Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 07:33 AM EDT

PDB ID	:	3AOC
Title	:	Structures of the multidrug exporter AcrB reveal a proximal multisite drug-binding pocket
Authors	:	Nakashima, R.; Sakurai, K.; Yamaguchi, A.
Deposited on	:	2010-09-23
Resolution	:	3.34 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

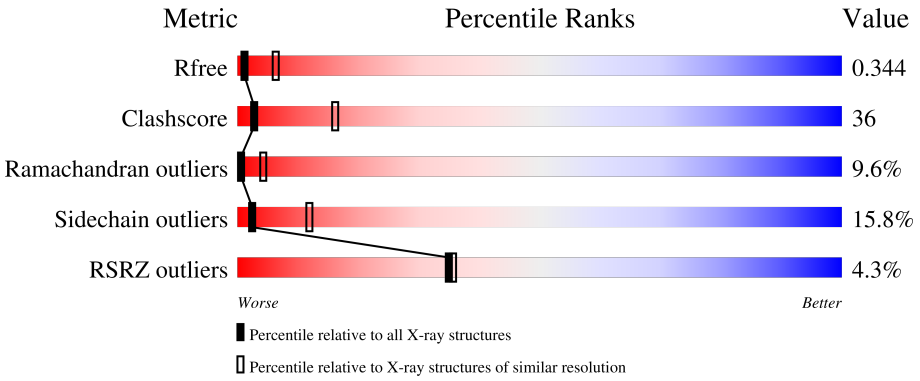
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.34 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1060 (3.38-3.30)
Clashscore	141614	1111 (3.38-3.30)
Ramachandran outliers	138981	1090 (3.38-3.30)
Sidechain outliers	138945	1089 (3.38-3.30)
RSRZ outliers	127900	1028 (3.38-3.30)

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 of 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1053	4% 38% 46% 12%
1	B	1053	5% 35% 47% 14%
1	C	1053	4% 39% 47% 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23378 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.

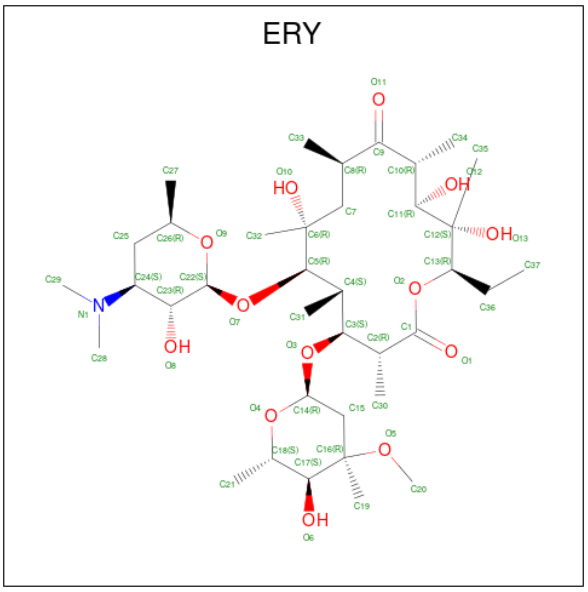
- Molecule 1 is a protein called Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	B	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			
1	C	1022	Total	C	N	O	S	0	0	0
			7774	5003	1283	1444	44			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C N O 51 37 1 13	0	0

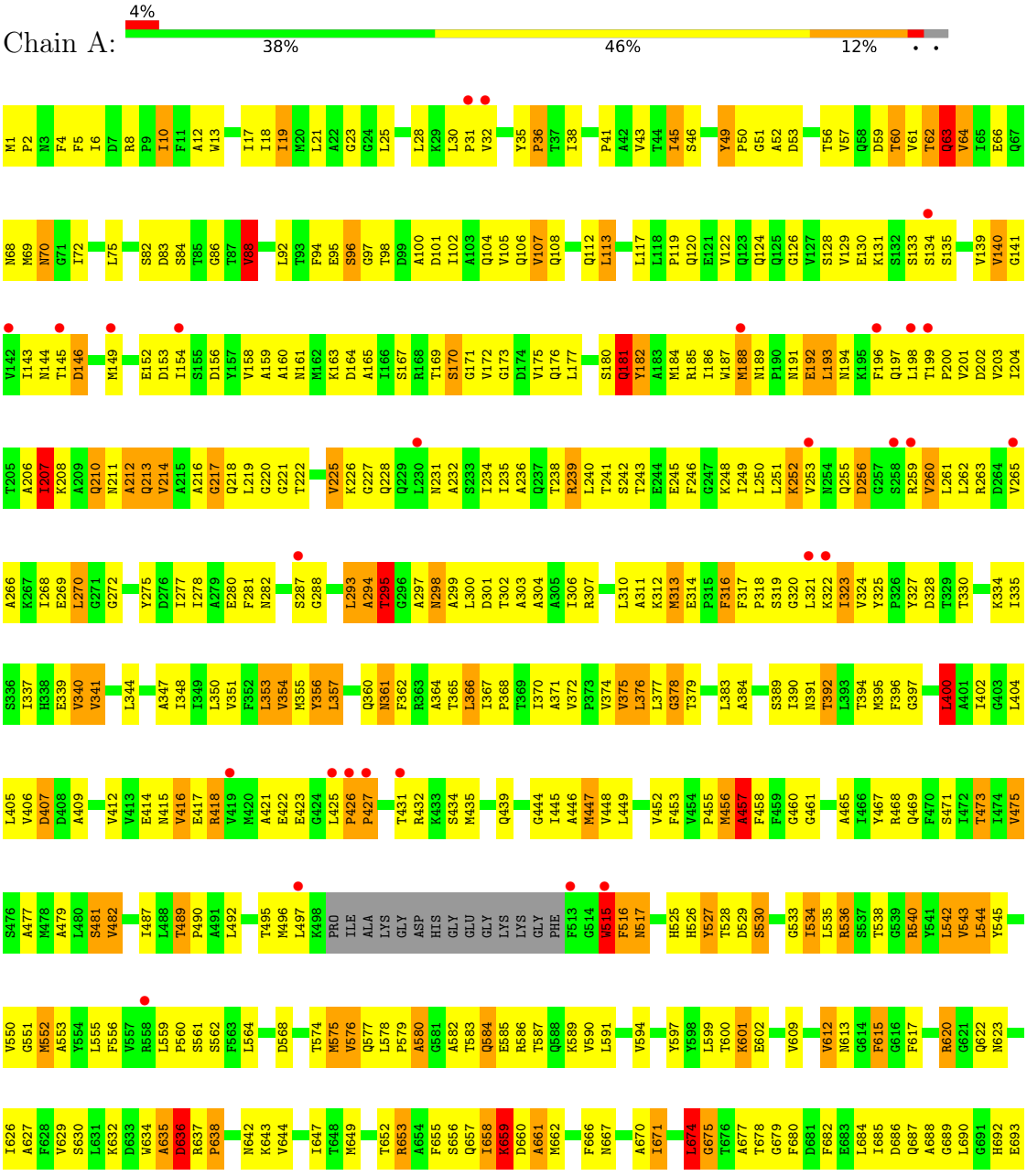
- Molecule 3 is water.

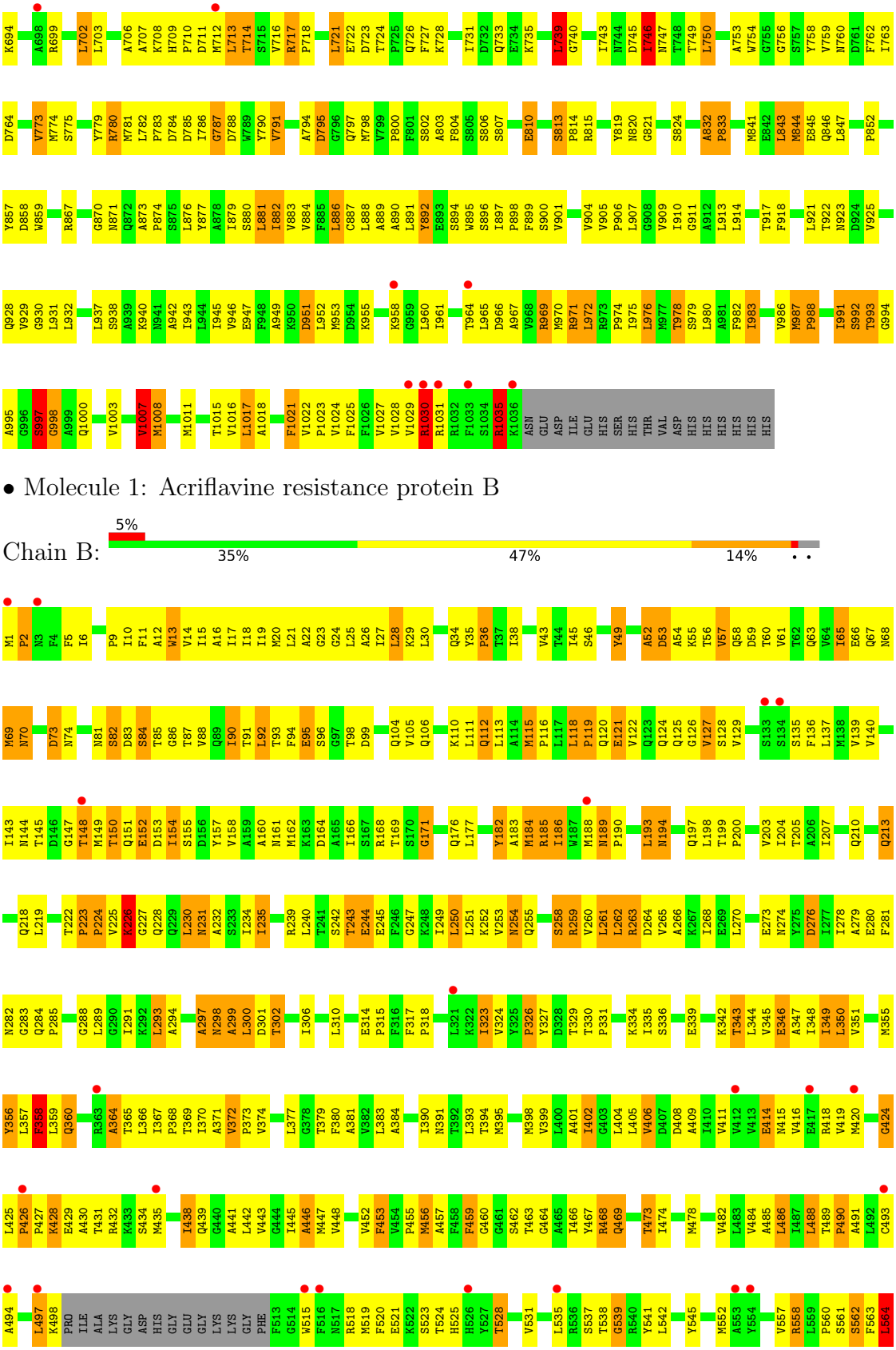
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total O 2 2	0	0
3	B	2	Total O 2 2	0	0
3	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

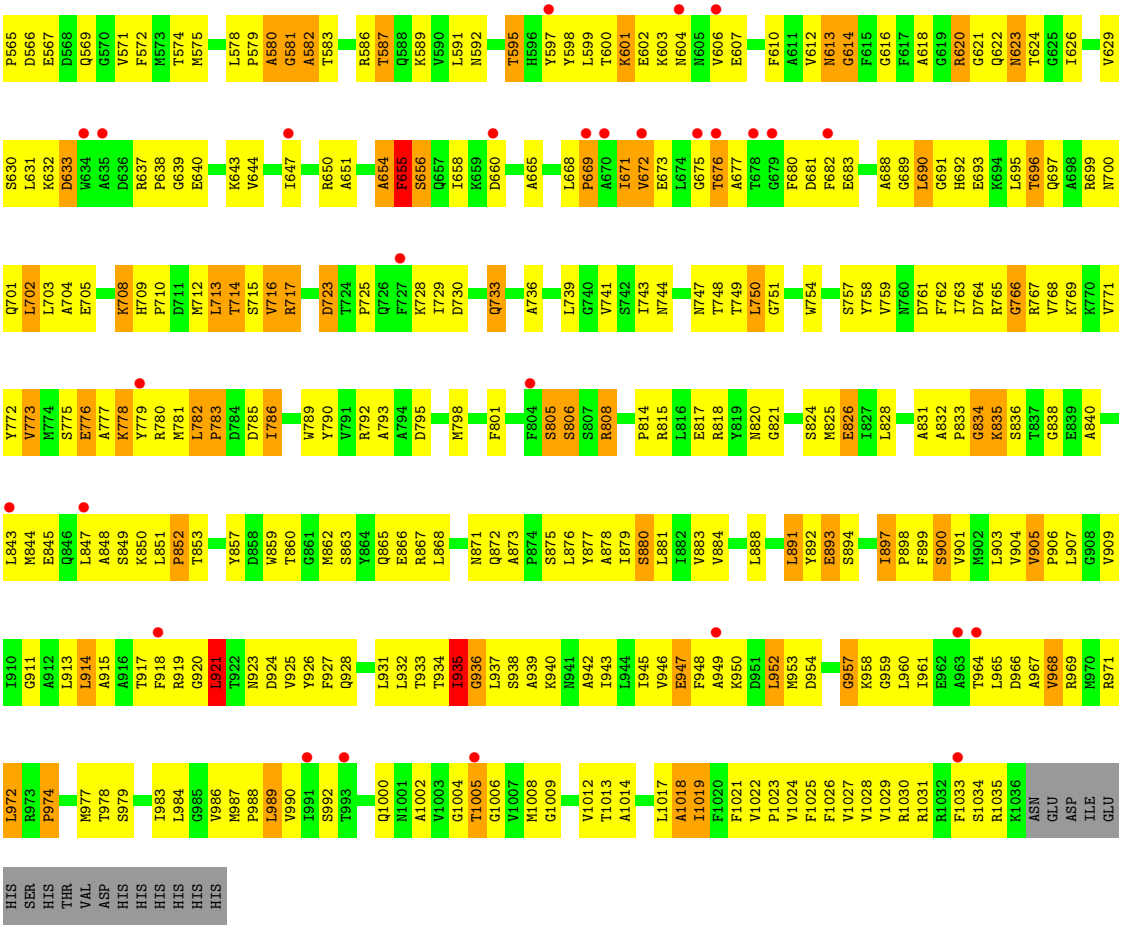
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Acriflavine resistance protein B

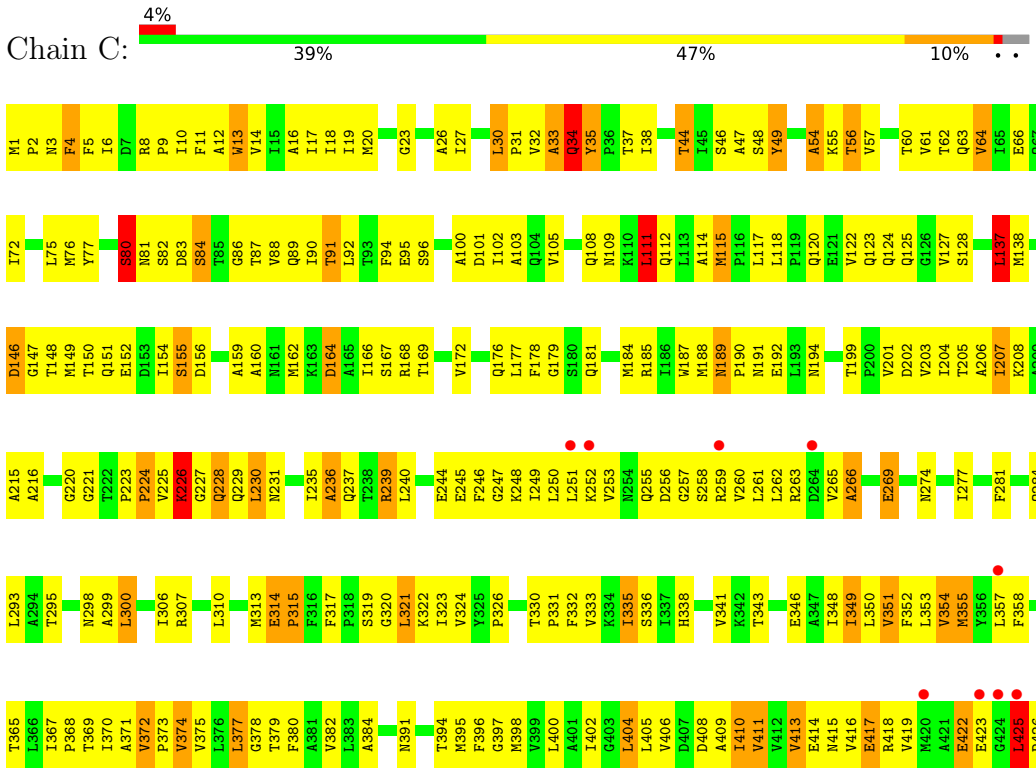


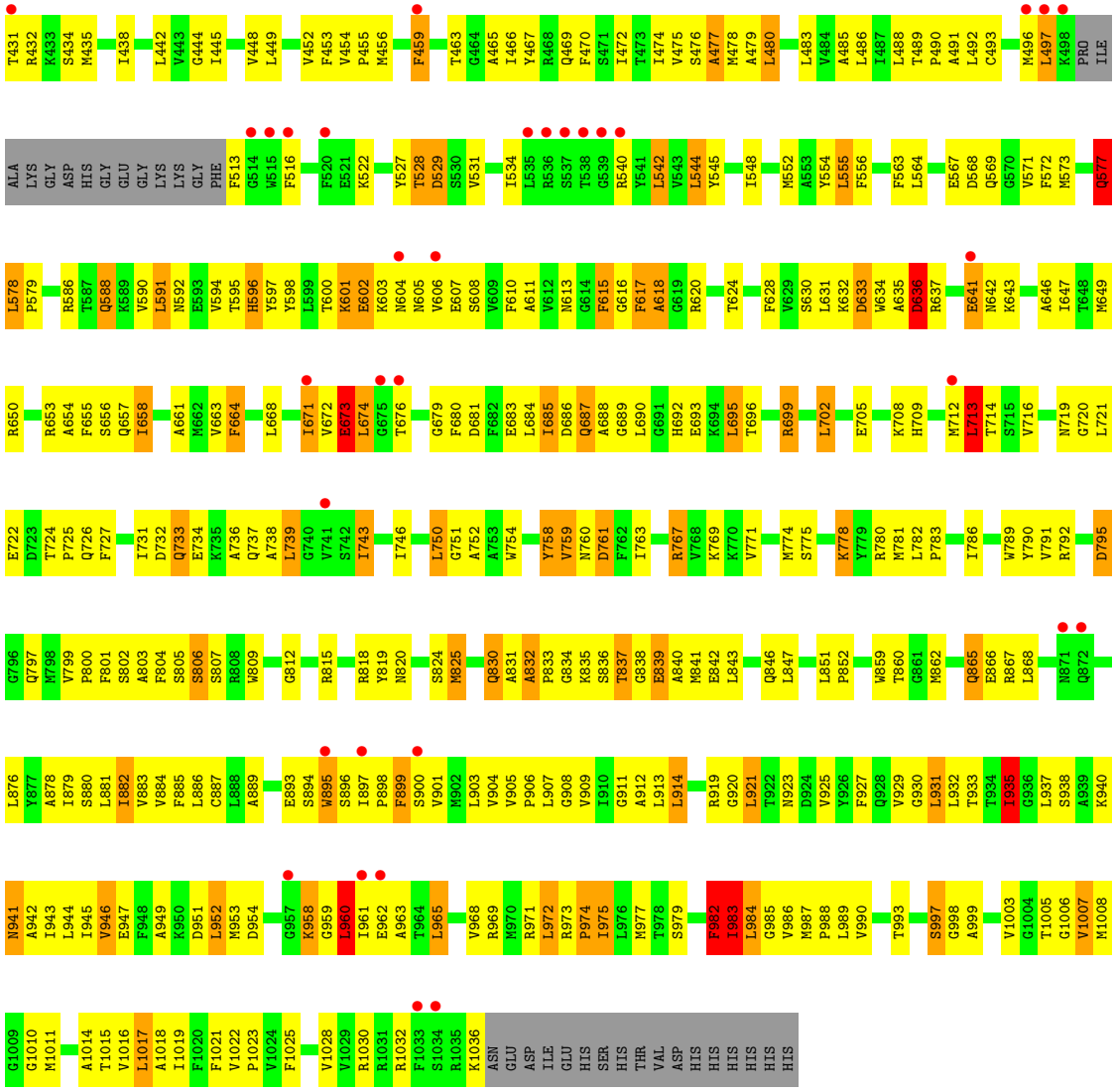


• Molecule 1: Acriflavine resistance protein B



• Molecule 1: Acriflavine resistance protein B




T431 R432 K433 S434 M435 I438 L442 V443 G444 I445 V448 L449 V452 F453 V454 P455 M456 F459 T463 G464 A465 I466 Y467 R468 Q469 F470 S471 I472 T473 I474 V475 S476 A477 M478 A479 L480 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492 C493 M496 L497 K498 PRO ILE
ALA LYS GLY ASP HIS GLY GLU GLY LYS LYS GLY PHE F513 G514 W515 F516 F520 E521 K522 Y527 T528 D529 S530 V531 I534 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 I548 M552 A553 Y554 L555 F556 F563 L564 E567 D568 Q569 G570 V571 F572 M573 Q577
L578 P579 R586 T587 Q588 K589 V590 L591 N592 E593 V594 T595 H596 Y597 Y598 L599 T600 K601 E602 K603 N604 N605 V606 E607 S608 V609 F610 A611 V612 N613 G614 F615 G616 F617 A618 G619 R620 T624 F628 V629 S630 L631 K632 D633 W634 A635 D636 R637 E641 N642 K643 A646 I647 T648 M649
R650 R653 A654 F655 S656 Q657 I658 A661 M662 V663 F664 L668 I671 V672 E673 L674 G675 T676 G679 F680 D681 F682 E683 L684 I685 D686 Q687 A688 G689 L690 G691 H692 E693 K694 L695 T696 R699 L702 E705 K708 H709 M712 L713 T714 S715 V716 N719 G720 L721
E722 D723 T724 P725 Q726 F727 I731 D732 Q733 E734 K735 A736 Q737 A738 L739 G740 V741 S742 I743 I746 L750 G751 A752 A753 W754 Y758 V759 N760 D761 F762 I763 R767 V768 K769 K770 V771 M774 S775 K778 Y779 R780 M781 L782 P783 I786 W789 Y790 V791 R792 D795
G796 Q797 M798 V799 P800 F801 S802 A803 F804 S805 S806 S807 R808 W809 G812 R815 R818 Y819 N820 S824 M825 Q830 A831 A832 P833 G834 K835 S836 T837 G838 E839 A840 M841 E842 L843 Q846 L847 L851 P852 W859 T860 G861 M862 Q865 E866 R867 L868 W871 Q872
L876 Y877 A878 I879 S880 L881 I882 V883 V884 F885 L886 C887 L888 A889 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 G911 A912 I913 L914 R919 G920 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 T933 T934 I935 G936 L937 S938 A939 K940
N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953 D954 G957 K958 G959 L960 I961 E962 A963 T964 L965 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 T978 S979 F982 I983 L984 G985 V986 M987 P988 L989 V990 T993 S997 G998 A999 V1003 G1004 T1005 G1006 V1007 M1008
G1009 G1010 M1011 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1026 V1028 V1029 R1030 R1031 R1032 F1033 S1034 R1035 K1036 ASN GLU ASP ILE GLU HIS SER HIS THR VAL ASP HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.28Å 134.21Å 162.05Å 90.00° 98.20° 90.00°	Depositor
Resolution (Å)	45.73 – 3.34 45.73 – 3.34	Depositor EDS
% Data completeness (in resolution range)	95.4 (45.73-3.34) 95.4 (45.73-3.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.91 (at 3.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.273 , 0.344 0.269 , 0.344	Depositor DCC
R_{free} test set	3329 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	97.8	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 74.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	23378	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.61	0/7920	0.77	6/10756 (0.1%)
1	B	0.59	0/7920	0.75	4/10756 (0.0%)
1	C	0.63	0/7920	0.78	6/10756 (0.1%)
All	All	0.61	0/23760	0.77	16/32268 (0.0%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	457	ALA	N-CA-CB	-19.94	82.18	110.10
1	A	456	MET	N-CA-C	7.14	130.27	111.00
1	C	960	LEU	CA-CB-CG	6.55	130.38	115.30
1	B	960	LEU	CA-CB-CG	6.32	129.83	115.30
1	C	578	LEU	CA-CB-CG	6.10	129.34	115.30
1	C	137	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	400	LEU	CA-CB-CG	5.83	128.70	115.30
1	A	674	LEU	CA-CB-CG	5.73	128.48	115.30
1	C	673	GLU	N-CA-C	-5.64	95.76	111.00
1	A	739	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	193	LEU	CA-CB-CG	5.33	127.55	115.30
1	A	88	VAL	CB-CA-C	-5.17	101.57	111.40
1	B	118	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	674	LEU	CA-CB-CG	5.13	127.10	115.30
1	C	111	LEU	CA-CB-CG	5.10	127.02	115.30
1	B	230	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7774	0	7931	510	0
1	B	7774	0	7931	626	0
1	C	7774	0	7931	611	0
2	C	51	0	67	10	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	23378	0	23860	1686	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 36.

