	1:A:385:LEU:HD12	1.47	0.79
1:A:842:ARG:HH11	1:A:856:VAL:HG23	1.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:C	1:A:112:GLN:HE21	1.85	0.79
1:A:28:ARG:NH1	1:A:241:ASP:OD2	2.14	0.78
1:A:822:VAL:HG22	1:A:839:THR:H	1.48	0.78
1:B:314:ALA:HB3	1:B:327:ARG:HE	1.48	0.78
1:B:586:ASN:HB3	1:B:589:LEU:CD1	2.12	0.78
1:A:292:PRO:HB2	1:A:297:GLN:CD	2.03	0.78
1:A:64:HIS:HA	1:A:103:ASP:OD1	1.83	0.78
1:A:468:LEU:HD22	1:A:469:TYR:CZ	2.18	0.78
1:A:123:MSE:HE2	1:A:961:ARG:NH2	1.97	0.78
1:A:616:THR:O	1:A:619:SER:HB3	1.82	0.78
1:B:493:TRP:CD1	1:B:494:LEU:HD12	2.18	0.78
1:A:859:GLU:CB	1:A:863:ARG:HH12	1.96	0.78
1:A:918:LEU:HD22	1:A:918:LEU:O	1.84	0.78
1:B:714:ASN:H	1:B:714:ASN:ND2	1.79	0.78
1:B:877:VAL:HG13	1:B:878:ASN:H	1.46	0.78
1:A:208:PRO:O	1:A:212:GLN:HG3	1.82	0.78
1:A:179:VAL:HG22	1:A:317:GLU:OE1	1.83	0.78
1:A:784:ILE:HG22	1:A:788:LEU:CD1	2.14	0.78
1:B:313:THR:C	1:B:315:THR:H	1.85	0.78
1:A:244:ASN:HB3	1:A:245:PRO:CD	2.14	0.78
1:A:962:LEU:H	1:A:962:LEU:CD1	1.97	0.78
1:B:599:ARG:NH1	1:B:599:ARG:HB3	1.98	0.78
1:A:123:MSE:HB3	1:A:865:LEU:HD13	1.66	0.78
1:B:729:ASN:H	1:B:743:SER:HB2	1.47	0.78
1:B:123:MSE:HB2	1:B:961:ARG:CZ	2.13	0.78
1:B:258:PHE:HD1	1:B:261:ARG:HE	1.31	0.78
1:B:246:PHE:CZ	1:B:268:HIS:HB2	2.18	0.78
1:A:161:ILE:HG23	1:A:165:VAL:HG21	1.64	0.78
1:A:751:PHE:CE1	1:A:782:PRO:HB3	2.17	0.78
1:A:612:TYR:HD2	1:A:619:SER:HA	1.48	0.78
1:B:431:ARG:HH22	1:B:635:THR:HA	1.49	0.78
1:A:194:GLN:NE2	1:A:199:ALA:HB3	1.98	0.78
1:A:184:THR:HB	1:A:222:ARG:HH22	1.48	0.78
1:B:627:GLU:HA	1:B:671:ARG:NH1	1.98	0.78
1:A:881:GLN:HG2	1:A:882:GLN:H	1.49	0.78
1:B:568:GLU:HB3	1:B:596:ARG:NE	1.99	0.78
1:A:373:LEU:HD23	1:A:374:GLY:H	1.47	0.78
1:A:383:GLU:H	1:A:384:PRO:HD3	1.47	0.77
1:B:494:LEU:O	1:B:498:LEU:HG	1.84	0.77
1:B:521:GLN:OE1	1:B:525:GLU:HG3	1.83	0.77
1:B:173:VAL:HG12	1:B:416:VAL:HA	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:ILE:HG22	1:B:788:LEU:CD1	2.14	0.77
1:B:521:GLN:HE22	1:B:525:GLU:CB	1.95	0.77
1:A:219:MSE:H	1:A:219:MSE:HE2	1.48	0.77
1:B:780:GLU:O	1:B:784:ILE:HG13	1.83	0.77
1:A:578:MSE:HE3	1:A:580:MSE:SE	2.34	0.77
1:A:202:ARG:HB3	1:A:274:TRP:HZ3	1.48	0.77
1:A:176:ALA:HA	1:A:313:THR:HG23	1.67	0.77
1:B:190:ILE:HD12	1:B:190:ILE:H	1.49	0.77
1:B:396:ALA:O	1:B:400:ARG:HD2	1.83	0.77
1:A:702:LEU:O	1:A:706:ILE:HD13	1.83	0.77
1:A:444:TYR:O	1:A:448:ILE:HG13	1.84	0.77
1:A:30:VAL:O	1:A:42:LEU:HD22	1.84	0.77
1:B:112:GLN:HE21	1:B:113:ASP:N	1.83	0.77
1:A:885:HIS:CA	1:A:888:LEU:HD23	2.13	0.77
1:B:125:ARG:CB	1:B:125:ARG:HH11	1.91	0.77
1:B:293:SER:O	1:B:297:GLN:HG3	1.85	0.77
1:B:573:GLN:HA	1:B:602:GLN:OE1	1.84	0.77
1:B:30:VAL:O	1:B:42:LEU:HD22	1.84	0.77
1:A:246:PHE:CZ	1:A:268:HIS:HB2	2.19	0.77
1:A:258:PHE:HD1	1:A:261:ARG:HE	1.31	0.77
1:A:431:ARG:HH22	1:A:635:THR:HA	1.48	0.77
1:A:472:ARG:HA	1:A:475:GLN:NE2	1.99	0.77
1:B:253:ILE:HD13	1:B:253:ILE:N	2.00	0.77
1:A:573:GLN:HA	1:A:602:GLN:OE1	1.84	0.77
1:A:627:GLU:HA	1:A:671:ARG:NH1	1.98	0.77
1:A:230:PHE:CE2	1:A:235:TYR:HA	2.19	0.77
1:A:780:GLU:HA	1:A:783:LEU:HD12	1.67	0.77
1:B:182:GLY:CA	1:B:185:ILE:HD13	2.15	0.77
1:A:905:ALA:O	1:A:909:GLU:HG2	1.85	0.77
1:B:161:ILE:HG23	1:B:165:VAL:HG21	1.67	0.77
1:B:801:ILE:HD11	1:B:814:LEU:HA	1.66	0.77
1:B:8:ARG:O	1:B:53:VAL:HG23	1.85	0.77
1:A:436:ILE:HD12	1:A:436:ILE:N	1.99	0.77
1:A:467:MSE:H	1:A:467:MSE:SE	2.17	0.77
1:B:485:TRP:HZ2	1:B:518:GLN:HE22	1.33	0.76
1:B:885:HIS:CA	1:B:888:LEU:HD23	2.15	0.76
1:A:446:THR:HA	1:A:449:LYS:HE2	1.68	0.76
1:A:752:PRO:HB2	1:A:779:TRP:NE1	2.00	0.76
1:B:785:ARG:O	1:B:789:ASP:HB2	1.83	0.76
1:A:859:GLU:HB3	1:A:863:ARG:CZ	2.14	0.76
1:A:553:GLU:HG2	1:A:554:ASP:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ALA:O	1:B:343:VAL:HG23	1.86	0.76
1:B:343:VAL:O	1:B:347:LYS:HG3	1.85	0.76
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.67	0.76
1:A:182:GLY:HA2	1:A:185:ILE:HD13	1.68	0.76
1:B:436:ILE:HD12	1:B:436:ILE:N	2.01	0.76
1:A:194:GLN:HE21	1:A:199:ALA:HB3	1.51	0.76
1:B:176:ALA:HB1	1:B:419:ARG:HB2	1.68	0.76
1:B:568:GLU:HB3	1:B:596:ARG:HE	1.50	0.76
1:A:881:GLN:HG2	1:A:882:GLN:N	2.00	0.76
1:A:599:ARG:HB3	1:A:599:ARG:NH1	2.00	0.76
1:B:918:LEU:HD22	1:B:918:LEU:O	1.86	0.76
1:A:52:ARG:O	1:A:54:MSE:HE2	1.86	0.76
1:A:123:MSE:HB2	1:A:961:ARG:CZ	2.16	0.76
1:B:859:GLU:HB3	1:B:863:ARG:NH1	2.01	0.76
1:B:409:ASP:O	1:B:927:VAL:HG11	1.85	0.75
1:A:110:LYS:HB3	1:A:112:GLN:HE22	1.51	0.75
1:A:826:ALA:HB3	1:A:832:LEU:HD13	1.68	0.75
1:B:881:GLN:HG2	1:B:882:GLN:H	1.50	0.75
1:B:798:SER:OG	1:B:962:LEU:HD11	1.86	0.75
1:B:530:ARG:NH1	1:B:555:THR:HB	2.01	0.75
1:A:105:LYS:H	1:A:105:LYS:HD3	1.49	0.75
1:A:176:ALA:HA	1:A:313:THR:CG2	2.17	0.75
1:A:521:GLN:HE22	1:A:525:GLU:CB	1.97	0.75
1:A:350:CYS:HB2	1:A:351:PRO:HD3	1.66	0.75
1:B:373:LEU:HD23	1:B:374:GLY:H	1.50	0.75
1:B:208:PRO:HD2	1:B:211:LEU:HD12	1.67	0.75
1:A:440:LEU:O	1:A:440:LEU:HD22	1.86	0.75
1:B:64:HIS:HA	1:B:103:ASP:OD1	1.86	0.75
1:A:446:THR:HA	1:A:449:LYS:CE	2.16	0.75
1:A:435:THR:HA	1:A:610:VAL:CG2	2.17	0.75
1:B:404:VAL:HG23	1:B:405:SER:N	2.01	0.75
1:B:205:ILE:HG23	1:B:278:VAL:HB	1.67	0.75
1:B:219:MSE:HE2	1:B:219:MSE:H	1.49	0.75
1:B:629:LEU:N	1:B:629:LEU:HD12	2.00	0.75
1:B:859:GLU:HB3	1:B:863:ARG:HH12	1.49	0.75
1:A:433:LEU:HG	1:A:434:HIS:H	1.52	0.75
1:A:404:VAL:HG23	1:A:405:SER:N	2.02	0.75
1:B:155:ILE:O	1:B:159:LEU:HG	1.86	0.75
1:B:473:ILE:HA	1:B:476:GLU:CD	2.07	0.75
1:B:919:SER:HA	1:B:922:GLU:OE1	1.87	0.75
1:A:313:THR:C	1:A:315:THR:H	1.90	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:751:PHE:CE1	1:B:782:PRO:HB3	2.21	0.75
1:A:473:ILE:HA	1:A:476:GLU:CD	2.08	0.75
1:A:161:ILE:H	1:A:161:ILE:HD12	1.52	0.75
1:B:826:ALA:HB3	1:B:832:LEU:HD13	1.69	0.75
1:B:446:THR:HA	1:B:449:LYS:HE2	1.69	0.74
1:A:521:GLN:OE1	1:A:525:GLU:HG3	1.86	0.74
1:B:52:ARG:O	1:B:54:MSE:HE2	1.87	0.74
1:B:752:PRO:HB2	1:B:779:TRP:NE1	2.02	0.74
1:B:780:GLU:CD	1:B:783:LEU:HD12	2.07	0.74
1:B:859:GLU:HB3	1:B:863:ARG:CZ	2.16	0.74
1:B:530:ARG:HH11	1:B:555:THR:HB	1.52	0.74
1:A:417:LEU:O	1:A:417:LEU:HD23	1.87	0.74
1:B:175:LEU:H	1:B:175:LEU:HD12	1.52	0.74
1:B:446:THR:HA	1:B:449:LYS:CE	2.17	0.74
1:A:433:LEU:HG	1:A:434:HIS:N	2.01	0.74
1:A:859:GLU:HB3	1:A:863:ARG:NH1	2.02	0.74
1:A:689:LEU:HD12	1:A:690:GLU:N	2.03	0.74
1:B:208:PRO:O	1:B:212:GLN:HG3	1.86	0.74
1:B:182:GLY:HA2	1:B:185:ILE:HD13	1.70	0.74
1:B:472:ARG:HA	1:B:475:GLN:NE2	2.02	0.74
1:B:228:ALA:HB1	1:B:234:ARG:NH1	2.03	0.74
1:A:155:ILE:O	1:A:159:LEU:HG	1.86	0.74
1:A:258:PHE:HA	1:A:261:ARG:HE	1.48	0.74
1:A:851:ASN:N	1:A:851:ASN:HD22	1.82	0.74
1:A:650:LEU:HD11	1:A:654:LEU:HD11	1.69	0.74
1:A:568:GLU:HB3	1:A:596:ARG:NE	2.01	0.74
1:A:921:LEU:HD22	1:A:921:LEU:H	1.51	0.74
1:A:780:GLU:HB3	1:A:784:ILE:HD11	1.70	0.74
1:B:845:LEU:N	1:B:845:LEU:HD23	2.03	0.74
1:B:385:LEU:H	1:B:385:LEU:HD12	1.52	0.74
1:A:399:ALA:O	1:A:403:LEU:HG	1.87	0.74
1:A:175:LEU:HD12	1:A:175:LEU:H	1.51	0.74
1:A:583:LEU:HB2	1:A:618:GLN:OE1	1.87	0.74
1:A:41:ARG:HB3	1:A:43:TYR:CE2	2.23	0.74
1:B:921:LEU:HD22	1:B:921:LEU:H	1.53	0.74
1:B:129:ARG:NH2	1:B:791:ILE:HA	2.02	0.73
1:B:515:THR:O	1:B:519:LEU:HG	1.88	0.73
1:B:881:GLN:HG2	1:B:882:GLN:N	2.03	0.73
1:B:816:VAL:O	1:B:844:LEU:HD23	1.87	0.73
1:A:348:ASN:C	1:A:351:PRO:HD2	2.09	0.73
1:A:801:ILE:HD11	1:A:814:LEU:HA	1.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HA	1:A:354:ASP:OD2	1.87	0.73
1:A:28:ARG:HH11	1:A:241:ASP:CG	1.90	0.73
1:A:780:GLU:CD	1:A:783:LEU:HD12	2.08	0.73
1:A:385:LEU:N	1:A:385:LEU:HD12	2.03	0.73
1:B:435:THR:HA	1:B:610:VAL:CG2	2.19	0.73
1:A:409:ASP:O	1:A:927:VAL:HG11	1.87	0.73
1:B:260:ARG:NH2	1:B:263:LYS:HE3	2.03	0.73
1:A:112:GLN:HE21	1:A:113:ASP:N	1.86	0.73
1:B:41:ARG:HB3	1:B:43:TYR:CE2	2.23	0.73
1:B:348:ASN:C	1:B:351:PRO:HD2	2.08	0.73
1:A:122:ARG:H	1:A:122:ARG:NE	1.85	0.73
1:B:597:LEU:HD23	1:B:602:GLN:HE22	1.53	0.73
1:A:330:LEU:N	1:A:330:LEU:HD12	2.03	0.73
1:B:145:SER:HA	1:B:148:ARG:CZ	2.18	0.73
1:B:772:GLU:OE2	1:B:778:THR:HG23	1.88	0.73
1:B:612:TYR:CD2	1:B:619:SER:HA	2.23	0.73
1:B:292:PRO:HB2	1:B:297:GLN:CD	2.08	0.73
1:A:568:GLU:HG3	1:A:596:ARG:NH2	2.03	0.73
1:B:112:GLN:NE2	1:B:113:ASP:N	2.37	0.73
1:A:427:GLY:C	1:A:600:ILE:HG23	2.09	0.73
1:A:578:MSE:HE1	1:A:594:ILE:HG12	1.70	0.73
1:A:678:LYS:HG3	1:A:679:ALA:N	2.02	0.73
1:B:440:LEU:HG	1:B:615:LYS:HD2	1.70	0.73
1:A:230:PHE:HE2	1:A:235:TYR:HA	1.52	0.73
1:B:781:HIS:CA	1:B:784:ILE:HD12	2.19	0.73
1:A:792:LEU:CA	1:A:795:ASP:HB2	2.19	0.73
1:A:383:GLU:HB2	1:A:387:GLN:CG	2.18	0.73
1:B:583:LEU:HB2	1:B:618:GLN:OE1	1.87	0.73
1:B:859:GLU:OE1	1:B:863:ARG:NH1	2.21	0.73
1:B:230:PHE:CE2	1:B:235:TYR:HA	2.24	0.73
1:B:701:ALA:O	1:B:704:GLU:HB2	1.88	0.73
1:A:214:GLN:O	1:A:217:VAL:HG12	1.88	0.73
1:A:253:ILE:HD13	1:A:253:ILE:N	2.03	0.73
1:A:114:ARG:O	1:A:114:ARG:HD3	1.89	0.73
1:B:574:PHE:H	1:B:574:PHE:HD1	1.37	0.73
1:B:568:GLU:HG3	1:B:596:ARG:NH2	2.04	0.72
1:B:677:LEU:HD12	1:B:677:LEU:O	1.87	0.72
1:A:340:ALA:O	1:A:343:VAL:HG23	1.88	0.72
1:A:574:PHE:HD1	1:A:574:PHE:H	1.37	0.72
1:A:173:VAL:HG12	1:A:416:VAL:HA	1.71	0.72
1:A:403:LEU:HD12	1:A:404:VAL:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HG23	1:A:278:VAL:HB	1.68	0.72
1:B:962:LEU:HD13	1:B:962:LEU:N	2.02	0.72
1:A:677:LEU:O	1:A:680:GLN:HB3	1.89	0.72
1:B:106:LEU:HD22	1:B:106:LEU:H	1.54	0.72
1:B:568:GLU:OE2	1:B:570:ARG:CZ	2.37	0.72
1:B:383:GLU:O	1:B:387:GLN:OE1	2.07	0.72
1:A:209:GLU:HA	1:A:212:GLN:NE2	2.04	0.72
1:A:568:GLU:HB3	1:A:596:ARG:HE	1.53	0.72
1:A:775:GLN:NE2	1:A:776:PHE:HB2	2.04	0.72
1:A:728:ILE:HA	1:A:743:SER:N	2.05	0.72
1:B:105:LYS:N	1:B:105:LYS:HD3	2.04	0.72
1:A:584:PRO:HD3	1:A:593:ARG:NE	2.04	0.72
1:A:877:VAL:HG13	1:A:878:ASN:N	2.04	0.72
1:B:330:LEU:N	1:B:330:LEU:HD12	2.04	0.72
1:B:506:VAL:CG1	1:B:507:LEU:H	1.90	0.72
1:A:859:GLU:HB3	1:A:863:ARG:HH12	1.52	0.72
1:A:403:LEU:HD12	1:A:404:VAL:N	2.04	0.72
1:B:253:ILE:O	1:B:254:CYS:SG	2.47	0.72
1:B:440:LEU:HD22	1:B:440:LEU:O	1.90	0.72
1:B:586:ASN:ND2	1:B:588:ASP:HB2	2.02	0.72
1:A:606:ILE:HD12	1:A:606:ILE:H	1.54	0.72
1:B:258:PHE:HA	1:B:261:ARG:HE	1.52	0.72
1:A:52:ARG:NH2	1:A:81:LEU:HG	2.04	0.72
1:B:209:GLU:HA	1:B:212:GLN:NE2	2.04	0.72
1:A:176:ALA:HB3	1:A:419:ARG:HB2	1.72	0.72
1:B:689:LEU:HD12	1:B:690:GLU:N	2.04	0.72
1:B:120:ILE:HD12	1:B:120:ILE:C	2.10	0.72
1:B:735:ASP:CG	1:B:736:ASN:N	2.43	0.72
1:A:383:GLU:O	1:A:387:GLN:OE1	2.08	0.72
1:B:383:GLU:H	1:B:384:PRO:HD3	1.54	0.72
1:A:202:ARG:HD3	1:A:273:GLU:HG2	1.72	0.72
1:A:266:LEU:HA	1:A:269:LEU:CD1	2.20	0.72
1:A:962:LEU:HD13	1:A:962:LEU:N	2.01	0.72
1:B:801:ILE:HG12	1:B:802:SER:N	2.04	0.72
1:B:865:LEU:HG	1:B:866:ASN:H	1.55	0.72
1:A:677:LEU:O	1:A:677:LEU:HD12	1.89	0.72
1:A:427:GLY:O	1:A:600:ILE:HG23	1.90	0.72
1:A:373:LEU:H	1:A:373:LEU:HD22	1.54	0.72
1:A:564:GLU:O	1:A:565:ILE:HG23	1.90	0.72
1:B:161:ILE:HD12	1:B:161:ILE:H	1.54	0.72
1:A:845:LEU:N	1:A:845:LEU:HD23	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:GLU:OE1	1:B:783:LEU:HD12	1.88	0.71
1:B:490:ARG:O	1:B:493:TRP:HB3	1.90	0.71
1:B:584:PRO:HD3	1:B:593:ARG:NE	2.03	0.71
1:B:689:LEU:C	1:B:691:ILE:H	1.92	0.71
1:A:343:VAL:O	1:A:347:LYS:HG3	1.90	0.71
1:B:374:GLY:HA2	1:B:378:GLY:O	1.91	0.71
1:B:110:LYS:HB3	1:B:112:GLN:NE2	2.05	0.71
1:B:220:LEU:O	1:B:220:LEU:HD12	1.90	0.71
1:B:837:PRO:HB2	1:B:838:PRO:CD	2.18	0.71
1:B:427:GLY:HA3	1:B:600:ILE:HG23	1.72	0.71
1:A:369:GLU:HA	1:A:372:MSE:HG2	1.71	0.71
1:A:431:ARG:NH2	1:A:591:GLU:OE2	2.23	0.71
1:B:403:LEU:HA	1:B:406:MSE:CG	2.20	0.71
1:A:112:GLN:NE2	1:A:113:ASP:N	2.38	0.71
1:B:735:ASP:CG	1:B:736:ASN:H	1.94	0.71
1:B:880:VAL:CG1	1:B:883:ASP:HB2	2.20	0.71
1:B:220:LEU:HA	1:B:225:LEU:H	1.56	0.71
1:A:427:GLY:HA3	1:A:600:ILE:HG23	1.73	0.71
1:A:10:ILE:HG12	1:A:53:VAL:HG22	1.72	0.71
1:A:506:VAL:CG1	1:A:507:LEU:H	1.87	0.71
1:B:287:TRP:HE3	1:B:292:PRO:HA	1.55	0.71
1:B:346:GLN:HA	1:B:349:TYR:HB2	1.71	0.71
1:B:261:ARG:HB2	1:B:265:ARG:NH2	2.05	0.71
1:A:202:ARG:HG2	1:A:202:ARG:HH11	1.54	0.71
1:A:728:ILE:HG22	1:A:728:ILE:O	1.90	0.71
1:B:444:TYR:O	1:B:448:ILE:HG13	1.90	0.71
1:B:564:GLU:O	1:B:565:ILE:HG23	1.91	0.71
1:A:650:LEU:O	1:A:650:LEU:HD22	1.91	0.71
1:B:620:VAL:HG23	1:B:621:LEU:HD23	1.72	0.71
1:A:403:LEU:HA	1:A:406:MSE:CG	2.21	0.71
1:B:541:ILE:HA	1:B:544:ASP:OD2	1.90	0.71
1:A:722:LEU:O	1:A:726:ILE:HG13	1.89	0.71
1:A:837:PRO:HB2	1:A:838:PRO:CD	2.19	0.71
1:B:433:LEU:HG	1:B:434:HIS:N	2.06	0.71
1:A:399:ALA:HB3	1:A:400:ARG:CZ	2.21	0.71
1:A:440:LEU:CD1	1:A:440:LEU:H	2.02	0.71
1:A:625:TYR:HA	1:A:629:LEU:HD11	1.72	0.71
1:A:541:ILE:HA	1:A:544:ASP:OD2	1.90	0.71
1:A:383:GLU:N	1:A:384:PRO:CD	2.54	0.70
1:B:351:PRO:HA	1:B:354:ASP:OD2	1.89	0.70
1:A:507:LEU:CD2	1:A:559:VAL:HG13	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:TRP:HE3	1:A:292:PRO:HA	1.56	0.70
1:A:8:ARG:HB3	1:A:19:LEU:CD2	2.20	0.70
1:A:738:ILE:HG22	1:A:739:VAL:N	2.06	0.70
1:B:190:ILE:HA	1:B:193:GLN:OE1	1.92	0.70
1:B:809:LEU:HD12	1:B:810:PRO:HD2	1.73	0.70
1:B:818:LEU:N	1:B:818:LEU:HD12	2.06	0.70
1:A:530:ARG:NH1	1:A:549:TRP:HE1	1.88	0.70
1:A:597:LEU:HD23	1:A:602:GLN:HE22	1.56	0.70
1:B:728:ILE:HA	1:B:743:SER:N	2.05	0.70
1:A:617:ALA:O	1:A:620:VAL:HG22	1.91	0.70
1:A:692:HIS:ND1	1:A:693:SER:N	2.39	0.70
1:A:950:LEU:HD12	1:A:951:ASP:OD1	1.91	0.70
1:A:221:ARG:HD3	1:A:770:ALA:HB1	1.72	0.70
1:A:311:LEU:HD23	1:A:311:LEU:N	2.06	0.70
1:B:220:LEU:HA	1:B:225:LEU:N	2.06	0.70
1:A:620:VAL:HG23	1:A:621:LEU:HD23	1.74	0.70
1:B:433:LEU:HG	1:B:434:HIS:H	1.56	0.70
1:B:586:ASN:HD21	1:B:588:ASP:CB	2.03	0.70
1:A:689:LEU:C	1:A:691:ILE:H	1.93	0.70
1:A:568:GLU:CG	1:A:596:ARG:HH21	2.04	0.70
1:B:221:ARG:HD3	1:B:770:ALA:HB1	1.72	0.70
1:A:612:TYR:CD2	1:A:619:SER:HA	2.26	0.70
1:B:98:ARG:HB2	1:B:101:PHE:CE1	2.27	0.70
1:B:403:LEU:C	1:B:407:LEU:HD22	2.11	0.70
1:A:685:ARG:HB2	1:A:687:ARG:CZ	2.22	0.70
1:A:106:LEU:H	1:A:106:LEU:HD22	1.56	0.70
1:A:220:LEU:O	1:A:220:LEU:HD12	1.91	0.70
1:A:762:THR:O	1:A:766:GLU:HB2	1.91	0.70
1:B:467:MSE:H	1:B:467:MSE:SE	2.25	0.70
1:A:522:VAL:O	1:A:526:ARG:HB2	1.90	0.70
1:A:411:HIS:CE1	1:A:413:THR:OG1	2.45	0.70
1:B:678:LYS:HG3	1:B:679:ALA:N	2.04	0.70
1:B:9:TRP:CE2	1:B:52:ARG:HD3	2.27	0.70
1:A:228:ALA:HB1	1:A:234:ARG:NH1	2.07	0.70
1:B:380:GLN:HE21	1:B:382:ILE:CB	1.94	0.70
1:B:877:VAL:HG13	1:B:878:ASN:N	2.07	0.70
1:A:820:TYR:H	1:A:841:VAL:HG12	1.56	0.70
1:A:190:ILE:N	1:A:190:ILE:HD12	2.07	0.70
1:B:722:LEU:O	1:B:726:ILE:HG13	1.91	0.70
1:B:578:MSE:HE1	1:B:594:ILE:HG12	1.74	0.70
1:A:493:TRP:HD1	1:A:494:LEU:HD12	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:SER:O	1:B:110:LYS:HB2	1.92	0.70
1:A:485:TRP:HZ2	1:A:518:GLN:HE22	1.40	0.69
1:A:227:PHE:HB3	1:A:253:ILE:HD12	1.73	0.69
1:B:19:LEU:H	1:B:106:LEU:HD11	1.54	0.69
1:A:521:GLN:NE2	1:A:525:GLU:HB2	2.02	0.69
1:B:52:ARG:NH1	1:B:54:MSE:HG3	2.07	0.69
1:B:792:LEU:CA	1:B:795:ASP:HB2	2.22	0.69
1:B:637:PRO:HG2	1:B:638:THR:H	1.57	0.69
1:B:277:LEU:HD12	1:B:278:VAL:H	1.57	0.69
1:A:780:GLU:O	1:A:784:ILE:HG13	1.93	0.69
1:B:617:ALA:O	1:B:620:VAL:HG22	1.92	0.69
1:B:761:ILE:HG12	1:B:774:ALA:HB3	1.74	0.69
1:B:558:GLN:CD	1:B:559:VAL:H	1.94	0.69
1:A:270:CYS:SG	1:A:305:HIS:HB2	2.32	0.69
1:B:775:GLN:OE1	1:B:777:ILE:HG12	1.92	0.69
1:B:618:GLN:O	1:B:622:VAL:HG23	1.93	0.69
1:A:190:ILE:HA	1:A:193:GLN:OE1	1.92	0.69
1:B:530:ARG:NH1	1:B:549:TRP:HE1	1.89	0.69
1:B:553:GLU:CG	1:B:554:ASP:H	2.01	0.69
1:A:490:ARG:O	1:A:493:TRP:HB3	1.93	0.69
1:A:403:LEU:C	1:A:407:LEU:HD22	2.13	0.69
1:A:110:LYS:HB3	1:A:112:GLN:NE2	2.07	0.69
1:A:176:ALA:O	1:A:419:ARG:CZ	2.41	0.69
1:A:261:ARG:HB2	1:A:265:ARG:NH2	2.07	0.69
1:B:844:LEU:C	1:B:845:LEU:HD23	2.12	0.69
1:A:637:PRO:HG2	1:A:638:THR:H	1.56	0.69
1:B:568:GLU:CG	1:B:596:ARG:HH21	2.05	0.69
1:B:369:GLU:HA	1:B:372:MSE:HG2	1.72	0.69
1:A:105:LYS:HD3	1:A:105:LYS:N	2.08	0.69
1:A:561:LEU:HD11	1:A:565:ILE:HG12	1.75	0.69
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.58	0.69
1:A:440:LEU:HG	1:A:615:LYS:HD2	1.75	0.69
1:A:188:GLY:CA	1:A:223:PHE:CE2	2.72	0.69
1:A:220:LEU:HA	1:A:225:LEU:H	1.58	0.69
1:B:738:ILE:HG22	1:B:739:VAL:N	2.07	0.69
1:B:453:ILE:HD12	1:B:453:ILE:N	2.07	0.69
1:B:580:MSE:HE1	1:B:593:ARG:CB	2.22	0.69
1:B:427:GLY:C	1:B:600:ILE:HG23	2.14	0.69
1:B:650:LEU:O	1:B:650:LEU:HD22	1.93	0.69
1:B:677:LEU:O	1:B:680:GLN:HB3	1.93	0.69
1:B:385:LEU:N	1:B:385:LEU:HD12	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ARG:O	1:A:528:GLY:HA2	1.93	0.69
1:B:73:GLU:HG2	1:B:84:ILE:HB	1.75	0.69
1:B:8:ARG:HB3	1:B:19:LEU:CD2	2.23	0.69
1:B:354:ASP:O	1:B:358:MSE:HG2	1.93	0.69
1:B:411:HIS:CE1	1:B:413:THR:OG1	2.46	0.69
1:A:880:VAL:CG1	1:A:883:ASP:HB2	2.22	0.69
1:A:738:ILE:CG2	1:A:739:VAL:N	2.56	0.68
1:B:129:ARG:NH1	1:B:791:ILE:O	2.27	0.68
1:B:565:ILE:HD13	1:B:596:ARG:HD3	1.75	0.68
1:B:507:LEU:CD2	1:B:559:VAL:HG13	2.22	0.68
1:B:822:VAL:HG22	1:B:839:THR:N	2.08	0.68
1:B:495:MSE:SE	1:B:498:LEU:HD12	2.42	0.68
1:B:625:TYR:HA	1:B:629:LEU:HD11	1.74	0.68
1:B:647:TYR:O	1:B:651:ILE:HG22	1.94	0.68
1:A:349:TYR:HE2	1:A:411:HIS:CE1	2.12	0.68
1:B:339:PHE:CE1	1:B:343:VAL:HG22	2.27	0.68
1:A:110:LYS:HB2	1:A:113:ASP:HB2	1.75	0.68
1:B:851:ASN:ND2	1:B:851:ASN:N	2.42	0.68
1:A:453:ILE:N	1:A:453:ILE:HD12	2.07	0.68
1:A:552:GLU:HB3	1:A:555:THR:OG1	1.94	0.68
1:A:346:GLN:HA	1:A:349:TYR:HB2	1.74	0.68
1:B:373:LEU:H	1:B:373:LEU:HD22	1.57	0.68
1:A:458:LYS:O	1:A:462:ASP:HB3	1.93	0.68
1:A:190:ILE:H	1:A:190:ILE:CD1	2.06	0.68
1:A:865:LEU:HG	1:A:866:ASN:H	1.59	0.68
1:B:738:ILE:CG2	1:B:739:VAL:N	2.57	0.68
1:B:650:LEU:HD11	1:B:654:LEU:HD11	1.74	0.68
1:A:927:VAL:HG12	1:A:929:PRO:HD3	1.74	0.68
1:B:114:ARG:HD3	1:B:114:ARG:O	1.93	0.68
1:A:369:GLU:HA	1:A:372:MSE:CG	2.23	0.68
1:B:729:ASN:ND2	1:B:741:THR:O	2.26	0.68
1:B:833:ASN:CG	1:B:837:PRO:HB3	2.14	0.68
1:A:432:GLU:HB2	1:A:607:GLN:HE21	1.58	0.68
1:A:843:MSE:HE2	1:A:850:ASN:CG	2.14	0.68
1:A:207:VAL:HG22	1:A:211:LEU:HB2	1.76	0.68
1:B:266:LEU:HA	1:B:269:LEU:CD1	2.24	0.68
1:B:708:GLU:C	1:B:710:ASP:H	1.95	0.68
1:A:801:ILE:HG12	1:A:802:SER:N	2.09	0.68
