Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:57 am BST

PDB ID	:	1TR2
Title	:	Crystal structure of human full-length vinculin (residues 1-1066)
Authors	:	Borgon, R.A.; Vonrhein, C.; Bricogne, G.; Bois, P.R.; Izard, T.
Deposited on	:	2004-06-19
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

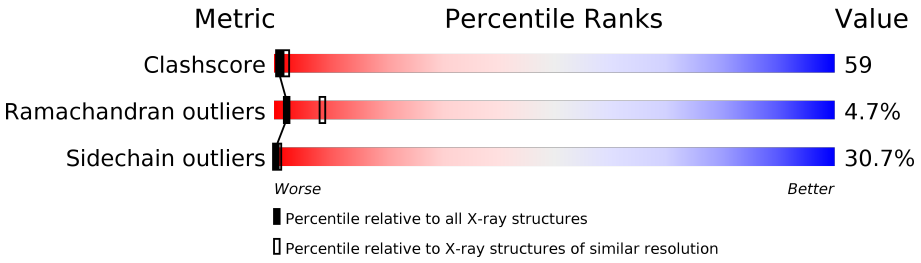
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1066	28% 48% 19%
1	B	1066	29% 48% 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16033 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 VINCULIN ISOFORM 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1028	Total	C	N	O	S	Se	99	8	0
			7908	4876	1436	1550	10	36			
1	B	1029	Total	C	N	O	S	Se	117	7	0
			7907	4873	1438	1550	10	36			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	INITIATING METHIONINE	UNP P18206
A	26	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	74	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	94	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	154	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	168	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	171	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	174	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	190	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	195	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	209	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	237	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	266	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	327	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	331	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	350	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	377	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	533	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	534	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	587	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	591	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	698	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	709	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	741	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	748	MSE	MET	MODIFIED RESIDUE	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
A	797	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	799	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	898	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	899	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	900	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	926	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	930	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	933	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1005	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1022	MSE	MET	MODIFIED RESIDUE	UNP P18206
A	1031	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1	MSE	MET	INITIATING METHIONINE	UNP P18206
B	26	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	74	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	94	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	154	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	168	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	171	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	174	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	190	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	195	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	209	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	237	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	266	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	327	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	331	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	350	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	377	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	533	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	534	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	587	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	591	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	698	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	709	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	741	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	748	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	797	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	799	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	898	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	899	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	900	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	926	MSE	MET	MODIFIED RESIDUE	UNP P18206

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Chain	Residue	Modelled	Actual	Comment	Reference
B	930	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	933	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1005	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1022	MSE	MET	MODIFIED RESIDUE	UNP P18206
B	1031	MSE	MET	MODIFIED RESIDUE	UNP P18206

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	108	Total O 108 108	0	0
2	B	110	Total O 110 110	0	0

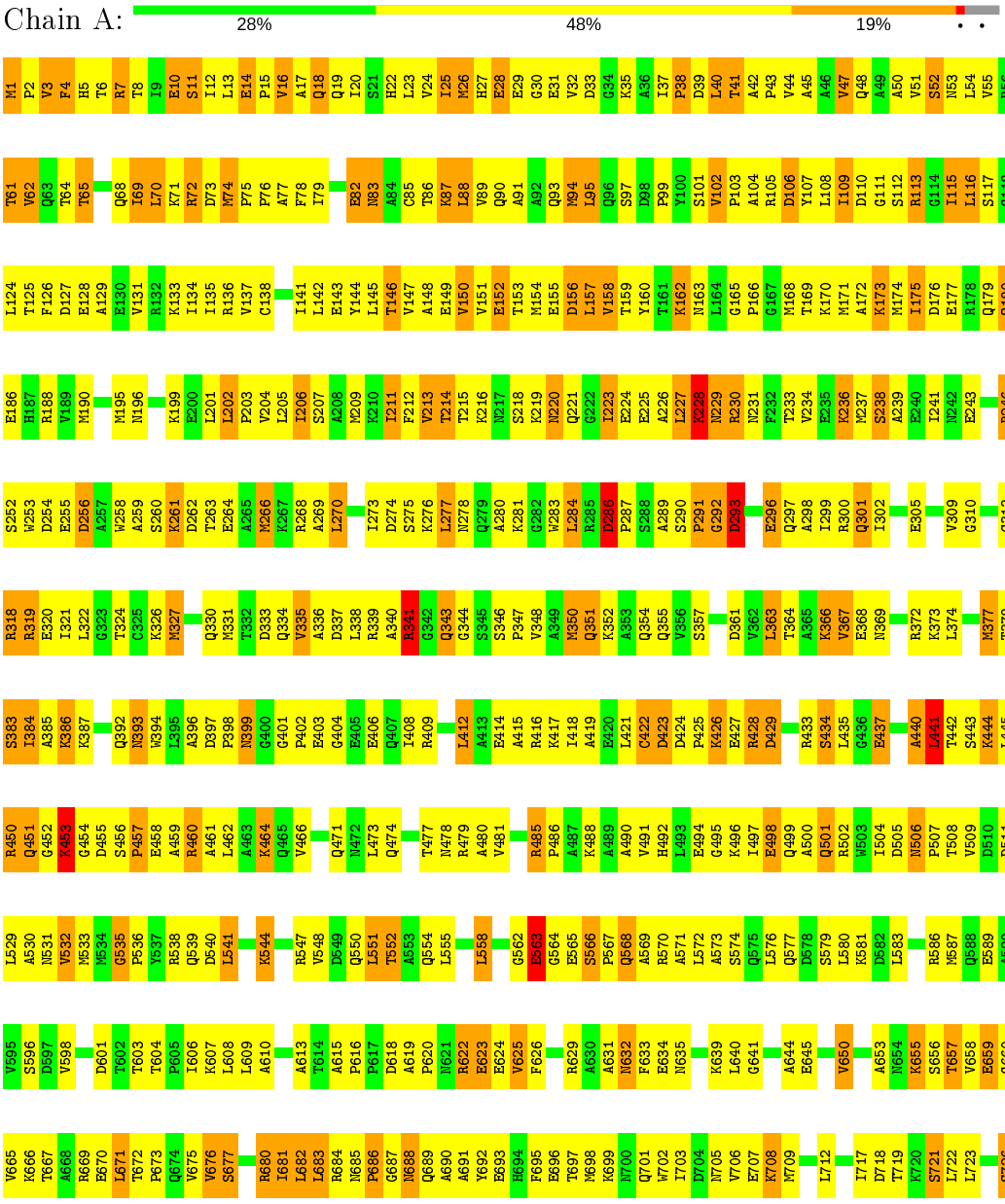
3 Residue-property plots (i)

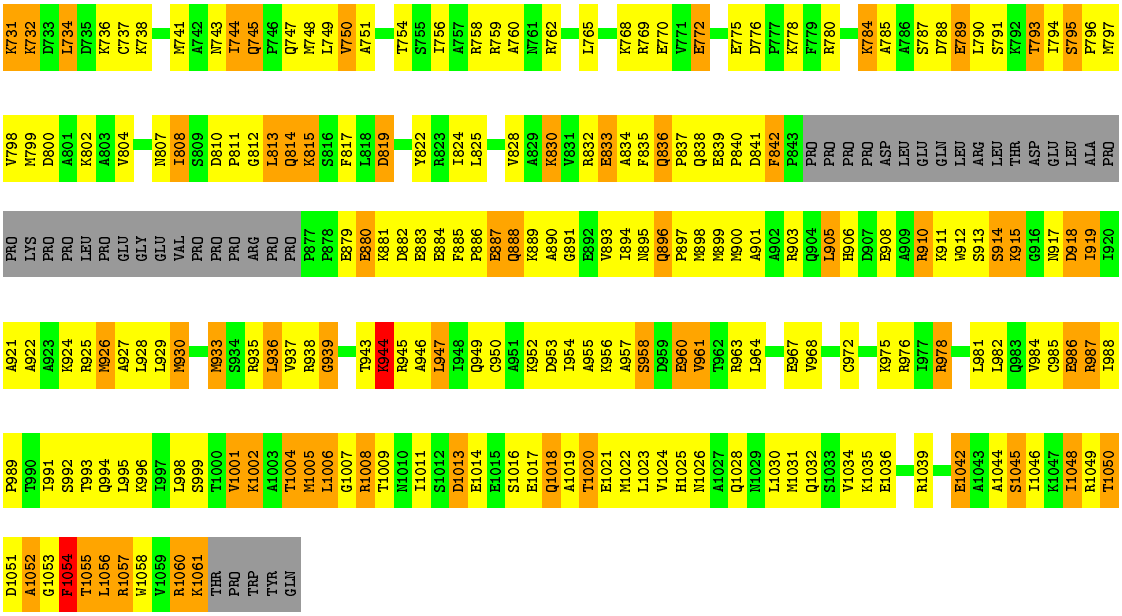
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

- Molecule 1: VINCULIN ISOFORM 1

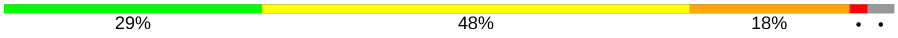
Chain A:

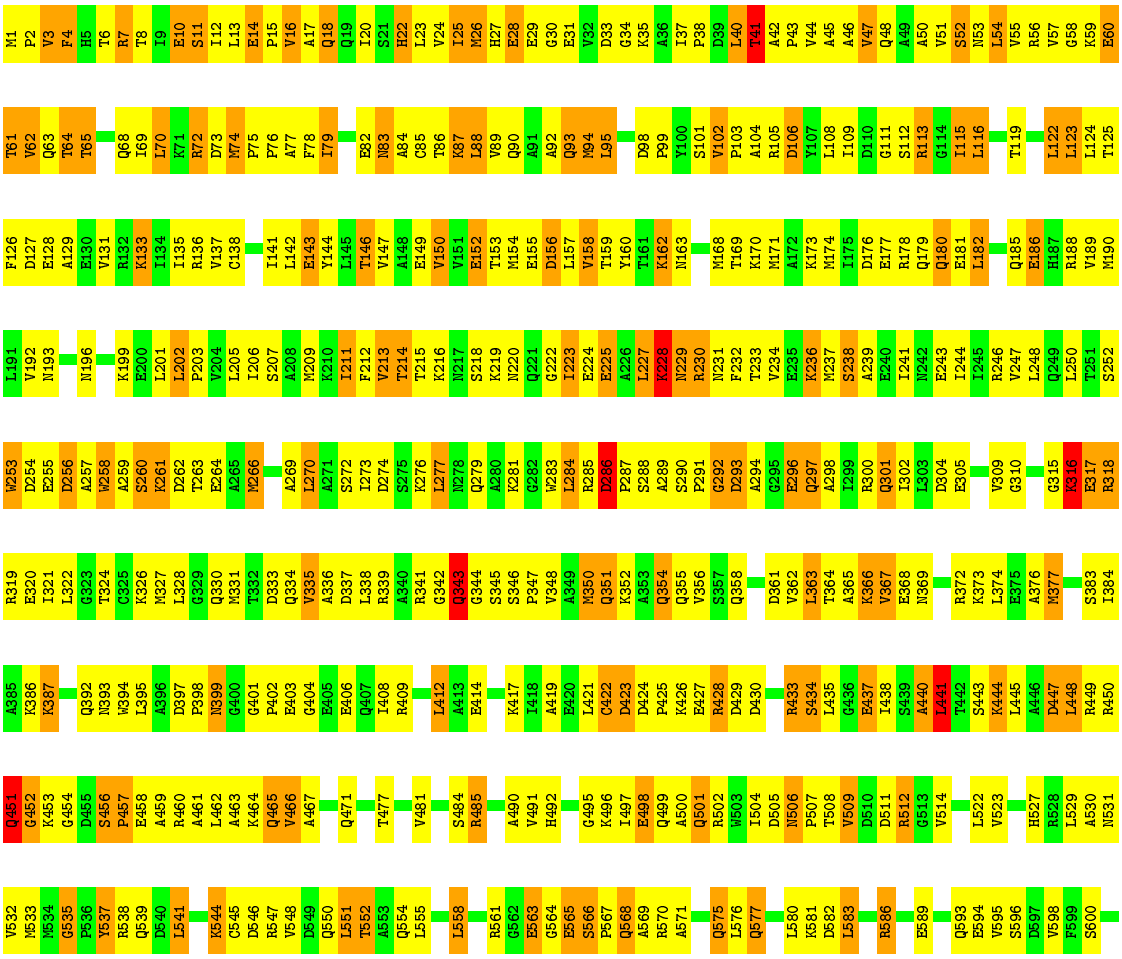


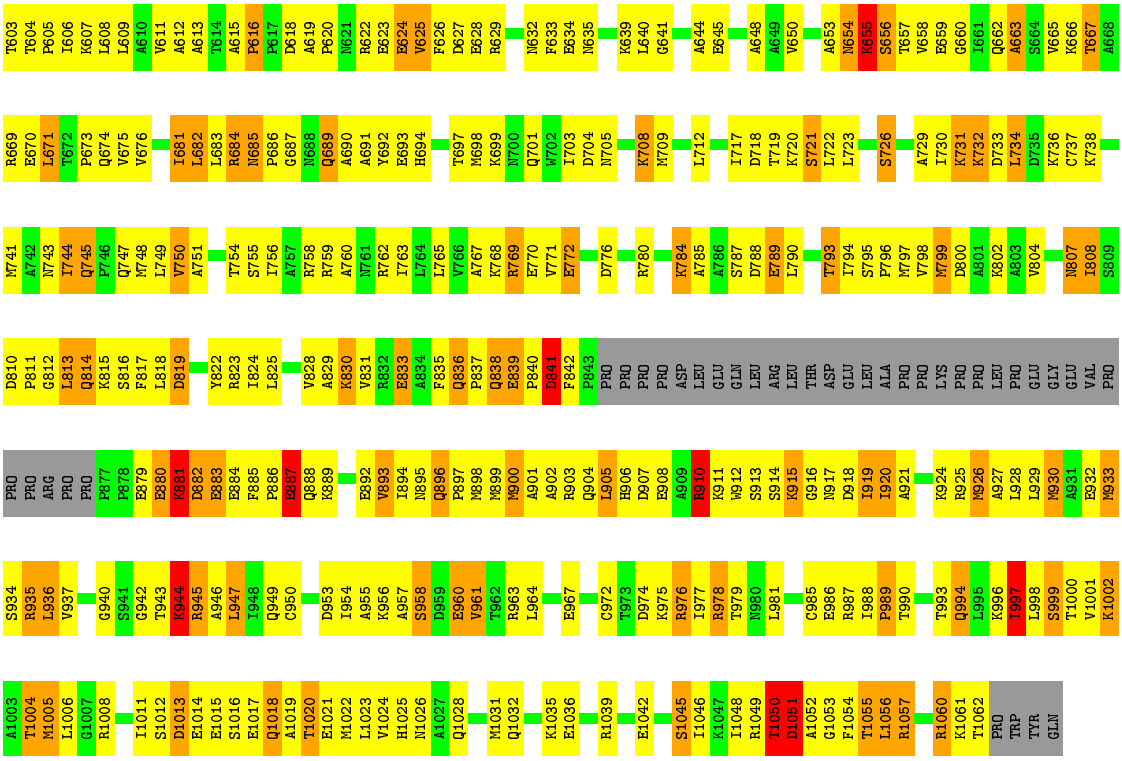


• Molecule 1: VINCULIN ISOFORM 1

Chain B:






T603 T604 P605 I606 K607 L608 L609 A610 V611 A612 A613 T614 A615 P616 P617 D618 A619 P620 N621 R622 E623 E624 V625 F626 D627 E628 R629 N632 F633 E634 N635 K639 L640 G641 A644 E645 A648 A649 V650 A653 N654 K655 S656 T657 V658 E659 G660 I661 Q662 A663 S664 V665 K666 T667 A668
R669 E670 L671 T672 P673 Q674 V675 V676 I681 L682 L683 R684 N685 P686 G687 N688 Q689 A690 A691 Y692 E693 H694 T697 M698 K699 N700 Q701 W702 I703 D704 N705 K708 M709 L712 I717 D718 T719 K720 S721 L722 L723 S726 A729 I730 K731 K732 D733 L734 D735 K736 C737 K738
M741 A742 N743 I744 Q745 F746 Q747 M748 L749 V750 A751 T754 S755 I756 A757 R758 R759 A760 N761 R762 I763 L764 L765 V766 A767 K768 R769 E770 V771 E772 D776 R780 K784 A785 A786 S787 D788 E789 L790 T793 I794 S795 P796 M797 V798 M799 D800 A801 K802 A803 V804 N807 I808 S809
D810 P811 G812 L813 Q814 K815 S816 F817 L818 D819 Y822 R823 I824 L825 V828 A829 K830 V831 R832 E833 A834 F835 Q836 P837 Q838 E839 P840 D841 F842 P843 PRO PRO PRO PRO ASP LEU GLU GLN LEU ARG LEU THR ASP GLU LEU ALA PRO PRO LYS PRO PRO LEU PRO GLU GLY GLU VAL PRO
PRO PRO ARG PRO PRO P877 P878 E879 E880 K881 D882 E883 E884 F885 P886 E887 Q888 K889 E892 V893 I894 N895 Q896 P897 M898 M899 N900 A901 A902 R903 Q904 L905 H906 D907 E908 A909 R910 K911 W912 S913 S914 K915 G916 N917 D918 I919 I920 A921 K924 R925 M926 A927 L928 L929 M930 A931 E932 M933
S934 R935 L936 V937 G940 S941 G942 T943 K944 R945 A946 L947 I948 Q949 C950 D953 I954 A955 K956 A957 S958 D959 E960 V961 T962 R963 L964 E967 C972 T973 D974 K975 R976 I977 R978 T979 N980 L981 C985 E986 R987 I988 P989 T990 T993 Q994 L995 K996 I997 L998 S999 T1000 V1001 K1002
A1003 T1004 M1005 L1006 G1007 R1008 I1011 S1012 D1013 E1014 E1015 S1016 E1017 Q1018 A1019 T1020 E1021 M1022 L1023 V1024 H1025 N1026 A1027 Q1028 M1031 Q1032 K1035 E1036 R1039 E1042 S1045 I1046 K1047 I1048 R1049 T1050 D1051 A1052 G1053 F1054 T1055 L1056 R1057 R1060 K1061 T1062 PRO TRP TYR GLN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.74Å 154.08Å 108.95Å 90.00° 90.44° 90.00°	Depositor
Resolution (Å)	56.86 – 2.90	Depositor
% Data completeness (in resolution range)	100.0 (56.86-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	BUSTER-TNT 1.1.1	Depositor
R, R_{free}	0.232 , 0.300	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16033	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.39	0/7994	0.61	2/10720 (0.0%)
1	B	0.38	0/7992	0.60	1/10717 (0.0%)
All	All	0.38	0/15986	0.61	3/21437 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1054	PHE	CB-CG-CD2	-10.78	113.25	120.80
1	A	1054	PHE	CB-CG-CD1	7.84	126.29	120.80
1	B	616	PRO	CA-N-CD	-5.02	104.48	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7908	0	8065	912	0
1	B	7907	0	8072	958	0
2	A	108	0	0	12	0
2	B	110	0	0	12	0
All	All	16033	0	16137	1865	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 59.