All (1686) 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:456:MET:HG3	1:B:467:TYR:HB3	1.24	1.16
1:A:145:THR:HG22	1:A:320:GLY:HA3	1.15	1.13
1:A:710:PRO:HA	1:A:713:LEU:HD22	1.19	1.12
1:A:638:PRO:HD2	1:A:642:ASN:HD22	1.04	1.07
1:A:714:THR:HG23	1:A:832:ALA:HA	1.33	1.06
1:A:317:PHE:HB3	1:A:321:LEU:HB2	1.36	1.05
1:A:414:GLU:HG2	1:A:974:PRO:HG3	1.35	1.05
1:A:94:PHE:HB3	1:A:98:THR:HG21	1.39	1.02
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.41	1.02
1:A:674:LEU:HD22	1:A:675:GLY:H	1.25	1.01
1:A:945:ILE:HG13	1:A:971:ARG:HG2	1.40	1.01
1:C:577:GLN:HB3	1:C:624:THR:HG22	1.41	1.01
1:C:415:ASN:HA	1:C:418:ARG:HE	1.23	1.01
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.24	1.00
1:B:52:ALA:HB2	1:B:86:GLY:N	1.76	1.00
1:B:879:ILE:O	1:B:883:VAL:HG23	1.58	1.00
1:C:34:GLN:HE22	1:C:299:ALA:HB3	1.26	0.99
1:B:445:ILE:HG23	1:B:940:LYS:HG3	1.44	0.99
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	1.43	0.98
1:A:140:VAL:HG12	1:A:141:GLY:H	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.44	0.98
1:A:447:MET:HB3	1:A:887:CYS:SG	2.04	0.98
1:C:901:VAL:HG11	1:C:943:ILE:HG13	1.43	0.97
1:C:26:ALA:O	1:C:30:LEU:HB2	1.63	0.96
1:A:659:LYS:HG2	1:A:660:ASP:H	1.27	0.96
1:C:418:ARG:HH12	1:C:971:ARG:HH11	1.06	0.95
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.46	0.95
1:C:240:LEU:HD12	1:C:245:GLU:HB3	1.48	0.94
1:A:246:PHE:O	1:A:249:ILE:HG12	1.68	0.94
1:A:145:THR:CG2	1:A:320:GLY:HA3	1.97	0.94
1:C:23:GLY:HA3	1:C:377:LEU:O	1.69	0.93
1:A:756:GLY:HA2	1:A:774:MET:HB2	1.52	0.92
1:B:574:THR:HG23	1:B:665:ALA:HB2	1.51	0.92
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.52	0.91
1:C:959:GLY:H	1:C:962:GLU:HB2	1.36	0.90
1:B:485:ALA:HA	1:B:489:THR:HB	1.54	0.90
1:A:638:PRO:HD2	1:A:642:ASN:ND2	1.87	0.89
1:B:26:ALA:O	1:B:30:LEU:HB2	1.73	0.89
1:A:710:PRO:CA	1:A:713:LEU:HD22	2.03	0.89
1:C:979:SER:O	1:C:983:ILE:HG12	1.72	0.88
1:A:795:ASP:HB2	1:A:797:GLN:HG2	1.54	0.88
1:B:743:ILE:HD12	1:B:743:ILE:H	1.37	0.88
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.55	0.87
1:B:631:LEU:HB3	1:B:637:ARG:HH12	1.39	0.87
1:B:222:THR:OG1	1:B:223:PRO:HD3	1.75	0.87
1:C:404:LEU:HD22	1:C:478:MET:HG3	1.56	0.87
1:C:409:ALA:O	1:C:413:VAL:HG12	1.72	0.87
1:C:972:LEU:H	1:C:974:PRO:HD2	1.39	0.87
1:A:140:VAL:HG12	1:A:141:GLY:N	1.88	0.86
1:B:986:VAL:O	1:B:990:VAL:HG23	1.75	0.86
1:C:11:PHE:O	1:C:14:VAL:HG12	1.76	0.86
1:C:513:PHE:HB2	1:C:516:PHE:HB2	1.58	0.85
1:C:692:HIS:HE1	1:C:721:LEU:HD21	1.38	0.85
1:A:612:VAL:HG23	1:A:626:ILE:HG22	1.58	0.85
1:A:525:HIS:HA	1:A:528:THR:HG22	1.59	0.85
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.56	0.85
1:B:607:GLU:HG2	1:B:632:LYS:HA	1.57	0.84
1:B:583:THR:HG22	1:B:586:ARG:HD3	1.59	0.84
1:A:141:GLY:HA2	1:A:288:GLY:HA2	1.58	0.84
1:B:591:LEU:O	1:B:595:THR:HG22	1.78	0.84
1:A:731:ILE:HD12	1:A:746:ILE:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HA	1:C:418:ARG:NE	1.93	0.83
1:B:24:GLY:H	1:B:27:ILE:HG23	1.44	0.83
1:C:176:GLN:NE2	1:C:620:ARG:NH1	2.26	0.83
1:C:767:ARG:HG3	1:C:767:ARG:HH11	1.43	0.83
1:C:545:TYR:OH	1:C:1021:PHE:HB3	1.78	0.83
1:B:143:ILE:HD12	1:B:144:ASN:H	1.43	0.82
1:B:736:ALA:HB1	1:B:741:VAL:CG2	2.08	0.82
1:A:13:TRP:O	1:A:17:ILE:HG12	1.77	0.82
1:B:193:LEU:HD23	1:B:265:VAL:HG11	1.59	0.82
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.62	0.82
1:C:713:LEU:CD1	1:C:834:GLY:HA3	2.09	0.82
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.60	0.82
1:B:157:TYR:HA	1:B:161:ASN:ND2	1.95	0.82
1:C:758:TYR:H	1:C:758:TYR:HD1	1.27	0.82
1:C:713:LEU:HD11	1:C:835:LYS:H	1.44	0.82
1:B:401:ALA:HA	1:B:404:LEU:HB2	1.61	0.82
1:C:265:VAL:O	1:C:265:VAL:HG23	1.79	0.81
1:B:235:ILE:HD13	1:B:235:ILE:N	1.96	0.81
1:A:750:LEU:O	1:A:754:TRP:HD1	1.64	0.81
1:A:51:GLY:O	1:C:215:ALA:HB1	1.80	0.80
1:B:715:SER:O	1:B:716:VAL:HG23	1.82	0.80
1:C:416:VAL:HG11	1:C:431:THR:HG22	1.63	0.80
1:A:140:VAL:CG1	1:A:141:GLY:H	1.94	0.80
1:A:591:LEU:CD1	1:A:613:ASN:HB3	2.11	0.80
1:B:563:PHE:HD1	1:B:866:GLU:HG3	1.46	0.80
1:B:359:LEU:HD23	1:B:365:THR:HA	1.62	0.80
1:C:932:LEU:HA	1:C:935:ILE:HG22	1.63	0.79
1:A:6:ILE:HD11	1:A:432:ARG:HD2	1.64	0.79
1:A:883:VAL:O	1:A:887:CYS:HB2	1.82	0.79
1:C:400:LEU:HD12	1:C:929:VAL:HG12	1.65	0.79
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.64	0.79
1:B:673:GLU:O	1:B:676:THR:HG22	1.82	0.79
1:B:143:ILE:HD13	1:B:285:PRO:O	1.83	0.78
1:C:552:MET:SD	1:C:909:VAL:HG21	2.22	0.78
1:C:672:VAL:CG1	1:C:673:GLU:H	1.96	0.78
1:C:983:ILE:HG23	1:C:1008:MET:HG2	1.65	0.78
1:A:396:PHE:CD2	1:A:1003:VAL:HG21	2.18	0.78
1:A:945:ILE:CG1	1:A:971:ARG:HG2	2.13	0.78
1:A:746:ILE:HD12	1:A:791:VAL:HG21	1.64	0.78
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.78
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:MET:HA	1:C:835:LYS:HG3	1.66	0.78
1:C:605:ASN:HB3	1:C:637:ARG:HD3	1.64	0.78
1:C:144:ASN:ND2	1:C:149:MET:H	1.81	0.77
1:A:552:MET:HE1	1:A:906:PRO:HA	1.65	0.77
1:B:552:MET:SD	1:B:909:VAL:HG21	2.24	0.77
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.15	0.77
1:B:225:VAL:H	1:C:781:MET:HE3	1.49	0.76
1:B:149:MET:HB3	1:B:154:ILE:HG22	1.67	0.76
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.66	0.76
1:A:278:ILE:HB	1:A:613:ASN:OD1	1.86	0.76
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.48	0.76
1:B:224:PRO:HA	1:C:781:MET:HE3	1.68	0.76
1:C:34:GLN:HE22	1:C:299:ALA:CB	1.99	0.76
1:C:894:SER:OG	1:C:897:ILE:HG12	1.86	0.76
1:A:890:ALA:HB1	1:C:11:PHE:HD1	1.50	0.76
1:B:343:THR:HG21	1:B:1000:GLN:OE1	1.84	0.76
1:B:399:VAL:O	1:B:402:ILE:HG22	1.85	0.76
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.65	0.76
1:C:588:GLN:HG2	1:C:613:ASN:HD22	1.51	0.76
1:A:702:LEU:HD21	1:A:844:MET:HE1	1.68	0.75
1:A:404:LEU:HD21	1:A:449:LEU:HD13	1.68	0.75
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.67	0.75
1:A:43:VAL:HG11	1:A:107:VAL:HG21	1.66	0.75
1:A:396:PHE:HD2	1:A:1003:VAL:HG21	1.51	0.75
1:B:552:MET:SD	1:B:909:VAL:CG2	2.74	0.75
2:C:3402:ERY:H302	2:C:3402:ERY:H14	1.68	0.75
1:A:354:VAL:HG12	1:A:355:MET:H	1.50	0.75
1:A:344:LEU:HD13	1:A:376:LEU:HD21	1.68	0.75
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.21	0.75
1:B:934:THR:C	1:B:936:GLY:H	1.90	0.74
1:B:934:THR:O	1:B:936:GLY:N	2.20	0.74
1:C:448:VAL:HG22	1:C:887:CYS:HB3	1.68	0.74
1:C:618:ALA:HB1	1:C:815:ARG:HH12	1.52	0.74
1:B:923:ASN:HD22	1:B:927:PHE:HD2	1.34	0.74
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.67	0.74
1:B:924:ASP:O	1:B:928:GLN:HG3	1.87	0.74
1:A:294:ALA:HB3	1:A:297:ALA:HB2	1.70	0.74
1:B:892:TYR:HB3	1:B:897:ILE:HD11	1.68	0.74
1:B:579:PRO:O	1:B:580:ALA:O	2.05	0.74
1:A:659:LYS:HG2	1:A:660:ASP:N	2.03	0.74
1:A:6:ILE:HG22	1:A:490:PRO:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLN:HG3	1:C:56:THR:HG23	1.69	0.74
1:C:176:GLN:HE22	1:C:620:ARG:NH1	1.84	0.73
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.70	0.73
1:A:707:ALA:HA	1:A:713:LEU:HD12	1.71	0.73
1:B:30:LEU:HD22	1:B:390:ILE:HG13	1.67	0.73
1:B:242:SER:HB2	1:B:245:GLU:OE2	1.87	0.73
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.24	0.73
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.23	0.73
1:A:921:LEU:HG	1:A:922:THR:H	1.51	0.73
1:B:36:PRO:HD3	1:B:391:ASN:ND2	2.04	0.73
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.69	0.73
1:B:203:VAL:O	1:B:207:ILE:HG12	1.88	0.73
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.70	0.73
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.70	0.73
1:A:144:ASN:HD22	1:A:149:MET:H	1.37	0.73
1:B:213:GLN:CG	1:C:56:THR:HG23	2.18	0.73
1:B:276:ASP:O	1:B:614:GLY:HA3	1.89	0.73
1:B:441:ALA:O	1:B:445:ILE:HG12	1.88	0.73
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.69	0.72
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.71	0.72
1:B:426:PRO:HB3	1:B:430:ALA:HB3	1.71	0.72
1:B:119:PRO:HB2	1:B:122:VAL:HG23	1.70	0.72
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.70	0.72
1:B:947:GLU:OE1	1:B:947:GLU:HA	1.88	0.72
1:C:92:LEU:HD12	1:C:92:LEU:H	1.53	0.72
1:A:728:LYS:HD2	1:C:235:ILE:O	1.89	0.72
1:C:681:ASP:HB3	1:C:860:THR:CG2	2.20	0.72
1:C:600:THR:O	1:C:603:LYS:HB2	1.90	0.72
1:A:597:TYR:O	1:A:601:LYS:HB3	1.89	0.72
1:A:188:MET:HA	1:A:266:ALA:HB2	1.72	0.72
1:B:560:PRO:HB2	1:B:836:SER:HB2	1.71	0.72
1:B:675:GLY:O	1:B:677:ALA:N	2.22	0.72
1:C:548:ILE:HD13	1:C:1017:LEU:HD21	1.72	0.71
1:C:203:VAL:O	1:C:207:ILE:HG12	1.90	0.71
1:A:753:ALA:HB3	1:A:754:TRP:CD1	2.26	0.71
1:C:617:PHE:O	2:C:3402:ERY:H332	1.90	0.71
1:C:709:HIS:HB3	1:C:712:MET:SD	2.31	0.71
1:A:170:SER:O	1:A:302:THR:HG22	1.90	0.71
1:C:137:LEU:HD23	1:C:293:LEU:HD13	1.73	0.71
1:A:4:PHE:HB3	1:A:8:ARG:NH2	2.05	0.71
1:C:795:ASP:OD1	1:C:797:GLN:HB2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.72	0.70
1:C:143:ILE:HD11	1:C:281:PHE:HB3	1.72	0.70
1:A:10:ILE:HG21	1:B:893:GLU:O	1.90	0.70
1:A:721:LEU:HD12	1:A:814:PRO:HG2	1.73	0.70
1:C:210:GLN:O	1:C:240:LEU:HD21	1.91	0.70
1:A:782:LEU:O	1:A:785:ASP:HB2	1.91	0.70
1:C:124:GLN:CB	1:C:758:TYR:HE2	2.05	0.70
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.56	0.70
1:A:471:SER:O	1:A:475:VAL:HG12	1.90	0.70
1:C:418:ARG:NH1	1:C:971:ARG:HH11	1.86	0.69
1:C:166:ILE:HG21	1:C:291:ILE:HD11	1.72	0.69
1:A:41:PRO:HB3	1:A:100:ALA:HB2	1.74	0.69
1:C:265:VAL:O	1:C:266:ALA:HB2	1.91	0.69
1:C:713:LEU:HD11	1:C:835:LYS:N	2.06	0.69
1:B:210:GLN:HG2	1:C:733:GLN:HE21	1.56	0.69
1:A:145:THR:HG21	1:A:322:LYS:HE2	1.73	0.69
1:A:591:LEU:HD12	1:A:613:ASN:HB3	1.74	0.69
1:A:714:THR:HG23	1:A:832:ALA:CA	2.19	0.69
1:B:932:LEU:HA	1:B:935:ILE:HG13	1.73	0.69
1:C:839:GLU:HA	1:C:842:GLU:HB3	1.74	0.69
1:A:314:GLU:HA	1:A:317:PHE:CD2	2.27	0.69
1:B:66:GLU:OE2	1:B:821:GLY:HA2	1.93	0.69
1:B:298:ASN:O	1:B:300:LEU:N	2.26	0.69
1:C:727:PHE:CE1	1:C:807:SER:HB2	2.28	0.69
1:B:460:GLY:HA2	1:B:872:GLN:HE22	1.58	0.69
1:A:674:LEU:CD2	1:A:675:GLY:H	2.04	0.69
1:A:707:ALA:HA	1:A:713:LEU:CD1	2.23	0.69
1:A:746:ILE:HG13	1:A:804:PHE:CE1	2.26	0.69
1:B:344:LEU:O	1:B:348:ILE:HG13	1.93	0.69
1:B:561:SER:O	1:B:838:GLY:HA3	1.93	0.69
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.58	0.69
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.23	0.68
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.75	0.68
1:C:146:ASP:HB3	1:C:148:THR:CG2	2.21	0.68
1:A:180:SER:O	1:A:181:GLN:HB3	1.91	0.68
1:B:671:ILE:HG22	1:B:676:THR:HB	1.75	0.68
1:C:190:PRO:HG3	1:C:789:TRP:CZ2	2.29	0.68
1:A:2:PRO:O	1:A:6:ILE:HG23	1.92	0.68
1:B:717:ARG:CG	1:B:717:ARG:HH11	2.06	0.68
1:A:895:TRP:HZ2	1:C:13:TRP:CE3	2.10	0.68
1:B:419:VAL:O	1:B:419:VAL:HG12	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:GLU:HA	1:C:708:LYS:HE2	1.75	0.68
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.75	0.68
1:A:1021:PHE:HD1	1:A:1025:PHE:CE1	2.11	0.68
1:B:68:ASN:C	1:B:70:ASN:H	1.96	0.68
1:B:326:PRO:HG2	1:B:610:PHE:CD1	2.28	0.68
1:B:775:SER:O	1:B:780:ARG:HD3	1.93	0.68
1:B:905:VAL:HG13	1:B:906:PRO:HD3	1.76	0.68
1:C:435:MET:HA	1:C:438:ILE:HG22	1.75	0.68
1:B:121:GLU:O	1:B:125:GLN:HG2	1.94	0.68
1:B:18:ILE:HG22	1:B:19:ILE:HD13	1.76	0.68
1:B:880:SER:O	1:B:884:VAL:HG23	1.94	0.68
1:C:973:ARG:O	1:C:977:MET:HB2	1.94	0.68
1:A:31:PRO:HB2	1:A:389:SER:HB2	1.74	0.68
1:B:456:MET:HG3	1:B:467:TYR:CB	2.13	0.68
1:C:2:PRO:O	1:C:6:ILE:HG12	1.92	0.68
1:C:672:VAL:HG12	1:C:673:GLU:H	1.59	0.68
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.76	0.68
1:C:759:VAL:HG23	1:C:771:VAL:O	1.94	0.68
1:A:23:GLY:HA3	1:A:378:GLY:HA2	1.77	0.67
1:A:299:ALA:O	1:A:303:ALA:HB2	1.94	0.67
1:A:643:LYS:O	1:A:647:ILE:HG13	1.93	0.67
1:A:844:MET:HA	1:A:844:MET:HE3	1.74	0.67
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.24	0.67
1:A:207:ILE:O	1:A:211:ASN:HB3	1.94	0.67
1:B:411:VAL:HB	1:B:438:ILE:HD11	1.76	0.67
1:B:717:ARG:HH11	1:B:717:ARG:HG2	1.58	0.67
1:C:66:GLU:OE2	1:C:80:SER:HB3	1.94	0.67
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.77	0.67
1:B:408:ASP:OD1	1:B:442:LEU:HA	1.94	0.67
1:C:244:GLU:HA	1:C:263:ARG:NH2	2.05	0.67
1:C:681:ASP:CB	1:C:860:THR:HG23	2.24	0.67
1:C:185:ARG:HB2	1:C:269:GLU:O	1.94	0.67
1:C:758:TYR:CD1	1:C:758:TYR:N	2.51	0.67
1:C:979:SER:O	1:C:983:ILE:CG1	2.41	0.67
1:B:94:PHE:CB	1:B:98:THR:HG21	2.24	0.67
1:B:416:VAL:O	1:B:426:PRO:HG2	1.95	0.67
1:B:915:ALA:CB	1:B:1009:GLY:HA3	2.24	0.67
1:B:55:LYS:HE2	1:B:59:ASP:OD1	1.94	0.67
1:B:298:ASN:HB3	1:B:301:ASP:HB2	1.76	0.67
1:B:582:ALA:O	1:B:583:THR:HB	1.94	0.67
1:C:925:VAL:O	1:C:929:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:CD1	1:A:1003:VAL:HG13	2.24	0.67
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.95	0.67
1:B:13:TRP:HE3	1:B:488:LEU:HD21	1.60	0.67
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.76	0.67
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.30	0.67
1:A:1:MET:SD	1:A:487:ILE:HD11	2.35	0.66
1:C:3:ASN:C	1:C:5:PHE:H	1.99	0.66
1:C:542:LEU:HD11	1:C:1028:VAL:HG11	1.76	0.66
1:B:188:MET:HB2	1:B:775:SER:HA	1.76	0.66
1:B:348:ILE:HG12	1:B:402:ILE:HD11	1.75	0.66
1:C:56:THR:O	1:C:60:THR:HB	1.95	0.66
1:C:610:PHE:HB3	1:C:628:PHE:HB2	1.76	0.66
1:C:636:ASP:OD1	1:C:636:ASP:N	2.27	0.66
1:B:149:MET:HB3	1:B:154:ILE:CG2	2.25	0.66
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.78	0.66
1:C:679:GLY:HA2	1:C:830:GLN:HA	1.76	0.66
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.66
1:A:94:PHE:CB	1:A:98:THR:HG21	2.22	0.66
1:A:294:ALA:O	1:A:295:THR:HB	1.93	0.66
1:C:616:GLY:HA3	1:C:624:THR:HB	1.76	0.66
1:B:419:VAL:O	1:B:426:PRO:HG3	1.95	0.66
1:A:69:MET:HE1	1:A:107:VAL:HG13	1.77	0.66
1:B:24:GLY:N	1:B:27:ILE:HG23	2.11	0.66
1:B:817:GLU:HB2	1:B:824:SER:O	1.96	0.66
1:C:986:VAL:O	1:C:986:VAL:HG12	1.96	0.66
1:B:13:TRP:CE3	1:B:488:LEU:HD21	2.30	0.65
1:B:859:TRP:HB3	1:B:863:SER:HB2	1.78	0.65
1:C:695:LEU:HD22	1:C:825:MET:SD	2.36	0.65
1:C:203:VAL:HG13	1:C:262:LEU:CD1	2.25	0.65
1:C:124:GLN:HB2	1:C:758:TYR:HE2	1.61	0.65
1:C:176:GLN:NE2	1:C:620:ARG:HH11	1.94	0.65
1:A:379:THR:HG21	1:A:477:ALA:HA	1.76	0.65
1:B:249:ILE:HB	1:B:262:LEU:HD12	1.78	0.65
1:B:632:LYS:O	1:B:633:ASP:O	2.15	0.65
1:C:522:LYS:HE2	1:C:522:LYS:HA	1.78	0.65
1:C:641:GLU:O	1:C:650:ARG:NH1	2.30	0.65
1:A:746:ILE:CD1	1:A:791:VAL:HG21	2.27	0.65
1:A:780:ARG:HG2	1:A:780:ARG:HH11	1.61	0.65
1:B:911:GLY:HA2	1:B:914:LEU:HB2	1.79	0.65
1:B:952:LEU:C	1:B:954:ASP:H	2.00	0.65
1:B:1009:GLY:O	1:B:1012:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.79	0.64
1:A:141:GLY:HA2	1:A:288:GLY:CA	2.28	0.64
1:B:925:VAL:HA	1:B:928:GLN:OE1	1.97	0.64
1:A:747:ASN:HD21	1:C:237:GLN:HE21	1.45	0.64
1:B:189:ASN:O	1:B:193:LEU:HB2	1.97	0.64
1:B:213:GLN:HB2	1:B:239:ARG:HG3	1.79	0.64
1:B:157:TYR:CA	1:B:161:ASN:HD22	2.10	0.64
1:A:591:LEU:HD11	1:A:613:ASN:HB3	1.77	0.64
1:B:563:PHE:CD1	1:B:866:GLU:HG3	2.32	0.64
1:A:171:GLY:HA3	1:A:302:THR:HG21	1.80	0.64
1:A:217:GLY:O	1:A:234:ILE:HG12	1.97	0.64
1:B:144:ASN:HD21	1:B:148:THR:H	1.44	0.64
1:B:683:GLU:OE1	1:B:826:GLU:HG3	1.98	0.64
1:B:931:LEU:O	1:B:935:ILE:HG12	1.97	0.64
1:A:714:THR:CG2	1:A:832:ALA:HA	2.19	0.64
1:B:5:PHE:HB3	1:B:12:ALA:HB2	1.80	0.64
1:C:752:ALA:O	1:C:774:MET:HA	1.98	0.64
1:A:159:ALA:HA	1:A:163:LYS:HB2	1.79	0.64
1:C:664:PHE:H	1:C:664:PHE:HD2	1.46	0.64
1:C:688:ALA:O	1:C:690:LEU:N	2.31	0.64
1:A:188:MET:HA	1:A:266:ALA:CB	2.27	0.64
1:B:356:TYR:CE2	1:B:365:THR:HG21	2.33	0.64
1:C:3:ASN:HD21	1:C:432:ARG:HG3	1.62	0.64
1:C:61:VAL:O	1:C:64:VAL:HG23	1.98	0.64
1:C:265:VAL:O	1:C:266:ALA:CB	2.46	0.64
1:A:102:ILE:HD11	1:C:101:ASP:HB3	1.80	0.63
1:A:277:ILE:HD11	1:A:615:PHE:HB3	1.80	0.63
1:B:339:GLU:O	1:B:342:LYS:HB3	1.98	0.63
1:C:713:LEU:HD11	1:C:834:GLY:CA	2.26	0.63
1:A:117:LEU:HD21	1:C:124:GLN:O	1.98	0.63
1:B:135:SER:HB2	1:B:676:THR:HG21	1.80	0.63
1:B:143:ILE:HD12	1:B:144:ASN:N	2.10	0.63
1:B:251:LEU:HD22	1:B:262:LEU:H	1.62	0.63
1:C:20:MET:HG3	1:C:374:VAL:HG23	1.80	0.63
1:A:895:TRP:HZ2	1:C:13:TRP:HE3	1.46	0.63
1:A:530:SER:O	1:A:534:ILE:HG13	1.97	0.63
1:A:886:LEU:CD1	1:C:14:VAL:HG23	2.28	0.63
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.64	0.63
1:A:731:ILE:HD12	1:A:746:ILE:CG2	2.27	0.63
1:A:154:ILE:O	1:A:158:VAL:HG23	1.99	0.63
1:C:144:ASN:HD22	1:C:149:MET:H	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:897:ILE:N	1:C:898:PRO:HD2	2.13	0.63
1:A:113:LEU:HG	1:C:127:VAL:HG23	1.81	0.63
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.80	0.63
1:A:620:ARG:HH11	1:A:620:ARG:CG	2.11	0.63
1:A:901:VAL:O	1:A:904:VAL:HG23	1.98	0.63
1:C:455:PRO:O	1:C:876:LEU:HD11	1.98	0.63
1:A:713:LEU:HD23	1:A:714:THR:H	1.63	0.62
1:B:359:LEU:CD2	1:B:365:THR:HA	2.29	0.62
1:A:890:ALA:HB1	1:C:11:PHE:CD1	2.32	0.62
1:B:111:LEU:HD22	1:B:129:VAL:CG2	2.29	0.62
1:A:145:THR:HG23	1:A:146:ASP:H	1.65	0.62
1:B:158:VAL:HA	1:B:162:MET:CG	2.28	0.62
1:B:326:PRO:O	1:B:630:SER:HB2	2.00	0.62
1:B:349:ILE:C	1:B:351:VAL:H	2.03	0.62
1:C:246:PHE:O	1:C:249:ILE:HG12	2.00	0.62
1:C:767:ARG:HH11	1:C:767:ARG:CG	2.11	0.62
1:A:182:TYR:HB3	1:A:270:LEU:HD11	1.82	0.62
1:A:330:THR:HG22	1:A:334:LYS:HE2	1.82	0.62
1:B:225:VAL:N	1:C:781:MET:HE3	2.15	0.62
1:A:144:ASN:HA	1:A:320:GLY:O	1.99	0.62
1:B:904:VAL:HG13	1:B:907:LEU:HD12	1.82	0.62
1:C:911:GLY:C	1:C:1010:GLY:HA2	2.20	0.62
1:A:717:ARG:HB2	1:A:718:PRO:HD2	1.82	0.62
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.99	0.62
1:B:346:GLU:O	1:B:988:PRO:HG3	2.00	0.62
1:C:211:ASN:HD22	1:C:240:LEU:HD23	1.65	0.62
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.82	0.62
1:A:241:THR:HG22	1:A:763:ILE:O	2.00	0.61
1:B:445:ILE:HD13	1:B:943:ILE:HG23	1.83	0.61
1:A:144:ASN:ND2	1:A:149:MET:H	1.97	0.61
1:A:888:LEU:HD21	1:A:901:VAL:HB	1.82	0.61
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.82	0.61
1:A:552:MET:CE	1:A:906:PRO:HA	2.29	0.61
1:C:372:VAL:HG21	1:C:406:VAL:HG22	1.82	0.61
1:A:713:LEU:HD23	1:A:714:THR:N	2.14	0.61
1:B:680:PHE:O	1:B:828:LEU:HD23	2.00	0.61
1:C:423:GLU:HB3	1:C:426:PRO:HD2	1.81	0.61
1:B:714:THR:HG22	1:B:831:ALA:HA	1.82	0.61
1:B:792:ARG:HG2	1:B:793:ALA:N	2.16	0.61
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.83	0.61
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:MET:SD	1:C:843:LEU:HD22	2.41	0.61
1:B:525:HIS:HA	1:B:528:THR:HG22	1.82	0.61
1:B:859:TRP:HB3	1:B:863:SER:CB	2.30	0.61
1:C:16:ALA:HB1	1:C:374:VAL:HG21	1.83	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61
1:A:568:ASP:O	1:A:634:TRP:CH2	2.54	0.61
1:B:485:ALA:HA	1:B:489:THR:CB	2.29	0.61
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.83	0.61
1:B:57:VAL:O	1:B:61:VAL:HG12	2.01	0.61
1:C:142:VAL:HG12	1:C:154:ILE:HG23	1.83	0.61
1:C:363:ARG:HB3	1:C:496:MET:HB2	1.83	0.61
2:C:3402:ERY:H14	2:C:3402:ERY:C30	2.29	0.61
1:A:746:ILE:HG22	1:A:747:ASN:N	2.16	0.60
1:A:124:GLN:HG2	1:A:758:TYR:CE2	2.36	0.60
1:A:298:ASN:HD22	1:A:300:LEU:H	1.47	0.60
1:B:456:MET:CG	1:B:467:TYR:HB3	2.14	0.60
1:A:965:LEU:O	1:A:969:ARG:HG3	2.01	0.60
1:B:10:ILE:HG13	1:C:893:GLU:O	2.01	0.60
1:B:28:LEU:HD12	1:B:29:LYS:HG3	1.82	0.60
1:C:672:VAL:HG21	1:C:676:THR:H	1.66	0.60
1:A:552:MET:HE3	1:A:906:PRO:HB3	1.83	0.60
1:A:750:LEU:O	1:A:754:TRP:CD1	2.51	0.60
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.37	0.60
1:C:672:VAL:HG12	1:C:673:GLU:N	2.16	0.60
1:C:673:GLU:O	1:C:674:LEU:HB3	2.01	0.60
1:C:958:LYS:HB3	1:C:962:GLU:CB	2.32	0.60
1:A:56:THR:O	1:A:60:THR:HB	2.01	0.60
1:B:139:VAL:O	1:B:139:VAL:HG12	2.00	0.60
1:B:680:PHE:HD1	1:B:859:TRP:HZ3	1.50	0.60
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.83	0.60
1:A:246:PHE:O	1:A:249:ILE:CG1	2.47	0.60
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.02	0.60
1:B:699:ARG:HG2	1:B:700:ASN:H	1.67	0.60
1:C:419:VAL:HG23	1:C:430:ALA:HB1	1.84	0.60
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.36	0.60
1:A:218:GLN:HB3	1:A:231:ASN:HD21	1.67	0.60
1:B:224:PRO:CA	1:C:781:MET:HE3	2.31	0.60
1:B:456:MET:HG2	1:B:457:ALA:N	2.17	0.60
1:B:575:MET:HA	1:B:626:ILE:HG22	1.83	0.60
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.17	0.60
1:C:355:MET:HB3	1:C:365:THR:HG23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PHE:CZ	1:A:366:LEU:HD13	2.36	0.60
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.25	0.60
1:A:921:LEU:HG	1:A:922:THR:N	2.17	0.59
1:C:322:LYS:HG2	1:C:323:ILE:O	2.02	0.59
1:C:358:PHE:HB3	1:C:977:MET:HE1	1.82	0.59
1:C:930:GLY:CA	1:C:1007:VAL:HG22	2.27	0.59
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.84	0.59
1:B:911:GLY:HA3	1:B:1013:THR:HG21	1.83	0.59
1:C:713:LEU:HB2	1:C:832:ALA:HB3	1.84	0.59
1:A:617:PHE:CE2	1:A:666:PHE:HZ	2.20	0.59
1:B:225:VAL:HG11	1:C:778:LYS:HB3	1.84	0.59
1:A:243:THR:O	1:A:268:ILE:HG21	2.02	0.59
1:B:1022:VAL:CG2	1:B:1023:PRO:HD3	2.31	0.59
1:B:957:GLY:O	1:B:958:LYS:HG3	2.02	0.59
1:C:156:ASP:HA	1:C:181:GLN:HA	1.84	0.59
1:C:882:ILE:O	1:C:882:ILE:HG22	2.03	0.59
1:C:932:LEU:HA	1:C:935:ILE:CG2	2.31	0.59
1:B:68:ASN:O	1:B:70:ASN:N	2.36	0.59
1:B:703:LEU:HD12	1:B:716:VAL:HG12	1.84	0.59
1:C:608:SER:HB3	1:C:630:SER:HB2	1.84	0.59
1:C:961:ILE:O	1:C:965:LEU:HB2	2.02	0.59
1:A:533:GLY:O	1:A:535:LEU:HG	2.02	0.59
1:B:370:ILE:HG22	1:B:370:ILE:O	2.02	0.59
1:C:354:VAL:O	1:C:354:VAL:HG12	2.02	0.59
1:C:899:PHE:N	1:C:899:PHE:HD1	2.00	0.59
1:C:1016:VAL:HA	1:C:1019:ILE:HG22	1.85	0.59
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.31	0.59
1:B:184:MET:H	1:B:762:PHE:HE2	1.50	0.59
1:B:364:ALA:CB	1:B:497:LEU:HG	2.32	0.59
1:A:620:ARG:HH11	1:A:620:ARG:HG2	1.68	0.59
1:B:258:SER:O	1:B:259:ARG:HG2	2.03	0.59
1:A:543:VAL:O	1:A:545:TYR:N	2.32	0.58
1:B:213:GLN:HB2	1:B:239:ARG:CD	2.31	0.58
1:B:225:VAL:H	1:C:781:MET:CE	2.16	0.58
1:B:235:ILE:N	1:B:235:ILE:CD1	2.65	0.58
1:B:729:ILE:HG12	1:B:730:ASP:H	1.68	0.58
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.85	0.58
1:B:345:VAL:HA	1:B:348:ILE:HD12	1.85	0.58
1:C:1:MET:HG3	1:C:3:ASN:H	1.68	0.58
1:B:197:GLN:HA	1:B:798:MET:SD	2.43	0.58
1:B:355:MET:O	1:B:365:THR:OG1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:THR:HG21	1:B:833:PRO:HD2	1.84	0.58
1:C:155:SER:OG	1:C:179:GLY:HA3	2.02	0.58
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.32	0.58
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.85	0.58
1:A:543:VAL:HG22	1:A:544:LEU:H	1.68	0.58
1:B:13:TRP:CE3	1:B:13:TRP:HA	2.37	0.58
1:B:23:GLY:N	1:B:381:ALA:HB2	2.18	0.58
1:B:99:ASP:C	1:B:99:ASP:OD2	2.40	0.58
1:C:149:MET:SD	1:C:321:LEU:HD23	2.44	0.58
1:C:331:PRO:O	1:C:335:ILE:HG12	2.04	0.58
1:C:527:TYR:HE2	1:C:968:VAL:O	1.86	0.58
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.38	0.58
1:A:212:ALA:O	1:A:213:GLN:HB2	2.02	0.58
1:A:240:LEU:HD23	1:A:246:PHE:HA	1.86	0.58
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.85	0.58
1:B:268:ILE:H	1:B:268:ILE:HD12	1.68	0.58
1:B:55:LYS:C	1:B:55:LYS:HD3	2.25	0.58
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.86	0.58
1:C:144:ASN:HA	1:C:320:GLY:O	2.04	0.58
1:B:115:MET:HE1	1:B:127:VAL:HG21	1.84	0.58
1:B:193:LEU:CD1	1:B:198:LEU:O	2.52	0.58
1:B:682:PHE:HD1	1:B:859:TRP:CH2	2.22	0.58
1:C:463:THR:C	1:C:465:ALA:H	2.07	0.58
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.86	0.57
1:A:1021:PHE:HD1	1:A:1025:PHE:HE1	1.52	0.57
1:B:728:LYS:HG2	1:B:808:ARG:HD3	1.86	0.57
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.84	0.57
1:C:986:VAL:O	1:C:990:VAL:HG23	2.03	0.57
1:A:10:ILE:HD12	1:A:10:ILE:O	2.04	0.57
1:A:75:LEU:HD13	1:A:92:LEU:HB3	1.87	0.57
1:A:348:ILE:HD11	1:A:372:VAL:CG1	2.33	0.57
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.86	0.57
1:C:489:THR:O	1:C:493:CYS:HB3	2.03	0.57
1:A:1035:ARG:HH11	1:A:1035:ARG:HA	1.69	0.57
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.34	0.57
1:C:554:TYR:O	1:C:556:PHE:N	2.29	0.57
1:C:643:LYS:NZ	1:C:997:SER:HB2	2.20	0.57
1:C:674:LEU:HD13	1:C:862:MET:HA	1.85	0.57
1:C:685:ILE:O	1:C:687:GLN:HG2	2.05	0.57
1:C:907:LEU:HD22	1:C:1017:LEU:HD23	1.86	0.57
1:A:820:ASN:ND2	3:A:4001:HOH:O	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:VAL:C	1:B:347:ALA:H	2.07	0.57
1:B:398:MET:HG3	1:B:473:THR:HG21	1.87	0.57
1:B:979:SER:O	1:B:983:ILE:HG12	2.03	0.57
1:B:57:VAL:CG1	1:B:58:GLN:N	2.67	0.57
1:C:146:ASP:C	1:C:148:THR:H	2.08	0.57
1:C:672:VAL:CG1	1:C:673:GLU:N	2.63	0.57
1:A:659:LYS:NZ	1:A:660:ASP:O	2.38	0.57
1:A:882:ILE:O	1:A:886:LEU:HB2	2.05	0.57
1:B:349:ILE:O	1:B:351:VAL:N	2.36	0.57
1:B:673:GLU:O	1:B:676:THR:CG2	2.51	0.57
1:C:144:ASN:HD21	1:C:148:THR:N	2.02	0.57
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.35	0.57
1:A:456:MET:O	1:A:458:PHE:N	2.35	0.57
1:B:425:LEU:HB2	1:B:498:LYS:O	2.04	0.57
1:C:899:PHE:N	1:C:899:PHE:CD1	2.72	0.57
1:C:395:MET:HA	1:C:395:MET:HE2	1.87	0.57
1:C:681:ASP:HB3	1:C:860:THR:HG23	1.87	0.57
1:B:792:ARG:HG2	1:B:793:ALA:H	1.70	0.57
1:C:88:VAL:HG12	1:C:90:ILE:HD12	1.86	0.57
1:A:871:ASN:O	1:A:874:PRO:HD2	2.04	0.56
1:B:453:PHE:HZ	1:B:933:THR:HG23	1.69	0.56
1:C:400:LEU:HD12	1:C:929:VAL:CG1	2.35	0.56
1:A:5:PHE:HD1	1:A:12:ALA:HB2	1.68	0.56
1:A:723:ASP:OD1	1:A:813:SER:N	2.38	0.56
1:B:537:SER:O	1:B:539:GLY:N	2.38	0.56
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.40	0.56
1:A:199:THR:CG2	1:A:791:VAL:HA	2.35	0.56
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.40	0.56
1:A:880:SER:O	1:A:884:VAL:HG23	2.06	0.56
1:A:911:GLY:H	1:A:914:LEU:HD13	1.70	0.56
1:B:298:ASN:ND2	1:B:301:ASP:OD1	2.39	0.56
1:B:314:GLU:HG2	1:B:317:PHE:CE2	2.40	0.56
1:B:900:SER:HB2	1:B:1026:PHE:CZ	2.40	0.56
1:B:934:THR:C	1:B:936:GLY:N	2.58	0.56
1:C:13:TRP:O	1:C:17:ILE:HG12	2.06	0.56
1:C:159:ALA:CB	1:C:181:GLN:HB2	2.35	0.56
1:B:149:MET:CB	1:B:154:ILE:HG22	2.35	0.56
1:B:213:GLN:HB2	1:B:239:ARG:CG	2.34	0.56
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.56
1:C:48:SER:HB2	1:C:87:THR:HG22	1.87	0.56
1:B:36:PRO:HD2	1:B:38:ILE:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:LEU:HD21	1:B:1023:PRO:HB2	1.87	0.56