1:A:647:TYR:O	1:A:651:ILE:HG22	1.93	0.68
1:A:530:ARG:NH1	1:A:555:THR:HB	2.08	0.68
1:B:403:LEU:O	1:B:407:LEU:HD13	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:TYR:HE2	1:B:411:HIS:CE1	2.11	0.68
1:A:565:ILE:HD13	1:A:596:ARG:HD3	1.76	0.68
1:B:202:ARG:HD3	1:B:273:GLU:HG2	1.74	0.68
1:A:716:ILE:CD1	1:A:716:ILE:H	2.06	0.68
1:B:410:ARG:CD	1:B:927:VAL:HG13	2.23	0.68
1:B:685:ARG:HB2	1:B:687:ARG:CZ	2.24	0.68
1:A:100:VAL:HG13	1:A:101:PHE:CE1	2.29	0.68
1:A:28:ARG:NH1	1:A:240:HIS:CE1	2.57	0.68
1:B:721:ASN:C	1:B:725:ILE:HD13	2.14	0.68
1:A:921:LEU:H	1:A:921:LEU:CD2	2.05	0.68
1:A:325:PHE:CA	1:A:328:LEU:HD23	2.24	0.67
1:B:777:ILE:HG13	1:B:778:THR:N	2.09	0.67
1:A:293:SER:O	1:A:297:GLN:HG3	1.94	0.67
1:A:494:LEU:O	1:A:498:LEU:HG	1.94	0.67
1:B:345:GLU:O	1:B:349:TYR:N	2.28	0.67
1:B:128:LEU:HD22	1:B:725:ILE:HG12	1.76	0.67
1:A:122:ARG:HE	1:A:122:ARG:N	1.87	0.67
1:A:663:PHE:CZ	1:A:667:ILE:HD11	2.29	0.67
1:B:9:TRP:NE1	1:B:52:ARG:HD3	2.09	0.67
1:A:701:ALA:O	1:A:704:GLU:HB2	1.94	0.67
1:A:762:THR:O	1:A:766:GLU:CB	2.43	0.67
1:B:584:PRO:HD3	1:B:593:ARG:NH2	2.10	0.67
1:A:686:ASP:OD1	1:A:689:LEU:HG	1.94	0.67
1:B:399:ALA:O	1:B:403:LEU:HG	1.94	0.67
1:B:692:HIS:ND1	1:B:693:SER:N	2.42	0.67
1:B:230:PHE:HE2	1:B:235:TYR:HA	1.58	0.67
1:A:80:LEU:HG	1:A:99:GLU:OE2	1.94	0.67
1:A:735:ASP:CG	1:A:736:ASN:H	1.98	0.67
1:A:174:LEU:HD11	1:A:176:ALA:HB2	1.75	0.67
1:A:229:LEU:HA	1:A:253:ILE:CG1	2.23	0.67
1:A:775:GLN:NE2	1:A:776:PHE:N	2.41	0.67
1:A:427:GLY:CA	1:A:600:ILE:HG23	2.24	0.67
1:B:927:VAL:HG12	1:B:929:PRO:HD3	1.76	0.67
1:A:618:GLN:O	1:A:622:VAL:HG23	1.93	0.67
1:A:792:LEU:HA	1:A:795:ASP:CB	2.24	0.67
1:B:728:ILE:HG22	1:B:728:ILE:O	1.94	0.67
1:B:100:VAL:HG13	1:B:101:PHE:CE1	2.29	0.67
1:B:522:VAL:O	1:B:526:ARG:HB2	1.94	0.67
1:B:369:GLU:HA	1:B:372:MSE:CG	2.25	0.67
1:B:207:VAL:HG22	1:B:211:LEU:HB2	1.77	0.67
1:A:781:HIS:CA	1:A:784:ILE:HD12	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:LEU:HD12	1:A:629:LEU:N	2.09	0.67
1:B:383:GLU:HB2	1:B:387:GLN:CG	2.19	0.67
1:A:446:THR:N	1:A:449:LYS:HE2	2.10	0.67
1:A:735:ASP:CG	1:A:736:ASN:N	2.47	0.67
1:A:142:MSE:HB3	1:A:148:ARG:HH22	1.60	0.67
1:A:620:VAL:HG23	1:A:621:LEU:N	2.08	0.67
1:B:599:ARG:CB	1:B:599:ARG:NH1	2.58	0.67
1:A:397:GLN:HA	1:A:400:ARG:HB2	1.76	0.67
1:B:410:ARG:HH11	1:B:927:VAL:HA	1.58	0.67
1:A:582:ASP:HA	1:A:618:GLN:HE22	1.58	0.67
1:A:183:LYS:HA	1:A:186:GLU:OE1	1.95	0.67
1:A:194:GLN:HG3	1:A:200:ALA:HB3	1.76	0.67
1:A:822:VAL:HG22	1:A:839:THR:N	2.09	0.67
1:A:453:ILE:H	1:A:453:ILE:CD1	2.07	0.67
1:B:411:HIS:CE1	1:B:413:THR:HG1	2.12	0.67
1:A:510:CYS:SG	1:A:562:CYS:CB	2.83	0.67
1:A:775:GLN:OE1	1:A:777:ILE:HG12	1.95	0.67
1:A:374:GLY:HA2	1:A:378:GLY:O	1.95	0.67
1:B:339:PHE:CZ	1:B:343:VAL:HG22	2.30	0.67
1:A:777:ILE:HG13	1:A:778:THR:H	1.60	0.67
1:B:72:GLU:CG	1:B:85:GLY:HA2	2.24	0.67
1:A:702:LEU:N	1:A:702:LEU:HD22	2.10	0.67
1:A:235:TYR:C	1:A:239:GLN:HE21	1.98	0.66
1:A:260:ARG:NH2	1:A:263:LYS:HE3	2.10	0.66
1:A:321:MSE:SE	1:A:322:GLU:H	2.28	0.66
1:A:324:HIS:O	1:A:327:ARG:NH1	2.28	0.66
1:B:123:MSE:HB3	1:B:865:LEU:HD13	1.76	0.66
1:B:183:LYS:HA	1:B:186:GLU:OE1	1.94	0.66
1:B:762:THR:O	1:B:766:GLU:HB2	1.95	0.66
1:B:918:LEU:HD13	1:B:918:LEU:C	2.15	0.66
1:B:458:LYS:O	1:B:462:ASP:HB3	1.95	0.66
1:A:872:THR:HG22	1:A:872:THR:O	1.95	0.66
1:B:517:LEU:O	1:B:520:GLU:HB3	1.95	0.66
1:B:521:GLN:NE2	1:B:525:GLU:HB2	2.01	0.66
1:B:561:LEU:HD11	1:B:565:ILE:HG12	1.78	0.66
1:B:383:GLU:N	1:B:384:PRO:CD	2.58	0.66
1:A:446:THR:CA	1:A:449:LYS:HE2	2.24	0.66
1:A:9:TRP:CE2	1:A:52:ARG:HD3	2.29	0.66
1:A:172:ARG:HD3	1:A:307:PRO:O	1.95	0.66
1:A:708:GLU:C	1:A:710:ASP:H	1.98	0.66
1:B:664:ASP:O	1:B:668:LYS:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:LEU:C	1:A:650:LEU:HD13	2.15	0.66
1:B:431:ARG:NH2	1:B:591:GLU:OE2	2.28	0.66
1:B:35:PRO:HB2	1:B:104:SER:OG	1.93	0.66
1:A:777:ILE:O	1:A:780:GLU:HB2	1.95	0.66
1:A:798:SER:OG	1:A:962:LEU:HD11	1.94	0.66
1:A:380:GLN:HE21	1:A:382:ILE:CB	1.96	0.66
1:A:103:ASP:HB3	1:A:105:LYS:HE2	1.77	0.66
1:A:919:SER:HA	1:A:922:GLU:OE1	1.95	0.66
1:A:28:ARG:HB2	1:A:241:ASP:CG	2.15	0.66
1:A:721:ASN:O	1:A:725:ILE:HD13	1.94	0.66
1:B:748:VAL:HG13	1:B:749:PRO:HD2	1.76	0.66
1:B:190:ILE:O	1:B:193:GLN:HG2	1.95	0.66
1:B:325:PHE:CA	1:B:328:LEU:HD23	2.26	0.66
1:B:103:ASP:HB3	1:B:105:LYS:HE2	1.77	0.66
1:B:427:GLY:O	1:B:600:ILE:HG23	1.95	0.66
1:A:403:LEU:O	1:A:407:LEU:HD13	1.94	0.66
1:A:120:ILE:C	1:A:120:ILE:HD12	2.16	0.66
1:A:228:ALA:C	1:A:253:ILE:HD11	2.15	0.66
1:A:257:ASP:O	1:A:261:ARG:HG3	1.96	0.66
1:B:762:THR:O	1:B:766:GLU:CB	2.44	0.66
1:B:432:GLU:HB2	1:B:607:GLN:HE21	1.59	0.66
1:B:640:ARG:HD3	1:B:643:TYR:HD2	1.61	0.66
1:A:411:HIS:CE1	1:A:413:THR:HG1	2.13	0.66
1:B:228:ALA:HB1	1:B:234:ARG:HH12	1.59	0.66
1:A:568:GLU:OE2	1:A:570:ARG:CZ	2.44	0.66
1:B:921:LEU:CD2	1:B:921:LEU:H	2.08	0.66
1:A:277:LEU:HD12	1:A:278:VAL:H	1.60	0.66
1:A:721:ASN:C	1:A:725:ILE:HD13	2.16	0.66
1:B:219:MSE:HE2	1:B:219:MSE:N	2.10	0.66
1:B:721:ASN:O	1:B:725:ILE:HD13	1.95	0.66
1:B:780:GLU:HB3	1:B:784:ILE:HD11	1.77	0.66
1:B:123:MSE:CE	1:B:961:ARG:HH22	2.02	0.66
1:A:438:LEU:HB2	1:A:613:LEU:HD23	1.78	0.66
1:A:383:GLU:N	1:A:384:PRO:HD3	2.11	0.66
1:B:399:ALA:HB3	1:B:400:ARG:CZ	2.26	0.66
1:B:227:PHE:HB3	1:B:253:ILE:HD12	1.76	0.66
1:B:235:TYR:C	1:B:239:GLN:HE21	1.98	0.66
1:B:524:ARG:O	1:B:528:GLY:HA2	1.96	0.66
1:A:98:ARG:HB2	1:A:101:PHE:CE1	2.30	0.66
1:B:175:LEU:N	1:B:175:LEU:HD12	2.10	0.66
1:B:190:ILE:N	1:B:190:ILE:HD12	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:TRP:HD1	1:B:494:LEU:HD12	1.59	0.66
1:B:620:VAL:HG23	1:B:621:LEU:N	2.09	0.66
1:A:686:ASP:OD1	1:A:688:LEU:HG	1.96	0.66
1:B:404:VAL:HA	1:B:407:LEU:HD22	1.78	0.66
1:A:9:TRP:NE1	1:A:52:ARG:HD3	2.11	0.66
1:A:73:GLU:HG2	1:A:84:ILE:HB	1.78	0.66
1:A:72:GLU:CG	1:A:85:GLY:HA2	2.26	0.66
1:A:729:ASN:ND2	1:A:741:THR:O	2.29	0.65
1:A:123:MSE:CB	1:A:865:LEU:HD13	2.26	0.65
1:B:379:GLU:O	1:B:381:ASP:N	2.29	0.65
1:A:748:VAL:HG13	1:A:749:PRO:HD2	1.77	0.65
1:B:759:ILE:HG13	1:B:760:THR:H	1.60	0.65
1:B:346:GLN:HE21	1:B:346:GLN:HA	1.60	0.65
1:B:714:ASN:H	1:B:714:ASN:HD22	1.44	0.65
1:A:185:ILE:HD12	1:A:185:ILE:H	1.62	0.65
1:A:761:ILE:HG12	1:A:774:ALA:HB3	1.77	0.65
1:B:722:LEU:HD21	1:B:726:ILE:HD11	1.77	0.65
1:B:427:GLY:CA	1:B:600:ILE:HG23	2.26	0.65
1:B:647:TYR:CE1	1:B:651:ILE:HD12	2.31	0.65
1:A:490:ARG:O	1:A:494:LEU:HD13	1.96	0.65
1:A:410:ARG:HH11	1:A:927:VAL:HA	1.60	0.65
1:B:686:ASP:OD1	1:B:689:LEU:HG	1.95	0.65
1:B:364:LYS:H	1:B:364:LYS:CD	2.02	0.65
1:A:722:LEU:C	1:A:722:LEU:HD22	2.16	0.65
1:B:465:ARG:CA	1:B:468:LEU:HD12	2.23	0.65
1:A:859:GLU:OE1	1:A:863:ARG:NH1	2.29	0.65
1:A:339:PHE:CZ	1:A:343:VAL:HG22	2.31	0.65
1:A:175:LEU:HD12	1:A:175:LEU:N	2.11	0.65
1:B:900:ARG:HG2	1:B:904:ASP:OD2	1.97	0.65
1:A:379:GLU:O	1:A:381:ASP:N	2.29	0.65
1:B:859:GLU:CG	1:B:863:ARG:HH12	2.08	0.65
1:A:530:ARG:HH11	1:A:555:THR:HB	1.62	0.65
1:A:344:GLU:OE1	1:A:347:LYS:HD3	1.96	0.65
1:A:404:VAL:HA	1:A:407:LEU:HD22	1.79	0.65
1:A:174:LEU:C	1:A:174:LEU:HD13	2.16	0.65
1:A:367:ASN:HB2	1:A:370:LEU:HD11	1.78	0.65
1:A:952:GLN:HE22	1:B:948:GLU:HB3	1.61	0.65
1:B:880:VAL:HG12	1:B:883:ASP:HB2	1.77	0.65
1:B:730:GLN:HG3	1:B:740:LEU:CD2	2.26	0.65
1:A:558:GLN:CD	1:A:559:VAL:H	1.99	0.65
1:B:24:ALA:HB3	1:B:31:THR:CB	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LEU:HA	1:A:225:LEU:N	2.12	0.65
1:B:775:GLN:NE2	1:B:776:PHE:HB2	2.10	0.65
1:B:815:LEU:HB3	1:B:844:LEU:HD22	1.77	0.65
1:A:620:VAL:CG2	1:A:621:LEU:N	2.60	0.65
1:A:24:ALA:HB3	1:A:31:THR:CB	2.27	0.65
1:A:614:GLU:OE1	1:A:615:LYS:HE3	1.97	0.65
1:A:194:GLN:HG3	1:A:200:ALA:CB	2.27	0.65
1:B:214:GLN:O	1:B:217:VAL:HG12	1.97	0.65
1:A:647:TYR:CE1	1:A:651:ILE:HD12	2.32	0.65
1:B:293:SER:HB3	1:B:296:TYR:HB3	1.79	0.65
1:B:367:ASN:HB2	1:B:370:LEU:HD11	1.79	0.65
1:B:597:LEU:HD23	1:B:602:GLN:NE2	2.11	0.65
1:B:440:LEU:H	1:B:440:LEU:CD1	2.08	0.65
1:B:735:ASP:OD1	1:B:736:ASN:N	2.30	0.65
1:A:759:ILE:HG13	1:A:760:THR:H	1.62	0.65
1:A:722:LEU:CD2	1:A:726:ILE:HD11	2.27	0.65
1:B:775:GLN:NE2	1:B:776:PHE:N	2.44	0.65
1:B:837:PRO:CB	1:B:838:PRO:HD2	2.22	0.65
1:B:620:VAL:CG2	1:B:621:LEU:N	2.60	0.65
1:A:329:ARG:O	1:A:333:PRO:HG3	1.97	0.65
1:B:151:ARG:HH21	1:B:771:ARG:N	1.85	0.64
1:B:194:GLN:HG3	1:B:200:ALA:HB3	1.79	0.64
1:B:324:HIS:O	1:B:327:ARG:NH1	2.30	0.64
1:B:133:ARG:CZ	1:B:788:LEU:HB3	2.27	0.64
1:A:440:LEU:N	1:A:440:LEU:HD13	2.12	0.64
1:B:329:ARG:O	1:B:333:PRO:HG3	1.97	0.64
1:A:586:ASN:ND2	1:A:588:ASP:HB2	2.08	0.64
1:A:52:ARG:NH1	1:A:53:VAL:O	2.30	0.64
1:B:730:GLN:HG3	1:B:740:LEU:HD21	1.79	0.64
1:B:311:LEU:N	1:B:311:LEU:HD23	2.13	0.64
1:A:443:GLN:O	1:A:446:THR:OG1	2.15	0.64
1:A:339:PHE:CE1	1:A:343:VAL:HG22	2.31	0.64
1:A:207:VAL:CG2	1:A:211:LEU:HB2	2.27	0.64
1:A:190:ILE:O	1:A:193:GLN:HG2	1.96	0.64
1:A:28:ARG:NH1	1:A:240:HIS:ND1	2.42	0.64
1:B:122:ARG:N	1:B:122:ARG:HE	1.89	0.64
1:B:207:VAL:CG2	1:B:211:LEU:HB2	2.28	0.64
1:B:386:LEU:HD23	1:B:386:LEU:C	2.17	0.64
1:A:129:ARG:NH2	1:A:791:ILE:HA	2.13	0.64
1:A:173:VAL:CA	1:A:416:VAL:HG13	2.23	0.64
1:A:722:LEU:HD21	1:A:726:ILE:HD11	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:LEU:C	1:A:845:LEU:HD23	2.18	0.64
1:A:380:GLN:HG3	1:A:384:PRO:HD3	1.78	0.64
1:B:383:GLU:O	1:B:387:GLN:HB2	1.98	0.64
1:B:298:ALA:O	1:B:302:LEU:HG	1.97	0.64
1:A:682:GLU:O	1:A:687:ARG:NH2	2.30	0.64
1:A:841:VAL:HG13	1:A:841:VAL:O	1.98	0.64
1:B:438:LEU:HB2	1:B:613:LEU:HD23	1.80	0.64
1:A:128:LEU:HD22	1:A:725:ILE:HG12	1.79	0.64
1:A:809:LEU:HD12	1:A:810:PRO:HD2	1.80	0.64
1:A:410:ARG:CD	1:A:927:VAL:HG13	2.26	0.64
1:A:219:MSE:N	1:A:219:MSE:HE2	2.11	0.64
1:A:816:VAL:O	1:A:844:LEU:HA	1.98	0.64
1:B:327:ARG:O	1:B:330:LEU:HD13	1.98	0.64
1:B:886:ALA:HA	1:B:889:GLN:CD	2.17	0.64
1:B:80:LEU:HG	1:B:99:GLU:OE2	1.98	0.64
1:A:340:ALA:C	1:A:343:VAL:HG23	2.17	0.64
1:A:345:GLU:O	1:A:349:TYR:N	2.30	0.64
1:B:872:THR:HG22	1:B:872:THR:O	1.98	0.64
1:A:129:ARG:NH1	1:A:791:ILE:O	2.31	0.64
1:B:176:ALA:HA	1:B:313:THR:HG23	1.80	0.64
1:B:279:VAL:O	1:B:311:LEU:HA	1.97	0.64
1:B:728:ILE:HG23	1:B:742:PRO:HA	1.79	0.64
1:A:399:ALA:CB	1:A:400:ARG:NH2	2.59	0.64
1:B:820:TYR:H	1:B:841:VAL:HG12	1.61	0.64
1:A:795:ASP:O	1:A:959:ALA:HA	1.98	0.64
1:A:726:ILE:HB	1:A:728:ILE:CD1	2.28	0.64
1:B:327:ARG:HA	1:B:330:LEU:HD13	1.79	0.64
1:B:582:ASP:HA	1:B:618:GLN:HE22	1.62	0.64
1:A:346:GLN:HE21	1:A:346:GLN:HA	1.62	0.64
1:B:686:ASP:OD1	1:B:688:LEU:HG	1.97	0.64
1:A:275:ASP:C	1:A:276:LEU:HD23	2.18	0.64
1:B:154:LEU:HD22	1:B:154:LEU:N	2.13	0.64
1:B:168:ARG:HH22	1:B:415:ARG:HD2	1.63	0.64
1:B:843:MSE:HE2	1:B:850:ASN:CG	2.19	0.64
1:B:453:ILE:H	1:B:453:ILE:CD1	2.10	0.64
1:B:519:LEU:HB2	1:B:560:LEU:HD13	1.80	0.64
1:A:386:LEU:C	1:A:386:LEU:HD23	2.18	0.64
1:B:174:LEU:HD13	1:B:174:LEU:C	2.17	0.63
1:B:650:LEU:HD13	1:B:650:LEU:C	2.19	0.63
1:A:835:PHE:CE2	1:A:910:ALA:HA	2.32	0.63
1:B:606:ILE:HD12	1:B:606:ILE:H	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLU:CG	1:A:554:ASP:H	2.04	0.63
1:B:340:ALA:C	1:B:343:VAL:HG23	2.17	0.63
1:B:880:VAL:HA	1:B:883:ASP:CG	2.18	0.63
1:A:168:ARG:HH22	1:A:415:ARG:HD2	1.63	0.63
1:A:900:ARG:HG2	1:A:904:ASP:OD2	1.98	0.63
1:B:190:ILE:CD1	1:B:190:ILE:H	2.11	0.63
1:B:172:ARG:HD3	1:B:307:PRO:O	1.98	0.63
1:A:669:ASN:O	1:A:672:GLU:HB2	1.99	0.63
1:A:154:LEU:N	1:A:154:LEU:HD22	2.13	0.63
1:A:640:ARG:HD3	1:A:643:TYR:HD2	1.63	0.63
1:A:772:GLU:OE2	1:A:778:THR:HG23	1.98	0.63
1:A:729:ASN:N	1:A:743:SER:HB2	2.13	0.63
1:A:799:SER:HB2	1:A:961:ARG:NE	2.13	0.63
1:B:151:ARG:HE	1:B:770:ALA:HA	1.63	0.63
1:A:620:VAL:HG21	1:A:654:LEU:CD2	2.29	0.63
1:B:620:VAL:HG21	1:B:654:LEU:CD2	2.29	0.63
1:A:599:ARG:NH1	1:A:599:ARG:CB	2.60	0.63
1:B:369:GLU:OE1	1:B:372:MSE:HG3	1.98	0.63
1:A:510:CYS:SG	1:A:562:CYS:HA	2.39	0.63
1:A:240:HIS:ND1	1:A:241:ASP:N	2.47	0.63
1:A:728:ILE:HG23	1:A:742:PRO:HA	1.80	0.63
1:B:495:MSE:SE	1:B:527:GLU:HG3	2.48	0.63
1:B:512:LYS:O	1:B:515:THR:HG22	1.98	0.63
1:A:918:LEU:HD13	1:A:918:LEU:C	2.19	0.63
1:A:151:ARG:HE	1:A:770:ALA:HA	1.63	0.63
1:B:570:ARG:NH1	1:B:570:ARG:HG3	2.14	0.63
1:B:124:ASP:HB2	1:B:125:ARG:NH2	2.13	0.63
1:B:325:PHE:HD2	1:B:342:PHE:HD2	1.47	0.63
1:B:446:THR:CA	1:B:449:LYS:HE2	2.27	0.63
1:B:380:GLN:HG3	1:B:384:PRO:HD3	1.80	0.63
1:A:714:ASN:HD22	1:A:714:ASN:H	1.47	0.63
1:A:799:SER:HB2	1:A:961:ARG:HE	1.63	0.63
1:A:818:LEU:HD12	1:A:818:LEU:N	2.14	0.63
1:B:490:ARG:O	1:B:494:LEU:HD13	1.99	0.63
1:A:293:SER:HB3	1:A:296:TYR:HB3	1.81	0.63
1:B:404:VAL:CA	1:B:407:LEU:HD22	2.28	0.63
1:A:952:GLN:NE2	1:B:948:GLU:CG	2.54	0.63
1:B:318:GLN:CA	1:B:318:GLN:HE21	2.11	0.63
1:A:777:ILE:HG13	1:A:778:THR:N	2.13	0.63
1:B:799:SER:HB2	1:B:961:ARG:NE	2.14	0.63
1:B:834:ARG:HG3	1:B:835:PHE:CD1	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:LEU:O	1:A:529:ILE:HD12	1.99	0.63
1:A:403:LEU:HA	1:A:406:MSE:HB2	1.80	0.63
1:A:580:MSE:HE1	1:A:593:ARG:CB	2.28	0.63
1:A:327:ARG:HA	1:A:330:LEU:HD13	1.80	0.62
1:A:726:ILE:HB	1:A:728:ILE:HD13	1.81	0.62
1:A:834:ARG:HG3	1:A:835:PHE:CD1	2.33	0.62
1:B:142:MSE:HB3	1:B:148:ARG:HH22	1.63	0.62
1:B:330:LEU:H	1:B:330:LEU:HD12	1.64	0.62
1:A:121:ASP:HA	1:A:122:ARG:HH21	1.63	0.62
1:A:318:GLN:CA	1:A:318:GLN:HE21	2.11	0.62
1:B:807:LYS:HB3	1:B:808:ALA:HA	1.81	0.62
1:B:176:ALA:O	1:B:177:ASP:C	2.38	0.62
1:B:722:LEU:CD2	1:B:726:ILE:HD11	2.28	0.62
1:B:644:ASP:C	1:B:646:VAL:H	2.01	0.62
1:B:552:GLU:HB3	1:B:555:THR:OG1	2.00	0.62
1:A:731:ASP:OD1	1:A:732:ASP:N	2.30	0.62
1:A:184:THR:OG1	1:A:185:ILE:HD12	1.99	0.62
1:B:220:LEU:C	1:B:224:ASN:HA	2.20	0.62
1:A:373:LEU:CD2	1:A:374:GLY:H	2.11	0.62
1:A:584:PRO:HD3	1:A:593:ARG:NH2	2.14	0.62
1:A:936:LEU:H	1:A:936:LEU:HD12	1.65	0.62
1:A:196:LEU:HD13	1:A:196:LEU:N	2.14	0.62
1:A:218:GLU:HB2	1:A:219:MSE:HE2	1.81	0.62
1:B:18:GLY:HA2	1:B:106:LEU:CD2	2.08	0.62
1:B:408:MSE:SE	1:B:692:HIS:HB3	2.50	0.62
1:A:807:LYS:HB3	1:A:808:ALA:HA	1.81	0.62
1:A:885:HIS:O	1:A:888:LEU:HB2	1.99	0.62
1:B:795:ASP:O	1:B:959:ALA:HA	2.00	0.62
1:B:586:ASN:HD22	1:B:589:LEU:CG	1.99	0.62
1:B:383:GLU:N	1:B:384:PRO:HD3	2.14	0.62
1:A:404:VAL:C	1:A:406:MSE:H	2.03	0.62
1:B:417:LEU:C	1:B:417:LEU:HD23	2.20	0.62
1:B:188:GLY:CA	1:B:223:PHE:CE2	2.78	0.62
1:B:523:LEU:O	1:B:529:ILE:HD12	2.00	0.62
1:B:570:ARG:HH11	1:B:570:ARG:HG3	1.65	0.62
1:A:356:VAL:HG21	1:A:688:LEU:HD22	1.82	0.62
1:A:465:ARG:CA	1:A:468:LEU:HD12	2.25	0.62
1:A:666:LEU:N	1:A:666:LEU:HD13	2.14	0.62
1:B:539:SER:HB3	1:B:542:GLU:CG	2.30	0.62
1:A:614:GLU:CD	1:A:615:LYS:HE3	2.20	0.62
1:B:843:MSE:HE1	1:B:894:GLN:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:HG3	1:A:612:TYR:OH	2.00	0.62
1:B:410:ARG:NH1	1:B:927:VAL:HA	2.14	0.62
1:A:516:ALA:HA	1:A:519:LEU:CD1	2.29	0.62
1:B:540:ILE:H	1:B:540:ILE:CD1	2.13	0.62
1:B:936:LEU:H	1:B:936:LEU:HD12	1.65	0.62
1:B:185:ILE:H	1:B:185:ILE:HD12	1.65	0.62
1:B:834:ARG:HG3	1:B:835:PHE:HD1	1.65	0.62
1:B:444:TYR:OH	1:B:490:ARG:NH2	2.33	0.62
1:A:371:ASN:O	1:A:375:GLU:HG3	2.00	0.62
1:B:121:ASP:HA	1:B:122:ARG:HH21	1.65	0.62
1:B:666:LEU:HD13	1:B:666:LEU:N	2.13	0.62
1:B:731:ASP:OD1	1:B:732:ASP:N	2.31	0.62
1:A:36:SER:HB3	1:A:104:SER:HB3	1.81	0.62
1:A:843:MSE:HE1	1:A:894:GLN:HG3	1.82	0.62
1:A:644:ASP:C	1:A:646:VAL:H	2.03	0.62
1:B:443:GLN:O	1:B:446:THR:OG1	2.17	0.62
1:A:860:THR:C	1:A:862:ASN:H	2.01	0.62
1:A:859:GLU:C	1:A:863:ARG:NH2	2.53	0.62
1:A:689:LEU:C	1:A:689:LEU:HD12	2.19	0.62
1:A:597:LEU:HD23	1:A:602:GLN:NE2	2.14	0.62
1:B:110:LYS:HB2	1:B:113:ASP:HB2	1.82	0.62
1:B:360:LEU:N	1:B:360:LEU:HD12	2.14	0.62
1:A:181:LEU:HD11	1:A:420:ASN:O	1.99	0.62
1:A:752:PRO:HB2	1:A:779:TRP:CD1	2.35	0.62
1:B:196:LEU:HD13	1:B:196:LEU:N	2.14	0.62
1:A:472:ARG:O	1:A:473:ILE:HD13	1.99	0.62
1:A:417:LEU:C	1:A:417:LEU:HD23	2.20	0.62
1:B:356:VAL:HG21	1:B:688:LEU:HD22	1.81	0.62
1:B:257:ASP:O	1:B:261:ARG:HG3	1.99	0.62
1:A:915:SER:HA	1:A:943:ARG:NH2	2.15	0.62
1:A:176:ALA:HB1	1:A:419:ARG:HB2	1.79	0.61
1:B:580:MSE:CE	1:B:593:ARG:HD2	2.30	0.61
1:B:860:THR:C	1:B:862:ASN:H	2.02	0.61
1:A:515:THR:OG1	1:A:519:LEU:HD11	1.98	0.61
1:B:702:LEU:HD22	1:B:702:LEU:N	2.15	0.61
1:A:574:PHE:CD1	1:A:574:PHE:N	2.68	0.61
1:B:182:GLY:O	1:B:186:GLU:HG3	1.99	0.61
1:B:176:ALA:HB3	1:B:419:ARG:HB2	1.81	0.61
1:B:397:GLN:HA	1:B:400:ARG:HB2	1.81	0.61
1:A:42:LEU:HD11	1:A:242:ALA:HB2	1.81	0.61
1:A:539:SER:HB3	1:A:542:GLU:CG	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:HIS:ND1	1:B:241:ASP:N	2.48	0.61
1:A:798:SER:HB3	1:A:962:LEU:HD21	1.81	0.61
1:B:783:LEU:HA	1:B:786:ASN:ND2	2.15	0.61
1:B:10:ILE:HD13	1:B:53:VAL:HG13	1.83	0.61
1:A:124:ASP:HB2	1:A:125:ARG:NH2	2.15	0.61
1:B:640:ARG:HA	1:B:643:TYR:HB3	1.83	0.61
1:B:355:ALA:O	1:B:359:LEU:HG	1.99	0.61
1:A:228:ALA:HB1	1:A:234:ARG:HH12	1.63	0.61
1:B:184:THR:OG1	1:B:185:ILE:HD12	1.99	0.61
1:B:173:VAL:CA	1:B:416:VAL:HG13	2.28	0.61
1:B:884:VAL:O	1:B:887:ILE:HB	2.01	0.61
1:B:126:PHE:HE2	1:B:961:ARG:HB2	1.64	0.61
1:B:446:THR:N	1:B:449:LYS:HE2	2.15	0.61
1:B:235:TYR:HB2	1:B:258:PHE:HZ	1.64	0.61
1:B:122:ARG:H	1:B:122:ARG:NE	1.89	0.61
1:B:244:ASN:HB3	1:B:245:PRO:HD3	1.81	0.61
1:A:766:GLU:HG3	1:A:773:ASP:OD2	1.98	0.61
1:A:123:MSE:CG	1:A:865:LEU:HD13	2.31	0.61
1:B:816:VAL:O	1:B:844:LEU:HA	2.00	0.61
1:B:962:LEU:HD22	1:B:962:LEU:O	2.01	0.61
1:A:948:GLU:HA	1:B:952:GLN:NE2	2.16	0.61
1:B:669:ASN:O	1:B:672:GLU:HB2	2.00	0.61
1:A:365:LEU:HD13	1:A:369:GLU:CG	2.30	0.61
1:A:169:HIS:C	1:A:171:PRO:HD3	2.21	0.61
1:A:775:GLN:HE22	1:A:776:PHE:CB	2.08	0.61
1:A:886:ALA:HA	1:A:889:GLN:CD	2.21	0.61
1:B:510:CYS:HB3	1:B:581:PHE:HD2	1.64	0.61
1:B:638:THR:HG22	1:B:677:LEU:HG	1.82	0.61
1:A:517:LEU:O	1:A:520:GLU:HB3	2.00	0.61
1:B:404:VAL:C	1:B:406:MSE:H	2.03	0.61
1:B:666:LEU:O	1:B:669:ASN:HB3	2.00	0.61
1:A:182:GLY:O	1:A:186:GLU:HG3	2.00	0.61
1:A:325:PHE:HD2	1:A:342:PHE:HD2	1.47	0.61
1:B:726:ILE:HB	1:B:728:ILE:HD13	1.83	0.61
1:A:579:VAL:HG22	1:A:609:HIS:O	2.01	0.61
1:A:355:ALA:O	1:A:359:LEU:HG	2.00	0.61
1:A:404:VAL:CG2	1:A:405:SER:N	2.64	0.61
