Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 10:03 AM EDT

PDB ID	:	3AOD
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	:	3.30 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:

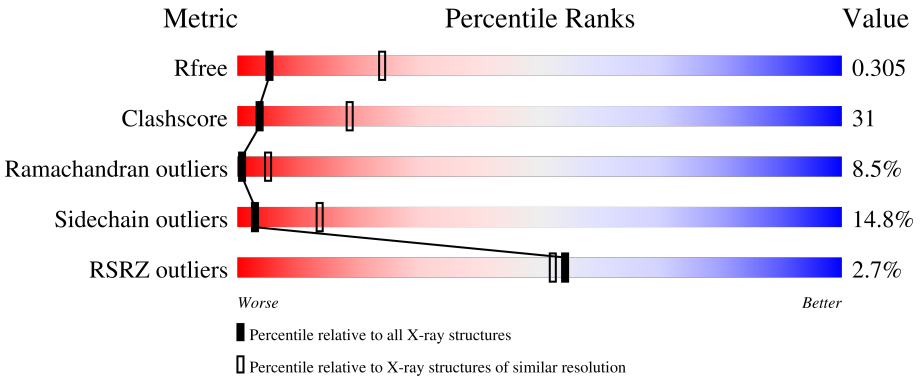
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	3% 43% 42% 11%
1	B	1053	2% 40% 45% 11%
1	C	1053	3% 44% 43% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23419 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.

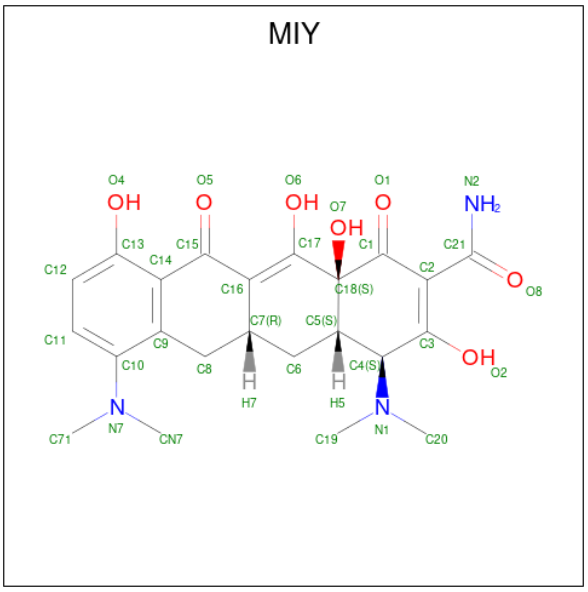
- Molecule 1 is a protein called Acriflavine resistance protein B.

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:

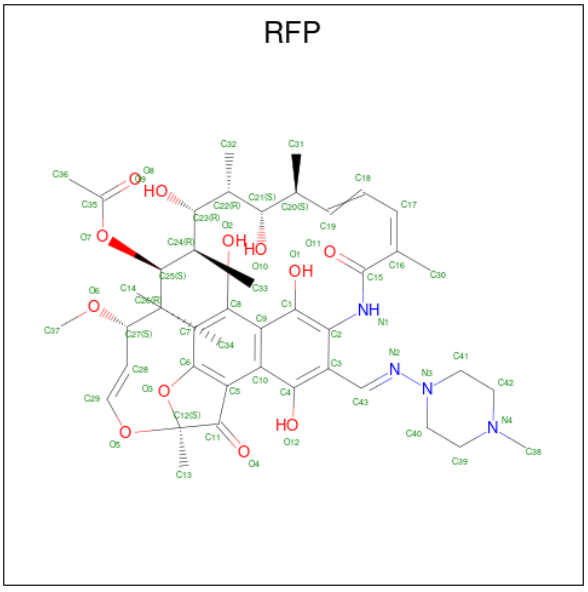
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression 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 (4S,4AS,5AR,12AS)-4,7-BIS(DIMETHYLAMINO)-3,10,12,12A-TETRAHYDROXY-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (three-letter code: MIY) (formula: $C_{23}H_{27}N_3O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	23	3	7	0	0

- Molecule 3 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	59	43	4	12	0	0

- Molecule 4 is water.

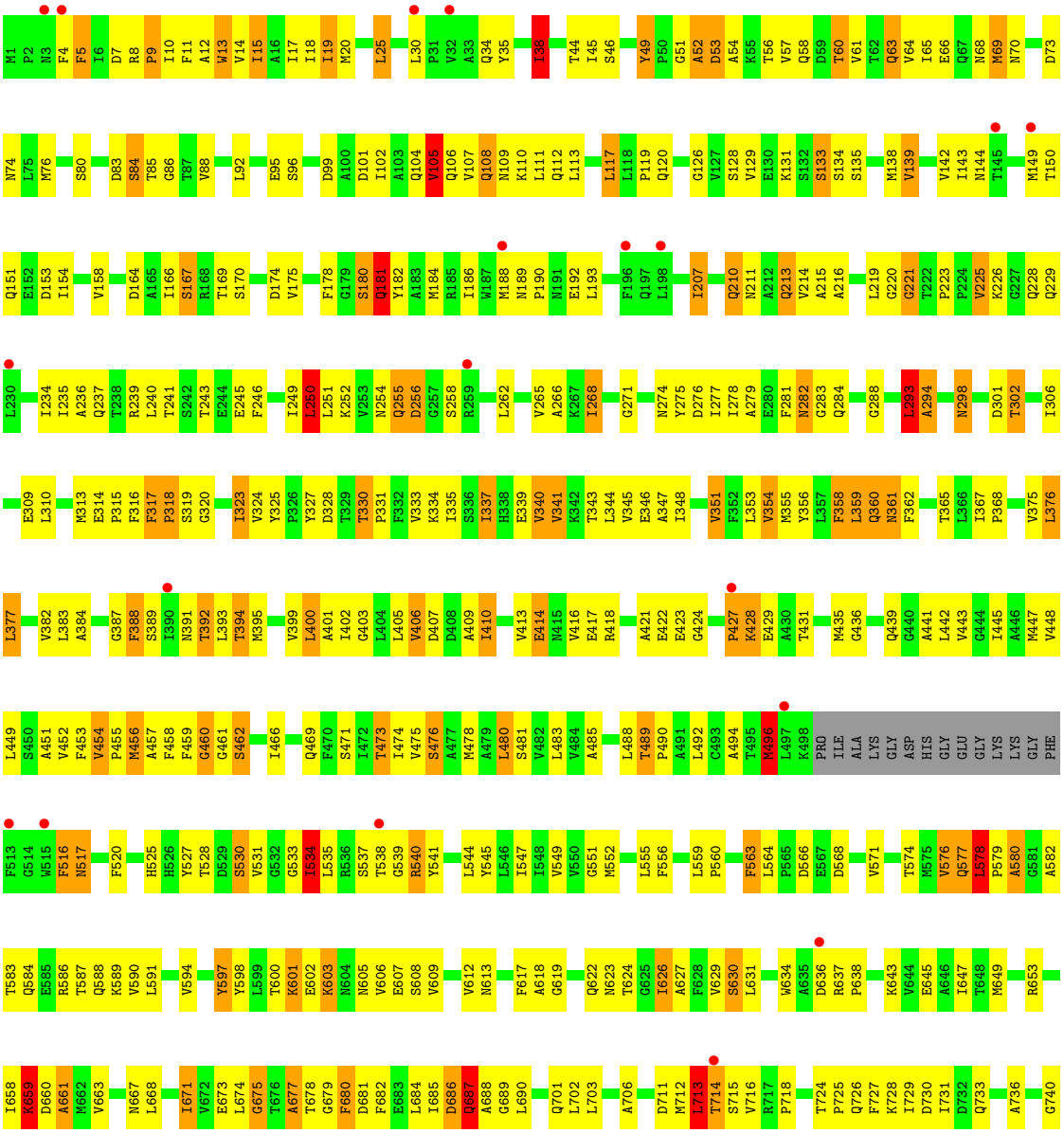
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total O 2 2	0	0
4	B	2	Total O 2 2	0	0
4	C	1	Total O 1 1	0	0

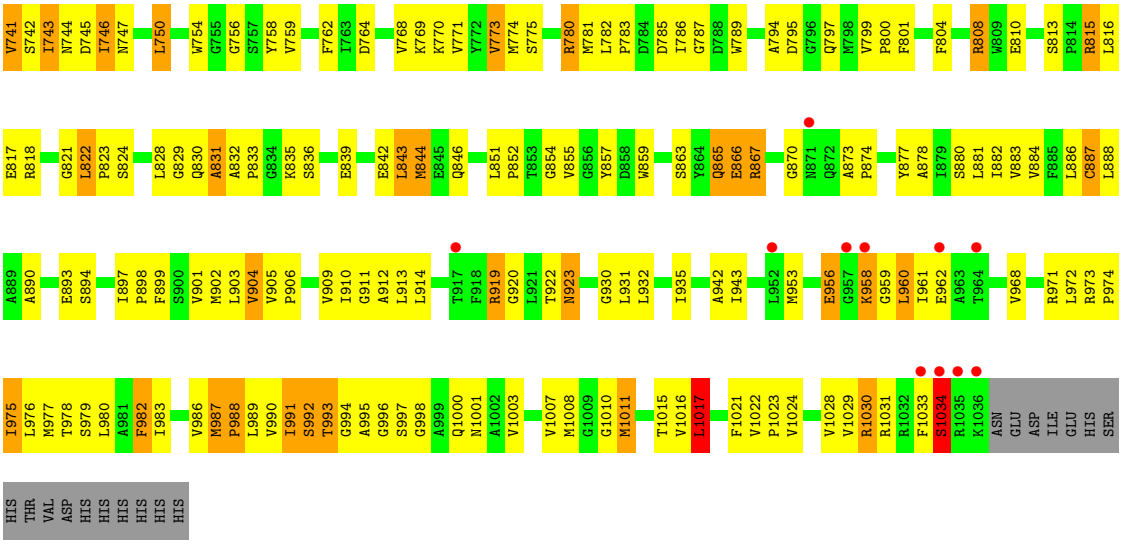
3 Residue-property plots (i)

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

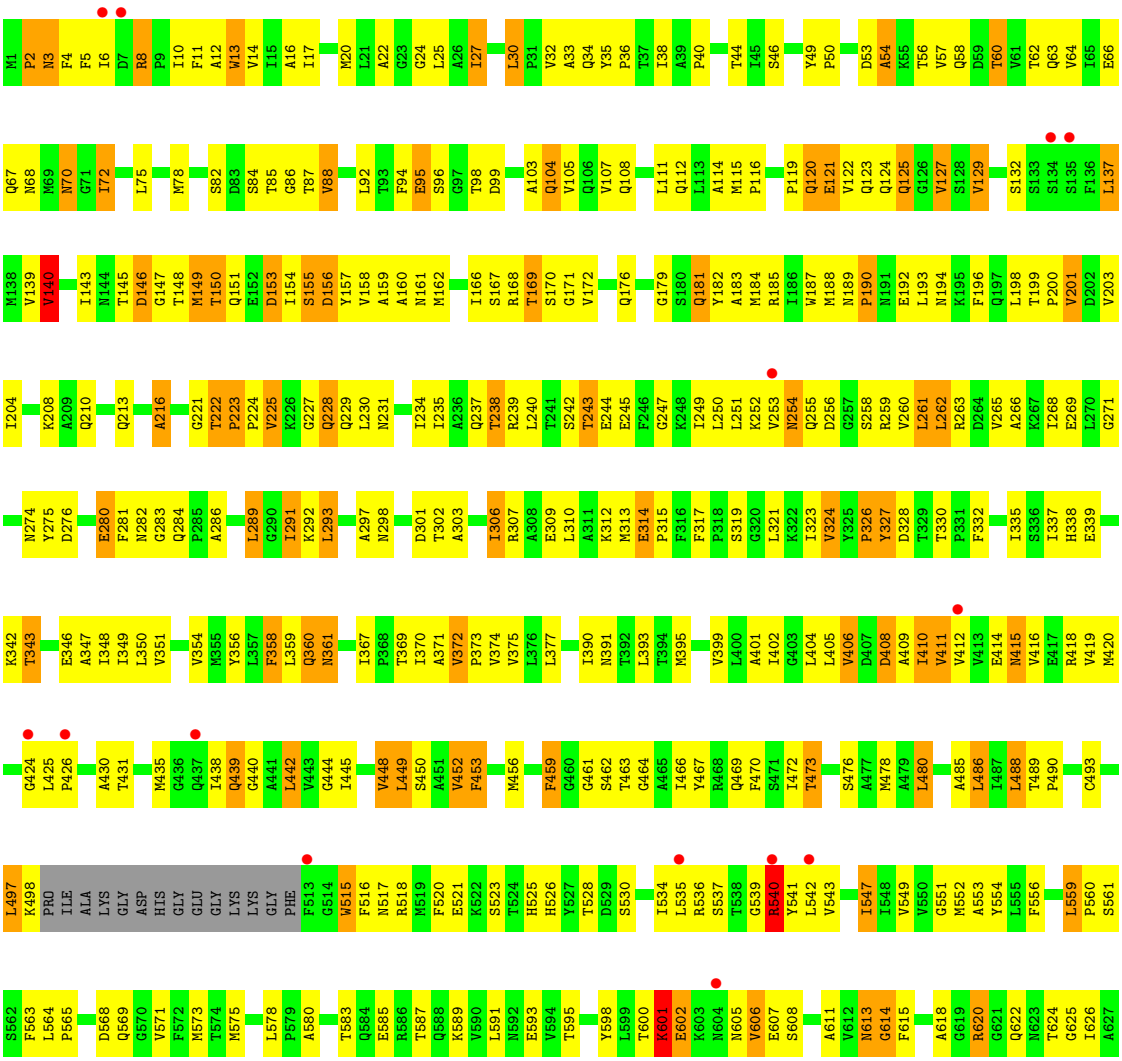
Chain A:

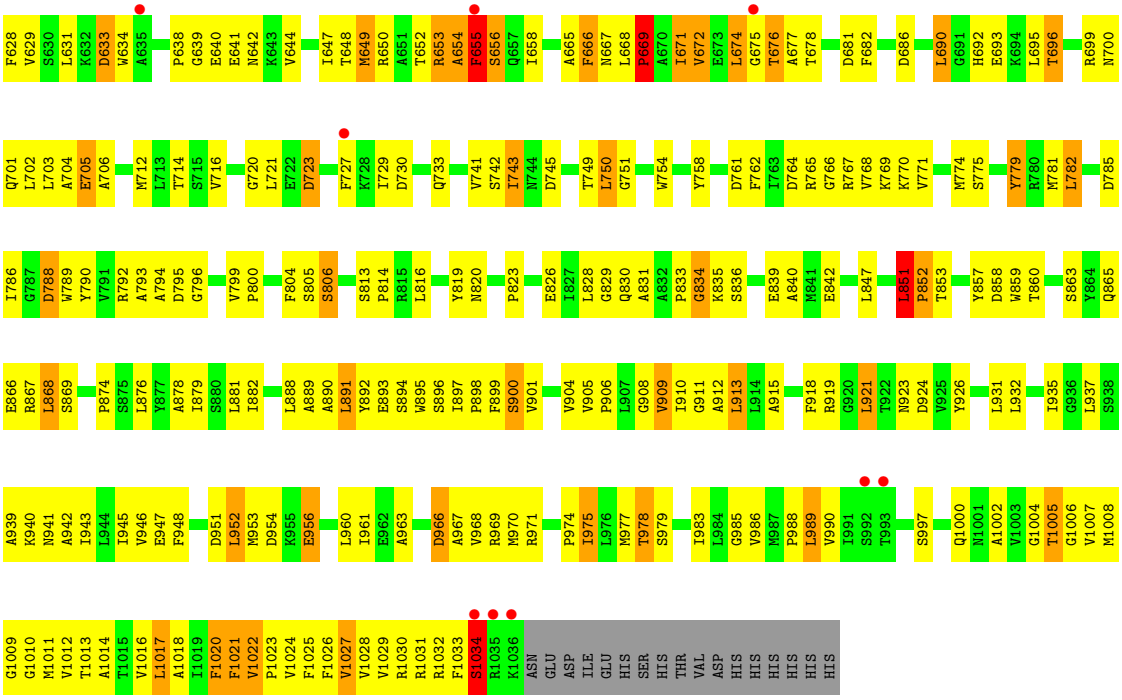




• Molecule 1: Acriflavine resistance protein B

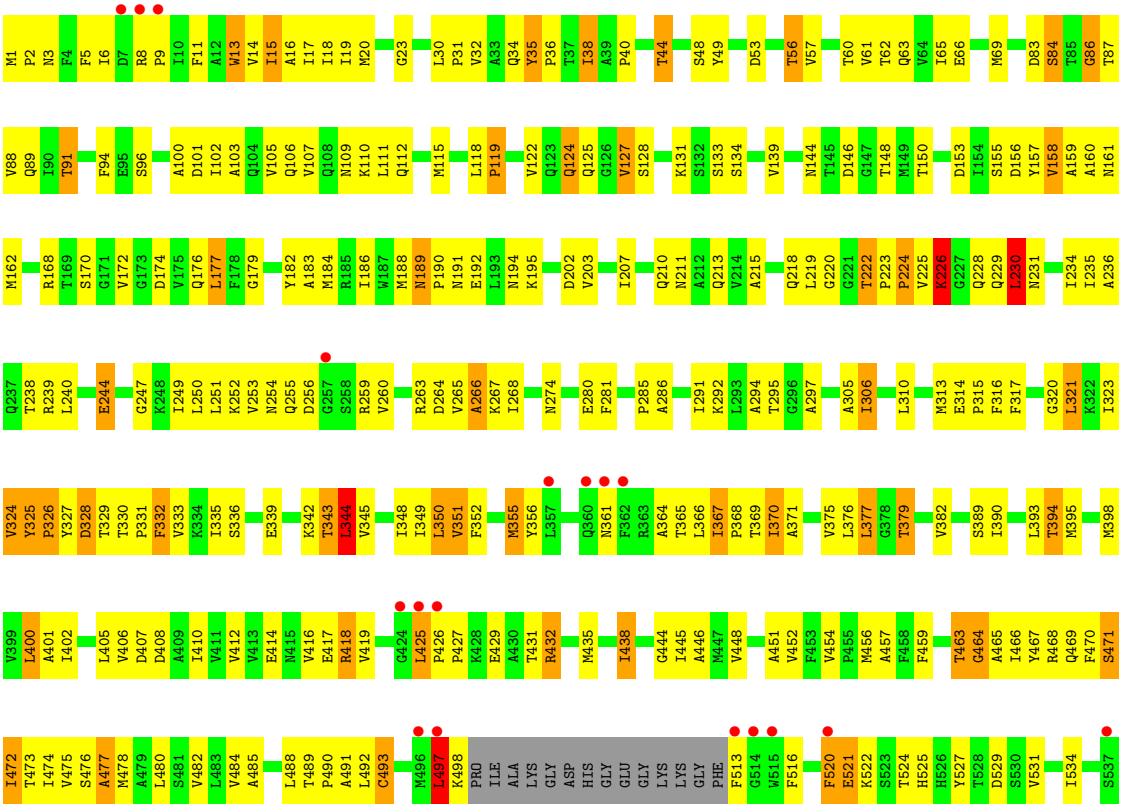
Chain B:

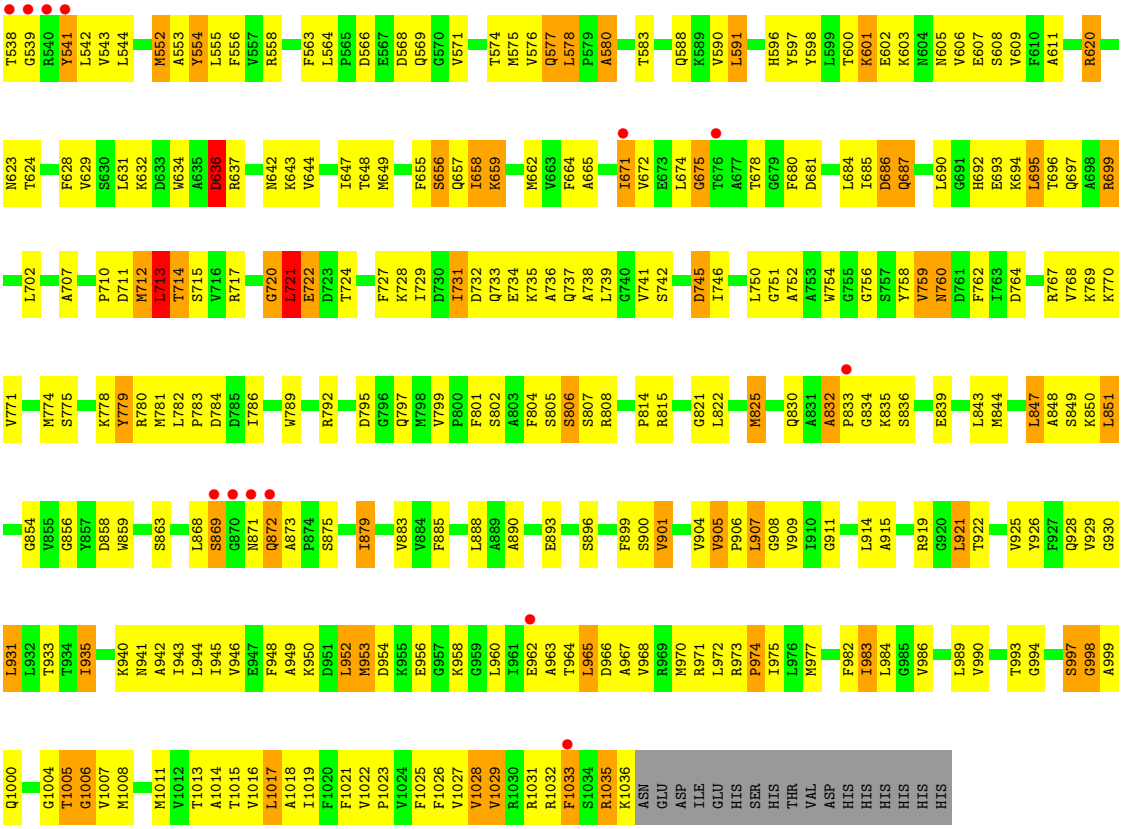




• Molecule 1: Acriflavine resistance protein B

Chain C:




T538 G539 R540 Y541 L542 V543 L544 M552 A553 Y554 L555 F556 V557 R558 F563 L564 P565 D566 E567 D568 Q569 G570 V571 T574 M575 V576 Q577 L578 P579 A580 T583 Q588 K589 V590 L591 H596 Y597 Y598 L599 T600 K601 E602 K603 N604 N605 V606 E607 S608 V609 F610 A611 R620
N623 T624 F628 V629 S630 L631 K632 D633 W634 A635 D636 R637 N642 K643 V644 I647 T648 M649 F655 S656 Q657 I658 K659 M662 V663 F664 A665 I671 V672 E673 L674 G675 T676 A677 T678 G679 F680 D681 L684 I685 D686 Q687 L690 G691 H692 E693 K694 L696 T696 Q697 A698 R699
L702 A707 P710 D711 M712 L713 T714 S715 V716 R717 G720 L721 E722 D723 T724 F727 K728 I729 D730 I731 D732 Q733 E734 K735 A736 Q737 A738 L739 G740 V741 S742 D745 I746 L750 G751 A752 A753 W754 G755 G756 S757 Y758 V759 N760 D761 F762 I763 D764 R767 V768 K769 K770
V771 M774 S775 K778 Y779 R780 M781 L782 P783 D784 D785 I786 W789 R792 D795 G796 Q797 M798 V799 P800 F801 S802 A803 F804 S805 S806 S807 R808 P814 R815 G821 L822 M825 Q830 A831 A832 P833 G834 K835 S836 E839 L843 M844 L847 A848 S849 K850 L851
G854 V855 G856 Y857 D858 W859 S863 L868 S869 G870 N871 Q872 A873 P874 S875 I879 V883 V884 F885 L888 A889 A890 E893 S896 F899 S900 V901 V904 V905 P906 L907 G908 V909 I910 G911 L914 A915 R919 G920 L921 T922 V925 Y926 F927 Q928 V929 G930
L931 L932 T933 T934 I935 K940 N941 A942 I943 L944 I945 V946 E947 F948 A949 K950 D951 L952 M953 D954 K955 E956 G957 K958 G959 L960 I961 E962 A963 T964 L965 D966 A967 V968 R969 M970 R971 L972 R973 P974 I975 L976 M977 F982 I983 L984 G985 V986 L989 V990 T993 G994 S997 G998 A999
Q1000 G1004 T1005 G1006 V1007 M1008 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 F1025 F1026 V1027 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	226.60Å 134.50Å 162.83Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	47.50 – 3.30 47.50 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.50-3.30) 97.3 (47.50-3.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.67 (at 3.33Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.258 , 0.318 0.251 , 0.305	Depositor DCC
R_{free} test set	3532 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	95.3	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 68.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23419	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: RFP, MIY

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	0.65	0/7920	0.77	4/10756 (0.0%)
1	B	0.60	0/7920	0.76	2/10756 (0.0%)
1	C	0.65	0/7920	0.79	5/10756 (0.0%)
All	All	0.64	0/23760	0.77	11/32268 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	321	LEU	CA-CB-CG	7.38	132.26	115.30
1	B	868	LEU	CA-CB-CG	6.60	130.48	115.30
1	C	721	LEU	CA-CB-CG	6.58	130.42	115.30
1	A	400	LEU	CA-CB-CG	6.09	129.30	115.30
1	C	344	LEU	CA-CB-CG	5.79	128.62	115.30
1	A	250	LEU	CA-CB-CG	5.68	128.35	115.30
1	A	578	LEU	CA-CB-CG	5.55	128.06	115.30
1	B	989	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	230	LEU	CA-CB-CG	5.30	127.49	115.30
1	C	720	GLY	N-CA-C	5.20	126.11	113.10
1	A	25	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7774	0	7931	510	0
1	B	7774	0	7931	537	0
1	C	7774	0	7931	503	0
2	A	33	0	24	0	0
3	C	59	0	56	4	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
All	All	23419	0	23873	1489	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 31.