1:B:539:GLY:C	1:B:541:TYR:H	2.07	0.56
1:A:204:ILE:CD1	1:A:773:VAL:HG11	2.35	0.56
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.40	0.56
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.20	0.56
1:B:921:LEU:HD21	1:B:1002:ALA:HA	1.87	0.56
1:C:947:GLU:C	1:C:949:ALA:H	2.09	0.56
1:B:589:LYS:HA	1:B:592:ASN:OD1	2.05	0.56
1:C:228:GLN:NE2	1:C:230:LEU:O	2.39	0.56
1:A:600:THR:O	1:A:601:LYS:HB2	2.06	0.56
1:A:747:ASN:HD21	1:C:237:GLN:NE2	2.04	0.56
1:B:73:ASP:HB2	1:B:106:GLN:HE22	1.71	0.56
1:B:356:TYR:HE2	1:B:365:THR:HG21	1.70	0.56
1:A:70:ASN:HB3	1:C:167:SER:HB3	1.88	0.56
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.41	0.56
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.88	0.56
1:B:281:PHE:CE2	1:B:324:VAL:HG11	2.41	0.56
1:C:20:MET:O	1:C:377:LEU:HD12	2.06	0.56
1:C:100:ALA:HB2	1:C:295:THR:HG21	1.88	0.56
1:C:367:ILE:HD11	1:C:489:THR:HA	1.87	0.56
1:C:958:LYS:HB3	1:C:962:GLU:HB3	1.87	0.55
1:C:1016:VAL:C	1:C:1018:ALA:H	2.09	0.55
1:A:240:LEU:HD12	1:A:240:LEU:N	2.20	0.55
1:A:1029:VAL:O	1:A:1030:ARG:HB2	2.05	0.55
1:B:23:GLY:HA2	1:B:26:ALA:HB3	1.89	0.55
1:B:445:ILE:HD13	1:B:943:ILE:CG2	2.36	0.55
1:C:818:ARG:HA	1:C:824:SER:H	1.71	0.55
1:A:582:ALA:HB3	1:A:623:ASN:HB2	1.88	0.55
1:C:655:PHE:C	1:C:657:GLN:H	2.09	0.55
1:A:4:PHE:HB3	1:A:8:ARG:HH21	1.72	0.55
1:B:231:ASN:C	1:B:231:ASN:ND2	2.60	0.55
1:B:778:LYS:HD3	1:B:778:LYS:H	1.71	0.55
1:B:881:LEU:HD21	1:B:905:VAL:HG21	1.89	0.55
1:C:351:VAL:O	1:C:355:MET:HB2	2.07	0.55
1:C:713:LEU:HG	1:C:833:PRO:C	2.27	0.55
1:B:224:PRO:HA	1:C:781:MET:CE	2.36	0.55
1:B:366:LEU:O	1:B:369:THR:N	2.36	0.55
1:B:712:MET:HA	1:B:834:GLY:HA3	1.87	0.55
1:B:892:TYR:CB	1:B:897:ILE:HD11	2.37	0.55
2:C:3402:ERY:C30	2:C:3402:ERY:C14	2.84	0.55
1:B:680:PHE:CD1	1:B:859:TRP:HZ3	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:LEU:O	1:B:850:LYS:HG2	2.06	0.55
1:C:353:LEU:C	1:C:355:MET:H	2.10	0.55
1:C:1032:ARG:HB3	1:C:1032:ARG:HH21	1.71	0.55
1:A:617:PHE:CE2	1:A:626:ILE:HD11	2.42	0.55
1:A:688:ALA:O	1:A:690:LEU:N	2.38	0.55
1:B:1023:PRO:O	1:B:1027:VAL:HG22	2.07	0.55
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.88	0.55
1:C:837:THR:O	1:C:841:MET:HG3	2.07	0.55
1:A:574:THR:HB	1:A:627:ALA:HB3	1.87	0.55
1:C:211:ASN:HA	1:C:240:LEU:HD23	1.89	0.55
1:A:156:ASP:OD1	1:A:182:TYR:HB2	2.07	0.55
1:B:415:ASN:ND2	1:B:434:SER:OG	2.36	0.55
1:B:709:HIS:N	1:B:710:PRO:HD3	2.22	0.55
1:B:987:MET:N	1:B:988:PRO:HD2	2.22	0.55
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.30	0.55
1:A:4:PHE:O	1:A:8:ARG:HG2	2.08	0.54
1:A:216:ALA:HA	1:B:751:GLY:HA2	1.89	0.54
1:B:13:TRP:HE3	1:B:13:TRP:HA	1.70	0.54
1:B:768:VAL:HG23	1:C:63:GLN:NE2	2.22	0.54
1:A:219:LEU:HD22	1:B:781:MET:O	2.06	0.54
1:A:418:ARG:HA	1:A:421:ALA:HB3	1.90	0.54
1:B:240:LEU:O	1:B:762:PHE:HB2	2.07	0.54
1:B:247:GLY:HA2	1:B:268:ILE:HD13	1.88	0.54
1:C:489:THR:N	1:C:490:PRO:HD2	2.22	0.54
1:A:991:ILE:O	1:A:992:SER:HB3	2.07	0.54
1:B:927:PHE:CE1	1:B:931:LEU:HG	2.42	0.54
1:A:609:VAL:HG12	1:A:629:VAL:HB	1.89	0.54
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.88	0.54
1:B:59:ASP:HA	1:B:63:GLN:CG	2.37	0.54
1:B:219:LEU:HD23	1:B:230:LEU:HD11	1.88	0.54
1:B:971:ARG:HA	1:B:974:PRO:HG2	1.89	0.54
1:C:607:GLU:HB2	1:C:632:LYS:CG	2.36	0.54
1:C:632:LYS:O	1:C:634:TRP:N	2.39	0.54
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.89	0.54
1:A:699:ARG:HH22	1:A:722:GLU:CD	2.10	0.54
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.88	0.54
1:B:913:LEU:O	1:B:917:THR:HB	2.08	0.54
1:C:326:PRO:HG3	1:C:610:PHE:CD1	2.43	0.54
1:C:909:VAL:HA	1:C:931:LEU:HD11	1.88	0.54
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.89	0.54
1:B:274:ASN:OD1	1:B:276:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:GLN:HE21	1:B:668:LEU:HB2	1.71	0.54
1:C:732:ASP:O	1:C:733:GLN:C	2.45	0.54
1:C:819:TYR:N	1:C:824:SER:HB3	2.23	0.54
1:C:9:PRO:HG3	1:C:491:ALA:HB1	1.89	0.54
1:C:912:ALA:C	1:C:914:LEU:H	2.11	0.54
1:A:302:THR:O	1:A:306:ILE:HG12	2.08	0.54
1:B:773:VAL:O	1:B:773:VAL:CG1	2.56	0.54
1:C:142:VAL:HG12	1:C:154:ILE:CG2	2.38	0.54
1:C:1018:ALA:O	1:C:1022:VAL:HG12	2.08	0.54
1:C:203:VAL:HG13	1:C:262:LEU:HD11	1.89	0.54
1:A:133:SER:O	1:A:135:SER:N	2.32	0.54
1:B:767:ARG:HA	1:C:63:GLN:HE22	1.73	0.54
1:B:699:ARG:O	1:B:701:GLN:N	2.40	0.53
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.29	0.53
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.90	0.53
1:C:938:SER:O	1:C:941:ASN:ND2	2.41	0.53
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.89	0.53
1:A:248:LYS:HA	1:A:261:LEU:HD22	1.90	0.53
1:B:16:ALA:HB2	1:B:488:LEU:HG	1.90	0.53
1:B:115:MET:HA	1:B:115:MET:CE	2.37	0.53
1:B:158:VAL:HA	1:B:162:MET:HG2	1.90	0.53
1:B:777:ALA:O	1:B:781:MET:HE2	2.08	0.53
1:B:892:TYR:O	1:B:894:SER:N	2.42	0.53
1:B:1017:LEU:O	1:B:1021:PHE:HD2	1.92	0.53
1:C:415:ASN:O	1:C:418:ARG:HG2	2.07	0.53
1:C:839:GLU:HA	1:C:842:GLU:CB	2.38	0.53
1:A:313:MET:HB2	1:A:317:PHE:CE1	2.44	0.53
1:A:740:GLY:HA3	1:A:794:ALA:H	1.73	0.53
1:A:754:TRP:CE3	1:A:780:ARG:HB2	2.44	0.53
1:A:781:MET:CE	1:C:228:GLN:OE1	2.56	0.53
1:C:601:LYS:C	1:C:603:LYS:H	2.11	0.53
1:C:594:VAL:HG13	1:C:598:TYR:HE1	1.73	0.53
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.43	0.53
1:A:987:MET:N	1:A:988:PRO:CD	2.72	0.53
1:B:152:GLU:O	1:B:182:TYR:HE1	1.90	0.53
1:B:428:LYS:O	1:B:432:ARG:HG3	2.07	0.53
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.90	0.53
1:C:265:VAL:O	1:C:265:VAL:CG2	2.50	0.53
1:C:358:PHE:HB3	1:C:977:MET:CE	2.39	0.53
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.90	0.53
1:C:444:GLY:O	1:C:448:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HB2	1:B:469:GLN:HG2	1.89	0.53
1:B:452:VAL:O	1:B:453:PHE:HB2	2.08	0.53
1:B:580:ALA:O	1:B:582:ALA:N	2.41	0.53
1:C:945:ILE:C	1:C:947:GLU:H	2.12	0.53
1:B:120:GLN:O	1:B:124:GLN:HG2	2.08	0.53
1:A:351:VAL:O	1:A:355:MET:HB2	2.08	0.53
1:A:578:LEU:HD21	1:A:587:THR:HA	1.91	0.53
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.91	0.53
1:B:339:GLU:OE1	1:B:339:GLU:HA	2.08	0.53
1:B:344:LEU:O	1:B:347:ALA:HB3	2.09	0.53
1:B:528:THR:O	1:B:531:VAL:HG12	2.08	0.53
1:B:1005:THR:O	1:B:1005:THR:HG22	2.09	0.53
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.89	0.53
1:C:164:ASP:O	1:C:168:ARG:HG3	2.09	0.53
1:C:655:PHE:HB3	1:C:663:VAL:CG2	2.38	0.53
1:C:761:ASP:HB3	1:C:769:LYS:O	2.09	0.53
1:A:35:TYR:CD1	1:A:671:ILE:HG22	2.44	0.53
1:A:164:ASP:HA	1:A:167:SER:HB2	1.91	0.53
1:A:242:SER:HB3	1:A:245:GLU:HB2	1.91	0.53
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.90	0.53
1:B:445:ILE:HG23	1:B:940:LYS:CG	2.29	0.53
1:B:888:LEU:HB2	1:B:898:PRO:HB3	1.90	0.53
1:C:851:LEU:HB3	1:C:852:PRO:HD2	1.91	0.53
1:A:128:SER:HB2	1:B:113:LEU:HD23	1.90	0.53
1:A:152:GLU:HG2	1:A:272:GLY:HA3	1.91	0.53
1:B:399:VAL:HG11	1:B:989:LEU:HG	1.90	0.53
1:C:591:LEU:HD12	1:C:611:ALA:HB1	1.89	0.53
1:A:235:ILE:O	1:A:235:ILE:HG22	2.09	0.52
1:A:947:GLU:O	1:A:951:ASP:N	2.40	0.52
1:B:1:MET:HG2	1:B:439:GLN:HE22	1.74	0.52
1:B:564:LEU:HD23	1:B:565:PRO:HD2	1.90	0.52
1:B:986:VAL:CG2	1:B:1008:MET:HB2	2.38	0.52
1:C:350:LEU:HD21	1:C:984:LEU:HD22	1.90	0.52
1:C:400:LEU:HD21	1:C:1003:VAL:HG13	1.91	0.52
1:B:57:VAL:HG12	1:B:58:GLN:H	1.74	0.52
1:B:434:SER:O	1:B:438:ILE:HG22	2.10	0.52
1:C:172:VAL:HG22	1:C:306:ILE:HD11	1.91	0.52
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.73	0.52
1:C:997:SER:O	1:C:999:ALA:N	2.43	0.52
1:A:193:LEU:HB2	1:A:265:VAL:HG13	1.91	0.52
1:A:576:VAL:HG11	1:A:591:LEU:CD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:ARG:HD2	1:B:772:TYR:HB2	1.91	0.52
1:B:409:ALA:HA	1:B:485:ALA:HB2	1.90	0.52
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.91	0.52
1:C:348:ILE:C	1:C:350:LEU:H	2.11	0.52
1:C:907:LEU:HD13	1:C:1018:ALA:HA	1.90	0.52
1:A:214:VAL:HG21	1:B:747:ASN:ND2	2.24	0.52
1:B:2:PRO:HB3	1:B:486:LEU:O	2.09	0.52
1:C:884:VAL:C	1:C:886:LEU:H	2.13	0.52
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.45	0.52
1:B:942:ALA:HA	1:B:1022:VAL:HG11	1.90	0.52
1:C:445:ILE:O	1:C:449:LEU:N	2.39	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:C:641:GLU:H	1:C:641:GLU:CD	2.13	0.52
1:C:831:ALA:HB2	1:C:840:ALA:CB	2.40	0.52
1:C:911:GLY:HA3	1:C:1010:GLY:HA2	1.91	0.52
1:A:395:MET:CE	1:A:395:MET:HA	2.40	0.52
1:B:5:PHE:O	1:B:9:PRO:HA	2.08	0.52
1:B:204:ILE:HG23	1:B:759:VAL:HG13	1.92	0.52
1:C:208:LYS:HA	1:C:760:ASN:HD21	1.75	0.52
1:C:899:PHE:HD1	1:C:899:PHE:H	1.57	0.52
1:A:200:PRO:HA	1:A:203:VAL:HG23	1.92	0.52
1:A:406:VAL:HG12	1:A:407:ASP:N	2.24	0.52
1:A:584:GLN:H	1:A:622:GLN:HG2	1.74	0.52
1:B:13:TRP:HD1	1:C:895:TRP:HZ2	1.57	0.52
1:B:193:LEU:HD11	1:B:198:LEU:O	2.09	0.52
1:C:378:GLY:O	1:C:382:VAL:HG23	2.10	0.52
1:C:527:TYR:OH	1:C:1019:ILE:HG13	2.09	0.52
1:C:646:ALA:HA	1:C:649:MET:HB2	1.92	0.52
1:A:62:THR:HG23	1:A:88:VAL:CG1	2.40	0.52
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.52
1:B:115:MET:HA	1:B:118:LEU:HD13	1.92	0.52
1:C:169:THR:O	1:C:172:VAL:HG23	2.10	0.52
1:B:52:ALA:HB2	1:B:85:THR:C	2.29	0.52
1:B:972:LEU:HD21	1:B:1019:ILE:HG12	1.91	0.52
1:C:124:GLN:HB3	1:C:758:TYR:HE2	1.74	0.52
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.43	0.52
1:C:736:ALA:C	1:C:738:ALA:H	2.12	0.52
1:B:45:ILE:HB	1:B:90:ILE:HB	1.92	0.52
1:B:459:PHE:O	1:B:464:GLY:HA3	2.10	0.52
1:B:873:ALA:HB1	1:B:877:TYR:CE2	2.45	0.52
1:B:911:GLY:HA2	1:B:914:LEU:CB	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.52
1:C:402:ILE:O	1:C:406:VAL:HG23	2.10	0.52
1:C:923:ASN:HD22	1:C:927:PHE:HD2	1.58	0.52
1:A:324:VAL:HG12	1:A:325:TYR:H	1.75	0.51
1:A:525:HIS:HA	1:A:528:THR:CG2	2.37	0.51
1:B:699:ARG:HA	1:B:702:LEU:HB2	1.92	0.51
1:B:729:ILE:CG1	1:B:730:ASP:H	2.23	0.51
1:B:1026:PHE:HB3	1:B:1030:ARG:HE	1.74	0.51
1:C:68:ASN:OD1	1:C:68:ASN:N	2.43	0.51
1:C:395:MET:O	1:C:398:MET:N	2.43	0.51
1:C:527:TYR:OH	1:C:968:VAL:HG12	2.10	0.51
1:C:615:PHE:C	1:C:615:PHE:CD2	2.83	0.51
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.91	0.51
1:A:550:VAL:O	1:A:553:ALA:N	2.43	0.51
1:A:886:LEU:HD12	1:C:14:VAL:HG23	1.90	0.51
1:B:280:GLU:CB	1:B:284:GLN:O	2.58	0.51
1:B:482:VAL:O	1:B:486:LEU:HB2	2.10	0.51
1:C:34:GLN:O	1:C:391:ASN:HB2	2.09	0.51
1:A:945:ILE:HG13	1:A:971:ARG:CG	2.27	0.51
1:B:291:ILE:HG21	1:B:306:ILE:HD11	1.91	0.51
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.51
1:B:897:ILE:HG13	1:B:898:PRO:HD3	1.92	0.51
1:C:176:GLN:HE22	1:C:620:ARG:HH12	1.58	0.51
1:C:210:GLN:O	1:C:240:LEU:CD2	2.58	0.51
1:A:63:GLN:O	1:A:64:VAL:C	2.48	0.51
1:A:204:ILE:HD11	1:A:773:VAL:HG11	1.93	0.51
1:B:776:GLU:HG2	1:B:777:ALA:H	1.75	0.51
1:C:102:ILE:O	1:C:103:ALA:C	2.47	0.51
1:C:731:ILE:HD13	1:C:746:ILE:HG21	1.92	0.51
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.39	0.51
1:A:886:LEU:HD13	1:C:14:VAL:HG23	1.91	0.51
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.25	0.51
1:B:13:TRP:O	1:B:16:ALA:HB3	2.11	0.51
1:B:418:ARG:HB3	1:B:418:ARG:HH11	1.76	0.51
1:C:326:PRO:CB	1:C:610:PHE:HB2	2.40	0.51
1:C:681:ASP:CB	1:C:860:THR:CG2	2.83	0.51
1:A:196:PHE:CG	1:A:260:VAL:HG11	2.45	0.51
1:A:431:THR:O	1:A:435:MET:HB2	2.11	0.51
1:C:423:GLU:CB	1:C:426:PRO:HD2	2.41	0.51
1:A:167:SER:HA	1:A:175:VAL:HG21	1.93	0.51
1:A:282:ASN:ND2	1:A:609:VAL:H	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:584:GLN:N	1:A:622:GLN:HG2	2.25	0.51
1:B:428:LYS:CB	1:B:494:ALA:HB1	2.40	0.51
1:A:585:GLU:OE2	1:C:227:GLY:HA2	2.10	0.51
1:A:601:LYS:O	1:A:602:GLU:HG2	2.11	0.51
1:A:671:ILE:CG1	1:A:674:LEU:HB3	2.41	0.51
1:C:176:GLN:HE21	1:C:620:ARG:HH11	1.55	0.51
1:C:326:PRO:HB3	1:C:610:PHE:HB2	1.93	0.51
1:C:352:PHE:HA	1:C:369:THR:HG21	1.93	0.51
1:C:465:ALA:O	1:C:469:GLN:HG2	2.10	0.51
1:C:712:MET:HB2	1:C:839:GLU:OE1	2.11	0.51
1:A:261:LEU:CD1	1:A:263:ARG:HH11	2.24	0.51
1:B:68:ASN:O	1:B:70:ASN:ND2	2.44	0.51
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.93	0.51
1:B:213:GLN:HE21	1:B:239:ARG:HD2	1.76	0.51
1:B:683:GLU:O	1:B:857:TYR:HA	2.10	0.51
1:C:181:GLN:CG	1:C:769:LYS:HE2	2.41	0.51
1:C:239:ARG:HB2	1:C:763:ILE:CD1	2.41	0.51
1:C:404:LEU:HD21	1:C:449:LEU:CD1	2.41	0.51
1:C:801:PHE:CD1	1:C:804:PHE:CE1	2.99	0.51
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.91	0.50
1:A:819:TYR:N	1:A:824:SER:HB3	2.25	0.50
1:B:552:MET:SD	1:B:909:VAL:HG23	2.50	0.50
1:B:764:ASP:HB3	1:B:769:LYS:HE3	1.93	0.50
1:B:899:PHE:O	1:B:899:PHE:CD1	2.64	0.50
1:B:900:SER:HA	1:B:903:LEU:HD12	1.92	0.50
1:C:485:ALA:HA	1:C:489:THR:OG1	2.11	0.50
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.92	0.50
1:A:92:LEU:H	1:A:92:LEU:HD12	1.75	0.50
1:A:185:ARG:HD3	1:A:272:GLY:O	2.10	0.50
1:A:780:ARG:HG2	1:A:780:ARG:NH1	2.25	0.50
1:B:46:SER:HA	1:B:88:VAL:O	2.12	0.50
1:B:49:TYR:HB3	1:B:57:VAL:HG23	1.92	0.50
1:B:213:GLN:HE21	1:B:239:ARG:CD	2.25	0.50
1:B:282:ASN:O	1:B:284:GLN:N	2.44	0.50
1:B:539:GLY:C	1:B:541:TYR:N	2.64	0.50
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.93	0.50
1:C:76:MET:SD	1:C:95:GLU:HG3	2.51	0.50
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.93	0.50
1:C:144:ASN:ND2	1:C:149:MET:N	2.57	0.50
1:C:189:ASN:ND2	1:C:192:GLU:H	2.09	0.50
1:C:463:THR:HA	1:C:466:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:MET:HE1	1:C:225:VAL:H	1.77	0.50
1:B:59:ASP:HA	1:B:63:GLN:HG2	1.93	0.50
1:B:876:LEU:HD22	1:B:932:LEU:HD13	1.93	0.50
1:C:946:VAL:O	1:C:946:VAL:HG12	2.12	0.50
1:A:877:TYR:O	1:A:881:LEU:HB2	2.12	0.50
1:C:47:ALA:HB2	1:C:127:VAL:HG12	1.92	0.50
1:C:382:VAL:HG11	1:C:476:SER:HB2	1.94	0.50
1:C:588:GLN:HG2	1:C:613:ASN:ND2	2.25	0.50
1:C:631:LEU:HB3	1:C:637:ARG:NH2	2.27	0.50
1:A:36:PRO:HG3	1:A:469:GLN:OE1	2.12	0.50
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.42	0.50
1:A:612:VAL:CG2	1:A:626:ILE:HG22	2.37	0.50
1:A:659:LYS:CG	1:A:660:ASP:H	2.05	0.50
1:B:261:LEU:O	1:B:263:ARG:N	2.44	0.50
1:B:714:THR:HG21	1:B:832:ALA:H	1.75	0.50
1:B:891:LEU:HD12	1:B:892:TYR:CE1	2.46	0.50
1:B:213:GLN:HG3	1:C:56:THR:CG2	2.41	0.50
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.94	0.50
1:B:699:ARG:HB3	1:B:699:ARG:HH11	1.77	0.50
1:B:814:PRO:O	1:B:815:ARG:HG2	2.12	0.50
1:C:239:ARG:HB2	1:C:763:ILE:HD13	1.92	0.50
1:C:477:ALA:HA	1:C:480:LEU:HB2	1.93	0.50
1:C:734:GLU:HA	1:C:737:GLN:HE21	1.76	0.50
1:C:912:ALA:O	1:C:914:LEU:N	2.44	0.50
1:C:920:GLY:O	1:C:921:LEU:O	2.28	0.50
1:A:677:ALA:O	1:A:679:GLY:N	2.31	0.50
1:A:904:VAL:HA	1:A:907:LEU:HD13	1.94	0.50
1:B:30:LEU:HD12	1:B:384:ALA:HB2	1.92	0.50
1:B:158:VAL:HB	1:B:289:LEU:HD21	1.93	0.50
1:B:391:ASN:HD21	1:B:393:LEU:HB2	1.77	0.50
1:B:964:THR:O	1:B:968:VAL:HG23	2.11	0.50
1:A:159:ALA:HB2	1:A:177:LEU:HD22	1.93	0.50
1:A:841:MET:O	1:A:845:GLU:HG3	2.12	0.50
1:B:135:SER:HB2	1:B:676:THR:CG2	2.42	0.50
1:B:261:LEU:O	1:B:261:LEU:HD23	2.12	0.50
1:B:323:ILE:HD12	1:B:323:ILE:N	2.27	0.50
1:B:428:LYS:HB2	1:B:494:ALA:HB1	1.93	0.50
1:B:905:VAL:HG13	1:B:906:PRO:CD	2.40	0.50
1:B:990:VAL:HG13	1:B:1005:THR:OG1	2.10	0.50
1:A:66:GLU:C	1:A:68:ASN:H	2.15	0.49
1:A:193:LEU:HD12	1:A:265:VAL:HG11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG21	1:A:745:ASP:OD2	2.12	0.49
1:A:543:VAL:C	1:A:545:TYR:N	2.65	0.49
1:A:832:ALA:O	1:A:833:PRO:C	2.49	0.49
1:A:1021:PHE:O	1:A:1024:VAL:HB	2.12	0.49
1:A:1022:VAL:HA	1:A:1025:PHE:HD1	1.77	0.49
1:B:729:ILE:HG12	1:B:730:ASP:N	2.25	0.49
1:A:311:ALA:O	1:A:312:LYS:HB2	2.11	0.49
1:A:583:THR:HG22	1:A:585:GLU:N	2.27	0.49
1:A:586:ARG:HA	1:A:589:LYS:HE3	1.94	0.49
1:A:590:VAL:O	1:A:594:VAL:HG23	2.12	0.49
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.76	0.49
1:C:941:ASN:HD22	1:C:942:ALA:N	2.10	0.49
1:A:187:TRP:HZ2	1:A:275:TYR:HE1	1.60	0.49
1:A:644:VAL:HG11	1:A:667:ASN:OD1	2.12	0.49
1:A:979:SER:O	1:A:983:ILE:HG23	2.12	0.49
1:B:741:VAL:HG12	1:B:792:ARG:O	2.12	0.49
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.76	0.49
1:C:1:MET:HB2	1:C:2:PRO:CD	2.38	0.49
1:C:414:GLU:HA	1:C:417:GLU:HG2	1.95	0.49
1:A:232:ALA:HB1	1:B:725:PRO:O	2.12	0.49
1:B:183:ALA:HB2	1:B:273:GLU:HB3	1.94	0.49
1:B:404:LEU:C	1:B:406:VAL:H	2.16	0.49
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.93	0.49
1:C:442:LEU:O	1:C:445:ILE:HG13	2.12	0.49
1:C:540:ARG:O	1:C:544:LEU:HB2	2.13	0.49
1:C:713:LEU:HD21	1:C:835:LYS:N	2.27	0.49
1:C:754:TRP:CZ3	1:C:780:ARG:HA	2.46	0.49
1:B:164:ASP:HB3	1:B:168:ARG:HH22	1.78	0.49
1:B:166:ILE:HD11	1:B:310:LEU:HG	1.94	0.49
1:C:713:LEU:HD21	1:C:835:LYS:H	1.78	0.49
1:B:623:ASN:OD1	1:B:623:ASN:N	2.37	0.49
1:B:708:LYS:HG2	1:B:708:LYS:O	2.12	0.49
1:C:26:ALA:O	1:C:30:LEU:HD12	2.12	0.49
1:C:726:GLN:CD	1:C:812:GLY:HA3	2.33	0.49
1:A:1:MET:SD	1:A:487:ILE:CD1	3.01	0.49
1:A:708:LYS:C	1:A:710:PRO:HD3	2.33	0.49
1:B:95:GLU:O	1:B:98:THR:HG22	2.12	0.49
1:B:897:ILE:N	1:B:898:PRO:CD	2.76	0.49
1:C:618:ALA:CB	1:C:815:ARG:HH12	2.23	0.49
1:C:681:ASP:HB3	1:C:860:THR:HG22	1.94	0.49
1:A:937:LEU:HD12	1:A:1011:MET:SD	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ALA:O	1:B:581:GLY:C	2.51	0.49
1:B:587:THR:HB	1:B:613:ASN:HD21	1.78	0.49
1:C:456:MET:O	1:C:459:PHE:HB2	2.13	0.49
1:A:253:VAL:HG23	1:A:259:ARG:HG2	1.94	0.49
1:A:416:VAL:HG22	1:A:434:SER:OG	2.12	0.49
1:B:49:TYR:HB3	1:B:57:VAL:CG2	2.43	0.49
1:B:764:ASP:O	1:B:766:GLY:N	2.39	0.49
1:B:831:ALA:CB	1:B:840:ALA:HB2	2.42	0.49
1:C:84:SER:C	1:C:86:GLY:N	2.65	0.49
1:C:395:MET:HE2	1:C:395:MET:CA	2.42	0.49
1:C:879:ILE:O	1:C:879:ILE:HG22	2.13	0.49
1:C:894:SER:C	1:C:896:SER:H	2.16	0.49
1:C:911:GLY:CA	1:C:1010:GLY:HA2	2.43	0.49
1:C:952:LEU:O	1:C:953:MET:HG3	2.13	0.49
1:A:561:SER:HA	1:A:923:ASN:HB3	1.95	0.49
1:B:16:ALA:O	1:B:374:VAL:HG23	2.13	0.49
1:B:1025:PHE:O	1:B:1029:VAL:HG12	2.13	0.49
1:C:33:ALA:HB1	1:C:34:GLN:HE21	1.78	0.49
1:C:349:ILE:HG23	1:C:349:ILE:O	2.13	0.49
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.78	0.49
1:C:713:LEU:CD1	1:C:835:LYS:H	2.18	0.49
1:C:968:VAL:HG11	1:C:1023:PRO:HG3	1.94	0.49
1:B:154:ILE:O	1:B:157:TYR:N	2.46	0.48
1:C:75:LEU:HD11	1:C:92:LEU:HD23	1.95	0.48
1:C:425:LEU:H	1:C:426:PRO:CD	2.26	0.48
1:C:590:VAL:O	1:C:592:ASN:O	2.30	0.48
1:C:975:ILE:HG21	1:C:1019:ILE:HD13	1.95	0.48
1:A:173:GLY:N	1:A:293:LEU:O	2.43	0.48
1:A:191:ASN:C	1:A:193:LEU:N	2.67	0.48
1:A:316:PHE:CD2	1:A:316:PHE:N	2.82	0.48
1:A:376:LEU:C	1:A:378:GLY:H	2.14	0.48
1:A:467:TYR:CE1	1:A:925:VAL:HG13	2.47	0.48
1:A:649:MET:HA	1:A:653:ARG:HH22	1.76	0.48
1:A:783:PRO:C	1:A:785:ASP:H	2.17	0.48
1:B:776:GLU:HG2	1:B:777:ALA:N	2.28	0.48
1:C:1032:ARG:HB3	1:C:1032:ARG:NH2	2.29	0.48
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.34	0.48
1:A:295:THR:HG22	1:A:295:THR:O	2.13	0.48
1:A:620:ARG:HG2	1:A:620:ARG:NH1	2.27	0.48
1:A:897:ILE:N	1:A:898:PRO:HD2	2.27	0.48
1:B:654:ALA:C	1:B:656:SER:H	2.16	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.48	0.48
1:C:577:GLN:HE21	1:C:577:GLN:H	1.60	0.48
1:C:750:LEU:HD23	1:C:754:TRP:CD1	2.49	0.48
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.95	0.48
1:A:57:VAL:HG12	1:A:82:SER:HB3	1.96	0.48
1:A:660:ASP:O	1:A:661:ALA:HB2	2.12	0.48
1:A:947:GLU:O	1:A:951:ASP:HB2	2.13	0.48
1:B:952:LEU:C	1:B:954:ASP:N	2.65	0.48
1:C:486:LEU:C	1:C:490:PRO:HG3	2.34	0.48
1:C:655:PHE:C	1:C:657:GLN:N	2.67	0.48
1:C:681:ASP:HB2	1:C:860:THR:HG23	1.94	0.48
1:A:45:ILE:HG23	1:A:129:VAL:CG2	2.43	0.48
1:B:157:TYR:C	1:B:161:ASN:HD22	2.16	0.48
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.93	0.48
1:B:219:LEU:CD1	1:B:234:ILE:HG12	2.44	0.48
1:B:420:MET:HG2	1:B:426:PRO:HD3	1.95	0.48
1:B:744:ASN:O	1:B:748:THR:N	2.40	0.48
1:B:989:LEU:HD13	1:B:1000:GLN:O	2.13	0.48
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.76	0.48
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.43	0.48
1:A:597:TYR:CD1	1:A:597:TYR:C	2.86	0.48
1:A:727:PHE:CZ	1:A:807:SER:HB3	2.49	0.48
1:A:991:ILE:O	1:A:992:SER:CB	2.61	0.48
1:B:446:ALA:O	1:B:447:MET:C	2.52	0.48
1:B:448:VAL:O	1:B:452:VAL:HG23	2.13	0.48
1:B:453:PHE:CE2	1:B:474:ILE:HG21	2.48	0.48
1:B:616:GLY:HA3	1:B:624:THR:HG22	1.95	0.48
1:B:913:LEU:O	1:B:917:THR:CB	2.62	0.48
1:C:114:ALA:HA	1:C:117:LEU:HD12	1.95	0.48
1:C:204:ILE:HG22	1:C:205:THR:N	2.28	0.48
1:C:313:MET:O	1:C:317:PHE:CE1	2.66	0.48
1:C:637:ARG:CB	1:C:642:ASN:HB3	2.44	0.48
1:C:889:ALA:HB2	1:C:898:PRO:HG3	1.94	0.48
1:A:194:ASN:ND2	1:A:790:TYR:CD2	2.82	0.48
1:A:425:LEU:HB3	1:A:426:PRO:HD2	1.95	0.48
1:A:471:SER:O	1:A:475:VAL:CG1	2.59	0.48
1:B:55:LYS:CE	1:B:59:ASP:OD1	2.61	0.48
1:B:111:LEU:HD22	1:B:129:VAL:HG23	1.96	0.48
1:B:717:ARG:CD	1:B:717:ARG:N	2.77	0.48
1:C:188:MET:HA	1:C:266:ALA:HB2	1.96	0.48
1:C:395:MET:C	1:C:397:GLY:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:GLN:HA	1:C:624:THR:HA	1.96	0.48
1:C:586:ARG:O	1:C:590:VAL:HG23	2.14	0.48
1:A:238:THR:OG1	1:A:239:ARG:N	2.47	0.48
1:A:527:TYR:HE2	1:A:972:LEU:HG	1.78	0.48
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.78	0.48
1:B:600:THR:C	1:B:602:GLU:H	2.17	0.48
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.44	0.48
1:A:896:SER:OG	1:A:897:ILE:N	2.47	0.48
1:B:306:ILE:HG23	1:B:310:LEU:HD12	1.96	0.48
1:B:364:ALA:HB2	1:B:497:LEU:HG	1.94	0.48
1:B:524:THR:O	1:B:528:THR:N	2.40	0.48
1:C:367:ILE:HD13	1:C:492:LEU:HD22	1.95	0.48
1:C:527:TYR:CZ	1:C:1019:ILE:HG13	2.49	0.48
1:C:655:PHE:HB3	1:C:663:VAL:HG23	1.95	0.48
1:A:367:ILE:HA	1:A:370:ILE:HG22	1.96	0.48
1:B:188:MET:HB3	1:B:789:TRP:HH2	1.79	0.48
1:B:518:ARG:HA	1:B:521:GLU:CD	2.34	0.48
1:B:640:GLU:H	1:B:643:LYS:HG2	1.79	0.48
1:B:940:LYS:HA	1:B:943:ILE:HG22	1.95	0.48
1:B:144:ASN:HD21	1:B:148:THR:N	2.10	0.47
1:B:372:VAL:HG13	1:B:405:LEU:HD21	1.96	0.47
1:B:452:VAL:HG11	1:B:932:LEU:O	2.14	0.47
1:C:33:ALA:HA	1:C:300:LEU:HD12	1.96	0.47
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.75	0.47
1:C:824:SER:OG	1:C:825:MET:N	2.47	0.47
1:C:982:PHE:O	1:C:984:LEU:N	2.47	0.47
1:A:449:LEU:O	1:A:453:PHE:HD1	1.97	0.47
1:A:550:VAL:O	1:A:551:GLY:C	2.53	0.47
1:A:685:ILE:HG22	1:A:686:ASP:N	2.29	0.47
1:A:901:VAL:HA	1:A:942:ALA:HB1	1.97	0.47
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.96	0.47
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.96	0.47
1:B:688:ALA:O	1:B:690:LEU:N	2.46	0.47
1:C:894:SER:HG	1:C:897:ILE:HG12	1.76	0.47
1:C:901:VAL:O	1:C:904:VAL:HG23	2.14	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HA	1.95	0.47
1:B:350:LEU:O	1:B:984:LEU:HB3	2.13	0.47
1:B:713:LEU:HD13	1:B:843:LEU:HD13	1.95	0.47
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.47	0.47
1:B:143:ILE:CD1	1:B:285:PRO:O	2.60	0.47
1:B:542:LEU:HD11	1:B:1028:VAL:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ILE:HD13	1:C:306:ILE:HD12	1.95	0.47
1:C:317:PHE:CD2	1:C:321:LEU:HD12	2.49	0.47
1:A:112:GLN:HE22	1:C:112:GLN:HG2	1.80	0.47
1:A:211:ASN:HB3	1:A:760:ASN:HD21	1.80	0.47
1:B:372:VAL:HB	1:B:373:PRO:CD	2.40	0.47
1:B:578:LEU:N	1:B:578:LEU:HD23	2.29	0.47
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.47
1:B:762:PHE:C	1:B:763:ILE:HD12	2.34	0.47
1:C:453:PHE:C	1:C:455:PRO:HD2	2.34	0.47
1:C:594:VAL:HG13	1:C:598:TYR:CE1	2.48	0.47
1:C:633:ASP:O	1:C:634:TRP:HB2	2.14	0.47
1:B:335:ILE:O	1:B:336:SER:C	2.53	0.47
1:B:463:THR:HA	1:B:466:ILE:HD12	1.97	0.47
1:B:843:LEU:HD23	1:B:847:LEU:HG	1.96	0.47
1:C:431:THR:O	1:C:434:SER:HB2	2.14	0.47
1:C:933:THR:O	1:C:937:LEU:HB2	2.14	0.47
1:A:250:LEU:CD2	1:A:259:ARG:HD2	2.45	0.47
1:A:542:LEU:HD23	1:A:1028:VAL:HG21	1.96	0.47
1:A:901:VAL:HG13	1:A:942:ALA:HB3	1.97	0.47
1:A:1021:PHE:CD1	1:A:1025:PHE:HE1	2.32	0.47
1:B:68:ASN:C	1:B:70:ASN:N	2.65	0.47
1:B:225:VAL:O	1:B:226:LYS:C	2.52	0.47
1:B:631:LEU:HB3	1:B:637:ARG:NH1	2.19	0.47
1:B:805:SER:OG	1:B:806:SER:N	2.47	0.47
1:B:866:GLU:O	1:B:867:ARG:C	2.52	0.47
1:C:4:PHE:O	1:C:8:ARG:NH1	2.48	0.47
1:C:18:ILE:O	1:C:19:ILE:C	2.53	0.47
1:C:34:GLN:NE2	1:C:299:ALA:HB3	2.11	0.47
1:C:62:THR:OG1	1:C:88:VAL:HG13	2.14	0.47
1:A:69:MET:CE	1:A:107:VAL:HG13	2.44	0.47
1:A:198:LEU:HD22	1:A:202:ASP:HB3	1.96	0.47
1:A:636:ASP:OD2	1:A:636:ASP:N	2.48	0.47
1:A:655:PHE:O	1:A:657:GLN:N	2.43	0.47
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.30	0.47
1:A:961:ILE:O	1:A:965:LEU:HD23	2.15	0.47
1:B:314:GLU:N	1:B:315:PRO:CD	2.77	0.47
1:B:490:PRO:O	1:B:493:CYS:N	2.48	0.47
1:B:1022:VAL:HG23	1:B:1023:PRO:CD	2.44	0.47
1:C:655:PHE:O	1:C:657:GLN:N	2.48	0.47
1:C:881:LEU:C	1:C:883:VAL:H	2.18	0.47
1:A:108:GLN:HG3	1:B:112:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HB	1:A:773:VAL:HG23	1.95	0.47
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.96	0.47
1:A:516:PHE:CG	1:A:517:ASN:N	2.82	0.47
1:A:780:ARG:O	1:A:780:ARG:HD2	2.14	0.47
1:B:45:ILE:HD13	1:B:65:ILE:CG2	2.45	0.47
1:B:445:ILE:HD12	1:B:940:LYS:CG	2.44	0.47
1:B:592:ASN:HA	1:B:595:THR:CG2	2.45	0.47
1:C:395:MET:C	1:C:397:GLY:N	2.69	0.47
1:C:882:ILE:O	1:C:882:ILE:CG2	2.63	0.47
1:C:958:LYS:HB3	1:C:962:GLU:HB2	1.96	0.47
1:A:671:ILE:HG13	1:A:674:LEU:CB	2.45	0.47
1:C:3:ASN:C	1:C:5:PHE:N	2.68	0.47
1:C:353:LEU:O	1:C:355:MET:N	2.48	0.47
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.50	0.47
1:C:615:PHE:HE2	2:C:3402:ERY:H341	1.80	0.47
1:C:912:ALA:HB1	1:C:927:PHE:CE1	2.50	0.47
1:A:104:GLN:OE1	1:A:131:LYS:HG3	2.15	0.46
1:A:609:VAL:HG23	1:A:609:VAL:O	2.15	0.46
1:B:356:TYR:O	1:B:358:PHE:N	2.35	0.46
1:B:1031:ARG:HD2	1:B:1035:ARG:HH21	1.80	0.46
1:C:120:GLN:O	1:C:124:GLN:HG2	2.15	0.46
1:A:41:PRO:HD3	1:A:96:SER:O	2.15	0.46
1:B:23:GLY:H	1:B:381:ALA:HB2	1.79	0.46
1:B:194:ASN:HB2	1:B:790:TYR:HB2	1.96	0.46
1:B:326:PRO:HB3	1:B:610:PHE:HB2	1.97	0.46
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.46
1:B:671:ILE:HB	1:B:672:VAL:H	1.50	0.46
1:B:681:ASP:CB	1:B:860:THR:CG2	2.93	0.46
1:C:34:GLN:HG2	1:C:35:TYR:H	1.79	0.46
1:C:146:ASP:C	1:C:148:THR:N	2.68	0.46
1:A:261:LEU:HD13	1:A:263:ARG:HH11	1.79	0.46
1:A:376:LEU:O	1:A:378:GLY:N	2.39	0.46
1:B:200:PRO:HA	1:B:203:VAL:HG23	1.97	0.46
1:B:356:TYR:O	1:B:360:GLN:HG2	2.15	0.46