1:A:510:CYS:HB3	1:A:581:PHE:HD2	1.66	0.61
1:A:894:GLN:HE22	1:A:897:LYS:HB2	1.66	0.61
1:B:178:GLU:HG3	1:B:422:ARG:HH22	1.65	0.61
1:B:472:ARG:O	1:B:473:ILE:HD13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:590:LEU:O	1:B:593:ARG:HB2	2.00	0.61
1:A:880:VAL:HA	1:A:883:ASP:CG	2.21	0.61
1:A:586:ASN:ND2	1:A:589:LEU:H	1.99	0.61
1:A:606:ILE:CD1	1:A:606:ILE:H	2.14	0.61
1:B:373:LEU:CD2	1:B:374:GLY:H	2.13	0.61
1:B:373:LEU:N	1:B:373:LEU:HD13	2.16	0.61
1:B:403:LEU:HA	1:B:406:MSE:HB2	1.83	0.61
1:A:820:TYR:H	1:A:841:VAL:CG1	2.14	0.61
1:A:185:ILE:HD12	1:A:185:ILE:N	2.15	0.61
1:A:848:ASN:HD21	1:A:851:ASN:ND2	1.98	0.61
1:A:296:TYR:CE2	1:A:297:GLN:HG2	2.36	0.61
1:A:582:ASP:HB3	1:A:593:ARG:HH22	1.64	0.61
1:B:274:TRP:O	1:B:307:PRO:HD2	2.01	0.61
1:B:161:ILE:HG23	1:B:165:VAL:CG2	2.31	0.61
1:A:421:THR:HA	1:A:422:ARG:NH1	2.16	0.60
1:B:421:THR:HA	1:B:422:ARG:NH1	2.16	0.60
1:B:722:LEU:O	1:B:725:ILE:HB	2.01	0.60
1:B:404:VAL:CG2	1:B:405:SER:N	2.64	0.60
1:A:161:ILE:HG23	1:A:165:VAL:CG2	2.31	0.60
1:A:168:ARG:NH2	1:A:415:ARG:HD2	2.16	0.60
1:A:126:PHE:CE2	1:A:961:ARG:HB2	2.36	0.60
1:A:851:ASN:ND2	1:A:851:ASN:N	2.45	0.60
1:B:139:GLN:HA	1:B:142:MSE:HG2	1.83	0.60
1:B:174:LEU:HD11	1:B:176:ALA:HB2	1.83	0.60
1:B:280:ASP:HB2	1:B:312:LEU:HD13	1.83	0.60
1:A:591:GLU:O	1:A:595:GLY:N	2.34	0.60
1:A:606:ILE:HD12	1:A:606:ILE:N	2.14	0.60
1:B:689:LEU:C	1:B:689:LEU:HD12	2.22	0.60
1:B:880:VAL:HA	1:B:883:ASP:OD1	2.02	0.60
1:A:880:VAL:HG12	1:A:883:ASP:HB2	1.83	0.60
1:B:371:ASN:O	1:B:375:GLU:HG3	2.02	0.60
1:B:663:PHE:CZ	1:B:667:ILE:HD11	2.36	0.60
1:A:833:ASN:CG	1:A:837:PRO:HB3	2.21	0.60
1:B:176:ALA:HA	1:B:313:THR:CG2	2.31	0.60
1:B:185:ILE:HD12	1:B:185:ILE:N	2.16	0.60
1:B:579:VAL:HG22	1:B:609:HIS:O	2.01	0.60
1:A:106:LEU:N	1:A:106:LEU:HD22	2.16	0.60
1:B:275:ASP:C	1:B:276:LEU:HD23	2.22	0.60
1:A:42:LEU:CD1	1:A:242:ALA:HB2	2.32	0.60
1:B:168:ARG:NH2	1:B:415:ARG:HD2	2.17	0.60
1:A:330:LEU:HD12	1:A:330:LEU:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:849:GLY:O	1:A:851:ASN:ND2	2.34	0.60
1:A:431:ARG:CB	1:A:633:GLU:HA	2.31	0.60
1:B:106:LEU:HD22	1:B:106:LEU:N	2.15	0.60
1:B:380:GLN:O	1:B:382:ILE:N	2.34	0.60
1:B:289:GLU:OE2	1:B:290:ASP:N	2.33	0.60
1:A:512:LYS:O	1:A:515:THR:HG22	2.00	0.60
1:A:516:ALA:HA	1:A:519:LEU:HD12	1.83	0.60
1:A:274:TRP:O	1:A:307:PRO:HD2	2.01	0.60
1:B:296:TYR:CE2	1:B:297:GLN:HG2	2.37	0.60
1:B:687:ARG:N	1:B:687:ARG:HD3	2.15	0.60
1:B:169:HIS:C	1:B:171:PRO:HD3	2.22	0.60
1:B:653:TYR:HD1	1:B:653:TYR:H	1.49	0.60
1:A:181:LEU:CD1	1:A:420:ASN:O	2.50	0.60
1:A:184:THR:CB	1:A:222:ARG:HH22	2.13	0.60
1:A:126:PHE:HE2	1:A:961:ARG:HB2	1.66	0.60
1:B:798:SER:HB3	1:B:962:LEU:HD21	1.82	0.60
1:B:914:LEU:HD12	1:B:914:LEU:N	2.17	0.60
1:B:469:TYR:OH	1:B:583:LEU:O	2.19	0.60
1:B:87:ARG:HD3	1:B:90:THR:OG1	2.01	0.60
1:B:155:ILE:HD12	1:B:155:ILE:H	1.66	0.60
1:A:365:LEU:HD13	1:A:369:GLU:HG3	1.83	0.60
1:B:874:SER:O	1:B:877:VAL:HG12	2.02	0.60
1:A:133:ARG:CZ	1:A:788:LEU:HB3	2.32	0.60
1:A:784:ILE:O	1:A:788:LEU:HG	2.02	0.60
1:A:816:VAL:HG11	1:A:884:VAL:CG1	2.32	0.60
1:B:769:LEU:HD13	1:B:771:ARG:HE	1.67	0.60
1:B:204:LEU:CD1	1:B:205:ILE:N	2.64	0.60
1:B:204:LEU:O	1:B:277:LEU:HD12	2.02	0.60
1:B:731:ASP:CG	1:B:732:ASP:N	2.54	0.60
1:A:875:LYS:O	1:A:876:LEU:HD23	2.02	0.60
1:A:810:PRO:C	1:A:812:GLY:H	2.05	0.60
1:A:444:TYR:OH	1:A:490:ARG:NH2	2.35	0.60
1:B:682:GLU:O	1:B:687:ARG:NH2	2.35	0.60
1:B:266:LEU:N	1:B:266:LEU:HD12	2.12	0.60
1:B:614:GLU:OE1	1:B:615:LYS:HE3	2.01	0.60
1:A:744:ASP:O	1:A:745:HIS:HB2	2.02	0.60
1:A:786:ASN:O	1:A:787:GLY:C	2.40	0.60
1:A:834:ARG:HG3	1:A:835:PHE:HD1	1.67	0.60
1:A:859:GLU:CG	1:A:863:ARG:HH12	2.14	0.60
1:A:834:ARG:NH2	1:A:913:LYS:HZ2	1.98	0.59
1:B:133:ARG:NH2	1:B:788:LEU:CB	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:ILE:HB	1:B:728:ILE:CD1	2.32	0.59
1:B:816:VAL:HG11	1:B:884:VAL:CG1	2.31	0.59
1:B:835:PHE:CE2	1:B:910:ALA:HA	2.37	0.59
1:A:380:GLN:O	1:A:382:ILE:N	2.35	0.59
1:B:516:ALA:HA	1:B:519:LEU:CD1	2.32	0.59
1:B:270:CYS:SG	1:B:305:HIS:HB2	2.41	0.59
1:A:527:GLU:HB3	1:A:529:ILE:HD11	1.84	0.59
1:B:126:PHE:CE2	1:B:961:ARG:HB2	2.36	0.59
1:B:357:ALA:C	1:B:359:LEU:H	2.06	0.59
1:A:161:ILE:CD1	1:A:161:ILE:H	2.15	0.59
1:A:440:LEU:H	1:A:440:LEU:HD13	1.67	0.59
1:B:875:LYS:O	1:B:876:LEU:HD23	2.02	0.59
1:A:279:VAL:O	1:A:311:LEU:HA	2.02	0.59
1:A:769:LEU:O	1:A:769:LEU:HD12	2.02	0.59
1:B:328:LEU:N	1:B:328:LEU:HD22	2.16	0.59
1:B:98:ARG:HB2	1:B:101:PHE:CD1	2.38	0.59
1:B:228:ALA:C	1:B:253:ILE:HD11	2.22	0.59
1:A:640:ARG:HA	1:A:643:TYR:HB3	1.85	0.59
1:A:178:GLU:HG2	1:A:419:ARG:NH1	2.17	0.59
1:A:688:LEU:CD2	1:A:688:LEU:H	2.13	0.59
1:B:614:GLU:CD	1:B:615:LYS:HE3	2.23	0.59
1:A:783:LEU:HA	1:A:786:ASN:ND2	2.18	0.59
1:A:884:VAL:O	1:A:887:ILE:HB	2.02	0.59
1:B:784:ILE:O	1:B:788:LEU:HD21	2.03	0.59
1:B:364:LYS:N	1:B:364:LYS:HD2	2.11	0.59
1:B:218:GLU:HB2	1:B:219:MSE:HE2	1.84	0.59
1:A:428:PHE:CZ	1:A:600:ILE:HG13	2.36	0.59
1:A:109:SER:O	1:A:110:LYS:HB2	2.02	0.59
1:A:178:GLU:HG3	1:A:422:ARG:HH22	1.67	0.59
1:B:194:GLN:NE2	1:B:199:ALA:CB	2.64	0.59
1:B:284:HIS:ND1	1:B:285:LEU:N	2.50	0.59
1:B:884:VAL:O	1:B:887:ILE:N	2.36	0.59
1:B:822:VAL:CG2	1:B:822:VAL:O	2.44	0.59
1:A:620:VAL:HG21	1:A:654:LEU:HD21	1.85	0.59
1:B:586:ASN:OD1	1:B:587:PRO:CD	2.50	0.59
1:A:373:LEU:N	1:A:373:LEU:HD13	2.17	0.59
1:B:803:LEU:H	1:B:803:LEU:HD23	1.68	0.59
1:A:284:HIS:ND1	1:A:285:LEU:N	2.50	0.59
1:A:769:LEU:HD13	1:A:771:ARG:HE	1.68	0.59
1:A:586:ASN:HD21	1:A:588:ASP:CB	2.10	0.59
1:B:99:GLU:HG3	1:B:100:VAL:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:ARG:HD3	1:A:687:ARG:N	2.16	0.59
1:A:465:ARG:HA	1:A:468:LEU:CD1	2.28	0.59
1:A:735:ASP:OD1	1:A:736:ASN:N	2.36	0.59
1:A:327:ARG:O	1:A:330:LEU:HD13	2.02	0.59
1:A:779:TRP:C	1:A:782:PRO:HD2	2.22	0.59
1:B:722:LEU:C	1:B:722:LEU:HD22	2.21	0.59
1:A:383:GLU:O	1:A:387:GLN:HB2	2.03	0.59
1:B:620:VAL:HG21	1:B:654:LEU:HD21	1.85	0.59
1:A:404:VAL:CA	1:A:407:LEU:HD22	2.31	0.59
1:A:731:ASP:CG	1:A:732:ASP:N	2.56	0.59
1:A:816:VAL:HG21	1:A:887:ILE:HG21	1.83	0.58
1:B:495:MSE:HA	1:B:498:LEU:CD1	2.33	0.58
1:B:580:MSE:HE1	1:B:593:ARG:HB2	1.84	0.58
1:B:431:ARG:CB	1:B:633:GLU:HA	2.32	0.58
1:A:689:LEU:O	1:A:691:ILE:N	2.36	0.58
1:B:371:ASN:HD22	1:B:371:ASN:N	1.97	0.58
1:A:100:VAL:HG13	1:A:101:PHE:CD1	2.39	0.58
1:A:360:LEU:N	1:A:360:LEU:HD12	2.17	0.58
1:A:766:GLU:C	1:A:766:GLU:CD	2.61	0.58
1:A:815:LEU:HB3	1:A:844:LEU:HD22	1.84	0.58
1:A:914:LEU:N	1:A:914:LEU:HD12	2.18	0.58
1:B:784:ILE:O	1:B:788:LEU:HG	2.03	0.58
1:B:428:PHE:HD1	1:B:429:PRO:HD2	1.67	0.58
1:B:465:ARG:HA	1:B:468:LEU:CD1	2.27	0.58
1:B:515:THR:OG1	1:B:519:LEU:HD11	2.02	0.58
1:B:519:LEU:HB2	1:B:560:LEU:CD1	2.32	0.58
1:A:950:LEU:C	1:A:950:LEU:HD13	2.23	0.58
1:A:298:ALA:O	1:A:302:LEU:HG	2.03	0.58
1:B:841:VAL:HG13	1:B:841:VAL:O	2.04	0.58
1:B:173:VAL:CG1	1:B:416:VAL:HA	2.32	0.58
1:B:814:LEU:HD23	1:B:814:LEU:N	2.18	0.58
1:B:900:ARG:HA	1:B:903:ILE:HD12	1.86	0.58
1:B:380:GLN:NE2	1:B:382:ILE:HD12	2.17	0.58
1:A:289:GLU:OE2	1:A:290:ASP:N	2.35	0.58
1:A:428:PHE:HD1	1:A:429:PRO:HD2	1.68	0.58
1:A:400:ARG:NE	1:A:400:ARG:N	2.51	0.58
1:B:344:GLU:OE1	1:B:347:LYS:HD3	2.04	0.58
1:A:318:GLN:HA	1:A:318:GLN:HE21	1.69	0.58
1:B:392:ASP:O	1:B:393:SER:HB3	2.03	0.58
1:A:797:GLY:O	1:A:961:ARG:HA	2.03	0.58
1:B:313:THR:C	1:B:315:THR:N	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ARG:NH1	1:A:927:VAL:HA	2.17	0.58
1:A:590:LEU:O	1:A:590:LEU:HD23	2.03	0.58
1:A:202:ARG:HG2	1:A:202:ARG:NH1	2.18	0.58
1:B:440:LEU:N	1:B:440:LEU:HD13	2.18	0.58
1:A:145:SER:C	1:A:147:LEU:H	2.07	0.58
1:B:849:GLY:O	1:B:851:ASN:ND2	2.37	0.58
1:B:435:THR:HG22	1:B:610:VAL:HG21	1.85	0.58
1:B:527:GLU:HB3	1:B:529:ILE:HD11	1.86	0.58
1:A:856:VAL:O	1:A:860:THR:N	2.37	0.58
1:B:365:LEU:HD13	1:B:369:GLU:CG	2.33	0.58
1:A:99:GLU:HG3	1:A:100:VAL:N	2.18	0.58
1:B:880:VAL:HG13	1:B:883:ASP:CB	2.34	0.58
1:A:664:ASP:O	1:A:668:LYS:HG3	2.04	0.58
1:B:847:LYS:HA	1:B:890:LEU:HD13	1.84	0.58
1:A:900:ARG:HA	1:A:903:ILE:HD12	1.85	0.58
1:B:330:LEU:H	1:B:330:LEU:CD1	2.17	0.58
1:B:894:GLN:HE22	1:B:897:LYS:HB2	1.68	0.58
1:B:19:LEU:HB2	1:B:106:LEU:CD1	2.33	0.58
1:A:516:ALA:CA	1:A:519:LEU:HG	2.33	0.58
1:A:202:ARG:HB3	1:A:274:TRP:CE3	2.39	0.58
1:A:87:ARG:HD3	1:A:90:THR:OG1	2.04	0.58
1:A:96:ALA:C	1:A:97:LEU:HD12	2.24	0.58
1:A:154:LEU:HD12	1:A:706:ILE:HG21	1.86	0.58
1:A:440:LEU:CD1	1:A:440:LEU:N	2.65	0.58
1:B:729:ASN:N	1:B:729:ASN:HD22	2.00	0.58
1:B:752:PRO:HB2	1:B:779:TRP:CD1	2.38	0.58
1:B:834:ARG:NH2	1:B:913:LYS:HZ2	2.01	0.58
1:B:516:ALA:CA	1:B:519:LEU:HG	2.34	0.58
1:B:856:VAL:HA	1:B:859:GLU:HB2	1.85	0.58
1:A:856:VAL:HA	1:A:859:GLU:HB2	1.85	0.58
1:B:848:ASN:HD21	1:B:851:ASN:ND2	2.01	0.58
1:A:348:ASN:O	1:A:351:PRO:HD2	2.04	0.58
1:B:403:LEU:CD1	1:B:404:VAL:N	2.65	0.58
1:A:8:ARG:O	1:A:53:VAL:HG23	2.04	0.58
1:A:36:SER:CB	1:A:104:SER:HB3	2.34	0.58
1:A:173:VAL:HA	1:A:416:VAL:CG1	2.27	0.58
1:A:722:LEU:O	1:A:725:ILE:HB	2.04	0.58
1:B:816:VAL:HG21	1:B:887:ILE:HG21	1.85	0.58
1:B:387:GLN:CD	1:B:387:GLN:H	2.06	0.58
1:B:261:ARG:CB	1:B:265:ARG:HH21	2.14	0.58
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLN:NE2	1:A:113:ASP:OD1	2.37	0.58
1:B:184:THR:CB	1:B:222:ARG:HH22	2.14	0.57
1:B:784:ILE:O	1:B:786:ASN:N	2.37	0.57
1:A:433:LEU:CG	1:A:434:HIS:N	2.66	0.57
1:B:689:LEU:O	1:B:691:ILE:N	2.37	0.57
1:A:519:LEU:HB2	1:A:560:LEU:HD13	1.86	0.57
1:A:392:ASP:O	1:A:393:SER:HB3	2.03	0.57
1:A:822:VAL:O	1:A:822:VAL:CG2	2.51	0.57
1:A:586:ASN:OD1	1:A:587:PRO:CD	2.52	0.57
1:B:516:ALA:HA	1:B:519:LEU:HD12	1.86	0.57
1:A:859:GLU:C	1:A:863:ARG:CZ	2.73	0.57
1:A:590:LEU:O	1:A:593:ARG:HB2	2.04	0.57
1:A:540:ILE:CD1	1:A:540:ILE:H	2.17	0.57
1:A:440:LEU:HD22	1:A:440:LEU:C	2.23	0.57
1:B:146:GLY:HA2	1:B:196:LEU:HD23	1.85	0.57
1:B:151:ARG:HH22	1:B:771:ARG:C	2.07	0.57
1:B:801:ILE:CD1	1:B:814:LEU:HA	2.34	0.57
1:B:913:LYS:O	1:B:913:LYS:HD3	2.04	0.57
1:B:510:CYS:HG	1:B:562:CYS:CB	2.17	0.57
1:A:435:THR:HA	1:A:610:VAL:HG22	1.85	0.57
1:B:367:ASN:O	1:B:370:LEU:HG	2.05	0.57
1:A:9:TRP:HA	1:A:53:VAL:HG23	1.86	0.57
1:A:653:TYR:HD1	1:A:653:TYR:H	1.51	0.57
1:A:187:ALA:O	1:A:191:LEU:HD13	2.04	0.57
1:A:846:ASP:C	1:A:848:ASN:H	2.08	0.57
1:B:606:ILE:CG2	1:B:607:GLN:N	2.67	0.57
1:A:34:PHE:N	1:A:34:PHE:CD1	2.72	0.57
1:A:462:ASP:OD1	1:A:463:ARG:NE	2.37	0.57
1:A:128:LEU:HD21	1:A:722:LEU:HA	1.87	0.57
1:B:816:VAL:HG11	1:B:884:VAL:HG11	1.86	0.57
1:A:344:GLU:HA	1:A:347:LYS:CD	2.29	0.57
1:A:510:CYS:HB2	1:A:562:CYS:HG	1.70	0.57
1:B:173:VAL:HA	1:B:416:VAL:CG1	2.31	0.57
1:B:779:TRP:O	1:B:783:LEU:CG	2.48	0.57
1:B:814:LEU:HD12	1:B:884:VAL:HG22	1.87	0.57
1:B:591:GLU:O	1:B:595:GLY:N	2.37	0.57
1:A:139:GLN:HA	1:A:142:MSE:HG2	1.87	0.57
1:A:729:ASN:H	1:A:743:SER:CB	2.15	0.57
1:A:816:VAL:CG2	1:A:818:LEU:HD11	2.31	0.57
1:B:886:ALA:O	1:B:889:GLN:HG3	2.04	0.57
1:B:100:VAL:HG13	1:B:101:PHE:CD1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:HIS:HA	1:A:888:LEU:CD2	2.26	0.57
1:B:145:SER:C	1:B:147:LEU:H	2.08	0.57
1:B:194:GLN:HG3	1:B:200:ALA:CB	2.34	0.57
1:B:769:LEU:O	1:B:769:LEU:HD12	2.04	0.57
1:B:580:MSE:HE1	1:B:593:ARG:HD2	1.86	0.57
1:A:520:GLU:OE2	1:A:524:ARG:HB2	2.05	0.57
1:A:529:ILE:HD12	1:A:529:ILE:N	2.20	0.57
1:B:685:ARG:HB2	1:B:687:ARG:HE	1.68	0.57
1:A:459:SER:O	1:A:462:ASP:OD1	2.22	0.57
1:A:176:ALA:O	1:A:177:ASP:C	2.42	0.57
1:B:421:THR:C	1:B:422:ARG:HD3	2.25	0.57
1:B:799:SER:HB2	1:B:961:ARG:HE	1.70	0.57
1:A:380:GLN:NE2	1:A:382:ILE:CB	2.61	0.57
1:B:435:THR:HA	1:B:610:VAL:HG22	1.86	0.57
1:A:860:THR:N	1:A:863:ARG:NH2	2.52	0.57
1:B:202:ARG:HB3	1:B:274:TRP:CE3	2.40	0.57
1:A:266:LEU:HA	1:A:269:LEU:HD12	1.87	0.57
1:B:816:VAL:CG2	1:B:818:LEU:HD11	2.33	0.57
1:B:123:MSE:CB	1:B:865:LEU:HD13	2.35	0.57
1:B:587:PRO:HA	1:B:625:TYR:HE1	1.70	0.57
1:A:515:THR:CG2	1:A:562:CYS:SG	2.93	0.57
1:B:627:GLU:CA	1:B:671:ARG:NH1	2.67	0.57
1:A:921:LEU:HD22	1:A:921:LEU:N	2.18	0.57
1:A:830:LEU:HD22	1:A:830:LEU:N	2.20	0.57
1:B:462:ASP:OD1	1:B:463:ARG:NE	2.38	0.57
1:A:730:GLN:HG3	1:A:740:LEU:CD2	2.34	0.57
1:A:729:ASN:N	1:A:729:ASN:HD22	2.01	0.56
1:B:569:GLY:O	1:B:570:ARG:C	2.42	0.56
1:B:644:ASP:O	1:B:646:VAL:N	2.38	0.56
1:B:120:ILE:HD13	1:B:121:ASP:O	2.05	0.56
1:A:510:CYS:HG	1:A:562:CYS:HB2	1.70	0.56
1:A:582:ASP:O	1:A:593:ARG:NH1	2.38	0.56
1:B:574:PHE:CD1	1:B:574:PHE:N	2.69	0.56
1:A:880:VAL:HG13	1:A:883:ASP:HB2	1.86	0.56
1:B:520:GLU:OE2	1:B:524:ARG:HB2	2.05	0.56
1:B:803:LEU:HG	1:B:803:LEU:O	2.05	0.56
1:B:151:ARG:HH22	1:B:772:GLU:N	2.03	0.56
1:B:193:GLN:HA	1:B:196:LEU:CD2	2.35	0.56
1:B:791:ILE:O	1:B:791:ILE:HG22	2.05	0.56
1:B:400:ARG:NE	1:B:400:ARG:N	2.53	0.56
1:A:880:VAL:HA	1:A:883:ASP:OD1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ALA:O	1:A:419:ARG:NH2	2.38	0.56
1:A:188:GLY:O	1:A:191:LEU:HB2	2.06	0.56
1:A:246:PHE:O	1:A:248:THR:N	2.37	0.56
1:A:280:ASP:HB2	1:A:312:LEU:HD13	1.88	0.56
1:A:884:VAL:HA	1:A:887:ILE:HG13	1.87	0.56
1:B:285:LEU:HB2	1:B:314:ALA:CB	2.24	0.56
1:B:727:GLY:C	1:B:728:ILE:HD12	2.25	0.56
1:B:729:ASN:N	1:B:729:ASN:ND2	2.52	0.56
1:B:174:LEU:HD21	1:B:313:THR:HG23	1.86	0.56
1:B:759:ILE:HD11	1:B:773:ASP:C	2.26	0.56
1:A:387:GLN:H	1:A:387:GLN:CD	2.08	0.56
1:B:103:ASP:OD1	1:B:105:LYS:NZ	2.37	0.56
1:B:446:THR:O	1:B:450:VAL:HG23	2.04	0.56
1:A:454:MSE:SE	1:A:457:ARG:HH21	2.39	0.56
1:A:400:ARG:C	1:A:402:GLU:H	2.07	0.56
1:A:692:HIS:HD1	1:A:693:SER:N	2.03	0.56
1:A:827:PRO:O	1:A:830:LEU:HD23	2.05	0.56
1:B:827:PRO:O	1:B:830:LEU:HD23	2.04	0.56
1:B:440:LEU:CG	1:B:615:LYS:HD2	2.35	0.56
1:B:459:SER:O	1:B:462:ASP:OD1	2.22	0.56
1:B:170:ALA:HB3	1:B:932:ARG:HH12	1.69	0.56
1:A:194:GLN:NE2	1:A:199:ALA:CB	2.67	0.56
1:A:192:HIS:O	1:A:196:LEU:HD22	2.05	0.56
1:A:751:PHE:HB3	1:A:752:PRO:CD	2.35	0.56
1:B:6:GLY:O	1:B:99:GLU:HG3	2.05	0.56
1:B:515:THR:CG2	1:B:562:CYS:SG	2.93	0.56
1:B:417:LEU:O	1:B:417:LEU:HD23	2.06	0.56
1:B:260:ARG:O	1:B:261:ARG:C	2.44	0.56
1:A:730:GLN:HG3	1:A:740:LEU:HD21	1.87	0.56
1:A:151:ARG:HH22	1:A:772:GLU:N	2.03	0.56
1:A:759:ILE:HG13	1:A:760:THR:N	2.20	0.56
1:A:784:ILE:O	1:A:786:ASN:N	2.38	0.56
1:B:779:TRP:C	1:B:782:PRO:HD2	2.25	0.56
1:B:885:HIS:O	1:B:888:LEU:HB2	2.05	0.56
1:A:446:THR:HA	1:A:449:LYS:HE3	1.87	0.56
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.70	0.56
1:A:627:GLU:CA	1:A:671:ARG:NH1	2.66	0.56
1:A:185:ILE:CD1	1:A:185:ILE:H	2.18	0.56
1:A:146:GLY:HA2	1:A:196:LEU:HD23	1.86	0.56
1:B:729:ASN:H	1:B:743:SER:CB	2.16	0.56
1:B:780:GLU:HA	1:B:783:LEU:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:885:HIS:HA	1:B:888:LEU:CD2	2.28	0.56
1:B:140:PHE:HB3	1:B:837:PRO:HG3	1.87	0.56
1:A:587:PRO:HA	1:A:625:TYR:HE1	1.71	0.56
1:B:404:VAL:HG23	1:B:405:SER:H	1.69	0.56
1:A:510:CYS:HG	1:A:562:CYS:CB	2.19	0.56
1:B:318:GLN:HA	1:B:318:GLN:HE21	1.70	0.56
1:A:847:LYS:HA	1:A:890:LEU:HD13	1.87	0.56
1:A:816:VAL:C	1:A:844:LEU:HD23	2.25	0.56
1:A:848:ASN:ND2	1:A:851:ASN:HD21	2.03	0.56
1:B:792:LEU:HA	1:B:795:ASP:CB	2.30	0.56
1:B:510:CYS:SG	1:B:562:CYS:HA	2.45	0.56
1:A:435:THR:HG22	1:A:610:VAL:HG21	1.87	0.56
1:B:229:LEU:HA	1:B:253:ILE:CG1	2.26	0.56
1:B:950:LEU:C	1:B:950:LEU:HD13	2.25	0.56
1:A:510:CYS:SG	1:A:562:CYS:CA	2.94	0.56
1:A:141:ARG:CZ	1:A:836:LEU:HA	2.35	0.56
1:B:759:ILE:HG13	1:B:760:THR:N	2.21	0.56
1:A:403:LEU:CA	1:A:406:MSE:HB2	2.36	0.56
1:B:161:ILE:H	1:B:161:ILE:CD1	2.18	0.56
1:A:133:ARG:NH2	1:A:788:LEU:CB	2.69	0.56
1:A:784:ILE:O	1:A:788:LEU:HD21	2.06	0.56
1:B:816:VAL:C	1:B:844:LEU:HD23	2.25	0.56
1:B:485:TRP:N	1:B:485:TRP:CD1	2.72	0.56
1:B:606:ILE:HG22	1:B:607:GLN:N	2.20	0.56
1:B:616:THR:HG22	1:B:617:ALA:N	2.21	0.56
1:B:946:VAL:O	1:B:947:MSE:C	2.44	0.56
1:A:874:SER:O	1:A:877:VAL:HG12	2.06	0.56
1:B:766:GLU:CD	1:B:766:GLU:C	2.65	0.56
1:B:510:CYS:SG	1:B:562:CYS:CB	2.94	0.56
1:A:343:VAL:O	1:A:347:LYS:N	2.24	0.56
1:B:345:GLU:O	1:B:349:TYR:HB2	2.06	0.56
1:B:921:LEU:N	1:B:921:LEU:HD22	2.20	0.56
1:A:886:ALA:O	1:A:889:GLN:HG3	2.06	0.55
1:B:738:ILE:O	1:B:759:ILE:N	2.36	0.55
1:A:638:THR:HG22	1:A:677:LEU:HG	1.87	0.55
1:B:606:ILE:CD1	1:B:606:ILE:H	2.18	0.55
1:A:170:ALA:HB3	1:A:932:ARG:HH12	1.71	0.55
1:B:339:PHE:CZ	1:B:343:VAL:HG13	2.41	0.55
1:B:399:ALA:CB	1:B:400:ARG:NH2	2.63	0.55
1:B:216:LEU:HD11	1:B:229:LEU:HB2	1.88	0.55
1:B:96:ALA:C	1:B:97:LEU:HD12	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:MSE:CB	1:A:148:ARG:HH22	2.18	0.55
1:A:719:ALA:O	1:A:720:MSE:C	2.45	0.55
1:B:850:ASN:C	1:B:851:ASN:HD22	2.09	0.55
1:B:895:ILE:HG13	1:B:896:GLU:OE1	2.06	0.55
1:B:856:VAL:O	1:B:860:THR:N	2.38	0.55
1:A:98:ARG:HB2	1:A:101:PHE:CD1	2.40	0.55
1:B:155:ILE:N	1:B:155:ILE:HD12	2.21	0.55
1:B:825:GLN:O	1:B:826:ALA:HB2	2.06	0.55
1:A:244:ASN:HB3	1:A:245:PRO:HD3	1.88	0.55
1:A:205:ILE:HA	1:A:278:VAL:O	2.06	0.55
1:A:722:LEU:O	1:A:722:LEU:HD22	2.06	0.55
1:B:784:ILE:O	1:B:788:LEU:CG	2.53	0.55
1:B:606:ILE:N	1:B:606:ILE:HD12	2.21	0.55
1:A:407:LEU:N	1:A:407:LEU:HD13	2.22	0.55
1:A:468:LEU:HD11	1:A:585:PHE:CD1	2.40	0.55
1:B:440:LEU:HD22	1:B:440:LEU:C	2.26	0.55
1:A:260:ARG:O	1:A:261:ARG:C	2.45	0.55
1:B:192:HIS:O	1:B:196:LEU:HD22	2.07	0.55
1:B:105:LYS:H	1:B:105:LYS:CD	2.16	0.55
1:B:586:ASN:ND2	1:B:589:LEU:H	2.05	0.55
1:A:820:TYR:CE1	1:A:957:LEU:HB2	2.41	0.55
1:A:880:VAL:HG13	1:A:883:ASP:CB	2.36	0.55
1:A:218:GLU:O	1:A:221:ARG:N	2.40	0.55
1:A:330:LEU:H	1:A:330:LEU:CD1	2.18	0.55
1:A:173:VAL:CG1	1:A:416:VAL:HA	2.36	0.55
1:A:784:ILE:O	1:A:788:LEU:CG	2.53	0.55
1:A:719:ALA:HB1	1:A:723:PHE:HE2	1.72	0.55
1:A:729:ASN:N	1:A:729:ASN:ND2	2.54	0.55
1:B:897:LYS:CD	1:B:897:LYS:H	1.89	0.55
1:A:570:ARG:HG3	1:A:570:ARG:NH1	2.20	0.55
1:B:202:ARG:HG2	1:B:202:ARG:NH1	2.21	0.55
1:A:110:LYS:O	1:A:113:ASP:HB2	2.06	0.55
1:B:34:PHE:CD1	1:B:34:PHE:N	2.74	0.55
1:B:154:LEU:HD12	1:B:706:ILE:HG21	1.89	0.55
1:A:458:LYS:N	1:A:458:LYS:HD2	2.22	0.55
1:A:163:HIS:O	1:A:167:ARG:HB2	2.06	0.55
1:B:784:ILE:C	1:B:788:LEU:HD11	2.26	0.55
1:B:468:LEU:HD22	1:B:469:TYR:CE1	2.42	0.55
1:B:410:ARG:HA	1:B:927:VAL:CG1	2.36	0.55