All (1865) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:HG21	1:B:70:LEU:HD22	1.21	1.18
1:A:74:MSE:HE3	1:A:122:LEU:HD21	1.18	1.18
1:B:913:SER:HB2	1:B:915:LYS:HG3	1.24	1.17
1:B:729:ALA:HA	1:B:732:LYS:HD3	1.24	1.16
1:B:215:THR:HG22	1:B:223:ILE:HG13	1.26	1.16
1:A:732:LYS:HE2	1:A:736:LYS:HE2	1.28	1.14
1:A:898:MSE:HE1	1:A:1023:LEU:HD23	1.30	1.14
1:A:65:THR:HG21	1:A:70:LEU:HD22	1.19	1.12
1:A:426:LYS:HE3	1:A:427:GLU:HG3	1.23	1.10
1:B:153:THR:HB	1:B:156:ASP:HB2	1.12	1.08
1:B:697:THR:HG22	1:B:698:MSE:HE2	1.35	1.08
1:A:153:THR:HB	1:A:156:ASP:HB2	1.10	1.08
1:A:807:ASN:HB3	1:A:810:ASP:HB3	1.37	1.07
1:B:20:ILE:HD11	1:B:115:ILE:HG12	1.09	1.06
1:B:807:ASN:ND2	1:B:807:ASN:H	1.45	1.06
1:A:53:ASN:HB3	1:B:288:SER:HB2	1.35	1.06
1:A:913:SER:HB2	1:A:915:LYS:HG2	1.35	1.03
1:B:613:ALA:HB1	1:B:682:LEU:HD12	1.41	1.02
1:A:158:VAL:HG13	1:A:162:LYS:HE3	1.41	1.02
1:B:216:LYS:HA	1:B:223:ILE:HG12	1.40	1.01
1:A:281:LYS:HA	1:A:284:LEU:HD12	1.40	1.01
1:A:74:MSE:CE	1:A:122:LEU:HD21	1.91	1.01
1:B:158:VAL:HG13	1:B:162:LYS:HE3	1.45	0.99
1:A:445:LEU:HB2	1:A:462:LEU:HD23	1.45	0.99
1:A:441:LEU:HA	1:A:444:LYS:HZ2	1.28	0.98
1:B:256:ASP:HA	1:B:258:TRP:CZ3	1.98	0.98
1:A:770:GLU:HG2	1:A:835:PHE:HE1	1.29	0.97
1:B:898:MSE:HE1	1:B:1023:LEU:HD23	1.47	0.96
1:A:491:VAL:HG11	1:A:658:VAL:HG11	1.44	0.96
1:A:215:THR:HG22	1:A:223:ILE:HG13	1.46	0.95
1:A:811:PRO:HB3	1:A:815:LYS:HE2	1.47	0.95
1:A:589:GLU:HG2	1:A:593:GLN:HE21	1.30	0.94
1:A:441:LEU:HD23	1:A:441:LEU:H	1.33	0.94
1:B:589:GLU:HG2	1:B:593:GLN:HE21	1.27	0.94
1:B:671:LEU:H	1:B:671:LEU:HD23	1.33	0.94
1:A:109:ILE:HD13	1:A:1008[B]:ARG:HH21	1.29	0.93
1:A:20:ILE:HD11	1:A:115:ILE:HG12	1.49	0.93
1:A:113:ARG:HB2	1:A:1004:THR:HG21	1.51	0.93
1:A:447:ASP:HA	1:A:450:ARG:HD2	1.50	0.93
1:B:897:PRO:HB2	1:B:1024:VAL:HG11	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:LYS:HA	1:B:741:MSE:HE2	1.50	0.93
1:B:22:HIS:HA	1:B:25:ILE:HG13	1.47	0.93
1:B:31:GLU:HA	1:B:105:ARG:NH2	1.84	0.92
1:B:936:LEU:HB3	1:B:943:THR:HG23	1.49	0.92
1:A:778:LYS:HD2	1:A:1049:ARG:HH12	1.35	0.92
1:B:913:SER:HB2	1:B:915:LYS:CG	2.00	0.92
1:B:448:LEU:HA	1:B:451:GLN:HG2	1.51	0.92
1:A:69:ILE:H	1:A:69:ILE:HD12	1.33	0.91
1:B:40:LEU:HB2	1:B:43:PRO:CG	1.98	0.91
1:A:453:LYS:HD2	1:A:453:LYS:H	1.34	0.91
1:B:1:MSE:HE1	1:B:1018:GLN:NE2	1.86	0.91
1:A:409[B]:ARG:NH2	1:A:442:THR:HB	1.86	0.91
1:B:75:PRO:HA	1:B:78:PHE:CD2	2.06	0.91
1:A:770:GLU:HG2	1:A:835:PHE:CE1	2.05	0.90
1:A:960:GLU:HG2	1:A:963:ARG:HH21	1.36	0.90
1:B:138:CYS:SG	1:B:171:MSE:HE3	2.10	0.90
1:B:74:MSE:HE3	1:B:122:LEU:HD21	1.54	0.90
1:A:51:VAL:HG11	1:A:115:ILE:HD12	1.53	0.90
1:B:906:HIS:HB2	1:B:927:ALA:HB1	1.52	0.90
1:B:926:MSE:HA	1:B:929:LEU:HB2	1.53	0.90
1:B:215:THR:HG23	1:B:220:ASN:HB2	1.52	0.90
1:B:40:LEU:HB2	1:B:43:PRO:HG2	1.50	0.90
1:B:116:LEU:HD13	1:B:1001:VAL:HG23	1.53	0.90
1:B:793:THR:HG23	1:B:824:ILE:HG12	1.52	0.90
1:B:179:GLN:HA	1:B:182:LEU:HD22	1.50	0.90
1:B:445:LEU:HB2	1:B:462:LEU:HD23	1.54	0.90
1:A:28:GLU:HG2	1:A:945:ARG:HE	1.37	0.90
1:A:491:VAL:CG1	1:A:658:VAL:HG11	2.01	0.89
1:A:138:CYS:SG	1:A:171:MSE:HE3	2.12	0.89
1:A:74:MSE:HE2	1:A:78:PHE:CZ	2.07	0.89
1:B:153:THR:HG22	1:B:154:MSE:H	1.36	0.89
1:B:533:MSE:CE	1:B:541:LEU:HD12	2.01	0.89
1:B:807:ASN:HD22	1:B:807:ASN:H	0.94	0.89
1:A:914:SER:N	1:A:915:LYS:HE2	1.88	0.89
1:A:675:VAL:HG22	1:A:698:MSE:HB3	1.54	0.88
1:A:789:GLU:HG2	1:A:830:LYS:NZ	1.88	0.88
1:B:281:LYS:HA	1:B:284:LEU:HD12	1.55	0.88
1:B:770:GLU:HG2	1:B:835:PHE:HE1	1.38	0.88
1:A:688:ASN:O	1:A:690:ALA:N	2.07	0.88
1:A:936:LEU:HB3	1:A:943:THR:HG23	1.56	0.88
1:A:75:PRO:HA	1:A:78:PHE:CD2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LYS:CA	1:B:223:ILE:HG12	2.03	0.87
1:A:641:GLY:HA2	1:A:709:MSE:HE1	1.56	0.87
1:B:69:ILE:HD12	1:B:69:ILE:H	1.40	0.87
1:B:807:ASN:HD22	1:B:807:ASN:N	1.73	0.87
1:A:558:LEU:HD22	1:A:569:ALA:HB2	1.53	0.87
1:A:153:THR:HB	1:A:156:ASP:CB	2.03	0.87
1:B:95:LEU:HD21	1:B:105:ARG:HG3	1.57	0.86
1:B:27:HIS:CD2	1:B:108:LEU:HD23	2.10	0.86
1:A:153:THR:HG22	1:A:154:MSE:H	1.39	0.86
1:B:898:MSE:HE1	1:B:1023:LEU:CD2	2.04	0.86
1:A:220:ASN:HD22	1:A:220:ASN:H	1.21	0.86
1:B:113:ARG:HB3	1:B:1004:THR:CG2	2.05	0.86
1:B:394:TRP:HE1	1:B:401:GLY:H	1.22	0.86
1:A:441:LEU:HA	1:A:444:LYS:NZ	1.90	0.86
1:B:558:LEU:HD22	1:B:569:ALA:HB2	1.56	0.86
1:B:276:LYS:HE3	1:B:301:GLN:HE21	1.40	0.86
1:B:94:MSE:HE2	1:B:104:ALA:HB2	1.55	0.86
1:A:926:MSE:HA	1:A:929:LEU:HB2	1.56	0.86
1:B:1005:MSE:HE1	1:B:1015:GLU:HG2	1.58	0.86
1:B:530:ALA:HA	1:B:533:MSE:HE3	1.58	0.85
1:A:70:LEU:HG	1:A:74:MSE:HG3	1.57	0.85
1:B:22:HIS:HA	1:B:25:ILE:CG1	2.06	0.85
1:B:412:LEU:HB3	1:B:435:LEU:HD22	1.58	0.85
1:A:259:ALA:HA	1:A:485:ARG:HH12	1.42	0.85
1:B:394:TRP:CD1	1:B:404:GLY:HA3	2.12	0.85
1:B:945:ARG:NH2	1:B:946:ALA:HB2	1.91	0.85
1:A:1024:VAL:O	1:A:1028:GLN:HG3	1.76	0.85
1:B:149:GLU:HA	1:B:230:ARG:NH2	1.92	0.84
1:A:65:THR:HG21	1:A:70:LEU:CD2	2.06	0.84
1:B:74:MSE:CE	1:B:122:LEU:HD21	2.06	0.84
1:B:738:LYS:HA	1:B:741:MSE:CE	2.07	0.84
1:B:729:ALA:CA	1:B:732:LYS:HD3	2.08	0.84
1:B:807:ASN:N	1:B:807:ASN:ND2	2.25	0.84
1:B:533:MSE:HE1	1:B:541:LEU:HD12	1.60	0.84
1:B:40:LEU:O	1:B:43:PRO:HD2	1.78	0.84
1:A:266:MSE:HG3	1:A:309:VAL:HG22	1.60	0.83
1:B:924:LYS:HZ1	1:B:1061:LYS:HE3	1.42	0.83
1:A:917:ASN:HA	1:A:1056:LEU:HD23	1.59	0.83
1:A:289:ALA:HB3	1:A:339:ARG:HH12	1.43	0.83
1:A:933:MSE:HG3	1:A:950:CYS:SG	2.18	0.83
1:B:441:LEU:HD23	1:B:441:LEU:H	1.42	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:HA	1:B:997:ILE:HD11	1.60	0.82
1:B:448:LEU:HA	1:B:451:GLN:CG	2.09	0.82
1:A:37:ILE:HD13	1:A:105:ARG:HG2	1.61	0.82
1:B:47:VAL:HG12	1:B:115:ILE:HD13	1.60	0.82
1:A:276:LYS:HE3	1:A:301:GLN:NE2	1.94	0.82
1:A:143:GLU:O	1:A:146:THR:HB	1.78	0.82
1:A:276:LYS:HE3	1:A:301:GLN:HE21	1.42	0.82
1:A:74:MSE:HE3	1:A:122:LEU:CD2	2.06	0.82
1:B:644:ALA:CB	1:B:709:MSE:HE2	2.09	0.82
1:A:448:LEU:HA	1:A:451:GLN:HG2	1.60	0.82
1:B:444:LYS:HZ2	1:B:444:LYS:HB2	1.43	0.82
1:B:75:PRO:HA	1:B:78:PHE:CE2	2.15	0.81
1:A:27:HIS:NE2	1:A:109:ILE:HB	1.94	0.81
1:B:936:LEU:HB3	1:B:943:THR:CG2	2.10	0.81
1:A:179:GLN:HA	1:A:182:LEU:HD22	1.63	0.81
1:A:297[B]:GLN:HG2	1:A:298:ALA:N	1.96	0.81
1:B:205:LEU:HB2	1:B:237:MSE:HE1	1.62	0.81
1:B:297:GLN:HA	1:B:297:GLN:NE2	1.94	0.81
1:A:732:LYS:CE	1:A:736:LYS:HE2	2.09	0.80
1:A:936:LEU:HB3	1:A:943:THR:CG2	2.10	0.80
1:A:836:GLN:NE2	1:A:837:PRO:HD2	1.96	0.80
1:B:594:GLU:O	1:B:598:VAL:HG23	1.82	0.80
1:B:563:GLU:HG3	1:B:564:GLY:N	1.96	0.80
1:B:53:ASN:O	1:B:57:VAL:HG22	1.81	0.80
1:B:216:LYS:HB2	1:B:223:ILE:CG2	2.11	0.80
1:B:506:ASN:HB2	1:B:509:VAL:HG13	1.64	0.80
1:B:932:GLU:HB2	2:B:1132:HOH:O	1.82	0.80
1:A:671:LEU:HD23	1:A:671:LEU:H	1.47	0.80
1:A:811:PRO:CB	1:A:815:LYS:HE2	2.12	0.79
1:A:708:LYS:O	1:A:712:LEU:HG	1.83	0.79
1:B:653:ALA:O	1:B:655:LYS:N	2.15	0.79
1:B:20:ILE:HD11	1:B:115:ILE:CG1	2.04	0.79
1:B:20:ILE:CD1	1:B:115:ILE:HG12	2.04	0.79
1:B:529:LEU:O	1:B:532:VAL:HG12	1.82	0.79
1:B:654:ASN:HB2	1:B:657:THR:CG2	2.12	0.79
1:A:220:ASN:HD22	1:A:220:ASN:N	1.78	0.79
1:A:215:THR:HG22	1:A:223:ILE:CG1	2.11	0.79
1:B:546:ASP:O	1:B:550[A]:GLN:HG3	1.82	0.79
1:A:547:ARG:O	1:A:551:LEU:HD23	1.83	0.79
1:A:793:THR:HG23	1:A:824:ILE:HG12	1.64	0.79
1:A:152:GLU:HB3	1:A:216:LYS:NZ	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:LEU:HD13	1:B:1001:VAL:CG2	2.13	0.79
1:B:895:ASN:HB2	1:B:937:VAL:HG11	1.63	0.79
1:B:913:SER:CB	1:B:915:LYS:HG3	2.10	0.79
1:A:914:SER:H	1:A:915:LYS:HE2	1.47	0.79
1:A:944:LYS:HD3	1:A:1007:GLY:HA2	1.63	0.78
1:A:149:GLU:HA	1:A:230:ARG:NH2	1.99	0.78
1:B:127:ASP:O	1:B:131:VAL:HG23	1.82	0.78
1:B:635:ASN:O	1:B:639:LYS:HE3	1.83	0.78
1:A:205:LEU:HB2	1:A:237:MSE:HE1	1.66	0.78
1:B:113:ARG:HB3	1:B:1004:THR:HG21	1.62	0.78
1:B:341[B]:ARG:HG3	1:B:343:GLN:CD	2.04	0.78
1:B:512:ARG:HH11	1:B:512:ARG:CB	1.95	0.78
1:B:113:ARG:HD2	1:B:1004:THR:HG23	1.64	0.78
1:B:324:THR:HG21	1:B:363:LEU:HG	1.62	0.78
1:A:75:PRO:HB2	1:A:76:PRO:HD3	1.65	0.78
1:B:1024:VAL:O	1:B:1028:GLN:HG3	1.82	0.78
1:B:247:VAL:HA	1:B:250:LEU:HD13	1.64	0.78
1:B:153:THR:HB	1:B:156:ASP:CB	2.06	0.78
1:B:770:GLU:HG2	1:B:835:PHE:CE1	2.18	0.78
1:A:529:LEU:O	1:A:532:VAL:HG12	1.84	0.78
1:A:608:LEU:HD23	1:A:629:ARG:CZ	2.14	0.78
1:B:202:LEU:HB3	1:B:203:PRO:HD3	1.65	0.78
1:B:836:GLN:NE2	1:B:837:PRO:HD2	1.99	0.78
1:A:283:TRP:HH2	1:A:336:ALA:HB2	1.48	0.78
1:B:729:ALA:HA	1:B:732:LYS:CD	2.10	0.78
1:A:429:ASP:O	1:A:433:ARG:HG2	1.83	0.77
1:A:4:PHE:HZ	1:A:998:LEU:HD21	1.49	0.77
1:B:563:GLU:HG3	1:B:565:GLU:H	1.48	0.77
1:B:741:MSE:HA	1:B:808:ILE:HD13	1.65	0.77
1:B:86:THR:O	1:B:90:GLN:HG2	1.84	0.77
1:A:635:ASN:O	1:A:639:LYS:HE3	1.84	0.77
1:A:1045:SER:O	1:A:1048:ILE:HD12	1.84	0.77
1:A:316:LYS:O	1:A:320:GLU:HG3	1.85	0.77
1:A:913:SER:HB2	1:A:915:LYS:CG	2.13	0.77
1:A:880:GLU:HG3	1:A:915:LYS:CE	2.13	0.77
1:A:906:HIS:HB2	1:A:927:ALA:HB1	1.65	0.77
1:B:216:LYS:HB2	1:B:223:ILE:HG21	1.63	0.77
1:B:789:GLU:HG2	1:B:830:LYS:NZ	1.99	0.77
1:B:211:ILE:CG1	1:B:690:ALA:O	2.31	0.77
1:B:457:PRO:CD	1:B:460:ARG:HG3	2.15	0.77
1:A:127:ASP:O	1:A:131:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:ARG:HH11	1:B:1057:ARG:HG2	1.49	0.76
1:B:4:PHE:HZ	1:B:998:LEU:HD21	1.50	0.76
1:B:760:ALA:CB	1:B:794:ILE:HD11	2.16	0.76
1:A:7:ARG:HG3	1:A:7:ARG:HH11	1.51	0.76
1:A:94:MSE:HG3	1:A:104:ALA:HB1	1.67	0.76
1:A:958:SER:HB3	2:A:1089:HOH:O	1.84	0.76
1:B:776:ASP:O	1:B:780:ARG:HG3	1.85	0.76
1:B:8:THR:O	1:B:12:ILE:HG13	1.86	0.76
1:A:550:GLN:O	1:A:554:GLN:HG3	1.84	0.76
1:B:944:LYS:HE2	1:B:1006:LEU:O	1.85	0.76
1:B:897:PRO:HB2	1:B:1024:VAL:CG1	2.16	0.76
1:B:424:ASP:HB3	1:B:427:GLU:HG2	1.66	0.76
1:A:555:LEU:HD23	1:A:555:LEU:O	1.86	0.76
1:A:568:GLN:HE21	1:A:568:GLN:H	1.33	0.76
1:B:495:GLY:O	1:B:499:GLN:HG3	1.86	0.76
1:B:653:ALA:HB1	1:B:658:VAL:HG23	1.68	0.76
1:A:40:LEU:HB2	1:A:43:PRO:HG2	1.67	0.75
1:A:506:ASN:HB2	1:A:509:VAL:HG13	1.67	0.75
1:A:906:HIS:CE1	1:A:910:ARG:HG3	2.21	0.75
1:B:29:GLU:HG2	1:B:945:ARG:HD3	1.67	0.75
1:B:563:GLU:CG	1:B:565:GLU:H	1.98	0.75
1:B:31:GLU:HG3	1:B:105:ARG:CZ	2.16	0.75
1:B:398:PRO:HB3	1:B:454:GLY:O	1.85	0.75
1:B:149:GLU:HA	1:B:230:ARG:CZ	2.16	0.75
1:A:287:PRO:HG3	1:A:350:MSE:HG2	1.68	0.75
1:B:59:LYS:HA	1:B:62:VAL:CG2	2.16	0.75
1:A:795:SER:O	1:A:798:VAL:HG22	1.87	0.75
1:A:1032:GLN:HA	1:A:1035:LYS:HD2	1.69	0.74
1:A:109:ILE:HD13	1:A:1008[B]:ARG:NH2	2.02	0.74
1:A:37:ILE:HB	1:A:95:LEU:HD11	1.69	0.74
1:B:28:GLU:OE1	1:B:942:GLY:HA2	1.85	0.74
1:A:702:TRP:CZ3	1:A:706:VAL:HG21	2.22	0.74
1:B:225:GLU:HB3	1:B:681:ILE:HG13	1.68	0.74
1:B:921:ALA:O	1:B:925:ARG:HG3	1.87	0.74
1:A:898:MSE:HE1	1:A:1023:LEU:CD2	2.13	0.74
1:B:507:PRO:CG	1:B:555:LEU:HD21	2.17	0.74
1:B:811:PRO:HB3	1:B:815:LYS:HE2	1.69	0.74
1:A:205:LEU:HD13	1:A:234:VAL:HG23	1.68	0.74
1:B:666:LYS:HE2	1:B:670:GLU:OE2	1.87	0.74
1:B:94:MSE:CE	1:B:104:ALA:HB2	2.18	0.74
1:B:793:THR:CG2	1:B:824:ILE:HG12	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:CG2	1:B:945:ARG:HG3	2.17	0.74
1:B:511:ASP:O	1:B:512:ARG:HB2	1.86	0.74
1:A:51:VAL:O	1:A:55:VAL:HG23	1.87	0.74
1:B:74:MSE:HE2	1:B:78:PHE:CZ	2.23	0.73
1:A:256:ASP:HB3	1:A:259:ALA:HB2	1.67	0.73
1:A:798:VAL:O	1:A:802:LYS:HG3	1.88	0.73
1:B:154:MSE:HE1	1:B:158:VAL:HG23	1.70	0.73
1:B:143:GLU:O	1:B:146:THR:HB	1.88	0.73
1:B:301:GLN:O	1:B:305:GLU:HG2	1.88	0.73
1:A:40:LEU:CB	1:A:43:PRO:HG2	2.17	0.73
1:A:75:PRO:HA	1:A:78:PHE:CE2	2.24	0.73
1:A:444:LYS:HB2	1:A:444:LYS:HZ2	1.53	0.73
1:A:447:ASP:HA	1:A:450:ARG:HH11	1.52	0.73
1:A:506:ASN:CB	1:A:509:VAL:HG13	2.18	0.73
1:A:670:GLU:O	1:A:673:PRO:HD2	1.89	0.73
1:A:793:THR:HG23	1:A:824:ILE:CG1	2.19	0.73
1:B:895:ASN:CB	1:B:937:VAL:HG11	2.19	0.73
1:A:738:LYS:HA	1:A:741:MSE:HE2	1.71	0.73
1:A:147:VAL:O	1:A:150:VAL:HG12	1.88	0.73
1:B:272:SER:O	1:B:276:LYS:HG3	1.89	0.73
1:A:608:LEU:HD23	1:A:629:ARG:NH2	2.03	0.73
1:B:142:LEU:HD23	1:B:238:SER:HB3	1.70	0.73
1:B:318:ARG:O	1:B:322:LEU:HG	1.87	0.73
1:B:394:TRP:HE1	1:B:401:GLY:N	1.87	0.73
1:A:202:LEU:HB3	1:A:203:PRO:HD3	1.71	0.73
1:A:53:ASN:HB3	1:B:288:SER:CB	2.18	0.73
1:B:152:GLU:HB3	1:B:216:LYS:NZ	2.04	0.73
1:B:908:GLU:O	1:B:911:LYS:HG3	1.89	0.73
1:B:154:MSE:O	1:B:154:MSE:HE3	1.88	0.72
1:B:558:LEU:CD2	1:B:569:ALA:HB2	2.19	0.72
1:B:65:THR:HG21	1:B:70:LEU:CD2	2.10	0.72
1:B:744:ILE:HA	1:B:808:ILE:HG21	1.70	0.72
1:A:201:LEU:HB3	1:A:237:MSE:HE2	1.70	0.72
1:A:281:LYS:HA	1:A:284:LEU:CD1	2.16	0.72
1:B:158:VAL:HG13	1:B:162:LYS:CE	2.19	0.72
1:B:201:LEU:HB3	1:B:237:MSE:HE2	1.71	0.72
1:A:448:LEU:HA	1:A:451:GLN:CG	2.17	0.72
1:A:511:ASP:O	1:A:512:ARG:HB2	1.88	0.72
1:B:911:LYS:O	1:B:1060:ARG:HG2	1.89	0.72
1:B:824:ILE:O	1:B:828:VAL:HG13	1.89	0.72
1:A:780:ARG:O	1:A:784:LYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:HIS:NE2	1:B:108:LEU:HB3	2.04	0.72
1:B:665:VAL:HG22	1:B:709:MSE:CE	2.19	0.72
1:A:225:GLU:OE1	1:A:677:SER:HB2	1.89	0.72
1:A:908:GLU:O	1:A:911:LYS:HG3	1.90	0.72
1:B:398:PRO:HB3	1:B:460:ARG:HH21	1.52	0.72
1:B:737:CYS:HG	1:B:817:PHE:HZ	1.36	0.72
1:A:209:MSE:O	1:A:213:VAL:HG23	1.89	0.72
1:A:769:ARG:NH1	1:A:976:ARG:NH2	2.37	0.72
1:B:445:LEU:HD21	1:B:449:ARG:NE	2.05	0.72
1:B:898:MSE:HE1	1:B:1023:LEU:CG	2.20	0.72
1:A:744:ILE:HA	1:A:808:ILE:HG21	1.72	0.72
1:B:215:THR:CG2	1:B:223:ILE:HG13	2.14	0.72
1:B:269:ALA:O	1:B:273:ILE:HG13	1.90	0.72
1:B:506:ASN:CB	1:B:509:VAL:HG13	2.20	0.72
1:A:37:ILE:CD1	1:A:105:ARG:HE	2.03	0.71
1:B:277:LEU:O	1:B:281:LYS:HG3	1.90	0.71
1:A:718:ASP:HB3	1:A:721:SER:OG	1.90	0.71
1:B:115:ILE:O	1:B:119:THR:HG23	1.90	0.71
1:B:266:MSE:HG3	1:B:309:VAL:HG22	1.70	0.71
1:B:211:ILE:HG21	1:B:681:ILE:HD13	1.72	0.71
1:B:906:HIS:HB2	1:B:927:ALA:CB	2.20	0.71
1:A:498:GLU:HG2	1:A:499:GLN:N	2.05	0.71
1:A:589:GLU:O	1:A:593:GLN:HG2	1.90	0.71
1:A:960:GLU:O	1:A:964:LEU:HG	1.91	0.71
1:B:324:THR:CG2	1:B:363:LEU:HG	2.20	0.71
1:A:776:ASP:O	1:A:780:ARG:HG3	1.90	0.71
1:A:86:THR:O	1:A:90:GLN:HG2	1.89	0.71
1:B:660:GLY:O	1:B:663:ALA:HB3	1.90	0.71
1:A:457:PRO:HB3	1:A:460:ARG:HG2	1.73	0.71
1:B:681:ILE:O	1:B:684:ARG:HG3	1.91	0.71
1:B:960:GLU:HG2	1:B:963[B]:ARG:NH2	2.06	0.71
1:A:434:SER:O	1:A:437:GLU:HG2	1.90	0.71
1:B:383:SER:OG	1:B:387:LYS:HE2	1.90	0.71
1:B:51:VAL:O	1:B:55:VAL:HG23	1.91	0.71
1:B:731:LYS:HG3	1:B:825:LEU:HD11	1.71	0.71
1:A:269:ALA:O	1:A:273:ILE:HG13	1.91	0.71
1:A:944:LYS:HD3	1:A:1007:GLY:CA	2.20	0.71
1:B:1045:SER:O	1:B:1048:ILE:HG13	1.91	0.71
1:B:211:ILE:HD11	1:B:691:ALA:HA	1.73	0.71
1:B:281:LYS:HA	1:B:284:LEU:CD1	2.21	0.71
1:B:504:ILE:CD1	1:B:576:LEU:HD23	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:HE2	1:A:107:TYR:HA	1.73	0.70
1:A:398:PRO:O	1:A:449:ARG:HG2	1.91	0.70
1:B:17:ALA:O	1:B:1000:THR:HG21	1.90	0.70
1:B:793:THR:HG23	1:B:824:ILE:CG1	2.20	0.70
1:B:960:GLU:O	1:B:964:LEU:HG	1.91	0.70
1:A:124:LEU:O	1:A:124:LEU:HD12	1.92	0.70
1:A:158:VAL:HG13	1:A:162:LYS:CE	2.19	0.70
1:A:154:MSE:HE3	1:A:154:MSE:O	1.91	0.70
1:A:789:GLU:HG2	1:A:830:LYS:HZ2	1.53	0.70
1:B:457:PRO:HD2	1:B:460:ARG:HG3	1.73	0.70
1:A:924:LYS:O	1:A:928:LEU:HD12	1.91	0.70
1:B:74:MSE:HG2	1:B:125:THR:HG21	1.73	0.70
1:B:341[B]:ARG:HG3	1:B:343:GLN:NE2	2.07	0.70
1:B:654:ASN:O	1:B:656:SER:N	2.25	0.70
1:B:95:LEU:CD1	1:B:104:ALA:HB1	2.22	0.70
1:B:589:GLU:O	1:B:593:GLN:HG2	1.91	0.70
1:A:113:ARG:HB2	1:A:1004:THR:CG2	2.21	0.70
1:A:812:GLY:N	1:A:815:LYS:HG2	2.06	0.70
1:B:26:MSE:HE3	1:B:40:LEU:HD23	1.73	0.70
1:B:936:LEU:N	1:B:936:LEU:HD23	2.06	0.70
1:A:671:LEU:HD23	1:A:671:LEU:N	2.06	0.70
1:A:530:ALA:HA	1:A:533:MSE:HE3	1.72	0.70
1:B:215:THR:HG22	1:B:223:ILE:CG1	2.12	0.70
1:B:653:ALA:CB	1:B:658:VAL:HG23	2.22	0.69
1:B:665:VAL:HG22	1:B:709:MSE:HE3	1.73	0.69
1:B:25:ILE:HG22	1:B:945:ARG:HG3	1.72	0.69
1:A:152:GLU:HB3	1:A:216:LYS:HZ2	1.55	0.69
1:A:372:ARG:NH1	2:A:1080:HOH:O	2.24	0.69
1:B:507:PRO:HG2	1:B:555:LEU:HD21	1.74	0.69
1:A:1013:ASP:O	1:A:1017:GLU:HG2	1.92	0.69
1:A:28:GLU:HG2	1:A:945:ARG:NE	2.06	0.69
1:A:37:ILE:CD1	1:A:105:ARG:HG2	2.23	0.69
1:A:440:ALA:C	1:A:444:LYS:HD3	2.12	0.69
1:B:1018:GLN:HG2	1:B:1019:ALA:N	2.05	0.69
1:B:608:LEU:H	1:B:608:LEU:HD12	1.57	0.69
1:A:58:GLY:O	1:A:62:VAL:HG22	1.92	0.69
1:A:613:ALA:HA	1:A:683:LEU:HD23	1.73	0.69
1:A:318:ARG:O	1:A:322:LEU:HG	1.93	0.69
1:B:124:LEU:O	1:B:124:LEU:HD12	1.92	0.69
1:B:26:MSE:CE	1:B:40:LEU:HD23	2.23	0.69
1:A:1054:PHE:HD1	1:A:1054:PHE:H	1.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:HD2	1:A:586:ARG:NE	2.08	0.69