1:B:669:PRO:HB2	1:B:862:MET:SD	2.55	0.46
1:B:848:ALA:O	1:B:850:LYS:N	2.39	0.46
1:B:937:LEU:O	1:B:940:LYS:HB3	2.16	0.46
1:B:121:GLU:H	1:B:121:GLU:HG2	1.59	0.46
1:B:213:GLN:CB	1:B:239:ARG:HD2	2.43	0.46
1:C:635:ALA:C	1:C:637:ARG:H	2.18	0.46
1:A:231:ASN:CB	1:B:622:GLN:HE22	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:N	1:A:316:PHE:HD2	2.14	0.46
1:A:456:MET:C	1:A:458:PHE:H	2.15	0.46
1:A:890:ALA:HB1	1:C:11:PHE:HA	1.97	0.46
1:B:69:MET:HB3	1:B:92:LEU:HD11	1.96	0.46
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.50	0.46
1:C:477:ALA:C	1:C:479:ALA:H	2.18	0.46
1:C:578:LEU:HD22	1:C:661:ALA:HB2	1.97	0.46
1:C:743:ILE:HA	1:C:746:ILE:HD12	1.97	0.46
1:C:912:ALA:HB1	1:C:927:PHE:HE1	1.80	0.46
1:A:391:ASN:O	1:A:392:THR:C	2.54	0.46
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.50	0.46
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.51	0.46
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.98	0.46
1:B:408:ASP:OD2	1:B:445:ILE:HB	2.16	0.46
1:B:416:VAL:HG22	1:B:431:THR:HA	1.96	0.46
1:C:527:TYR:CE2	1:C:968:VAL:O	2.67	0.46
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.51	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.98	0.46
1:A:426:PRO:CB	1:A:427:PRO:CD	2.94	0.46
1:A:444:GLY:HA3	1:A:891:LEU:HD22	1.97	0.46
1:A:527:TYR:C	1:A:529:ASP:H	2.17	0.46
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.98	0.46
1:A:652:THR:HB	1:A:653:ARG:HH21	1.81	0.46
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.97	0.46
1:B:183:ALA:CB	1:B:273:GLU:HB3	2.45	0.46
1:B:398:MET:HG3	1:B:473:THR:CG2	2.46	0.46
1:B:729:ILE:CG1	1:B:730:ASP:N	2.79	0.46
1:B:833:PRO:C	1:B:835:LYS:H	2.18	0.46
1:C:49:TYR:N	1:C:122:VAL:HG23	2.31	0.46
1:C:563:PHE:CE2	1:C:564:LEU:HD12	2.51	0.46
1:A:240:LEU:N	1:A:240:LEU:CD1	2.79	0.46
1:A:575:MET:CE	1:A:577:GLN:HE21	2.29	0.46
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.97	0.46
1:B:671:ILE:C	1:B:673:GLU:N	2.69	0.46
1:C:111:LEU:HD13	1:C:115:MET:HE3	1.97	0.46
1:C:346:GLU:O	1:C:350:LEU:HB2	2.16	0.46
1:C:683:GLU:HG3	1:C:819:TYR:CD2	2.51	0.46
1:C:947:GLU:C	1:C:949:ALA:N	2.68	0.46
1:C:951:ASP:C	1:C:953:MET:H	2.19	0.46
1:C:1016:VAL:O	1:C:1018:ALA:N	2.42	0.46
1:B:13:TRP:CD1	1:C:895:TRP:HZ2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:HB3	1:B:814:PRO:HA	1.98	0.46
1:B:151:GLN:NE2	1:B:279:ALA:H	2.14	0.46
1:B:833:PRO:O	1:B:835:LYS:N	2.49	0.46
1:B:919:ARG:NH2	1:B:990:VAL:O	2.46	0.46
1:C:102:ILE:O	1:C:105:VAL:N	2.49	0.46
1:C:164:ASP:O	1:C:167:SER:HB2	2.16	0.46
1:C:592:ASN:HA	1:C:595:THR:OG1	2.16	0.46
1:A:671:ILE:HG13	1:A:674:LEU:HB3	1.96	0.46
1:B:36:PRO:HD3	1:B:391:ASN:HD21	1.77	0.46
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.46
1:C:220:GLY:H	1:C:231:ASN:HD22	1.64	0.46
1:C:348:ILE:HG13	1:C:349:ILE:N	2.31	0.46
1:C:912:ALA:C	1:C:914:LEU:N	2.69	0.46
1:A:317:PHE:HB3	1:A:321:LEU:CB	2.26	0.45
1:A:354:VAL:O	1:A:356:TYR:N	2.48	0.45
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.45
1:B:414:GLU:OE2	1:B:974:PRO:HD3	2.16	0.45
1:B:464:GLY:O	1:B:468:ARG:HD3	2.16	0.45
1:B:602:GLU:C	1:B:604:ASN:H	2.18	0.45
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.98	0.45
1:C:357:LEU:HD23	1:C:358:PHE:CE2	2.51	0.45
1:C:367:ILE:HG21	1:C:497:LEU:HD23	1.98	0.45
1:C:973:ARG:HG2	1:C:977:MET:HE3	1.97	0.45
1:A:95:GLU:O	1:A:96:SER:C	2.55	0.45
1:A:189:ASN:ND2	1:A:779:TYR:CZ	2.84	0.45
1:A:228:GLN:O	1:B:583:THR:HG21	2.16	0.45
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.82	0.45
1:B:197:GLN:O	1:B:792:ARG:NH2	2.50	0.45
1:B:349:ILE:C	1:B:351:VAL:N	2.69	0.45
1:B:356:TYR:C	1:B:358:PHE:H	2.17	0.45
1:B:427:PRO:C	1:B:429:GLU:H	2.20	0.45
1:B:843:LEU:HD23	1:B:847:LEU:CD2	2.46	0.45
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.95	0.45
1:B:935:ILE:O	1:B:935:ILE:HG22	2.17	0.45
1:B:984:LEU:HA	1:B:987:MET:HB2	1.97	0.45
1:C:3:ASN:O	1:C:5:PHE:N	2.45	0.45
1:C:54:ALA:HB2	1:C:84:SER:CA	2.46	0.45
1:C:91:THR:HG21	2:C:3402:ERY:H272	1.98	0.45
1:C:330:THR:N	1:C:331:PRO:CD	2.79	0.45
1:C:578:LEU:HB3	1:C:579:PRO:CD	2.41	0.45
1:C:898:PRO:HG2	1:C:899:PHE:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:NH2	1:A:328:ASP:OD2	2.49	0.45
1:B:15:ILE:O	1:B:19:ILE:HG12	2.17	0.45
1:C:32:VAL:O	1:C:33:ALA:C	2.54	0.45
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.99	0.45
1:C:373:PRO:O	1:C:377:LEU:HB2	2.15	0.45
1:C:733:GLN:OE1	1:C:733:GLN:HA	2.16	0.45
1:A:199:THR:HG22	1:A:791:VAL:HA	1.96	0.45
1:A:447:MET:CB	1:A:887:CYS:SG	2.91	0.45
1:A:786:ILE:O	1:A:787:GLY:C	2.54	0.45
1:A:974:PRO:C	1:A:976:LEU:H	2.18	0.45
1:B:198:LEU:HD23	1:B:792:ARG:HH22	1.81	0.45
1:B:639:GLY:HA2	1:B:643:LYS:NZ	2.31	0.45
1:C:176:GLN:HE21	1:C:620:ARG:NH1	2.11	0.45
1:C:408:ASP:OD2	1:C:940:LYS:NZ	2.46	0.45
1:C:801:PHE:CD1	1:C:804:PHE:HE1	2.35	0.45
1:C:1015:THR:O	1:C:1019:ILE:HB	2.17	0.45
2:C:3402:ERY:H343	2:C:3402:ERY:H353	1.98	0.45
1:A:239:ARG:CD	1:A:763:ILE:HG13	2.47	0.45
1:A:714:THR:H	1:A:832:ALA:HB2	1.80	0.45
1:C:54:ALA:HB2	1:C:84:SER:CB	2.46	0.45
1:C:937:LEU:HD12	1:C:937:LEU:HA	1.88	0.45
1:A:216:ALA:O	1:A:217:GLY:O	2.35	0.45
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.52	0.45
1:A:800:PRO:O	1:A:803:ALA:HB3	2.17	0.45
1:A:901:VAL:HG13	1:A:942:ALA:CB	2.46	0.45
1:A:909:VAL:O	1:A:913:LEU:HD23	2.17	0.45
1:B:327:TYR:CG	1:B:327:TYR:O	2.70	0.45
1:B:414:GLU:CD	1:B:974:PRO:HG3	2.37	0.45
1:C:6:ILE:O	1:C:9:PRO:HD3	2.16	0.45
1:C:27:ILE:HD11	1:C:380:PHE:CE2	2.52	0.45
1:C:251:LEU:CD1	1:C:262:LEU:HA	2.47	0.45
1:A:96:SER:OG	1:A:97:GLY:N	2.48	0.45
1:A:180:SER:O	1:A:181:GLN:CB	2.63	0.45
1:A:489:THR:HG22	1:A:490:PRO:HD3	1.98	0.45
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.98	0.45
1:B:409:ALA:HA	1:B:485:ALA:CB	2.47	0.45
1:B:934:THR:HA	1:B:937:LEU:HB2	1.98	0.45
1:B:967:ALA:C	1:B:969:ARG:N	2.68	0.45
1:C:314:GLU:N	1:C:315:PRO:HD2	2.32	0.45
1:C:463:THR:HA	1:C:466:ILE:CG1	2.46	0.45
1:C:527:TYR:C	1:C:529:ASP:H	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:734:GLU:HA	1:C:737:GLN:CG	2.46	0.45
1:C:801:PHE:O	1:C:803:ALA:N	2.38	0.45
1:C:986:VAL:O	1:C:986:VAL:CG1	2.64	0.45
1:B:27:ILE:HG22	1:B:380:PHE:CD2	2.51	0.45
1:B:399:VAL:O	1:B:402:ILE:CG2	2.59	0.45
1:B:892:TYR:OH	1:B:947:GLU:HB2	2.17	0.45
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.16	0.45
1:C:474:ILE:HG22	1:C:475:VAL:N	2.30	0.45
1:A:200:PRO:HG2	1:A:749:THR:HG23	1.98	0.45
1:A:240:LEU:CD1	1:A:240:LEU:H	2.30	0.45
1:A:250:LEU:HD23	1:A:259:ARG:HD2	1.99	0.45
1:A:735:LYS:O	1:A:739:LEU:HD22	2.15	0.45
1:A:949:ALA:O	1:A:953:MET:HB2	2.16	0.45
1:B:57:VAL:HG12	1:B:82:SER:HB2	1.98	0.45
1:B:177:LEU:HD12	1:B:288:GLY:O	2.17	0.45
1:B:232:ALA:HB1	1:C:725:PRO:O	2.17	0.45
1:B:306:ILE:CG2	1:B:310:LEU:HD12	2.47	0.45
1:B:343:THR:HA	1:B:346:GLU:HG2	1.99	0.45
1:C:176:GLN:NE2	1:C:620:ARG:HH12	2.09	0.45
1:C:672:VAL:HG13	1:C:673:GLU:H	1.77	0.45
1:A:61:VAL:HG21	1:A:122:VAL:HG21	1.98	0.45
1:B:356:TYR:O	1:B:360:GLN:N	2.50	0.45
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.51	0.45
1:B:420:MET:SD	1:B:425:LEU:HA	2.57	0.45
1:B:484:VAL:HG12	1:B:489:THR:OG1	2.16	0.45
1:B:525:HIS:HA	1:B:528:THR:CG2	2.47	0.45
1:B:564:LEU:HG	1:B:925:VAL:HG11	1.98	0.45
1:B:967:ALA:C	1:B:969:ARG:H	2.20	0.45
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.52	0.45
1:C:528:THR:CG2	1:C:969:ARG:HG3	2.47	0.45
1:A:18:ILE:O	1:A:19:ILE:C	2.54	0.44
1:A:66:GLU:OE2	1:A:821:GLY:HA2	2.17	0.44
1:A:197:GLN:HA	1:A:798:MET:SD	2.57	0.44
1:A:367:ILE:CG1	1:A:368:PRO:HD3	2.46	0.44
1:B:204:ILE:O	1:B:205:THR:C	2.55	0.44
1:B:230:LEU:HD21	1:C:809:TRP:CH2	2.53	0.44
1:C:653:ARG:HG3	1:C:654:ALA:N	2.32	0.44
1:C:684:LEU:HD21	1:C:699:ARG:HA	1.99	0.44
1:C:838:GLY:O	1:C:842:GLU:HB2	2.17	0.44
1:A:165:ALA:O	1:A:169:THR:HG23	2.17	0.44
1:B:57:VAL:HG12	1:B:58:GLN:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:LEU:O	1:B:113:LEU:N	2.51	0.44
1:B:680:PHE:CD1	1:B:859:TRP:CZ3	3.05	0.44
1:B:712:MET:HA	1:B:834:GLY:CA	2.47	0.44
1:B:717:ARG:N	1:B:717:ARG:HD3	2.31	0.44
1:B:919:ARG:HG3	1:B:920:GLY:H	1.82	0.44
1:C:57:VAL:CG1	1:C:88:VAL:HG22	2.46	0.44
1:C:69:MET:CG	1:C:92:LEU:HD21	2.47	0.44
1:C:145:THR:C	1:C:147:GLY:H	2.19	0.44
1:C:350:LEU:HD23	1:C:350:LEU:O	2.17	0.44
1:C:367:ILE:CD1	1:C:492:LEU:HD22	2.48	0.44
1:C:452:VAL:HG11	1:C:935:ILE:HG23	1.98	0.44
1:C:767:ARG:CG	1:C:767:ARG:NH1	2.77	0.44
1:A:355:MET:HB3	1:A:365:THR:HG22	2.00	0.44
1:B:343:THR:O	1:B:347:ALA:HB2	2.17	0.44
1:B:696:THR:HG23	1:B:825:MET:HE1	1.99	0.44
1:C:5:PHE:HD2	1:C:12:ALA:HB2	1.81	0.44
1:C:44:THR:HB	1:C:91:THR:HB	1.99	0.44
1:C:191:ASN:O	1:C:194:ASN:N	2.48	0.44
1:C:428:LYS:O	1:C:428:LYS:HG2	2.17	0.44
1:A:207:ILE:CB	1:A:759:VAL:HG11	2.46	0.44
1:A:415:ASN:O	1:A:434:SER:HB2	2.17	0.44
1:B:34:GLN:OE1	1:B:35:TYR:CD1	2.71	0.44
1:B:35:TYR:HB3	1:B:38:ILE:HG13	1.99	0.44
1:B:87:THR:HG21	1:B:620:ARG:CZ	2.47	0.44
1:C:330:THR:N	1:C:331:PRO:HD2	2.33	0.44
1:C:410:ILE:O	1:C:411:VAL:C	2.55	0.44
1:C:467:TYR:OH	1:C:925:VAL:HG12	2.17	0.44
1:C:686:ASP:CG	1:C:690:LEU:HB2	2.38	0.44
1:C:763:ILE:HD12	1:C:763:ILE:N	2.33	0.44
1:A:324:VAL:HG12	1:A:325:TYR:N	2.33	0.44
1:A:552:MET:HB2	1:A:910:ILE:HG23	1.99	0.44
1:A:930:GLY:C	1:A:932:LEU:H	2.21	0.44
1:B:768:VAL:HG23	1:C:63:GLN:CD	2.38	0.44
1:B:945:ILE:HG13	1:B:946:VAL:HG23	2.00	0.44
1:B:972:LEU:N	1:B:974:PRO:HD2	2.32	0.44
1:C:72:ILE:HB	1:C:75:LEU:HD12	2.00	0.44
1:C:544:LEU:O	1:C:548:ILE:HG13	2.17	0.44
1:C:830:GLN:OE1	1:C:832:ALA:HA	2.18	0.44
1:C:912:ALA:N	1:C:1010:GLY:HA2	2.33	0.44
1:C:1030:ARG:C	1:C:1032:ARG:H	2.21	0.44
1:A:355:MET:HG2	1:A:365:THR:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:THR:O	1:A:587:THR:N	2.49	0.44
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.98	0.44
1:A:879:ILE:O	1:A:883:VAL:HG23	2.18	0.44
1:A:942:ALA:O	1:A:946:VAL:HB	2.17	0.44
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.99	0.44
1:C:115:MET:HA	1:C:115:MET:HE2	1.98	0.44
1:C:255:GLN:C	1:C:257:GLY:N	2.71	0.44
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.99	0.44
1:C:449:LEU:HA	1:C:452:VAL:HG23	2.00	0.44
1:C:919:ARG:HG2	1:C:1005:THR:HG21	1.99	0.44
1:A:45:ILE:HD11	1:A:92:LEU:HD11	2.00	0.44
1:A:124:GLN:HG2	1:A:758:TYR:HE2	1.81	0.44
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.52	0.44
1:B:859:TRP:HB3	1:B:863:SER:HB3	2.00	0.44
1:C:68:ASN:O	1:C:70:ASN:N	2.51	0.44
1:C:228:GLN:NE2	1:C:229:GLN:O	2.37	0.44
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.53	0.44
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.99	0.44
1:A:750:LEU:HD13	1:C:216:ALA:HB1	1.99	0.44
1:A:773:VAL:O	1:A:773:VAL:CG1	2.66	0.44
1:B:455:PRO:HG3	1:B:880:SER:HA	1.99	0.44
1:B:897:ILE:O	1:B:901:VAL:HG23	2.18	0.44
1:C:467:TYR:O	1:C:470:PHE:N	2.51	0.44
1:C:684:LEU:HD22	1:C:702:LEU:HD23	2.00	0.44
1:C:866:GLU:C	1:C:867:ARG:HG2	2.38	0.44
1:C:885:PHE:CG	1:C:885:PHE:O	2.70	0.44
1:A:375:VAL:O	1:A:379:THR:N	2.51	0.44
1:A:583:THR:HG22	1:A:585:GLU:H	1.82	0.44
1:A:634:TRP:CZ3	1:A:995:ALA:HA	2.52	0.44
1:A:894:SER:C	1:A:896:SER:H	2.20	0.44
1:B:151:GLN:O	1:B:153:ASP:N	2.43	0.44
1:C:210:GLN:HB2	1:C:249:ILE:HD12	1.99	0.44
1:C:564:LEU:HD13	1:C:671:ILE:HB	2.00	0.44
1:C:896:SER:C	1:C:898:PRO:HD2	2.38	0.44
1:C:953:MET:HG3	1:C:963:ALA:HB2	2.00	0.44
2:C:3402:ERY:H321	2:C:3402:ERY:H8	1.78	0.44
1:A:515:TRP:O	1:A:516:PHE:HB2	2.18	0.43
1:A:781:MET:HE2	1:C:228:GLN:OE1	2.17	0.43
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.18	0.43
1:B:111:LEU:HD22	1:B:129:VAL:HG21	1.99	0.43
1:B:560:PRO:CB	1:B:836:SER:HB2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:THR:HA	1:B:665:ALA:HA	1.98	0.43
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.53	0.43
1:B:843:LEU:O	1:B:847:LEU:HD23	2.18	0.43
1:C:332:PHE:O	1:C:336:SER:HB2	2.17	0.43
1:C:897:ILE:N	1:C:898:PRO:CD	2.80	0.43
1:A:635:ALA:C	1:A:637:ARG:H	2.22	0.43
1:B:704:ALA:O	1:B:705:GLU:HB3	2.17	0.43
1:B:950:LYS:O	1:B:954:ASP:HB3	2.18	0.43
1:C:181:GLN:HG2	1:C:769:LYS:HE2	2.00	0.43
1:C:395:MET:O	1:C:397:GLY:N	2.51	0.43
1:A:193:LEU:HD21	1:A:199:THR:HA	2.00	0.43
1:A:886:LEU:HD11	1:C:17:ILE:HB	1.99	0.43
1:B:26:ALA:HB1	1:B:384:ALA:HB2	2.00	0.43
1:B:262:LEU:O	1:B:265:VAL:N	2.51	0.43
1:B:293:LEU:HD22	1:B:294:ALA:N	2.33	0.43
1:B:355:MET:SD	1:B:369:THR:HG23	2.58	0.43
1:B:419:VAL:O	1:B:419:VAL:CG1	2.65	0.43
1:C:137:LEU:HD12	1:C:138:MET:HB3	2.01	0.43
1:C:191:ASN:O	1:C:192:GLU:C	2.56	0.43
1:C:824:SER:O	1:C:825:MET:HB2	2.18	0.43
1:A:367:ILE:CD1	1:A:368:PRO:HD3	2.48	0.43
1:A:682:PHE:HD1	1:A:859:TRP:CH2	2.36	0.43
1:A:966:ASP:HA	1:A:969:ARG:HD2	1.99	0.43
1:B:25:LEU:O	1:B:28:LEU:HG	2.18	0.43
1:B:367:ILE:N	1:B:368:PRO:HD2	2.33	0.43
1:C:208:LYS:HA	1:C:760:ASN:ND2	2.32	0.43
1:C:314:GLU:N	1:C:315:PRO:CD	2.82	0.43
1:C:353:LEU:C	1:C:355:MET:N	2.72	0.43
1:A:535:LEU:HB3	1:A:961:ILE:HD12	2.00	0.43
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.49	0.43
1:B:298:ASN:O	1:B:298:ASN:ND2	2.49	0.43
1:B:699:ARG:HB3	1:B:699:ARG:NH1	2.33	0.43
1:C:72:ILE:HG22	1:C:94:PHE:HE2	1.83	0.43
1:C:80:SER:HA	1:C:90:ILE:HA	2.00	0.43
1:C:674:LEU:HD11	1:C:865:GLN:HB2	2.01	0.43
1:C:983:ILE:HD11	1:C:1011:MET:HG2	2.00	0.43
1:A:72:ILE:HG23	1:A:106:GLN:HB3	1.99	0.43
1:A:186:ILE:HG22	1:A:186:ILE:O	2.18	0.43
1:A:225:VAL:O	1:A:226:LYS:C	2.56	0.43
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.00	0.43
1:B:901:VAL:HG22	1:B:1026:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:LEU:H	1:A:231:ASN:ND2	2.17	0.43
1:A:886:LEU:HD21	1:C:17:ILE:HG21	2.01	0.43
1:A:970:MET:O	1:A:971:ARG:HB2	2.19	0.43
1:B:242:SER:C	1:B:244:GLU:N	2.72	0.43
1:B:393:LEU:CB	1:B:469:GLN:HG2	2.49	0.43
1:B:651:ALA:HB1	1:B:655:PHE:CE2	2.53	0.43
1:B:964:THR:HG22	1:B:1023:PRO:HB3	2.01	0.43
1:C:77:TYR:N	1:C:77:TYR:CD2	2.87	0.43
1:C:162:MET:HG2	1:C:313:MET:SD	2.59	0.43
1:C:214:VAL:HG23	1:C:236:ALA:HB3	2.00	0.43
1:A:997:SER:HB2	1:A:998:GLY:H	1.62	0.43
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.48	0.43
1:B:219:LEU:HD12	1:B:234:ILE:HD11	2.00	0.43
1:B:778:LYS:C	1:B:780:ARG:H	2.22	0.43
1:B:961:ILE:O	1:B:965:LEU:HD23	2.18	0.43
1:B:967:ALA:O	1:B:969:ARG:N	2.52	0.43
1:C:34:GLN:CG	1:C:35:TYR:H	2.32	0.43
1:C:124:GLN:HB2	1:C:758:TYR:CE2	2.47	0.43
1:C:189:ASN:HA	1:C:190:PRO:HD3	1.84	0.43
1:C:199:THR:OG1	1:C:201:VAL:N	2.51	0.43
1:C:244:GLU:O	1:C:263:ARG:NH2	2.52	0.43
1:C:713:LEU:HD13	1:C:713:LEU:N	2.33	0.43
1:A:405:LEU:HD23	1:A:477:ALA:HB1	1.99	0.43
1:B:448:VAL:HG21	1:B:888:LEU:HD21	2.01	0.43
1:B:453:PHE:HA	1:B:456:MET:SD	2.59	0.43
1:B:566:ASP:O	1:B:567:GLU:HG2	2.18	0.43
1:B:946:VAL:C	1:B:948:PHE:H	2.22	0.43
1:B:1014:ALA:O	1:B:1018:ALA:HB2	2.19	0.43
1:A:584:GLN:H	1:A:622:GLN:HE21	1.66	0.43
1:B:226:LYS:HA	1:B:226:LYS:NZ	2.33	0.43
1:B:949:ALA:HB3	1:B:1030:ARG:HH22	1.84	0.43
1:C:605:ASN:CB	1:C:637:ARG:HD3	2.42	0.43
1:C:941:ASN:HD22	1:C:941:ASN:C	2.23	0.43
1:C:1030:ARG:HE	1:C:1030:ARG:HB3	1.52	0.43
1:A:189:ASN:HB3	1:A:192:GLU:HB2	2.00	0.42
1:A:199:THR:HG21	1:A:791:VAL:HA	2.00	0.42
1:A:457:ALA:O	1:A:458:PHE:HD2	2.02	0.42
1:A:536:ARG:H	1:A:536:ARG:HG2	1.56	0.42
1:B:110:LYS:HZ3	1:B:110:LYS:HG3	1.72	0.42
1:B:240:LEU:HB3	1:B:245:GLU:HB2	2.00	0.42
1:B:520:PHE:O	1:B:523:SER:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:SER:O	1:B:924:ASP:HA	2.19	0.42
1:C:637:ARG:HB3	1:C:642:ASN:CB	2.48	0.42
1:A:146:ASP:OD2	1:A:146:ASP:N	2.52	0.42
1:A:298:ASN:C	1:A:300:LEU:H	2.22	0.42
1:A:364:ALA:O	1:A:367:ILE:HG13	2.20	0.42
1:A:961:ILE:HD11	1:A:1031:ARG:NH1	2.34	0.42
1:B:43:VAL:N	1:B:92:LEU:O	2.48	0.42
1:B:612:VAL:HG22	1:B:626:ILE:O	2.19	0.42
1:C:188:MET:HA	1:C:266:ALA:CB	2.49	0.42
1:C:982:PHE:O	1:C:985:GLY:N	2.51	0.42
1:A:30:LEU:HD21	1:A:384:ALA:HB2	2.01	0.42
1:A:105:VAL:HG22	1:B:105:VAL:HG13	2.01	0.42
1:A:206:ALA:C	1:A:208:LYS:N	2.73	0.42
1:A:368:PRO:HA	1:A:371:ALA:HB3	2.00	0.42
1:A:843:LEU:O	1:A:846:GLN:N	2.51	0.42
1:A:876:LEU:HA	1:A:879:ILE:HD12	2.01	0.42
1:A:894:SER:HB2	1:A:896:SER:OG	2.19	0.42
1:C:202:ASP:O	1:C:203:VAL:C	2.58	0.42
1:C:596:HIS:O	1:C:597:TYR:C	2.57	0.42
1:A:35:TYR:CG	1:A:671:ILE:HG22	2.55	0.42
1:A:479:ALA:O	1:A:482:VAL:HG12	2.20	0.42
1:B:53:ASP:HB2	1:B:56:THR:OG1	2.20	0.42
1:B:58:GLN:O	1:B:59:ASP:HB2	2.19	0.42
1:B:122:VAL:O	1:B:125:GLN:HB2	2.18	0.42
1:B:545:TYR:CE1	1:B:1025:PHE:HZ	2.37	0.42
1:B:717:ARG:CG	1:B:717:ARG:NH1	2.73	0.42
1:C:9:PRO:C	1:C:11:PHE:H	2.21	0.42
1:C:203:VAL:HG12	1:C:207:ILE:HD11	2.02	0.42
1:C:643:LYS:O	1:C:647:ILE:HG13	2.20	0.42
1:C:758:TYR:HD1	1:C:758:TYR:N	2.04	0.42
1:A:198:LEU:HD22	1:A:202:ASP:CB	2.50	0.42
1:A:354:VAL:HG12	1:A:355:MET:N	2.27	0.42
1:A:361:ASN:HB2	1:A:364:ALA:HB3	2.02	0.42
1:B:300:LEU:HD21	1:B:334:LYS:HG3	2.01	0.42
1:B:924:ASP:HB3	1:B:926:TYR:N	2.34	0.42
1:C:251:LEU:HD11	1:C:262:LEU:HA	2.01	0.42
1:C:324:VAL:O	1:C:326:PRO:HD2	2.20	0.42
1:B:262:LEU:C	1:B:264:ASP:N	2.72	0.42
1:B:380:PHE:O	1:B:383:LEU:N	2.53	0.42
1:B:697:GLN:O	1:B:699:ARG:O	2.38	0.42
1:B:733:GLN:HE22	1:B:743:ILE:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:ILE:H	1:C:534:ILE:HG13	1.74	0.42
1:C:545:TYR:CZ	1:C:1025:PHE:CZ	3.07	0.42
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.55	0.42
1:B:420:MET:SD	1:B:424:GLY:O	2.78	0.42
1:B:852:PRO:HB2	1:B:853:THR:H	1.52	0.42
1:B:1025:PHE:HA	1:B:1028:VAL:HG12	2.01	0.42
1:C:144:ASN:ND2	1:C:148:THR:N	2.67	0.42
1:C:379:THR:HB	1:C:398:MET:CE	2.50	0.42
1:C:415:ASN:O	1:C:419:VAL:HG22	2.19	0.42
1:C:818:ARG:HA	1:C:824:SER:N	2.33	0.42
1:C:905:VAL:HG22	1:C:935:ILE:HD11	2.02	0.42
1:A:282:ASN:HD21	1:A:609:VAL:H	1.68	0.42
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.85	0.42
1:A:889:ALA:HA	1:A:898:PRO:HG3	2.01	0.42
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.67	0.42
1:B:452:VAL:HG12	1:B:932:LEU:HG	2.02	0.42
1:B:733:GLN:HE22	1:B:743:ILE:HG21	1.85	0.42
1:B:986:VAL:HG23	1:B:1008:MET:HB2	2.00	0.42
1:B:1004:GLY:O	1:B:1006:GLY:N	2.53	0.42
1:C:178:PHE:HA	1:C:277:ILE:HG21	2.02	0.42
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.52	0.42
1:C:249:ILE:CG2	1:C:250:LEU:N	2.83	0.42
1:C:615:PHE:C	1:C:615:PHE:HD2	2.21	0.42
1:A:102:ILE:HA	1:A:105:VAL:HG23	2.02	0.42
1:A:412:VAL:O	1:A:416:VAL:HG23	2.20	0.42
1:A:978:THR:CG2	1:A:979:SER:N	2.83	0.42
1:B:20:MET:HG2	1:B:374:VAL:HA	2.02	0.42
1:B:136:PHE:HD1	1:B:136:PHE:H	1.65	0.42
1:B:150:THR:H	1:B:153:ASP:HB3	1.84	0.42
1:B:647:ILE:H	1:B:647:ILE:HG12	1.65	0.42
1:B:876:LEU:HD22	1:B:932:LEU:CD1	2.49	0.42
1:C:142:VAL:CG1	1:C:154:ILE:HG23	2.50	0.42
1:A:72:ILE:CD1	1:A:107:VAL:HA	2.50	0.41
1:A:446:ALA:HB2	1:A:482:VAL:HG21	2.01	0.41
1:B:57:VAL:HG21	1:B:86:GLY:HA2	2.01	0.41
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.85	0.41
1:B:268:ILE:HD12	1:B:268:ILE:N	2.34	0.41
1:B:602:GLU:C	1:B:604:ASN:N	2.73	0.41
1:B:924:ASP:HB3	1:B:926:TYR:H	1.84	0.41
1:C:248:LYS:HA	1:C:261:LEU:HD13	2.01	0.41
1:C:680:PHE:CD2	1:C:680:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:LEU:HD12	1:C:739:LEU:HA	1.82	0.41
1:A:46:SER:HA	1:A:88:VAL:O	2.20	0.41
1:A:304:ALA:O	1:A:307:ARG:N	2.53	0.41
1:A:658:ILE:H	1:A:658:ILE:HG12	1.63	0.41
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.50	0.41
1:C:83:ASP:HA	1:C:815:ARG:HA	2.02	0.41
1:C:615:PHE:CE2	2:C:3402:ERY:H341	2.55	0.41
1:A:901:VAL:HG11	1:A:943:ILE:HG13	2.01	0.41
1:B:9:PRO:HD2	1:C:893:GLU:OE1	2.20	0.41
1:B:65:ILE:HD11	1:B:118:LEU:HD21	2.02	0.41
1:B:572:PHE:HE2	1:B:631:LEU:HD21	1.84	0.41
1:B:602:GLU:OE2	1:B:650:ARG:NH2	2.54	0.41
1:B:696:THR:O	1:B:699:ARG:HB3	2.20	0.41
1:B:699:ARG:HG2	1:B:700:ASN:N	2.35	0.41
1:C:247:GLY:HA3	1:C:263:ARG:NE	2.35	0.41
1:A:31:PRO:HB2	1:A:389:SER:CB	2.48	0.41
1:A:193:LEU:HG	1:A:198:LEU:O	2.20	0.41
1:A:218:GLN:O	1:A:234:ILE:HD11	2.20	0.41
1:A:347:ALA:HA	1:A:350:LEU:HD23	2.02	0.41
1:A:892:TYR:CE1	1:A:947:GLU:OE2	2.73	0.41
1:A:943:ILE:O	1:A:947:GLU:HB2	2.20	0.41
1:A:1015:THR:C	1:A:1017:LEU:H	2.23	0.41
1:B:218:GLN:HB2	1:B:232:ALA:O	2.20	0.41
1:B:782:LEU:HD23	1:B:782:LEU:H	1.84	0.41
1:B:785:ASP:O	1:B:786:ILE:C	2.59	0.41
1:B:845:GLU:HG3	1:B:857:TYR:OH	2.19	0.41
1:B:1021:PHE:O	1:B:1025:PHE:CD1	2.72	0.41
1:C:9:PRO:O	1:C:10:ILE:HB	2.20	0.41
1:C:125:GLN:NE2	1:C:758:TYR:CZ	2.85	0.41
1:C:310:LEU:O	1:C:313:MET:HG2	2.20	0.41
1:C:545:TYR:CE1	1:C:1025:PHE:CZ	3.08	0.41
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.56	0.41
1:A:417:GLU:OE2	1:A:497:LEU:HD22	2.20	0.41
1:A:527:TYR:C	1:A:529:ASP:N	2.74	0.41
1:B:14:VAL:HG21	1:C:886:LEU:O	2.21	0.41
1:B:219:LEU:HD13	1:B:234:ILE:HG12	2.02	0.41
1:B:355:MET:SD	1:B:368:PRO:HB2	2.60	0.41
1:B:911:GLY:HA3	1:B:1013:THR:CG2	2.49	0.41
1:C:137:LEU:CD1	1:C:138:MET:HB3	2.50	0.41
1:C:463:THR:C	1:C:465:ALA:N	2.73	0.41
1:A:251:LEU:O	1:A:252:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ILE:HG22	1:B:69:MET:HE3	2.02	0.41
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.36	0.41
1:B:938:SER:C	1:B:940:LYS:H	2.24	0.41
1:C:30:LEU:CD1	1:C:384:ALA:HB2	2.50	0.41
1:C:144:ASN:CB	1:C:154:ILE:HD11	2.51	0.41
1:C:298:ASN:O	1:C:299:ALA:C	2.58	0.41
1:C:602:GLU:O	1:C:604:ASN:N	2.54	0.41
1:A:239:ARG:HD3	1:A:763:ILE:HG13	2.03	0.41
1:A:692:HIS:C	1:A:694:LYS:H	2.23	0.41
1:A:1007:VAL:O	1:A:1008:MET:C	2.59	0.41
1:B:61:VAL:HG23	1:B:118:LEU:HD23	2.03	0.41
1:B:330:THR:N	1:B:331:PRO:CD	2.84	0.41
1:B:420:MET:HG2	1:B:426:PRO:CD	2.50	0.41
1:C:5:PHE:CD2	1:C:12:ALA:HB2	2.55	0.41
1:C:226:LYS:HB3	1:C:227:GLY:H	1.74	0.41
1:C:394:THR:HG22	1:C:395:MET:CE	2.50	0.41
1:C:413:VAL:O	1:C:413:VAL:HG22	2.20	0.41
1:C:431:THR:O	1:C:435:MET:HG2	2.21	0.41
1:C:463:THR:HG22	1:C:467:TYR:CD1	2.55	0.41
1:C:1017:LEU:HD23	1:C:1017:LEU:O	2.21	0.41
1:A:465:ALA:O	1:A:469:GLN:HG2	2.20	0.41
1:A:551:GLY:O	1:A:555:LEU:HB2	2.21	0.41
1:A:674:LEU:HD13	1:A:675:GLY:N	2.36	0.41
1:B:58:GLN:HB2	1:B:82:SER:HB3	2.02	0.41
1:B:189:ASN:HD22	1:B:190:PRO:HD2	1.85	0.41
1:B:282:ASN:C	1:B:284:GLN:H	2.23	0.41
1:B:851:LEU:N	1:B:852:PRO:HD3	2.35	0.41
1:C:404:LEU:HD21	1:C:449:LEU:HD12	2.01	0.41
1:C:423:GLU:HB3	1:C:426:PRO:HG2	2.03	0.41
1:C:672:VAL:CG2	1:C:676:THR:H	2.31	0.41
1:A:191:ASN:C	1:A:193:LEU:H	2.23	0.41
1:A:294:ALA:HB3	1:A:297:ALA:CB	2.46	0.41
1:A:365:THR:O	1:A:368:PRO:HD2	2.21	0.41
1:A:781:MET:HE1	1:C:225:VAL:N	2.36	0.41
1:B:18:ILE:HD12	1:C:886:LEU:HD13	2.02	0.41
1:B:46:SER:O	1:B:127:VAL:HA	2.20	0.41
1:B:57:VAL:CG1	1:B:82:SER:HB2	2.51	0.41
1:B:186:ILE:HB	1:B:773:VAL:HG23	2.02	0.41
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.36	0.41
1:B:262:LEU:O	1:B:266:ALA:N	2.44	0.41
1:B:298:ASN:O	1:B:299:ALA:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:SER:N	1:B:865:GLN:OE1	2.37	0.41
1:B:782:LEU:HB2	1:B:783:PRO:HD2	2.03	0.41
1:C:115:MET:CE	1:C:127:VAL:HG21	2.51	0.41
1:C:160:ALA:HA	1:C:767:ARG:NE	2.36	0.41
1:C:255:GLN:O	1:C:257:GLY:N	2.54	0.41
1:C:617:PHE:CZ	2:C:3402:ERY:H312	2.55	0.41
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.68	0.41
1:C:719:ASN:O	1:C:721:LEU:N	2.53	0.41
1:A:231:ASN:OD1	1:B:622:GLN:NE2	2.53	0.41
1:A:579:PRO:O	1:A:580:ALA:C	2.59	0.41
1:B:200:PRO:HD2	1:B:749:THR:CG2	2.51	0.41
1:B:213:GLN:CG	1:C:56:THR:CG2	2.96	0.41
1:B:310:LEU:HD22	1:B:323:ILE:HG21	2.03	0.41
1:C:249:ILE:HG22	1:C:250:LEU:N	2.36	0.41
1:C:251:LEU:HB2	1:C:260:VAL:O	2.20	0.41
1:C:961:ILE:O	1:C:961:ILE:HG22	2.20	0.41
1:A:53:ASP:HA	1:A:84:SER:HA	2.03	0.40
1:A:153:ASP:HA	1:A:182:TYR:CE1	2.56	0.40
1:A:172:VAL:HG23	1:A:172:VAL:O	2.21	0.40
1:A:353:LEU:C	1:A:354:VAL:O	2.59	0.40
1:A:538:THR:HG23	1:A:540:ARG:NH2	2.37	0.40
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.02	0.40
1:B:52:ALA:HB2	1:B:86:GLY:H	1.74	0.40
1:B:701:GLN:HE22	1:B:851:LEU:HB2	1.86	0.40
1:C:142:VAL:HG13	1:C:321:LEU:HD13	2.03	0.40
1:C:527:TYR:OH	1:C:968:VAL:CG1	2.69	0.40
1:C:655:PHE:HB3	1:C:663:VAL:HG21	2.03	0.40
1:A:952:LEU:HD11	1:A:966:ASP:HB3	2.03	0.40
1:B:13:TRP:O	1:B:17:ILE:HG12	2.21	0.40
1:B:193:LEU:HD13	1:B:198:LEU:O	2.21	0.40
1:B:230:LEU:HD21	1:C:809:TRP:HH2	1.86	0.40
1:B:293:LEU:HD22	1:B:294:ALA:H	1.85	0.40
1:B:377:LEU:O	1:B:380:PHE:HB2	2.21	0.40
1:B:383:LEU:O	1:B:384:ALA:C	2.59	0.40
1:B:644:VAL:HA	1:B:647:ILE:HG13	2.03	0.40
1:C:184:MET:HA	1:C:184:MET:HE3	2.01	0.40
1:A:184:MET:HB2	1:A:762:PHE:CE2	2.57	0.40
1:A:426:PRO:HB3	1:A:427:PRO:CD	2.51	0.40
1:A:686:ASP:OD1	1:A:690:LEU:HB2	2.21	0.40
1:B:115:MET:CE	1:B:127:VAL:HG21	2.50	0.40
1:B:445:ILE:HD12	1:B:940:LYS:HG3	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLU:HB3	1:C:426:PRO:CD	2.49	0.40
1:C:944:LEU:O	1:C:971:ARG:HD2	2.20	0.40
1:C:1022:VAL:O	1:C:1022:VAL:HG22	2.21	0.40
1:A:375:VAL:HG21	1:A:481:SER:HA	2.03	0.40
1:A:406:VAL:O	1:A:409:ALA:N	2.51	0.40
1:A:620:ARG:CG	1:A:620:ARG:NH1	2.78	0.40
1:A:897:ILE:O	1:A:900:SER:OG	2.29	0.40
1:B:158:VAL:HA	1:B:162:MET:HG3	2.00	0.40
1:B:231:ASN:ND2	1:B:232:ALA:N	2.70	0.40
1:B:443:VAL:O	1:B:447:MET:N	2.54	0.40
1:B:681:ASP:CB	1:B:860:THR:HG23	2.51	0.40
1:C:878:ALA:C	1:C:880:SER:H	2.24	0.40
1:A:325:TYR:N	1:A:325:TYR:CD1	2.90	0.40
1:A:708:LYS:C	1:A:709:HIS:HD2	2.24	0.40
1:A:713:LEU:H	1:A:832:ALA:HB2	1.86	0.40
1:A:726:GLN:N	1:A:810:GLU:O	2.53	0.40
1:B:150:THR:HG22	1:B:151:GLN:H	1.86	0.40
1:B:231:ASN:HD22	1:B:232:ALA:N	2.20	0.40
1:B:240:LEU:HD13	1:B:245:GLU:HB3	2.02	0.40
1:B:240:LEU:HD22	1:B:245:GLU:HG2	2.03	0.40
1:B:416:VAL:HG21	1:B:431:THR:HG22	2.03	0.40
1:B:459:PHE:HB2	1:B:460:GLY:H	1.59	0.40
1:B:897:ILE:HA	1:B:900:SER:OG	2.21	0.40
1:B:935:ILE:HG12	1:B:935:ILE:H	1.58	0.40
1:C:33:ALA:HB2	1:C:298:ASN:ND2	2.36	0.40
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	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	1018/1053 (97%)	715 (70%)	198 (19%)	105 (10%)	0 3
1	B	1018/1053 (97%)	694 (68%)	214 (21%)	110 (11%)	0 3
1	C	1018/1053 (97%)	734 (72%)	207 (20%)	77 (8%)	1 7
All	All	3054/3159 (97%)	2143 (70%)	619 (20%)	292 (10%)	0 4