All (1489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:CB	1:A:832:ALA:HA	1.80	1.11
1:C:44:THR:HG23	1:C:91:THR:HB	1.33	1.10
1:C:909:VAL:HG12	1:C:931:LEU:HD21	1.11	1.09
1:B:95:GLU:O	1:B:98:THR:HG22	1.50	1.09
1:C:115:MET:HE3	1:C:127:VAL:HG11	1.33	1.08
1:A:713:LEU:HB3	1:A:832:ALA:HA	1.09	1.03
1:B:1026:PHE:HB3	1:B:1030:ARG:HH21	1.23	1.02
1:A:901:VAL:O	1:A:904:VAL:HG23	1.60	1.02
1:A:210:GLN:HG3	1:A:249:ILE:HG23	1.42	1.01
1:A:225:VAL:H	1:B:781:MET:HE2	1.25	1.01
1:C:713:LEU:HD11	1:C:834:GLY:HA3	1.02	1.01
1:B:222:THR:HB	1:B:223:PRO:HD3	1.38	1.01
1:A:713:LEU:HB3	1:A:832:ALA:CA	1.89	1.01
1:C:760:ASN:O	1:C:771:VAL:HG23	1.61	1.01
1:B:919:ARG:HD2	1:B:1005:THR:HG21	1.42	1.00
1:A:671:ILE:H	1:A:671:ILE:CD1	1.74	1.00
1:C:713:LEU:CD1	1:C:834:GLY:HA3	1.92	0.98
1:C:974:PRO:HA	1:C:977:MET:HE2	1.44	0.98
1:B:831:ALA:HB2	1:B:840:ALA:HB2	1.44	0.98
1:C:190:PRO:HD2	1:C:779:TYR:CD1	1.99	0.97
1:A:30:LEU:HD21	1:A:384:ALA:HB2	1.46	0.96
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.47	0.96
1:A:731:ILE:HG12	1:A:746:ILE:HG21	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:659:LYS:HD2	1:A:660:ASP:H	1.33	0.93
1:A:139:VAL:HG12	1:A:327:TYR:HB3	1.50	0.93
1:A:356:TYR:HD1	1:A:361:ASN:H	1.17	0.93
1:A:713:LEU:HG	1:A:833:PRO:HD3	1.50	0.92
1:A:911:GLY:H	1:A:914:LEU:HD13	1.34	0.92
1:C:184:MET:HA	1:C:184:MET:HE3	1.52	0.91
1:B:835:LYS:HB2	1:B:839:GLU:OE2	1.70	0.91
1:A:73:ASP:H	1:A:106:GLN:HE22	1.10	0.91
1:C:1025:PHE:O	1:C:1029:VAL:HB	1.70	0.91
1:C:115:MET:CE	1:C:127:VAL:HG11	2.00	0.91
1:A:832:ALA:HB3	1:A:835:LYS:HB2	1.52	0.90
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.50	0.89
1:C:758:TYR:HE2	1:C:770:LYS:HB3	1.34	0.89
1:C:564:LEU:HD13	1:C:671:ILE:HD12	1.54	0.89
1:A:713:LEU:HB2	1:A:833:PRO:HD3	1.54	0.89
1:C:211:ASN:HD22	1:C:240:LEU:HG	1.38	0.89
1:C:758:TYR:CE2	1:C:770:LYS:HB3	2.08	0.88
1:A:302:THR:O	1:A:306:ILE:HG12	1.73	0.88
1:A:462:SER:HB2	1:A:865:GLN:HG2	1.56	0.88
1:B:222:THR:HB	1:B:223:PRO:CD	2.03	0.88
1:C:848:ALA:HA	1:C:851:LEU:HD22	1.56	0.88
1:B:456:MET:HG3	1:B:467:TYR:HB3	1.56	0.88
1:B:463:THR:HG21	1:B:869:SER:HB2	1.54	0.88
1:B:729:ILE:HG13	1:B:730:ASP:H	1.37	0.88
1:A:886:LEU:HD21	1:C:17:ILE:HG22	1.54	0.87
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.56	0.87
1:B:897:ILE:HB	1:B:1026:PHE:HE1	1.40	0.87
1:C:1:MET:HB2	1:C:2:PRO:CD	2.04	0.86
1:C:418:ARG:HH12	1:C:970:MET:HG2	1.39	0.86
1:C:758:TYR:CE2	1:C:770:LYS:HD3	2.09	0.86
1:A:447:MET:HB3	1:A:887:CYS:SG	2.16	0.86
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.55	0.86
1:A:15:ILE:O	1:A:19:ILE:HD13	1.73	0.86
1:C:281:PHE:CZ	1:C:324:VAL:HG21	2.11	0.86
1:B:150:THR:H	1:B:153:ASP:HB2	1.41	0.85
1:A:310:LEU:HD12	1:A:325:TYR:OH	1.76	0.85
1:C:848:ALA:HA	1:C:851:LEU:CD2	2.07	0.85
1:A:886:LEU:HG	1:C:14:VAL:HG23	1.57	0.85
1:A:886:LEU:HD21	1:C:17:ILE:CG2	2.06	0.84
1:A:454:VAL:HG12	1:A:455:PRO:HD3	1.57	0.84
1:B:560:PRO:HB2	1:B:836:SER:HB3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ALA:O	1:C:490:PRO:HD3	1.77	0.84
1:B:459:PHE:HZ	1:B:876:LEU:HG	1.40	0.83
1:B:416:VAL:HG11	1:B:431:THR:HG22	1.59	0.83
1:C:713:LEU:HD11	1:C:834:GLY:CA	1.98	0.83
1:B:70:ASN:H	1:B:70:ASN:HD22	1.27	0.83
1:B:84:SER:HB3	1:B:814:PRO:HA	1.59	0.83
1:A:11:PHE:CD1	1:B:890:ALA:HB1	2.13	0.83
1:B:1020:PHE:O	1:B:1021:PHE:HB2	1.76	0.83
1:C:729:ILE:HD11	1:C:786:ILE:CD1	2.09	0.82
1:C:901:VAL:O	1:C:904:VAL:HG23	1.81	0.80
1:A:852:PRO:O	1:A:855:VAL:HG22	1.81	0.80
1:C:38:ILE:HD13	1:C:38:ILE:H	1.45	0.80
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.63	0.80
1:B:743:ILE:HD13	1:B:743:ILE:H	1.44	0.80
1:B:906:PRO:HA	1:B:909:VAL:HG22	1.63	0.80
1:C:729:ILE:HD11	1:C:786:ILE:HD13	1.63	0.79
1:C:34:GLN:HB3	1:C:333:VAL:CG2	2.12	0.79
1:A:843:LEU:HA	1:A:846:GLN:HE21	1.47	0.79
1:C:696:THR:O	1:C:699:ARG:HG3	1.82	0.79
1:A:367:ILE:HG13	1:A:368:PRO:HD3	1.64	0.79
1:B:252:LYS:HB3	1:B:260:VAL:CG1	2.13	0.79
1:C:418:ARG:HH22	1:C:970:MET:CE	1.96	0.78
1:C:909:VAL:HG12	1:C:931:LEU:CD2	2.05	0.78
1:B:894:SER:HB3	1:B:897:ILE:HG12	1.65	0.78
1:A:4:PHE:O	1:A:8:ARG:NH2	2.16	0.78
1:A:713:LEU:CB	1:A:833:PRO:HD3	2.14	0.78
1:A:690:LEU:HD11	1:A:854:GLY:HA3	1.65	0.78
1:A:671:ILE:H	1:A:671:ILE:HD13	1.47	0.78
1:A:756:GLY:HA2	1:A:774:MET:HB3	1.65	0.78
1:B:104:GLN:HE21	1:B:104:GLN:C	1.87	0.78
1:A:886:LEU:O	1:C:14:VAL:HG21	1.84	0.77
1:A:601:LYS:O	1:A:601:LYS:HG3	1.83	0.77
1:A:104:GLN:HE21	1:A:131:LYS:HD3	1.50	0.77
1:A:878:ALA:O	1:A:882:ILE:HD13	1.85	0.77
1:A:987:MET:H	1:A:988:PRO:HD3	1.47	0.77
1:A:126:GLY:HA3	1:B:116:PRO:HB3	1.66	0.77
1:A:832:ALA:CB	1:A:835:LYS:HB2	2.14	0.77
1:B:94:PHE:HB3	1:B:98:THR:HG21	1.65	0.77
1:B:743:ILE:HD13	1:B:743:ILE:N	2.00	0.77
1:A:383:LEU:HD21	1:A:473:THR:HG23	1.66	0.77
1:B:139:VAL:HG12	1:B:139:VAL:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:LEU:O	1:B:595:THR:HG22	1.85	0.76
1:C:343:THR:HG21	1:C:989:LEU:HD13	1.65	0.76
1:B:171:GLY:HA3	1:B:302:THR:CG2	2.15	0.76
1:B:54:ALA:HB1	1:B:816:LEU:HD12	1.67	0.76
1:B:1020:PHE:N	1:B:1020:PHE:HD2	1.84	0.76
1:A:219:LEU:HD22	1:B:781:MET:O	1.86	0.76
1:A:987:MET:N	1:A:988:PRO:HD3	2.01	0.76
1:B:867:ARG:HG2	1:B:868:LEU:HD22	1.68	0.76
1:B:1026:PHE:HB3	1:B:1030:ARG:NH2	2.01	0.76
1:A:713:LEU:HD22	1:A:714:THR:H	1.51	0.75
1:A:466:ILE:O	1:A:469:GLN:HB2	1.86	0.75
1:A:729:ILE:HG22	1:A:730:ASP:N	2.01	0.75
1:A:775:SER:O	1:A:780:ARG:HD3	1.86	0.75
1:A:538:THR:H	1:A:540:ARG:NH2	1.84	0.75
1:A:457:ALA:O	1:A:458:PHE:HD1	1.68	0.75
1:C:444:GLY:O	1:C:448:VAL:HG23	1.87	0.75
1:A:13:TRP:O	1:A:17:ILE:HG12	1.86	0.75
1:A:367:ILE:HD11	1:A:413:VAL:HB	1.68	0.74
1:A:987:MET:O	1:A:987:MET:HG2	1.86	0.74
1:C:184:MET:HA	1:C:184:MET:CE	2.17	0.74
1:C:189:ASN:C	1:C:189:ASN:HD22	1.90	0.74
1:B:699:ARG:O	1:B:701:GLN:N	2.20	0.74
1:A:268:ILE:O	1:A:268:ILE:HG22	1.86	0.74
1:B:6:ILE:HD11	1:B:490:PRO:HB2	1.68	0.74
1:C:643:LYS:O	1:C:647:ILE:HG13	1.87	0.74
1:C:909:VAL:CG1	1:C:931:LEU:HD21	2.06	0.74
1:A:11:PHE:HD1	1:B:890:ALA:HB1	1.51	0.73
1:A:52:ALA:HB3	1:A:86:GLY:HA2	1.71	0.73
1:B:171:GLY:HA3	1:B:302:THR:CB	2.19	0.73
1:B:652:THR:O	1:B:656:SER:HB3	1.88	0.73
1:A:574:THR:HG1	1:A:598:TYR:HE1	1.37	0.73
1:B:171:GLY:HA3	1:B:302:THR:HG21	1.70	0.73
1:C:244:GLU:HA	1:C:263:ARG:HH22	1.54	0.73
1:C:252:LYS:HG2	1:C:260:VAL:CG1	2.18	0.73
1:A:52:ALA:HB1	1:A:57:VAL:HG23	1.71	0.72
1:B:280:GLU:HB2	1:B:284:GLN:O	1.88	0.72
1:B:699:ARG:HH11	1:B:699:ARG:HB3	1.54	0.72
1:C:758:TYR:HE2	1:C:770:LYS:HD3	1.54	0.72
1:B:171:GLY:HA3	1:B:302:THR:HB	1.71	0.72
1:B:1020:PHE:N	1:B:1020:PHE:CD2	2.55	0.72
1:C:554:TYR:O	1:C:556:PHE:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:950:LYS:HA	1:C:953:MET:CE	2.19	0.72
1:B:671:ILE:HG22	1:B:672:VAL:N	2.03	0.72
1:A:584:GLN:HB2	1:A:622:GLN:HG2	1.70	0.72
1:A:808:ARG:H	1:A:808:ARG:HD2	1.53	0.72
1:C:950:LYS:HA	1:C:953:MET:HE2	1.70	0.72
1:A:80:SER:OG	1:A:818:ARG:HG3	1.90	0.72
1:A:795:ASP:OD1	1:A:797:GLN:HG2	1.88	0.72
1:A:873:ALA:HB3	1:A:874:PRO:HD3	1.71	0.71
1:A:990:VAL:O	1:A:991:ILE:HG12	1.90	0.71
1:A:5:PHE:CE1	1:A:12:ALA:HB2	2.25	0.71
1:A:216:ALA:HB2	1:B:750:LEU:HD13	1.72	0.71
1:A:1029:VAL:O	1:A:1030:ARG:HB2	1.89	0.71
1:B:986:VAL:O	1:B:990:VAL:HG23	1.90	0.71
1:B:158:VAL:HA	1:B:162:MET:CG	2.20	0.71
1:B:701:GLN:HB3	1:B:851:LEU:HD13	1.73	0.71
1:A:142:VAL:O	1:A:154:ILE:HG21	1.90	0.71
1:A:671:ILE:H	1:A:671:ILE:HD12	1.53	0.71
1:A:733:GLN:OE1	1:A:743:ILE:HD11	1.91	0.71
1:B:979:SER:O	1:B:983:ILE:HG13	1.90	0.71
1:A:53:ASP:HA	1:A:84:SER:HA	1.73	0.71
1:A:73:ASP:H	1:A:106:GLN:NE2	1.87	0.71
1:C:115:MET:CE	1:C:118:LEU:HD23	2.20	0.71
1:C:524:THR:HG22	1:C:972:LEU:HD12	1.73	0.71
1:A:178:PHE:HB2	1:A:288:GLY:H	1.55	0.70
1:C:911:GLY:HA3	1:C:1013:THR:HG21	1.73	0.70
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.25	0.70
1:C:552:MET:SD	1:C:909:VAL:HG23	2.30	0.70
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.72	0.70
1:A:713:LEU:CG	1:A:833:PRO:HD3	2.20	0.70
1:C:202:ASP:OD2	1:C:792:ARG:NH2	2.25	0.70
1:C:527:TYR:OH	1:C:968:VAL:HG12	1.91	0.70
1:A:533:GLY:C	1:A:535:LEU:H	1.95	0.70
1:A:1033:PHE:O	1:A:1034:SER:HB2	1.91	0.70
1:B:5:PHE:HE2	1:B:11:PHE:HD2	1.40	0.70
1:C:695:LEU:HB3	1:C:825:MET:HE1	1.74	0.70
1:A:400:LEU:HD11	1:A:930:GLY:HA2	1.72	0.70
1:C:375:VAL:HG11	1:C:405:LEU:HD22	1.74	0.70