1:B:185:GLN:OE1	1:B:188:ARG:HD3	1.93	0.69
1:B:444:LYS:NZ	1:B:444:LYS:HB2	2.07	0.69
1:B:726:SER:O	1:B:730:ILE:HG13	1.93	0.69
1:B:926:MSE:HE1	1:B:958:SER:HA	1.74	0.69
1:A:936:LEU:N	1:A:936:LEU:HD23	2.07	0.69
1:A:964:LEU:O	1:A:968:VAL:HG23	1.92	0.69
1:B:147:VAL:O	1:B:150:VAL:HG12	1.92	0.69
1:B:441:LEU:HA	1:B:444:LYS:NZ	2.07	0.69
1:B:670:GLU:O	1:B:673:PRO:HD2	1.93	0.68
1:A:444:LYS:HB2	1:A:444:LYS:NZ	2.07	0.68
1:A:613:ALA:HB1	1:A:682:LEU:HD21	1.76	0.68
1:B:457:PRO:O	1:B:460:ARG:HB2	1.93	0.68
1:B:1013:ASP:O	1:B:1017:GLU:HG2	1.92	0.68
1:A:343:GLN:NE2	2:A:1141:HOH:O	2.27	0.68
1:A:364:THR:O	1:A:368[A]:GLU:HG3	1.93	0.68
1:A:40:LEU:HD23	1:A:40:LEU:N	2.08	0.68
1:A:929:LEU:HD11	1:A:953:ASP:HB3	1.76	0.68
1:B:276:LYS:HE3	1:B:301:GLN:NE2	2.07	0.68
1:B:289:ALA:HB3	1:B:339:ARG:HH12	1.58	0.68
1:B:563:GLU:HG3	1:B:564:GLY:H	1.57	0.68
1:A:667:THR:HG23	1:A:671:LEU:HD21	1.76	0.68
1:A:812:GLY:H	1:A:815:LYS:CG	2.06	0.68
1:A:412:LEU:HB3	1:A:435:LEU:HD22	1.76	0.68
1:A:452:GLY:O	1:A:454:GLY:N	2.27	0.68
1:B:498:GLU:HG2	1:B:499:GLN:N	2.06	0.68
1:A:318:ARG:HH11	1:A:318:ARG:HG3	1.59	0.68
1:A:381:LYS:HE2	1:A:478:ASN:OD1	1.93	0.68
1:A:74:MSE:HG2	1:A:125:THR:HG21	1.74	0.68
1:A:960:GLU:HG2	1:A:963:ARG:NH2	2.08	0.68
1:B:330:GLN:O	1:B:333:ASP:HB2	1.94	0.68
1:B:408:ILE:O	1:B:412:LEU:HG	1.94	0.68
1:B:895:ASN:HB2	1:B:937:VAL:CG1	2.23	0.68
1:A:1048:ILE:HD13	1:A:1048:ILE:O	1.95	0.67
1:B:233:THR:HG22	1:B:237:MSE:HE3	1.76	0.67
1:B:943:THR:O	1:B:945:ARG:N	2.27	0.67
1:B:1050:THR:O	1:B:1052:ALA:N	2.27	0.67
1:B:74:MSE:HE3	1:B:122:LEU:CD2	2.23	0.67
1:B:47:VAL:HG12	1:B:115:ILE:CD1	2.24	0.67
1:A:563:GLU:HB3	1:A:566:SER:OG	1.94	0.67
1:B:924:LYS:HZ1	1:B:1061:LYS:CE	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HB	1:A:95:LEU:CD1	2.24	0.67
1:A:533:MSE:CE	1:A:541:LEU:HD12	2.24	0.67
1:A:95:LEU:HD13	1:A:99:PRO:HA	1.75	0.67
1:B:671:LEU:HD23	1:B:671:LEU:N	2.07	0.67
1:A:153:THR:HG22	1:A:154:MSE:N	2.08	0.67
1:A:283:TRP:CH2	1:A:336:ALA:HB2	2.29	0.67
1:A:403:GLU:CD	1:A:403:GLU:H	1.98	0.67
1:A:75:PRO:HA	1:A:78:PHE:HD2	1.53	0.67
1:B:124:LEU:O	1:B:128:GLU:HG3	1.95	0.67
1:B:47:VAL:CG1	1:B:115:ILE:HD13	2.23	0.67
1:B:756:ILE:CG2	1:B:797:MSE:HE2	2.24	0.67
1:A:263:THR:HG21	1:A:378:THR:OG1	1.94	0.67
1:A:793:THR:HG21	1:A:824:ILE:HA	1.75	0.67
1:B:129:ALA:O	1:B:133:LYS:HE3	1.95	0.67
1:A:27:HIS:HE2	1:A:109:ILE:HB	1.58	0.67
1:B:654:ASN:HB2	1:B:657:THR:HG23	1.76	0.67
1:A:215:THR:CG2	1:A:223:ILE:HG13	2.21	0.67
1:A:926:MSE:HE1	1:A:958:SER:HA	1.76	0.67
1:B:70:LEU:O	1:B:74:MSE:HB2	1.94	0.67
1:B:75:PRO:HA	1:B:78:PHE:HD2	1.57	0.67
1:A:149:GLU:HA	1:A:230:ARG:CZ	2.25	0.67
1:A:551:LEU:HB2	1:A:576:LEU:HD13	1.77	0.67
1:A:812:GLY:H	1:A:815:LYS:HG2	1.59	0.67
1:B:153:THR:HG22	1:B:154:MSE:N	2.09	0.67
1:A:87:LYS:CE	1:A:107:TYR:HA	2.24	0.67
1:A:887:GLU:HB3	1:A:903:ARG:HH21	1.60	0.67
1:B:930:MSE:HG3	1:B:1031:MSE:SE	2.44	0.67
1:B:454:GLY:O	1:B:460:ARG:NE	2.27	0.67
1:B:283:TRP:HH2	1:B:336:ALA:HB2	1.58	0.66
1:B:398:PRO:O	1:B:449:ARG:HG2	1.94	0.66
1:B:717:ILE:HG21	1:B:722:LEU:HB2	1.77	0.66
1:A:811:PRO:HB3	1:A:815:LYS:CE	2.23	0.66
1:A:893:VAL:HG22	1:A:938:ARG:HD3	1.76	0.66
1:B:566:SER:HB3	1:B:567:PRO:HD2	1.77	0.66
1:B:613:ALA:CB	1:B:682:LEU:HD12	2.21	0.66
1:B:812:GLY:N	1:B:815:LYS:HG2	2.10	0.66
1:A:47:VAL:HG12	1:A:115:ILE:HD13	1.76	0.66
1:A:807:ASN:HB3	1:A:810:ASP:CB	2.20	0.66
1:B:236:LYS:HE3	1:B:236:LYS:N	2.10	0.66
1:B:839:GLU:OE1	1:B:839:GLU:HA	1.95	0.66
1:A:898:MSE:CE	1:A:1024:VAL:HA	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ALA:HA	1:B:339:ARG:HD2	1.76	0.66
1:B:684:ARG:NE	1:B:684:ARG:O	2.28	0.66
1:A:327:MSE:O	1:A:331:MSE:HG3	1.95	0.66
1:B:316:LYS:O	1:B:320:GLU:HG3	1.95	0.66
1:B:406:GLU:OE1	1:B:409:ARG:NH1	2.28	0.66
1:B:658:VAL:HG13	1:B:662:GLN:NE2	2.11	0.66
1:A:644:ALA:HB2	1:A:709:MSE:HE2	1.77	0.66
1:A:943:THR:O	1:A:945:ARG:N	2.29	0.66
1:B:40:LEU:HD22	1:B:44:VAL:HG23	1.77	0.66
1:B:58:GLY:O	1:B:62:VAL:HG22	1.95	0.66
1:B:717:ILE:CG2	1:B:722:LEU:HB2	2.26	0.66
1:B:910:ARG:HD3	2:B:1167:HOH:O	1.94	0.66
1:A:289:ALA:HB3	1:A:339:ARG:NH1	2.10	0.66
1:A:490:ALA:O	1:A:496:LYS:HE3	1.95	0.66
1:B:364:THR:O	1:B:368:GLU:HG3	1.96	0.66
1:B:772:GLU:O	1:B:975:LYS:NZ	2.29	0.66
1:B:1:MSE:HE1	1:B:1018:GLN:HE22	1.57	0.66
1:B:457:PRO:HG2	1:B:460:ARG:CG	2.26	0.65
1:B:512:ARG:HH11	1:B:512:ARG:CG	2.08	0.65
1:B:554:GLN:NE2	2:B:1176:HOH:O	2.29	0.65
1:A:233:THR:CG2	1:A:237:MSE:HE3	2.26	0.65
1:A:422:CYS:O	1:A:428:ARG:NH2	2.29	0.65
1:B:317:GLU:O	1:B:321:ILE:HG13	1.96	0.65
1:B:65:THR:CG2	1:B:70:LEU:HD22	2.14	0.65
1:A:1004:THR:O	1:A:1008[B]:ARG:NH2	2.29	0.65
1:A:608:LEU:H	1:A:608:LEU:HD12	1.61	0.65
1:B:760:ALA:HB3	1:B:794:ILE:HD11	1.78	0.65
1:A:613:ALA:HB1	1:A:682:LEU:CD2	2.25	0.65
1:B:27:HIS:NE2	1:B:108:LEU:HD23	2.11	0.65
1:B:266:MSE:HE3	1:B:309:VAL:HG13	1.78	0.65
1:A:660:GLY:O	1:A:663:ALA:HB3	1.96	0.65
1:A:20:ILE:O	1:A:24:VAL:HG23	1.97	0.65
1:A:500:ALA:O	1:A:504:ILE:HG12	1.96	0.65
1:B:16:VAL:HG12	1:B:17:ALA:N	2.10	0.65
1:B:22:HIS:HA	1:B:25:ILE:CD1	2.26	0.65
1:B:297:GLN:NE2	2:B:1099:HOH:O	2.29	0.65
1:B:459:ALA:O	1:B:462:LEU:HB2	1.96	0.65
1:A:626:PHE:CZ	1:A:680:ARG:HG2	2.32	0.65
1:A:635:ASN:C	1:A:639:LYS:HE3	2.16	0.65
1:B:186:GLU:O	1:B:190:MSE:HG3	1.97	0.65
1:B:216:LYS:N	1:B:223:ILE:HG12	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:MSE:CE	1:B:309:VAL:HG13	2.27	0.65
1:B:628:GLU:O	1:B:632:ASN:ND2	2.30	0.65
1:B:62:VAL:HA	1:B:70:LEU:HD21	1.77	0.65
1:A:319:ARG:HD3	2:A:1134:HOH:O	1.96	0.65
1:A:589:GLU:HG2	1:A:593:GLN:NE2	2.09	0.65
1:B:343:GLN:N	1:B:343:GLN:OE1	2.29	0.65
1:B:544:LYS:HD2	1:B:586:ARG:NE	2.10	0.65
1:B:760:ALA:HB1	1:B:794:ILE:HD11	1.78	0.65
1:A:205:LEU:O	1:A:209:MSE:HG3	1.97	0.65
1:A:256:ASP:OD1	1:A:485:ARG:NH2	2.29	0.65
1:A:53:ASN:O	1:A:57:VAL:HG22	1.97	0.65
1:B:547:ARG:NH2	1:B:575:GLN:HG2	2.12	0.65
1:B:719:THR:HG22	1:B:723:LEU:CD2	2.26	0.65
1:B:960:GLU:HG2	1:B:963[A]:ARG:HH21	1.62	0.65
1:A:880:GLU:HG3	1:A:915:LYS:HD2	1.78	0.65
1:A:91:ALA:HB2	1:A:107:TYR:CB	2.27	0.65
1:B:40:LEU:HD22	1:B:43:PRO:HG2	1.79	0.65
1:B:533:MSE:HE3	1:B:541:LEU:HD12	1.78	0.65
1:B:608:LEU:HD23	1:B:629:ARG:NH2	2.12	0.65
1:B:207:SER:HB3	1:B:694:HIS:CE1	2.31	0.65
1:B:733:ASP:OD2	1:B:759:ARG:NH1	2.29	0.65
1:A:37:ILE:HD12	1:A:105:ARG:HE	1.62	0.64
1:B:1005:MSE:CE	1:B:1015:GLU:HG2	2.26	0.64
1:B:441:LEU:HA	1:B:444:LYS:HZ2	1.60	0.64
1:B:644:ALA:HB3	1:B:709:MSE:HE2	1.79	0.64
1:A:403:GLU:O	1:A:406:GLU:N	2.30	0.64
1:A:74:MSE:O	1:A:77:ALA:HB3	1.97	0.64
1:B:403:GLU:CD	1:B:403:GLU:H	2.01	0.64
1:B:589:GLU:HG2	1:B:593:GLN:NE2	2.06	0.64
1:B:667:THR:CG2	1:B:671:LEU:HD21	2.26	0.64
1:B:793:THR:HG21	1:B:824:ILE:HA	1.78	0.64
1:A:27:HIS:ND1	2:A:1154:HOH:O	2.30	0.64
1:A:409[B]:ARG:HH22	1:A:442:THR:HB	1.60	0.64
1:A:512:ARG:HH11	1:A:512:ARG:CB	2.11	0.64
1:A:566:SER:HB3	1:A:567:PRO:HD2	1.80	0.64
1:A:594:GLU:O	1:A:598:VAL:HG23	1.98	0.64
1:B:440:ALA:O	1:B:443:SER:N	2.30	0.64
1:B:789:GLU:HG2	1:B:830:LYS:HZ1	1.62	0.64
1:A:944:LYS:CD	1:A:1007:GLY:HA2	2.27	0.64
1:A:211:ILE:HD11	1:A:690:ALA:O	1.96	0.64
1:A:898:MSE:HE3	1:A:1024:VAL:HG22	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:898:MSE:CE	1:B:1023:LEU:HD23	2.24	0.64
1:B:812:GLY:H	1:B:815:LYS:CG	2.10	0.64
1:A:287:PRO:HB3	1:A:344:GLY:O	1.96	0.64
1:B:635:ASN:C	1:B:639:LYS:HE3	2.17	0.64
1:B:798:VAL:O	1:B:802:LYS:HG3	1.97	0.64
1:A:62:VAL:HA	1:A:70:LEU:HD21	1.79	0.64
1:A:815:LYS:O	1:A:819:ASP:HB3	1.97	0.64
1:B:815:LYS:O	1:B:819:ASP:HB3	1.98	0.64
1:A:266:MSE:HE3	1:A:309:VAL:HG13	1.80	0.64
1:A:619:ALA:O	1:A:622:ARG:HB2	1.98	0.64
1:A:756:ILE:CG2	1:A:797:MSE:HE2	2.27	0.64
1:B:341[B]:ARG:NE	1:B:343:GLN:NE2	2.46	0.64
1:B:837:PRO:O	1:B:839:GLU:N	2.31	0.64
1:A:158:VAL:O	1:A:162:LYS:HG3	1.97	0.64
1:A:247:VAL:HA	1:A:250:LEU:HD13	1.79	0.64
1:A:281:LYS:NZ	1:A:361:ASP:OD2	2.31	0.64
1:B:1057:ARG:NH1	1:B:1057:ARG:HG2	2.13	0.64
1:B:209:MSE:O	1:B:212:PHE:HB3	1.98	0.64
1:B:412:LEU:N	1:B:412:LEU:HD23	2.12	0.64
1:B:564:GLY:HA2	1:B:569:ALA:HB1	1.79	0.64
1:B:207:SER:OG	1:B:694:HIS:ND1	2.29	0.64
1:A:1:MSE:HB2	1:A:1018:GLN:CD	2.18	0.64
1:B:1014:GLU:HA	1:B:1017:GLU:CG	2.27	0.64
1:B:281:LYS:NZ	1:B:361:ASP:OD2	2.31	0.63
1:B:708:LYS:O	1:B:712:LEU:HG	1.98	0.63
1:A:152:GLU:O	1:A:213:VAL:HG13	1.98	0.63
1:A:449:ARG:HA	1:A:453:LYS:HA	1.80	0.63
1:B:795:SER:OG	1:B:796:PRO:HD3	1.98	0.63
1:A:108:LEU:O	1:A:112:SER:N	2.32	0.63
1:A:233:THR:HG22	1:A:237:MSE:HE3	1.79	0.63
1:B:901:ALA:HB1	1:B:1031:MSE:HG3	1.79	0.63
1:B:83:ASN:OD1	1:B:83:ASN:N	2.31	0.63
1:B:28:GLU:HG2	1:B:944:LYS:HB2	1.80	0.63
1:A:453:LYS:N	1:A:453:LYS:HD2	2.10	0.63
1:B:682:LEU:O	1:B:682:LEU:HD22	1.98	0.63
1:A:18:GLN:NE2	1:A:22[B]:HIS:NE2	2.47	0.63
1:A:448:LEU:CD1	1:A:448:LEU:H	2.11	0.63
1:A:633:PHE:CD2	1:A:676:VAL:HG23	2.32	0.63
1:B:236:LYS:HE3	1:B:236:LYS:CA	2.29	0.63
1:B:257:ALA:HB2	2:B:1115:HOH:O	1.97	0.63
1:B:718:ASP:HB3	1:B:721:SER:OG	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ASP:C	1:B:507:PRO:HD3	2.18	0.63
1:B:811:PRO:CB	1:B:815:LYS:HE2	2.28	0.63
1:B:394:TRP:CG	1:B:404:GLY:HA3	2.34	0.63
1:B:734:LEU:O	1:B:738:LYS:HG3	1.98	0.63
1:B:335:VAL:HG12	1:B:336:ALA:N	2.14	0.63
1:A:266:MSE:CE	1:A:309:VAL:HG13	2.29	0.63
1:A:880:GLU:HG3	1:A:915:LYS:NZ	2.14	0.63
1:B:905:LEU:HD12	1:B:1031:MSE:SE	2.49	0.63
1:B:318:ARG:HG3	1:B:318:ARG:HH11	1.63	0.63
1:B:441:LEU:N	1:B:441:LEU:HD23	2.14	0.63
1:B:499:GLN:NE2	1:B:514:VAL:HG11	2.14	0.63
1:B:731:LYS:HG3	1:B:825:LEU:CD1	2.29	0.63
1:A:258:TRP:HB3	1:A:488:LYS:HE2	1.81	0.62
1:A:812:GLY:CA	1:A:815:LYS:HG2	2.28	0.62
1:B:440:ALA:C	1:B:444:LYS:HD3	2.19	0.62
1:B:667:THR:O	1:B:670:GLU:N	2.26	0.62
1:A:833:GLU:O	1:A:835:PHE:N	2.32	0.62
1:B:14:GLU:N	1:B:15:PRO:HD2	2.14	0.62
1:B:70:LEU:HG	1:B:74:MSE:HG3	1.81	0.62
1:B:907:ASP:O	1:B:910:ARG:HG3	1.98	0.62
1:A:947:LEU:O	1:A:947:LEU:HD22	1.99	0.62
1:B:59:LYS:HA	1:B:62:VAL:HG23	1.81	0.62
1:A:22[A]:HIS:HD2	1:A:23:LEU:HD23	1.63	0.62
1:B:215:THR:HG21	1:B:222:GLY:CA	2.29	0.62
1:B:886:PRO:CG	1:B:928:LEU:HD23	2.29	0.62
1:B:29:GLU:CG	1:B:945:ARG:HD3	2.30	0.62
1:A:2:PRO:O	1:A:1022:MSE:HE1	2.00	0.62
1:A:610:ALA:HA	1:A:695:PHE:CZ	2.35	0.62
1:B:283:TRP:CZ2	1:B:296:GLU:HG2	2.33	0.62
1:B:347:PRO:HA	1:B:350:MSE:HE1	1.82	0.62
1:B:551:LEU:HB2	1:B:576:LEU:HD13	1.80	0.62
1:A:109:ILE:CD1	1:A:1008[B]:ARG:HH21	2.10	0.62
1:A:91:ALA:HB2	1:A:107:TYR:HB3	1.82	0.62
1:A:283:TRP:CZ2	1:A:296:GLU:HG2	2.34	0.62
1:A:613:ALA:CB	1:A:682:LEU:HD21	2.29	0.62
1:A:70:LEU:O	1:A:74:MSE:HB2	1.99	0.62
1:A:115:ILE:O	1:A:119:THR:HG23	2.00	0.62
1:A:1:MSE:O	1:A:1:MSE:HE2	1.99	0.62
1:A:205:LEU:CD1	1:A:234:VAL:HG23	2.29	0.62
1:A:793:THR:CG2	1:A:824:ILE:HG12	2.29	0.62
1:A:944:LYS:CE	1:A:1007:GLY:HA2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:GLU:HA	1:B:225:GLU:OE1	1.98	0.62
1:B:2:PRO:O	1:B:1022:MSE:HE1	1.98	0.62
1:A:330:GLN:O	1:A:333:ASP:HB2	2.00	0.62
1:A:445:LEU:HD12	1:A:462:LEU:HB3	1.80	0.62
1:A:7:ARG:CG	1:A:7:ARG:HH11	2.10	0.62
1:A:90:GLN:C	1:A:94:MSE:HE3	2.20	0.62
1:B:613:ALA:HB1	1:B:682:LEU:CD1	2.23	0.62
1:B:795:SER:O	1:B:798:VAL:HG22	2.00	0.62
1:A:958:SER:O	1:A:961:VAL:HG23	2.00	0.62
1:B:701:GLN:O	1:B:704:ASP:HB2	2.00	0.62
1:B:940:GLY:O	1:B:944:LYS:NZ	2.31	0.62
1:A:441:LEU:CD2	1:A:441:LEU:H	2.05	0.62
1:B:667:THR:HG23	1:B:671:LEU:HD21	1.81	0.62
1:A:369:ASN:O	1:A:373:LYS:HG3	2.00	0.61
1:A:910:ARG:O	1:A:1061:LYS:HD3	2.00	0.61
1:B:960:GLU:HG2	1:B:963[B]:ARG:HH21	1.64	0.61
1:A:408:ILE:O	1:A:412:LEU:HG	2.00	0.61
1:A:290:SER:O	1:A:292:GLY:N	2.33	0.61
1:A:884:GLU:HG3	1:A:885:PHE:H	1.65	0.61
1:B:51:VAL:HG11	1:B:115:ILE:HD12	1.82	0.61
1:B:684:ARG:NH2	1:B:686:PRO:HB3	2.16	0.61
1:A:335:VAL:HG12	1:A:336:ALA:N	2.15	0.61
1:A:944:LYS:HE2	1:A:1007:GLY:HA2	1.81	0.61
1:B:176:ASP:O	1:B:179:GLN:HG3	2.00	0.61
1:B:310:GLY:O	1:B:318:ARG:HG2	2.00	0.61
1:B:444:LYS:O	1:B:448:LEU:HD13	1.99	0.61
1:B:74:MSE:O	1:B:77:ALA:HB3	2.01	0.61
1:B:93:GLN:HG2	1:B:94:MSE:H	1.65	0.61
1:B:958:SER:O	1:B:961:VAL:HG23	2.01	0.61
1:A:424:ASP:OD1	1:A:427:GLU:HB2	2.01	0.61
1:A:69:ILE:N	1:A:69:ILE:HD12	2.11	0.61
1:B:95:LEU:HD11	1:B:104:ALA:HB1	1.81	0.61
1:A:558:LEU:CD2	1:A:569:ALA:HB2	2.27	0.61
1:A:666:LYS:HE2	1:A:670:GLU:OE2	2.01	0.61
1:A:756:ILE:HG22	1:A:797:MSE:HE2	1.83	0.61
1:A:885:PHE:CZ	1:A:899:MSE:HE3	2.36	0.61
1:B:168:MSE:CE	1:B:202:LEU:HB2	2.31	0.61
1:B:744:ILE:HD12	1:B:744:ILE:N	2.14	0.61
1:B:769:ARG:NH1	1:B:976:ARG:NH2	2.49	0.61
1:A:447:ASP:CA	1:A:450:ARG:HD2	2.29	0.61
1:B:1014:GLU:HA	1:B:1017:GLU:HG2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:LEU:HD13	1:B:126:PHE:HE1	1.64	0.61
1:B:547:ARG:HD2	1:B:551:LEU:HD21	1.83	0.61
1:A:170:LYS:O	1:A:174:MSE:HG3	2.00	0.61
1:A:227:LEU:CD1	1:A:230:ARG:HH12	2.14	0.61
1:A:374:LEU:O	1:A:374:LEU:HD12	2.01	0.60
1:A:825:LEU:O	1:A:828:VAL:HG22	2.01	0.60
1:B:59:LYS:O	1:B:62:VAL:HG23	2.01	0.60
1:A:41:THR:O	1:A:45:ALA:HB2	2.00	0.60
1:A:65:THR:CG2	1:A:70:LEU:HD22	2.13	0.60
1:A:258:TRP:CD1	1:A:488:LYS:HD2	2.36	0.60
1:A:573:ALA:O	1:A:577:GLN:HG2	2.01	0.60
1:A:1049:ARG:HG3	1:A:1050:THR:H	1.67	0.60
1:A:719:THR:O	1:A:723:LEU:HD23	2.01	0.60
1:B:218:SER:OG	1:B:220:ASN:ND2	2.35	0.60
1:B:898:MSE:HE1	1:B:1023:LEU:HG	1.84	0.60
1:B:913:SER:CB	1:B:915:LYS:HE3	2.31	0.60
1:B:300:ARG:HG3	2:B:1099:HOH:O	2.01	0.60
1:A:808:ILE:O	1:A:814:GLN:NE2	2.35	0.60
1:B:87:LYS:O	1:B:87:LYS:HG3	2.02	0.60
1:A:286:ASP:O	1:A:339:ARG:NH2	2.35	0.60
1:A:37:ILE:H	1:A:37:ILE:HD12	1.67	0.60
1:A:444:LYS:O	1:A:448:LEU:HD13	2.01	0.60
1:A:4:PHE:HZ	1:A:998:LEU:CD2	2.15	0.60
1:A:683:LEU:HD13	1:A:683:LEU:O	2.00	0.60
1:B:327:MSE:O	1:B:331:MSE:HG3	2.02	0.60
1:A:533:MSE:HE1	1:A:541:LEU:HD12	1.84	0.60
1:B:152:GLU:HB3	1:B:216:LYS:HZ2	1.65	0.60
1:B:445:LEU:HD23	1:B:445:LEU:O	2.02	0.60
1:A:972:CYS:SG	1:A:1044:ALA:HB1	2.42	0.59
1:A:87:LYS:O	1:A:87:LYS:HG3	2.01	0.59
1:A:880:GLU:HG3	1:A:915:LYS:CD	2.31	0.59
1:B:697:THR:HG22	1:B:698:MSE:CE	2.21	0.59
1:A:512:ARG:CG	1:A:512:ARG:HH11	2.16	0.59
1:A:48:GLN:O	1:A:52:SER:HB3	2.01	0.59
1:A:69:ILE:HG22	1:A:73:ASP:OD2	2.01	0.59
1:A:734:LEU:O	1:A:738:LYS:HG3	2.01	0.59
1:A:930:MSE:HG3	1:A:1031:MSE:SE	2.52	0.59
1:B:211:ILE:HG12	1:B:690:ALA:O	2.00	0.59
1:B:75:PRO:HB2	1:B:76:PRO:HD3	1.84	0.59
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.67	0.59
1:A:459:ALA:O	1:A:462:LEU:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HA	1:A:62:VAL:CG2	2.32	0.59
1:A:760:ALA:CB	1:A:794:ILE:HD11	2.32	0.59
1:B:209:MSE:O	1:B:213:VAL:HG23	2.01	0.59
1:A:1:MSE:HB2	1:A:1018:GLN:NE2	2.17	0.59
1:A:666:LYS:O	1:A:669:ARG:HB2	2.02	0.59
1:B:1001:VAL:HG12	1:B:1002:LYS:N	2.16	0.59
1:B:113:ARG:HB3	1:B:1004:THR:HG23	1.83	0.59
1:B:211:ILE:HD11	1:B:690:ALA:O	2.02	0.59
1:B:40:LEU:HB2	1:B:43:PRO:HG3	1.82	0.59
1:B:69:ILE:HG22	1:B:73:ASP:OD2	2.03	0.59
1:A:681:ILE:HG22	1:A:682:LEU:N	2.16	0.59
1:A:839:GLU:HA	2:A:1161:HOH:O	2.02	0.59
1:A:564:GLY:O	1:A:565:GLU:HG3	2.02	0.59
1:A:738:LYS:HA	1:A:741:MSE:CE	2.31	0.59
1:A:83:ASN:N	1:A:83:ASN:OD1	2.35	0.59
1:B:253:TRP:CD1	1:B:1025:HIS:HD2	2.21	0.59
1:B:7:ARG:CG	1:B:7:ARG:HH11	2.16	0.59
1:A:16:VAL:HG12	1:A:17:ALA:N	2.17	0.59
1:A:185:GLN:OE1	1:A:188:ARG:HD3	2.02	0.59
1:B:256:ASP:OD1	1:B:258:TRP:HZ3	1.86	0.59
1:B:28:GLU:CD	1:B:942:GLY:HA2	2.23	0.59
1:B:317:GLU:CD	1:B:317:GLU:H	2.03	0.59
1:B:887:GLU:OE1	1:B:887:GLU:HA	2.01	0.59
1:A:336:ALA:HA	1:A:339:ARG:HD2	1.84	0.59
1:A:377:MSE:HE3	1:A:421:LEU:HD23	1.83	0.59
1:A:42:ALA:N	1:A:43:PRO:HD2	2.18	0.59
1:B:897:PRO:CB	1:B:1024:VAL:HG11	2.26	0.59
1:B:215:THR:HG21	1:B:222:GLY:HA3	1.84	0.59
1:A:1052:ALA:O	1:A:1053:GLY:C	2.40	0.58
1:A:215:THR:HG23	1:A:220:ASN:ND2	2.17	0.58
1:A:641:GLY:HA2	1:A:709:MSE:CE	2.31	0.58
1:A:79:ILE:HG12	2:A:1097:HOH:O	2.03	0.58
1:B:22:HIS:CE1	1:B:23:LEU:HD23	2.38	0.58
1:B:40:LEU:O	1:B:43:PRO:CD	2.48	0.58
1:B:720:LYS:HD3	1:B:837:PRO:HD3	1.84	0.58
1:B:917:ASN:HA	1:B:1056:LEU:HD23	1.84	0.58
1:A:216:LYS:HA	1:A:223:ILE:HG12	1.84	0.58
1:B:293:ASP:OD1	1:B:293:ASP:N	2.33	0.58
1:A:1001:VAL:HG12	1:A:1002:LYS:N	2.18	0.58
1:A:94:MSE:HG3	1:A:104:ALA:CB	2.33	0.58
1:A:129:ALA:O	1:A:133:LYS:HE3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLY:C	1:B:457:PRO:HD2	2.23	0.58
1:B:667:THR:O	1:B:670:GLU:HB2	2.02	0.58
1:A:51:VAL:HG11	1:A:115:ILE:CD1	2.30	0.58