All (292) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	SER
1	A	134	SER
1	A	160	ALA
1	A	170	SER
1	A	188	MET
1	A	212	ALA
1	A	256	ASP
1	A	293	LEU
1	A	319	SER
1	A	375	VAL
1	A	426	PRO
1	A	516	PHE
1	A	580	ALA
1	A	601	LYS
1	A	638	PRO
1	A	659	LYS
1	A	661	ALA
1	A	678	THR
1	A	775	SER
1	A	788	ASP
1	A	870	GLY
1	A	958	LYS
1	A	971	ARG
1	A	997	SER
1	A	998	GLY
1	A	1008	MET
1	B	2	PRO
1	B	54	ALA
1	B	69	MET
1	B	262	LEU
1	B	299	ALA
1	B	426	PRO
1	B	538	THR
1	B	580	ALA

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Mol	Chain	Res	Type
1	B	581	GLY
1	B	582	ALA
1	B	633	ASP
1	B	656	SER
1	B	671	ILE
1	B	676	THR
1	B	690	LEU
1	B	691	GLY
1	B	805	SER
1	B	806	SER
1	B	820	ASN
1	B	849	SER
1	B	893	GLU
1	B	918	PHE
1	B	921	LEU
1	B	935	ILE
1	B	1033	PHE
1	C	34	GLN
1	C	152	GLU
1	C	226	LYS
1	C	256	ASP
1	C	266	ALA
1	C	319	SER
1	C	427	PRO
1	C	633	ASP
1	C	673	GLU
1	C	713	LEU
1	C	720	GLY
1	C	806	SER
1	C	825	MET
1	C	832	ALA
1	C	836	SER
1	C	837	THR
1	C	921	LEU
1	C	958	LYS
1	C	965	LEU
1	A	64	VAL
1	A	181	GLN
1	A	213	GLN
1	A	217	GLY
1	A	220	GLY
1	A	221	GLY