1:A:818:ARG:HA	1:A:824:SER:H	1.57	0.70
1:B:347:ALA:HB1	1:B:402:ILE:HG21	1.72	0.70
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.27	0.70
1:A:389:SER:O	1:A:394:THR:HG21	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:OD2	1:A:978:THR:HG21	1.91	0.69
1:B:727:PHE:HE1	1:B:786:ILE:HD11	1.57	0.69
1:C:465:ALA:O	1:C:469:GLN:HG2	1.91	0.69
1:C:538:THR:HG22	1:C:539:GLY:H	1.56	0.69
1:B:87:THR:HG21	1:B:620:ARG:NH1	2.07	0.69
1:B:332:PHE:CD1	1:B:569:GLN:HA	2.26	0.69
1:C:417:GLU:OE2	1:C:417:GLU:HA	1.90	0.69
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.73	0.69
1:B:459:PHE:O	1:B:464:GLY:HA3	1.92	0.69
1:C:332:PHE:CD2	1:C:569:GLN:HA	2.28	0.69
1:A:781:MET:HE2	1:C:225:VAL:H	1.58	0.69
1:B:898:PRO:C	1:B:900:SER:H	1.96	0.69
1:A:603:LYS:H	1:A:603:LYS:HD3	1.58	0.69
1:B:729:ILE:HG13	1:B:730:ASP:N	2.07	0.69
1:C:600:THR:O	1:C:603:LYS:HB2	1.92	0.69
1:A:69:MET:O	1:C:168:ARG:HG2	1.93	0.69
1:A:901:VAL:O	1:A:904:VAL:CG2	2.40	0.68
1:C:454:VAL:HG23	1:C:475:VAL:HG21	1.75	0.68
1:A:7:ASP:O	1:A:9:PRO:HD3	1.93	0.68
1:B:523:SER:HA	1:B:526:HIS:CD2	2.28	0.68
1:B:704:ALA:O	1:B:705:GLU:HB2	1.94	0.68
1:C:727:PHE:CE2	1:C:807:SER:HB2	2.27	0.68
1:C:190:PRO:HD2	1:C:779:TYR:HD1	1.54	0.68
1:C:418:ARG:HD2	1:C:419:VAL:HG22	1.74	0.68
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.74	0.68
1:C:445:ILE:HG13	1:C:446:ALA:H	1.57	0.68
1:C:476:SER:O	1:C:478:MET:N	2.25	0.68
1:A:818:ARG:HB3	1:A:823:PRO:HA	1.74	0.68
1:C:34:GLN:HB3	1:C:333:VAL:HG22	1.76	0.68
1:A:10:ILE:HG12	1:B:895:TRP:HB2	1.74	0.68
1:C:101:ASP:O	1:C:105:VAL:HG23	1.93	0.68
1:C:265:VAL:O	1:C:266:ALA:HB2	1.93	0.68
1:B:190:PRO:HD3	1:B:779:TYR:CE2	2.28	0.68
1:A:387:GLY:O	1:A:388:PHE:O	2.12	0.68
1:B:648:THR:HG23	1:B:665:ALA:HB3	1.76	0.68
1:C:554:TYR:HB3	1:C:558:ARG:HH21	1.57	0.68
1:B:213:GLN:HB2	1:B:239:ARG:HD2	1.76	0.67
1:C:1:MET:HB2	1:C:2:PRO:HD2	1.75	0.67
1:C:552:MET:SD	1:C:909:VAL:CG2	2.82	0.67
1:A:83:ASP:HB3	1:A:815:ARG:HG3	1.75	0.67
1:B:591:LEU:HD12	1:B:611:ALA:HB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:LYS:HB3	1:B:260:VAL:HG12	1.76	0.67
1:B:851:LEU:N	1:B:852:PRO:HD3	2.09	0.67
1:A:104:GLN:NE2	1:A:131:LYS:HD3	2.10	0.67
1:B:20:MET:HG2	1:B:377:LEU:HD12	1.77	0.67
1:B:229:GLN:HA	1:C:583:THR:HG21	1.77	0.67
1:B:696:THR:HG22	1:B:699:ARG:HH12	1.60	0.67
1:C:190:PRO:CD	1:C:779:TYR:CD1	2.77	0.67
1:A:276:ASP:HB3	1:C:222:THR:HG23	1.76	0.67
1:A:188:MET:HA	1:A:266:ALA:HB2	1.76	0.66
1:A:560:PRO:HB2	1:A:922:THR:HG22	1.77	0.66
1:A:643:LYS:O	1:A:647:ILE:HG12	1.95	0.66
1:B:897:ILE:HB	1:B:1026:PHE:CE1	2.27	0.66
1:B:699:ARG:HG2	1:B:700:ASN:H	1.58	0.66
1:A:746:ILE:HD12	1:A:804:PHE:CE1	2.30	0.66
1:B:324:VAL:HG23	1:B:326:PRO:HD3	1.77	0.66
1:B:898:PRO:HA	1:B:901:VAL:HG23	1.77	0.66
1:B:1028:VAL:O	1:B:1032:ARG:HB2	1.96	0.66
1:A:340:VAL:HG13	1:A:399:VAL:CG2	2.25	0.66
1:B:692:HIS:HE1	1:B:723:ASP:OD1	1.78	0.66
1:A:842:GLU:O	1:A:846:GLN:HG3	1.95	0.66
1:C:189:ASN:ND2	1:C:191:ASN:H	1.93	0.66
1:A:298:ASN:HD22	1:A:301:ASP:H	1.43	0.66
1:B:727:PHE:CE1	1:B:786:ILE:HD11	2.31	0.66
1:A:403:GLY:HA3	1:A:982:PHE:CZ	2.32	0.65
1:A:525:HIS:HA	1:A:528:THR:HG22	1.76	0.65
1:C:712:MET:O	1:C:713:LEU:HD22	1.96	0.65
1:A:685:ILE:HG22	1:A:686:ASP:H	1.62	0.65
1:C:115:MET:HE1	1:C:118:LEU:HD23	1.76	0.65
1:B:714:THR:CG2	1:B:830:GLN:HG3	2.26	0.65
1:C:445:ILE:HG13	1:C:446:ALA:N	2.11	0.65
1:C:945:ILE:HG13	1:C:946:VAL:H	1.62	0.65
1:B:404:LEU:HD13	1:B:449:LEU:HD21	1.78	0.65
1:C:489:THR:O	1:C:493:CYS:HB2	1.96	0.65
1:C:174:ASP:HB3	1:C:292:LYS:HB2	1.78	0.65
1:C:491:ALA:C	1:C:493:CYS:H	2.00	0.65
1:A:178:PHE:HB2	1:A:288:GLY:N	2.11	0.65
1:B:255:GLN:HG3	1:B:256:ASP:H	1.61	0.65
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.32	0.65
1:C:252:LYS:HG2	1:C:260:VAL:HG12	1.79	0.65
1:C:34:GLN:HB3	1:C:333:VAL:HG21	1.79	0.64
1:A:601:LYS:O	1:A:602:GLU:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1018:ALA:O	1:C:1022:VAL:HG12	1.96	0.64
1:A:391:ASN:O	1:A:392:THR:C	2.36	0.64
1:B:1022:VAL:HG23	1:B:1023:PRO:HD3	1.79	0.64
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.28	0.64
1:A:441:ALA:O	1:A:445:ILE:HG23	1.97	0.64
1:B:1027:VAL:O	1:B:1031:ARG:HB3	1.97	0.64
1:A:911:GLY:HA2	1:A:914:LEU:HB2	1.79	0.64
1:B:425:LEU:HB3	1:B:498:LYS:C	2.18	0.64
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.78	0.64
1:A:729:ILE:CG2	1:A:730:ASP:N	2.60	0.64
1:C:445:ILE:HD13	1:C:940:LYS:HE3	1.79	0.64
1:B:459:PHE:CZ	1:B:876:LEU:HG	2.28	0.64
1:C:815:ARG:HG2	1:C:815:ARG:HH11	1.62	0.64
1:A:677:ALA:C	1:A:679:GLY:H	2.01	0.64
1:B:242:SER:HB2	1:B:245:GLU:HG3	1.80	0.64
1:C:213:GLN:NE2	1:C:238:THR:HA	2.13	0.64
1:C:729:ILE:CD1	1:C:786:ILE:HD13	2.27	0.64
1:A:14:VAL:O	1:A:17:ILE:N	2.31	0.64
1:B:36:PRO:O	1:B:38:ILE:HG12	1.98	0.64
1:C:158:VAL:CG1	1:C:177:LEU:HD21	2.28	0.64
1:C:418:ARG:NH2	1:C:970:MET:CE	2.60	0.64
1:A:117:LEU:HD11	1:C:124:GLN:O	1.97	0.63
1:A:836:SER:OG	1:A:839:GLU:HG2	1.98	0.63
1:B:792:ARG:HG2	1:B:793:ALA:H	1.63	0.63
1:A:328:ASP:OD1	1:A:330:THR:HB	1.98	0.63
1:C:102:ILE:HA	1:C:105:VAL:HG23	1.79	0.63
1:A:9:PRO:HD2	1:B:893:GLU:OE2	1.98	0.63
1:B:298:ASN:HB2	1:B:301:ASP:HB2	1.79	0.63
1:C:832:ALA:HB1	1:C:833:PRO:CD	2.29	0.63
1:A:886:LEU:HG	1:C:14:VAL:CG2	2.26	0.63
1:A:166:ILE:HD11	1:A:310:LEU:HD21	1.78	0.63
1:A:351:VAL:HG12	1:A:351:VAL:O	1.98	0.63
1:A:367:ILE:HG22	1:A:496:MET:CE	2.29	0.63
1:C:53:ASP:OD1	1:C:56:THR:HB	1.99	0.63
1:B:72:ILE:N	1:B:72:ILE:HD13	2.14	0.63
1:B:706:ALA:HB1	1:B:716:VAL:HG21	1.80	0.63
1:B:2:PRO:HB3	1:B:486:LEU:O	1.99	0.62
1:A:351:VAL:HG21	1:A:406:VAL:HG21	1.81	0.62
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	1.81	0.62
1:A:968:VAL:HG21	1:A:1023:PRO:HB3	1.80	0.62
1:A:354:VAL:HG11	1:A:980:LEU:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:O	1:A:714:THR:HG23	1.99	0.62
1:B:281:PHE:HE1	1:B:608:SER:HB2	1.62	0.62
1:B:444:GLY:HA2	1:B:891:LEU:HD11	1.81	0.62
1:B:667:ASN:O	1:B:678:THR:HB	1.99	0.62
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.34	0.62
1:A:702:LEU:HB2	1:A:851:LEU:HD11	1.81	0.62
1:B:228:GLN:NE2	1:C:781:MET:HB3	2.14	0.62
1:B:966:ASP:O	1:B:970:MET:HG3	1.98	0.62
1:A:894:SER:OG	1:A:897:ILE:HB	1.99	0.62
1:B:94:PHE:CB	1:B:98:THR:HG21	2.30	0.62
1:B:274:ASN:HD22	1:B:276:ASP:HB2	1.64	0.62
1:B:671:ILE:CG2	1:B:672:VAL:H	2.12	0.62
1:A:139:VAL:CG1	1:A:327:TYR:HB3	2.27	0.62
1:C:15:ILE:O	1:C:19:ILE:HG12	1.99	0.62
1:C:222:THR:HG22	1:C:223:PRO:HD3	1.81	0.62
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.81	0.62
1:A:773:VAL:CG1	1:A:773:VAL:O	2.47	0.62
1:B:198:LEU:HD23	1:B:792:ARG:NH2	2.15	0.62
1:C:361:ASN:HB2	1:C:364:ALA:HB3	1.82	0.62
1:C:836:SER:HB3	1:C:839:GLU:HG2	1.82	0.62
1:A:60:THR:CG2	1:A:119:PRO:HG3	2.30	0.62
1:B:158:VAL:HA	1:B:162:MET:HG3	1.81	0.62
1:B:255:GLN:HG3	1:B:256:ASP:N	2.14	0.62
1:B:255:GLN:CG	1:B:256:ASP:H	2.12	0.62
1:B:14:VAL:HG11	1:C:890:ALA:HB2	1.82	0.61
1:C:23:GLY:HA3	1:C:377:LEU:O	1.99	0.61
1:A:228:GLN:HG3	1:A:229:GLN:N	2.15	0.61
1:B:671:ILE:HG22	1:B:672:VAL:H	1.65	0.61
1:C:343:THR:O	1:C:343:THR:HG22	1.99	0.61
1:C:990:VAL:HG13	1:C:1005:THR:HG22	1.82	0.61
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.18	0.61
1:C:418:ARG:HH22	1:C:970:MET:HE2	1.63	0.61
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.35	0.61
1:B:671:ILE:CG2	1:B:672:VAL:N	2.63	0.61
1:C:945:ILE:HG13	1:C:946:VAL:N	2.16	0.61
1:A:367:ILE:HG22	1:A:496:MET:HE1	1.83	0.61
1:A:993:THR:HG21	1:A:1000:GLN:OE1	2.00	0.61
1:A:246:PHE:O	1:A:249:ILE:HG12	2.01	0.61
1:A:883:VAL:O	1:A:887:CYS:HB2	2.00	0.61
1:A:339:GLU:O	1:A:341:VAL:N	2.33	0.61
1:A:375:VAL:HG21	1:A:481:SER:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:ILE:H	1:B:743:ILE:CD1	2.09	0.61
1:A:354:VAL:O	1:A:354:VAL:HG12	2.00	0.61
1:C:974:PRO:HA	1:C:977:MET:CE	2.28	0.61
1:A:73:ASP:N	1:A:106:GLN:HE22	1.92	0.61
1:A:108:GLN:CD	1:B:112:GLN:HG3	2.21	0.61
1:A:403:GLY:HA3	1:A:982:PHE:CE1	2.36	0.61
1:C:228:GLN:HG3	1:C:229:GLN:O	2.01	0.61
1:C:1:MET:HB2	1:C:2:PRO:HD3	1.82	0.61
1:A:485:ALA:HA	1:A:489:THR:OG1	2.02	0.60
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.31	0.60
1:C:38:ILE:CD1	1:C:38:ILE:N	2.64	0.60
1:A:344:LEU:HD23	1:A:402:ILE:HD12	1.82	0.60
1:B:68:ASN:HD22	1:B:114:ALA:HB2	1.66	0.60