1:A:536:PRO:O	1:A:540:ASP:N	2.34	0.58
1:B:253:TRP:O	1:B:255:GLU:HG2	2.03	0.58
1:B:563:GLU:HG2	1:B:565:GLU:HB2	1.84	0.58
1:A:14:GLU:N	1:A:15:PRO:HD2	2.19	0.58
1:A:505:ASP:C	1:A:507:PRO:HD3	2.23	0.58
1:A:530:ALA:CA	1:A:533:MSE:HE3	2.33	0.58
1:B:933:MSE:HG3	1:B:950:CYS:SG	2.43	0.58
1:B:137:VAL:O	1:B:141:ILE:HG12	2.04	0.58
1:A:53:ASN:CB	1:B:288:SER:HB2	2.21	0.58
1:B:270:LEU:HD21	1:B:367:VAL:HG23	1.84	0.58
1:A:206:ILE:HG22	1:A:207:SER:N	2.17	0.58
1:A:209:MSE:O	1:A:212:PHE:HB3	2.04	0.58
1:A:644:ALA:CB	1:A:709:MSE:HE2	2.32	0.58
1:A:658:VAL:HG13	1:A:662:GLN:NE2	2.18	0.58
1:A:906:HIS:O	1:A:910:ARG:HB2	2.04	0.58
1:A:898:MSE:CG	1:A:1024:VAL:HG13	2.34	0.58
1:A:112:SER:O	1:A:115:ILE:HG23	2.03	0.58
1:A:394:TRP:CD1	1:A:404:GLY:HA3	2.39	0.58
1:A:702:TRP:CH2	1:A:706:VAL:HG21	2.38	0.58
1:A:896:GLN:HG3	1:A:897:PRO:N	2.18	0.58
1:A:926:MSE:HE2	1:A:957:ALA:CB	2.34	0.58
1:A:986:GLU:HG2	2:A:1151:HOH:O	2.02	0.58
1:A:176:ASP:O	1:A:179:GLN:HG3	2.03	0.58
1:A:726:SER:O	1:A:730:ILE:HG13	2.02	0.58
1:B:154:MSE:CE	1:B:158:VAL:HB	2.34	0.58
1:B:202:LEU:CB	1:B:203:PRO:HD3	2.34	0.58
1:B:741:MSE:SE	1:B:814:GLN:HB3	2.53	0.58
1:A:548:VAL:HG13	1:A:576:LEU:HD11	1.84	0.58
1:A:885:PHE:CE2	1:A:903:ARG:HG3	2.39	0.58
1:B:227:LEU:HD21	1:B:230:ARG:NH2	2.19	0.58
1:B:756:ILE:HG22	1:B:797:MSE:HE2	1.85	0.58
1:B:896:GLN:HG3	1:B:897:PRO:N	2.18	0.58
1:A:1054:PHE:N	1:A:1054:PHE:CD1	2.71	0.57
1:A:653:ALA:HB1	1:A:657:THR:OG1	2.04	0.57
1:A:87:LYS:HE2	1:A:107:TYR:CA	2.33	0.57
1:A:882:ASP:OD2	1:A:924:LYS:NZ	2.30	0.57
1:B:4:PHE:HZ	1:B:998:LEU:CD2	2.15	0.57
1:A:473:LEU:O	1:A:477:THR:HG23	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LYS:CA	1:B:284:LEU:HD12	2.33	0.57
1:B:548:VAL:O	1:B:552:THR:OG1	2.23	0.57
1:B:902:ALA:HB2	1:B:930:MSE:HB3	1.86	0.57
1:A:154:MSE:HE1	1:A:158:VAL:HG23	1.86	0.57
1:A:1:MSE:HE3	1:A:3:VAL:HG23	1.85	0.57
1:A:456:SER:O	1:A:458:GLU:N	2.37	0.57
1:A:717:ILE:CG2	1:A:722:LEU:HB2	2.34	0.57
1:B:924:LYS:NZ	1:B:1061:LYS:HE3	2.17	0.57
1:B:133:LYS:HD3	1:B:136:ARG:NH2	2.20	0.57
1:B:244:ILE:O	1:B:248:LEU:HD12	2.04	0.57
1:B:69:ILE:HD12	1:B:69:ILE:N	2.16	0.57
1:A:440:ALA:O	1:A:443:SER:N	2.30	0.57
1:A:530:ALA:C	1:A:532:VAL:H	2.08	0.57
1:A:667:THR:O	1:A:670:GLU:N	2.35	0.57
1:B:1050:THR:C	1:B:1052:ALA:H	2.07	0.57
1:B:216:LYS:HB2	1:B:223:ILE:HG23	1.86	0.57
1:B:523:VAL:HG13	1:B:545:CYS:HB3	1.85	0.57
1:B:886:PRO:HD3	1:B:928:LEU:HD23	1.86	0.57
1:A:338:LEU:HD23	1:A:338:LEU:N	2.20	0.57
1:A:501:GLN:NE2	1:A:501:GLN:HA	2.20	0.57
1:A:576:LEU:O	1:A:579:SER:N	2.38	0.57
1:B:790:LEU:O	1:B:793:THR:HG22	2.04	0.57
1:A:741:MSE:HA	1:A:808:ILE:HD13	1.85	0.57
1:B:1020:THR:O	1:B:1024:VAL:HG23	2.04	0.57
1:B:227:LEU:HD13	1:B:230:ARG:HH12	1.70	0.57
1:B:362:VAL:O	1:B:365:ALA:HB3	2.04	0.57
1:B:477:THR:O	1:B:481:VAL:HG23	2.03	0.57
1:B:501:GLN:HA	1:B:501:GLN:NE2	2.18	0.57
1:B:882:ASP:CG	1:B:1061:LYS:HZ1	2.07	0.57
1:B:88:LEU:HD11	1:B:111:GLY:O	2.04	0.57
1:B:930:MSE:HG2	1:B:954:ILE:CD1	2.35	0.57
1:A:437:GLU:O	1:A:441:LEU:HG	2.04	0.57
1:B:227:LEU:HD22	1:B:230:ARG:NH1	2.20	0.57
1:B:812:GLY:CA	1:B:815:LYS:HG2	2.35	0.57
1:A:905:LEU:HD12	1:A:1031:MSE:SE	2.55	0.57
1:A:568:GLN:NE2	1:A:568:GLN:H	2.03	0.57
1:B:945:ARG:CZ	1:B:946:ALA:HB2	2.35	0.57
1:A:69:ILE:H	1:A:69:ILE:CD1	2.10	0.57
1:B:732:LYS:HG2	1:B:733:ASP:N	2.19	0.57
1:A:897:PRO:HB2	1:A:1024:VAL:HG11	1.87	0.57
1:A:441:LEU:HD23	1:A:441:LEU:N	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:HIS:HB3	1:B:655:LYS:HD3	1.85	0.57
1:A:8:THR:O	1:A:12:ILE:HG13	2.05	0.56
1:B:1002:LYS:HZ1	1:B:1020:THR:HG1	1.49	0.56
1:B:985:CYS:O	1:B:989:PRO:HD2	2.04	0.56
1:A:40:LEU:HB2	1:A:44:VAL:HG23	1.88	0.56
1:A:568:GLN:C	1:A:570:ARG:H	2.08	0.56
1:B:170:LYS:O	1:B:174:MSE:HG3	2.04	0.56
1:B:665:VAL:CG2	1:B:709:MSE:HE3	2.35	0.56
1:B:671:LEU:HD13	1:B:701:GLN:HG2	1.86	0.56
1:A:293:ASP:OD1	1:A:293:ASP:N	2.33	0.56
1:A:610:ALA:HA	1:A:695:PHE:HZ	1.70	0.56
1:A:778:LYS:HD2	1:A:1049:ARG:NH1	2.14	0.56
1:A:898:MSE:HE2	1:A:1024:VAL:HA	1.87	0.56
1:B:152:GLU:O	1:B:213:VAL:HG13	2.05	0.56
1:B:376:ALA:CB	1:B:421:LEU:HD21	2.36	0.56
1:A:604:THR:HA	1:A:607:LYS:HD3	1.86	0.56
1:A:685:ASN:N	1:A:686:PRO:HD3	2.20	0.56
1:B:608:LEU:N	1:B:608:LEU:HD12	2.21	0.56
1:A:258:TRP:CB	1:A:488:LYS:HE2	2.35	0.56
1:B:205:LEU:O	1:B:209:MSE:HG3	2.04	0.56
1:B:289:ALA:HB3	1:B:339:ARG:NH1	2.20	0.56
1:B:547:ARG:O	1:B:551:LEU:HD23	2.06	0.56
1:B:604:THR:O	1:B:607:LYS:HB2	2.06	0.56
1:B:807:ASN:HB2	1:B:810:ASP:HB3	1.87	0.56
1:B:812:GLY:H	1:B:815:LYS:HG2	1.66	0.56
1:A:20:ILE:HD12	1:A:116:LEU:CD2	2.36	0.56
1:A:347:PRO:HA	1:A:350:MSE:HE1	1.88	0.56
1:A:760:ALA:HB3	1:A:794:ILE:HD11	1.86	0.56
1:A:744:ILE:HA	1:A:808:ILE:CG2	2.35	0.56
1:B:224:GLU:OE1	1:B:228:LYS:NZ	2.38	0.56
1:B:886:PRO:HG3	1:B:928:LEU:HD23	1.88	0.56
1:B:893:VAL:HG13	1:B:893:VAL:O	2.06	0.56
1:B:398:PRO:CB	1:B:460:ARG:HH21	2.19	0.56
1:B:913:SER:HB3	1:B:915:LYS:HE3	1.87	0.56
1:A:412:LEU:N	1:A:412:LEU:HD23	2.20	0.56
1:A:533:MSE:O	1:A:538:ARG:NH1	2.39	0.56
1:A:566:SER:CB	1:A:567:PRO:HD2	2.36	0.56
1:A:744:ILE:HG22	1:A:744:ILE:O	2.04	0.56
1:B:452:GLY:C	1:B:454:GLY:H	2.08	0.56
1:B:458:GLU:HG2	1:B:459:ALA:N	2.21	0.56
1:A:281:LYS:CA	1:A:284:LEU:HD12	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:H	1:A:317:GLU:CD	2.07	0.56
1:B:1032:GLN:HA	1:B:1035:LYS:HD2	1.88	0.56
1:B:1049:ARG:O	1:B:1051:ASP:N	2.39	0.56
1:B:122:LEU:HD22	1:B:122:LEU:O	2.05	0.56
1:B:675:VAL:HG22	1:B:698:MSE:HB3	1.86	0.56
1:B:85:CYS:O	1:B:89:VAL:HG23	2.05	0.56
1:A:258:TRP:CG	1:A:488:LYS:HE2	2.40	0.56
1:A:447:ASP:O	1:A:449:ARG:N	2.38	0.56
1:B:447:ASP:O	1:B:451:GLN:HG2	2.06	0.56
1:A:337:ASP:O	1:A:340:ALA:HB3	2.06	0.56
1:A:887:GLU:HB3	1:A:903:ARG:NH2	2.20	0.56
1:A:913:SER:HB2	1:A:915:LYS:CE	2.36	0.56
1:B:836:GLN:C	1:B:838:GLN:H	2.07	0.56
1:A:212:PHE:CE1	1:A:227:LEU:HD23	2.40	0.55
1:B:13:LEU:HD11	1:B:119:THR:OG1	2.05	0.55
1:A:124:LEU:O	1:A:128:GLU:HG3	2.06	0.55
1:B:227:LEU:CD1	1:B:230:ARG:HH12	2.19	0.55
1:B:334:GLN:O	1:B:337:ASP:HB3	2.06	0.55
1:B:216:LYS:HA	1:B:223:ILE:CG1	2.25	0.55
1:B:373:LYS:O	1:B:376:ALA:HB3	2.07	0.55
1:B:41:THR:O	1:B:45:ALA:HB2	2.06	0.55
1:B:744:ILE:HG22	1:B:744:ILE:O	2.06	0.55
1:A:25:ILE:O	1:A:29:GLU:HB2	2.06	0.55
1:A:441:LEU:N	1:A:444:LYS:HD3	2.20	0.55
1:A:719:THR:HG22	1:A:723:LEU:HD23	1.88	0.55
1:B:112:SER:O	1:B:115:ILE:HG23	2.07	0.55
1:B:501:GLN:OE1	1:B:577:GLN:HG3	2.06	0.55
1:A:1055:THR:HG22	1:A:1056:LEU:H	1.71	0.55
1:A:2:PRO:HB2	1:A:4:PHE:CE2	2.42	0.55
1:A:276:LYS:CE	1:A:301:GLN:HE21	2.17	0.55
1:A:401:GLY:O	1:A:403:GLU:N	2.40	0.55
1:A:665:VAL:O	1:A:669:ARG:HD2	2.07	0.55
1:B:253:TRP:CD1	1:B:1025:HIS:CD2	2.94	0.55
1:B:253:TRP:CE2	1:B:1025:HIS:CD2	2.95	0.55
1:A:236:LYS:HA	1:A:236:LYS:HE3	1.89	0.55
1:A:377:MSE:HE3	1:A:421:LEU:CD2	2.37	0.55
1:B:22:HIS:HB2	1:B:25:ILE:CD1	2.35	0.55
1:B:316:LYS:HB2	1:B:317:GLU:OE2	2.07	0.55
1:B:374:LEU:O	1:B:374:LEU:HD12	2.07	0.55
1:B:266:MSE:SE	1:B:374:LEU:HD23	2.56	0.55
1:B:461:ALA:HB1	2:B:1084:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:LEU:HD12	1:B:462:LEU:HB3	1.89	0.55
1:A:570:ARG:HH22	1:A:577:GLN:HE22	1.54	0.55
1:B:290:SER:O	1:B:292:GLY:N	2.40	0.55
1:B:351:GLN:HA	1:B:351:GLN:NE2	2.21	0.55
1:B:456:SER:N	1:B:457:PRO:CD	2.70	0.55
1:B:737:CYS:SG	1:B:817:PHE:HZ	2.28	0.55
1:A:744:ILE:N	1:A:744:ILE:HD12	2.21	0.55
1:A:833:GLU:O	1:A:836:GLN:HB2	2.07	0.55
1:B:924:LYS:O	1:B:928:LEU:HD12	2.06	0.55
1:A:922:ALA:O	1:A:926:MSE:HG2	2.07	0.55
1:B:346:SER:OG	1:B:347:PRO:HD2	2.06	0.55
1:B:767:ALA:O	1:B:771:VAL:HG23	2.06	0.55
1:B:800:ASP:O	1:B:804:VAL:HG23	2.07	0.55
1:B:641:GLY:HA2	1:B:709:MSE:HE1	1.90	0.54
1:B:899:MSE:HB2	1:B:934:SER:OG	2.06	0.54
1:B:990:THR:HA	2:B:1128:HOH:O	2.06	0.54
1:A:26:MSE:HE3	1:A:40:LEU:HD13	1.89	0.54
1:A:570:ARG:HH12	1:A:577:GLN:NE2	2.06	0.54
1:A:775:GLU:HG3	1:A:975:LYS:HE3	1.88	0.54
1:B:158:VAL:O	1:B:162:LYS:HG3	2.07	0.54
1:A:227:LEU:HD11	1:A:230:ARG:HH12	1.72	0.54
1:A:789:GLU:HG2	1:A:830:LYS:HZ1	1.71	0.54
1:A:790:LEU:O	1:A:790:LEU:HD12	2.06	0.54
1:B:744:ILE:HA	1:B:808:ILE:CG2	2.34	0.54
1:A:939:GLY:HA2	1:A:1006:LEU:CG	2.37	0.54
1:A:1014:GLU:HA	1:A:1017:GLU:CG	2.38	0.54
1:A:152:GLU:HB3	1:A:216:LYS:HZ1	1.70	0.54
1:A:246:ARG:NH2	1:A:254:ASP:OD1	2.41	0.54
1:A:492:HIS:CD2	1:A:495:GLY:H	2.26	0.54
1:A:885:PHE:CE2	1:A:899:MSE:HE3	2.43	0.54
1:A:893:VAL:HG13	1:A:893:VAL:O	2.08	0.54
1:A:896:GLN:CB	1:A:897:PRO:HD3	2.38	0.54
1:B:136:ARG:HD2	2:B:1126:HOH:O	2.07	0.54
1:B:237:MSE:O	1:B:241:ILE:HG13	2.08	0.54
1:B:22:HIS:CB	1:B:25:ILE:HD11	2.37	0.54
1:B:789:GLU:HG2	1:B:830:LYS:HZ2	1.70	0.54
1:A:501:GLN:O	1:A:504:ILE:HB	2.08	0.54
1:A:507:PRO:HG2	1:A:555:LEU:HD21	1.88	0.54
1:A:717:ILE:HG21	1:A:722:LEU:HB2	1.89	0.54
1:B:13:LEU:CD2	1:B:123:LEU:HD23	2.37	0.54
1:A:511:ASP:N	1:A:511:ASP:OD1	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:PHE:CE1	1:A:680:ARG:HG2	2.43	0.54
1:A:719:THR:HG22	1:A:723:LEU:CD2	2.38	0.54
1:B:233:THR:CG2	1:B:237:MSE:HE3	2.37	0.54
1:B:260:SER:OG	1:B:261:LYS:N	2.40	0.54
1:B:69:ILE:CD1	1:B:69:ILE:H	2.18	0.54
1:A:318:ARG:NH1	1:A:318:ARG:HG3	2.21	0.54
1:A:457:PRO:CB	1:A:460:ARG:HG2	2.37	0.54
1:A:409[B]:ARG:HH21	1:A:442:THR:HB	1.71	0.54
1:A:913:SER:CA	1:A:915:LYS:HE2	2.38	0.54
1:B:1018:GLN:O	1:B:1021:GLU:HB2	2.08	0.54
1:B:457:PRO:CG	1:B:460:ARG:HG3	2.38	0.54
1:A:533:MSE:HE3	1:A:541:LEU:HD12	1.89	0.54
1:A:898:MSE:HE3	1:A:1024:VAL:CA	2.37	0.54
1:B:910:ARG:O	1:B:1061:LYS:HD2	2.08	0.54
1:B:279:GLN:OE1	1:B:294:ALA:HB1	2.08	0.54
1:B:457:PRO:HG2	1:B:460:ARG:HG3	1.90	0.54
1:B:211:ILE:CD1	1:B:690:ALA:O	2.56	0.54
1:B:276:LYS:CE	1:B:301:GLN:HE21	2.16	0.54
1:B:490:ALA:O	1:B:496:LYS:HE3	2.08	0.54
1:A:898:MSE:HE3	1:A:1024:VAL:HA	1.89	0.53
1:A:74:MSE:HG2	1:A:125:THR:CG2	2.38	0.53
1:A:237:MSE:O	1:A:241:ILE:HG13	2.08	0.53
1:B:338:LEU:HD23	1:B:338:LEU:N	2.23	0.53
1:B:430:ASP:OD1	1:B:433[B]:ARG:NH2	2.41	0.53
1:A:1054:PHE:HD1	1:A:1054:PHE:N	2.04	0.53
1:A:384:ILE:HG12	1:A:414:GLU:HB3	1.90	0.53
1:A:393:ASN:ND2	1:A:393:ASN:N	2.55	0.53
1:A:495:GLY:O	1:A:499:GLN:HG3	2.08	0.53
1:A:171:MSE:O	1:A:175:ILE:HG13	2.09	0.53
1:A:298:ALA:O	1:A:302:ILE:HD12	2.08	0.53
1:B:341[B]:ARG:CZ	1:B:343:GLN:HE21	2.20	0.53
1:B:732:LYS:NZ	1:B:733:ASP:OD1	2.40	0.53
1:A:186:GLU:CD	1:A:186:GLU:H	2.12	0.53
1:A:567:PRO:HD2	1:A:568:GLN:NE2	2.23	0.53
1:A:807:ASN:ND2	1:A:810:ASP:HB2	2.23	0.53
1:A:14:GLU:HG2	1:A:993:THR:HG23	1.90	0.53
1:B:152:GLU:HB3	1:B:216:LYS:HZ1	1.72	0.53
1:A:641:GLY:CA	1:A:709:MSE:HE1	2.32	0.53
1:A:918:ASP:HB2	1:A:964:LEU:HD13	1.90	0.53
1:A:842:PHE:N	1:A:842:PHE:CD1	2.77	0.53
1:A:97:SER:O	1:A:99:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:O	1:B:219:LYS:HB2	2.08	0.53
1:B:547:ARG:HD2	1:B:551:LEU:CD2	2.39	0.53
1:B:544:LYS:HD2	1:B:586:ARG:HE	1.73	0.53
1:B:57:VAL:HA	1:B:60:GLU:HG3	1.90	0.53
1:A:144:TYR:CE2	1:A:160:TYR:CD1	2.97	0.53
1:A:26:MSE:O	1:A:29:GLU:N	2.42	0.53
1:A:28:GLU:HA	2:A:1154:HOH:O	2.08	0.53
1:A:448:LEU:CD1	1:A:448:LEU:N	2.72	0.53
1:A:453:LYS:HB2	1:A:455:ASP:OD1	2.09	0.53
1:A:772:GLU:O	1:A:975:LYS:NZ	2.35	0.53
1:A:811:PRO:C	1:A:813:LEU:H	2.12	0.53
1:B:608:LEU:HD23	1:B:629:ARG:CZ	2.38	0.53
1:A:917:ASN:OD1	1:A:1056:LEU:HD22	2.09	0.53
1:A:151:VAL:O	1:A:212:PHE:HE2	1.92	0.53
1:A:7:ARG:CG	1:A:7:ARG:NH1	2.72	0.53
1:B:256:ASP:HA	1:B:258:TRP:CE3	2.42	0.53
1:B:363:LEU:O	1:B:367:VAL:HG13	2.09	0.53
1:B:530:ALA:C	1:B:532:VAL:H	2.12	0.53
1:B:760:ALA:HB3	1:B:794:ILE:CD1	2.38	0.53
1:B:880:GLU:O	1:B:881:LYS:HD2	2.09	0.53
1:B:947:LEU:O	1:B:947:LEU:HD22	2.09	0.53
1:A:91:ALA:HB2	1:A:107:TYR:HB2	1.91	0.53
1:A:236:LYS:CA	1:A:236:LYS:HE3	2.39	0.53
1:A:334:GLN:O	1:A:337:ASP:HB3	2.08	0.52
1:B:318:ARG:HG3	1:B:318:ARG:NH1	2.23	0.52
1:B:906:HIS:CB	1:B:927:ALA:HB1	2.32	0.52
1:B:963[B]:ARG:HG3	2:B:1095:HOH:O	2.09	0.52
1:A:216:LYS:HB2	1:A:223:ILE:HG21	1.92	0.52
1:B:1048:ILE:HD12	1:B:1048:ILE:O	2.09	0.52
1:B:563:GLU:CG	1:B:565:GLU:HB2	2.39	0.52
1:A:898:MSE:HG3	1:A:1024:VAL:HG13	1.90	0.52
1:A:419:ALA:O	1:A:422:CYS:HB2	2.09	0.52
1:A:603:THR:O	1:A:606:ILE:HG22	2.08	0.52
1:A:655:LYS:HG2	1:A:659:GLU:OE2	2.09	0.52
1:A:688:ASN:O	1:A:691:ALA:N	2.27	0.52
1:B:144:TYR:CE2	1:B:160:TYR:CD1	2.97	0.52
1:B:402:PRO:HD2	1:B:403:GLU:OE2	2.09	0.52
1:B:454:GLY:C	1:B:460:ARG:HE	2.11	0.52
1:B:654:ASN:HB2	1:B:657:THR:HG21	1.90	0.52
1:B:919:ILE:HD11	1:B:964:LEU:HB2	1.92	0.52
1:A:698:MSE:HA	1:A:698:MSE:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:GLN:O	1:B:72:ARG:HG2	2.10	0.52
1:B:74:MSE:HG2	1:B:125:THR:CG2	2.38	0.52
1:A:224:GLU:O	1:A:228:LYS:HD3	2.09	0.52
1:A:253:TRP:CD2	1:A:1025:HIS:CD2	2.98	0.52
1:A:604:THR:O	1:A:607:LYS:HB2	2.09	0.52
1:A:987:ARG:O	1:A:991:ILE:HG13	2.10	0.52
1:B:551:LEU:CD1	1:B:575:GLN:HB3	2.40	0.52
1:A:883:GLU:OE1	1:A:883:GLU:HA	2.09	0.52
1:B:551:LEU:CD2	1:B:551:LEU:N	2.73	0.52
1:B:734:LEU:HD13	1:B:822:TYR:CE1	2.44	0.52
1:A:144:TYR:CE2	1:A:160:TYR:CE1	2.98	0.52
1:A:220:ASN:OD1	1:A:685:ASN:OD1	2.27	0.52
1:A:424:ASP:OD1	1:A:424:ASP:O	2.27	0.52
1:B:218:SER:HB3	1:B:220:ASN:CG	2.29	0.52
1:B:283:TRP:CH2	1:B:336:ALA:HB2	2.41	0.52
1:B:457:PRO:HG2	1:B:460:ARG:HG2	1.91	0.52
1:B:530:ALA:CA	1:B:533:MSE:HE3	2.34	0.52
1:B:555:LEU:HD23	1:B:555:LEU:O	2.10	0.52
1:A:87:LYS:NZ	1:A:107:TYR:HA	2.24	0.52
1:A:75:PRO:HB2	1:A:76:PRO:CD	2.36	0.52
1:B:113:ARG:CZ	1:B:1005:MSE:HB3	2.40	0.52
1:B:15:PRO:O	1:B:18:GLN:N	2.39	0.52
1:B:535:GLY:O	1:B:539:GLN:OE1	2.28	0.52
1:A:142:LEU:HD23	1:A:238:SER:HB3	1.91	0.52
1:A:692:TYR:O	1:A:696:GLU:HB2	2.09	0.52
1:B:144:TYR:CE2	1:B:160:TYR:CE1	2.98	0.52
1:B:653:ALA:O	1:B:654:ASN:C	2.48	0.52
1:B:93:GLN:HG2	1:B:94:MSE:HG3	1.91	0.52
1:A:218:SER:O	1:A:219:LYS:HB2	2.11	0.52
1:A:341:ARG:CB	1:A:343:GLN:HE21	2.23	0.52
1:A:42:ALA:H	1:A:43:PRO:HD2	1.75	0.52
1:A:458:GLU:CG	1:A:459:ALA:N	2.73	0.52
1:B:538[A]:ARG:HH11	1:B:539:GLN:HE22	1.57	0.52
1:A:574:SER:HA	1:A:577:GLN:HG2	1.92	0.51
1:A:800:ASP:O	1:A:804:VAL:HG23	2.10	0.51
1:B:205:LEU:HD13	1:B:234:VAL:HG23	1.90	0.51
1:B:808:ILE:O	1:B:814:GLN:NE2	2.43	0.51
1:B:926:MSE:HE2	1:B:957:ALA:C	2.31	0.51
1:B:933:MSE:HE2	1:B:947:LEU:HD21	1.92	0.51
1:A:1020:THR:O	1:A:1024:VAL:HG23	2.10	0.51
1:A:220:ASN:H	1:A:220:ASN:ND2	2.00	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:GLU:HA	1:B:997:ILE:CD1	2.34	0.51
1:B:154:MSE:O	1:B:157:LEU:N	2.43	0.51
1:B:754:THR:HG22	1:B:758:ARG:HH21	1.76	0.51
1:B:780:ARG:O	1:B:784:LYS:HB2	2.09	0.51
1:B:93:GLN:CG	1:B:94:MSE:N	2.72	0.51
1:A:30:GLY:O	1:A:105:ARG:NH2	2.43	0.51
1:A:535:GLY:O	1:A:539:GLN:OE1	2.28	0.51
1:A:59:LYS:O	1:A:62:VAL:HG23	2.10	0.51
1:A:793:THR:CG2	1:A:824:ILE:HA	2.40	0.51
1:B:1014:GLU:HA	1:B:1017:GLU:CD	2.29	0.51
1:B:236:LYS:HA	1:B:236:LYS:HE3	1.90	0.51
1:B:142:LEU:CD2	1:B:238:SER:HB3	2.39	0.51
1:B:328:LEU:HD22	1:B:356:VAL:HG13	1.92	0.51
1:B:910:ARG:HA	1:B:924:LYS:HE2	1.91	0.51
1:A:896:GLN:HB3	1:A:897:PRO:HD3	1.93	0.51
1:B:634:GLU:HG3	1:B:676:VAL:HG21	1.92	0.51
1:A:1014:GLU:HA	1:A:1017:GLU:HG2	1.91	0.51
1:A:123:LEU:HA	1:A:126:PHE:HD1	1.75	0.51
1:A:548:VAL:O	1:A:552:THR:OG1	2.29	0.51
1:B:22:HIS:HA	1:B:25:ILE:HD11	1.91	0.51
1:B:22:HIS:CA	1:B:25:ILE:HG13	2.30	0.51
1:B:290:SER:O	1:B:293:ASP:OD1	2.28	0.51
1:B:563:GLU:HG3	1:B:565:GLU:N	2.24	0.51
1:B:886:PRO:CD	1:B:928:LEU:HD23	2.41	0.51
1:A:165:GLY:N	1:A:166:PRO:HD2	2.26	0.51
1:A:363:LEU:O	1:A:367:VAL:HG13	2.11	0.51
1:A:731:LYS:HB3	1:A:731:LYS:NZ	2.25	0.51
1:A:985:CYS:O	1:A:989:PRO:HD2	2.10	0.51
1:A:895:ASN:O	1:A:895:ASN:OD1	2.28	0.51
1:A:445:LEU:HD21	1:A:449:ARG:NE	2.25	0.51
1:A:947:LEU:HD22	1:A:947:LEU:C	2.30	0.51
1:B:684:ARG:HH22	1:B:686:PRO:HB3	1.76	0.51
1:B:885:PHE:CZ	1:B:899:MSE:HE3	2.46	0.51
1:A:460:ARG:O	1:A:464:LYS:HB2	2.11	0.51
1:B:297:GLN:HA	1:B:297:GLN:HE21	1.71	0.51
1:B:423:ASP:O	1:B:425:PRO:HD3	2.11	0.51
1:B:454:GLY:HA3	1:B:460:ARG:HE	1.75	0.51
1:A:998:LEU:HB3	1:A:1023:LEU:HD12	1.93	0.51
1:A:790:LEU:O	1:A:793:THR:HG22	2.11	0.51
1:A:955:ALA:HA	1:A:958:SER:HB2	1.93	0.51
1:B:1004:THR:HG22	1:B:1005:MSE:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:LEU:HD23	1:B:157:LEU:C	2.31	0.51
1:B:885:PHE:CE2	1:B:899:MSE:HE3	2.46	0.51
1:A:506:ASN:HB3	1:A:509:VAL:HG13	1.91	0.50
1:A:667:THR:CG2	1:A:671:LEU:HD21	2.41	0.50
1:A:75:PRO:O	1:A:79:ILE:HD13	2.11	0.50
1:B:898:MSE:HE3	1:B:1024:VAL:N	2.26	0.50
1:B:179:GLN:O	1:B:188:ARG:NE	2.45	0.50