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Mol	Chain	Res	Type
1	A	227	GLY
1	A	294	ALA
1	A	318	PRO
1	A	354	VAL
1	A	376	LEU
1	A	457	ALA
1	A	460	GLY
1	A	534	ILE
1	A	599	LEU
1	A	656	SER
1	A	670	ALA
1	A	675	GLY
1	A	784	ASP
1	A	787	GLY
1	A	917	THR
1	A	931	LEU
1	A	969	ARG
1	A	992	SER
1	A	1016	VAL
1	A	1017	LEU
1	A	1030	ARG
1	A	1035	ARG
1	B	22	ALA
1	B	84	SER
1	B	140	VAL
1	B	147	GLY
1	B	226	LYS
1	B	243	THR
1	B	263	ARG
1	B	283	GLY
1	B	358	PHE
1	B	360	GLN
1	B	424	GLY
1	B	453	PHE
1	B	486	LEU
1	B	490	PRO
1	B	558	ARG
1	B	601	LYS
1	B	618	ALA
1	B	638	PRO
1	B	658	ILE
1	B	669	PRO

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Mol	Chain	Res	Type
1	B	672	VAL
1	B	689	GLY
1	B	693	GLU
1	B	834	GLY
1	B	852	PRO
1	B	878	ALA
1	B	953	MET
1	B	1005	THR
1	C	4	PHE
1	C	221	GLY
1	C	285	PRO
1	C	411	VAL
1	C	577	GLN
1	C	601	LYS
1	C	602	GLU
1	C	618	ALA
1	C	733	GLN
1	C	802	SER
1	C	820	ASN
1	C	913	LEU
1	C	946	VAL
1	C	960	LEU
1	C	975	ILE
1	C	983	ILE
1	C	997	SER
1	C	998	GLY
1	C	1017	LEU
1	A	182	TYR
1	A	192	GLU
1	A	295	THR
1	A	374	VAL
1	A	377	LEU
1	A	378	GLY
1	A	427	PRO
1	A	517	ASN
1	A	636	ASP
1	A	689	GLY
1	A	714	THR
1	A	847	LEU
1	A	975	ILE
1	A	988	PRO
1	A	991	ILE