1:A:660:ASP:O	1:A:661:ALA:HB2	2.00	0.60
1:A:597:TYR:O	1:A:601:LYS:HB3	2.02	0.60
1:B:204:ILE:CG2	1:B:208:LYS:HE2	2.30	0.60
1:B:274:ASN:ND2	1:B:276:ASP:HB2	2.16	0.60
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.84	0.60
1:B:539:GLY:C	1:B:541:TYR:H	2.05	0.60
1:B:983:ILE:HD13	1:B:1012:VAL:HG12	1.83	0.60
1:C:38:ILE:HD13	1:C:38:ILE:N	2.15	0.60
1:A:293:LEU:O	1:A:294:ALA:CB	2.49	0.60
1:A:597:TYR:CD1	1:A:597:TYR:C	2.74	0.60
1:A:661:ALA:O	1:A:663:VAL:HG23	2.02	0.60
1:C:379:THR:HB	1:C:398:MET:CE	2.31	0.60
1:C:836:SER:HB3	1:C:839:GLU:CG	2.31	0.60
1:A:993:THR:HB	1:A:997:SER:CB	2.32	0.60
1:B:665:ALA:O	1:B:666:PHE:HB2	2.01	0.60
1:C:162:MET:HA	1:C:313:MET:CE	2.32	0.60
1:B:282:ASN:O	1:B:284:GLN:N	2.34	0.60
1:C:973:ARG:N	1:C:974:PRO:HD2	2.17	0.60
1:A:578:LEU:HB3	1:A:579:PRO:HD2	1.82	0.60
1:B:146:ASP:O	1:B:148:THR:N	2.32	0.60
1:C:310:LEU:HD13	1:C:323:ILE:HD13	1.83	0.60
1:C:767:ARG:HD3	1:C:769:LYS:HE3	1.81	0.60
1:B:10:ILE:HG13	1:C:893:GLU:O	2.02	0.59
1:B:30:LEU:HD13	1:B:390:ILE:HD11	1.83	0.59
1:C:40:PRO:HB2	1:C:94:PHE:O	2.02	0.59
1:C:762:PHE:CE1	1:C:769:LYS:HB2	2.37	0.59
1:B:476:SER:O	1:B:480:LEU:HB2	2.03	0.59
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:945:ILE:HD11	1:C:1022:VAL:HG22	1.84	0.59
1:B:151:GLN:O	1:B:155:SER:HB2	2.02	0.59
1:A:919:ARG:HG3	1:A:920:GLY:N	2.16	0.59
1:B:193:LEU:HD22	1:B:198:LEU:HB2	1.83	0.59
1:C:795:ASP:OD2	1:C:797:GLN:HB3	2.02	0.59
1:C:948:PHE:HE1	1:C:971:ARG:HE	1.48	0.59
1:A:685:ILE:HG22	1:A:686:ASP:N	2.18	0.59
1:B:276:ASP:O	1:B:614:GLY:HA3	2.02	0.59
1:B:552:MET:SD	1:B:909:VAL:HG23	2.43	0.59
1:C:220:GLY:HA3	1:C:231:ASN:HD22	1.68	0.59
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.83	0.59
1:C:958:LYS:HG2	1:C:962:GLU:HB3	1.85	0.59
1:A:254:ASN:ND2	1:A:258:SER:OG	2.36	0.59
1:C:1:MET:CB	1:C:2:PRO:CD	2.80	0.59
1:C:418:ARG:NH2	1:C:970:MET:HE3	2.17	0.59
1:C:466:ILE:HG13	1:C:563:PHE:HZ	1.65	0.59
1:A:612:VAL:HG22	1:A:626:ILE:HG22	1.83	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59
1:C:1017:LEU:O	1:C:1021:PHE:HB2	2.03	0.59
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.84	0.59
1:A:293:LEU:O	1:A:294:ALA:HB2	2.03	0.59
1:A:649:MET:O	1:A:653:ARG:HD3	2.02	0.59
1:A:680:PHE:CE1	1:A:829:GLY:HA3	2.38	0.59
1:B:418:ARG:HB3	1:B:418:ARG:HH11	1.66	0.59
1:B:876:LEU:CD2	1:B:932:LEU:HD11	2.32	0.59
1:C:759:VAL:HB	1:C:760:ASN:ND2	2.17	0.59
1:A:169:THR:HG22	1:A:309:GLU:HG3	1.85	0.59
1:A:671:ILE:HD13	1:A:671:ILE:N	2.15	0.59
1:B:375:VAL:HG13	1:B:480:LEU:HB3	1.85	0.59
1:B:876:LEU:HD22	1:B:932:LEU:HD11	1.85	0.59
1:B:910:ILE:HG23	1:B:911:GLY:H	1.67	0.59
1:C:38:ILE:H	1:C:38:ILE:CD1	2.16	0.59
1:C:44:THR:CG2	1:C:91:THR:HB	2.22	0.59
1:A:448:VAL:HG22	1:A:884:VAL:HG13	1.85	0.58
1:B:104:GLN:C	1:B:104:GLN:NE2	2.56	0.58
1:B:169:THR:O	1:B:172:VAL:HG23	2.02	0.58
1:A:239:ARG:HD3	1:A:762:PHE:HA	1.85	0.58
1:A:919:ARG:HG3	1:A:920:GLY:H	1.69	0.58
1:A:987:MET:N	1:A:988:PRO:CD	2.66	0.58
1:B:240:LEU:O	1:B:762:PHE:HB2	2.03	0.58
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.85	0.58
1:A:671:ILE:HG12	1:A:674:LEU:HB3	1.85	0.58
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.34	0.58
1:B:449:LEU:HB3	1:B:478:MET:HG3	1.85	0.58
1:C:474:ILE:O	1:C:478:MET:HB2	2.03	0.58
1:C:997:SER:O	1:C:999:ALA:N	2.36	0.58
1:B:782:LEU:N	1:B:785:ASP:OD1	2.36	0.58
1:B:70:ASN:HD22	1:B:70:ASN:N	1.99	0.58
1:A:216:ALA:CB	1:B:750:LEU:HD13	2.33	0.58
1:B:183:ALA:N	1:B:271:GLY:O	2.36	0.58
1:B:213:GLN:CG	1:C:56:THR:OG1	2.51	0.58
1:B:525:HIS:HA	1:B:528:THR:HG22	1.86	0.58
1:C:1022:VAL:HA	1:C:1025:PHE:CD2	2.39	0.58
1:A:401:ALA:HB2	1:A:474:ILE:HG13	1.85	0.58
1:B:70:ASN:H	1:B:70:ASN:ND2	2.01	0.58
1:C:412:VAL:HG12	1:C:412:VAL:O	2.04	0.58
1:C:16:ALA:O	1:C:20:MET:HG3	2.04	0.58
1:C:355:MET:HB3	1:C:365:THR:HG23	1.86	0.58
1:A:688:ALA:O	1:A:690:LEU:N	2.37	0.58
1:A:713:LEU:HB3	1:A:832:ALA:CB	2.34	0.58
1:B:537:SER:HB2	1:B:540:ARG:HE	1.68	0.58
1:B:593:GLU:OE2	1:B:658:ILE:HD13	2.04	0.58
1:B:911:GLY:HA3	1:B:1013:THR:HB	1.86	0.58
1:B:1012:VAL:HG23	1:B:1013:THR:N	2.18	0.58
1:C:158:VAL:HG11	1:C:177:LEU:HD21	1.86	0.58
1:C:577:GLN:HA	1:C:577:GLN:HE21	1.68	0.58
1:A:154:ILE:O	1:A:158:VAL:HG23	2.04	0.57
1:B:201:VAL:HG21	1:B:745:ASP:OD1	2.03	0.57
1:B:948:PHE:HB2	1:B:971:ARG:NH2	2.19	0.57
1:C:84:SER:HB2	1:C:814:PRO:HA	1.86	0.57
1:A:671:ILE:HG12	1:A:674:LEU:HD12	1.85	0.57
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.85	0.57
1:A:742:SER:OG	1:A:745:ASP:HB2	2.05	0.57
1:A:746:ILE:HG22	1:A:747:ASN:N	2.19	0.57
1:C:945:ILE:HG22	1:C:971:ARG:HB2	1.86	0.57
1:A:340:VAL:HG13	1:A:399:VAL:HG23	1.85	0.57
1:A:731:ILE:CG1	1:A:746:ILE:HG21	2.30	0.57
1:A:773:VAL:O	1:A:773:VAL:HG12	2.04	0.57
1:B:605:ASN:HD21	1:B:642:ASN:ND2	2.01	0.57
1:C:531:VAL:O	1:C:534:ILE:HG12	2.04	0.57
1:C:746:ILE:HD12	1:C:804:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:972:LEU:H	1:C:974:PRO:HD2	1.69	0.57
1:C:327:TYR:HB2	1:C:628:PHE:HB3	1.85	0.57
1:A:979:SER:OG	1:A:1015:THR:HG21	2.05	0.57
1:B:742:SER:OG	1:B:745:ASP:HB2	2.05	0.57
1:A:108:GLN:HG2	1:A:129:VAL:HB	1.86	0.57
1:B:49:TYR:CE1	1:B:60:THR:HG21	2.40	0.57
1:B:633:ASP:OD1	1:B:634:TRP:N	2.36	0.57
1:C:580:ALA:HA	1:C:623:ASN:ND2	2.20	0.57
1:C:935:ILE:HG22	1:C:935:ILE:O	2.05	0.57
1:A:365:THR:O	1:A:368:PRO:HD2	2.05	0.56
1:A:712:MET:SD	1:A:835:LYS:HG2	2.45	0.56
1:A:713:LEU:CG	1:A:832:ALA:HA	2.34	0.56
1:B:204:ILE:HG22	1:B:208:LYS:HE2	1.86	0.56
1:B:356:TYR:O	1:B:360:GLN:N	2.37	0.56
1:C:331:PRO:O	1:C:335:ILE:HG12	2.05	0.56
1:A:395:MET:HA	1:A:395:MET:CE	2.35	0.56
1:B:187:TRP:O	1:B:266:ALA:HB1	2.04	0.56
1:B:911:GLY:HA3	1:B:1013:THR:CB	2.35	0.56
1:C:35:TYR:CD1	1:C:671:ILE:HG12	2.40	0.56
1:C:568:ASP:HB2	1:C:643:LYS:HG3	1.88	0.56
1:A:324:VAL:HG12	1:A:325:TYR:H	1.71	0.56
1:A:563:PHE:O	1:A:564:LEU:HD12	2.05	0.56
1:A:780:ARG:HH22	1:C:223:PRO:HD2	1.69	0.56
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.88	0.56
1:A:30:LEU:HD21	1:A:384:ALA:CB	2.27	0.56
1:A:180:SER:O	1:A:181:GLN:HB2	2.05	0.56
1:B:192:GLU:O	1:B:196:PHE:HD2	1.89	0.56
1:B:225:VAL:HG23	1:C:781:MET:SD	2.46	0.56
1:A:756:GLY:HA2	1:A:774:MET:CB	2.36	0.56
1:A:780:ARG:NH2	1:C:223:PRO:HD2	2.19	0.56
1:A:813:SER:HB3	1:A:816:LEU:HD21	1.88	0.56
1:A:1015:THR:O	1:A:1017:LEU:N	2.34	0.56
1:B:238:THR:HG23	1:B:239:ARG:N	2.20	0.56
1:B:898:PRO:C	1:B:900:SER:N	2.59	0.56
1:A:298:ASN:O	1:A:302:THR:HG23	2.05	0.56
1:C:911:GLY:HA3	1:C:1013:THR:CG2	2.36	0.56
1:A:449:LEU:O	1:A:453:PHE:HD1	1.89	0.56
1:A:740:GLY:HA3	1:A:794:ALA:H	1.71	0.56
1:B:159:ALA:HB1	1:B:181:GLN:HG3	1.87	0.56
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.41	0.56
1:C:686:ASP:OD1	1:C:686:ASP:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.88	0.56
1:A:740:GLY:HA3	1:A:794:ALA:CB	2.36	0.56
1:B:188:MET:HA	1:B:266:ALA:HB2	1.88	0.56
1:B:947:GLU:O	1:B:951:ASP:HB2	2.06	0.56
1:C:247:GLY:HA3	1:C:263:ARG:CZ	2.36	0.56
1:C:909:VAL:CG1	1:C:935:ILE:HD11	2.36	0.56
1:A:534:ILE:O	1:A:534:ILE:HG13	2.06	0.56
1:A:706:ALA:HB3	1:A:716:VAL:HG21	1.88	0.56
1:B:314:GLU:N	1:B:315:PRO:CD	2.69	0.56
1:B:979:SER:HA	1:B:1011:MET:HE3	1.88	0.56
1:B:1020:PHE:O	1:B:1021:PHE:CB	2.48	0.56
1:C:418:ARG:HH22	1:C:970:MET:HE3	1.71	0.56
1:A:1022:VAL:N	1:A:1023:PRO:HD2	2.20	0.55
1:B:57:VAL:HG23	1:B:82:SER:HB2	1.87	0.55
1:C:220:GLY:HA3	1:C:231:ASN:ND2	2.21	0.55
1:C:962:GLU:HA	1:C:965:LEU:HD13	1.87	0.55
1:A:729:ILE:CG2	1:A:730:ASP:H	2.20	0.55
1:B:237:GLN:HG2	1:B:238:THR:N	2.21	0.55
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.86	0.55
1:C:5:PHE:HE2	1:C:11:PHE:HD2	1.54	0.55
1:A:353:LEU:C	1:A:355:MET:H	2.09	0.55
1:C:183:ALA:HB1	1:C:770:LYS:O	2.07	0.55
1:A:986:VAL:O	1:A:986:VAL:HG13	2.06	0.55
1:B:4:PHE:O	1:B:5:PHE:HB2	2.07	0.55
1:B:682:PHE:CE1	1:B:857:TYR:CD1	2.95	0.55
1:A:108:GLN:NE2	1:B:112:GLN:HG3	2.21	0.55
1:A:150:THR:N	1:A:153:ASP:OD2	2.35	0.55
1:A:167:SER:OG	1:A:175:VAL:CG2	2.55	0.55
1:A:184:MET:HG3	1:A:186:ILE:HD11	1.88	0.55
1:B:119:PRO:C	1:B:121:GLU:H	2.09	0.55
1:C:190:PRO:CD	1:C:779:TYR:HD1	2.17	0.55
1:B:900:SER:OG	1:B:1029:VAL:HG11	2.07	0.55
1:A:583:THR:CG2	1:A:584:GLN:N	2.70	0.55
1:B:24:GLY:HA2	1:B:27:ILE:HG23	1.89	0.55
1:A:588:GLN:HG2	1:A:613:ASN:OD1	2.07	0.55
1:A:606:VAL:HA	1:A:631:LEU:HD23	1.89	0.55