1:B:72:GLU:HG3	1:B:85:GLY:CA	2.33	0.55
1:B:112:GLN:NE2	1:B:113:ASP:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:941:SER:O	1:B:945:GLN:HG2	2.07	0.55
1:A:196:LEU:H	1:A:196:LEU:HD22	1.71	0.55
1:A:895:ILE:HG13	1:A:896:GLU:OE1	2.06	0.55
1:B:330:LEU:N	1:B:330:LEU:CD1	2.69	0.55
1:B:141:ARG:CZ	1:B:836:LEU:HA	2.37	0.55
1:B:380:GLN:NE2	1:B:382:ILE:CB	2.60	0.55
1:B:382:ILE:O	1:B:385:LEU:HD13	2.07	0.55
1:B:548:ALA:O	1:B:552:GLU:HB2	2.07	0.55
1:A:417:LEU:HD21	1:A:689:LEU:HD13	1.88	0.55
1:A:929:PRO:O	1:A:931:ILE:HG12	2.06	0.55
1:B:402:GLU:O	1:B:406:MSE:HG2	2.07	0.55
1:A:580:MSE:CE	1:A:593:ARG:HD2	2.36	0.55
1:B:11:SER:HB3	1:B:14:GLU:O	2.07	0.55
1:A:315:THR:N	1:A:316:PRO:CD	2.70	0.55
1:A:784:ILE:C	1:A:788:LEU:HD11	2.27	0.55
1:A:814:LEU:HD12	1:A:884:VAL:HG22	1.89	0.55
1:B:327:ARG:HG3	1:B:327:ARG:NH1	2.21	0.55
1:B:810:PRO:C	1:B:812:GLY:H	2.09	0.55
1:A:382:ILE:N	1:A:384:PRO:HD2	2.22	0.55
1:A:432:GLU:CB	1:A:607:GLN:HE21	2.19	0.55
1:A:64:HIS:CE1	1:A:101:PHE:HB3	2.42	0.55
1:A:515:THR:OG1	1:A:519:LEU:HD21	2.07	0.55
1:B:52:ARG:HG3	1:B:52:ARG:HH11	1.72	0.55
1:B:458:LYS:N	1:B:458:LYS:HD2	2.22	0.55
1:A:875:LYS:C	1:A:876:LEU:HD23	2.27	0.55
1:A:144:TYR:HB3	1:A:147:LEU:HD12	1.88	0.55
1:A:28:ARG:HD2	1:A:237:GLU:HB3	1.88	0.55
1:B:149:GLY:HA3	1:B:775:GLN:HG3	1.89	0.55
1:B:817:GLU:O	1:B:960:LEU:HG	2.07	0.55
1:B:797:GLY:O	1:B:961:ARG:HA	2.07	0.55
1:A:650:LEU:C	1:A:650:LEU:HD22	2.26	0.55
1:A:677:LEU:HD12	1:A:680:GLN:HB3	1.87	0.55
1:B:582:ASP:HB3	1:B:593:ARG:HH22	1.70	0.55
1:B:287:TRP:CZ3	1:B:292:PRO:HA	2.42	0.55
1:A:357:ALA:C	1:A:359:LEU:H	2.10	0.55
1:B:346:GLN:CA	1:B:346:GLN:HE21	2.15	0.55
1:B:689:LEU:C	1:B:691:ILE:N	2.59	0.55
1:B:880:VAL:HG13	1:B:883:ASP:HB2	1.87	0.55
1:B:11:SER:OG	1:B:14:GLU:HB2	2.06	0.55
1:B:163:HIS:O	1:B:167:ARG:HB2	2.06	0.55
1:A:789:ASP:C	1:A:791:ILE:HD12	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:VAL:HG11	1:A:884:VAL:HG11	1.89	0.55
1:B:751:PHE:HB3	1:B:752:PRO:CD	2.36	0.55
1:A:380:GLN:NE2	1:A:382:ILE:HD12	2.22	0.55
1:B:437:LYS:N	1:B:437:LYS:HD2	2.22	0.55
1:B:446:THR:HA	1:B:449:LYS:HE3	1.87	0.55
1:B:859:GLU:C	1:B:863:ARG:NH2	2.61	0.55
1:A:404:VAL:HG23	1:A:405:SER:H	1.72	0.55
1:B:120:ILE:C	1:B:120:ILE:CD1	2.74	0.55
1:A:466:ASP:HB2	1:A:467:MSE:SE	2.56	0.55
1:A:702:LEU:N	1:A:702:LEU:CD2	2.70	0.55
1:B:659:GLN:CD	1:B:660:THR:H	2.10	0.55
1:A:146:GLY:C	1:A:148:ARG:H	2.11	0.54
1:A:261:ARG:CB	1:A:265:ARG:HH21	2.18	0.54
1:A:141:ARG:NH2	1:A:839:THR:OG1	2.39	0.54
1:A:913:LYS:HD3	1:A:913:LYS:O	2.07	0.54
1:B:327:ARG:HH11	1:B:327:ARG:HG3	1.72	0.54
1:B:719:ALA:O	1:B:720:MSE:C	2.45	0.54
1:B:846:ASP:C	1:B:848:ASN:H	2.09	0.54
1:B:529:ILE:N	1:B:529:ILE:HD12	2.22	0.54
1:B:437:LYS:HG3	1:B:612:TYR:OH	2.07	0.54
1:A:428:PHE:CE1	1:A:600:ILE:HG13	2.42	0.54
1:A:371:ASN:HD22	1:A:371:ASN:N	2.02	0.54
1:A:371:ASN:HB3	1:A:375:GLU:CG	2.37	0.54
1:A:930:ASN:O	1:A:931:ILE:HG23	2.06	0.54
1:B:365:LEU:HD13	1:B:369:GLU:HG3	1.87	0.54
1:B:259:ALA:O	1:B:265:ARG:HB3	2.07	0.54
1:A:580:MSE:HE1	1:A:593:ARG:HD2	1.89	0.54
1:B:313:THR:O	1:B:315:THR:N	2.38	0.54
1:B:507:LEU:CA	1:B:558:GLN:HE22	2.09	0.54
1:A:520:GLU:OE2	1:A:524:ARG:HD3	2.08	0.54
1:B:404:VAL:CG2	1:B:405:SER:H	2.20	0.54
1:A:582:ASP:CA	1:A:618:GLN:HE22	2.19	0.54
1:A:803:LEU:O	1:A:803:LEU:HG	2.07	0.54
1:B:322:GLU:HA	1:B:324:HIS:NE2	2.22	0.54
1:A:354:ASP:O	1:A:358:MSE:HG2	2.08	0.54
1:A:210:THR:O	1:A:212:GLN:N	2.41	0.54
1:A:42:LEU:HD13	1:A:42:LEU:C	2.28	0.54
1:B:884:VAL:O	1:B:888:LEU:HD23	2.07	0.54
1:B:10:ILE:CD1	1:B:53:VAL:HG13	2.36	0.54
1:B:98:ARG:O	1:B:101:PHE:HD1	1.90	0.54
1:A:6:GLY:HA3	1:A:80:LEU:HD21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PHE:CE1	1:A:265:ARG:NH1	2.75	0.54
1:A:235:TYR:HB2	1:A:258:PHE:HZ	1.71	0.54
1:A:260:ARG:HD3	1:A:260:ARG:C	2.28	0.54
1:A:141:ARG:NH2	1:A:836:LEU:HG	2.23	0.54
1:A:837:PRO:CB	1:A:838:PRO:HD2	2.23	0.54
1:A:137:SER:HB2	1:A:838:PRO:O	2.08	0.54
1:B:219:MSE:O	1:B:224:ASN:N	2.41	0.54
1:B:174:LEU:HD23	1:B:313:THR:H	1.71	0.54
1:B:766:GLU:HG3	1:B:773:ASP:OD2	2.07	0.54
1:B:884:VAL:HA	1:B:887:ILE:HG13	1.90	0.54
1:A:485:TRP:CD1	1:A:485:TRP:N	2.74	0.54
1:A:401:GLN:C	1:A:404:VAL:HG22	2.27	0.54
1:B:236:ALA:CA	1:B:239:GLN:NE2	2.69	0.54
1:B:828:LYS:HA	1:B:832:LEU:CD2	2.38	0.54
1:B:830:LEU:HD22	1:B:830:LEU:N	2.21	0.54
1:B:415:ARG:HH11	1:B:415:ARG:HG3	1.73	0.54
1:A:762:THR:HG21	1:A:765:ARG:HB3	1.90	0.54
1:A:850:ASN:C	1:A:851:ASN:HD22	2.11	0.54
1:A:798:SER:O	1:A:865:LEU:HD12	2.08	0.54
1:B:186:GLU:HA	1:B:189:MSE:SE	2.58	0.54
1:B:192:HIS:O	1:B:195:LEU:HB2	2.07	0.54
1:B:817:GLU:C	1:B:818:LEU:HD12	2.28	0.54
1:B:629:LEU:HD12	1:B:629:LEU:H	1.68	0.54
1:A:98:ARG:O	1:A:101:PHE:HD1	1.91	0.54
1:A:161:ILE:N	1:A:161:ILE:HD12	2.20	0.54
1:A:176:ALA:N	1:A:418:PHE:O	2.41	0.54
1:A:177:ASP:O	1:A:183:LYS:HD3	2.08	0.54
1:A:327:ARG:HG3	1:A:327:ARG:NH1	2.22	0.54
1:B:146:GLY:C	1:B:148:ARG:H	2.11	0.54
1:B:798:SER:O	1:B:865:LEU:HD12	2.08	0.54
1:A:385:LEU:H	1:A:385:LEU:CD1	2.16	0.54
1:B:8:ARG:HA	1:B:20:GLY:O	2.08	0.54
1:B:472:ARG:O	1:B:472:ARG:HG2	2.08	0.54
1:B:467:MSE:HE2	1:B:655:ALA:O	2.08	0.54
1:A:495:MSE:HA	1:A:498:LEU:CD1	2.37	0.54
1:B:347:LYS:O	1:B:351:PRO:HD3	2.08	0.54
1:A:11:SER:OG	1:A:14:GLU:HB2	2.08	0.54
1:A:216:LEU:HD11	1:A:229:LEU:HB2	1.90	0.54
1:A:259:ALA:O	1:A:265:ARG:HB3	2.08	0.54
1:A:759:ILE:HD11	1:A:773:ASP:C	2.28	0.54
1:A:151:ARG:HH22	1:A:771:ARG:C	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:786:ASN:O	1:A:788:LEU:N	2.41	0.54
1:A:616:THR:HG22	1:A:617:ALA:N	2.23	0.54
1:A:125:ARG:CB	1:A:125:ARG:NH1	2.63	0.54
1:A:689:LEU:C	1:A:691:ILE:N	2.61	0.54
1:A:948:GLU:HA	1:B:952:GLN:HE22	1.73	0.54
1:A:663:PHE:CE1	1:A:667:ILE:HD11	2.43	0.54
1:A:110:LYS:HB3	1:A:112:GLN:OE1	2.08	0.54
1:B:744:ASP:O	1:B:745:HIS:HB2	2.07	0.54
1:A:789:ASP:O	1:A:791:ILE:HD12	2.08	0.54
1:A:801:ILE:CD1	1:A:814:LEU:HA	2.35	0.54
1:A:644:ASP:O	1:A:646:VAL:N	2.41	0.54
1:B:579:VAL:O	1:B:579:VAL:HG12	2.08	0.54
1:A:210:THR:C	1:A:212:GLN:H	2.11	0.54
1:A:8:ARG:NH2	1:A:19:LEU:HD13	2.23	0.54
1:A:11:SER:HB3	1:A:14:GLU:O	2.07	0.54
1:A:328:LEU:HD22	1:A:328:LEU:N	2.19	0.54
1:A:728:ILE:N	1:A:743:SER:HB3	2.23	0.54
1:B:403:LEU:CA	1:B:406:MSE:HB2	2.38	0.54
1:A:580:MSE:O	1:A:581:PHE:C	2.46	0.54
1:B:321:MSE:SE	1:B:321:MSE:O	2.76	0.54
1:B:729:ASN:N	1:B:743:SER:HB2	2.20	0.53
1:A:648:ASN:O	1:A:652:ASN:OD1	2.26	0.53
1:B:474:TYR:O	1:B:478:GLU:HB3	2.07	0.53
1:B:270:CYS:SG	1:B:302:LEU:HA	2.48	0.53
1:B:353:ALA:O	1:B:356:VAL:HB	2.08	0.53
1:B:365:LEU:HD23	1:B:366:SER:H	1.73	0.53
1:B:253:ILE:C	1:B:254:CYS:SG	2.87	0.53
1:A:155:ILE:H	1:A:155:ILE:HD12	1.73	0.53
1:B:440:LEU:CD1	1:B:440:LEU:N	2.70	0.53
1:B:392:ASP:O	1:B:395:ASP:OD2	2.25	0.53
1:A:185:ILE:O	1:A:189:MSE:HG3	2.06	0.53
1:A:285:LEU:HB2	1:A:314:ALA:CB	2.26	0.53
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.72	0.53
1:B:173:VAL:HG12	1:B:416:VAL:HG13	1.90	0.53
1:B:444:TYR:O	1:B:445:GLN:C	2.46	0.53
1:A:552:GLU:HG2	1:A:553:GLU:OE2	2.09	0.53
1:A:345:GLU:O	1:A:349:TYR:HB2	2.07	0.53
1:A:403:LEU:HA	1:A:406:MSE:CB	2.37	0.53
1:B:348:ASN:O	1:B:351:PRO:HD2	2.07	0.53
1:B:417:LEU:HD21	1:B:689:LEU:HD13	1.90	0.53
1:A:193:GLN:HA	1:A:196:LEU:CD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HA	1:A:837:PRO:CG	2.39	0.53
1:A:123:MSE:CE	1:A:961:ARG:HH22	2.06	0.53
1:B:123:MSE:CG	1:B:865:LEU:HD13	2.38	0.53
1:B:144:TYR:HB3	1:B:147:LEU:HD12	1.89	0.53
1:B:188:GLY:O	1:B:191:LEU:HB2	2.09	0.53
1:B:196:LEU:HD22	1:B:196:LEU:H	1.73	0.53
1:B:328:LEU:CD2	1:B:328:LEU:H	2.17	0.53
1:B:325:PHE:HD2	1:B:342:PHE:CD2	2.26	0.53
1:A:437:LYS:N	1:A:437:LYS:HD2	2.23	0.53
1:B:349:TYR:OH	1:B:411:HIS:HA	2.09	0.53
1:B:277:LEU:HD12	1:B:278:VAL:N	2.23	0.53
1:B:950:LEU:C	1:B:952:GLN:H	2.12	0.53
1:A:509:ILE:HA	1:A:561:LEU:O	2.07	0.53
1:A:962:LEU:HD22	1:A:962:LEU:O	2.08	0.53
1:B:775:GLN:C	1:B:777:ILE:H	2.12	0.53
1:A:446:THR:O	1:A:450:VAL:HG23	2.08	0.53
1:A:579:VAL:HG13	1:A:611:PRO:HD3	1.91	0.53
1:B:349:TYR:CE2	1:B:411:HIS:CE1	2.96	0.53
1:B:832:LEU:H	1:B:832:LEU:HD23	1.72	0.53
1:B:13:THR:O	1:B:13:THR:HG22	2.08	0.53
1:A:119:GLN:HB2	1:A:870:ARG:NH2	2.23	0.53
1:A:123:MSE:HG2	1:A:865:LEU:HD13	1.90	0.53
1:A:367:ASN:O	1:A:370:LEU:HG	2.09	0.53
1:A:403:LEU:O	1:A:406:MSE:N	2.41	0.53
1:A:465:ARG:HA	1:A:468:LEU:HB2	1.91	0.53
1:A:275:ASP:O	1:A:307:PRO:HG2	2.08	0.53
1:A:791:ILE:HG22	1:A:791:ILE:O	2.06	0.53
1:A:137:SER:O	1:A:141:ARG:HG3	2.09	0.53
1:B:148:ARG:N	1:B:150:GLN:HE22	2.06	0.53
1:B:178:GLU:HG2	1:B:419:ARG:NH1	2.23	0.53
1:B:187:ALA:O	1:B:191:LEU:HD13	2.09	0.53
1:B:519:LEU:HD23	1:B:519:LEU:N	2.23	0.53
1:B:859:GLU:C	1:B:863:ARG:CZ	2.77	0.53
1:A:482:ALA:O	1:A:483:THR:HB	2.09	0.53
1:A:685:ARG:HB2	1:A:687:ARG:HE	1.67	0.53
1:A:170:ALA:CB	1:A:932:ARG:HH12	2.20	0.53
1:B:918:LEU:HB2	1:B:939:ILE:HG21	1.90	0.53
1:B:947:MSE:O	1:B:950:LEU:HB3	2.08	0.53
1:A:519:LEU:N	1:A:519:LEU:HD23	2.23	0.53
1:B:540:ILE:HD12	1:B:540:ILE:N	2.19	0.53
1:B:170:ALA:CB	1:B:932:ARG:HH12	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:VAL:O	1:A:888:LEU:HD23	2.08	0.53
1:B:142:MSE:CB	1:B:148:ARG:HH22	2.21	0.53
1:B:762:THR:HG21	1:B:765:ARG:HB3	1.90	0.53
1:B:775:GLN:HE22	1:B:776:PHE:CB	2.15	0.53
1:A:638:THR:O	1:A:639:GLY:C	2.46	0.53
1:A:287:TRP:CZ3	1:A:292:PRO:HA	2.44	0.53
1:B:344:GLU:HA	1:B:347:LYS:CD	2.34	0.53
1:B:373:LEU:H	1:B:373:LEU:HD13	1.73	0.53
1:A:465:ARG:HG2	1:A:468:LEU:HD12	1.90	0.53
1:A:937:THR:HA	1:A:940:GLU:OE1	2.09	0.53
1:A:192:HIS:O	1:A:195:LEU:HB2	2.09	0.53
1:A:175:LEU:HD13	1:A:312:LEU:HA	1.91	0.53
1:B:185:ILE:CD1	1:B:185:ILE:H	2.20	0.53
1:B:128:LEU:HD21	1:B:722:LEU:HA	1.91	0.53
1:B:510:CYS:HG	1:B:562:CYS:HB2	1.74	0.53
1:A:339:PHE:CZ	1:A:343:VAL:HG13	2.43	0.53
1:A:400:ARG:O	1:A:403:LEU:CD1	2.55	0.53
1:A:8:ARG:HA	1:A:20:GLY:O	2.08	0.53
1:A:156:PRO:HA	1:A:159:LEU:HD12	1.89	0.53
1:A:34:PHE:CZ	1:A:41:ARG:HB2	2.43	0.53
1:A:877:VAL:CG1	1:A:878:ASN:H	2.19	0.53
1:B:820:TYR:H	1:B:841:VAL:CG1	2.21	0.53
1:A:659:GLN:CD	1:A:660:THR:H	2.12	0.53
1:B:833:ASN:O	1:B:837:PRO:HD3	2.08	0.53
1:A:650:LEU:HD13	1:A:651:ILE:CA	2.38	0.53
1:B:382:ILE:N	1:B:384:PRO:HD2	2.24	0.53
1:A:346:GLN:CA	1:A:346:GLN:HE21	2.17	0.53
1:A:404:VAL:CG2	1:A:405:SER:H	2.21	0.53
1:B:400:ARG:C	1:B:402:GLU:H	2.10	0.53
1:B:261:ARG:CB	1:B:265:ARG:NH2	2.71	0.53
1:B:73:GLU:HG3	1:B:84:ILE:HD12	1.89	0.53
1:A:504:GLN:NE2	1:A:504:GLN:H	2.07	0.53
1:A:253:ILE:O	1:A:254:CYS:SG	2.64	0.53
1:B:178:GLU:HG3	1:B:422:ARG:NH2	2.24	0.53
1:B:403:LEU:HA	1:B:406:MSE:CB	2.38	0.53
1:B:688:LEU:H	1:B:688:LEU:CD2	2.16	0.53
1:A:469:TYR:OH	1:A:583:LEU:O	2.25	0.53
1:B:33:LEU:O	1:B:35:PRO:HD3	2.09	0.53
1:A:775:GLN:C	1:A:777:ILE:H	2.13	0.52
1:A:140:PHE:HB3	1:A:837:PRO:HG3	1.91	0.52
1:A:843:MSE:HE2	1:A:850:ASN:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:MSE:HE2	1:B:850:ASN:CB	2.39	0.52
1:A:434:HIS:CD2	1:A:607:GLN:HE22	2.26	0.52
1:B:370:LEU:O	1:B:373:LEU:HD21	2.09	0.52
1:B:210:THR:C	1:B:212:GLN:H	2.12	0.52
1:B:210:THR:O	1:B:212:GLN:N	2.43	0.52
1:B:949:SER:HA	1:B:952:GLN:OE1	2.09	0.52
1:A:515:THR:C	1:A:519:LEU:HG	2.29	0.52
1:B:161:ILE:HD12	1:B:161:ILE:N	2.22	0.52
1:A:141:ARG:CZ	1:A:837:PRO:HD2	2.32	0.52
1:B:728:ILE:HG13	1:B:746:MSE:SE	2.59	0.52
1:B:677:LEU:HD12	1:B:680:GLN:HB3	1.90	0.52
1:B:287:TRP:CH2	1:B:289:GLU:HA	2.42	0.52
1:B:859:GLU:C	1:B:862:ASN:HB3	2.29	0.52
1:B:530:ARG:CD	1:B:549:TRP:HZ2	2.22	0.52
1:A:582:ASP:CA	1:A:618:GLN:NE2	2.71	0.52
1:A:627:GLU:C	1:A:671:ARG:HH11	2.13	0.52
1:B:735:ASP:O	1:B:737:MSE:N	2.42	0.52
1:A:791:ILE:O	1:A:795:ASP:HB2	2.10	0.52
1:A:727:GLY:C	1:A:728:ILE:HD12	2.30	0.52
1:B:434:HIS:CD2	1:B:607:GLN:HE22	2.27	0.52
1:B:585:PHE:N	1:B:585:PHE:CD1	2.77	0.52
1:A:606:ILE:CG2	1:A:607:GLN:N	2.71	0.52
1:A:859:GLU:C	1:A:862:ASN:HB3	2.29	0.52
1:A:99:GLU:CG	1:A:100:VAL:N	2.72	0.52
1:A:662:GLY:C	1:A:666:LEU:HD22	2.29	0.52
1:B:169:HIS:O	1:B:171:PRO:HD3	2.09	0.52
1:A:803:LEU:HD23	1:A:803:LEU:H	1.74	0.52
1:A:151:ARG:NE	1:A:770:ALA:HA	2.24	0.52
1:A:277:LEU:HD12	1:A:278:VAL:N	2.24	0.52
1:A:814:LEU:N	1:A:814:LEU:HD23	2.24	0.52
1:B:177:ASP:O	1:B:183:LYS:HD3	2.08	0.52
1:B:719:ALA:HB1	1:B:723:PHE:HE2	1.74	0.52
1:B:782:PRO:O	1:B:785:ARG:HB3	2.09	0.52
1:B:64:HIS:CE1	1:B:101:PHE:HB3	2.44	0.52
1:B:590:LEU:HD23	1:B:590:LEU:O	2.09	0.52
1:A:606:ILE:HG22	1:A:607:GLN:N	2.25	0.52
1:B:346:GLN:CA	1:B:349:TYR:HB2	2.38	0.52
1:A:510:CYS:CB	1:A:562:CYS:HG	2.22	0.52
1:B:266:LEU:H	1:B:266:LEU:CD1	2.14	0.52
1:B:44:ALA:O	1:B:48:SER:HB3	2.09	0.52
1:B:119:GLN:HB2	1:B:870:ARG:NH2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLY:HA3	1:A:775:GLN:HG3	1.91	0.52
1:A:884:VAL:HG12	1:A:888:LEU:CD2	2.39	0.52
1:B:315:THR:N	1:B:316:PRO:CD	2.72	0.52
1:B:721:ASN:O	1:B:722:LEU:C	2.48	0.52
1:A:382:ILE:O	1:A:385:LEU:HD13	2.09	0.52
1:B:428:PHE:CZ	1:B:600:ILE:HG13	2.45	0.52
1:B:692:HIS:HD1	1:B:693:SER:N	2.07	0.52
1:A:468:LEU:HD22	1:A:469:TYR:CE1	2.44	0.52
1:B:273:GLU:O	1:B:273:GLU:HG2	2.09	0.52
1:B:246:PHE:O	1:B:248:THR:N	2.40	0.52
1:A:275:ASP:O	1:A:276:LEU:HD23	2.08	0.52
1:B:34:PHE:CE1	1:B:41:ARG:HB2	2.45	0.52
1:B:728:ILE:N	1:B:743:SER:HB3	2.23	0.52
1:A:287:TRP:CH2	1:A:289:GLU:HA	2.42	0.52
1:A:495:MSE:HE1	1:A:523:LEU:CD2	2.39	0.52
1:B:918:LEU:HD13	1:B:919:SER:N	2.25	0.52
1:B:939:ILE:O	1:B:940:GLU:C	2.48	0.52
1:A:266:LEU:HD12	1:A:266:LEU:N	2.18	0.52
1:A:73:GLU:HG3	1:A:84:ILE:HD12	1.91	0.52
1:A:828:LYS:C	1:A:830:LEU:H	2.13	0.52
1:A:392:ASP:O	1:A:395:ASP:OD2	2.27	0.52
1:A:204:LEU:CD1	1:A:205:ILE:N	2.66	0.52
1:A:28:ARG:NH1	1:A:241:ASP:CG	2.57	0.52
1:A:313:THR:C	1:A:315:THR:N	2.61	0.52
1:B:123:MSE:HG2	1:B:865:LEU:HD13	1.92	0.52
1:B:137:SER:HA	1:B:837:PRO:CG	2.39	0.52
1:B:468:LEU:HD11	1:B:585:PHE:CD1	2.44	0.52
1:B:432:GLU:CB	1:B:607:GLN:HE21	2.20	0.52
1:B:646:VAL:HG23	1:B:647:TYR:N	2.24	0.52
1:A:859:GLU:O	1:A:863:ARG:CZ	2.58	0.52
1:B:407:LEU:N	1:B:407:LEU:HD13	2.25	0.52
1:A:832:LEU:H	1:A:832:LEU:HD23	1.73	0.52
1:A:220:LEU:C	1:A:224:ASN:HA	2.30	0.52
1:B:150:GLN:HB2	1:B:152:THR:HG22	1.91	0.52
1:B:786:ASN:O	1:B:787:GLY:C	2.47	0.52
1:A:629:LEU:H	1:A:629:LEU:HD12	1.73	0.52
1:A:474:TYR:O	1:A:478:GLU:HB3	2.10	0.52
1:A:530:ARG:CD	1:A:549:TRP:HZ2	2.23	0.52
1:A:114:ARG:CZ	1:A:117:ALA:CB	2.83	0.52
1:A:52:ARG:HH11	1:A:54:MSE:HG3	1.69	0.52
1:A:34:PHE:CE1	1:A:41:ARG:HB2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG22	1:A:13:THR:O	2.10	0.52
1:A:795:ASP:OD2	1:A:796:THR:HG23	2.10	0.52
1:B:848:ASN:ND2	1:B:851:ASN:HD21	2.08	0.52
1:A:648:ASN:HA	1:A:651:ILE:HG21	1.92	0.52
1:A:349:TYR:OH	1:A:411:HIS:HA	2.10	0.52
1:A:400:ARG:C	1:A:402:GLU:N	2.63	0.52
1:A:410:ARG:HA	1:A:927:VAL:CG1	2.39	0.52
1:B:403:LEU:O	1:B:407:LEU:CD2	2.55	0.52
1:B:205:ILE:HA	1:B:278:VAL:O	2.09	0.52
1:A:270:CYS:SG	1:A:302:LEU:HA	2.50	0.52
1:A:666:LEU:O	1:A:669:ASN:HB3	2.09	0.52
1:A:541:ILE:HD13	1:A:544:ASP:OD2	2.09	0.52
1:B:828:LYS:C	1:B:830:LEU:H	2.12	0.52
1:A:150:GLN:HB2	1:A:152:THR:HG22	1.91	0.52
1:B:629:LEU:O	1:B:630:ASP:C	2.49	0.52
1:B:205:ILE:HD11	1:B:227:PHE:CZ	2.44	0.52
1:B:875:LYS:C	1:B:876:LEU:HD23	2.30	0.52
1:A:653:TYR:CE2	1:A:660:THR:HB	2.45	0.52
1:A:884:VAL:O	1:A:887:ILE:N	2.40	0.51
1:B:313:THR:CB	1:B:316:PRO:HD2	2.25	0.51
1:B:644:ASP:C	1:B:646:VAL:N	2.64	0.51
1:A:353:ALA:O	1:A:356:VAL:HB	2.09	0.51
1:B:404:VAL:HA	1:B:407:LEU:CD2	2.40	0.51
1:B:235:TYR:O	1:B:238:ALA:HB3	2.11	0.51
1:A:230:PHE:CE1	1:A:234:ARG:HB3	2.45	0.51
1:B:784:ILE:O	1:B:788:LEU:CD2	2.58	0.51
1:A:558:GLN:NE2	1:A:559:VAL:O	2.40	0.51
1:B:4:THR:CG2	1:B:80:LEU:HD13	2.40	0.51
1:B:646:VAL:O	1:B:649:ASP:N	2.42	0.51
1:A:579:VAL:O	1:A:579:VAL:HG12	2.10	0.51
1:B:343:VAL:O	1:B:347:LYS:N	2.26	0.51
1:B:682:GLU:C	1:B:684:GLY:H	2.14	0.51
1:A:782:PRO:O	1:A:785:ARG:HB3	2.09	0.51
1:B:722:LEU:HD13	1:B:723:PHE:CA	2.40	0.51
1:B:892:GLU:HA	1:B:895:ILE:HD13	1.92	0.51
1:B:260:ARG:HD3	1:B:260:ARG:C	2.31	0.51
1:A:266:LEU:CD1	1:A:266:LEU:H	2.19	0.51
1:B:466:ASP:HB2	1:B:467:MSE:SE	2.61	0.51
1:B:648:ASN:HA	1:B:651:ILE:HG21	1.93	0.51
1:B:266:LEU:HA	1:B:269:LEU:HD12	1.92	0.51
1:A:426:LYS:O	1:A:426:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:LEU:HD13	1:B:722:LEU:C	2.30	0.51
1:B:515:THR:OG1	1:B:519:LEU:HD21	2.11	0.51
1:B:648:ASN:O	1:B:652:ASN:OD1	2.27	0.51
1:A:371:ASN:HB3	1:A:375:GLU:HG3	1.93	0.51
1:B:230:PHE:CE1	1:B:234:ARG:HB3	2.45	0.51
1:B:202:ARG:NH2	1:B:274:TRP:CH2	2.78	0.51
1:A:218:GLU:O	1:A:219:MSE:C	2.49	0.51
1:B:219:MSE:HE1	1:B:222:ARG:NH1	2.26	0.51
1:B:284:HIS:CG	1:B:285:LEU:H	2.28	0.51
1:A:647:TYR:HE1	1:A:651:ILE:HD12	1.75	0.51
1:A:507:LEU:CA	1:A:558:GLN:HE22	2.07	0.51
1:B:469:TYR:OH	1:B:584:PRO:HA	2.10	0.51
1:A:444:TYR:O	1:A:445:GLN:C	2.48	0.51
1:A:169:HIS:O	1:A:171:PRO:HD3	2.09	0.51
1:A:160:ASN:HD22	1:A:695:GLY:HA2	1.76	0.51
1:A:174:LEU:HD21	1:A:313:THR:HG23	1.91	0.51
1:A:324:HIS:HA	1:A:327:ARG:NH1	2.26	0.51
1:A:691:ILE:C	1:A:693:SER:N	2.59	0.51
1:B:277:LEU:HG	1:B:278:VAL:N	2.25	0.51
1:A:8:ARG:CZ	1:A:19:LEU:HD13	2.40	0.51
1:A:569:GLY:O	1:A:570:ARG:C	2.48	0.51
1:B:274:TRP:CA	1:B:274:TRP:CE3	2.88	0.51
1:B:34:PHE:CZ	1:B:41:ARG:HB2	2.45	0.51
1:B:154:LEU:HD22	1:B:154:LEU:H	1.72	0.51
1:B:877:VAL:CG1	1:B:878:ASN:H	2.20	0.51
1:B:160:ASN:HD22	1:B:695:GLY:HA2	1.75	0.51
1:A:175:LEU:CD2	1:A:312:LEU:HG	2.28	0.51
1:A:324:HIS:O	1:A:325:PHE:C	2.49	0.51
1:A:137:SER:CB	1:A:837:PRO:HG2	2.41	0.51
1:B:795:ASP:OD2	1:B:796:THR:HG23	2.11	0.51
1:B:885:HIS:O	1:B:889:GLN:HG2	2.10	0.51
1:B:99:GLU:CG	1:B:100:VAL:N	2.74	0.51
1:B:582:ASP:CA	1:B:618:GLN:HE22	2.23	0.51
1:A:610:VAL:HG23	1:A:610:VAL:O	2.10	0.51
1:A:856:VAL:O	1:A:863:ARG:NH2	2.44	0.51
1:A:371:ASN:O	1:A:375:GLU:CG	2.58	0.51
1:A:403:LEU:C	1:A:406:MSE:HB2	2.30	0.51
1:B:232:ASP:O	1:B:235:TYR:HB3	2.10	0.51
1:B:114:ARG:CZ	1:B:117:ALA:CB	2.83	0.51
1:A:8:ARG:HE	1:A:19:LEU:CD2	2.19	0.51
1:B:828:LYS:HA	1:B:832:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:LEU:H	1:B:440:LEU:HD13	1.73	0.51
1:A:325:PHE:HD2	1:A:342:PHE:CD2	2.28	0.51