1:B:232:PHE:CE1	1:B:674:GLN:NE2	2.79	0.50
1:A:1050:THR:O	1:A:1050:THR:HG23	2.12	0.50
1:A:74:MSE:HB2	1:A:75:PRO:HD3	1.94	0.50
1:A:794:ILE:O	1:A:798:VAL:HG13	2.11	0.50
1:A:929:LEU:CD1	1:A:953:ASP:HB3	2.41	0.50
1:B:445:LEU:HD23	1:B:445:LEU:C	2.31	0.50
1:A:301:GLN:O	1:A:305:GLU:HG2	2.10	0.50
1:A:754:THR:HG22	1:A:758:ARG:HH21	1.76	0.50
1:A:915:LYS:H	1:A:915:LYS:CD	2.22	0.50
1:B:747:GLN:HG3	1:B:748:MSE:N	2.25	0.50
1:A:258:TRP:CE3	1:A:261:LYS:HE2	2.47	0.50
1:A:316:LYS:HB2	1:A:317:GLU:OE2	2.09	0.50
1:A:569:ALA:HB1	2:A:1138:HOH:O	2.12	0.50
1:B:665:VAL:O	1:B:669:ARG:HD2	2.10	0.50
1:B:606:ILE:CD1	1:B:699:LYS:HG3	2.41	0.50
1:B:881:LYS:HG2	2:B:1136:HOH:O	2.12	0.50
1:A:157:LEU:HD23	1:A:158:VAL:N	2.25	0.50
1:A:270:LEU:N	1:A:270:LEU:HD23	2.26	0.50
1:A:79:ILE:O	1:A:83:ASN:OD1	2.29	0.50
1:A:935:ARG:HB2	1:A:936:LEU:HD23	1.94	0.50
1:B:207:SER:CB	1:B:694:HIS:ND1	2.75	0.50
1:B:756:ILE:HG21	1:B:797:MSE:HE2	1.92	0.50
1:B:61:THR:O	1:B:65:THR:HB	2.10	0.50
1:B:333:ASP:O	1:B:337:ASP:HB2	2.11	0.50
1:B:460:ARG:NH1	1:B:460:ARG:HB3	2.27	0.50
1:B:785:ALA:O	1:B:788:ASP:HB2	2.11	0.50
1:B:896:GLN:CB	1:B:897:PRO:HD3	2.42	0.50
1:B:913:SER:HB2	1:B:915:LYS:HE3	1.93	0.50
1:A:568:GLN:O	1:A:572:LEU:HB2	2.11	0.50
1:A:785:ALA:O	1:A:788:ASP:HB2	2.12	0.50
1:B:287:PRO:HG3	1:B:350:MSE:HG2	1.94	0.50
1:B:895:ASN:O	1:B:895:ASN:OD1	2.29	0.50
1:A:108:LEU:O	1:A:112:SER:OG	2.29	0.50
1:A:618:ASP:OD1	1:A:618:ASP:O	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:THR:HG21	1:B:223:ILE:N	2.26	0.50
1:B:454:GLY:CA	1:B:460:ARG:HE	2.25	0.50
1:B:608:LEU:H	1:B:608:LEU:CD1	2.25	0.50
1:B:839:GLU:N	1:B:840:PRO:CD	2.75	0.50
1:A:939:GLY:HA2	1:A:1006:LEU:HG	1.92	0.49
1:B:403:GLU:O	1:B:406:GLU:N	2.44	0.49
1:A:113:ARG:NH1	1:A:1005:MSE:HE2	2.27	0.49
1:A:1004:THR:HG22	1:A:1005:MSE:HG3	1.93	0.49
1:A:1013:ASP:N	1:A:1013:ASP:OD1	2.44	0.49
1:A:234:VAL:O	1:A:238:SER:OG	2.29	0.49
1:A:952:LYS:NZ	1:B:623[B]:GLU:OE2	2.44	0.49
1:B:342:GLY:C	1:B:344:GLY:H	2.15	0.49
1:B:558:LEU:HD22	1:B:569:ALA:CB	2.37	0.49
1:A:136:ARG:HG3	1:A:136:ARG:NH1	2.26	0.49
1:A:682:LEU:O	1:A:682:LEU:HD12	2.11	0.49
1:A:737:CYS:HG	1:A:817:PHE:HZ	1.60	0.49
1:A:157:LEU:HD23	1:A:157:LEU:C	2.32	0.49
1:A:313:CYS:O	1:A:486:PRO:HG3	2.12	0.49
1:B:10:GLU:HG2	1:B:11:SER:N	2.26	0.49
1:A:122:LEU:O	1:A:122:LEU:HD22	2.12	0.49
1:A:626:PHE:CZ	1:A:680:ARG:CG	2.95	0.49
1:A:68:GLN:O	1:A:72:ARG:HG2	2.11	0.49
1:B:229:ASN:OD1	1:B:229:ASN:N	2.45	0.49
1:B:885:PHE:CE2	1:B:903:ARG:HG3	2.46	0.49
1:B:894:ILE:CG2	1:B:895:ASN:N	2.75	0.49
1:B:932:GLU:O	1:B:936:LEU:HG	2.13	0.49
1:A:1018:GLN:HG2	1:A:1019:ALA:N	2.24	0.49
1:A:898:MSE:HE3	1:A:1024:VAL:CG2	2.43	0.49
1:A:426:LYS:HG2	1:A:427:GLU:N	2.27	0.49
1:A:745:GLN:HG3	1:A:748:MSE:HB2	1.95	0.49
1:A:747:GLN:HG3	1:A:748:MSE:N	2.27	0.49
1:A:85:CYS:O	1:A:89:VAL:HG23	2.12	0.49
1:A:901:ALA:HB1	1:A:1031:MSE:HG3	1.93	0.49
1:A:90:GLN:O	1:A:94:MSE:HE3	2.12	0.49
1:B:79:ILE:O	1:B:83:ASN:OD1	2.29	0.49
1:A:453:LYS:CD	1:A:453:LYS:H	2.09	0.49
1:A:479:ARG:HB3	2:A:1164:HOH:O	2.11	0.49
1:B:31:GLU:HG3	1:B:105:ARG:NH1	2.27	0.49
1:B:580:LEU:O	1:B:583:LEU:N	2.46	0.49
1:B:790:LEU:O	1:B:790:LEU:HD12	2.13	0.49
1:B:836:GLN:C	1:B:838:GLN:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD13	1:A:1008[B]:ARG:HE	1.78	0.49
1:A:631:ALA:O	1:A:633:PHE:N	2.45	0.49
1:B:14:GLU:HB3	1:B:15:PRO:HD3	1.94	0.49
1:B:212:PHE:C	1:B:214:THR:H	2.16	0.49
1:A:136:ARG:HG3	1:A:136:ARG:HH11	1.78	0.49
1:A:333:ASP:O	1:A:337:ASP:HB2	2.13	0.49
1:A:498:GLU:CG	1:A:499:GLN:N	2.75	0.49
1:A:912:TRP:O	1:A:1061:LYS:HD2	2.13	0.49
1:B:654:ASN:O	1:B:657:THR:N	2.36	0.49
1:A:944:LYS:HE2	1:A:1006:LEU:O	2.13	0.49
1:A:168:MSE:CE	1:A:202:LEU:HB2	2.43	0.49
1:A:216:LYS:HB2	1:A:223:ILE:CG2	2.43	0.49
1:A:769:ARG:HH11	1:A:976:ARG:NH2	2.08	0.49
1:B:258:TRP:HE3	1:B:258:TRP:C	2.15	0.49
1:B:376:ALA:HB1	1:B:421:LEU:HD21	1.95	0.49
1:B:799:MSE:HB2	1:B:799:MSE:HE2	1.77	0.49
1:B:815:LYS:CD	1:B:815:LYS:N	2.76	0.49
1:A:911:LYS:O	1:A:1060:ARG:HG2	2.13	0.48
1:B:898:MSE:CE	1:B:1024:VAL:HA	2.43	0.48
1:B:43:PRO:O	1:B:46:ALA:HB3	2.13	0.48
1:B:811:PRO:C	1:B:813:LEU:H	2.15	0.48
1:B:894:ILE:HD13	1:B:934:SER:O	2.13	0.48
1:A:310:GLY:O	1:A:318:ARG:HG2	2.13	0.48
1:A:555:LEU:C	1:A:555:LEU:HD23	2.34	0.48
1:A:634:GLU:HG3	1:A:676:VAL:HG21	1.96	0.48
1:A:665:VAL:HG22	1:A:709:MSE:HE3	1.95	0.48
1:B:1014:GLU:CA	1:B:1017:GLU:HG2	2.43	0.48
1:B:1055:THR:HG22	1:B:1056:LEU:H	1.78	0.48
1:B:641:GLY:O	1:B:645:GLU:HG3	2.13	0.48
1:B:841:ASP:N	1:B:841:ASP:OD1	2.40	0.48
1:A:457:PRO:CA	1:A:460:ARG:HG2	2.44	0.48
1:A:477:THR:O	1:A:481:VAL:HG23	2.12	0.48
1:B:2:PRO:HB2	1:B:1022:MSE:SE	2.63	0.48
1:B:22:HIS:HB2	1:B:25:ILE:HD12	1.94	0.48
1:B:530:ALA:O	1:B:532:VAL:N	2.45	0.48
1:B:744:ILE:CD1	1:B:744:ILE:N	2.75	0.48
1:A:898:MSE:CE	1:A:1023:LEU:HD23	2.23	0.48
1:A:448:LEU:HD13	1:A:448:LEU:H	1.77	0.48
1:A:530:ALA:O	1:A:532:VAL:N	2.45	0.48
1:B:14:GLU:HG2	1:B:993:THR:CG2	2.43	0.48
1:B:566:SER:CB	1:B:567:PRO:HD2	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:PHE:O	1:A:129:ALA:HB3	2.13	0.48
1:A:769:ARG:NH1	1:A:976:ARG:HH22	2.12	0.48
1:A:833:GLU:C	1:A:835:PHE:H	2.17	0.48
1:B:29:GLU:HG2	1:B:945:ARG:CD	2.38	0.48
1:B:434:SER:O	1:B:438:ILE:HG13	2.14	0.48
1:B:437:GLU:O	1:B:441:LEU:HG	2.14	0.48
1:B:903:ARG:O	1:B:907:ASP:OD2	2.31	0.48
1:A:544:LYS:HD2	1:A:586:ARG:HE	1.76	0.48
1:A:74:MSE:CE	1:A:78:PHE:CZ	2.91	0.48
1:B:253:TRP:CD2	1:B:1025:HIS:CD2	3.02	0.48
1:B:341[B]:ARG:CZ	1:B:343:GLN:NE2	2.77	0.48
1:B:384:ILE:HG12	1:B:414:GLU:HB3	1.95	0.48
1:B:422:CYS:O	1:B:428:ARG:NH2	2.45	0.48
1:B:673:PRO:C	1:B:675:VAL:H	2.17	0.48
1:A:622:ARG:NH1	1:A:683:LEU:HD13	2.28	0.48
1:A:741:MSE:SE	1:A:814:GLN:HB3	2.64	0.48
1:A:906:HIS:HB2	1:A:927:ALA:CB	2.40	0.48
1:A:913:SER:C	1:A:915:LYS:HE2	2.33	0.48
1:B:159:THR:HA	1:B:162:LYS:NZ	2.29	0.48
1:B:42:ALA:N	1:B:43:PRO:HD2	2.29	0.48
1:B:807:ASN:CB	1:B:810:ASP:HB3	2.42	0.48
1:A:173:LYS:O	1:A:177:GLU:HG3	2.14	0.48
1:A:644:ALA:CB	1:A:709:MSE:CE	2.91	0.48
1:A:898:MSE:HG2	1:A:1024:VAL:HG13	1.96	0.48
1:A:921:ALA:O	1:A:925:ARG:HG3	2.14	0.48
1:B:104:ALA:C	1:B:106:ASP:H	2.17	0.48
1:B:502:ARG:O	1:B:505:ASP:HB2	2.14	0.48
1:A:123:LEU:HA	1:A:126:PHE:CD1	2.49	0.48
1:A:697:THR:HG22	1:A:698:MSE:HE2	1.95	0.48
1:A:838:GLN:HA	1:A:838:GLN:NE2	2.27	0.48
1:B:377:MSE:HB3	1:B:481:VAL:HG13	1.95	0.48
1:B:466:VAL:HG12	1:B:467:ALA:N	2.29	0.48
1:B:262:ASP:OD2	1:B:485:ARG:HD2	2.12	0.48
1:B:754:THR:HG22	1:B:758:ARG:NH2	2.29	0.48
1:B:880:GLU:CG	1:B:881:LYS:N	2.77	0.48
1:A:146:THR:HG22	1:A:147:VAL:N	2.27	0.48
1:A:460:ARG:NH2	2:A:1097:HOH:O	2.43	0.48
1:A:836:GLN:HA	1:A:836:GLN:OE1	2.13	0.48
1:A:919:ILE:CD1	1:A:964:LEU:HB2	2.44	0.48
1:B:321:ILE:HG12	1:B:366:LYS:HD2	1.96	0.48
1:B:667:THR:HG22	1:B:671:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:ASN:C	1:B:687:GLY:H	2.16	0.48
1:B:833:GLU:O	1:B:836:GLN:HB2	2.14	0.48
1:B:902:ALA:HB1	1:B:927:ALA:O	2.13	0.48
1:B:947:LEU:C	1:B:947:LEU:HD22	2.33	0.48
1:A:60:GLU:O	1:A:64:THR:OG1	2.31	0.47
1:A:744:ILE:HG13	1:A:808:ILE:CG2	2.44	0.47
1:A:769:ARG:NH1	1:A:976:ARG:HH21	2.11	0.47
1:B:331:MSE:HE1	1:B:355:GLN:HG2	1.95	0.47
1:B:551:LEU:H	1:B:551:LEU:HD23	1.77	0.47
1:A:1008[A]:ARG:CZ	1:A:1008[A]:ARG:HB2	2.44	0.47
1:A:253:TRP:CZ3	1:A:1022:MSE:HG2	2.49	0.47
1:A:321:ILE:HG12	1:A:366:LYS:HD2	1.96	0.47
1:A:682:LEU:HB2	1:A:691:ALA:HB1	1.95	0.47
1:B:294:ALA:O	1:B:297:GLN:HB2	2.15	0.47
1:B:598:VAL:HG12	1:B:640:LEU:HD23	1.95	0.47
1:A:512:ARG:CG	1:A:512:ARG:NH1	2.77	0.47
1:A:658:VAL:CG1	1:A:662:GLN:NE2	2.77	0.47
1:A:685:ASN:N	1:A:686:PRO:CD	2.77	0.47
1:A:94:MSE:H	1:A:94:MSE:HG2	1.46	0.47
1:B:750:VAL:CG1	1:B:751:ALA:N	2.77	0.47
1:B:972:CYS:O	1:B:978:ARG:NH2	2.47	0.47
1:A:142:LEU:O	1:A:145:LEU:HB2	2.14	0.47
1:B:454:GLY:HA2	1:B:457:PRO:CG	2.44	0.47
1:A:1:MSE:HE3	1:A:3:VAL:CG2	2.44	0.47
1:A:566:SER:CB	1:A:567:PRO:CD	2.93	0.47
1:B:74:MSE:HE1	1:B:122:LEU:HD21	1.94	0.47
1:B:48:GLN:O	1:B:52:SER:HB3	2.13	0.47
1:B:564:GLY:CA	1:B:569:ALA:HB1	2.45	0.47
1:A:1014:GLU:CA	1:A:1017:GLU:HG2	2.45	0.47
1:A:153:THR:CG2	1:A:154:MSE:H	2.18	0.47
1:A:223:ILE:HA	1:A:226:ALA:HB3	1.95	0.47
1:A:429:ASP:OD2	1:A:433:ARG:NH2	2.47	0.47
1:A:675:VAL:CG2	1:A:698:MSE:HB3	2.36	0.47
1:B:456:SER:N	1:B:457:PRO:HD2	2.30	0.47
1:B:603:THR:O	1:B:606:ILE:HG22	2.14	0.47
1:A:122:LEU:HD13	1:A:126:PHE:HE1	1.80	0.47
1:A:337:ASP:O	1:A:340:ALA:N	2.35	0.47
1:A:913:SER:CB	1:A:915:LYS:HG2	2.25	0.47
1:A:936:LEU:HD12	1:A:947:LEU:HA	1.96	0.47
1:B:211:ILE:CD1	1:B:681:ILE:HG21	2.45	0.47
1:B:253:TRP:CG	1:B:1025:HIS:CD2	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:LEU:HD22	1:B:685:ASN:HB3	1.96	0.47
1:B:929:LEU:O	1:B:950:CYS:SG	2.73	0.47
1:A:324:THR:HG21	1:A:363:LEU:HG	1.96	0.47
1:A:626:PHE:CE1	1:A:680:ARG:CG	2.97	0.47
1:A:744:ILE:HG13	1:A:808:ILE:HG22	1.97	0.47
1:B:13:LEU:CD2	1:B:123:LEU:CD2	2.93	0.47
1:B:31:GLU:HA	1:B:105:ARG:HH21	1.73	0.47
1:B:377:MSE:HE3	1:B:421:LEU:HD23	1.96	0.47
1:A:131:VAL:O	1:A:135:ILE:HG13	2.15	0.47
1:A:215:THR:HG23	1:A:220:ASN:HD21	1.78	0.47
1:A:82:GLU:O	1:A:86:THR:HG23	2.15	0.47
1:B:122:LEU:HD22	1:B:122:LEU:C	2.35	0.47
1:B:448:LEU:HA	1:B:451:GLN:HG3	1.94	0.47
1:A:227:LEU:CD1	1:A:230:ARG:NH1	2.78	0.47
1:A:227:LEU:HA	1:A:227:LEU:HD22	1.61	0.47
1:A:394:TRP:CG	1:A:404:GLY:HA3	2.50	0.47
1:A:447:ASP:O	1:A:450:ARG:HG3	2.15	0.47
1:A:563:GLU:HG2	1:A:563:GLU:H	1.45	0.47
1:A:619:ALA:HA	1:A:620:PRO:HD3	1.81	0.47
1:A:885:PHE:CZ	1:A:899:MSE:CE	2.98	0.47
1:B:563:GLU:HG2	1:B:565:GLU:H	1.76	0.47
1:B:595:VAL:HG11	1:B:717:ILE:HD11	1.97	0.47
1:B:611:VAL:HG12	1:B:612:ALA:N	2.29	0.47
1:B:790:LEU:HD12	1:B:793:THR:CG2	2.45	0.47
1:A:1014:GLU:HA	1:A:1017:GLU:CD	2.36	0.47
1:A:202:LEU:CB	1:A:203:PRO:HD3	2.44	0.47
1:A:243:GLU:OE1	1:A:243:GLU:HA	2.15	0.47
1:A:622:ARG:CZ	1:A:683:LEU:HD13	2.44	0.47
1:B:10:GLU:O	1:B:14:GLU:HB2	2.15	0.47
1:B:227:LEU:O	1:B:231:ASN:HB2	2.15	0.47
1:B:402:PRO:O	1:B:406:GLU:HB2	2.15	0.47
1:B:544:LYS:HD3	1:B:582:ASP:OD2	2.14	0.47
1:B:93:GLN:HG2	1:B:94:MSE:N	2.29	0.47
1:A:216:LYS:HD3	1:A:216:LYS:C	2.35	0.46
1:A:815:LYS:CD	1:A:815:LYS:N	2.78	0.46
1:A:894:ILE:CG2	1:A:895:ASN:N	2.77	0.46
1:B:216:LYS:HD3	1:B:216:LYS:C	2.36	0.46
1:B:24:VAL:O	1:B:27:HIS:HB2	2.15	0.46
1:B:247:VAL:CA	1:B:250:LEU:HD13	2.39	0.46
1:B:929:LEU:HD11	1:B:953:ASP:HB3	1.97	0.46
1:A:270:LEU:HA	1:A:270:LEU:HD22	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ASN:OD1	1:A:372:ARG:NH2	2.48	0.46
1:A:440:ALA:O	1:A:442:THR:N	2.48	0.46
1:A:460:ARG:C	1:A:462:LEU:H	2.19	0.46
1:B:277:LEU:HD23	1:B:277:LEU:HA	1.68	0.46
1:B:460:ARG:HA	1:B:460:ARG:HH11	1.80	0.46
1:B:74:MSE:CE	1:B:78:PHE:CZ	2.97	0.46
1:A:427:GLU:OE1	1:A:480:ALA:HA	2.15	0.46
1:A:688:ASN:C	1:A:690:ALA:H	2.17	0.46
1:A:749:LEU:HD13	1:A:749:LEU:C	2.36	0.46
1:A:74:MSE:CB	1:A:75:PRO:HD3	2.46	0.46
1:B:143:GLU:HG2	1:B:144:TYR:N	2.29	0.46
1:B:223:ILE:HG13	1:B:223:ILE:H	1.50	0.46
1:B:6:THR:HG22	1:B:182:LEU:HD12	1.96	0.46
1:A:110:ASP:OD1	1:A:1008[B]:ARG:NH1	2.49	0.46
1:A:47:VAL:HG12	1:A:115:ILE:CD1	2.44	0.46
1:A:10:GLU:HG2	1:A:11:SER:N	2.29	0.46
1:A:743:ASN:HB2	1:A:745:GLN:NE2	2.31	0.46
1:B:223:ILE:C	1:B:225:GLU:H	2.17	0.46
1:B:885:PHE:CE2	1:B:899:MSE:CE	2.99	0.46
1:B:84:ALA:O	1:B:88:LEU:HD12	2.15	0.46
1:B:919:ILE:CD1	1:B:964:LEU:HB2	2.46	0.46
1:A:5:HIS:CD2	1:A:6:THR:HG23	2.50	0.46
1:A:28:GLU:OE1	1:A:944:LYS:HD2	2.15	0.46
1:B:397:ASP:C	1:B:399:ASN:H	2.19	0.46
1:B:45:ALA:O	1:B:48:GLN:HB3	2.16	0.46
1:B:619:ALA:HA	1:B:620:PRO:HD3	1.79	0.46
1:A:793:THR:HG23	1:A:824:ILE:HG13	1.97	0.46
1:A:930:MSE:HG2	1:A:954:ILE:CD1	2.46	0.46
1:B:190:MSE:HE2	1:B:247:VAL:HG21	1.97	0.46
1:B:343:GLN:H	1:B:343:GLN:CD	2.14	0.46
1:B:568:GLN:C	1:B:570:ARG:H	2.19	0.46
1:B:754:THR:CG2	1:B:758:ARG:HH21	2.29	0.46
1:A:20:ILE:CD1	1:A:115:ILE:HG23	2.45	0.46
1:A:346:SER:O	1:A:350:MSE:HE2	2.16	0.46
1:A:744:ILE:N	1:A:744:ILE:CD1	2.78	0.46
1:A:915:LYS:CD	1:A:915:LYS:N	2.78	0.46
1:A:769:ARG:HH11	1:A:976:ARG:HH21	1.64	0.46
1:B:943:THR:C	1:B:945:ARG:H	2.18	0.46
1:A:150:VAL:O	1:A:150:VAL:HG13	2.14	0.46
1:A:324:THR:CG2	1:A:363:LEU:HG	2.45	0.46
1:A:59:LYS:HA	1:A:62:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:LYS:CB	1:A:731:LYS:NZ	2.78	0.46
1:A:824:ILE:HG22	1:A:825:LEU:N	2.30	0.46
1:B:102:VAL:N	1:B:103:PRO:CD	2.79	0.46
1:B:225:GLU:HB3	1:B:681:ILE:CG1	2.41	0.46
1:B:22:HIS:CE1	1:B:23:LEU:CD2	2.99	0.46
1:B:369:ASN:OD1	1:B:372:ARG:NH2	2.49	0.46
1:B:40:LEU:CD2	1:B:43:PRO:HG2	2.45	0.46
1:B:452:GLY:O	1:B:454:GLY:N	2.49	0.46
1:B:512:ARG:NH1	1:B:512:ARG:CG	2.71	0.46
1:A:448:LEU:N	1:A:448:LEU:HD12	2.30	0.46
1:A:741:MSE:O	1:A:744:ILE:HD12	2.16	0.46
1:B:623[B]:GLU:OE2	1:B:624:GLU:HG3	2.16	0.46
1:B:648:ALA:O	1:B:658:VAL:HG22	2.15	0.46
1:A:401:GLY:HA3	1:A:403:GLU:OE1	2.15	0.46
1:A:601:ASP:OD2	1:A:604:THR:OG1	2.22	0.46
1:A:988:ILE:HB	1:A:989:PRO:HD3	1.98	0.46
1:B:458:GLU:O	1:B:459:ALA:HB3	2.15	0.46
1:B:54:LEU:HD13	1:B:122:LEU:HD12	1.96	0.46
1:B:604:THR:HA	1:B:607:LYS:HD3	1.98	0.46
1:B:811:PRO:HB3	1:B:815:LYS:CE	2.43	0.46
1:B:933:MSE:HE2	1:B:947:LEU:CD2	2.45	0.46
1:A:377:MSE:CE	1:A:418:ILE:HA	2.46	0.45
1:A:760:ALA:HB3	1:A:794:ILE:CD1	2.46	0.45
1:A:906:HIS:NE2	1:A:910:ARG:HG3	2.31	0.45
1:A:995:LEU:HD13	1:A:995:LEU:O	2.16	0.45
1:B:625:VAL:CG1	1:B:626:PHE:N	2.80	0.45
1:B:734:LEU:HD22	1:B:818:LEU:CD2	2.45	0.45
1:B:936:LEU:N	1:B:936:LEU:CD2	2.77	0.45
1:A:122:LEU:HD22	1:A:122:LEU:C	2.36	0.45
1:A:220:ASN:N	1:A:220:ASN:ND2	2.51	0.45
1:A:350:MSE:HE3	1:A:350:MSE:HB2	1.61	0.45
1:A:623:GLU:OE1	1:A:623:GLU:HA	2.16	0.45
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.63	0.45
1:A:506:ASN:O	1:A:508:THR:N	2.50	0.45
1:A:622:ARG:NH1	1:A:683:LEU:CD1	2.80	0.45
1:A:644:ALA:HB3	1:A:709:MSE:CE	2.46	0.45
1:A:20:ILE:HD11	1:A:115:ILE:CG2	2.46	0.45
1:A:343:GLN:HG3	1:A:343:GLN:H	1.55	0.45
1:A:593:GLN:H	1:A:593:GLN:HG2	1.58	0.45
1:A:87:LYS:HZ1	1:A:107:TYR:HA	1.82	0.45
1:B:189:VAL:O	1:B:192:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:LEU:HD22	1:B:227:LEU:HA	1.71	0.45
1:B:354[A]:GLN:HG2	1:B:355:GLN:N	2.32	0.45
1:B:731:LYS:CB	1:B:731:LYS:NZ	2.79	0.45
1:A:172:ALA:HB2	1:A:195:MSE:HE2	1.98	0.45
1:A:615:ALA:HA	1:A:616:PRO:HD2	1.59	0.45
1:A:893:VAL:CG2	1:A:938:ARG:HD3	2.44	0.45
1:B:108:LEU:O	1:B:112:SER:N	2.49	0.45
1:B:131:VAL:O	1:B:135:ILE:HG13	2.17	0.45
1:B:157:LEU:HD23	1:B:158:VAL:N	2.32	0.45
1:B:168:MSE:HE3	1:B:202:LEU:HB2	1.98	0.45
1:B:419:ALA:O	1:B:422:CYS:HB2	2.16	0.45
1:B:836:GLN:HE22	1:B:837:PRO:HD2	1.79	0.45
1:A:87:LYS:NZ	1:A:107:TYR:O	2.45	0.45
1:A:225:GLU:O	1:A:229:ASN:OD1	2.34	0.45
1:A:277:LEU:HD23	1:A:277:LEU:HA	1.43	0.45
1:A:331:MSE:HE1	1:A:355:GLN:HG2	1.97	0.45
1:A:456:SER:O	1:A:458:GLU:HG2	2.16	0.45
1:A:61:THR:O	1:A:65:THR:HB	2.16	0.45
1:A:756:ILE:HG22	1:A:797:MSE:CE	2.46	0.45
1:A:880:GLU:HG3	1:A:915:LYS:HE3	1.97	0.45
1:A:933:MSE:C	1:A:935:ARG:H	2.20	0.45
1:B:154:MSE:HE3	1:B:158:VAL:HB	1.97	0.45
1:B:499:GLN:NE2	1:B:514:VAL:CG1	2.80	0.45
1:B:618:ASP:OD1	1:B:618:ASP:O	2.35	0.45
1:A:341:ARG:HB3	1:A:343:GLN:HE21	1.82	0.45
1:A:351:GLN:HA	1:A:351:GLN:NE2	2.32	0.45
1:B:819:ASP:OD1	1:B:823:ARG:NH1	2.50	0.45
1:A:280:ALA:HB1	1:A:299:ILE:HG13	1.99	0.45
1:B:258:TRP:C	1:B:258:TRP:CE3	2.90	0.45
1:B:277:LEU:HD13	1:B:281:LYS:HE2	1.99	0.45
1:B:40:LEU:C	1:B:43:PRO:HD2	2.35	0.45
1:B:458:GLU:C	1:B:460:ARG:H	2.20	0.45
1:A:101:SER:O	1:A:105:ARG:HD2	2.17	0.45
1:A:270:LEU:HD21	1:A:367:VAL:HG23	1.99	0.45
1:A:266:MSE:CG	1:A:309:VAL:HG22	2.41	0.45
1:A:70:LEU:HD23	1:A:70:LEU:C	2.37	0.45
1:A:836:GLN:CD	1:A:837:PRO:HD2	2.37	0.45
1:B:523:VAL:HG12	1:B:527:HIS:CE1	2.51	0.45
1:A:734:LEU:HD13	1:A:822:TYR:CE1	2.52	0.45
1:A:993:THR:O	1:A:996:LYS:HB2	2.17	0.45
1:B:1005:MSE:HE1	1:B:1015:GLU:CG	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1053:GLY:O	1:B:1054:PHE:HD1	1.99	0.45
1:B:16:VAL:CG1	1:B:17:ALA:N	2.77	0.45
1:B:615:ALA:HA	1:B:616:PRO:HD2	1.71	0.45
1:A:95:LEU:HD21	1:A:105:ARG:HG3	1.99	0.44
1:A:544:LYS:H	1:A:544:LYS:HG2	1.42	0.44
1:B:95:LEU:HD11	1:B:104:ALA:CB	2.45	0.44
1:B:190:MSE:HE1	1:B:246:ARG:HH12	1.83	0.44
1:A:444:LYS:CB	1:A:444:LYS:NZ	2.78	0.44
1:A:551:LEU:CB	1:A:576:LEU:HD13	2.45	0.44
1:A:633:PHE:HD2	1:A:676:VAL:HG23	1.79	0.44
1:B:445:LEU:HD23	1:B:449:ARG:HD2	1.99	0.44
1:B:551:LEU:HD11	1:B:575:GLN:HB3	1.98	0.44