1:A:713:LEU:HG	1:A:833:PRO:CD	2.29	0.55
1:B:730:ASP:HB3	1:B:806:SER:HB3	1.89	0.55
1:C:601:LYS:C	1:C:603:LYS:H	2.10	0.55
1:A:52:ALA:CB	1:A:57:VAL:HG23	2.36	0.55
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:PHE:CE2	1:B:11:PHE:HD2	2.23	0.55
1:B:375:VAL:HB	1:B:405:LEU:HD22	1.89	0.55
1:C:577:GLN:HB2	3:C:2002:RFP:H402	1.89	0.55
1:A:207:ILE:HB	1:A:759:VAL:HG11	1.89	0.54
1:A:733:GLN:OE1	1:A:743:ILE:CD1	2.56	0.54
1:B:452:VAL:O	1:B:453:PHE:HB2	2.07	0.54
1:A:782:LEU:O	1:A:785:ASP:HB2	2.07	0.54
1:B:123:GLN:O	1:B:125:GLN:N	2.40	0.54
1:B:139:VAL:O	1:B:139:VAL:CG1	2.54	0.54
1:A:102:ILE:O	1:A:106:GLN:HG3	2.08	0.54
1:A:531:VAL:HG12	1:A:535:LEU:HD11	1.89	0.54
1:B:686:ASP:HB2	1:B:695:LEU:HD23	1.89	0.54
1:B:239:ARG:NH2	1:B:761:ASP:HB2	2.21	0.54
1:B:1033:PHE:O	1:B:1034:SER:HB2	2.07	0.54
1:C:401:ALA:O	1:C:405:LEU:HG	2.08	0.54
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.42	0.54
1:A:880:SER:O	1:A:884:VAL:HG23	2.08	0.54
1:B:343:THR:HG21	1:B:1000:GLN:OE1	2.08	0.54
1:B:541:TYR:C	1:B:543:VAL:H	2.11	0.54
1:B:978:THR:HG22	1:B:979:SER:N	2.22	0.54
1:C:729:ILE:HD11	1:C:786:ILE:HD11	1.88	0.54
1:A:991:ILE:O	1:A:992:SER:CB	2.56	0.54
1:B:411:VAL:O	1:B:415:ASN:HB2	2.06	0.54
1:B:551:GLY:HA2	1:B:554:TYR:HB3	1.90	0.54
1:B:888:LEU:C	1:B:890:ALA:H	2.11	0.54
1:B:898:PRO:O	1:B:900:SER:N	2.40	0.54
1:C:265:VAL:O	1:C:265:VAL:HG23	2.06	0.54
1:C:365:THR:O	1:C:368:PRO:HD2	2.07	0.54
1:C:974:PRO:O	1:C:977:MET:HB2	2.08	0.54
1:A:315:PRO:O	1:A:316:PHE:HB2	2.08	0.54
1:A:750:LEU:O	1:A:754:TRP:HD1	1.90	0.54
1:B:99:ASP:C	1:B:99:ASP:OD2	2.46	0.54
1:B:255:GLN:CG	1:B:256:ASP:N	2.70	0.54
1:B:948:PHE:HB2	1:B:971:ARG:CZ	2.37	0.54
1:B:552:MET:C	1:B:554:TYR:H	2.11	0.54
1:C:144:ASN:HD21	1:C:148:THR:H	1.54	0.54
1:C:662:MET:HG3	1:C:664:PHE:CE1	2.43	0.54
1:B:84:SER:HB3	1:B:814:PRO:CA	2.33	0.54
1:B:258:SER:C	1:B:259:ARG:HG2	2.28	0.54
1:C:325:TYR:N	1:C:325:TYR:CD1	2.76	0.54
1:B:792:ARG:HG2	1:B:793:ALA:N	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:952:LEU:HG	1:B:956:GLU:OE2	2.08	0.53
1:C:210:GLN:HE22	1:C:249:ILE:HA	1.73	0.53
1:C:265:VAL:O	1:C:266:ALA:CB	2.55	0.53
1:C:552:MET:O	1:C:554:TYR:N	2.41	0.53
1:A:360:GLN:HE22	1:A:517:ASN:HD21	1.56	0.53
1:B:335:ILE:HG13	1:B:634:TRP:CD1	2.43	0.53
1:B:518:ARG:HA	1:B:521:GLU:CD	2.28	0.53
1:C:211:ASN:ND2	1:C:240:LEU:HG	2.16	0.53
1:C:815:ARG:HG2	1:C:815:ARG:NH1	2.23	0.53
1:A:214:VAL:HG23	1:A:237:GLN:HB3	1.89	0.53
1:A:1029:VAL:HG12	1:A:1030:ARG:H	1.72	0.53
1:C:906:PRO:HA	1:C:909:VAL:HG22	1.91	0.53
1:A:38:ILE:HG12	1:A:674:LEU:HD23	1.89	0.53
1:A:617:PHE:O	1:A:619:GLY:N	2.42	0.53
1:B:351:VAL:HG12	1:B:351:VAL:O	2.08	0.53
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.91	0.53
1:B:598:TYR:HB3	1:B:606:VAL:HG11	1.90	0.53
1:C:153:ASP:OD2	1:C:182:TYR:OH	2.27	0.53
1:C:702:LEU:HB2	1:C:851:LEU:HD21	1.90	0.53
1:B:360:GLN:O	1:B:361:ASN:HB3	2.09	0.53
1:C:379:THR:HB	1:C:398:MET:HE1	1.90	0.53
1:A:456:MET:O	1:A:458:PHE:N	2.42	0.53
1:A:688:ALA:C	1:A:690:LEU:H	2.12	0.53
1:B:188:MET:CE	1:B:203:VAL:HG21	2.37	0.53
1:C:146:ASP:HB3	1:C:148:THR:HG23	1.90	0.53
1:B:419:VAL:HG12	1:B:419:VAL:O	2.09	0.53
1:C:692:HIS:CE1	1:C:721:LEU:HD21	2.43	0.53
1:C:907:LEU:HG	1:C:1017:LEU:HB3	1.91	0.53
1:B:282:ASN:C	1:B:284:GLN:H	2.12	0.53
1:B:699:ARG:HG2	1:B:700:ASN:N	2.24	0.53
1:B:878:ALA:O	1:B:882:ILE:HG12	2.09	0.53
1:C:139:VAL:HG12	1:C:326:PRO:HG2	1.90	0.53
1:C:176:GLN:HE22	1:C:620:ARG:NH1	2.07	0.53
1:A:8:ARG:HB3	1:B:893:GLU:OE1	2.08	0.53
1:A:600:THR:O	1:A:601:LYS:CB	2.57	0.53
1:B:420:MET:SD	1:B:424:GLY:HA2	2.49	0.53
1:A:818:ARG:HA	1:A:824:SER:N	2.23	0.52
1:B:238:THR:CG2	1:B:239:ARG:N	2.71	0.52
1:B:967:ALA:C	1:B:969:ARG:N	2.61	0.52
1:C:418:ARG:NH2	1:C:970:MET:HE2	2.23	0.52
1:C:552:MET:SD	1:C:909:VAL:HG21	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:O	1:A:904:VAL:N	2.41	0.52
1:B:63:GLN:O	1:B:66:GLU:N	2.42	0.52
1:B:154:ILE:HG23	1:B:321:LEU:HD11	1.92	0.52
1:B:351:VAL:HA	1:B:354:VAL:HG22	1.91	0.52
1:C:314:GLU:HB2	1:C:315:PRO:HD3	1.91	0.52
1:C:847:LEU:HA	1:C:850:LYS:HG2	1.90	0.52
1:A:442:LEU:HA	1:A:445:ILE:HG13	1.92	0.52
1:B:20:MET:HG3	1:B:374:VAL:HA	1.90	0.52
1:C:66:GLU:O	1:C:69:MET:N	2.38	0.52
1:C:714:THR:HG23	1:C:830:GLN:O	2.08	0.52
1:B:185:ARG:HB2	1:B:269:GLU:O	2.10	0.52
1:B:967:ALA:C	1:B:969:ARG:H	2.12	0.52
1:C:2:PRO:O	1:C:6:ILE:N	2.42	0.52
1:C:329:THR:C	1:C:331:PRO:HD2	2.30	0.52
1:A:451:ALA:O	1:A:453:PHE:N	2.42	0.52
1:B:788:ASP:N	1:B:788:ASP:OD1	2.43	0.52
1:C:351:VAL:HG13	1:C:369:THR:HG22	1.91	0.52
1:C:963:ALA:C	1:C:965:LEU:H	2.11	0.52
1:A:909:VAL:CG1	1:A:913:LEU:HD22	2.40	0.52
1:C:110:LYS:O	1:C:111:LEU:C	2.47	0.52
1:C:280:GLU:HA	1:C:286:ALA:HB3	1.92	0.52
1:C:953:MET:SD	1:C:963:ALA:HB2	2.50	0.52
1:A:255:GLN:O	1:A:256:ASP:HB2	2.09	0.52
1:B:251:LEU:HB2	1:B:261:LEU:HA	1.92	0.52
1:B:565:PRO:HD3	1:B:924:ASP:OD1	2.09	0.52
1:A:459:PHE:O	1:A:460:GLY:O	2.27	0.52
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.92	0.52
1:C:680:PHE:HE1	1:C:844:MET:HE3	1.74	0.52
1:C:1028:VAL:HA	1:C:1031:ARG:HB3	1.90	0.52
1:A:682:PHE:HE2	1:A:684:LEU:HD12	1.74	0.52
1:A:1011:MET:HA	1:A:1011:MET:CE	2.40	0.52
1:B:405:LEU:HD12	1:B:406:VAL:HG13	1.92	0.52
1:B:412:VAL:HG21	1:B:485:ALA:HB1	1.91	0.52
1:A:210:GLN:CG	1:A:249:ILE:HG23	2.27	0.51
1:A:993:THR:HB	1:A:997:SER:HB2	1.92	0.51
1:B:251:LEU:HD22	1:B:262:LEU:H	1.75	0.51
1:B:785:ASP:O	1:B:786:ILE:C	2.49	0.51
1:B:894:SER:CB	1:B:897:ILE:HG12	2.38	0.51
1:B:919:ARG:HD3	1:B:921:LEU:HD13	1.91	0.51
1:B:1021:PHE:O	1:B:1024:VAL:HB	2.11	0.51
1:C:448:VAL:O	1:C:452:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:897:ILE:O	1:B:900:SER:OG	2.18	0.51
1:B:213:GLN:HG2	1:C:56:THR:OG1	2.10	0.51
1:B:692:HIS:CE1	1:B:723:ASP:OD1	2.60	0.51
1:C:3:ASN:OD1	1:C:432:ARG:HG3	2.10	0.51
1:C:342:LYS:C	1:C:344:LEU:H	2.13	0.51
1:C:580:ALA:HA	1:C:623:ASN:HD22	1.74	0.51
1:C:727:PHE:CE2	1:C:807:SER:CB	2.93	0.51
1:A:169:THR:CG2	1:A:309:GLU:HG3	2.40	0.51
1:A:902:MET:O	1:A:905:VAL:HG23	2.11	0.51
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.92	0.51
1:B:568:ASP:OD2	1:B:634:TRP:HH2	1.93	0.51
1:C:131:LYS:HB2	1:C:295:THR:HG21	1.93	0.51
1:A:281:PHE:O	1:A:282:ASN:C	2.47	0.51
1:A:703:LEU:HD11	1:A:718:PRO:HD3	1.93	0.51
1:B:530:SER:O	1:B:534:ILE:HG12	2.10	0.51
1:C:3:ASN:C	1:C:5:PHE:H	2.14	0.51
1:C:472:ILE:HG22	1:C:473:THR:N	2.25	0.51
1:A:151:GLN:NE2	1:A:279:ALA:H	2.07	0.51
1:A:151:GLN:NE2	1:A:279:ALA:N	2.59	0.51
1:A:189:ASN:CG	1:A:192:GLU:HB2	2.31	0.51
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.93	0.51
1:B:360:GLN:O	1:B:361:ASN:CB	2.59	0.51
1:A:265:VAL:O	1:A:265:VAL:CG1	2.58	0.51
1:B:518:ARG:HA	1:B:521:GLU:HB2	1.92	0.51
1:B:626:ILE:HD11	1:B:628:PHE:CZ	2.45	0.51
1:B:701:GLN:HB3	1:B:851:LEU:CD1	2.39	0.51
1:C:607:GLU:HB2	1:C:632:LYS:HG2	1.93	0.51
1:A:605:ASN:OD1	1:A:637:ARG:HG2	2.11	0.51
1:B:456:MET:HG3	1:B:467:TYR:CB	2.35	0.51
1:C:762:PHE:CZ	1:C:764:ASP:HB2	2.46	0.51
1:A:99:ASP:OD1	1:A:101:ASP:HB2	2.11	0.51
1:B:445:ILE:HG13	1:B:940:LYS:HG3	1.93	0.51
1:C:281:PHE:HE1	1:C:608:SER:HG	1.59	0.51
1:A:391:ASN:O	1:A:393:LEU:N	2.43	0.51
1:A:993:THR:HB	1:A:997:SER:HB3	1.92	0.51
1:A:1015:THR:C	1:A:1017:LEU:H	2.13	0.51
1:C:225:VAL:O	1:C:226:LYS:C	2.48	0.51
1:C:1028:VAL:HG12	1:C:1032:ARG:HB2	1.92	0.51
1:A:298:ASN:ND2	1:A:301:ASP:H	2.09	0.50
1:A:886:LEU:HD21	1:C:17:ILE:HG21	1.91	0.50
1:B:139:VAL:O	1:B:140:VAL:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:GLU:N	1:C:315:PRO:HD2	2.26	0.50
1:C:467:TYR:CZ	1:C:925:VAL:HG12	2.46	0.50
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.94	0.50
1:B:291:ILE:HD12	1:B:291:ILE:N	2.27	0.50
1:B:939:ALA:O	1:B:943:ILE:HG12	2.11	0.50
1:B:1027:VAL:O	1:B:1031:ARG:CB	2.59	0.50
1:C:144:ASN:ND2	1:C:148:THR:N	2.58	0.50
1:A:281:PHE:CZ	1:A:324:VAL:HG11	2.47	0.50
1:B:373:PRO:O	1:B:377:LEU:HG	2.11	0.50
1:B:600:THR:C	1:B:602:GLU:H	2.15	0.50
1:C:115:MET:HE2	1:C:118:LEU:HD23	1.93	0.50
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.46	0.50
1:C:218:GLN:HE21	1:C:231:ASN:HD21	1.60	0.50
1:C:956:GLU:OE2	1:C:956:GLU:HA	2.11	0.50
1:A:456:MET:HB2	1:A:471:SER:HB2	1.94	0.50
1:A:909:VAL:HG12	1:A:913:LEU:HD22	1.93	0.50
1:B:1010:GLY:HA2	1:B:1013:THR:HG22	1.93	0.50
1:C:158:VAL:HG12	1:C:177:LEU:HD21	1.93	0.50