1:A:834:ARG:HH22	1:A:913:LYS:NZ	2.09	0.51
1:A:884:VAL:HG22	1:A:887:ILE:HD12	1.92	0.51
1:A:897:LYS:CD	1:A:897:LYS:H	1.88	0.51
1:B:507:LEU:CA	1:B:558:GLN:NE2	2.72	0.51
1:B:433:LEU:CG	1:B:434:HIS:N	2.72	0.51
1:B:842:ARG:HH11	1:B:856:VAL:CG2	2.19	0.51
1:A:402:GLU:O	1:A:406:MSE:HG2	2.11	0.51
1:A:349:TYR:CE2	1:A:411:HIS:CE1	2.95	0.51
1:B:403:LEU:O	1:B:406:MSE:N	2.44	0.51
1:A:120:ILE:CD1	1:A:120:ILE:C	2.79	0.51
1:A:302:LEU:O	1:A:306:VAL:HG23	2.11	0.51
1:A:698:LYS:O	1:A:701:ALA:HB3	2.10	0.51
1:A:174:LEU:HD23	1:A:313:THR:H	1.75	0.51
1:B:151:ARG:NE	1:B:770:ALA:HA	2.26	0.51
1:B:915:SER:HA	1:B:943:ARG:NH2	2.26	0.51
1:B:586:ASN:OD1	1:B:588:ASP:OD1	2.29	0.51
1:B:650:LEU:HD13	1:B:651:ILE:CA	2.40	0.51
1:B:552:GLU:O	1:B:553:GLU:C	2.48	0.51
1:A:472:ARG:HG2	1:A:472:ARG:O	2.10	0.51
1:A:120:ILE:HD13	1:A:121:ASP:O	2.11	0.51
1:A:155:ILE:HD12	1:A:155:ILE:N	2.26	0.51
1:B:733:ARG:HD3	1:B:733:ARG:O	2.11	0.51
1:A:733:ARG:HD3	1:A:733:ARG:O	2.11	0.51
1:A:722:LEU:HD13	1:A:723:PHE:CA	2.41	0.50
1:B:176:ALA:O	1:B:419:ARG:CZ	2.59	0.50
1:B:136:SER:O	1:B:140:PHE:HB2	2.11	0.50
1:A:629:LEU:O	1:A:630:ASP:C	2.50	0.50
1:B:19:LEU:CA	1:B:106:LEU:HD11	2.42	0.50
1:B:475:GLN:HG2	1:B:476:GLU:N	2.26	0.50
1:B:860:THR:N	1:B:863:ARG:NH2	2.59	0.50
1:A:347:LYS:O	1:A:351:PRO:HD3	2.11	0.50
1:B:365:LEU:HD22	1:B:368:ASP:OD1	2.11	0.50
1:B:401:GLN:C	1:B:404:VAL:HG22	2.31	0.50
1:A:952:GLN:NE2	1:B:948:GLU:HA	2.27	0.50
1:A:590:LEU:C	1:A:590:LEU:HD23	2.31	0.50
1:A:467:MSE:HE2	1:A:655:ALA:O	2.11	0.50
1:B:520:GLU:OE2	1:B:524:ARG:HD3	2.11	0.50
1:A:239:GLN:O	1:A:243:TYR:HB3	2.11	0.50
1:A:325:PHE:O	1:A:326:ALA:C	2.48	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:VAL:HG12	1:A:416:VAL:HG13	1.93	0.50
1:B:833:ASN:C	1:B:835:PHE:H	2.15	0.50
1:B:7:GLN:HA	1:B:99:GLU:OE2	2.11	0.50
1:B:465:ARG:HA	1:B:468:LEU:HB2	1.93	0.50
1:B:582:ASP:O	1:B:593:ARG:NH1	2.45	0.50
1:A:519:LEU:HB2	1:A:560:LEU:CD1	2.42	0.50
1:B:275:ASP:O	1:B:276:LEU:HD23	2.11	0.50
1:B:110:LYS:O	1:B:113:ASP:HB2	2.10	0.50
1:B:708:GLU:C	1:B:710:ASP:N	2.61	0.50
1:A:939:ILE:O	1:A:940:GLU:C	2.49	0.50
1:A:735:ASP:O	1:A:737:MSE:N	2.45	0.50
1:A:126:PHE:C	1:A:128:LEU:H	2.14	0.50
1:B:715:LEU:HD23	1:B:715:LEU:C	2.32	0.50
1:B:141:ARG:CZ	1:B:837:PRO:HD2	2.36	0.50
1:B:650:LEU:HD22	1:B:650:LEU:C	2.31	0.50
1:B:400:ARG:C	1:B:402:GLU:N	2.65	0.50
1:B:244:ASN:CB	1:B:245:PRO:CD	2.87	0.50
1:A:369:GLU:CD	1:A:372:MSE:HG3	2.31	0.50
1:B:218:GLU:O	1:B:221:ARG:N	2.45	0.50
1:A:507:LEU:CA	1:A:558:GLN:NE2	2.71	0.50
1:B:493:TRP:CD1	1:B:611:PRO:HB3	2.47	0.50
1:A:427:GLY:HA3	1:A:600:ILE:CG2	2.42	0.50
1:A:552:GLU:O	1:A:553:GLU:C	2.49	0.50
1:A:683:GLN:HA	1:A:687:ARG:HH22	1.76	0.50
1:A:687:ARG:O	1:A:691:ILE:HG13	2.11	0.50
1:B:357:ALA:O	1:B:359:LEU:N	2.44	0.50
1:B:678:LYS:CG	1:B:679:ALA:N	2.75	0.50
1:B:234:ARG:HA	1:B:237:GLU:OE2	2.12	0.50
1:A:34:PHE:HD1	1:A:39:GLU:O	1.95	0.50
1:A:365:LEU:HD23	1:A:366:SER:H	1.76	0.50
1:A:700:GLN:NE2	1:A:700:GLN:O	2.44	0.50
1:B:11:SER:HB3	1:B:14:GLU:C	2.32	0.50
1:A:277:LEU:HG	1:A:278:VAL:N	2.25	0.50
1:A:136:SER:O	1:A:140:PHE:HB2	2.10	0.50
1:A:833:ASN:C	1:A:835:PHE:H	2.15	0.50
1:A:833:ASN:O	1:A:837:PRO:HD3	2.12	0.50
1:A:646:VAL:HG23	1:A:647:TYR:N	2.27	0.50
1:B:428:PHE:CD1	1:B:429:PRO:HD2	2.46	0.50
1:B:437:LYS:H	1:B:437:LYS:HD2	1.76	0.50
1:A:493:TRP:CD1	1:A:611:PRO:HB3	2.46	0.50
1:B:916:ALA:O	1:B:920:ARG:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:PHE:HD1	1:B:39:GLU:O	1.95	0.50
1:A:223:PHE:HB2	1:A:225:LEU:HG	1.93	0.50
1:A:248:THR:O	1:A:249:GLU:OE1	2.30	0.50
1:A:261:ARG:HD2	1:A:265:ARG:NH2	2.26	0.50
1:A:788:LEU:H	1:A:788:LEU:HD23	1.75	0.50
1:B:884:VAL:HG12	1:B:888:LEU:CD2	2.41	0.50
1:B:19:LEU:HB2	1:B:106:LEU:HD11	1.94	0.50
1:B:552:GLU:HG2	1:B:553:GLU:OE2	2.11	0.50
1:A:548:ALA:O	1:A:552:GLU:HB2	2.12	0.50
1:A:346:GLN:CA	1:A:349:TYR:HB2	2.41	0.50
1:A:105:LYS:CD	1:A:105:LYS:H	2.19	0.50
1:A:202:ARG:CZ	1:A:274:TRP:CZ3	2.95	0.50
1:A:154:LEU:H	1:A:154:LEU:HD22	1.74	0.50
1:B:832:LEU:N	1:B:832:LEU:HD23	2.27	0.50
1:A:281:GLU:OE1	1:A:314:ALA:HA	2.11	0.50
1:A:775:GLN:OE1	1:A:777:ILE:HG23	2.10	0.50
1:A:780:GLU:O	1:A:781:HIS:C	2.50	0.50
1:A:836:LEU:HD23	1:A:836:LEU:O	2.11	0.50
1:B:134:LYS:O	1:B:138:GLU:HB2	2.12	0.50
1:A:648:ASN:HA	1:A:651:ILE:CG2	2.41	0.50
1:B:466:ASP:C	1:B:468:LEU:H	2.14	0.50
1:A:289:GLU:HG3	1:A:290:ASP:OD1	2.12	0.50
1:B:371:ASN:O	1:B:375:GLU:CG	2.59	0.50
1:A:103:ASP:OD1	1:A:105:LYS:NZ	2.44	0.50
1:A:44:ALA:O	1:A:48:SER:HB3	2.12	0.50
1:A:469:TYR:OH	1:A:584:PRO:HA	2.11	0.50
1:A:568:GLU:O	1:A:596:ARG:NH2	2.45	0.50
1:B:426:LYS:HG2	1:B:426:LYS:O	2.12	0.50
1:A:229:LEU:HD12	1:A:253:ILE:O	2.12	0.50
1:B:219:MSE:O	1:B:225:LEU:N	2.42	0.50
1:B:778:THR:HG22	1:B:779:TRP:N	2.27	0.50
1:B:884:VAL:HG13	1:B:887:ILE:CD1	2.39	0.50
1:B:429:PRO:HB2	1:B:606:ILE:HD13	1.94	0.50
1:A:533:VAL:HG12	1:A:534:PHE:N	2.27	0.50
1:A:561:LEU:CD1	1:A:565:ILE:HG12	2.42	0.50
1:B:156:PRO:HA	1:B:159:LEU:HD12	1.93	0.50
1:B:42:LEU:C	1:B:42:LEU:HD13	2.31	0.50
1:A:72:GLU:HG3	1:A:85:GLY:CA	2.36	0.50
1:A:538:MSE:H	1:A:543:ARG:NH2	2.10	0.50
1:A:253:ILE:N	1:A:253:ILE:CD1	2.70	0.50
1:B:385:LEU:H	1:B:385:LEU:CD1	2.21	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PRO:HD3	1:A:599:ARG:O	2.12	0.50
1:B:403:LEU:O	1:B:407:LEU:N	2.45	0.50
1:A:678:LYS:CG	1:A:679:ALA:N	2.73	0.50
1:A:832:LEU:N	1:A:832:LEU:HD23	2.27	0.50
1:A:783:LEU:O	1:A:786:ASN:ND2	2.45	0.49
1:A:721:ASN:O	1:A:722:LEU:C	2.50	0.49
1:B:108:PHE:CZ	1:B:791:ILE:HD13	2.47	0.49
1:B:137:SER:HB2	1:B:838:PRO:O	2.11	0.49
1:A:586:ASN:OD1	1:A:587:PRO:HD2	2.12	0.49
1:A:635:THR:O	1:A:637:PRO:HD3	2.12	0.49
1:B:471:GLU:C	1:B:473:ILE:H	2.15	0.49
1:B:474:TYR:O	1:B:478:GLU:CB	2.60	0.49
1:A:453:ILE:C	1:A:455:GLY:H	2.14	0.49
1:A:403:LEU:O	1:A:407:LEU:CD2	2.57	0.49
1:B:371:ASN:HB3	1:B:375:GLU:CG	2.41	0.49
1:A:828:LYS:HA	1:A:832:LEU:CD2	2.42	0.49
1:B:820:TYR:CE1	1:B:957:LEU:HB2	2.47	0.49
1:A:33:LEU:O	1:A:35:PRO:HD3	2.11	0.49
1:A:204:LEU:O	1:A:277:LEU:HD12	2.12	0.49
1:A:313:THR:O	1:A:315:THR:N	2.42	0.49
1:A:775:GLN:NE2	1:A:776:PHE:CB	2.73	0.49
1:A:791:ILE:CG2	1:A:791:ILE:O	2.59	0.49
1:A:848:ASN:ND2	1:A:851:ASN:ND2	2.58	0.49
1:B:173:VAL:HG11	1:B:418:PHE:HE2	1.76	0.49
1:B:722:LEU:O	1:B:722:LEU:HD22	2.13	0.49
1:A:431:ARG:HH22	1:A:635:THR:CA	2.23	0.49
1:B:8:ARG:NH2	1:B:19:LEU:HD13	2.27	0.49
1:B:465:ARG:HG2	1:B:468:LEU:HD12	1.93	0.49
1:B:465:ARG:C	1:B:468:LEU:HB2	2.33	0.49
1:B:586:ASN:OD1	1:B:587:PRO:N	2.44	0.49
1:A:403:LEU:CD1	1:A:404:VAL:N	2.73	0.49
1:B:878:ASN:CG	1:B:878:ASN:O	2.50	0.49
1:B:829:GLN:O	1:B:829:GLN:HG2	2.13	0.49
1:A:218:GLU:CB	1:A:219:MSE:HE2	2.42	0.49
1:A:886:ALA:O	1:A:889:GLN:CG	2.60	0.49
1:B:332:ASP:OD1	1:B:335:ARG:N	2.39	0.49
1:B:141:ARG:NH2	1:B:839:THR:OG1	2.44	0.49
1:B:647:TYR:HE1	1:B:651:ILE:HD12	1.75	0.49
1:A:266:LEU:O	1:A:269:LEU:HB2	2.11	0.49
1:A:623:ARG:O	1:A:627:GLU:HB3	2.12	0.49
1:B:702:LEU:C	1:B:706:ILE:HD13	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:N	1:A:150:GLN:HE22	2.11	0.49
1:A:822:VAL:CG2	1:A:837:PRO:O	2.60	0.49
1:B:215:TRP:CD1	1:B:215:TRP:N	2.80	0.49
1:B:281:GLU:OE1	1:B:314:ALA:HA	2.11	0.49
1:B:140:PHE:HB3	1:B:833:ASN:OD1	2.12	0.49
1:A:646:VAL:O	1:A:649:ASP:N	2.44	0.49
1:B:596:ARG:HA	1:B:596:ARG:HH11	1.78	0.49
1:A:494:LEU:CD1	1:A:494:LEU:H	2.25	0.49
1:A:859:GLU:O	1:A:863:ARG:NH1	2.45	0.49
1:A:408:MSE:SE	1:A:692:HIS:HB3	2.63	0.49
1:B:685:ARG:NH2	1:B:687:ARG:HD2	2.27	0.49
1:B:691:ILE:C	1:B:693:SER:N	2.62	0.49
1:B:227:PHE:HB3	1:B:253:ILE:CD1	2.43	0.49
1:B:261:ARG:HD2	1:B:265:ARG:NH2	2.26	0.49
1:A:585:PHE:N	1:A:585:PHE:CD1	2.80	0.49
1:A:202:ARG:NH2	1:A:274:TRP:CH2	2.81	0.49
1:B:702:LEU:O	1:B:706:ILE:HB	2.12	0.49
1:B:168:ARG:CZ	1:B:415:ARG:CZ	2.90	0.49
1:A:960:LEU:HD23	1:A:960:LEU:C	2.31	0.49
1:B:780:GLU:O	1:B:781:HIS:C	2.50	0.49
1:B:137:SER:O	1:B:141:ARG:HG3	2.12	0.49
1:B:567:SER:O	1:B:568:GLU:C	2.50	0.49
1:B:580:MSE:O	1:B:581:PHE:C	2.50	0.49
1:A:530:ARG:CZ	1:A:549:TRP:HE1	2.25	0.49
1:A:8:ARG:NH2	1:A:19:LEU:HB3	2.20	0.49
1:A:155:ILE:CD1	1:A:158:GLN:HB2	2.33	0.49
1:B:623:ARG:O	1:B:627:GLU:HB3	2.13	0.49
1:B:539:SER:HB3	1:B:542:GLU:HG3	1.95	0.49
1:A:702:LEU:H	1:A:702:LEU:CD2	2.25	0.49
1:A:40:ASN:HD21	1:B:304:GLU:HG2	1.78	0.49
1:A:377:ILE:O	1:A:377:ILE:HG22	2.13	0.49
1:A:784:ILE:O	1:A:788:LEU:CD2	2.60	0.49
1:A:845:LEU:CD2	1:A:845:LEU:N	2.75	0.49
1:B:223:PHE:HB2	1:B:225:LEU:HG	1.93	0.49
1:B:716:ILE:H	1:B:716:ILE:CD1	2.05	0.49
1:B:775:GLN:OE1	1:B:777:ILE:HG23	2.12	0.49
1:B:106:LEU:N	1:B:106:LEU:HD13	2.28	0.49
1:B:646:VAL:O	1:B:647:TYR:C	2.50	0.49
1:B:530:ARG:CG	1:B:549:TRP:HZ2	2.25	0.49
1:B:235:TYR:HB2	1:B:258:PHE:CZ	2.47	0.49
1:B:114:ARG:NH1	1:B:117:ALA:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:950:LEU:C	1:A:952:GLN:H	2.14	0.49
1:B:907:ARG:HD2	1:B:950:LEU:CD1	2.42	0.49
1:A:9:TRP:CZ3	1:A:50:VAL:HG23	2.47	0.49
1:A:540:ILE:HD12	1:A:540:ILE:N	2.20	0.49
1:A:700:GLN:CA	1:A:700:GLN:HE21	2.26	0.49
1:A:702:LEU:C	1:A:704:GLU:N	2.66	0.49
1:A:702:LEU:C	1:A:706:ILE:HD13	2.32	0.49
1:B:735:ASP:C	1:B:737:MSE:N	2.65	0.49
1:A:244:ASN:HB3	1:A:245:PRO:HD2	1.94	0.49
1:B:777:ILE:O	1:B:780:GLU:HB2	2.12	0.49
1:B:960:LEU:C	1:B:960:LEU:HD23	2.32	0.49
1:A:437:LYS:HA	1:A:612:TYR:CE1	2.48	0.49
1:A:637:PRO:HG2	1:A:638:THR:N	2.25	0.49
1:B:599:ARG:CZ	1:B:599:ARG:CB	2.90	0.49
1:B:930:ASN:O	1:B:931:ILE:HG23	2.13	0.49
1:A:510:CYS:SG	1:A:562:CYS:HB2	2.51	0.49
1:A:873:GLY:C	1:A:875:LYS:H	2.16	0.49
1:A:390:ASN:OD1	1:A:391:SER:N	2.45	0.49
1:A:261:ARG:CB	1:A:265:ARG:NH2	2.74	0.49
1:A:175:LEU:O	1:A:313:THR:HG23	2.12	0.49
1:B:791:ILE:O	1:B:791:ILE:CG2	2.61	0.49
1:B:568:GLU:O	1:B:596:ARG:NH2	2.45	0.49
1:A:429:PRO:HB2	1:A:606:ILE:HD13	1.95	0.49
1:B:346:GLN:CA	1:B:346:GLN:NE2	2.75	0.49
1:B:266:LEU:O	1:B:269:LEU:HB2	2.12	0.49
1:B:702:LEU:CD2	1:B:702:LEU:N	2.75	0.49
1:A:941:SER:O	1:A:945:GLN:HG2	2.12	0.49
1:A:235:TYR:O	1:A:238:ALA:HB3	2.13	0.49
1:A:328:LEU:CD2	1:A:328:LEU:H	2.20	0.49
1:A:810:PRO:O	1:A:812:GLY:N	2.45	0.49
1:B:783:LEU:O	1:B:786:ASN:ND2	2.46	0.49
1:B:821:VAL:O	1:B:955:TRP:HA	2.13	0.49
1:B:475:GLN:HG2	1:B:476:GLU:H	1.78	0.49
1:A:52:ARG:HG3	1:A:54:MSE:SE	2.62	0.49
1:A:568:GLU:O	1:A:569:GLY:C	2.50	0.49
1:B:627:GLU:C	1:B:671:ARG:HH11	2.16	0.49
1:A:415:ARG:HG3	1:A:415:ARG:HH11	1.76	0.49
1:A:11:SER:HB3	1:A:14:GLU:C	2.33	0.49
1:A:178:GLU:HA	1:A:419:ARG:HH12	1.78	0.49
1:A:757:ASP:O	1:A:758:GLY:C	2.51	0.49
1:A:126:PHE:C	1:A:128:LEU:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:GLU:CB	1:B:219:MSE:HE2	2.43	0.49
1:B:834:ARG:HH22	1:B:913:LYS:NZ	2.11	0.49
1:A:644:ASP:C	1:A:646:VAL:N	2.65	0.49
1:A:381:ASP:C	1:A:384:PRO:HD2	2.33	0.49
1:B:523:LEU:CB	1:B:529:ILE:HD13	2.37	0.49
1:B:648:ASN:HA	1:B:651:ILE:CG2	2.43	0.49
1:B:937:THR:HA	1:B:940:GLU:OE1	2.12	0.49
1:A:950:LEU:HD13	1:A:951:ASP:N	2.27	0.49
1:A:465:ARG:C	1:A:468:LEU:HB2	2.34	0.49
1:A:567:SER:O	1:A:568:GLU:C	2.51	0.49
1:A:580:MSE:HE1	1:A:593:ARG:HB2	1.95	0.49
1:B:110:LYS:HB3	1:B:112:GLN:OE1	2.13	0.49
1:A:829:GLN:O	1:A:829:GLN:HG2	2.12	0.49
1:A:880:VAL:O	1:A:880:VAL:HG12	2.13	0.49
1:A:890:LEU:O	1:A:893:ALA:HB3	2.13	0.49
1:B:884:VAL:HG22	1:B:887:ILE:HD12	1.94	0.48
1:A:642:ILE:C	1:A:644:ASP:H	2.16	0.48
1:B:287:TRP:CZ3	1:B:292:PRO:CA	2.96	0.48
1:A:466:ASP:C	1:A:468:LEU:H	2.15	0.48
1:B:70:GLN:O	1:B:85:GLY:HA3	2.13	0.48
1:B:536:GLU:C	1:B:543:ARG:HH21	2.16	0.48
1:B:81:LEU:HD12	1:B:83:TYR:OH	2.13	0.48
1:A:145:SER:CA	1:A:148:ARG:HE	2.19	0.48
1:A:751:PHE:CB	1:A:752:PRO:CD	2.91	0.48
1:A:821:VAL:O	1:A:955:TRP:HA	2.13	0.48
1:B:174:LEU:HD22	1:B:175:LEU:C	2.33	0.48
1:B:192:HIS:CD2	1:B:196:LEU:HD21	2.49	0.48
1:B:292:PRO:HA	1:B:296:TYR:CE2	2.49	0.48
1:A:495:MSE:HE1	1:A:523:LEU:HD23	1.95	0.48
1:A:932:ARG:H	1:A:932:ARG:HG3	1.44	0.48
1:B:687:ARG:O	1:B:691:ILE:HG13	2.13	0.48
1:A:949:SER:HA	1:A:952:GLN:OE1	2.13	0.48
1:A:539:SER:HB3	1:A:542:GLU:HG3	1.95	0.48
1:B:390:ASN:OD1	1:B:391:SER:N	2.46	0.48
1:B:12:ASP:OD2	1:B:785:ARG:NH2	2.46	0.48
1:B:788:LEU:HD23	1:B:788:LEU:H	1.77	0.48
1:A:431:ARG:HH11	1:A:632:PHE:C	2.17	0.48
1:B:610:VAL:O	1:B:610:VAL:HG23	2.13	0.48
1:B:637:PRO:HG2	1:B:638:THR:N	2.26	0.48
1:A:373:LEU:HD13	1:A:373:LEU:H	1.76	0.48
1:B:700:GLN:HG3	1:B:701:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:GLN:C	1:A:700:GLN:NE2	2.67	0.48
1:A:284:HIS:CG	1:A:285:LEU:H	2.31	0.48
1:A:779:TRP:HA	1:A:779:TRP:CE3	2.48	0.48
1:B:123:MSE:CB	1:B:961:ARG:CZ	2.89	0.48
1:B:455:GLY:C	1:B:457:ARG:H	2.16	0.48
1:B:642:ILE:C	1:B:644:ASP:H	2.16	0.48
1:B:530:ARG:HH11	1:B:555:THR:CB	2.21	0.48
1:A:475:GLN:HG2	1:A:476:GLU:N	2.28	0.48
1:A:842:ARG:HH11	1:A:856:VAL:CG2	2.21	0.48
1:A:947:MSE:O	1:A:950:LEU:HB3	2.12	0.48
1:A:178:GLU:HG3	1:A:422:ARG:NH2	2.28	0.48
1:B:218:GLU:O	1:B:219:MSE:C	2.52	0.48
1:B:886:ALA:O	1:B:889:GLN:CG	2.62	0.48
1:A:511:ALA:O	1:A:563:SER:HA	2.13	0.48
1:A:728:ILE:HG23	1:A:742:PRO:CA	2.43	0.48
1:A:507:LEU:HD23	1:A:559:VAL:HG11	1.95	0.48
1:B:244:ASN:HB3	1:B:245:PRO:HD2	1.93	0.48
1:A:150:GLN:N	1:A:150:GLN:CD	2.67	0.48
1:A:174:LEU:C	1:A:174:LEU:HD22	2.34	0.48
1:A:137:SER:HA	1:A:837:PRO:HG3	1.95	0.48
1:B:475:GLN:HA	1:B:480:ASP:O	2.12	0.48
1:A:402:GLU:O	1:A:405:SER:OG	2.24	0.48
1:A:409:ASP:N	1:A:409:ASP:OD1	2.41	0.48
1:A:369:GLU:HA	1:A:372:MSE:HG3	1.96	0.48
1:B:751:PHE:CB	1:B:752:PRO:CD	2.92	0.48
1:B:895:ILE:HG13	1:B:955:TRP:CZ3	2.49	0.48
1:B:103:ASP:HB3	1:B:105:LYS:CE	2.43	0.48
1:B:431:ARG:HH22	1:B:635:THR:CA	2.21	0.48
1:B:515:THR:C	1:B:519:LEU:HG	2.33	0.48
1:B:533:VAL:HG12	1:B:534:PHE:N	2.29	0.48
1:B:429:PRO:HD3	1:B:599:ARG:O	2.14	0.48
1:B:381:ASP:C	1:B:384:PRO:HD2	2.34	0.48
1:A:474:TYR:O	1:A:478:GLU:CB	2.62	0.48
1:B:403:LEU:C	1:B:406:MSE:HB2	2.33	0.48
1:A:952:GLN:NE2	1:B:948:GLU:CB	2.68	0.48
1:A:81:LEU:HD12	1:A:83:TYR:OH	2.13	0.48
1:B:803:LEU:HD23	1:B:803:LEU:N	2.28	0.48
1:A:322:GLU:HG2	1:A:324:HIS:CD2	2.49	0.48
1:A:723:PHE:HA	1:A:726:ILE:HD12	1.95	0.48
1:B:315:THR:HA	1:B:317:GLU:OE2	2.14	0.48
1:B:324:HIS:O	1:B:325:PHE:C	2.52	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:ILE:HG23	1:B:742:PRO:CA	2.42	0.48
1:B:770:ALA:C	1:B:771:ARG:HG3	2.35	0.48
1:B:896:GLU:O	1:B:900:ARG:N	2.47	0.48
1:B:137:SER:HA	1:B:837:PRO:HG3	1.95	0.48
1:B:453:ILE:C	1:B:455:GLY:H	2.16	0.48
1:B:590:LEU:HD23	1:B:590:LEU:C	2.34	0.48
1:B:929:PRO:O	1:B:931:ILE:HG12	2.14	0.48
1:B:950:LEU:HD13	1:B:951:ASP:N	2.28	0.48
1:A:272:ALA:O	1:A:273:GLU:C	2.53	0.48
1:B:9:TRP:CZ3	1:B:50:VAL:HG23	2.49	0.48
1:B:880:VAL:O	1:B:880:VAL:HG12	2.14	0.48
1:A:735:ASP:C	1:A:737:MSE:N	2.67	0.48
1:B:77:GLU:O	1:B:78:ASN:HB2	2.14	0.48
1:B:435:THR:HA	1:B:610:VAL:HG23	1.93	0.48
1:A:367:ASN:HB2	1:A:370:LEU:CD1	2.43	0.48
1:B:356:VAL:HA	1:B:359:LEU:CD1	2.44	0.48
1:A:210:THR:C	1:A:212:GLN:N	2.68	0.48
1:A:110:LYS:HB3	1:A:112:GLN:CD	2.34	0.48
1:A:95:VAL:HG12	1:A:97:LEU:HD11	1.96	0.48
1:A:702:LEU:O	1:A:706:ILE:HB	2.14	0.48
1:B:73:GLU:CG	1:B:84:ILE:HB	2.43	0.48
1:B:386:LEU:O	1:B:389:ALA:N	2.42	0.48
1:A:227:PHE:HB3	1:A:253:ILE:CD1	2.42	0.47
1:A:232:ASP:O	1:A:235:TYR:HB3	2.13	0.47
1:A:311:LEU:N	1:A:311:LEU:CD2	2.74	0.47
1:A:321:MSE:SE	1:A:321:MSE:CG	3.12	0.47
1:A:738:ILE:O	1:A:759:ILE:N	2.37	0.47
1:B:324:HIS:HA	1:B:327:ARG:NH1	2.29	0.47
1:B:510:CYS:HB3	1:B:581:PHE:CD2	2.47	0.47
1:B:616:THR:HG22	1:B:617:ALA:H	1.78	0.47
1:B:431:ARG:NH2	1:B:635:THR:HA	2.24	0.47
1:A:428:PHE:CD1	1:A:429:PRO:HD2	2.47	0.47
1:A:445:GLN:C	1:A:449:LYS:HE2	2.33	0.47
1:B:403:LEU:HA	1:B:406:MSE:HG2	1.95	0.47
1:B:232:ASP:HA	1:B:258:PHE:CE1	2.48	0.47
1:B:208:PRO:O	1:B:209:GLU:C	2.52	0.47
1:B:700:GLN:C	1:B:700:GLN:NE2	2.67	0.47
1:A:825:GLN:O	1:A:826:ALA:HB2	2.13	0.47
1:A:440:LEU:CG	1:A:615:LYS:HD2	2.41	0.47
1:A:392:ASP:O	1:A:393:SER:CB	2.62	0.47
1:A:313:THR:HG21	1:A:419:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ARG:NH2	1:A:913:LYS:NZ	2.62	0.47
1:B:174:LEU:HD21	1:B:313:THR:CG2	2.43	0.47
1:B:762:THR:O	1:B:766:GLU:HB3	2.13	0.47
1:B:140:PHE:CD2	1:B:837:PRO:HB2	2.49	0.47
1:B:914:LEU:CD1	1:B:914:LEU:N	2.77	0.47
1:B:570:ARG:HH11	1:B:570:ARG:CG	2.26	0.47
1:B:549:TRP:HE1	1:B:555:THR:HB	1.79	0.47
1:A:358:MSE:O	1:A:359:LEU:HD23	2.14	0.47
1:B:367:ASN:HB2	1:B:370:LEU:CD1	2.44	0.47
1:A:509:ILE:HG21	1:A:593:ARG:HD3	1.95	0.47
1:B:125:ARG:NH1	1:B:125:ARG:CB	2.63	0.47
1:B:328:LEU:HB3	1:B:336:PHE:HE2	1.73	0.47
1:B:381:ASP:HA	1:B:384:PRO:HD2	1.96	0.47
1:B:245:PRO:C	1:B:246:PHE:CD1	2.88	0.47
1:A:300:GLU:O	1:A:302:LEU:N	2.47	0.47
1:B:700:GLN:O	1:B:700:GLN:NE2	2.47	0.47
1:B:541:ILE:HD13	1:B:544:ASP:OD2	2.14	0.47
1:B:827:PRO:HG2	1:B:830:LEU:HD21	1.94	0.47
1:B:803:LEU:C	1:B:805:LYS:H	2.15	0.47
1:B:392:ASP:O	1:B:393:SER:CB	2.62	0.47
1:B:504:GLN:NE2	1:B:504:GLN:H	2.13	0.47
1:B:511:ALA:O	1:B:563:SER:HA	2.14	0.47
1:A:193:GLN:CG	1:A:194:GLN:N	2.78	0.47
1:B:213:HIS:O	1:B:214:GLN:C	2.52	0.47
1:B:152:THR:O	1:B:763:PHE:CE1	2.67	0.47
1:B:509:ILE:HA	1:B:561:LEU:O	2.14	0.47
1:A:455:GLY:C	1:A:457:ARG:H	2.16	0.47
1:B:662:GLY:O	1:B:665:ASP:N	2.47	0.47
1:A:536:GLU:C	1:A:543:ARG:HH21	2.17	0.47
1:B:9:TRP:CH2	1:B:52:ARG:HB2	2.49	0.47
1:A:829:GLN:O	1:A:830:LEU:HD13	2.13	0.47
1:B:458:LYS:N	1:B:458:LYS:CD	2.77	0.47
1:A:896:GLU:HB3	1:A:900:ARG:NH2	2.29	0.47
1:B:786:ASN:O	1:B:788:LEU:N	2.48	0.47
1:B:884:VAL:O	1:B:887:ILE:CB	2.61	0.47
1:B:140:PHE:CB	1:B:837:PRO:HG3	2.44	0.47
1:A:646:VAL:O	1:A:647:TYR:C	2.53	0.47
1:B:442:THR:HA	1:B:445:GLN:HG3	1.97	0.47
1:B:516:ALA:HA	1:B:519:LEU:HG	1.96	0.47
1:B:592:GLN:O	1:B:593:ARG:C	2.53	0.47
1:B:289:GLU:HG3	1:B:290:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HG22	1:A:68:GLN:HG2	1.96	0.47
1:B:673:GLN:O	1:B:676:ALA:HB3	2.14	0.47
1:A:236:ALA:CA	1:A:239:GLN:NE2	2.71	0.47
1:A:719:ALA:O	1:A:722:LEU:HB3	2.15	0.47
1:B:176:ALA:HB3	1:B:418:PHE:C	2.35	0.47
1:A:437:LYS:H	1:A:437:LYS:HD2	1.79	0.47
1:A:558:GLN:NE2	1:A:559:VAL:N	2.57	0.47
1:B:561:LEU:CD1	1:B:565:ILE:HG12	2.44	0.47
1:B:580:MSE:SE	1:B:593:ARG:HD2	2.65	0.47