1:B:604:THR:N	1:B:605:PRO:HD2	2.32	0.44
1:B:633:PHE:CE2	1:B:676:VAL:HG23	2.52	0.44
1:B:734:LEU:CD2	1:B:818:LEU:HD23	2.47	0.44
1:B:978:ARG:HG3	1:B:979:THR:N	2.31	0.44
1:A:102:VAL:N	1:A:103:PRO:CD	2.80	0.44
1:A:943:THR:O	1:A:946:ALA:N	2.50	0.44
1:B:369:ASN:O	1:B:373:LYS:HG3	2.16	0.44
1:B:743:ASN:HB2	1:B:745:GLN:NE2	2.32	0.44
1:B:744:ILE:HG13	1:B:808:ILE:CG2	2.47	0.44
1:B:836:GLN:OE1	1:B:836:GLN:HA	2.07	0.44
1:B:924:LYS:HZ1	1:B:1061:LYS:NZ	2.16	0.44
1:A:622:ARG:O	1:A:623:GLU:CB	2.64	0.44
1:A:87:LYS:NZ	1:A:107:TYR:CA	2.81	0.44
1:A:880:GLU:CG	1:A:915:LYS:NZ	2.81	0.44
1:A:926:MSE:HE2	1:A:957:ALA:C	2.38	0.44
1:A:14:GLU:HG2	1:A:993:THR:CG2	2.48	0.44
1:B:1004:THR:HG22	1:B:1005:MSE:CG	2.46	0.44
1:B:904:GLN:HB3	1:B:1035:LYS:HE2	2.00	0.44
1:B:88:LEU:HD11	1:B:111:GLY:C	2.38	0.44
1:B:331:MSE:HE2	1:B:331:MSE:HB3	1.95	0.44
1:B:501:GLN:NE2	1:B:501:GLN:CA	2.78	0.44
1:B:595:VAL:HG11	1:B:717:ILE:CD1	2.48	0.44
1:B:658:VAL:HG13	1:B:662:GLN:HE21	1.81	0.44
1:A:706:VAL:O	1:A:709:MSE:N	2.51	0.44
1:B:153:THR:CG2	1:B:154:MSE:H	2.18	0.44
1:B:512:ARG:HB3	1:B:512:ARG:HH11	1.77	0.44
1:B:63:GLN:O	1:B:65:THR:N	2.44	0.44
1:B:990:THR:O	1:B:994:GLN:HG2	2.18	0.44
1:A:1004:THR:HG22	1:A:1005:MSE:CG	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:HIS:ND1	1:A:27:HIS:O	2.50	0.44
1:A:204:VAL:HG22	1:A:698:MSE:HE1	1.99	0.44
1:A:71:LYS:O	1:A:75:PRO:HG2	2.18	0.44
1:B:1014:GLU:HA	1:B:1017:GLU:OE2	2.18	0.44
1:A:1030:LEU:O	1:A:1034:VAL:HG23	2.18	0.44
1:B:448:LEU:N	1:B:448:LEU:CD1	2.80	0.44
1:A:838:GLN:CD	1:A:839:GLU:H	2.21	0.44
1:B:27:HIS:CE1	1:B:108:LEU:HB3	2.53	0.44
1:B:266:MSE:HE2	1:B:309:VAL:HG13	2.00	0.44
1:B:341[B]:ARG:CG	1:B:343:GLN:NE2	2.79	0.44
1:B:538[A]:ARG:HD2	1:B:539:GLN:NE2	2.33	0.44
1:B:570:ARG:HA	1:B:570:ARG:HD2	1.72	0.44
1:B:912:TRP:HB2	1:B:920:ILE:HG13	2.00	0.44
1:A:898:MSE:HE3	1:A:1024:VAL:N	2.33	0.44
1:A:159:THR:HA	1:A:162:LYS:NZ	2.32	0.44
1:A:45:ALA:O	1:A:48:GLN:HB3	2.18	0.44
1:A:580:LEU:O	1:A:583:LEU:N	2.51	0.44
1:B:445:LEU:HD21	1:B:449:ARG:HE	1.80	0.44
1:B:211:ILE:HG13	1:B:690:ALA:O	2.16	0.44
1:B:795:SER:N	1:B:796:PRO:CD	2.80	0.44
1:B:930:MSE:HG2	1:B:954:ILE:HD11	1.98	0.44
1:A:317:GLU:O	1:A:321:ILE:HG13	2.18	0.43
1:A:383:SER:O	1:A:386:LYS:HG3	2.17	0.43
1:A:448:LEU:HA	1:A:451:GLN:HG3	1.98	0.43
1:A:898:MSE:CE	1:A:1024:VAL:CA	2.96	0.43
1:A:899:MSE:HG3	1:A:903:ARG:NH1	2.33	0.43
1:A:4:PHE:CZ	1:A:998:LEU:HD21	2.40	0.43
1:B:1057:ARG:NH1	1:B:1057:ARG:CG	2.81	0.43
1:B:177:GLU:O	1:B:180:GLN:HB2	2.18	0.43
1:B:233:THR:CG2	1:B:237:MSE:CE	2.96	0.43
1:B:626:PHE:CD1	1:B:627:ASP:N	2.86	0.43
1:B:885:PHE:HA	1:B:886:PRO:HD3	1.67	0.43
1:B:943:THR:O	1:B:946:ALA:N	2.50	0.43
1:B:974:ASP:CG	1:B:977:ILE:HG13	2.39	0.43
1:A:384:ILE:HD11	1:A:415:ALA:CA	2.48	0.43
1:A:68:GLN:HB3	1:A:396:ALA:HB1	2.00	0.43
1:A:530:ALA:C	1:A:532:VAL:N	2.71	0.43
1:A:591:MSE:HE3	1:A:591:MSE:HB3	1.96	0.43
1:A:769:ARG:HH12	1:A:976:ARG:NH2	2.14	0.43
1:B:653:ALA:HB1	1:B:658:VAL:CG2	2.42	0.43
1:B:666:LYS:O	1:B:669:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASP:HA	1:A:450:ARG:NH1	2.29	0.43
1:A:606:ILE:CD1	1:A:699:LYS:HG3	2.48	0.43
1:A:914:SER:H	1:A:915:LYS:CE	2.26	0.43
1:B:369:ASN:CG	1:B:373:LYS:HE2	2.38	0.43
1:B:40:LEU:CD2	1:B:44:VAL:HG23	2.46	0.43
1:B:547:ARG:O	1:B:550[A]:GLN:HB2	2.17	0.43
1:B:656:SER:O	1:B:659:GLU:HB2	2.18	0.43
1:B:94:MSE:H	1:B:94:MSE:HG3	1.40	0.43
1:A:227:LEU:HD13	1:A:230:ARG:NH1	2.33	0.43
1:A:227:LEU:O	1:A:231:ASN:HB2	2.18	0.43
1:A:236:LYS:O	1:A:239:ALA:HB3	2.19	0.43
1:A:280:ALA:HB1	1:A:299:ILE:CG1	2.48	0.43
1:A:40:LEU:N	1:A:40:LEU:CD2	2.79	0.43
1:A:760:ALA:HB1	1:A:794:ILE:HD11	2.00	0.43
1:A:825:LEU:HA	1:A:828:VAL:HG22	2.00	0.43
1:A:885:PHE:CE2	1:A:899:MSE:CE	3.01	0.43
1:B:395:LEU:HD13	1:B:467:ALA:HB2	2.01	0.43
1:B:59:LYS:CA	1:B:62:VAL:HG23	2.48	0.43
1:B:793:THR:CG2	1:B:824:ILE:HA	2.47	0.43
1:A:223:ILE:H	1:A:223:ILE:HG13	1.44	0.43
1:A:229:ASN:N	1:A:229:ASN:OD1	2.50	0.43
1:A:291:PRO:HB3	1:A:336:ALA:HB1	2.01	0.43
1:A:501:GLN:NE2	1:A:501:GLN:CA	2.82	0.43
1:A:625:VAL:CG1	1:A:626:PHE:N	2.81	0.43
1:A:633:PHE:CE2	1:A:676:VAL:HG23	2.53	0.43
1:A:750:VAL:CG1	1:A:751:ALA:N	2.80	0.43
1:B:158:VAL:HG12	1:B:159:THR:N	2.34	0.43
1:B:185:GLN:O	1:B:189:VAL:HG23	2.18	0.43
1:B:227:LEU:CD2	1:B:230:ARG:NH1	2.82	0.43
1:B:350:MSE:HB2	1:B:350:MSE:HE3	1.80	0.43
1:B:406:GLU:OE1	1:B:406:GLU:HA	2.17	0.43
1:B:42:ALA:H	1:B:43:PRO:HD2	1.83	0.43
1:B:896:GLN:HB3	1:B:897:PRO:HD3	2.01	0.43
1:A:1002:LYS:NZ	1:A:1020:THR:OG1	2.51	0.43
1:A:14:GLU:HB3	1:A:15:PRO:HD3	2.01	0.43
1:A:186:GLU:O	1:A:190:MSE:HG3	2.18	0.43
1:A:212:PHE:O	1:A:214:THR:N	2.41	0.43
1:A:309:VAL:HG11	1:A:367:VAL:HB	2.01	0.43
1:A:258:TRP:CE2	1:A:488:LYS:HD3	2.53	0.43
1:A:728:GLU:OE2	1:A:731:LYS:HE3	2.18	0.43
1:B:216:LYS:CB	1:B:223:ILE:HG21	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ARG:CA	1:B:460:ARG:HH11	2.31	0.43
1:B:738:LYS:CA	1:B:741:MSE:HE2	2.36	0.43
1:B:838:GLN:O	1:B:838:GLN:HG2	2.18	0.43
1:B:840:PRO:C	1:B:842:PHE:H	2.20	0.43
1:B:933:MSE:C	1:B:935:ARG:H	2.21	0.43
1:A:496:LYS:HD2	1:A:522:LEU:HD13	2.01	0.43
1:A:568:GLN:HA	1:A:571:ALA:HB3	2.01	0.43
1:A:836:GLN:HE22	1:A:837:PRO:HD2	1.81	0.43
1:A:950:CYS:O	1:A:954:ILE:HG13	2.18	0.43
1:B:123:LEU:HA	1:B:126:PHE:HD1	1.82	0.43
1:B:154:MSE:HE1	1:B:158:VAL:CG2	2.42	0.43
1:B:301:GLN:O	1:B:304:ASP:HB3	2.19	0.43
1:B:335:VAL:C	1:B:337:ASP:N	2.72	0.43
1:B:537:TYR:HD1	1:B:537:TYR:O	2.00	0.43
1:B:56:ARG:HG2	1:B:57:VAL:N	2.34	0.43
1:B:719:THR:HG22	1:B:723:LEU:HD21	1.97	0.43
1:B:955:ALA:HA	1:B:958:SER:HB2	2.01	0.43
1:A:541:LEU:HA	1:A:541:LEU:HD23	1.80	0.43
1:A:756:ILE:HG21	1:A:797:MSE:HE2	1.97	0.43
1:B:144:TYR:HE2	1:B:160:TYR:CD1	2.37	0.43
1:B:15:PRO:O	1:B:18:GLN:CB	2.67	0.43
1:B:285:ARG:O	1:B:286:ASP:HB2	2.19	0.43
1:B:263:THR:HG22	1:B:374:LEU:HG	2.00	0.43
1:B:98:ASP:HA	1:B:99:PRO:HD2	1.69	0.43
1:B:994:GLN:HG2	1:B:994:GLN:H	1.56	0.43
1:A:1042:GLU:HA	1:A:1045:SER:HB3	2.00	0.43
1:A:10:GLU:O	1:A:14:GLU:HB2	2.19	0.43
1:A:641:GLY:O	1:A:645:GLU:HG3	2.19	0.43
1:A:936:LEU:H	1:A:936:LEU:HD23	1.83	0.43
1:B:177:GLU:H	1:B:177:GLU:HG3	1.62	0.43
1:B:202:LEU:N	1:B:203:PRO:CD	2.82	0.43
1:B:270:LEU:HD21	1:B:367:VAL:CG2	2.49	0.43
1:B:61:THR:CG2	1:B:70:LEU:HD11	2.48	0.43
1:B:900:MSE:HE3	1:B:904:GLN:HE22	1.84	0.43
1:A:683:LEU:HD13	1:A:683:LEU:C	2.40	0.43
1:A:698:MSE:O	1:A:701:GLN:HB3	2.19	0.43
1:B:122:LEU:HA	1:B:122:LEU:HD23	1.83	0.43
1:B:270:LEU:HD22	1:B:270:LEU:HA	1.71	0.43
1:B:466:VAL:CG1	1:B:467:ALA:N	2.82	0.43
1:B:7:ARG:CG	1:B:7:ARG:NH1	2.78	0.43
1:B:926:MSE:HE2	1:B:957:ALA:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:LEU:HD12	1:B:947:LEU:HA	2.01	0.43
1:A:613:ALA:O	1:A:682:LEU:HD11	2.18	0.42
1:A:978:ARG:O	1:A:982:LEU:HG	2.19	0.42
1:B:759:ARG:O	1:B:763:ILE:HG13	2.19	0.42
1:A:1042:GLU:HB2	1:A:1058:TRP:CD2	2.54	0.42
1:A:650:VAL:O	1:A:650:VAL:CG2	2.66	0.42
1:A:221:GLN:O	1:A:684:ARG:HB3	2.19	0.42
1:B:15:PRO:O	1:B:18:GLN:HB2	2.18	0.42
1:B:212:PHE:CE1	1:B:227:LEU:HD23	2.53	0.42
1:B:22:HIS:O	1:B:26:MSE:HG2	2.18	0.42
1:B:882:ASP:O	1:B:883:GLU:O	2.37	0.42
1:B:950:CYS:O	1:B:954:ILE:HG13	2.20	0.42
1:A:1049:ARG:HG3	1:A:1050:THR:N	2.33	0.42
1:A:122:LEU:HD13	1:A:126:PHE:CE1	2.53	0.42
1:A:343:GLN:HB2	1:A:346:SER:HB2	2.01	0.42
1:A:485:ARG:HE	1:A:485:ARG:HB2	1.60	0.42
1:A:607:LYS:O	1:A:610:ALA:N	2.52	0.42
1:A:61:THR:CG2	1:A:70:LEU:HD11	2.50	0.42
1:A:1018:GLN:O	1:A:1021:GLU:HB2	2.20	0.42
1:A:88:LEU:HD11	1:A:111:GLY:C	2.39	0.42
1:A:423:ASP:O	1:A:425:PRO:HD3	2.19	0.42
1:A:566:SER:HB3	1:A:567:PRO:CD	2.49	0.42
1:A:658:VAL:HG13	1:A:662:GLN:HE21	1.85	0.42
1:A:804:VAL:HG12	1:A:804:VAL:O	2.20	0.42
1:A:899:MSE:HE2	1:A:903:ARG:NH2	2.34	0.42
1:B:501:GLN:O	1:B:502:ARG:C	2.58	0.42
1:B:60:GLU:O	1:B:64:THR:OG1	2.37	0.42
1:A:331:MSE:HE2	1:A:331:MSE:HB3	1.88	0.42
1:A:447:ASP:C	1:A:449:ARG:H	2.23	0.42
1:A:268:ARG:CZ	1:A:669:ARG:HH11	2.32	0.42
1:B:126:PHE:O	1:B:129:ALA:HB3	2.19	0.42
1:B:445:LEU:HD11	1:B:463:ALA:HB2	2.01	0.42
1:A:104:ALA:C	1:A:106:ASP:H	2.22	0.42
1:A:37:ILE:CG2	1:A:38:PRO:CD	2.97	0.42
1:A:262:ASP:OD2	1:A:485:ARG:HD2	2.20	0.42
1:A:671:LEU:CD2	1:A:671:LEU:H	2.19	0.42
1:A:804:VAL:HG12	1:A:808:ILE:HA	2.02	0.42
1:A:915:LYS:HD3	1:A:915:LYS:N	2.35	0.42
1:B:1001:VAL:CG1	1:B:1002:LYS:N	2.81	0.42
1:B:1002:LYS:NZ	1:B:1020:THR:OG1	2.29	0.42
1:B:555:LEU:HD23	1:B:555:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:571:ALA:O	1:B:575:GLN:HB2	2.19	0.42
1:B:883:GLU:CG	1:B:884:GLU:H	2.32	0.42
1:B:14:GLU:CA	1:B:997:ILE:HD11	2.41	0.42
1:A:152:GLU:OE1	1:A:216:LYS:NZ	2.30	0.42
1:A:284:LEU:HD13	1:A:357:SER:HB2	2.01	0.42
1:A:440:ALA:HB3	1:A:441:LEU:HD23	2.00	0.42
1:B:898:MSE:HE3	1:B:1024:VAL:CA	2.49	0.42
1:B:28:GLU:OE2	1:B:944:LYS:NZ	2.30	0.42
1:B:512:ARG:NH1	1:B:512:ARG:HG3	2.34	0.42
1:B:94:MSE:HE2	1:B:94:MSE:HB2	1.96	0.42
1:A:212:PHE:C	1:A:214:THR:H	2.19	0.42
1:A:529:LEU:CD1	1:A:587:MSE:HB3	2.49	0.42
1:A:650:VAL:HG22	1:A:650:VAL:O	2.18	0.42
1:A:685:ASN:O	1:A:686:PRO:O	2.37	0.42
1:A:886:PRO:C	1:A:887:GLU:HG3	2.39	0.42
1:B:815:LYS:N	1:B:815:LYS:HD3	2.34	0.42
1:B:896:GLN:CG	1:B:897:PRO:HD3	2.50	0.42
1:B:988:ILE:HG22	1:B:989:PRO:N	2.34	0.42
1:A:137:VAL:O	1:A:141:ILE:HG12	2.19	0.42
1:A:14:GLU:HB3	1:A:15:PRO:CD	2.50	0.42
1:A:168:MSE:HE2	1:A:202:LEU:HD12	2.01	0.42
1:A:185:GLN:O	1:A:188:ARG:HB2	2.20	0.42
1:A:397:ASP:C	1:A:399:ASN:H	2.22	0.42
1:A:440:ALA:HB1	1:A:444:LYS:HD2	2.02	0.42
1:A:745:GLN:O	1:A:748:MSE:N	2.52	0.42
1:A:754:THR:HG22	1:A:758:ARG:NH2	2.35	0.42
1:A:833:GLU:C	1:A:835:PHE:N	2.74	0.42
1:B:924:LYS:NZ	1:B:1061:LYS:NZ	2.67	0.42
1:B:256:ASP:CG	1:B:259:ALA:HB2	2.39	0.42
1:B:54:LEU:HA	1:B:54:LEU:HD23	1.73	0.42
1:B:504:ILE:HD12	1:B:576:LEU:HD23	2.01	0.42
1:B:756:ILE:HG22	1:B:797:MSE:CE	2.49	0.42
1:A:148:ALA:O	1:A:209:MSE:HE1	2.19	0.42
1:A:278:ASN:O	1:A:281:LYS:N	2.51	0.42
1:A:785:ALA:O	1:A:788:ASP:N	2.49	0.42
1:A:795:SER:N	1:A:796:PRO:CD	2.83	0.42
1:B:236:LYS:O	1:B:239:ALA:HB3	2.20	0.42
1:B:505:ASP:O	1:B:507:PRO:HD3	2.20	0.42
1:B:79:ILE:N	1:B:79:ILE:CD1	2.83	0.42
1:B:974:ASP:OD1	1:B:977:ILE:HG13	2.20	0.42
1:A:1:MSE:HA	1:A:1018:GLN:OE1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:MSE:HE2	1:A:957:ALA:HB3	2.01	0.41
1:A:984:VAL:O	1:A:984:VAL:HG12	2.20	0.41
1:B:182:LEU:HD13	1:B:182:LEU:N	2.35	0.41
1:B:189:VAL:HG12	1:B:193:ASN:OD1	2.19	0.41
1:B:205:LEU:CD1	1:B:234:VAL:HG23	2.50	0.41
1:B:582:ASP:O	1:B:586:ARG:HB2	2.20	0.41
1:B:737:CYS:SG	1:B:817:PHE:CZ	3.09	0.41
1:A:807:ASN:CB	1:A:810:ASP:HB3	2.27	0.41
1:A:896:GLN:CG	1:A:897:PRO:HD3	2.49	0.41
1:A:919:ILE:HD11	1:A:964:LEU:HB2	2.02	0.41
1:B:196:ASN:O	1:B:199:LYS:HB2	2.19	0.41
1:B:458:GLU:HG2	1:B:459:ALA:H	1.83	0.41
1:A:162:LYS:H	1:A:162:LYS:HG3	1.68	0.41
1:A:287:PRO:HG3	1:A:350:MSE:CG	2.45	0.41
1:A:78:PHE:O	1:A:82:GLU:OE1	2.38	0.41
1:A:888:GLN:H	1:A:888:GLN:HG2	1.37	0.41
1:B:1018:GLN:O	1:B:1021:GLU:N	2.53	0.41
1:B:227:LEU:HD22	1:B:230:ARG:CZ	2.50	0.41
1:B:298:ALA:O	1:B:302:ILE:HD12	2.20	0.41
1:B:444:LYS:CB	1:B:444:LYS:NZ	2.81	0.41
1:A:458:GLU:HG2	1:A:459:ALA:N	2.36	0.41
1:A:506:ASN:HB3	1:A:509:VAL:CG1	2.51	0.41
1:B:14:GLU:N	1:B:15:PRO:CD	2.82	0.41
1:B:202:LEU:CB	1:B:203:PRO:CD	2.98	0.41
1:B:376:ALA:HB3	1:B:421:LEU:HD21	2.02	0.41
1:B:566:SER:CB	1:B:567:PRO:CD	2.98	0.41
1:B:655:LYS:HA	1:B:655:LYS:HD2	1.34	0.41
1:B:63:GLN:C	1:B:65:THR:H	2.22	0.41
1:B:811:PRO:HA	1:B:814:GLN:HG3	2.02	0.41
1:B:930:MSE:O	1:B:933:MSE:N	2.42	0.41
1:B:894:ILE:HA	1:B:934:SER:O	2.20	0.41
1:A:19:GLN:O	1:A:22[A]:HIS:HB3	2.20	0.41
1:A:441:LEU:HA	1:A:444:LYS:CE	2.51	0.41
1:A:445:LEU:HD23	1:A:445:LEU:C	2.40	0.41
1:A:385:ALA:HA	1:A:474:GLN:HE22	1.86	0.41
1:A:506:ASN:C	1:A:508:THR:H	2.22	0.41
1:A:919:ILE:HG23	1:A:961:VAL:HG12	2.02	0.41
1:B:1050:THR:C	1:B:1052:ALA:N	2.72	0.41
1:B:916:GLY:O	1:B:1057:ARG:HB2	2.20	0.41
1:B:14:GLU:HB3	1:B:15:PRO:CD	2.50	0.41
1:B:159:THR:HA	1:B:162:LYS:HZ1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:CB	1:B:25:ILE:CD1	2.95	0.41
1:A:290:SER:O	1:A:293:ASP:OD1	2.38	0.41
1:B:174:MSE:HE2	1:B:174:MSE:HB3	1.73	0.41
1:B:178:ARG:HD2	1:B:178:ARG:HA	1.89	0.41
1:B:501:GLN:O	1:B:504:ILE:N	2.53	0.41
1:B:732:LYS:O	1:B:736:LYS:HG3	2.21	0.41
1:B:829:ALA:O	1:B:833:GLU:OE2	2.39	0.41
1:B:894:ILE:HD13	1:B:894:ILE:HA	1.95	0.41
1:A:88:LEU:CD2	1:A:108:LEU:CD1	2.99	0.41
1:A:377:MSE:HE1	1:A:418:ILE:HA	2.02	0.41
1:A:633:PHE:HD2	1:A:676:VAL:CG2	2.34	0.41
1:A:74:MSE:HE2	1:A:74:MSE:HB3	1.98	0.41
1:A:939:GLY:HA2	1:A:1006:LEU:HD11	2.03	0.41
1:B:20:ILE:CD1	1:B:115:ILE:CG2	2.99	0.41
1:B:212:PHE:O	1:B:214:THR:N	2.44	0.41
1:B:22:HIS:CA	1:B:25:ILE:HD11	2.51	0.41
1:B:40:LEU:O	1:B:43:PRO:HG2	2.21	0.41
1:B:461:ALA:O	1:B:465:GLN:HB3	2.21	0.41
1:B:506:ASN:HB3	1:B:509:VAL:HG13	1.97	0.41
1:B:996:LYS:O	1:B:999:SER:N	2.54	0.41
1:A:196:ASN:O	1:A:199:LYS:HB2	2.21	0.41
1:A:460:ARG:HG3	1:A:461:ALA:N	2.36	0.41
1:A:491:VAL:HG11	1:A:658:VAL:CG1	2.32	0.41
1:A:512:ARG:NH1	1:A:512:ARG:HG3	2.35	0.41
1:A:75:PRO:CA	1:A:78:PHE:CE2	3.00	0.41
1:B:1001:VAL:O	1:B:1004:THR:N	2.51	0.41
1:B:583:LEU:HA	1:B:583:LEU:HD23	1.72	0.41
1:B:70:LEU:HD23	1:B:70:LEU:C	2.40	0.41
1:B:733:ASP:HB3	1:B:756:ILE:HG13	2.03	0.41
1:A:201:LEU:HD23	1:A:201:LEU:HA	1.86	0.41
1:B:1:MSE:O	1:B:3:VAL:N	2.54	0.41
1:B:253:TRP:C	1:B:255:GLU:H	2.21	0.41
1:B:731:LYS:CB	1:B:731:LYS:HZ2	2.33	0.41
1:B:749:LEU:C	1:B:749:LEU:HD13	2.41	0.41
1:A:20:ILE:HD12	1:A:116:LEU:HD21	2.02	0.41
1:A:190:MSE:HE2	1:A:247:VAL:HG21	2.02	0.41
1:A:744:ILE:HD12	1:A:744:ILE:H	1.86	0.41
1:A:896:GLN:HG3	1:A:897:PRO:CD	2.51	0.41
1:A:933:MSE:HE2	1:A:947:LEU:HD21	2.03	0.41
1:B:152:GLU:OE1	1:B:216:LYS:NZ	2.35	0.41
1:B:153:THR:O	1:B:213:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASN:C	1:B:508:THR:N	2.74	0.41
1:B:626:PHE:O	1:B:629:ARG:N	2.43	0.41
1:B:644:ALA:HB2	1:B:709:MSE:HE2	1.95	0.41
1:A:13:LEU:HD13	1:A:13:LEU:HA	1.84	0.41
1:A:69:ILE:N	1:A:69:ILE:CD1	2.80	0.41
1:B:14:GLU:CB	1:B:15:PRO:CD	2.99	0.41
1:B:154:MSE:CE	1:B:158:VAL:CG2	2.98	0.41
1:B:243:GLU:OE2	1:B:246:ARG:NH1	2.53	0.41
1:B:500:ALA:O	1:B:504:ILE:HG12	2.21	0.41
1:A:218:SER:HB3	1:A:220:ASN:ND2	2.36	0.40
1:A:37:ILE:CD1	1:A:105:ARG:NE	2.80	0.40
1:A:501:GLN:O	1:A:502:ARG:C	2.59	0.40
1:A:731:LYS:HB3	1:A:731:LYS:HZ2	1.86	0.40
1:A:880:GLU:HG3	1:A:915:LYS:HZ2	1.83	0.40
1:A:895:ASN:HB2	1:A:937:VAL:HG11	2.04	0.40
1:B:335:VAL:O	1:B:337:ASP:N	2.54	0.40
1:B:734:LEU:CD2	1:B:818:LEU:CD2	2.99	0.40
1:B:811:PRO:CA	1:B:815:LYS:HE2	2.51	0.40
1:A:460:ARG:HG3	1:A:461:ALA:H	1.86	0.40
1:A:640:LEU:HA	1:A:640:LEU:HD23	1.93	0.40
1:B:133:LYS:CD	1:B:136:ARG:HH21	2.34	0.40
1:B:347:PRO:HA	1:B:350:MSE:CE	2.49	0.40
1:B:434:SER:O	1:B:437:GLU:HG2	2.21	0.40
1:B:40:LEU:CB	1:B:43:PRO:HG2	2.36	0.40
1:B:697:THR:CG2	1:B:698:MSE:HE2	2.26	0.40
1:A:20:ILE:CD1	1:A:115:ILE:CG2	2.99	0.40
1:A:154:MSE:O	1:A:157:LEU:N	2.55	0.40
1:A:574:SER:HA	1:A:577:GLN:HE21	1.85	0.40
1:A:658:VAL:CG1	1:A:662:GLN:HE22	2.34	0.40
1:A:672:THR:O	1:A:676:VAL:HB	2.22	0.40
1:B:190:MSE:HE2	1:B:247:VAL:CG2	2.52	0.40
1:B:733:ASP:OD2	1:B:755:SER:OG	2.35	0.40
1:B:880:GLU:HG2	1:B:881:LYS:N	2.34	0.40
1:A:180:GLN:HE21	1:B:358:GLN:CD	2.24	0.40
1:A:26:MSE:HA	1:A:29:GLU:HB2	2.02	0.40
1:A:506:ASN:C	1:A:508:THR:N	2.75	0.40
1:A:717:ILE:HG22	1:A:722:LEU:HB2	2.03	0.40
1:A:896:GLN:CB	1:A:897:PRO:CD	2.99	0.40
1:B:227:LEU:CD2	1:B:230:ARG:CZ	2.99	0.40
1:B:377:MSE:HG2	1:B:421:LEU:HD23	2.04	0.40
1:B:412:LEU:N	1:B:412:LEU:CD2	2.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:VAL:CG1	1:B:658:VAL:HG11	2.51	0.40
1:B:506:ASN:O	1:B:508:THR:N	2.54	0.40
1:B:882:ASP:OD2	1:B:1061:LYS:NZ	2.48	0.40
1:B:901:ALA:HB1	1:B:1031:MSE:CG	2.49	0.40
1:A:583:LEU:HA	1:A:583:LEU:HD12	1.93	0.40
1:A:910:ARG:HH12	1:A:1061:LYS:HE2	1.86	0.40
1:B:898:MSE:HE3	1:B:1024:VAL:HA	2.03	0.40
1:B:108:LEU:O	1:B:112:SER:OG	2.34	0.40
1:B:316:LYS:CB	2:B:1108:HOH:O	2.68	0.40
1:B:566:SER:HB3	1:B:567:PRO:CD	2.48	0.40
1:B:731:LYS:NZ	1:B:731:LYS:HB3	2.36	0.40
1:B:919:ILE:HG23	1:B:961:VAL:HG12	2.04	0.40
1:B:996:LYS:O	1:B:998:LEU:N	2.55	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	1032/1066 (97%)	849 (82%)	140 (14%)	43 (4%)	3 10
1	B	1032/1066 (97%)	849 (82%)	130 (13%)	53 (5%)	2 7
All	All	2064/2132 (97%)	1698 (82%)	270 (13%)	96 (5%)	2 8