1:C:983:ILE:HD11	1:C:1011:MET:HB3	1.92	0.50
1:A:278:ILE:HB	1:A:613:ASN:HB3	1.92	0.50
1:A:591:LEU:HD12	1:A:613:ASN:HB2	1.94	0.50
1:A:728:LYS:NZ	1:C:236:ALA:O	2.45	0.50
1:A:888:LEU:HD11	1:A:943:ILE:HG12	1.94	0.50
1:C:513:PHE:CG	1:C:516:PHE:HB3	2.47	0.50
1:C:948:PHE:O	1:C:952:LEU:HB3	2.11	0.50
1:A:367:ILE:HG13	1:A:368:PRO:CD	2.41	0.50
1:A:671:ILE:CG1	1:A:674:LEU:HD12	2.41	0.50
1:C:470:PHE:CD2	1:C:929:VAL:HG11	2.47	0.50
1:A:686:ASP:OD1	1:A:686:ASP:C	2.50	0.50
1:A:780:ARG:HH21	1:C:222:THR:H	1.58	0.50
1:B:493:CYS:O	1:B:497:LEU:CB	2.59	0.50
1:B:631:LEU:HD11	1:B:644:VAL:HG12	1.93	0.50
1:B:681:ASP:OD2	1:B:826:GLU:OE1	2.29	0.50
1:C:350:LEU:HD22	1:C:984:LEU:HB3	1.92	0.50
1:C:752:ALA:O	1:C:774:MET:HA	2.11	0.50
1:A:813:SER:HB3	1:A:816:LEU:CD2	2.42	0.50
1:B:150:THR:HG23	1:B:153:ASP:OD1	2.11	0.50
1:B:166:ILE:C	1:B:168:ARG:H	2.14	0.50
1:B:338:HIS:HE1	1:B:342:LYS:HE3	1.76	0.50
1:C:220:GLY:HA2	1:C:228:GLN:HE21	1.77	0.50
1:A:181:GLN:O	1:A:181:GLN:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:O	1:A:211:ASN:HB3	2.12	0.50
1:A:221:GLY:H	1:B:622:GLN:HE22	1.60	0.50
1:A:607:GLU:HB3	1:A:630:SER:O	2.12	0.50
1:B:103:ALA:O	1:B:107:VAL:HG23	2.12	0.50
1:B:149:MET:HG2	1:B:153:ASP:HB3	1.94	0.50
1:C:189:ASN:C	1:C:189:ASN:ND2	2.58	0.50
1:A:931:LEU:O	1:A:935:ILE:HG12	2.12	0.49
1:B:372:VAL:HG22	1:B:373:PRO:HD3	1.93	0.49
1:C:56:THR:O	1:C:60:THR:HB	2.12	0.49
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.42	0.49
1:C:914:LEU:O	1:C:915:ALA:HB3	2.11	0.49
1:A:317:PHE:HE2	1:A:323:ILE:HG23	1.77	0.49
1:B:104:GLN:HE21	1:B:105:VAL:N	2.10	0.49
1:B:213:GLN:HG3	1:C:56:THR:OG1	2.11	0.49
1:B:967:ALA:O	1:B:969:ARG:N	2.44	0.49
1:C:451:ALA:CB	1:C:883:VAL:HG12	2.42	0.49
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.74	0.49
1:C:908:GLY:CA	1:C:1014:ALA:HB2	2.39	0.49
1:C:911:GLY:HA3	1:C:1013:THR:CB	2.42	0.49
1:A:271:GLY:HA3	1:A:275:TYR:OH	2.12	0.49
1:A:400:LEU:HD13	1:A:1003:VAL:HG13	1.95	0.49
1:B:221:GLY:HA3	1:C:780:ARG:NH1	2.28	0.49
1:B:420:MET:SD	1:B:425:LEU:N	2.77	0.49
1:B:462:SER:H	1:B:865:GLN:NE2	2.10	0.49
1:C:389:SER:O	1:C:394:THR:HG21	2.12	0.49
1:C:986:VAL:O	1:C:990:VAL:HG23	2.12	0.49
1:A:393:LEU:HD11	1:A:466:ILE:HG12	1.95	0.49
1:B:985:GLY:O	1:B:988:PRO:HD2	2.13	0.49
1:B:1018:ALA:O	1:B:1022:VAL:HG22	2.12	0.49
1:C:161:ASN:O	1:C:313:MET:HE2	2.13	0.49
1:C:805:SER:O	1:C:806:SER:HB3	2.13	0.49
1:A:214:VAL:HG12	1:A:215:ALA:N	2.28	0.49
1:A:228:GLN:HG3	1:A:229:GLN:H	1.77	0.49
1:A:235:ILE:HG22	1:A:235:ILE:O	2.13	0.49
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.94	0.49
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.94	0.49
1:B:649:MET:O	1:B:653:ARG:HB2	2.11	0.49
1:B:906:PRO:HA	1:B:909:VAL:CG2	2.39	0.49
1:C:11:PHE:O	1:C:14:VAL:HG12	2.12	0.49
1:C:655:PHE:O	1:C:657:GLN:N	2.46	0.49
1:C:859:TRP:HB3	1:C:863:SER:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:MET:SD	1:A:490:PRO:HB3	2.52	0.49
1:B:182:TYR:O	1:B:769:LYS:HD2	2.13	0.49
1:B:291:ILE:N	1:B:291:ILE:CD1	2.76	0.49
1:C:636:ASP:N	1:C:636:ASP:OD2	2.44	0.49
1:A:38:ILE:N	1:A:38:ILE:HD13	2.28	0.49
1:A:746:ILE:CD1	1:A:804:PHE:CE1	2.96	0.49
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.95	0.49
1:B:119:PRO:HG2	1:B:122:VAL:HG23	1.95	0.49
1:B:332:PHE:HB2	1:B:569:GLN:O	2.12	0.49
1:B:573:MET:HB2	1:B:575:MET:HE1	1.94	0.49
1:C:131:LYS:HB2	1:C:295:THR:CG2	2.42	0.49
1:A:167:SER:OG	1:A:175:VAL:HG22	2.13	0.49
1:A:223:PRO:HD3	1:B:275:TYR:HB2	1.95	0.49
1:B:539:GLY:H	1:B:540:ARG:NH2	2.10	0.49
1:B:561:SER:HA	1:B:923:ASN:HB3	1.95	0.49
1:B:894:SER:C	1:B:896:SER:H	2.16	0.49
1:C:106:GLN:O	1:C:107:VAL:C	2.50	0.49
1:C:186:ILE:HG13	1:C:268:ILE:CD1	2.42	0.49
1:A:323:ILE:HG12	1:A:325:TYR:HE1	1.78	0.49
1:A:447:MET:CB	1:A:887:CYS:SG	2.97	0.49
1:A:571:VAL:HG12	1:A:630:SER:HB3	1.94	0.48
1:A:578:LEU:HB3	1:A:579:PRO:CD	2.43	0.48
1:A:990:VAL:C	1:A:991:ILE:HG12	2.33	0.48
1:A:1007:VAL:O	1:A:1011:MET:HB2	2.13	0.48
1:B:250:LEU:HA	1:B:261:LEU:HB3	1.94	0.48
1:A:102:ILE:HA	1:A:105:VAL:HG23	1.96	0.48
1:A:343:THR:HG21	1:A:399:VAL:HG13	1.94	0.48
1:B:193:LEU:HD23	1:B:265:VAL:HG21	1.95	0.48
1:B:401:ALA:O	1:B:405:LEU:HG	2.13	0.48
1:B:931:LEU:O	1:B:935:ILE:HG12	2.13	0.48
1:C:162:MET:HA	1:C:313:MET:HE1	1.95	0.48
1:C:844:MET:O	1:C:847:LEU:HD22	2.13	0.48
1:B:404:LEU:HD22	1:B:449:LEU:HD11	1.93	0.48
1:B:665:ALA:O	1:B:666:PHE:CB	2.61	0.48
1:C:431:THR:O	1:C:435:MET:HG2	2.13	0.48
1:C:466:ILE:HG13	1:C:563:PHE:CZ	2.47	0.48
1:C:727:PHE:HE2	1:C:807:SER:CB	2.26	0.48
1:C:962:GLU:HA	1:C:965:LEU:HB2	1.95	0.48
1:B:34:GLN:O	1:B:391:ASN:HB2	2.13	0.48
1:B:404:LEU:HD21	1:B:937:LEU:HD21	1.95	0.48
1:B:963:ALA:HA	1:B:966:ASP:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:712:MET:CB	1:C:835:LYS:HG3	2.44	0.48
1:C:935:ILE:O	1:C:935:ILE:CG2	2.61	0.48
1:A:443:VAL:HG12	1:A:443:VAL:O	2.13	0.48
1:B:193:LEU:CD2	1:B:198:LEU:HB2	2.44	0.48
1:B:1022:VAL:HA	1:B:1025:PHE:CD1	2.48	0.48
1:C:192:GLU:HB3	1:C:265:VAL:HG12	1.96	0.48
1:C:244:GLU:O	1:C:263:ARG:NH2	2.46	0.48
1:C:732:ASP:O	1:C:733:GLN:C	2.51	0.48
1:A:178:PHE:HB2	1:A:288:GLY:CA	2.44	0.48
1:B:314:GLU:OE2	1:B:323:ILE:HD12	2.14	0.48
1:B:754:TRP:HH2	1:B:785:ASP:HB2	1.76	0.48
1:B:945:ILE:HG23	1:B:975:ILE:HD11	1.94	0.48
1:C:144:ASN:HD21	1:C:148:THR:N	2.12	0.48
1:C:211:ASN:ND2	1:C:240:LEU:H	2.12	0.48
1:C:229:GLN:O	1:C:230:LEU:HB3	2.13	0.48
1:C:463:THR:O	1:C:465:ALA:N	2.47	0.48
1:C:491:ALA:O	1:C:493:CYS:N	2.46	0.48
1:A:780:ARG:NH2	1:C:223:PRO:O	2.47	0.48
1:A:912:ALA:HB2	1:A:1010:GLY:HA3	1.95	0.48
1:B:44:THR:OG1	1:B:132:SER:HB3	2.13	0.48
1:B:158:VAL:HA	1:B:162:MET:HG2	1.93	0.48
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.47	0.48
1:C:931:LEU:HD22	1:C:931:LEU:O	2.14	0.48
1:B:200:PRO:HD2	1:B:749:THR:HG23	1.94	0.48
1:B:324:VAL:CG2	1:B:326:PRO:HD3	2.43	0.48
1:B:372:VAL:HB	1:B:405:LEU:HD11	1.96	0.48
1:B:408:ASP:OD1	1:B:442:LEU:HA	2.13	0.48
1:B:720:GLY:O	1:B:721:LEU:HD12	2.14	0.48
1:C:158:VAL:HG12	1:C:159:ALA:N	2.27	0.48
1:C:190:PRO:HB3	1:C:789:TRP:CE3	2.49	0.48
1:C:858:ASP:OD1	1:C:859:TRP:N	2.47	0.48
1:A:211:ASN:CG	1:A:211:ASN:O	2.52	0.48
1:A:729:ILE:HG22	1:A:730:ASP:H	1.76	0.48
1:B:200:PRO:HG2	1:B:749:THR:HG23	1.96	0.48
1:C:119:PRO:HG2	1:C:122:VAL:HG23	1.96	0.48
1:A:574:THR:HB	1:A:627:ALA:HB3	1.95	0.48
1:B:426:PRO:HB3	1:B:430:ALA:CB	2.44	0.48
1:B:655:PHE:O	1:B:658:ILE:HG13	2.13	0.48
1:B:990:VAL:HG21	1:B:1008:MET:SD	2.54	0.48
1:C:366:LEU:O	1:C:370:ILE:N	2.42	0.48
1:C:379:THR:CG2	1:C:477:ALA:HB2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:948:PHE:HE1	1:C:971:ARG:NE	2.12	0.48
1:A:5:PHE:CD1	1:A:12:ALA:HB2	2.48	0.47
1:A:533:GLY:C	1:A:535:LEU:N	2.65	0.47
1:A:1033:PHE:O	1:A:1034:SER:CB	2.60	0.47
1:B:940:LYS:NZ	1:B:978:THR:CG2	2.77	0.47
1:A:144:ASN:HB2	1:A:149:MET:HE3	1.96	0.47
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.49	0.47
1:A:649:MET:HG2	1:A:653:ARG:NH1	2.29	0.47
1:A:897:ILE:N	1:A:898:PRO:HD2	2.29	0.47
1:A:987:MET:HA	1:A:990:VAL:O	2.14	0.47
1:B:157:TYR:HA	1:B:161:ASN:ND2	2.29	0.47
1:B:762:PHE:HD2	1:B:771:VAL:HG22	1.78	0.47
1:B:940:LYS:HZ2	1:B:978:THR:CG2	2.28	0.47
1:B:1024:VAL:O	1:B:1028:VAL:HG23	2.14	0.47
1:C:294:ALA:HB3	1:C:297:ALA:HB2	1.96	0.47
1:C:909:VAL:HG11	1:C:935:ILE:HD11	1.96	0.47
1:C:973:ARG:O	1:C:977:MET:HG3	2.14	0.47
1:A:324:VAL:HG12	1:A:325:TYR:N	2.29	0.47
1:B:314:GLU:N	1:B:315:PRO:HD3	2.29	0.47
1:A:51:GLY:O	1:C:215:ALA:HB1	2.13	0.47
1:A:54:ALA:HB1	1:A:816:LEU:HG	1.95	0.47
1:B:221:GLY:HA3	1:C:780:ARG:HH12	1.79	0.47
1:B:342:LYS:O	1:B:346:GLU:HG3	2.13	0.47
1:B:921:LEU:HD22	1:B:1005:THR:HB	1.97	0.47
1:A:674:LEU:HD13	1:A:675:GLY:N	2.29	0.47
1:A:818:ARG:NH1	1:A:821:GLY:O	2.47	0.47
1:A:991:ILE:O	1:A:992:SER:OG	2.26	0.47
1:B:210:GLN:NE2	1:B:249:ILE:HA	2.28	0.47
1:B:692:HIS:O	1:B:692:HIS:ND1	2.48	0.47
1:B:881:LEU:O	1:B:882:ILE:C	2.53	0.47
1:C:736:ALA:C	1:C:738:ALA:H	2.18	0.47
1:C:778:LYS:HG3	1:C:779:TYR:CE2	2.50	0.47
1:A:552:MET:HA	1:A:555:LEU:HB2	1.97	0.47
1:A:597:TYR:HD1	1:A:598:TYR:N	2.12	0.47
1:B:13:TRP:O	1:B:17:ILE:HG12	2.14	0.47
1:B:222:THR:CB	1:B:223:PRO:HD3	2.26	0.47
1:B:456:MET:CG	1:B:467:TYR:HB3	2.36	0.47
1:B:518:ARG:HA	1:B:521:GLU:CG	2.45	0.47
1:B:681:ASP:O	1:B:859:TRP:HE3	1.98	0.47