1:B:586:ASN:ND2	1:B:640:ARG:HH21	2.12	0.47
1:B:579:VAL:HG13	1:B:611:PRO:HD3	1.97	0.47
1:A:599:ARG:CB	1:A:599:ARG:CZ	2.92	0.47
1:B:670:CYS:C	1:B:672:GLU:N	2.68	0.47
1:A:678:LYS:HG3	1:A:679:ALA:H	1.77	0.47
1:B:698:LYS:O	1:B:701:ALA:HB3	2.14	0.47
1:B:827:PRO:O	1:B:830:LEU:CD2	2.62	0.47
1:A:803:LEU:C	1:A:805:LYS:H	2.17	0.47
1:A:256:LEU:HD13	1:A:256:LEU:H	1.80	0.47
1:A:816:VAL:HG11	1:A:884:VAL:HG13	1.97	0.47
1:B:126:PHE:C	1:B:128:LEU:N	2.68	0.47
1:B:728:ILE:C	1:B:729:ASN:HD22	2.18	0.47
1:B:848:ASN:ND2	1:B:851:ASN:ND2	2.61	0.47
1:B:311:LEU:HD11	1:B:327:ARG:HB3	1.96	0.47
1:B:314:ALA:CB	1:B:327:ARG:HE	2.24	0.47
1:B:507:LEU:HD23	1:B:559:VAL:HG11	1.96	0.47
1:B:8:ARG:NH2	1:B:19:LEU:HB3	2.22	0.47
1:B:64:HIS:ND1	1:B:64:HIS:N	2.63	0.47
1:B:8:ARG:HE	1:B:19:LEU:CD2	2.22	0.47
1:A:125:ARG:HG3	1:A:794:GLY:HA2	1.97	0.47
1:B:482:ALA:O	1:B:483:THR:HB	2.15	0.47
1:B:568:GLU:O	1:B:569:GLY:C	2.52	0.47
1:B:642:ILE:O	1:B:644:ASP:N	2.48	0.47
1:B:380:GLN:HE22	1:B:382:ILE:HD12	1.79	0.47
1:B:288:SER:O	1:B:291:ALA:HB3	2.15	0.47
1:A:442:THR:HA	1:A:445:GLN:HG3	1.97	0.47
1:A:471:GLU:C	1:A:473:ILE:H	2.17	0.47
1:A:494:LEU:N	1:A:494:LEU:HD12	2.29	0.47
1:B:549:TRP:NE1	1:B:555:THR:HB	2.29	0.47
1:B:925:ARG:HA	1:B:931:ILE:CD1	2.36	0.47
1:A:346:GLN:CA	1:A:346:GLN:NE2	2.77	0.47
1:A:400:ARG:O	1:A:402:GLU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:GLU:C	1:A:684:GLY:H	2.17	0.47
1:B:120:ILE:HD12	1:B:120:ILE:O	2.15	0.47
1:B:69:MSE:HG2	1:B:70:GLN:N	2.30	0.47
1:A:70:GLN:O	1:A:85:GLY:HA3	2.15	0.47
1:A:538:MSE:HG2	1:A:542:GLU:OE1	2.15	0.47
1:B:700:GLN:HE21	1:B:700:GLN:CA	2.28	0.47
1:B:829:GLN:O	1:B:830:LEU:HD13	2.13	0.47
1:B:873:GLY:C	1:B:875:LYS:H	2.18	0.47
1:A:151:ARG:HH21	1:A:771:ARG:N	1.91	0.47
1:A:175:LEU:CD1	1:A:175:LEU:H	2.25	0.47
1:A:184:THR:O	1:A:222:ARG:NH1	2.48	0.47
1:B:191:LEU:O	1:B:192:HIS:C	2.53	0.47
1:B:137:SER:CB	1:B:837:PRO:HG2	2.45	0.47
1:B:299:ILE:O	1:B:300:GLU:C	2.53	0.47
1:A:356:VAL:HA	1:A:359:LEU:CD1	2.45	0.47
1:B:253:ILE:CD1	1:B:253:ILE:N	2.69	0.47
1:A:580:MSE:HE1	1:A:593:ARG:HB3	1.97	0.47
1:A:274:TRP:CA	1:A:274:TRP:CE3	2.92	0.47
1:A:161:ILE:O	1:A:165:VAL:N	2.47	0.47
1:A:828:LYS:HA	1:A:832:LEU:HD21	1.96	0.47
1:B:800:THR:OG1	1:B:864:GLN:HB2	2.15	0.47
1:B:377:ILE:O	1:B:377:ILE:HG22	2.14	0.47
1:A:716:ILE:O	1:A:720:MSE:HG3	2.14	0.47
1:A:833:ASN:O	1:A:835:PHE:N	2.47	0.47
1:B:186:GLU:O	1:B:190:ILE:CD1	2.63	0.47
1:B:578:MSE:HE2	1:B:608:ILE:CD1	2.30	0.47
1:B:629:LEU:N	1:B:629:LEU:CD1	2.72	0.47
1:B:638:THR:O	1:B:639:GLY:C	2.52	0.47
1:A:370:LEU:O	1:A:373:LEU:HD21	2.15	0.47
1:A:907:ARG:HD2	1:A:950:LEU:CD1	2.45	0.47
1:A:467:MSE:N	1:A:467:MSE:SE	2.94	0.47
1:A:364:LYS:HD2	1:A:364:LYS:N	2.16	0.47
1:A:670:CYS:C	1:A:672:GLU:N	2.69	0.47
1:A:365:LEU:HD22	1:A:368:ASP:OD1	2.15	0.47
1:A:440:LEU:HD12	1:A:440:LEU:H	1.78	0.47
1:B:36:SER:OG	1:B:104:SER:HB3	2.14	0.47
1:A:895:ILE:HG13	1:A:955:TRP:CZ3	2.49	0.47
1:B:217:VAL:CG1	1:B:218:GLU:N	2.78	0.47
1:B:322:GLU:HG2	1:B:324:HIS:CD2	2.50	0.47
1:B:178:GLU:HA	1:B:419:ARG:HH12	1.79	0.47
1:B:834:ARG:NH2	1:B:913:LYS:NZ	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:LEU:HD23	1:B:836:LEU:O	2.15	0.47
1:B:10:ILE:HG12	1:B:53:VAL:HG22	1.96	0.47
1:B:635:THR:O	1:B:637:PRO:HD3	2.15	0.47
1:B:856:VAL:O	1:B:863:ARG:NH2	2.48	0.47
1:A:435:THR:HA	1:A:610:VAL:HG23	1.92	0.47
1:A:208:PRO:O	1:A:212:GLN:CG	2.60	0.47
1:A:946:VAL:O	1:A:947:MSE:C	2.51	0.47
1:A:519:LEU:H	1:A:519:LEU:HD23	1.80	0.47
1:A:386:LEU:O	1:A:389:ALA:N	2.45	0.47
1:B:125:ARG:HG3	1:B:794:GLY:HA2	1.97	0.46
1:A:637:PRO:CG	1:A:638:THR:H	2.27	0.46
1:B:519:LEU:HD23	1:B:519:LEU:H	1.80	0.46
1:B:530:ARG:CZ	1:B:549:TRP:HE1	2.28	0.46
1:A:523:LEU:CB	1:A:529:ILE:HD13	2.39	0.46
1:A:596:ARG:HH11	1:A:596:ARG:HA	1.80	0.46
1:B:708:GLU:N	1:B:710:ASP:OD1	2.48	0.46
1:B:539:SER:HB3	1:B:542:GLU:CB	2.45	0.46
1:B:168:ARG:NH2	1:B:415:ARG:CD	2.78	0.46
1:A:77:GLU:O	1:A:78:ASN:HB2	2.15	0.46
1:A:174:LEU:HD22	1:A:175:LEU:C	2.36	0.46
1:A:186:GLU:O	1:A:189:MSE:HB2	2.16	0.46
1:A:728:ILE:C	1:A:729:ASN:HD22	2.19	0.46
1:B:325:PHE:O	1:B:326:ALA:C	2.53	0.46
1:A:651:ILE:HA	1:A:654:LEU:HD12	1.97	0.46
1:B:565:ILE:HB	1:B:568:GLU:HB2	1.96	0.46
1:B:431:ARG:HH11	1:B:632:PHE:C	2.18	0.46
1:A:294:ARG:HB2	1:A:295:GLU:OE2	2.14	0.46
1:B:272:ALA:O	1:B:273:GLU:C	2.54	0.46
1:A:273:GLU:HG2	1:A:273:GLU:O	2.14	0.46
1:B:662:GLY:C	1:B:666:LEU:HD22	2.33	0.46
1:A:708:GLU:N	1:A:710:ASP:OD1	2.49	0.46
1:A:168:ARG:CZ	1:A:415:ARG:CZ	2.93	0.46
1:B:653:TYR:N	1:B:653:TYR:CD1	2.83	0.46
1:A:175:LEU:HD13	1:A:312:LEU:CA	2.45	0.46
1:A:174:LEU:CD2	1:A:313:THR:H	2.27	0.46
1:A:884:VAL:O	1:A:887:ILE:CB	2.63	0.46
1:A:816:VAL:HG21	1:A:887:ILE:CG2	2.45	0.46
1:A:495:MSE:SE	1:A:498:LEU:CD1	3.07	0.46
1:A:288:SER:O	1:A:291:ALA:HB3	2.15	0.46
1:A:892:GLU:HA	1:A:895:ILE:HD13	1.97	0.46
1:B:531:ALA:HA	1:B:558:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:THR:HG22	1:A:617:ALA:H	1.80	0.46
1:B:599:ARG:CZ	1:B:599:ARG:HB2	2.45	0.46
1:B:637:PRO:CG	1:B:638:THR:H	2.27	0.46
1:A:293:SER:H	1:A:297:GLN:HG3	1.81	0.46
1:A:403:LEU:O	1:A:406:MSE:CB	2.57	0.46
1:B:688:LEU:HD23	1:B:688:LEU:N	2.22	0.46
1:B:277:LEU:CG	1:B:278:VAL:N	2.79	0.46
1:A:52:ARG:NH1	1:A:52:ARG:HG3	2.31	0.46
1:A:727:GLY:O	1:A:743:SER:HB3	2.14	0.46
1:B:193:GLN:HA	1:B:196:LEU:HD23	1.98	0.46
1:B:335:ARG:C	1:B:336:PHE:CD1	2.88	0.46
1:B:898:SER:O	1:B:902:LEU:HG	2.15	0.46
1:B:833:ASN:O	1:B:835:PHE:N	2.49	0.46
1:B:822:VAL:CG1	1:B:839:THR:HB	2.46	0.46
1:A:381:ASP:CA	1:A:384:PRO:HD2	2.46	0.46
1:B:494:LEU:CD1	1:B:494:LEU:H	2.29	0.46
1:B:620:VAL:CG2	1:B:621:LEU:H	2.27	0.46
1:B:371:ASN:HB3	1:B:375:GLU:HG3	1.97	0.46
1:B:400:ARG:O	1:B:403:LEU:CD1	2.57	0.46
1:A:64:HIS:ND1	1:A:64:HIS:N	2.62	0.46
1:A:516:ALA:HA	1:A:519:LEU:HG	1.96	0.46
1:A:918:LEU:HB2	1:A:939:ILE:HG21	1.97	0.46
1:A:653:TYR:CD1	1:A:653:TYR:N	2.84	0.46
1:B:95:VAL:HG12	1:B:97:LEU:HD11	1.96	0.46
1:A:256:LEU:CD1	1:A:256:LEU:H	2.29	0.46
1:B:181:LEU:HD11	1:B:420:ASN:O	2.16	0.46
1:B:777:ILE:O	1:B:778:THR:C	2.52	0.46
1:A:381:ASP:HA	1:A:384:PRO:HD2	1.96	0.46
1:B:62:THR:HG22	1:B:68:GLN:HG2	1.98	0.46
1:A:287:TRP:CZ3	1:A:292:PRO:CA	2.99	0.46
1:B:539:SER:H	1:B:542:GLU:HB2	1.80	0.46
1:A:700:GLN:HG3	1:A:701:ALA:N	2.30	0.46
1:A:708:GLU:C	1:A:710:ASP:N	2.64	0.46
1:A:744:ASP:O	1:A:745:HIS:CB	2.64	0.46
1:B:754:LEU:HB3	1:B:755:SER:H	1.44	0.46
1:A:192:HIS:CD2	1:A:196:LEU:HD21	2.51	0.46
1:A:234:ARG:HA	1:A:237:GLU:OE2	2.15	0.46
1:A:239:GLN:HG3	1:A:239:GLN:H	1.56	0.46
1:B:910:ALA:O	1:B:914:LEU:HB2	2.15	0.46
1:A:636:CYS:HA	1:A:637:PRO:HD2	1.75	0.46
1:A:403:LEU:O	1:A:407:LEU:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ALA:O	1:B:358:MSE:N	2.49	0.46
1:B:210:THR:C	1:B:212:GLN:N	2.69	0.46
1:A:52:ARG:HH22	1:A:81:LEU:HG	1.77	0.46
1:A:583:LEU:HA	1:A:583:LEU:HD23	1.74	0.46
1:A:594:ILE:HG22	1:A:598:ASP:HB2	1.96	0.46
1:B:202:ARG:CZ	1:B:274:TRP:CZ3	2.99	0.46
1:B:828:LYS:O	1:B:830:LEU:N	2.49	0.46
1:A:846:ASP:C	1:A:848:ASN:N	2.69	0.46
1:B:311:LEU:N	1:B:311:LEU:CD2	2.78	0.46
1:B:888:LEU:O	1:B:891:GLY:N	2.48	0.46
1:B:381:ASP:CA	1:B:384:PRO:HD2	2.46	0.46
1:B:302:LEU:O	1:B:306:VAL:HG23	2.15	0.46
1:A:470:PRO:O	1:A:473:ILE:HB	2.16	0.46
1:A:434:HIS:O	1:A:609:HIS:HA	2.15	0.46
1:B:202:ARG:HD3	1:B:273:GLU:CG	2.44	0.46
1:A:539:SER:HB3	1:A:542:GLU:CB	2.46	0.46
1:B:702:LEU:C	1:B:704:GLU:N	2.69	0.46
1:B:708:GLU:O	1:B:710:ASP:N	2.48	0.46
1:B:52:ARG:HH11	1:B:54:MSE:HG3	1.76	0.46
1:B:440:LEU:HD11	1:B:615:LYS:NZ	2.30	0.46
1:A:119:GLN:HG3	1:A:870:ARG:HH21	1.80	0.46
1:A:213:HIS:O	1:A:214:GLN:C	2.53	0.46
1:A:217:VAL:CG1	1:A:218:GLU:N	2.79	0.46
1:B:177:ASP:OD1	1:B:420:ASN:ND2	2.49	0.46
1:B:844:LEU:C	1:B:845:LEU:CD2	2.84	0.46
1:B:558:GLN:NE2	1:B:559:VAL:O	2.42	0.46
1:B:515:THR:O	1:B:516:ALA:C	2.54	0.46
1:B:592:GLN:O	1:B:595:GLY:N	2.49	0.46
1:B:288:SER:O	1:B:289:GLU:C	2.53	0.46
1:A:682:GLU:C	1:A:682:GLU:CD	2.74	0.46
1:A:686:ASP:OD1	1:A:688:LEU:CD2	2.64	0.46
1:B:371:ASN:ND2	1:B:371:ASN:N	2.61	0.46
1:B:683:GLN:HA	1:B:687:ARG:HH22	1.80	0.46
1:A:828:LYS:O	1:A:830:LEU:N	2.49	0.46
1:A:168:ARG:NH2	1:A:415:ARG:CD	2.79	0.46
1:A:740:LEU:HD23	1:A:740:LEU:HA	1.69	0.46
1:A:253:ILE:C	1:A:254:CYS:SG	2.94	0.46
1:A:260:ARG:O	1:A:260:ARG:HD3	2.16	0.46
1:A:884:VAL:HG13	1:A:887:ILE:CD1	2.41	0.46
1:A:531:ALA:HA	1:A:558:GLN:O	2.16	0.46
1:A:530:ARG:CG	1:A:549:TRP:HZ2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ARG:CZ	1:B:120:ILE:HG22	2.46	0.46
1:A:510:CYS:HB3	1:A:581:PHE:CD2	2.49	0.46
1:B:248:THR:O	1:B:249:GLU:OE1	2.34	0.46
1:A:269:LEU:O	1:A:272:ALA:HB3	2.16	0.46
1:A:69:MSE:SE	1:A:97:LEU:HD13	2.66	0.46
1:B:129:ARG:HH11	1:B:795:ASP:HA	1.81	0.45
1:B:510:CYS:SG	1:B:562:CYS:CA	3.03	0.45
1:B:568:GLU:OE2	1:B:570:ARG:NE	2.48	0.45
1:B:587:PRO:HA	1:B:625:TYR:CE1	2.50	0.45
1:B:293:SER:H	1:B:297:GLN:HG3	1.81	0.45
1:A:860:THR:C	1:A:862:ASN:N	2.69	0.45
1:A:404:VAL:C	1:A:406:MSE:N	2.69	0.45
1:B:227:PHE:HA	1:B:251:LEU:CB	2.46	0.45
1:B:209:GLU:C	1:B:212:GLN:HG3	2.37	0.45
1:B:52:ARG:HG3	1:B:54:MSE:CG	2.39	0.45
1:B:161:ILE:O	1:B:165:VAL:N	2.49	0.45
1:B:318:GLN:HB2	1:B:319:LEU:HD12	1.99	0.45
1:B:858:PHE:CD1	1:B:861:PHE:CZ	3.04	0.45
1:A:235:TYR:C	1:A:239:GLN:NE2	2.67	0.45
1:A:123:MSE:HB2	1:A:961:ARG:NH2	2.31	0.45
1:B:175:LEU:HD12	1:B:311:LEU:O	2.15	0.45
1:A:431:ARG:HD2	1:A:632:PHE:O	2.15	0.45
1:B:445:GLN:C	1:B:449:LYS:HE2	2.35	0.45
1:A:494:LEU:H	1:A:494:LEU:HD12	1.81	0.45
1:B:253:ILE:HD13	1:B:253:ILE:H	1.81	0.45
1:B:256:LEU:C	1:B:256:LEU:HD22	2.36	0.45
1:A:918:LEU:HD13	1:A:919:SER:N	2.32	0.45
1:A:174:LEU:HD21	1:A:313:THR:CG2	2.46	0.45
1:A:777:ILE:CG1	1:A:778:THR:H	2.28	0.45
1:A:141:ARG:HH22	1:A:836:LEU:HG	1.81	0.45
1:B:176:ALA:O	1:B:419:ARG:NH2	2.49	0.45
1:B:215:TRP:HD1	1:B:215:TRP:H	1.63	0.45
1:B:777:ILE:CG1	1:B:778:THR:H	2.21	0.45
1:B:788:LEU:HD12	1:B:789:ASP:OD2	2.16	0.45
1:B:896:GLU:O	1:B:897:LYS:C	2.53	0.45
1:B:300:GLU:O	1:B:302:LEU:N	2.49	0.45
1:B:707:GLU:C	1:B:710:ASP:OD1	2.54	0.45
1:A:458:LYS:CD	1:A:458:LYS:N	2.79	0.45
1:A:148:ARG:HD3	1:A:148:ARG:HA	1.66	0.45
1:A:256:LEU:HD13	1:A:256:LEU:N	2.31	0.45
1:A:780:GLU:HA	1:A:783:LEU:CD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:GLU:O	1:A:960:LEU:HG	2.16	0.45
1:A:896:GLU:O	1:A:900:ARG:N	2.48	0.45
1:B:316:PRO:HB3	1:B:327:ARG:NH2	2.32	0.45
1:B:757:ASP:O	1:B:758:GLY:C	2.54	0.45
1:B:779:TRP:HA	1:B:779:TRP:CE3	2.52	0.45
1:B:816:VAL:HG11	1:B:884:VAL:HG13	1.98	0.45
1:A:475:GLN:HG2	1:A:476:GLU:H	1.81	0.45
1:A:106:LEU:N	1:A:106:LEU:HD13	2.30	0.45
1:A:565:ILE:HB	1:A:568:GLU:HB2	1.97	0.45
1:A:916:ALA:O	1:A:920:ARG:HG3	2.16	0.45
1:B:536:GLU:C	1:B:543:ARG:NH2	2.70	0.45
1:A:322:GLU:HG2	1:A:324:HIS:HD2	1.81	0.45
1:A:140:PHE:HB3	1:A:833:ASN:OD1	2.17	0.45
1:B:760:THR:CG2	1:B:766:GLU:HG2	2.39	0.45
1:B:822:VAL:CG2	1:B:837:PRO:O	2.65	0.45
1:B:494:LEU:HD12	1:B:494:LEU:N	2.31	0.45
1:B:640:ARG:HD3	1:B:643:TYR:CD2	2.45	0.45
1:A:927:VAL:CG1	1:A:929:PRO:HD3	2.43	0.45
1:B:358:MSE:O	1:B:359:LEU:HD23	2.17	0.45
1:A:7:GLN:HA	1:A:99:GLU:OE2	2.16	0.45
1:A:7:GLN:HG3	1:A:80:LEU:HD12	1.97	0.45
1:B:86:THR:HA	1:B:92:GLU:O	2.16	0.45
1:B:663:PHE:HA	1:B:666:LEU:HD23	1.98	0.45
1:A:662:GLY:O	1:A:665:ASP:N	2.50	0.45
1:B:110:LYS:HB3	1:B:112:GLN:CD	2.36	0.45
1:A:73:GLU:CG	1:A:84:ILE:HB	2.45	0.45
1:A:536:GLU:HA	1:A:543:ARG:HH21	1.81	0.45
1:B:538:MSE:H	1:B:543:ARG:NH2	2.14	0.45
1:A:572:PHE:HA	1:A:574:PHE:CE1	2.52	0.45
1:B:517:LEU:O	1:B:520:GLU:CB	2.64	0.45
1:B:890:LEU:O	1:B:893:ALA:HB3	2.16	0.45
1:B:932:ARG:H	1:B:932:ARG:HG3	1.41	0.45
1:A:186:GLU:O	1:A:187:ALA:C	2.54	0.45
1:B:176:ALA:HB3	1:B:419:ARG:CA	2.47	0.45
1:B:185:ILE:O	1:B:189:MSE:HG3	2.17	0.45
1:B:521:GLN:O	1:B:523:LEU:N	2.49	0.45
1:B:437:LYS:HA	1:B:612:TYR:CE1	2.52	0.45
1:A:692:HIS:CE1	1:A:693:SER:HB3	2.52	0.45
1:B:206:ILE:HD13	1:B:206:ILE:HA	1.65	0.45
1:B:227:PHE:HA	1:B:251:LEU:HB2	1.98	0.45
1:A:103:ASP:HB3	1:A:105:LYS:CE	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:LEU:O	1:A:602:GLN:HG3	2.16	0.45
1:B:917:GLU:O	1:B:921:LEU:HD23	2.16	0.45
1:A:827:PRO:O	1:A:830:LEU:CD2	2.65	0.45
1:A:640:ARG:HD3	1:A:643:TYR:CD2	2.48	0.45
1:A:215:TRP:CD1	1:A:215:TRP:N	2.82	0.45
1:A:277:LEU:CG	1:A:278:VAL:N	2.79	0.45
1:A:335:ARG:C	1:A:336:PHE:CD1	2.90	0.45
1:A:726:ILE:O	1:A:747:LEU:HD23	2.17	0.45
1:A:885:HIS:O	1:A:889:GLN:HG2	2.16	0.45
1:A:914:LEU:N	1:A:914:LEU:CD1	2.79	0.45
1:B:279:VAL:O	1:B:279:VAL:HG13	2.17	0.45
1:B:327:ARG:CA	1:B:330:LEU:HD13	2.45	0.45
1:B:799:SER:HB2	1:B:961:ARG:CZ	2.46	0.45
1:B:586:ASN:OD1	1:B:587:PRO:HD2	2.16	0.45
1:A:475:GLN:HA	1:A:480:ASP:O	2.17	0.45
1:A:599:ARG:CZ	1:A:599:ARG:HB2	2.47	0.45
1:A:663:PHE:HA	1:A:666:LEU:HD23	1.99	0.45
1:A:256:LEU:C	1:A:256:LEU:HD22	2.37	0.45
1:A:173:VAL:HG11	1:A:418:PHE:HE2	1.81	0.45
1:A:728:ILE:O	1:A:729:ASN:C	2.55	0.45
1:A:817:GLU:C	1:A:818:LEU:HD12	2.37	0.45
1:A:845:LEU:HB2	1:A:848:ASN:O	2.17	0.45
1:A:834:ARG:HH12	1:A:913:LYS:HZ1	1.65	0.45
1:B:281:GLU:CD	1:B:314:ALA:CA	2.79	0.45
1:B:789:ASP:O	1:B:791:ILE:HD12	2.17	0.45
1:B:959:ALA:O	1:B:960:LEU:HB2	2.16	0.45
1:A:650:LEU:CD1	1:A:651:ILE:N	2.72	0.45
1:B:450:VAL:O	1:B:453:ILE:HD13	2.17	0.45
1:B:640:ARG:O	1:B:644:ASP:CG	2.55	0.45
1:B:293:SER:N	1:B:296:TYR:HD2	2.14	0.45
1:A:521:GLN:O	1:A:523:LEU:N	2.49	0.45
1:A:355:ALA:O	1:A:358:MSE:N	2.49	0.45
1:A:592:GLN:O	1:A:593:ARG:C	2.55	0.45
1:A:42:LEU:HG	1:A:242:ALA:HB1	1.99	0.45
1:A:90:THR:OG1	1:A:92:GLU:HG3	2.16	0.45
1:A:235:TYR:HB2	1:A:258:PHE:CZ	2.52	0.45
1:A:322:GLU:HA	1:A:324:HIS:NE2	2.31	0.45
1:A:799:SER:HB2	1:A:961:ARG:CZ	2.47	0.45
1:B:186:GLU:O	1:B:189:MSE:HB2	2.17	0.45
1:B:217:VAL:HG12	1:B:218:GLU:N	2.32	0.45
1:B:174:LEU:CD2	1:B:313:THR:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ASN:OD1	1:A:588:ASP:OD1	2.35	0.45
1:A:613:LEU:O	1:A:619:SER:HB2	2.17	0.45
1:A:925:ARG:HA	1:A:931:ILE:CD1	2.39	0.45
1:B:689:LEU:O	1:B:693:SER:OG	2.17	0.45
1:A:114:ARG:CZ	1:A:120:ILE:HG22	2.47	0.45
1:A:62:THR:OG1	1:A:103:ASP:HB2	2.17	0.45
1:A:512:LYS:O	1:A:513:ALA:C	2.55	0.45
1:A:156:PRO:N	1:A:159:LEU:HD12	2.32	0.45
1:B:275:ASP:O	1:B:307:PRO:HG2	2.17	0.45
1:B:112:GLN:O	1:B:115:LEU:HD12	2.17	0.45
1:A:86:THR:HA	1:A:92:GLU:O	2.17	0.45
1:B:551:ALA:HA	1:B:574:PHE:CE2	2.52	0.45
1:A:799:SER:HB2	1:A:961:ARG:NH2	2.31	0.45
1:B:177:ASP:N	1:B:419:ARG:HA	2.31	0.45
1:B:191:LEU:H	1:B:191:LEU:CD1	2.30	0.45
1:B:896:GLU:HG3	1:B:955:TRP:CZ3	2.51	0.45
1:A:650:LEU:O	1:A:652:ASN:N	2.49	0.45
1:B:8:ARG:CZ	1:B:19:LEU:HD13	2.46	0.45
1:B:530:ARG:CD	1:B:549:TRP:CZ2	3.00	0.45
1:A:686:ASP:OD1	1:A:688:LEU:CG	2.64	0.45
1:B:373:LEU:N	1:B:373:LEU:HD22	2.28	0.45
1:B:403:LEU:O	1:B:406:MSE:CB	2.59	0.45
1:A:103:ASP:CG	1:A:105:LYS:HZ3	2.20	0.45
1:A:508:VAL:O	1:A:561:LEU:N	2.49	0.45
1:A:156:PRO:CA	1:A:159:LEU:HD12	2.46	0.45
1:B:662:GLY:O	1:B:666:LEU:CD2	2.57	0.45
1:A:917:GLU:O	1:A:921:LEU:HD23	2.16	0.45
1:B:536:GLU:O	1:B:543:ARG:NH2	2.50	0.45
1:B:820:TYR:HA	1:B:956:ARG:O	2.17	0.45
1:A:800:THR:OG1	1:A:864:GLN:HB2	2.17	0.45
1:A:315:THR:HA	1:A:317:GLU:OE2	2.16	0.44
1:A:177:ASP:OD1	1:A:420:ASN:ND2	2.50	0.44
1:B:126:PHE:C	1:B:128:LEU:H	2.19	0.44
1:B:193:GLN:CG	1:B:194:GLN:N	2.80	0.44
1:B:726:ILE:O	1:B:747:LEU:HD23	2.17	0.44
1:B:726:ILE:C	1:B:728:ILE:HD12	2.38	0.44
1:B:558:GLN:CD	1:B:559:VAL:N	2.67	0.44
1:B:485:TRP:NE1	1:B:518:GLN:OE1	2.39	0.44
1:B:404:VAL:N	1:B:407:LEU:HD22	2.33	0.44
1:A:48:SER:O	1:A:50:VAL:N	2.45	0.44
1:A:565:ILE:HD12	1:A:566:GLY:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:GLU:HA	1:B:543:ARG:HH21	1.82	0.44
1:A:386:LEU:O	1:A:389:ALA:HB3	2.17	0.44
1:B:728:ILE:HD12	1:B:728:ILE:N	2.33	0.44
1:A:485:TRP:CZ3	1:A:526:ARG:NH2	2.86	0.44
1:A:685:ARG:NH2	1:A:687:ARG:HD2	2.33	0.44
1:B:950:LEU:C	1:B:952:GLN:N	2.69	0.44
1:A:565:ILE:HD13	1:A:596:ARG:CD	2.44	0.44
1:A:921:LEU:O	1:A:924:LEU:N	2.47	0.44
1:A:178:GLU:HB2	1:A:422:ARG:NH1	2.32	0.44
1:A:191:LEU:H	1:A:191:LEU:CD1	2.31	0.44
1:A:281:GLU:HG3	1:A:314:ALA:CA	2.39	0.44
1:A:325:PHE:O	1:A:328:LEU:N	2.50	0.44
1:A:129:ARG:HH11	1:A:795:ASP:HA	1.83	0.44
1:A:722:LEU:C	1:A:722:LEU:HD13	2.35	0.44
1:B:108:PHE:CE2	1:B:791:ILE:HD13	2.52	0.44
1:A:642:ILE:O	1:A:644:ASP:N	2.50	0.44
1:B:534:PHE:HB3	1:B:561:LEU:HD22	1.99	0.44
1:A:928:ASN:N	1:A:929:PRO:CD	2.80	0.44
1:A:42:LEU:CD1	1:A:242:ALA:CB	2.95	0.44
1:B:245:PRO:O	1:B:246:PHE:CD1	2.70	0.44
1:B:663:PHE:CE1	1:B:667:ILE:HD11	2.52	0.44
1:A:826:ALA:O	1:A:832:LEU:CD1	2.66	0.44
1:B:807:LYS:CB	1:B:808:ALA:HA	2.47	0.44
1:A:898:SER:O	1:A:902:LEU:HG	2.17	0.44
1:A:760:THR:CG2	1:A:766:GLU:HG2	2.40	0.44
1:B:788:LEU:CD2	1:B:788:LEU:H	2.30	0.44
1:B:62:THR:OG1	1:B:103:ASP:HB2	2.16	0.44
1:A:400:ARG:HA	1:A:403:LEU:HD11	1.99	0.44
1:A:687:ARG:HA	1:A:690:GLU:HB3	1.99	0.44
1:B:258:PHE:CE1	1:B:265:ARG:NH1	2.85	0.44
1:A:516:ALA:HA	1:A:519:LEU:CG	2.47	0.44
1:A:112:GLN:HE22	1:A:113:ASP:CG	2.21	0.44
1:A:878:ASN:CG	1:A:878:ASN:O	2.56	0.44
1:B:440:LEU:HA	1:B:441:PRO:HD3	1.82	0.44
1:A:182:GLY:HA3	1:A:185:ILE:HD13	1.98	0.44
1:B:845:LEU:HB2	1:B:848:ASN:O	2.17	0.44
1:B:846:ASP:C	1:B:848:ASN:N	2.70	0.44
1:A:650:LEU:C	1:A:652:ASN:N	2.69	0.44
1:A:549:TRP:NE1	1:A:555:THR:HB	2.31	0.44
1:A:688:LEU:N	1:A:688:LEU:HD23	2.19	0.44
1:A:692:HIS:HD1	1:A:693:SER:H	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:CYS:HB2	1:B:351:PRO:CD	2.40	0.44
1:B:678:LYS:HG3	1:B:679:ALA:H	1.81	0.44
1:B:239:GLN:H	1:B:239:GLN:HG3	1.54	0.44
1:B:917:GLU:OE2	1:B:920:ARG:NH1	2.49	0.44
1:A:627:GLU:C	1:A:671:ARG:NH1	2.71	0.44
1:A:536:GLU:C	1:A:543:ARG:NH2	2.71	0.44
1:B:702:LEU:O	1:B:706:ILE:CD1	2.60	0.44
1:B:538:MSE:HG2	1:B:542:GLU:OE1	2.17	0.44
1:B:462:ASP:OD1	1:B:463:ARG:CZ	2.65	0.44
1:B:520:GLU:CD	1:B:520:GLU:C	2.76	0.44
1:A:327:ARG:CA	1:A:330:LEU:HD13	2.47	0.44
1:A:884:VAL:C	1:A:888:LEU:HD23	2.38	0.44
1:B:143:PRO:C	1:B:144:TYR:CD1	2.91	0.44
1:B:174:LEU:HD22	1:B:174:LEU:C	2.36	0.44
1:B:311:LEU:CD1	1:B:327:ARG:HB3	2.48	0.44
1:B:775:GLN:NE2	1:B:776:PHE:CB	2.79	0.44