All (96) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	402	PRO
1	A	441	LEU
1	A	453	LYS
1	A	686	PRO

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Mol	Chain	Res	Type
1	A	689	GLN
1	A	834	ALA
1	A	896	GLN
1	A	944	LYS
1	B	456	SER
1	B	531	ASN
1	B	655	LYS
1	B	838	GLN
1	B	881	LYS
1	B	883	GLU
1	B	887	GLU
1	B	893	VAL
1	B	896	GLN
1	B	944	LYS
1	B	1050	THR
1	B	1051	ASP
1	A	213	VAL
1	A	291	PRO
1	A	315	GLY
1	A	316	LYS
1	A	440	ALA
1	A	448	LEU
1	A	457	PRO
1	A	531	ASN
1	A	535	GLY
1	A	563	GLU
1	A	632	ASN
1	A	687	GLY
1	A	688	ASN
1	A	705	ASN
1	A	890	ALA
1	A	939	GLY
1	B	34	GLY
1	B	41	THR
1	B	101	SER
1	B	213	VAL
1	B	291	PRO
1	B	335	VAL
1	B	440	ALA
1	B	441	LEU
1	B	535	GLY
1	B	622	ARG

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Mol	Chain	Res	Type
1	B	654	ASN
1	B	656	SER
1	B	997	ILE
1	A	50	ALA
1	A	116	LEU
1	A	150	VAL
1	A	228	LYS
1	A	335	VAL
1	A	341	ARG
1	A	512	ARG
1	A	656	SER
1	B	30	GLY
1	B	38	PRO
1	B	116	LEU
1	B	253	TRP
1	B	254	ASP
1	B	316	LYS
1	B	451	GLN
1	B	600	SER
1	B	667	THR
1	B	689	GLN
1	B	892	GLU
1	A	38	PRO
1	A	1051	ASP
1	A	1052	ALA
1	B	64	THR
1	B	228	LYS
1	B	315	GLY
1	B	343	GLN
1	B	452	GLY
1	B	453	LYS
1	B	841	ASP
1	A	293	ASP
1	B	50	ALA
1	B	150	VAL
1	B	286	ASP
1	B	663	ALA
1	B	92	ALA
1	B	457	PRO
1	B	910	ARG
1	A	286	ASP
1	A	840	PRO