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Mol	Chain	Res	Type
1	B	52	ALA
1	B	223	PRO
1	B	258	SER
1	B	318	PRO
1	B	357	LEU
1	B	364	ALA
1	B	597	TYR
1	B	603	LYS
1	B	654	ALA
1	B	708	LYS
1	B	765	ARG
1	B	835	LYS
1	B	936	GLY
1	B	1018	ALA
1	B	1019	ILE
1	C	33	ALA
1	C	69	MET
1	C	81	ASN
1	C	146	ASP
1	C	224	PRO
1	C	230	LEU
1	C	354	VAL
1	C	477	ALA
1	C	555	LEU
1	C	656	SER
1	C	972	LEU
1	A	236	ALA
1	A	252	LYS
1	A	287	SER
1	A	335	ILE
1	A	357	LEU
1	A	392	THR
1	A	407	ASP
1	A	416	VAL
1	A	423	GLU
1	A	439	GLN
1	A	635	ALA
1	A	693	GLU
1	A	746	ILE
1	A	892	TYR
1	A	994	GLY
1	A	1007	VAL

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Mol	Chain	Res	Type
1	B	36	PRO
1	B	82	SER
1	B	112	GLN
1	B	127	VAL
1	B	350	LEU
1	B	428	LYS
1	B	491	ALA
1	B	655	PHE
1	B	733	GLN
1	B	766	GLY
1	B	776	GLU
1	B	959	GLY
1	C	54	ALA
1	C	80	SER
1	C	206	ALA
1	C	236	ALA
1	C	372	VAL
1	C	396	PHE
1	C	410	ILE
1	C	413	VAL
1	C	425	LEU
1	C	531	VAL
1	C	617	PHE
1	C	882	ILE
1	C	895	TRP
1	C	974	PRO
1	C	982	PHE
1	A	19	ILE
1	A	50	PRO
1	A	63	GLN
1	A	120	GLN
1	A	397	GLY
1	A	832	ALA
1	A	967	ALA
1	B	171	GLY
1	B	184	MET
1	B	228	GLN
1	B	254	ASN
1	B	297	ALA
1	B	346	GLU
1	B	446	ALA
1	B	539	GLY

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Mol	Chain	Res	Type
1	B	564	LEU
1	B	713	LEU
1	B	716	VAL
1	B	723	ASP
1	B	871	ASN
1	B	957	GLY
1	B	974	PRO
1	B	992	SER
1	C	187	TRP
1	C	335	ILE
1	C	422	GLU
1	C	528	THR
1	C	636	ASP
1	C	1006	GLY
1	A	340	VAL
1	A	361	ASN
1	A	422	GLU
1	A	452	VAL
1	A	515	TRP
1	B	73	ASP
1	B	126	GLY
1	B	326	PRO
1	B	438	ILE
1	B	557	VAL
1	B	614	GLY
1	B	939	ALA
1	C	349	ILE
1	C	751	GLY
1	A	207	ILE
1	A	543	VAL
1	A	833	PRO
1	B	119	PRO
1	B	783	PRO
1	B	968	VAL
1	C	315	PRO
1	A	107	VAL
1	B	227	GLY
1	B	786	ILE
1	C	658	ILE
1	C	671	ILE
1	A	461	GLY
1	B	224	PRO

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Mol	Chain	Res	Type
1	B	621	GLY
1	A	36	PRO
1	A	140	VAL
1	C	689	GLY
1	C	935	ILE
1	A	987	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	833/859 (97%)	699 (84%)	134 (16%)	2 11
1	B	833/859 (97%)	700 (84%)	133 (16%)	2 11
1	C	833/859 (97%)	705 (85%)	128 (15%)	2 13
All	All	2499/2577 (97%)	2104 (84%)	395 (16%)	2 12

All (395) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	21	LEU
1	A	25	LEU
1	A	28	LEU
1	A	38	ILE
1	A	45	ILE
1	A	49	TYR
1	A	59	ASP
1	A	60	THR
1	A	62	THR
1	A	63	GLN
1	A	70	ASN
1	A	88	VAL
1	A	101	ASP
1	A	113	LEU
1	A	130	GLU

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Mol	Chain	Res	Type
1	A	146	ASP
1	A	161	ASN
1	A	176	GLN
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	210	GLN
1	A	214	VAL
1	A	222	THR
1	A	225	VAL
1	A	239	ARG
1	A	255	GLN
1	A	256	ASP
1	A	260	VAL
1	A	269	GLU
1	A	270	LEU
1	A	280	GLU
1	A	295	THR
1	A	298	ASN
1	A	301	ASP
1	A	310	LEU
1	A	313	MET
1	A	316	PHE
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	353	LEU
1	A	356	TYR
1	A	357	LEU
1	A	360	GLN
1	A	366	LEU
1	A	400	LEU
1	A	402	ILE
1	A	418	ARG
1	A	447	MET
1	A	448	VAL
1	A	473	THR
1	A	475	VAL
1	A	481	SER
1	A	482	VAL
1	A	489	THR
1	A	495	THR

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Mol	Chain	Res	Type
1	A	496	MET
1	A	515	TRP
1	A	526	HIS
1	A	527	TYR
1	A	530	SER
1	A	536	ARG
1	A	540	ARG
1	A	542	LEU
1	A	544	LEU
1	A	552	MET
1	A	556	PHE
1	A	562	SER
1	A	564	LEU
1	A	575	MET
1	A	576	VAL
1	A	584	GLN
1	A	612	VAL
1	A	615	PHE
1	A	620	ARG
1	A	630	SER
1	A	632	LYS
1	A	636	ASP
1	A	653	ARG
1	A	658	ILE
1	A	659	LYS
1	A	662	MET
1	A	671	ILE
1	A	674	LEU
1	A	687	GLN
1	A	702	LEU
1	A	711	ASP
1	A	712	MET
1	A	713	LEU
1	A	717	ARG
1	A	721	LEU
1	A	724	THR
1	A	739	LEU
1	A	746	ILE
1	A	750	LEU
1	A	764	ASP
1	A	773	VAL
1	A	780	ARG