1:B:814:LEU:CD2	1:B:814:LEU:N	2.81	0.44
1:B:834:ARG:HH12	1:B:913:LYS:HZ1	1.66	0.44
1:A:586:ASN:OD1	1:A:587:PRO:N	2.50	0.44
1:A:587:PRO:HA	1:A:625:TYR:CE1	2.51	0.44
1:B:427:GLY:HA3	1:B:600:ILE:CG2	2.43	0.44
1:B:565:ILE:HD13	1:B:596:ARG:CD	2.44	0.44
1:A:292:PRO:HA	1:A:296:TYR:CE2	2.52	0.44
1:A:549:TRP:CD1	1:A:555:THR:HB	2.53	0.44
1:A:568:GLU:OE2	1:A:570:ARG:NE	2.49	0.44
1:A:762:THR:O	1:A:766:GLU:HB3	2.15	0.44
1:A:802:SER:HA	1:A:812:GLY:HA2	2.00	0.44
1:B:781:HIS:HB2	1:B:782:PRO:CD	2.36	0.44
1:B:865:LEU:HG	1:B:866:ASN:N	2.28	0.44
1:B:865:LEU:CG	1:B:866:ASN:H	2.25	0.44
1:B:105:LYS:C	1:B:106:LEU:HD13	2.38	0.44
1:B:582:ASP:HA	1:B:618:GLN:HE21	1.81	0.44
1:B:642:ILE:C	1:B:644:ASP:N	2.71	0.44
1:B:651:ILE:HA	1:B:654:LEU:HD12	1.98	0.44
1:A:350:CYS:HB2	1:A:351:PRO:CD	2.43	0.44
1:A:683:GLN:HA	1:A:687:ARG:NH2	2.32	0.44
1:B:918:LEU:HD22	1:B:918:LEU:C	2.36	0.44
1:A:42:LEU:HG	1:A:242:ALA:CB	2.47	0.44
1:A:627:GLU:HB3	1:A:667:ILE:HG21	1.99	0.44
1:A:77:GLU:OE1	1:A:77:GLU:HA	2.17	0.44
1:A:46:SER:OG	1:A:47:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ALA:C	1:A:771:ARG:HG3	2.38	0.44
1:B:123:MSE:HB2	1:B:961:ARG:NH2	2.32	0.44
1:B:181:LEU:CD1	1:B:420:ASN:O	2.65	0.44
1:B:103:ASP:CG	1:B:105:LYS:NZ	2.71	0.44
1:B:493:TRP:CG	1:B:494:LEU:N	2.84	0.44
1:A:436:ILE:CD1	1:A:436:ILE:N	2.72	0.44
1:B:406:MSE:C	1:B:409:ASP:OD1	2.56	0.44
1:B:687:ARG:HA	1:B:690:GLU:HB3	2.00	0.44
1:B:256:LEU:CD1	1:B:256:LEU:H	2.31	0.44
1:B:256:LEU:HD13	1:B:256:LEU:H	1.82	0.44
1:B:950:LEU:O	1:B:952:GLN:N	2.51	0.44
1:B:112:GLN:HE21	1:B:112:GLN:CA	2.30	0.44
1:A:539:SER:H	1:A:542:GLU:HB2	1.82	0.44
1:B:539:SER:HB2	1:B:542:GLU:OE2	2.18	0.44
1:B:77:GLU:HA	1:B:77:GLU:OE1	2.18	0.44
1:B:63:SER:OG	1:B:65:ASP:OD2	2.35	0.44
1:A:206:ILE:HD13	1:A:206:ILE:HA	1.71	0.44
1:A:726:ILE:C	1:A:728:ILE:HD12	2.38	0.44
1:B:175:LEU:HD13	1:B:312:LEU:HA	2.00	0.44
1:B:849:GLY:O	1:B:850:ASN:C	2.55	0.44
1:B:884:VAL:O	1:B:888:LEU:CD2	2.66	0.44
1:B:910:ALA:O	1:B:914:LEU:HD13	2.17	0.44
1:B:473:ILE:HG23	1:B:476:GLU:OE1	2.18	0.44
1:B:515:THR:HG23	1:B:562:CYS:HG	1.82	0.44
1:A:427:GLY:O	1:A:600:ILE:HA	2.18	0.44
1:A:707:GLU:C	1:A:710:ASP:OD1	2.57	0.44
1:B:119:GLN:HG3	1:B:870:ARG:HH21	1.83	0.44
1:A:150:GLN:H	1:A:150:GLN:CD	2.21	0.43
1:A:227:PHE:HA	1:A:251:LEU:CB	2.48	0.43
1:A:316:PRO:HB3	1:A:327:ARG:NH2	2.33	0.43
1:B:123:MSE:CB	1:B:961:ARG:NH2	2.81	0.43
1:B:215:TRP:O	1:B:218:GLU:N	2.51	0.43
1:A:620:VAL:CG2	1:A:621:LEU:H	2.28	0.43
1:A:383:GLU:C	1:A:385:LEU:H	2.21	0.43
1:B:568:GLU:HB3	1:B:596:ARG:CZ	2.48	0.43
1:B:428:PHE:CE1	1:B:600:ILE:HG13	2.53	0.43
1:B:620:VAL:CG2	1:B:621:LEU:HD23	2.44	0.43
1:B:682:GLU:CD	1:B:682:GLU:C	2.76	0.43
1:B:109:SER:O	1:B:110:LYS:CB	2.63	0.43
1:A:773:ASP:OD1	1:A:774:ALA:O	2.35	0.43
1:B:722:LEU:CD1	1:B:723:PHE:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:884:VAL:C	1:B:888:LEU:HD23	2.38	0.43
1:A:629:LEU:CD1	1:A:629:LEU:N	2.79	0.43
1:B:521:GLN:O	1:B:522:VAL:C	2.57	0.43
1:B:381:ASP:N	1:B:384:PRO:HG2	2.33	0.43
1:B:530:ARG:NH1	1:B:555:THR:CB	2.78	0.43
1:A:931:ILE:HA	1:A:935:GLU:OE1	2.18	0.43
1:B:944:GLN:O	1:B:948:GLU:HG3	2.18	0.43
1:A:566:GLY:O	1:A:596:ARG:HD3	2.18	0.43
1:A:307:PRO:HG2	1:A:308:GLY:H	1.83	0.43
1:A:715:LEU:C	1:A:715:LEU:HD23	2.38	0.43
1:A:229:LEU:N	1:A:253:ILE:HD11	2.33	0.43
1:A:788:LEU:CD2	1:A:788:LEU:H	2.29	0.43
1:B:176:ALA:HB3	1:B:419:ARG:CB	2.48	0.43
1:A:625:TYR:HB3	1:A:632:PHE:CE2	2.53	0.43
1:B:636:CYS:HA	1:B:637:PRO:HD2	1.75	0.43
1:A:476:GLU:HB2	1:A:477:PHE:H	1.59	0.43
1:A:406:MSE:C	1:A:407:LEU:HD13	2.38	0.43
1:A:407:LEU:CD1	1:A:407:LEU:N	2.81	0.43
1:A:932:ARG:HD3	1:A:935:GLU:HG3	2.00	0.43
1:B:402:GLU:O	1:B:405:SER:OG	2.25	0.43
1:B:922:GLU:O	1:B:925:ARG:HB3	2.19	0.43
1:B:205:ILE:O	1:B:206:ILE:HD13	2.17	0.43
1:B:258:PHE:HA	1:B:261:ARG:CZ	2.45	0.43
1:A:208:PRO:O	1:A:209:GLU:C	2.56	0.43
1:B:917:GLU:CD	1:B:920:ARG:HH11	2.20	0.43
1:B:386:LEU:CD2	1:B:386:LEU:C	2.86	0.43
1:A:177:ASP:N	1:A:419:ARG:HA	2.34	0.43
1:A:815:LEU:HD23	1:A:815:LEU:HA	1.84	0.43
1:A:896:GLU:O	1:A:897:LYS:C	2.56	0.43
1:A:896:GLU:HG3	1:A:955:TRP:CZ3	2.53	0.43
1:B:150:GLN:N	1:B:150:GLN:CD	2.72	0.43
1:B:183:LYS:HG2	2:B:1001:SO4:S	2.58	0.43
1:B:188:GLY:HA2	1:B:191:LEU:HD13	2.00	0.43
1:B:184:THR:O	1:B:222:ARG:NH1	2.51	0.43
1:B:728:ILE:O	1:B:729:ASN:C	2.56	0.43
1:A:380:GLN:HE22	1:A:382:ILE:HD12	1.82	0.43
1:A:530:ARG:HD3	1:A:555:THR:O	2.18	0.43
1:A:356:VAL:O	1:A:359:LEU:HG	2.18	0.43
1:B:404:VAL:C	1:B:406:MSE:N	2.71	0.43
1:B:572:PHE:HA	1:B:574:PHE:CE1	2.53	0.43
1:A:460:ALA:HA	1:A:463:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:ILE:H	1:A:784:ILE:HG13	1.56	0.43
1:B:757:ASP:O	1:B:759:ILE:N	2.51	0.43
1:B:802:SER:HA	1:B:812:GLY:HA2	2.00	0.43
1:B:899:ALA:O	1:B:900:ARG:C	2.57	0.43
1:A:642:ILE:C	1:A:644:ASP:N	2.72	0.43
1:A:652:ASN:OD1	1:A:652:ASN:N	2.51	0.43
1:A:558:GLN:CD	1:A:559:VAL:N	2.70	0.43
1:B:7:GLN:HG3	1:B:80:LEU:HD12	1.99	0.43
1:B:512:LYS:O	1:B:513:ALA:C	2.56	0.43
1:B:582:ASP:CA	1:B:618:GLN:NE2	2.73	0.43
1:B:201:GLU:O	1:B:275:ASP:CG	2.57	0.43
1:A:201:GLU:O	1:A:275:ASP:CG	2.57	0.43
1:A:69:MSE:HG2	1:A:70:GLN:N	2.34	0.43
1:A:640:ARG:O	1:A:643:TYR:HB3	2.19	0.43
1:B:95:VAL:HG12	1:B:97:LEU:CD1	2.48	0.43
1:A:152:THR:O	1:A:763:PHE:CE1	2.71	0.43
1:A:258:PHE:HA	1:A:261:ARG:CZ	2.44	0.43
1:A:810:PRO:C	1:A:812:GLY:N	2.72	0.43
1:B:897:LYS:N	1:B:897:LYS:CD	2.65	0.43
1:B:799:SER:HB2	1:B:961:ARG:NH2	2.33	0.43
1:B:510:CYS:HB2	1:B:562:CYS:HG	1.83	0.43
1:B:566:GLY:O	1:B:596:ARG:HD3	2.18	0.43
1:A:351:PRO:CA	1:A:354:ASP:OD2	2.62	0.43
1:A:405:SER:O	1:A:409:ASP:OD2	2.37	0.43
1:B:376:MSE:C	1:B:378:GLY:H	2.22	0.43
1:A:661:GLU:C	1:A:663:PHE:N	2.70	0.43
1:A:918:LEU:HD11	1:A:922:GLU:OE2	2.18	0.43
1:A:708:GLU:O	1:A:710:ASP:N	2.51	0.43
1:A:143:PRO:C	1:A:144:TYR:CD1	2.91	0.43
1:B:186:GLU:O	1:B:187:ALA:C	2.57	0.43
1:B:715:LEU:O	1:B:716:ILE:C	2.57	0.43
1:B:133:ARG:NH2	1:B:788:LEU:HB2	2.33	0.43
1:B:141:ARG:NH2	1:B:836:LEU:HG	2.34	0.43
1:A:124:ASP:HB2	1:A:125:ARG:HH22	1.83	0.43
1:B:485:TRP:CZ3	1:B:526:ARG:NH2	2.87	0.43
1:B:640:ARG:O	1:B:643:TYR:HB3	2.19	0.43
1:A:373:LEU:N	1:A:373:LEU:HD22	2.24	0.43
1:A:404:VAL:HA	1:A:407:LEU:CD2	2.45	0.43
1:A:691:ILE:HA	1:A:694:ASN:OD1	2.19	0.43
1:B:396:ALA:O	1:B:398:SER:N	2.52	0.43
1:A:568:GLU:HB3	1:A:596:ARG:CZ	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:SER:HB3	1:A:104:SER:CB	2.48	0.43
1:B:360:LEU:CD1	1:B:360:LEU:N	2.80	0.43
1:A:134:LYS:O	1:A:138:GLU:HB2	2.19	0.43
1:A:28:ARG:HD2	1:A:241:ASP:OD2	2.19	0.43
1:A:798:SER:HG	1:A:962:LEU:HD11	1.83	0.43
1:B:194:GLN:HE21	1:B:199:ALA:CB	2.22	0.43
1:B:325:PHE:O	1:B:328:LEU:N	2.51	0.43
1:B:558:GLN:NE2	1:B:559:VAL:N	2.55	0.43
1:B:294:ARG:HB2	1:B:295:GLU:OE2	2.17	0.43
1:B:856:VAL:CA	1:B:859:GLU:HB2	2.48	0.43
1:B:692:HIS:HD1	1:B:693:SER:H	1.67	0.43
1:B:256:LEU:N	1:B:256:LEU:HD13	2.33	0.43
1:A:583:LEU:N	1:A:618:GLN:HE22	2.17	0.43
1:B:665:ASP:O	1:B:669:ASN:HB2	2.17	0.43
1:A:69:MSE:HG3	1:A:86:THR:C	2.39	0.43
1:A:917:GLU:CD	1:A:920:ARG:HH11	2.21	0.43
1:A:918:LEU:HD22	1:A:918:LEU:C	2.35	0.43
1:A:138:GLU:HG3	1:A:139:GLN:OE1	2.19	0.43
1:A:193:GLN:HA	1:A:196:LEU:HD23	2.01	0.43
1:A:777:ILE:CG1	1:A:778:THR:N	2.81	0.43
1:B:719:ALA:O	1:B:722:LEU:HB3	2.19	0.43
1:B:646:VAL:CG2	1:B:647:TYR:N	2.82	0.43
1:A:530:ARG:HH11	1:A:555:THR:CB	2.29	0.43
1:A:530:ARG:CD	1:A:549:TRP:CZ2	3.01	0.43
1:A:549:TRP:HE1	1:A:555:THR:HB	1.84	0.43
1:B:378:GLY:HA2	1:B:410:ARG:HE	1.84	0.43
1:B:414:SER:HB3	1:B:692:HIS:CD2	2.54	0.43
1:B:686:ASP:CG	1:B:688:LEU:CD2	2.88	0.43
1:A:209:GLU:C	1:A:212:GLN:HG3	2.39	0.43
1:B:702:LEU:CD2	1:B:702:LEU:H	2.32	0.43
1:B:48:SER:O	1:B:50:VAL:N	2.45	0.43
1:A:551:ALA:HA	1:A:574:PHE:CE2	2.54	0.43
1:B:735:ASP:C	1:B:737:MSE:H	2.21	0.43
1:A:735:ASP:C	1:A:737:MSE:H	2.22	0.43
1:A:754:LEU:HB3	1:A:755:SER:H	1.42	0.43
1:A:186:GLU:O	1:A:190:ILE:CD1	2.67	0.43
1:A:244:ASN:ND2	1:B:267:GLU:OE2	2.52	0.43
1:A:788:LEU:HD12	1:A:789:ASP:OD2	2.19	0.43
1:B:834:ARG:CZ	1:B:913:LYS:HZ2	2.31	0.43
1:B:482:ALA:HB1	1:B:518:GLN:OE1	2.19	0.43
1:A:948:GLU:HG2	1:B:952:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:THR:O	1:A:516:ALA:C	2.56	0.43
1:A:826:ALA:O	1:A:832:LEU:HD13	2.18	0.43
1:B:828:LYS:C	1:B:830:LEU:N	2.71	0.43
1:A:746:MSE:HG3	1:A:748:VAL:O	2.19	0.43
1:A:318:GLN:CA	1:A:318:GLN:NE2	2.81	0.43
1:B:932:ARG:HD3	1:B:935:GLU:HG3	2.01	0.43
1:B:325:PHE:O	1:B:328:LEU:CD2	2.67	0.42
1:B:558:GLN:CG	1:B:559:VAL:N	2.81	0.42
1:B:141:ARG:NH2	1:B:836:LEU:HA	2.34	0.42
1:B:516:ALA:HA	1:B:519:LEU:CG	2.49	0.42
1:A:450:VAL:O	1:A:453:ILE:HD13	2.19	0.42
1:A:474:TYR:OH	1:A:480:ASP:HB2	2.19	0.42
1:B:683:GLN:HA	1:B:687:ARG:NH2	2.33	0.42
1:B:918:LEU:HD11	1:B:922:GLU:OE2	2.18	0.42
1:B:235:TYR:C	1:B:239:GLN:NE2	2.68	0.42
1:B:252:VAL:CG2	1:B:253:ILE:N	2.82	0.42
1:A:466:ASP:HB2	1:A:467:MSE:H	1.58	0.42
1:A:663:PHE:HA	1:A:666:LEU:CD2	2.49	0.42
1:A:541:ILE:O	1:A:542:GLU:C	2.57	0.42
1:A:462:ASP:OD1	1:A:463:ARG:CZ	2.67	0.42
1:A:145:SER:C	1:A:147:LEU:N	2.71	0.42
1:A:176:ALA:HB3	1:A:419:ARG:CB	2.44	0.42
1:A:728:ILE:HD12	1:A:728:ILE:N	2.35	0.42
1:B:835:PHE:O	1:B:836:LEU:HB2	2.19	0.42
1:A:586:ASN:CB	1:A:589:LEU:HD12	2.19	0.42
1:A:431:ARG:NH2	1:A:635:THR:HA	2.23	0.42
1:B:650:LEU:C	1:B:652:ASN:N	2.70	0.42
1:B:383:GLU:C	1:B:385:LEU:H	2.22	0.42
1:B:859:GLU:O	1:B:863:ARG:CZ	2.67	0.42
1:A:406:MSE:HB2	1:A:407:LEU:HD13	2.00	0.42
1:B:348:ASN:CA	1:B:351:PRO:HD2	2.48	0.42
1:B:369:GLU:HA	1:B:372:MSE:HG3	1.97	0.42
1:B:686:ASP:OD2	1:B:688:LEU:HD21	2.19	0.42
1:A:55:PHE:O	1:A:83:TYR:HE2	2.02	0.42
1:A:202:ARG:NE	1:A:274:TRP:CZ3	2.87	0.42
1:A:702:LEU:O	1:A:704:GLU:N	2.52	0.42
1:B:460:ALA:HA	1:B:463:ARG:HH21	1.83	0.42
1:A:215:TRP:HD1	1:A:215:TRP:H	1.64	0.42
1:A:219:MSE:O	1:A:224:ASN:N	2.52	0.42
1:A:205:ILE:HD11	1:A:227:PHE:CZ	2.54	0.42
1:A:327:ARG:H	1:A:327:ARG:HG3	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:VAL:HG21	1:B:887:ILE:CG2	2.50	0.42
1:B:845:LEU:N	1:B:845:LEU:CD2	2.74	0.42
1:B:889:GLN:HG2	1:B:889:GLN:H	1.57	0.42
1:A:381:ASP:N	1:A:384:PRO:HG2	2.34	0.42
1:A:686:ASP:CG	1:A:688:LEU:CD2	2.88	0.42
1:B:691:ILE:O	1:B:692:HIS:C	2.57	0.42
1:B:234:ARG:HA	1:B:237:GLU:CD	2.39	0.42
1:A:7:GLN:HA	1:A:99:GLU:CD	2.39	0.42
1:A:465:ARG:HG2	1:A:468:LEU:CD1	2.49	0.42
1:A:515:THR:O	1:A:519:LEU:CG	2.61	0.42
1:A:299:ILE:O	1:A:300:GLU:C	2.57	0.42
1:B:52:ARG:NH1	1:B:52:ARG:HG3	2.33	0.42
1:A:191:LEU:N	1:A:191:LEU:CD1	2.83	0.42
1:A:175:LEU:HD12	1:A:311:LEU:O	2.20	0.42
1:A:816:VAL:CG2	1:A:887:ILE:HG21	2.47	0.42
1:B:281:GLU:HG3	1:B:314:ALA:CA	2.39	0.42
1:B:723:PHE:HA	1:B:726:ILE:HD12	2.00	0.42
1:B:759:ILE:HD12	1:B:772:GLU:C	2.38	0.42
1:B:762:THR:HG23	1:B:762:THR:O	2.19	0.42
1:B:884:VAL:CG1	1:B:887:ILE:HD12	2.38	0.42
1:B:896:GLU:HB3	1:B:900:ARG:NH2	2.34	0.42
1:B:580:MSE:HE1	1:B:593:ARG:HB3	1.97	0.42
1:B:583:LEU:HA	1:B:584:PRO:HD2	1.68	0.42
1:B:588:ASP:C	1:B:592:GLN:HE21	2.23	0.42
1:B:357:ALA:C	1:B:359:LEU:N	2.72	0.42
1:B:407:LEU:O	1:B:408:MSE:C	2.58	0.42
1:B:679:ALA:HA	1:B:682:GLU:CB	2.50	0.42
1:A:208:PRO:CD	1:A:211:LEU:HD12	2.43	0.42
1:B:112:GLN:HE22	1:B:113:ASP:CG	2.22	0.42
1:B:39:GLU:CD	1:B:41:ARG:HH12	2.23	0.42
1:A:69:MSE:SE	1:A:95:VAL:HB	2.68	0.42
1:A:877:VAL:CG1	1:A:878:ASN:N	2.75	0.42
1:A:539:SER:HB2	1:A:542:GLU:OE2	2.20	0.42
1:A:883:ASP:OD1	1:A:883:ASP:N	2.43	0.42
1:A:458:LYS:O	1:A:462:ASP:CB	2.66	0.42
1:B:175:LEU:H	1:B:175:LEU:CD1	2.28	0.42
1:B:718:PHE:O	1:B:719:ALA:C	2.57	0.42
1:B:473:ILE:HA	1:B:476:GLU:OE1	2.20	0.42
1:B:652:ASN:OD1	1:B:652:ASN:N	2.53	0.42
1:B:114:ARG:NH1	1:B:120:ILE:CG2	2.83	0.42
1:A:950:LEU:C	1:A:952:GLN:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:TRP:HB3	1:A:306:VAL:HG13	2.01	0.42
1:B:706:ILE:N	1:B:706:ILE:HD12	2.35	0.42
1:B:744:ASP:O	1:B:745:HIS:CB	2.68	0.42
1:A:111:PRO:HG2	1:A:958:ASP:HA	2.01	0.42
1:A:777:ILE:O	1:A:778:THR:C	2.57	0.42
1:A:818:LEU:HD13	1:A:845:LEU:HD21	2.01	0.42
1:A:849:GLY:O	1:A:850:ASN:C	2.58	0.42
1:B:185:ILE:CD1	1:B:185:ILE:N	2.80	0.42
1:B:178:GLU:HB2	1:B:422:ARG:NH1	2.35	0.42
1:B:513:ALA:O	1:B:514:ALA:C	2.58	0.42
1:B:434:HIS:O	1:B:609:HIS:HA	2.20	0.42
1:A:521:GLN:O	1:A:522:VAL:C	2.58	0.42
1:A:338:ASP:O	1:A:339:PHE:C	2.58	0.42
1:B:927:VAL:CG1	1:B:929:PRO:HD3	2.45	0.42
1:B:236:ALA:HA	1:B:239:GLN:HE22	1.80	0.42
1:B:277:LEU:CD1	1:B:278:VAL:N	2.82	0.42
1:A:623:ARG:O	1:A:627:GLU:CB	2.68	0.42
1:B:733:ARG:C	1:B:735:ASP:N	2.72	0.42
1:A:640:ARG:O	1:A:641:THR:C	2.58	0.42
1:A:757:ASP:O	1:A:759:ILE:N	2.52	0.42
1:B:814:LEU:HD12	1:B:884:VAL:CG2	2.50	0.42
1:A:438:LEU:N	1:A:438:LEU:HD22	2.35	0.42
1:B:565:ILE:HD12	1:B:566:GLY:N	2.33	0.42
1:A:428:PHE:CE1	1:A:600:ILE:N	2.88	0.42
1:A:378:GLY:HA2	1:A:410:ARG:NE	2.34	0.42
1:B:661:GLU:C	1:B:663:PHE:N	2.71	0.42
1:B:55:PHE:O	1:B:83:TYR:HE2	2.01	0.42
1:A:245:PRO:C	1:A:246:PHE:CD1	2.93	0.42
1:B:219:MSE:C	1:B:225:LEU:H	2.21	0.42
1:B:133:ARG:NH2	1:B:788:LEU:HB3	2.34	0.42
1:B:434:HIS:HB2	1:B:608:ILE:O	2.19	0.42
1:B:385:LEU:N	1:B:385:LEU:CD1	2.77	0.42
1:A:548:ALA:O	1:A:552:GLU:N	2.52	0.42
1:A:465:ARG:CG	1:A:468:LEU:HD12	2.50	0.42
1:A:95:VAL:HG12	1:A:97:LEU:CD1	2.50	0.42
1:A:801:ILE:CG1	1:A:802:SER:N	2.82	0.42
1:B:125:ARG:HG3	1:B:794:GLY:CA	2.50	0.42
1:B:454:MSE:SE	1:B:457:ARG:HH21	2.52	0.42
1:B:466:ASP:C	1:B:468:LEU:N	2.73	0.42
1:B:473:ILE:O	1:B:476:GLU:HG3	2.19	0.42
1:B:509:ILE:HG22	1:B:510:CYS:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:THR:C	1:B:862:ASN:N	2.70	0.42
1:A:485:TRP:NE1	1:A:518:GLN:OE1	2.41	0.42
1:A:856:VAL:CA	1:A:859:GLU:HB2	2.49	0.42
1:A:411:HIS:HE2	1:A:689:LEU:HD23	1.85	0.42
1:B:405:SER:O	1:B:409:ASP:OD2	2.38	0.42
1:A:509:ILE:O	1:A:581:PHE:HB3	2.20	0.42
1:B:161:ILE:O	1:B:162:ALA:C	2.59	0.42
1:B:826:ALA:O	1:B:832:LEU:CD1	2.68	0.42
1:A:819:ILE:HA	1:A:841:VAL:O	2.20	0.42
1:B:461:GLU:O	1:B:464:ALA:HB3	2.20	0.42
1:B:281:GLU:OE2	1:B:313:THR:O	2.38	0.42
1:B:327:ARG:C	1:B:330:LEU:HD13	2.38	0.42
1:B:884:VAL:HA	1:B:887:ILE:CD1	2.50	0.42
1:B:568:GLU:OE1	1:B:570:ARG:NH2	2.53	0.42
1:B:586:ASN:OD1	1:B:587:PRO:HG2	2.19	0.42
1:B:625:TYR:HB3	1:B:632:PHE:CE2	2.55	0.42
1:A:293:SER:N	1:A:296:TYR:HD2	2.17	0.42
1:A:293:SER:O	1:A:294:ARG:C	2.58	0.42
1:B:549:TRP:CD1	1:B:555:THR:HB	2.55	0.42
1:A:435:THR:C	1:A:436:ILE:HD12	2.39	0.42
1:A:417:LEU:CD2	1:A:689:LEU:HD13	2.49	0.42
1:B:411:HIS:HE2	1:B:689:LEU:HD23	1.85	0.42
1:B:679:ALA:HA	1:B:682:GLU:HB3	2.02	0.42
1:B:686:ASP:OD1	1:B:688:LEU:CG	2.66	0.42
1:B:663:PHE:HA	1:B:666:LEU:CD2	2.50	0.42
1:A:110:LYS:CB	1:A:112:GLN:HE22	2.28	0.42
1:B:52:ARG:HH12	1:B:54:MSE:HA	1.84	0.42
1:A:702:LEU:HA	1:A:702:LEU:HD13	1.83	0.42
1:A:825:GLN:N	1:A:825:GLN:OE1	2.53	0.42
1:B:868:VAL:HG11	1:B:872:THR:HG22	2.02	0.42
1:A:803:LEU:HD23	1:A:803:LEU:N	2.34	0.42
1:A:790:LEU:HB2	1:A:793:SER:OG	2.19	0.42
1:A:246:PHE:CZ	1:A:268:HIS:CB	2.99	0.41
1:A:762:THR:CG2	1:A:765:ARG:HB3	2.50	0.41
1:A:884:VAL:O	1:A:888:LEU:CD2	2.67	0.41
1:A:910:ALA:O	1:A:911:ASP:C	2.58	0.41
1:B:191:LEU:N	1:B:191:LEU:CD1	2.83	0.41
1:A:621:LEU:O	1:A:625:TYR:HB2	2.19	0.41
1:B:103:ASP:CG	1:B:105:LYS:HZ3	2.24	0.41
1:A:292:PRO:HB2	1:A:297:GLN:CG	2.50	0.41
1:A:352:VAL:HG23	1:A:353:ALA:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:O	1:B:339:PHE:C	2.58	0.41
1:B:155:ILE:C	1:B:159:LEU:HG	2.39	0.41
1:B:39:GLU:CD	1:B:41:ARG:NH1	2.73	0.41
1:B:714:ASN:ND2	1:B:714:ASN:N	2.56	0.41
1:A:673:GLN:O	1:A:676:ALA:HB3	2.20	0.41
1:A:193:GLN:CG	1:A:194:GLN:H	2.33	0.41
1:A:232:ASP:HA	1:A:258:PHE:CE1	2.54	0.41
1:A:884:VAL:CG1	1:A:887:ILE:HD12	2.40	0.41
1:B:191:LEU:N	1:B:191:LEU:HD12	2.35	0.41
1:B:780:GLU:CA	1:B:780:GLU:OE1	2.49	0.41
1:B:815:LEU:HA	1:B:815:LEU:HD23	1.79	0.41
1:A:379:GLU:O	1:A:381:ASP:OD2	2.37	0.41
1:B:640:ARG:O	1:B:641:THR:C	2.59	0.41
1:B:650:LEU:O	1:B:652:ASN:N	2.52	0.41
1:A:356:VAL:HA	1:A:359:LEU:HD11	2.01	0.41
1:A:356:VAL:O	1:A:359:LEU:HD12	2.20	0.41
1:B:688:LEU:HG	1:B:689:LEU:H	1.85	0.41
1:B:926:ALA:O	1:B:928:ASN:ND2	2.53	0.41
1:B:154:LEU:N	1:B:154:LEU:CD2	2.83	0.41
1:B:539:SER:HB3	1:B:542:GLU:HB2	2.01	0.41
1:A:828:LYS:C	1:A:830:LEU:N	2.72	0.41
1:A:440:LEU:HA	1:A:441:PRO:HD3	1.80	0.41
1:B:827:PRO:HG2	1:B:830:LEU:CD2	2.50	0.41
1:B:730:GLN:CG	1:B:740:LEU:HD21	2.48	0.41
1:A:318:GLN:HB2	1:A:319:LEU:HD12	2.02	0.41
1:A:33:LEU:HD12	1:A:33:LEU:HA	1.90	0.41
1:A:188:GLY:C	1:A:223:PHE:CE2	2.94	0.41
1:B:910:ALA:O	1:B:911:ASP:C	2.58	0.41
1:A:493:TRP:CG	1:A:494:LEU:N	2.84	0.41
1:A:357:ALA:O	1:A:359:LEU:N	2.51	0.41
1:A:376:MSE:C	1:A:378:GLY:H	2.23	0.41
1:A:378:GLY:HA2	1:A:410:ARG:HE	1.86	0.41
1:B:356:VAL:O	1:B:359:LEU:HG	2.20	0.41
1:A:120:ILE:HD12	1:A:120:ILE:O	2.19	0.41
1:A:534:PHE:HB3	1:A:561:LEU:HD22	2.03	0.41
1:A:570:ARG:CG	1:A:570:ARG:HH11	2.32	0.41
1:A:820:TYR:HA	1:A:956:ARG:O	2.19	0.41
1:A:215:TRP:O	1:A:216:LEU:C	2.59	0.41
1:A:718:PHE:O	1:A:719:ALA:C	2.58	0.41
1:A:884:VAL:HA	1:A:887:ILE:CG1	2.49	0.41
1:B:184:THR:HG23	2:B:1001:SO4:O4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:ILE:H	1:B:784:ILE:HG13	1.51	0.41
1:B:833:ASN:ND2	1:B:837:PRO:HB3	2.34	0.41
1:B:640:ARG:O	1:B:644:ASP:OD1	2.39	0.41
1:A:396:ALA:O	1:A:398:SER:N	2.53	0.41
1:A:404:VAL:N	1:A:407:LEU:HD22	2.36	0.41
1:B:343:VAL:C	1:B:347:LYS:HG3	2.38	0.41
1:A:8:ARG:NE	1:A:19:LEU:HD13	2.34	0.41
1:A:202:ARG:CB	1:A:274:TRP:HZ3	2.27	0.41
1:B:706:ILE:C	1:B:708:GLU:H	2.24	0.41
1:B:877:VAL:C	1:B:879:ALA:H	2.24	0.41
1:B:732:ASP:C	1:B:734:GLY:H	2.24	0.41
1:A:145:SER:O	1:A:147:LEU:N	2.50	0.41
1:A:325:PHE:O	1:A:328:LEU:CD2	2.68	0.41
1:A:751:PHE:HB3	1:A:752:PRO:HD2	2.02	0.41
1:A:140:PHE:CB	1:A:837:PRO:HG3	2.49	0.41
1:B:175:LEU:HB2	1:B:312:LEU:HA	2.03	0.41
1:B:895:ILE:O	1:B:898:SER:OG	2.38	0.41
1:B:510:CYS:HG	1:B:562:CYS:HG	1.63	0.41
1:B:586:ASN:CG	1:B:640:ARG:HH21	2.23	0.41
1:B:583:LEU:N	1:B:618:GLN:HE22	2.19	0.41
1:B:346:GLN:OE1	1:B:350:CYS:SG	2.79	0.41
1:B:378:GLY:HA2	1:B:410:ARG:NE	2.35	0.41
1:B:928:ASN:N	1:B:929:PRO:CD	2.83	0.41