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Mol	Chain	Res	Type
1	B	292	GLY
1	B	989	PRO
1	A	562	GLY
1	A	292	GLY
1	A	744	ILE
1	A	891	GLY
1	B	744	ILE

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	850/842 (101%)	587 (69%)	263 (31%)	0 1
1	B	850/842 (101%)	590 (69%)	260 (31%)	0 1
All	All	1700/1684 (101%)	1177 (69%)	523 (31%)	0 1

All (523) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	3	VAL
1	A	4	PHE
1	A	7	ARG
1	A	10	GLU
1	A	11	SER
1	A	14	GLU
1	A	16	VAL
1	A	18	GLN
1	A	25	ILE
1	A	26	MSE
1	A	28	GLU
1	A	31	GLU
1	A	32	VAL
1	A	35	LYS
1	A	39	ASP

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Mol	Chain	Res	Type
1	A	40	LEU
1	A	41	THR
1	A	47	VAL
1	A	52	SER
1	A	54	LEU
1	A	60	GLU
1	A	61	THR
1	A	62	VAL
1	A	65	THR
1	A	69	ILE
1	A	70	LEU
1	A	72	ARG
1	A	74	MSE
1	A	82	GLU
1	A	83	ASN
1	A	87	LYS
1	A	88	LEU
1	A	93	GLN
1	A	94	MSE
1	A	95	LEU
1	A	102	VAL
1	A	106	ASP
1	A	109	ILE
1	A	113	ARG
1	A	115	ILE
1	A	117	SER
1	A	122	LEU
1	A	123	LEU
1	A	134	ILE
1	A	146	THR
1	A	152	GLU
1	A	155	GLU
1	A	156	ASP
1	A	157	LEU
1	A	158	VAL
1	A	162	LYS
1	A	163	ASN
1	A	169	THR
1	A	173	LYS
1	A	175	ILE
1	A	180	GLN
1	A	181	GLU

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	202	LEU
1	A	206	ILE
1	A	211	ILE
1	A	214	THR
1	A	220	ASN
1	A	223	ILE
1	A	227	LEU
1	A	228	LYS
1	A	229	ASN
1	A	230	ARG
1	A	236	LYS
1	A	238	SER
1	A	246	ARG
1	A	252	SER
1	A	255	GLU
1	A	256	ASP
1	A	260	SER
1	A	261	LYS
1	A	264	GLU
1	A	266	MSE
1	A	270	LEU
1	A	274	ASP
1	A	275	SER
1	A	277	LEU
1	A	284	LEU
1	A	286	ASP
1	A	293	ASP
1	A	296	GLU
1	A	301	GLN
1	A	316	LYS
1	A	317	GLU
1	A	318	ARG
1	A	319	ARG
1	A	326	LYS
1	A	327	MSE
1	A	341	ARG
1	A	343	GLN
1	A	348	VAL
1	A	350	MSE
1	A	351	GLN
1	A	352	LYS

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Mol	Chain	Res	Type
1	A	354[A]	GLN
1	A	354[B]	GLN
1	A	363	LEU
1	A	366	LYS
1	A	367	VAL
1	A	377	MSE
1	A	380	SER
1	A	383	SER
1	A	384	ILE
1	A	386	LYS
1	A	387	LYS
1	A	392	GLN
1	A	393	ASN
1	A	399	ASN
1	A	412	LEU
1	A	416	ARG
1	A	417	LYS
1	A	422	CYS
1	A	423	ASP
1	A	426	LYS
1	A	428	ARG
1	A	429	ASP
1	A	434	SER
1	A	437	GLU
1	A	441	LEU
1	A	444	LYS
1	A	448	LEU
1	A	450	ARG
1	A	451	GLN
1	A	453	LYS
1	A	460	ARG
1	A	464	LYS
1	A	466	VAL
1	A	471	GLN
1	A	485	ARG
1	A	497	ILE
1	A	498	GLU
1	A	501	GLN
1	A	506	ASN
1	A	512	ARG
1	A	522	LEU
1	A	532	VAL

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Mol	Chain	Res	Type
1	A	541	LEU
1	A	544	LYS
1	A	551	LEU
1	A	552	THR
1	A	558	LEU
1	A	563	GLU
1	A	566	SER
1	A	568	GLN
1	A	581	LYS
1	A	596	SER
1	A	609	LEU
1	A	622	ARG
1	A	623	GLU
1	A	624	GLU
1	A	625	VAL
1	A	632	ASN
1	A	650	VAL
1	A	655	LYS
1	A	657	THR
1	A	659	GLU
1	A	671	LEU
1	A	676	VAL
1	A	677	SER
1	A	680	ARG
1	A	681	ILE
1	A	682	LEU
1	A	683	LEU
1	A	693	GLU
1	A	703	ILE
1	A	707	GLU
1	A	708	LYS
1	A	721	SER
1	A	726	SER
1	A	731	LYS
1	A	732	LYS
1	A	734	LEU
1	A	745	GLN
1	A	750	VAL
1	A	759	ARG
1	A	762	ARG
1	A	765	LEU
1	A	768	LYS

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Mol	Chain	Res	Type
1	A	772	GLU
1	A	784	LYS
1	A	787	SER
1	A	789	GLU
1	A	791	SER
1	A	793	THR
1	A	795	SER
1	A	799	MSE
1	A	808	ILE
1	A	813	LEU
1	A	814	GLN
1	A	815	LYS
1	A	819	ASP
1	A	830	LYS
1	A	832	ARG
1	A	833	GLU
1	A	836	GLN
1	A	841	ASP
1	A	842	PHE
1	A	879	GLU
1	A	880	GLU
1	A	881	LYS
1	A	887	GLU
1	A	888	GLN
1	A	889	LYS
1	A	900	MSE
1	A	905	LEU
1	A	910	ARG
1	A	914	SER
1	A	915	LYS
1	A	918	ASP
1	A	919	ILE
1	A	926	MSE
1	A	930	MSE
1	A	933	MSE
1	A	936	LEU
1	A	944	LYS
1	A	947	LEU
1	A	949	GLN
1	A	956	LYS
1	A	958	SER
1	A	960	GLU

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Mol	Chain	Res	Type
1	A	961	VAL
1	A	967	GLU
1	A	978	ARG
1	A	981	LEU
1	A	986	GLU
1	A	987	ARG
1	A	992	SER
1	A	994	GLN
1	A	999	SER
1	A	1001	VAL
1	A	1002	LYS
1	A	1004	THR
1	A	1005	MSE
1	A	1006	LEU
1	A	1008[A]	ARG
1	A	1008[B]	ARG
1	A	1009	THR
1	A	1011	ILE
1	A	1013	ASP
1	A	1016	SER
1	A	1018	GLN
1	A	1020	THR
1	A	1026	ASN
1	A	1036	GLU
1	A	1039	ARG
1	A	1042	GLU
1	A	1045	SER
1	A	1046	ILE
1	A	1048	ILE
1	A	1050	THR
1	A	1054	PHE
1	A	1055	THR
1	A	1056	LEU
1	A	1057[A]	ARG
1	A	1057[B]	ARG
1	A	1060	ARG
1	A	1061	LYS
1	B	3	VAL
1	B	4	PHE
1	B	7	ARG
1	B	10	GLU
1	B	11	SER

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Mol	Chain	Res	Type
1	B	14	GLU
1	B	16	VAL
1	B	18	GLN
1	B	22	HIS
1	B	25	ILE
1	B	26	MSE
1	B	28	GLU
1	B	33	ASP
1	B	35	LYS
1	B	37	ILE
1	B	40	LEU
1	B	41	THR
1	B	47	VAL
1	B	52	SER
1	B	54	LEU
1	B	60	GLU
1	B	61	THR
1	B	62	VAL
1	B	65	THR
1	B	70	LEU
1	B	72	ARG
1	B	74	MSE
1	B	79	ILE
1	B	82	GLU
1	B	83	ASN
1	B	87	LYS
1	B	88	LEU
1	B	93	GLN
1	B	94	MSE
1	B	95	LEU
1	B	102	VAL
1	B	106	ASP
1	B	109	ILE
1	B	113	ARG
1	B	115	ILE
1	B	122	LEU
1	B	123	LEU
1	B	133	LYS
1	B	143	GLU
1	B	146	THR
1	B	152	GLU
1	B	155	GLU

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Mol	Chain	Res	Type
1	B	156	ASP
1	B	158	VAL
1	B	162	LYS
1	B	163	ASN
1	B	169	THR
1	B	173	LYS
1	B	180	GLN
1	B	181	GLU
1	B	182	LEU
1	B	186	GLU
1	B	202	LEU
1	B	206	ILE
1	B	211	ILE
1	B	214	THR
1	B	223	ILE
1	B	225	GLU
1	B	227	LEU
1	B	228	LYS
1	B	229	ASN
1	B	230	ARG
1	B	236	LYS
1	B	238	SER
1	B	252	SER
1	B	256	ASP
1	B	258	TRP
1	B	260	SER
1	B	261	LYS
1	B	264	GLU
1	B	266	MSE
1	B	270	LEU
1	B	274	ASP
1	B	277	LEU
1	B	284	LEU
1	B	286	ASP
1	B	293	ASP
1	B	296	GLU
1	B	297	GLN
1	B	301	GLN
1	B	316	LYS
1	B	317	GLU
1	B	318	ARG
1	B	319	ARG

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Mol	Chain	Res	Type
1	B	326	LYS
1	B	343	GLN
1	B	345	SER
1	B	348	VAL
1	B	350	MSE
1	B	351	GLN
1	B	352	LYS
1	B	354[A]	GLN
1	B	354[B]	GLN
1	B	363	LEU
1	B	366	LYS
1	B	367	VAL
1	B	377	MSE
1	B	386	LYS
1	B	387	LYS
1	B	392	GLN
1	B	393	ASN
1	B	399	ASN
1	B	412	LEU
1	B	417	LYS
1	B	422	CYS
1	B	423	ASP
1	B	426	LYS
1	B	428	ARG
1	B	429	ASP
1	B	433[A]	ARG
1	B	433[B]	ARG
1	B	434	SER
1	B	437	GLU
1	B	441	LEU
1	B	444	LYS
1	B	447	ASP
1	B	448	LEU
1	B	450	ARG
1	B	451	GLN
1	B	464	LYS
1	B	465	GLN
1	B	466	VAL
1	B	471	GLN
1	B	484	SER
1	B	485	ARG
1	B	497	ILE

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Mol	Chain	Res	Type
1	B	498	GLU
1	B	501	GLN
1	B	506	ASN
1	B	509	VAL
1	B	512	ARG
1	B	522	LEU
1	B	537	TYR
1	B	541	LEU
1	B	544	LYS
1	B	551	LEU
1	B	552	THR
1	B	558	LEU
1	B	561	ARG
1	B	563	GLU
1	B	565	GLU
1	B	566	SER
1	B	568	GLN
1	B	575	GLN
1	B	577	GLN
1	B	581	LYS
1	B	583	LEU
1	B	586	ARG
1	B	596	SER
1	B	609	LEU
1	B	624	GLU
1	B	625	VAL
1	B	650	VAL
1	B	655	LYS
1	B	671	LEU
1	B	681	ILE
1	B	682	LEU
1	B	683	LEU
1	B	684	ARG
1	B	685	ASN
1	B	689	GLN
1	B	692	TYR
1	B	693	GLU
1	B	703	ILE
1	B	705	ASN
1	B	708	LYS
1	B	721	SER
1	B	726	SER

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Mol	Chain	Res	Type
1	B	731	LYS
1	B	732	LYS
1	B	734	LEU
1	B	745	GLN
1	B	750	VAL
1	B	762	ARG
1	B	765	LEU
1	B	768	LYS
1	B	769	ARG
1	B	772	GLU
1	B	784	LYS
1	B	787	SER
1	B	789	GLU
1	B	793	THR
1	B	799	MSE
1	B	807	ASN
1	B	808	ILE
1	B	813	LEU
1	B	814	GLN
1	B	816	SER
1	B	819	ASP
1	B	830	LYS
1	B	831	VAL
1	B	833	GLU
1	B	836	GLN
1	B	839	GLU
1	B	841	ASP
1	B	879	GLU
1	B	880	GLU
1	B	881	LYS
1	B	882	ASP
1	B	887	GLU
1	B	888	GLN
1	B	889	LYS
1	B	900	MSE
1	B	905	LEU
1	B	910	ARG
1	B	914	SER
1	B	915	LYS
1	B	918	ASP
1	B	919	ILE
1	B	920	ILE

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Mol	Chain	Res	Type
1	B	926	MSE
1	B	930	MSE
1	B	933	MSE
1	B	935	ARG
1	B	936	LEU
1	B	944	LYS
1	B	945	ARG
1	B	947	LEU
1	B	949	GLN
1	B	956	LYS
1	B	958	SER
1	B	960	GLU
1	B	961	VAL
1	B	967	GLU
1	B	976	ARG
1	B	978	ARG
1	B	981	LEU
1	B	986	GLU
1	B	987	ARG
1	B	994	GLN
1	B	997	ILE
1	B	999	SER
1	B	1002	LYS
1	B	1004	THR
1	B	1005	MSE
1	B	1008	ARG
1	B	1011	ILE
1	B	1012	SER
1	B	1013	ASP
1	B	1016	SER
1	B	1018	GLN
1	B	1020	THR
1	B	1026	ASN
1	B	1036	GLU
1	B	1039	ARG
1	B	1042	GLU
1	B	1045	SER
1	B	1046	ILE
1	B	1050	THR
1	B	1051	ASP
1	B	1055	THR
1	B	1056	LEU

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Mol	Chain	Res	Type
1	B	1057	ARG
1	B	1060	ARG
1	B	1062	THR

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	180	GLN
1	A	193	ASN
1	A	220	ASN
1	A	279	GLN
1	A	301	GLN
1	A	343	GLN
1	A	351	GLN
1	A	379	ASN
1	A	393	ASN
1	A	472	ASN
1	A	474	GLN
1	A	492	HIS
1	A	550	GLN
1	A	568	GLN
1	A	577	GLN
1	A	593	GLN
1	A	632	ASN
1	A	662	GLN
1	A	701	GLN
1	A	895	ASN
1	A	904	GLN
1	A	949	GLN
1	A	1025	HIS
1	B	93	GLN
1	B	220	ASN
1	B	297	GLN
1	B	301	GLN
1	B	351	GLN
1	B	472	ASN
1	B	539	GLN
1	B	575	GLN
1	B	593	GLN
1	B	662	GLN
1	B	701	GLN

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Mol	Chain	Res	Type
1	B	807	ASN
1	B	836	GLN
1	B	888	GLN
1	B	895	ASN
1	B	904	GLN
1	B	949	GLN
1	B	1018	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.