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Mol	Chain	Res	Type
1	A	791	VAL
1	A	795	ASP
1	A	802	SER
1	A	806	SER
1	A	810	GLU
1	A	813	SER
1	A	843	LEU
1	A	844	MET
1	A	852	PRO
1	A	858	ASP
1	A	867	ARG
1	A	881	LEU
1	A	882	ILE
1	A	886	LEU
1	A	899	PHE
1	A	918	PHE
1	A	928	GLN
1	A	929	VAL
1	A	951	ASP
1	A	955	LYS
1	A	960	LEU
1	A	972	LEU
1	A	976	LEU
1	A	978	THR
1	A	980	LEU
1	A	982	PHE
1	A	983	ILE
1	A	986	VAL
1	A	993	THR
1	A	997	SER
1	A	1007	VAL
1	A	1021	PHE
1	A	1030	ARG
1	A	1035	ARG
1	B	11	PHE
1	B	13	TRP
1	B	21	LEU
1	B	28	LEU
1	B	49	TYR
1	B	53	ASP
1	B	57	VAL
1	B	60	THR

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Mol	Chain	Res	Type
1	B	65	ILE
1	B	67	GLN
1	B	70	ASN
1	B	74	ASN
1	B	81	ASN
1	B	83	ASP
1	B	90	ILE
1	B	91	THR
1	B	92	LEU
1	B	93	THR
1	B	95	GLU
1	B	96	SER
1	B	104	GLN
1	B	115	MET
1	B	121	GLU
1	B	128	SER
1	B	137	LEU
1	B	145	THR
1	B	148	THR
1	B	150	THR
1	B	152	GLU
1	B	154	ILE
1	B	155	SER
1	B	169	THR
1	B	176	GLN
1	B	182	TYR
1	B	185	ARG
1	B	186	ILE
1	B	189	ASN
1	B	194	ASN
1	B	199	THR
1	B	213	GLN
1	B	226	LYS
1	B	231	ASN
1	B	235	ILE
1	B	243	THR
1	B	244	GLU
1	B	250	LEU
1	B	253	VAL
1	B	254	ASN
1	B	255	GLN
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	261	LEU
1	B	270	LEU
1	B	276	ASP
1	B	293	LEU
1	B	298	ASN
1	B	300	LEU
1	B	302	THR
1	B	323	ILE
1	B	329	THR
1	B	343	THR
1	B	349	ILE
1	B	356	TYR
1	B	358	PHE
1	B	372	VAL
1	B	379	THR
1	B	394	THR
1	B	395	MET
1	B	402	ILE
1	B	406	VAL
1	B	414	GLU
1	B	435	MET
1	B	456	MET
1	B	459	PHE
1	B	468	ARG
1	B	469	GLN
1	B	473	THR
1	B	478	MET
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	519	MET
1	B	528	THR
1	B	558	ARG
1	B	562	SER
1	B	564	LEU
1	B	571	VAL
1	B	587	THR
1	B	595	THR
1	B	599	LEU
1	B	601	LYS
1	B	613	ASN
1	B	620	ARG

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Mol	Chain	Res	Type
1	B	623	ASN
1	B	629	VAL
1	B	655	PHE
1	B	660	ASP
1	B	692	HIS
1	B	695	LEU
1	B	696	THR
1	B	702	LEU
1	B	714	THR
1	B	717	ARG
1	B	723	ASP
1	B	739	LEU
1	B	750	LEU
1	B	757	SER
1	B	758	TYR
1	B	773	VAL
1	B	778	LYS
1	B	779	TYR
1	B	782	LEU
1	B	795	ASP
1	B	801	PHE
1	B	808	ARG
1	B	818	ARG
1	B	826	GLU
1	B	844	MET
1	B	875	SER
1	B	880	SER
1	B	891	LEU
1	B	897	ILE
1	B	900	SER
1	B	905	VAL
1	B	914	LEU
1	B	921	LEU
1	B	935	ILE
1	B	947	GLU
1	B	952	LEU
1	B	966	ASP
1	B	972	LEU
1	B	978	THR
1	B	989	LEU
1	B	1034	SER
1	C	13	TRP

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Mol	Chain	Res	Type
1	C	30	LEU
1	C	34	GLN
1	C	35	TYR
1	C	37	THR
1	C	44	THR
1	C	46	SER
1	C	49	TYR
1	C	55	LYS
1	C	56	THR
1	C	64	VAL
1	C	68	ASN
1	C	80	SER
1	C	82	SER
1	C	84	SER
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	108	GLN
1	C	109	ASN
1	C	111	LEU
1	C	115	MET
1	C	118	LEU
1	C	123	GLN
1	C	128	SER
1	C	137	LEU
1	C	150	THR
1	C	151	GLN
1	C	155	SER
1	C	164	ASP
1	C	177	LEU
1	C	189	ASN
1	C	207	ILE
1	C	226	LYS
1	C	228	GLN
1	C	239	ARG
1	C	253	VAL
1	C	258	SER
1	C	259	ARG
1	C	269	GLU
1	C	274	ASN
1	C	284	GLN
1	C	285	PRO

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Mol	Chain	Res	Type
1	C	300	LEU
1	C	307	ARG
1	C	314	GLU
1	C	321	LEU
1	C	338	HIS
1	C	341	VAL
1	C	351	VAL
1	C	355	MET
1	C	370	ILE
1	C	374	VAL
1	C	377	LEU
1	C	404	LEU
1	C	417	GLU
1	C	422	GLU
1	C	425	LEU
1	C	454	VAL
1	C	459	PHE
1	C	472	ILE
1	C	480	LEU
1	C	483	LEU
1	C	497	LEU
1	C	529	ASP
1	C	542	LEU
1	C	544	LEU
1	C	555	LEU
1	C	567	GLU
1	C	571	VAL
1	C	573	MET
1	C	577	GLN
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	615	PHE
1	C	636	ASP
1	C	641	GLU
1	C	658	ILE
1	C	664	PHE
1	C	668	LEU
1	C	685	ILE
1	C	687	GLN
1	C	693	GLU
1	C	695	LEU

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Mol	Chain	Res	Type
1	C	696	THR
1	C	699	ARG
1	C	702	LEU
1	C	713	LEU
1	C	714	THR
1	C	716	VAL
1	C	722	GLU
1	C	724	THR
1	C	739	LEU
1	C	743	ILE
1	C	750	LEU
1	C	758	TYR
1	C	759	VAL
1	C	761	ASP
1	C	767	ARG
1	C	778	LYS
1	C	791	VAL
1	C	795	ASP
1	C	799	VAL
1	C	805	SER
1	C	806	SER
1	C	830	GLN
1	C	839	GLU
1	C	846	GLN
1	C	847	LEU
1	C	865	GLN
1	C	868	LEU
1	C	899	PHE
1	C	900	SER
1	C	903	LEU
1	C	914	LEU
1	C	931	LEU
1	C	935	ILE
1	C	941	ASN
1	C	952	LEU
1	C	954	ASP
1	C	960	LEU
1	C	982	PHE
1	C	983	ILE
1	C	984	LEU
1	C	993	THR
1	C	1007	VAL

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Mol	Chain	Res	Type
1	C	1036	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	58	GLN
1	A	112	GLN
1	A	120	GLN
1	A	123	GLN
1	A	124	GLN
1	A	144	ASN
1	A	210	GLN
1	A	229	GLN
1	A	231	ASN
1	A	282	ASN
1	A	298	ASN
1	A	360	GLN
1	A	577	GLN
1	A	584	GLN
1	A	622	GLN
1	A	623	ASN
1	A	709	HIS
1	A	719	ASN
1	A	726	GLN
1	A	846	GLN
1	A	865	GLN
1	A	928	GLN
1	A	1001	ASN
1	B	70	ASN
1	B	74	ASN
1	B	104	GLN
1	B	106	GLN
1	B	108	GLN
1	B	109	ASN
1	B	112	GLN
1	B	144	ASN
1	B	151	GLN
1	B	161	ASN
1	B	176	GLN
1	B	189	ASN
1	B	191	ASN

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Mol	Chain	Res	Type
1	B	210	GLN
1	B	213	GLN
1	B	218	GLN
1	B	228	GLN
1	B	231	ASN
1	B	254	ASN
1	B	391	ASN
1	B	415	ASN
1	B	517	ASN
1	B	613	ASN
1	B	622	GLN
1	B	700	ASN
1	B	709	HIS
1	B	726	GLN
1	B	733	GLN
1	B	846	GLN
1	B	872	GLN
1	B	941	ASN
1	C	3	ASN
1	C	34	GLN
1	C	58	GLN
1	C	63	GLN
1	C	89	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	237	GLN
1	C	274	ASN
1	C	284	GLN
1	C	360	GLN
1	C	439	GLN
1	C	577	GLN
1	C	588	GLN
1	C	605	ASN
1	C	700	ASN
1	C	737	GLN
1	C	923	ASN
1	C	941	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ERY	C	3402	-	53,53,53	1.01	1 (1%)	82,82,82	1.64	18 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ERY	C	3402	-	-	4/72/107/107	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3402	ERY	O2-C1	4.97	1.45	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3402	ERY	C20-O5-C16	4.16	126.23	117.55
2	C	3402	ERY	C29-N1-C24	3.74	124.37	113.11
2	C	3402	ERY	O2-C1-C2	3.52	119.29	111.56
2	C	3402	ERY	C15-C16-C17	3.41	113.78	107.67
2	C	3402	ERY	C13-O2-C1	-3.24	112.42	118.18
2	C	3402	ERY	O7-C5-C6	3.16	110.29	106.39
2	C	3402	ERY	C25-C24-N1	-3.15	106.77	115.67
2	C	3402	ERY	C33-C8-C7	-3.12	104.06	109.81
2	C	3402	ERY	O12-C11-C10	3.12	115.38	110.71
2	C	3402	ERY	O12-C11-C12	-2.67	101.69	106.68
2	C	3402	ERY	O7-C5-C4	-2.60	107.65	111.54
2	C	3402	ERY	O4-C18-C21	2.52	112.15	106.70
2	C	3402	ERY	O2-C1-O1	-2.48	119.31	123.94
2	C	3402	ERY	C34-C10-C11	-2.27	111.55	114.38
2	C	3402	ERY	C29-N1-C28	2.18	116.81	110.38
2	C	3402	ERY	C25-C24-C23	2.17	113.08	109.97
2	C	3402	ERY	C19-C16-C15	-2.07	106.80	110.49
2	C	3402	ERY	O7-C22-C23	2.03	113.35	108.10

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3402	ERY	C32-C6-C7-C8
2	C	3402	ERY	C23-C24-N1-C29
2	C	3402	ERY	C25-C24-N1-C28
2	C	3402	ERY	C19-C16-O5-C20

There are no ring outliers.

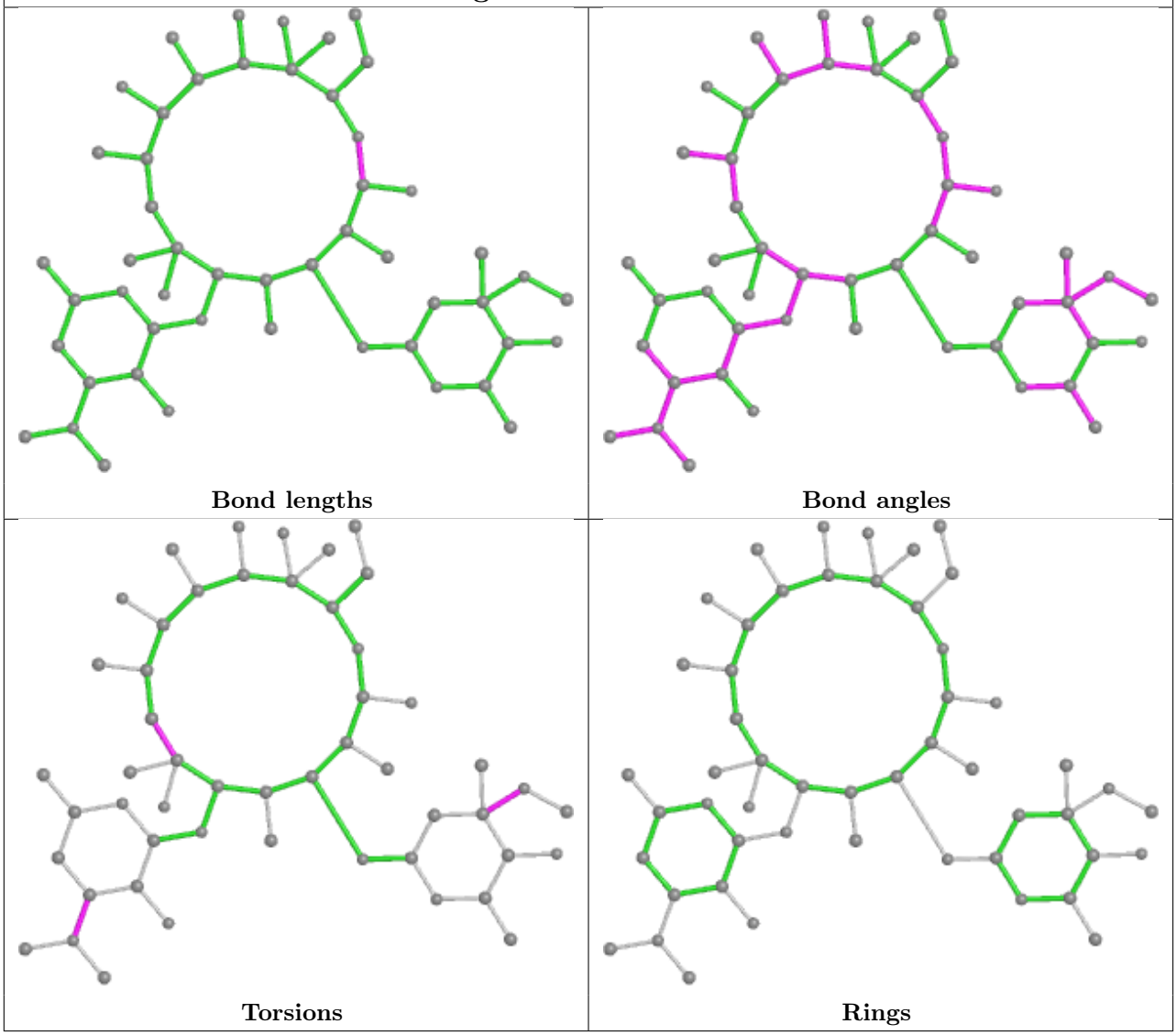
1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3402	ERY	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ERY C 3402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1022/1053 (97%)	0.15	37 (3%)	42	41	58, 111, 150, 192	0
1	B	1022/1053 (97%)	0.22	50 (4%)	29	29	69, 115, 154, 179	0
1	C	1022/1053 (97%)	0.17	45 (4%)	34	35	55, 109, 160, 188	0
All	All	3066/3159 (97%)	0.18	132 (4%)	35	36	55, 113, 155, 192	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	520	PHE	9.4
1	A	497	LEU	5.7
1	B	963	ALA	5.4
1	C	537	SER	5.1
1	A	259	ARG	4.5
1	C	540	ARG	4.5
1	C	712	MET	4.1
1	C	1034	SER	4.1
1	B	675	GLY	4.1
1	A	515	TRP	4.1
1	B	1033	PHE	3.8
1	A	1036	LYS	3.8
1	C	425	LEU	3.7
1	C	538	THR	3.7
1	B	515	TRP	3.7
1	C	872	GLN	3.7
1	B	676	THR	3.7
1	A	513	PHE	3.7
1	C	671	ILE	3.6
1	C	535	LEU	3.5
1	C	497	LEU	3.5
1	C	962	GLU	3.5
1	A	198	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	539	GLY	3.4
1	B	420	MET	3.4
1	C	1033	PHE	3.4
1	B	526	HIS	3.3
1	B	635	ALA	3.3
1	B	727	PHE	3.2
1	A	425	LEU	3.1
1	B	435	MET	3.1
1	A	419	VAL	3.1
1	C	604	ASN	3.0
1	A	253	VAL	3.0
1	B	426	PRO	3.0
1	C	420	MET	3.0
1	C	496	MET	2.9
1	B	779	TYR	2.9
1	A	145	THR	2.9
1	A	1029	VAL	2.8
1	C	515	TRP	2.8
1	C	516	PHE	2.8
1	A	258	SER	2.8
1	B	497	LEU	2.8
1	B	188	MET	2.8
1	C	675	GLY	2.8
1	C	961	ILE	2.7
1	C	430	ALA	2.7
1	C	252	LYS	2.7
1	A	427	PRO	2.7
1	B	670	ALA	2.7
1	B	949	ALA	2.7
1	B	964	THR	2.6
1	B	634	TRP	2.6
1	A	1030	ARG	2.6
1	A	1033	PHE	2.6
1	B	669	PRO	2.6
1	B	494	ALA	2.6
1	A	149	MET	2.6
1	A	322	LYS	2.5
1	C	251	LEU	2.5
1	A	431	THR	2.5
1	A	712	MET	2.5
1	B	597	TYR	2.5
1	A	230	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	514	GLY	2.5
1	B	516	PHE	2.5
1	A	154	ILE	2.5
1	C	957	GLY	2.5
1	B	679	GLY	2.5
1	C	606	VAL	2.5
1	A	199	THR	2.4
1	A	31	PRO	2.4
1	A	134	SER	2.4
1	C	424	GLY	2.4
1	C	431	THR	2.4
1	B	535	LEU	2.4
1	C	423	GLU	2.4
1	A	558	ARG	2.4
1	B	363	ARG	2.4
1	C	900	SER	2.4
1	B	804	PHE	2.3
1	C	357	LEU	2.3
1	A	698	ALA	2.3
1	C	427	PRO	2.3
1	C	459	PHE	2.3
1	A	142	VAL	2.3
1	B	493	CYS	2.3
1	B	672	VAL	2.3
1	B	3	ASN	2.3
1	C	641	GLU	2.3
1	C	361	ASN	2.3
1	B	606	VAL	2.3
1	A	287	SER	2.2
1	C	871	ASN	2.2
1	B	554	TYR	2.2
1	A	964	THR	2.2
1	B	918	PHE	2.2
1	B	847	LEU	2.2
1	C	895	TRP	2.2
1	B	660	ASP	2.2
1	B	412	VAL	2.2
1	A	196	PHE	2.2
1	B	991	ILE	2.2
1	A	32	VAL	2.2
1	C	264	ASP	2.2
1	A	265	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	134	SER	2.1
1	B	647	ILE	2.1
1	C	897	ILE	2.1
1	C	676	THR	2.1
1	B	604	ASN	2.1
1	C	259	ARG	2.1
1	A	188	MET	2.1
1	A	958	LYS	2.1
1	B	993	THR	2.1
1	A	321	LEU	2.1
1	A	426	PRO	2.1
1	B	133	SER	2.1
1	B	321	LEU	2.1
1	B	1	MET	2.1
1	C	741	VAL	2.1
1	C	498	LYS	2.1
1	B	843	LEU	2.0
1	B	553	ALA	2.0
1	B	1005	THR	2.0
1	A	1031	ARG	2.0
1	B	417	GLU	2.0
1	B	148	THR	2.0
1	B	682	PHE	2.0
1	B	678	THR	2.0
1	C	536	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

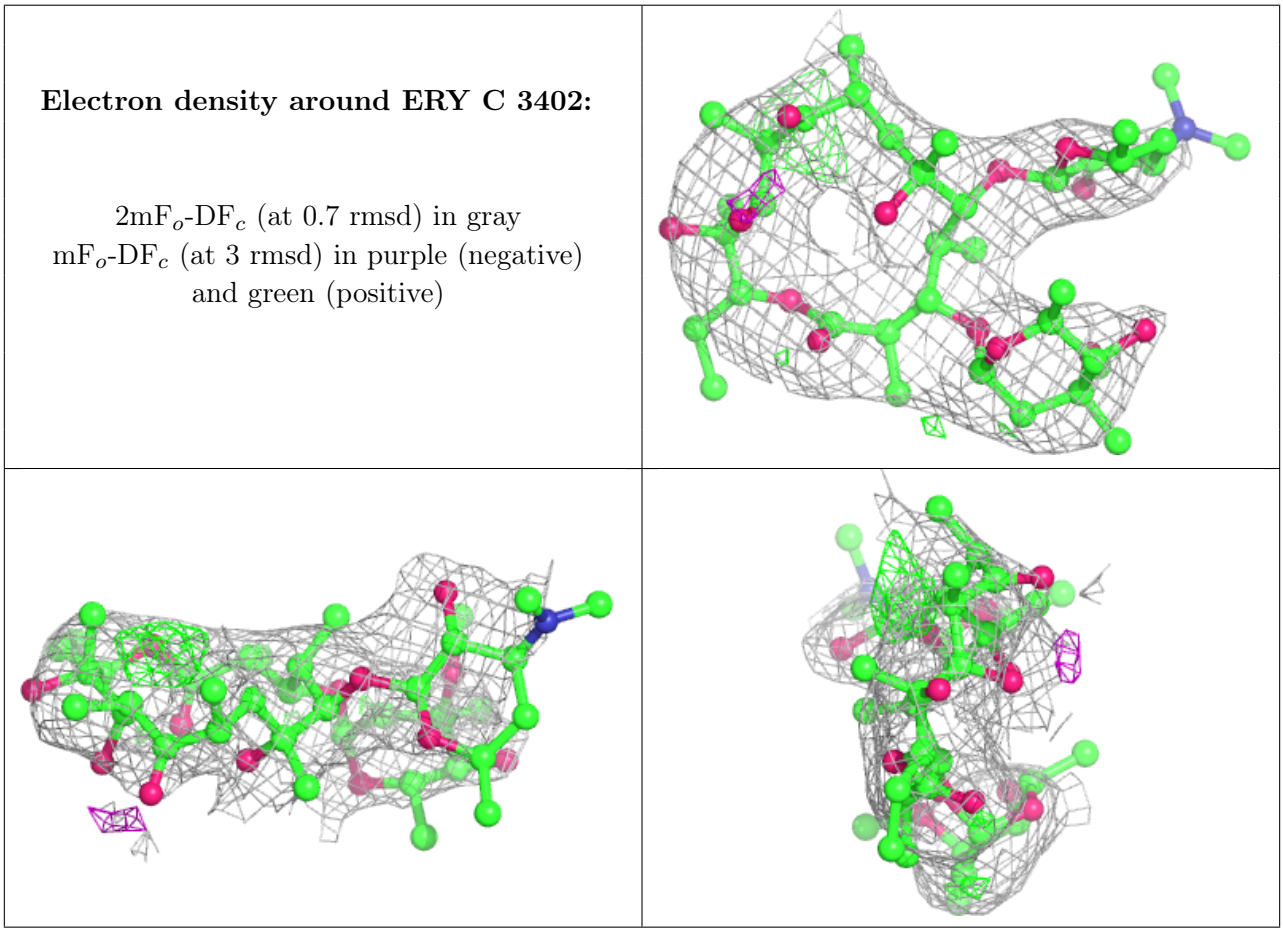
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ERY	C	3402	51/51	0.85	0.33	58,68,74,79	51

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ERY C 3402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.