1:A:9:TRP:CH2	1:A:52:ARG:HB2	2.55	0.41
1:A:829:GLN:C	1:A:830:LEU:HD22	2.40	0.41
1:B:168:ARG:NH1	1:B:415:ARG:NH1	2.68	0.41
1:A:807:LYS:CB	1:A:808:ALA:HA	2.45	0.41
1:B:696:GLY:O	1:B:697:GLU:C	2.57	0.41
1:A:144:TYR:HD1	1:A:163:HIS:HE2	1.68	0.41
1:A:196:LEU:C	1:A:198:GLY:N	2.74	0.41
1:A:779:TRP:O	1:A:782:PRO:CD	2.46	0.41
1:A:780:GLU:O	1:A:783:LEU:N	2.53	0.41
1:A:141:ARG:HE	1:A:837:PRO:CG	2.31	0.41
1:A:834:ARG:CZ	1:A:913:LYS:HZ2	2.33	0.41
1:B:837:PRO:CB	1:B:838:PRO:CD	2.92	0.41
1:A:453:ILE:O	1:A:455:GLY:N	2.49	0.41
1:A:523:LEU:O	1:A:529:ILE:CD1	2.68	0.41
1:A:343:VAL:C	1:A:347:LYS:HG3	2.41	0.41
1:A:376:MSE:O	1:A:378:GLY:N	2.54	0.41
1:B:353:ALA:HA	1:B:356:VAL:CG2	2.50	0.41
1:B:411:HIS:NE2	1:B:689:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ARG:NH1	1:A:120:ILE:CG2	2.83	0.41
1:B:69:MSE:HG3	1:B:86:THR:C	2.41	0.41
1:A:191:LEU:O	1:A:192:HIS:C	2.58	0.41
1:A:243:TYR:HB2	1:A:244:ASN:H	1.64	0.41
1:A:281:GLU:CD	1:A:314:ALA:CA	2.76	0.41
1:A:759:ILE:HD12	1:A:772:GLU:C	2.40	0.41
1:A:884:VAL:HA	1:A:887:ILE:CD1	2.50	0.41
1:B:148:ARG:HD3	1:B:148:ARG:HA	1.67	0.41
1:B:332:ASP:C	1:B:334:ASN:H	2.24	0.41
1:B:474:TYR:OH	1:B:480:ASP:HB2	2.20	0.41
1:B:521:GLN:HE22	1:B:525:GLU:CG	2.32	0.41
1:B:859:GLU:O	1:B:863:ARG:NH1	2.53	0.41
1:A:371:ASN:N	1:A:371:ASN:ND2	2.64	0.41
1:A:688:LEU:HG	1:A:689:LEU:H	1.86	0.41
1:B:356:VAL:HA	1:B:359:LEU:HD11	2.02	0.41
1:B:365:LEU:CD2	1:B:366:SER:H	2.33	0.41
1:B:407:LEU:N	1:B:407:LEU:CD1	2.84	0.41
1:B:944:GLN:HA	1:B:947:MSE:CG	2.51	0.41
1:A:582:ASP:HA	1:A:618:GLN:HE21	1.80	0.41
1:A:39:GLU:CD	1:A:41:ARG:NH1	2.74	0.41
1:B:710:ASP:N	1:B:710:ASP:OD1	2.53	0.41
1:A:733:ARG:C	1:A:735:ASP:N	2.73	0.41
1:A:141:ARG:NH2	1:A:836:LEU:HA	2.36	0.41
1:B:325:PHE:CD2	1:B:342:PHE:HD2	2.33	0.41
1:A:646:VAL:CG2	1:A:647:TYR:N	2.84	0.41
1:A:648:ASN:C	1:A:651:ILE:HG22	2.41	0.41
1:B:494:LEU:O	1:B:498:LEU:CG	2.63	0.41
1:B:523:LEU:O	1:B:529:ILE:CD1	2.68	0.41
1:B:427:GLY:O	1:B:600:ILE:HA	2.20	0.41
1:A:289:GLU:CD	1:A:290:ASP:H	2.24	0.41
1:A:691:ILE:O	1:A:692:HIS:C	2.57	0.41
1:B:352:VAL:HG23	1:B:353:ALA:N	2.36	0.41
1:B:369:GLU:CD	1:B:372:MSE:HG3	2.41	0.41
1:B:399:ALA:HA	1:B:402:GLU:HB3	2.02	0.41
1:B:406:MSE:HB2	1:B:407:LEU:HD13	2.01	0.41
1:A:155:ILE:O	1:A:155:ILE:CD1	2.68	0.41
1:B:662:GLY:O	1:B:663:PHE:C	2.59	0.41
1:A:539:SER:HB3	1:A:542:GLU:HB2	2.03	0.41
1:B:52:ARG:NH2	1:B:81:LEU:HG	2.34	0.41
1:A:161:ILE:O	1:A:162:ALA:C	2.59	0.41
1:A:706:ILE:C	1:A:708:GLU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:GLY:O	1:A:697:GLU:C	2.58	0.41
1:A:858:PHE:CD1	1:A:861:PHE:CZ	3.09	0.41
1:A:147:LEU:C	1:A:150:GLN:HE22	2.24	0.41
1:A:191:LEU:N	1:A:191:LEU:HD12	2.36	0.41
1:A:281:GLU:CG	1:A:314:ALA:CA	2.86	0.41
1:A:311:LEU:HD11	1:A:327:ARG:HB3	2.02	0.41
1:A:910:ALA:O	1:A:914:LEU:HB2	2.21	0.41
1:B:126:PHE:C	1:B:126:PHE:CD1	2.93	0.41
1:B:182:GLY:HA3	1:B:185:ILE:HD13	2.00	0.41
1:B:769:LEU:CD2	1:B:771:ARG:HH21	2.08	0.41
1:B:12:ASP:OD2	1:B:785:ARG:CZ	2.69	0.41
1:B:149:GLY:H	1:B:777:ILE:HD13	1.86	0.41
1:B:914:LEU:O	1:B:915:SER:C	2.59	0.41
1:B:425:VAL:HG21	1:B:600:ILE:HD11	2.03	0.41
1:B:621:LEU:O	1:B:625:TYR:HB2	2.21	0.41
1:B:296:TYR:CG	1:B:297:GLN:N	2.87	0.41
1:B:842:ARG:NH1	1:B:856:VAL:HG23	2.24	0.41
1:B:530:ARG:HD3	1:B:555:THR:O	2.21	0.41
1:A:436:ILE:HD13	1:A:610:VAL:C	2.42	0.41
1:A:521:GLN:O	1:A:524:ARG:N	2.54	0.41
1:B:376:MSE:O	1:B:378:GLY:N	2.54	0.41
1:A:355:ALA:O	1:A:356:VAL:C	2.58	0.41
1:B:344:GLU:O	1:B:347:LYS:HB2	2.21	0.41
1:B:233:GLU:C	1:B:235:TYR:N	2.74	0.41
1:B:239:GLN:O	1:B:243:TYR:HA	2.21	0.41
1:B:209:GLU:O	1:B:212:GLN:HG3	2.21	0.41
1:B:209:GLU:CA	1:B:212:GLN:HG3	2.51	0.41
1:A:952:GLN:HE21	1:B:948:GLU:HA	1.85	0.41
1:A:105:LYS:C	1:A:106:LEU:HD13	2.41	0.41
1:A:155:ILE:C	1:A:159:LEU:HG	2.38	0.41
1:A:662:GLY:O	1:A:665:ASP:HB2	2.21	0.41
1:A:665:ASP:O	1:A:669:ASN:HB2	2.19	0.41
1:A:112:GLN:O	1:A:115:LEU:HD12	2.21	0.41
1:B:111:PRO:C	1:B:113:ASP:H	2.24	0.41
1:B:111:PRO:HG2	1:B:958:ASP:HA	2.03	0.41
1:B:436:ILE:CD1	1:B:436:ILE:N	2.74	0.41
1:B:832:LEU:H	1:B:832:LEU:CD2	2.33	0.41
1:B:803:LEU:C	1:B:805:LYS:N	2.73	0.41
1:A:133:ARG:NH2	1:A:788:LEU:HB2	2.36	0.41
1:A:215:TRP:O	1:A:218:GLU:N	2.54	0.41
1:A:277:LEU:CD1	1:A:278:VAL:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:MSE:HB3	1:A:322:GLU:H	1.63	0.41
1:A:817:GLU:HA	1:A:817:GLU:OE1	2.21	0.41
1:A:955:TRP:HD1	1:A:955:TRP:O	2.03	0.41
1:B:125:ARG:O	1:B:128:LEU:HB3	2.20	0.41
1:B:196:LEU:C	1:B:198:GLY:N	2.75	0.41
1:B:892:GLU:HA	1:B:895:ILE:CD1	2.49	0.41
1:B:509:ILE:O	1:B:581:PHE:HB3	2.21	0.41
1:B:587:PRO:HD2	1:B:643:TYR:CE2	2.56	0.41
1:B:648:ASN:C	1:B:651:ILE:HG22	2.42	0.41
1:A:520:GLU:C	1:A:520:GLU:CD	2.80	0.41
1:A:337:HIS:HB2	1:A:338:ASP:H	1.76	0.41
1:B:409:ASP:OD1	1:B:409:ASP:N	2.44	0.41
1:B:686:ASP:OD1	1:B:688:LEU:CD2	2.68	0.41
1:A:8:ARG:HG2	1:A:99:GLU:HG3	2.03	0.41
1:B:202:ARG:NH1	1:B:250:GLN:OE1	2.50	0.41
1:B:829:GLN:C	1:B:830:LEU:HD22	2.40	0.41
1:A:176:ALA:HB3	1:A:418:PHE:C	2.41	0.40
1:A:325:PHE:CD2	1:A:342:PHE:HD2	2.34	0.40
1:A:831:GLN:C	1:A:833:ASN:H	2.24	0.40
1:A:489:PRO:HG2	1:A:613:LEU:HD21	2.02	0.40
1:B:485:TRP:CZ2	1:B:518:GLN:NE2	2.85	0.40
1:B:289:GLU:CD	1:B:290:ASP:H	2.23	0.40
1:B:296:TYR:O	1:B:299:ILE:HB	2.21	0.40
1:A:948:GLU:CB	1:B:952:GLN:HE22	2.34	0.40
1:A:19:LEU:N	1:A:106:LEU:HD11	2.36	0.40
1:A:509:ILE:HG22	1:A:510:CYS:N	2.36	0.40
1:B:363:ASN:CB	1:B:364:LYS:HD2	2.51	0.40
1:A:39:GLU:CD	1:A:41:ARG:HH12	2.23	0.40
1:B:156:PRO:CA	1:B:159:LEU:HD12	2.50	0.40
1:A:827:PRO:HG2	1:A:830:LEU:HD21	2.02	0.40
1:B:458:LYS:O	1:B:462:ASP:CB	2.67	0.40
1:A:174:LEU:C	1:A:174:LEU:CD1	2.85	0.40
1:A:281:GLU:OE2	1:A:313:THR:O	2.38	0.40
1:A:123:MSE:CB	1:A:961:ARG:NH2	2.84	0.40
1:A:821:VAL:HA	1:A:839:THR:O	2.22	0.40
1:B:727:GLY:O	1:B:743:SER:HB3	2.20	0.40
1:B:769:LEU:HD13	1:B:771:ARG:NE	2.35	0.40
1:B:287:TRP:CE3	1:B:291:ALA:O	2.75	0.40
1:A:471:GLU:HG3	1:A:490:ARG:HH12	1.86	0.40
1:A:482:ALA:HB1	1:A:518:GLN:OE1	2.21	0.40
1:A:53:VAL:HG12	1:A:55:PHE:CZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ASP:C	1:A:468:LEU:N	2.74	0.40
1:B:90:THR:OG1	1:B:92:GLU:HG3	2.21	0.40
1:B:541:ILE:O	1:B:542:GLU:C	2.58	0.40
1:A:702:LEU:O	1:A:706:ILE:CD1	2.63	0.40
1:A:710:ASP:OD1	1:A:710:ASP:N	2.50	0.40
1:B:941:SER:O	1:B:942:ASN:C	2.59	0.40
1:A:332:ASP:C	1:A:334:ASN:H	2.23	0.40
1:A:219:MSE:O	1:A:225:LEU:N	2.49	0.40
1:B:138:GLU:HG3	1:B:139:GLN:OE1	2.21	0.40
1:B:145:SER:C	1:B:147:LEU:N	2.73	0.40
1:B:716:ILE:O	1:B:720:MSE:HG3	2.21	0.40
1:B:751:PHE:HB3	1:B:752:PRO:HD2	2.02	0.40
1:B:884:VAL:HA	1:B:887:ILE:CG1	2.51	0.40
1:A:506:VAL:HA	1:A:577:HIS:HB2	2.04	0.40
1:B:4:THR:HG22	1:B:80:LEU:HD13	2.04	0.40
1:B:293:SER:O	1:B:294:ARG:C	2.59	0.40
1:A:353:ALA:HA	1:A:356:VAL:CG2	2.51	0.40
1:B:366:SER:HB3	1:B:367:ASN:H	1.77	0.40
1:B:685:ARG:CZ	1:B:687:ARG:NH1	2.85	0.40
1:A:269:LEU:O	1:A:272:ALA:N	2.45	0.40
1:A:84:ILE:HA	1:A:95:VAL:O	2.22	0.40
1:A:705:SER:OG	1:A:706:ILE:HD12	2.21	0.40
1:B:386:LEU:O	1:B:389:ALA:HB3	2.20	0.40
1:A:724:ASP:CA	1:A:730:GLN:HE22	2.34	0.40
1:A:327:ARG:C	1:A:330:LEU:HD13	2.41	0.40
1:B:773:ASP:OD1	1:B:774:ALA:O	2.39	0.40
1:B:780:GLU:O	1:B:783:LEU:N	2.54	0.40
1:A:473:ILE:HA	1:A:476:GLU:OE1	2.22	0.40
1:A:352:VAL:O	1:A:356:VAL:HG23	2.21	0.40
1:A:413:THR:OG1	1:A:414:SER:N	2.55	0.40
1:B:661:GLU:O	1:B:663:PHE:N	2.55	0.40
1:A:661:GLU:O	1:A:663:PHE:N	2.54	0.40
1:B:627:GLU:C	1:B:671:ARG:NH1	2.75	0.40
1:B:156:PRO:N	1:B:159:LEU:HD12	2.37	0.40
1:B:705:SER:OG	1:B:706:ILE:HD12	2.22	0.40
1:B:54:MSE:HG2	1:B:81:LEU:HD11	2.02	0.40
1:B:826:ALA:O	1:B:832:LEU:HD13	2.21	0.40
1:A:386:LEU:HD23	1:A:386:LEU:O	2.20	0.40
1:B:653:TYR:CE2	1:B:660:THR:HB	2.56	0.40
1:A:194:GLN:HG3	1:A:200:ALA:HB2	2.01	0.40
1:A:261:ARG:HD2	1:A:265:ARG:CZ	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:LEU:N	1:A:814:LEU:CD2	2.85	0.40
1:A:888:LEU:O	1:A:891:GLY:N	2.52	0.40
1:B:147:LEU:C	1:B:150:GLN:HE22	2.24	0.40
1:B:284:HIS:CG	1:B:285:LEU:N	2.89	0.40
1:A:646:VAL:O	1:A:650:LEU:N	2.49	0.40
1:B:471:GLU:HG3	1:B:490:ARG:HH12	1.86	0.40
1:B:300:GLU:C	1:B:302:LEU:N	2.75	0.40
1:A:434:HIS:CD2	1:A:607:GLN:NE2	2.89	0.40
1:A:485:TRP:HZ3	1:A:526:ARG:NH2	2.19	0.40
1:A:407:LEU:O	1:A:408:MSE:C	2.60	0.40
1:B:396:ALA:C	1:B:398:SER:N	2.75	0.40
1:B:692:HIS:CE1	1:B:693:SER:HB3	2.56	0.40
1:B:230:PHE:HB3	1:B:254:CYS:SG	2.62	0.40
1:B:269:LEU:O	1:B:272:ALA:N	2.46	0.40
1:A:939:ILE:O	1:A:942:ASN:N	2.55	0.40
1:B:440:LEU:H	1:B:440:LEU:HD12	1.84	0.40
1:B:800:THR:CG2	1:B:803:LEU:HD21	2.52	0.40
1:A:803:LEU:C	1:A:805:LYS:N	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	959/968 (99%)	607 (63%)	238 (25%)	114 (12%)	0 3
1	B	959/968 (99%)	602 (63%)	235 (24%)	122 (13%)	0 2
All	All	1918/1936 (99%)	1209 (63%)	473 (25%)	236 (12%)	0 2

All (236) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ARG
1	A	241	ASP
1	A	273	GLU
1	A	377	ILE
1	A	380	GLN
1	A	381	ASP
1	A	393	SER
1	A	466	ASP
1	A	476	GLU
1	A	483	THR
1	A	511	ALA
1	A	513	ALA
1	A	553	GLU
1	A	565	ILE
1	A	639	GLY
1	A	647	TYR
1	A	690	GLU
1	A	772	GLU
1	A	778	THR
1	A	785	ARG
1	A	786	ASN
1	A	791	ILE
1	A	810	PRO
1	A	811	VAL
1	A	853	ALA
1	A	855	GLN
1	A	928	ASN
1	B	148	ARG
1	B	241	ASP
1	B	273	GLU
1	B	321	MSE
1	B	377	ILE
1	B	380	GLN
1	B	381	ASP
1	B	393	SER
1	B	466	ASP
1	B	476	GLU
1	B	483	THR
1	B	511	ALA
1	B	513	ALA
1	B	553	GLU
1	B	565	ILE
1	B	639	GLY

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Mol	Chain	Res	Type
1	B	647	TYR
1	B	690	GLU
1	B	772	GLU
1	B	778	THR
1	B	785	ARG
1	B	786	ASN
1	B	791	ILE
1	B	810	PRO
1	B	811	VAL
1	B	853	ALA
1	B	928	ASN
1	A	118	GLY
1	A	178	GLU
1	A	211	LEU
1	A	214	GLN
1	A	244	ASN
1	A	245	PRO
1	A	261	ARG
1	A	301	GLN
1	A	313	THR
1	A	315	THR
1	A	318	GLN
1	A	325	PHE
1	A	337	HIS
1	A	339	PHE
1	A	340	ALA
1	A	356	VAL
1	A	358	MSE
1	A	379	GLU
1	A	396	ALA
1	A	522	VAL
1	A	528	GLY
1	A	530	ARG
1	A	568	GLU
1	A	569	GLY
1	A	606	ILE
1	A	643	TYR
1	A	645	SER
1	A	657	PRO
1	A	660	THR
1	A	719	ALA
1	A	729	ASN

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Mol	Chain	Res	Type
1	A	736	ASN
1	A	787	GLY
1	A	800	THR
1	A	834	ARG
1	A	841	VAL
1	A	865	LEU
1	A	883	ASP
1	A	931	ILE
1	A	933	ASP
1	B	118	GLY
1	B	178	GLU
1	B	211	LEU
1	B	214	GLN
1	B	222	ARG
1	B	244	ASN
1	B	245	PRO
1	B	261	ARG
1	B	301	GLN
1	B	313	THR
1	B	318	GLN
1	B	322	GLU
1	B	325	PHE
1	B	337	HIS
1	B	339	PHE
1	B	340	ALA
1	B	356	VAL
1	B	358	MSE
1	B	379	GLU
1	B	396	ALA
1	B	522	VAL
1	B	528	GLY
1	B	530	ARG
1	B	568	GLU
1	B	606	ILE
1	B	643	TYR
1	B	645	SER
1	B	657	PRO
1	B	719	ALA
1	B	729	ASN
1	B	736	ASN
1	B	763	PHE
1	B	776	PHE

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Mol	Chain	Res	Type
1	B	787	GLY
1	B	800	THR
1	B	829	GLN
1	B	834	ARG
1	B	841	VAL
1	B	855	GLN
1	B	865	LEU
1	B	883	ASP
1	B	931	ILE
1	B	933	ASP
1	A	192	HIS
1	A	202	ARG
1	A	218	GLU
1	A	222	ARG
1	A	307	PRO
1	A	314	ALA
1	A	324	HIS
1	A	326	ALA
1	A	397	GLN
1	A	459	SER
1	A	478	GLU
1	A	526	ARG
1	A	709	GLN
1	A	720	MSE
1	A	763	PHE
1	A	776	PHE
1	A	829	GLN
1	A	929	PRO
1	B	160	ASN
1	B	177	ASP
1	B	192	HIS
1	B	202	ARG
1	B	218	GLU
1	B	307	PRO
1	B	314	ALA
1	B	315	THR
1	B	324	HIS
1	B	326	ALA
1	B	397	GLN
1	B	459	SER
1	B	478	GLU
1	B	526	ARG

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Mol	Chain	Res	Type
1	B	569	GLY
1	B	630	ASP
1	B	660	THR
1	B	709	GLN
1	B	720	MSE
1	B	929	PRO
1	B	943	ARG
1	B	951	ASP
1	A	110	LYS
1	A	160	ASN
1	A	177	ASP
1	A	247	ASP
1	A	292	PRO
1	A	321	MSE
1	A	474	TYR
1	A	484	TRP
1	A	498	LEU
1	A	527	GLU
1	A	602	GLN
1	A	625	TYR
1	A	630	ASP
1	A	651	ILE
1	A	680	GLN
1	A	756	GLU
1	A	943	ARG
1	B	110	LYS
1	B	187	ALA
1	B	292	PRO
1	B	465	ARG
1	B	474	TYR
1	B	498	LEU
1	B	527	GLU
1	B	625	TYR
1	B	756	GLU
1	B	758	GLY
1	B	762	THR
1	B	803	LEU
1	B	948	GLU
1	A	269	LEU
1	A	320	GLY
1	A	471	GLU
1	A	514	ALA

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Mol	Chain	Res	Type
1	A	758	GLY
1	B	269	LEU
1	B	317	GLU
1	B	471	GLU
1	B	514	ALA
1	B	570	ARG
1	B	602	GLN
1	B	629	LEU
1	B	680	GLN
1	B	895	ILE
1	A	161	ILE
1	A	243	TYR
1	A	895	ILE
1	A	948	GLU
1	B	161	ILE
1	B	651	ILE
1	B	682	GLU
1	B	826	ALA
1	B	960	LEU
1	A	826	ALA
1	A	506	VAL
1	B	506	VAL
1	B	749	PRO
1	B	856	VAL
1	A	856	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	822/805 (102%)	697 (85%)	125 (15%)	3 17
1	B	822/805 (102%)	696 (85%)	126 (15%)	3 17
All	All	1644/1610 (102%)	1393 (85%)	251 (15%)	3 17

All (251) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	19	LEU
1	A	34	PHE
1	A	36	SER
1	A	53	VAL
1	A	54	MSE
1	A	64	HIS
1	A	67	TRP
1	A	70	GLN
1	A	100	VAL
1	A	105	LYS
1	A	106	LEU
1	A	112	GLN
1	A	114	ARG
1	A	115	LEU
1	A	122	ARG
1	A	123	MSE
1	A	124	ASP
1	A	125	ARG
1	A	126	PHE
1	A	140	PHE
1	A	154	LEU
1	A	155	ILE
1	A	174	LEU
1	A	175	LEU
1	A	177	ASP
1	A	178	GLU
1	A	196	LEU
1	A	217	VAL
1	A	219	MSE
1	A	230	PHE
1	A	237	GLU
1	A	243	TYR
1	A	247	ASP
1	A	253	ILE
1	A	256	LEU
1	A	260	ARG
1	A	262	SER
1	A	268	HIS
1	A	274	TRP
1	A	275	ASP
1	A	276	LEU
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	287	TRP
1	A	290	ASP
1	A	296	TYR
1	A	315	THR
1	A	318	GLN
1	A	319	LEU
1	A	321	MSE
1	A	337	HIS
1	A	343	VAL
1	A	346	GLN
1	A	349	TYR
1	A	360	LEU
1	A	365	LEU
1	A	373	LEU
1	A	381	ASP
1	A	385	LEU
1	A	400	ARG
1	A	401	GLN
1	A	403	LEU
1	A	407	LEU
1	A	409	ASP
1	A	422	ARG
1	A	440	LEU
1	A	444	TYR
1	A	466	ASP
1	A	467	MSE
1	A	468	LEU
1	A	475	GLN
1	A	476	GLU
1	A	485	TRP
1	A	504	GLN
1	A	510	CYS
1	A	515	THR
1	A	519	LEU
1	A	527	GLU
1	A	529	ILE
1	A	553	GLU
1	A	561	LEU
1	A	574	PHE
1	A	585	PHE
1	A	588	ASP
1	A	605	ASP

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	647	TYR
1	A	650	LEU
1	A	652	ASN
1	A	660	THR
1	A	666	LEU
1	A	675	GLU
1	A	682	GLU
1	A	688	LEU
1	A	692	HIS
1	A	694	ASN
1	A	700	GLN
1	A	714	ASN
1	A	722	LEU
1	A	729	ASN
1	A	732	ASP
1	A	733	ARG
1	A	750	ASP
1	A	751	PHE
1	A	763	PHE
1	A	779	TRP
1	A	780	GLU
1	A	788	LEU
1	A	801	ILE
1	A	802	SER
1	A	806	ASN
1	A	830	LEU
1	A	831	GLN
1	A	845	LEU
1	A	851	ASN
1	A	859	GLU
1	A	868	VAL
1	A	883	ASP
1	A	912	GLU
1	A	918	LEU
1	A	931	ILE
1	A	932	ARG
1	A	951	ASP
1	A	955	TRP
1	A	962	LEU
1	B	12	ASP
1	B	19	LEU

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Mol	Chain	Res	Type
1	B	34	PHE
1	B	36	SER
1	B	53	VAL
1	B	54	MSE
1	B	64	HIS
1	B	67	TRP
1	B	70	GLN
1	B	81	LEU
1	B	100	VAL
1	B	105	LYS
1	B	106	LEU
1	B	108	PHE
1	B	112	GLN
1	B	114	ARG
1	B	115	LEU
1	B	122	ARG
1	B	123	MSE
1	B	124	ASP
1	B	125	ARG
1	B	126	PHE
1	B	140	PHE
1	B	154	LEU
1	B	155	ILE
1	B	174	LEU
1	B	175	LEU
1	B	177	ASP
1	B	178	GLU
1	B	196	LEU
1	B	217	VAL
1	B	219	MSE
1	B	230	PHE
1	B	237	GLU
1	B	243	TYR
1	B	247	ASP
1	B	253	ILE
1	B	256	LEU
1	B	260	ARG
1	B	262	SER
1	B	268	HIS
1	B	274	TRP
1	B	275	ASP
1	B	276	LEU

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Mol	Chain	Res	Type
1	B	285	LEU
1	B	287	TRP
1	B	290	ASP
1	B	296	TYR
1	B	315	THR
1	B	318	GLN
1	B	319	LEU
1	B	337	HIS
1	B	343	VAL
1	B	346	GLN
1	B	349	TYR
1	B	360	LEU
1	B	364	LYS
1	B	365	LEU
1	B	371	ASN
1	B	373	LEU
1	B	385	LEU
1	B	400	ARG
1	B	401	GLN
1	B	403	LEU
1	B	407	LEU
1	B	409	ASP
1	B	422	ARG
1	B	440	LEU
1	B	444	TYR
1	B	466	ASP
1	B	467	MSE
1	B	468	LEU
1	B	475	GLN
1	B	476	GLU
1	B	485	TRP
1	B	503	SER
1	B	504	GLN
1	B	510	CYS
1	B	515	THR
1	B	519	LEU
1	B	527	GLU
1	B	529	ILE
1	B	553	GLU
1	B	561	LEU
1	B	574	PHE
1	B	585	PHE

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Mol	Chain	Res	Type
1	B	588	ASP
1	B	605	ASP
1	B	629	LEU
1	B	650	LEU
1	B	652	ASN
1	B	659	GLN
1	B	660	THR
1	B	666	LEU
1	B	675	GLU
1	B	682	GLU
1	B	688	LEU
1	B	692	HIS
1	B	694	ASN
1	B	700	GLN
1	B	714	ASN
1	B	722	LEU
1	B	729	ASN
1	B	732	ASP
1	B	733	ARG
1	B	737	MSE
1	B	751	PHE
1	B	763	PHE
1	B	779	TRP
1	B	788	LEU
1	B	801	ILE
1	B	806	ASN
1	B	830	LEU
1	B	831	GLN
1	B	845	LEU
1	B	851	ASN
1	B	859	GLU
1	B	868	VAL
1	B	883	ASP
1	B	912	GLU
1	B	918	LEU
1	B	931	ILE
1	B	932	ARG
1	B	951	ASP
1	B	955	TRP
1	B	962	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	78	ASN
1	A	112	GLN
1	A	150	GLN
1	A	194	GLN
1	A	212	GLN
1	A	224	ASN
1	A	239	GLN
1	A	244	ASN
1	A	301	GLN
1	A	318	GLN
1	A	341	GLN
1	A	348	ASN
1	A	371	ASN
1	A	380	GLN
1	A	397	GLN
1	A	401	GLN
1	A	504	GLN
1	A	521	GLN
1	A	558	GLN
1	A	573	GLN
1	A	577	HIS
1	A	586	ASN
1	A	592	GLN
1	A	607	GLN
1	A	618	GLN
1	A	674	HIS
1	A	700	GLN
1	A	714	ASN
1	A	721	ASN
1	A	729	ASN
1	A	786	ASN
1	A	851	ASN
1	A	889	GLN
1	A	908	ASN
1	A	944	GLN
1	A	952	GLN
1	B	78	ASN
1	B	112	GLN
1	B	150	GLN
1	B	194	GLN
1	B	212	GLN
1	B	224	ASN

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Mol	Chain	Res	Type
1	B	239	GLN
1	B	301	GLN
1	B	318	GLN
1	B	341	GLN
1	B	346	GLN
1	B	348	ASN
1	B	371	ASN
1	B	380	GLN
1	B	397	GLN
1	B	401	GLN
1	B	504	GLN
1	B	521	GLN
1	B	558	GLN
1	B	573	GLN
1	B	577	HIS
1	B	586	ASN
1	B	592	GLN
1	B	602	GLN
1	B	607	GLN
1	B	674	HIS
1	B	700	GLN
1	B	714	ASN
1	B	721	ASN
1	B	729	ASN
1	B	786	ASN
1	B	851	ASN
1	B	889	GLN
1	B	908	ASN
1	B	944	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	SO4	A	1001	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	B	1001	-	4,4,4	0.45	0	6,6,6	0.11	0

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	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1001	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SO4	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	938/968 (96%)	-0.42	8 (0%)	85	78	15, 62, 87, 88	0
1	B	938/968 (96%)	-0.42	10 (1%)	82	72	15, 60, 86, 88	0
All	All	1876/1936 (96%)	-0.42	18 (0%)	84	75	15, 61, 87, 88	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	84	ILE	4.2
1	B	10	ILE	3.3
1	A	74	VAL	2.8
1	A	49	PRO	2.7
1	B	82	THR	2.7
1	A	71	VAL	2.6
1	B	102	LEU	2.6
1	B	9	TRP	2.5
1	A	22	VAL	2.5
1	A	48	SER	2.4
1	A	61	ILE	2.3
1	B	959	ALA	2.3
1	B	25	VAL	2.2
1	B	49	PRO	2.2
1	A	75	LYS	2.1
1	B	32	LEU	2.1
1	B	44	ALA	2.1
1	B	561	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	1001	5/5	0.97	0.14	-0.83	63,65,67,67	0
2	SO4	A	1001	5/5	0.96	0.14	-1.01	63,65,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.