1:B:703:LEU:HA	1:B:706:ALA:HB3	1.96	0.47
1:C:713:LEU:HD23	1:C:832:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:GLN:HG3	1:A:249:ILE:CG2	2.29	0.47
1:A:228:GLN:HB2	1:B:781:MET:HE1	1.96	0.47
1:A:314:GLU:O	1:A:317:PHE:HB2	2.15	0.47
1:A:337:ILE:HG12	1:A:395:MET:SD	2.54	0.47
1:A:688:ALA:C	1:A:690:LEU:N	2.68	0.47
1:B:371:ALA:HA	1:B:374:VAL:HG12	1.96	0.47
1:B:666:PHE:HB3	1:B:678:THR:CG2	2.45	0.47
1:B:910:ILE:HG23	1:B:911:GLY:N	2.28	0.47
1:C:2:PRO:O	1:C:6:ILE:HG13	2.14	0.47
1:C:186:ILE:O	1:C:186:ILE:HG22	2.13	0.47
1:A:608:SER:O	1:A:629:VAL:HG23	2.15	0.47
1:A:1029:VAL:HG12	1:A:1030:ARG:N	2.30	0.47
1:B:123:GLN:C	1:B:125:GLN:H	2.17	0.47
1:B:549:VAL:O	1:B:552:MET:HB3	2.14	0.47
1:B:860:THR:O	1:B:863:SER:HB2	2.14	0.47
1:B:1012:VAL:CG2	1:B:1013:THR:N	2.78	0.47
1:C:328:ASP:OD1	1:C:330:THR:HB	2.15	0.47
1:C:376:LEU:O	1:C:379:THR:N	2.44	0.47
1:C:457:ALA:HB2	1:C:471:SER:CB	2.45	0.47
1:C:926:TYR:CE2	1:C:999:ALA:HB1	2.50	0.47
1:C:949:ALA:HB1	1:C:1026:PHE:CE2	2.50	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CD2	2.49	0.47
1:A:974:PRO:O	1:A:975:ILE:C	2.53	0.47
1:B:78:MET:HG3	1:B:92:LEU:HG	1.97	0.47
1:B:160:ALA:HB1	1:B:767:ARG:HD3	1.96	0.47
1:B:452:VAL:O	1:B:453:PHE:CB	2.63	0.47
1:C:497:LEU:HD12	1:C:498:LYS:HG3	1.96	0.47
1:A:150:THR:OG1	1:A:153:ASP:OD2	2.31	0.47
1:A:351:VAL:HG21	1:A:406:VAL:CG2	2.45	0.47
1:A:431:THR:HB	1:A:494:ALA:HB2	1.95	0.47
1:A:673:GLU:O	1:A:673:GLU:HG3	2.15	0.47
1:A:808:ARG:N	1:A:808:ARG:HH11	2.12	0.47
1:B:997:SER:HA	1:B:1000:GLN:HB2	1.97	0.47
1:C:350:LEU:CD2	1:C:984:LEU:HB3	2.45	0.47
1:C:713:LEU:HD13	1:C:713:LEU:N	2.29	0.47
1:A:66:GLU:C	1:A:68:ASN:H	2.18	0.46
1:A:309:GLU:O	1:A:313:MET:HG2	2.15	0.46
1:A:681:ASP:H	1:A:863:SER:CB	2.28	0.46
1:B:115:MET:HB2	1:B:116:PRO:HD3	1.96	0.46
1:C:305:ALA:O	1:C:306:ILE:C	2.53	0.46
1:C:463:THR:HG22	1:C:464:GLY:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LEU:HD23	1:A:587:THR:HG23	1.97	0.46
1:B:62:THR:O	1:B:66:GLU:HB2	2.14	0.46
1:B:72:ILE:HD13	1:B:72:ILE:H	1.79	0.46
1:B:469:GLN:O	1:B:473:THR:OG1	2.33	0.46
1:B:472:ILE:HG23	1:B:473:THR:N	2.30	0.46
1:C:484:VAL:HG13	1:C:488:LEU:HB3	1.98	0.46
1:C:778:LYS:HG3	1:C:779:TYR:HE2	1.81	0.46
1:C:821:GLY:O	1:C:822:LEU:HD23	2.15	0.46
1:C:966:ASP:O	1:C:970:MET:N	2.29	0.46
1:A:255:GLN:O	1:A:256:ASP:CB	2.63	0.46
1:A:367:ILE:HG12	1:A:413:VAL:HG21	1.97	0.46
1:A:545:TYR:HB2	1:A:1021:PHE:HE1	1.79	0.46
1:A:680:PHE:CZ	1:A:844:MET:HE1	2.50	0.46
1:B:2:PRO:O	1:B:4:PHE:N	2.48	0.46
1:C:655:PHE:C	1:C:657:GLN:N	2.68	0.46
1:C:899:PHE:HD1	1:C:899:PHE:H	1.62	0.46
1:A:281:PHE:O	1:A:283:GLY:N	2.48	0.46
1:A:711:ASP:C	1:A:713:LEU:H	2.17	0.46
1:C:371:ALA:HB2	1:C:488:LEU:HD23	1.97	0.46
1:C:734:GLU:HA	1:C:737:GLN:HG2	1.97	0.46
1:C:1032:ARG:HG3	1:C:1036:LYS:HE2	1.97	0.46
1:A:973:ARG:O	1:A:977:MET:HG3	2.16	0.46
1:B:50:PRO:HG2	1:B:125:GLN:HE22	1.80	0.46
1:B:613:ASN:O	1:B:625:GLY:HA2	2.15	0.46
1:B:654:ALA:C	1:B:656:SER:H	2.18	0.46
1:B:828:LEU:HB3	1:B:829:GLY:H	1.59	0.46
1:B:1009:GLY:O	1:B:1012:VAL:HG22	2.16	0.46
1:C:160:ALA:HA	1:C:767:ARG:NE	2.31	0.46
1:C:435:MET:HA	1:C:438:ILE:HG22	1.98	0.46
1:C:601:LYS:O	1:C:603:LYS:N	2.48	0.46
1:C:680:PHE:CE1	1:C:844:MET:HE3	2.50	0.46
1:A:221:GLY:HA2	1:B:622:GLN:OE1	2.16	0.46
1:A:682:PHE:CZ	1:A:857:TYR:HB2	2.51	0.46
1:A:702:LEU:O	1:A:702:LEU:HG	2.16	0.46
1:B:111:LEU:HD21	1:B:127:VAL:HG13	1.97	0.46
1:B:445:ILE:O	1:B:449:LEU:HB2	2.16	0.46
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.98	0.46
1:C:658:ILE:HD12	1:C:658:ILE:H	1.81	0.46
1:A:274:ASN:OD1	1:A:275:TYR:N	2.49	0.46
1:A:395:MET:HA	1:A:395:MET:HE2	1.97	0.46
1:C:317:PHE:CG	1:C:321:LEU:HD12	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:PRO:O	1:A:429:GLU:N	2.48	0.46
1:A:883:VAL:O	1:A:883:VAL:CG1	2.64	0.46
1:B:587:THR:HG22	1:B:591:LEU:HD23	1.98	0.46
1:C:379:THR:O	1:C:382:VAL:N	2.49	0.46
1:C:767:ARG:HH11	1:C:767:ARG:HG3	1.81	0.46
1:C:911:GLY:CA	1:C:1013:THR:HG21	2.44	0.46
1:A:167:SER:OG	1:A:175:VAL:HG21	2.16	0.46
1:A:391:ASN:H	1:A:394:THR:HG22	1.80	0.46
1:A:427:PRO:C	1:A:429:GLU:H	2.18	0.46
1:A:677:ALA:C	1:A:679:GLY:N	2.69	0.46
1:B:328:ASP:OD2	1:B:328:ASP:C	2.54	0.46
1:B:671:ILE:HD13	1:B:676:THR:HG22	1.98	0.46
1:C:759:VAL:HG23	1:C:771:VAL:HB	1.98	0.46
1:C:997:SER:O	1:C:1000:GLN:N	2.41	0.46
1:A:729:ILE:HD13	1:C:234:ILE:CG2	2.44	0.45
1:A:799:VAL:CG1	1:A:800:PRO:HD2	2.46	0.45
1:B:764:ASP:O	1:B:766:GLY:N	2.49	0.45
1:C:30:LEU:HD23	1:C:31:PRO:HD2	1.98	0.45
1:C:144:ASN:ND2	1:C:148:THR:H	2.14	0.45
1:C:531:VAL:HA	1:C:534:ILE:HG23	1.97	0.45
1:C:731:ILE:HG12	1:C:746:ILE:HG21	1.98	0.45
1:A:389:SER:OG	1:A:391:ASN:ND2	2.48	0.45
1:A:428:LYS:HG3	1:A:429:GLU:HG3	1.98	0.45
1:B:1022:VAL:HA	1:B:1025:PHE:HD1	1.80	0.45
1:C:14:VAL:HG13	1:C:15:ILE:N	2.31	0.45
1:C:457:ALA:HB2	1:C:471:SER:OG	2.17	0.45
1:A:56:THR:O	1:A:60:THR:HB	2.16	0.45
1:A:317:PHE:HE2	1:A:323:ILE:CG2	2.29	0.45
1:C:156:ASP:O	1:C:157:TYR:C	2.55	0.45
1:A:431:THR:CB	1:A:494:ALA:HB2	2.46	0.45
1:A:530:SER:O	1:A:534:ILE:HG23	2.15	0.45
1:B:58:GLN:O	1:B:63:GLN:HG2	2.17	0.45
1:B:66:GLU:HG3	1:B:78:MET:SD	2.56	0.45
1:B:104:GLN:HE22	1:B:108:GLN:HE21	1.64	0.45
1:B:228:GLN:HE22	1:C:781:MET:HB3	1.79	0.45
1:B:399:VAL:O	1:B:402:ILE:HB	2.16	0.45
1:B:418:ARG:HB3	1:B:418:ARG:NH1	2.31	0.45
1:C:9:PRO:O	1:C:11:PHE:N	2.46	0.45
1:C:65:ILE:HD13	1:C:111:LEU:HD21	1.97	0.45
1:C:332:PHE:O	1:C:333:VAL:C	2.54	0.45
1:C:758:TYR:HE2	1:C:770:LYS:CB	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:VAL:O	1:C:348:ILE:N	2.48	0.45
1:A:60:THR:HG23	1:A:119:PRO:HG3	1.97	0.45
1:A:727:PHE:CZ	1:A:783:PRO:HB3	2.51	0.45
1:A:909:VAL:O	1:A:912:ALA:HB3	2.16	0.45
1:A:911:GLY:N	1:A:914:LEU:HD13	2.16	0.45
1:B:314:GLU:HG3	1:B:317:PHE:CE2	2.51	0.45
1:C:352:PHE:HA	1:C:369:THR:HG21	1.98	0.45
1:C:598:TYR:HB3	1:C:606:VAL:HG11	1.99	0.45
1:A:456:MET:C	1:A:458:PHE:N	2.69	0.45
1:B:154:ILE:C	1:B:156:ASP:N	2.70	0.45
1:B:348:ILE:HG12	1:B:372:VAL:HG21	1.98	0.45
1:B:805:SER:O	1:B:806:SER:HB2	2.16	0.45
1:B:986:VAL:HG12	1:B:990:VAL:CG2	2.47	0.45
1:C:414:GLU:HG2	1:C:974:PRO:HB3	1.98	0.45
1:C:418:ARG:HD2	1:C:419:VAL:CG2	2.42	0.45
1:C:872:GLN:HE21	1:C:875:SER:HB2	1.81	0.45
1:C:901:VAL:HG11	1:C:943:ILE:HA	1.98	0.45
1:B:34:GLN:HG2	1:B:35:TYR:CD2	2.51	0.45
1:B:669:PRO:HG3	1:B:678:THR:HA	1.99	0.45
1:A:576:VAL:HG11	1:A:591:LEU:HD23	1.98	0.45
1:B:639:GLY:O	1:B:641:GLU:N	2.50	0.45
1:C:155:SER:OG	1:C:179:GLY:HA3	2.17	0.45
1:C:491:ALA:C	1:C:493:CYS:N	2.68	0.45
1:B:5:PHE:HA	1:B:8:ARG:HB2	1.99	0.45
1:B:44:THR:OG1	1:B:132:SER:CB	2.64	0.45
1:B:493:CYS:O	1:B:497:LEU:HB2	2.17	0.45
1:C:38:ILE:HG21	1:C:466:ILE:HD11	1.98	0.45
1:C:188:MET:HA	1:C:266:ALA:HB2	1.98	0.45
1:C:367:ILE:HG23	1:C:368:PRO:HD3	1.99	0.45
1:A:623:ASN:O	1:A:623:ASN:CG	2.54	0.44
1:A:750:LEU:O	1:A:754:TRP:CD1	2.70	0.44
1:B:410:ILE:HD13	1:B:977:MET:HG3	1.99	0.44
1:B:891:LEU:HD13	1:B:892:TYR:CE2	2.52	0.44
1:C:712:MET:C	1:C:713:LEU:HD22	2.37	0.44
1:C:925:VAL:HG23	1:C:926:TYR:N	2.32	0.44
1:A:69:MET:CG	1:A:92:LEU:HD21	2.48	0.44
1:A:83:ASP:O	1:A:85:THR:N	2.49	0.44
1:A:713:LEU:HB2	1:A:833:PRO:CD	2.36	0.44
1:B:261:LEU:O	1:B:263:ARG:N	2.50	0.44
1:B:291:ILE:CD1	1:B:291:ILE:H	2.30	0.44
1:B:601:LYS:HE2	1:B:601:LYS:HB2	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:GLY:CA	1:B:1013:THR:HG21	2.46	0.44
1:C:102:ILE:O	1:C:103:ALA:C	2.54	0.44
1:C:314:GLU:N	1:C:315:PRO:CD	2.80	0.44
1:C:577:GLN:HE21	1:C:577:GLN:CA	2.25	0.44
1:C:1004:GLY:C	1:C:1006:GLY:H	2.20	0.44
1:A:241:THR:N	1:A:245:GLU:OE1	2.40	0.44
1:A:250:LEU:HD22	1:A:250:LEU:H	1.81	0.44
1:A:971:ARG:O	1:A:974:PRO:HD2	2.17	0.44
1:B:238:THR:HG23	1:B:239:ARG:H	1.82	0.44
1:B:280:GLU:HA	1:B:286:ALA:HB3	1.99	0.44
1:B:339:GLU:O	1:B:342:LYS:HB2	2.16	0.44
1:C:859:TRP:CE3	1:C:863:SER:HB3	2.53	0.44
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.99	0.44
1:B:863:SER:O	1:B:866:GLU:N	2.50	0.44
1:B:891:LEU:HD13	1:B:892:TYR:CZ	2.52	0.44
1:B:892:TYR:CD1	1:B:897:ILE:HD11	2.51	0.44
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.99	0.44
1:C:219:LEU:CD2	1:C:234:ILE:HD11	2.47	0.44
1:A:359:LEU:O	1:A:360:GLN:HB2	2.17	0.44
1:A:540:ARG:HD2	1:A:541:TYR:CE2	2.52	0.44
1:A:574:THR:HG21	1:A:594:VAL:CG1	2.48	0.44
1:B:57:VAL:CG2	1:B:82:SER:HB2	2.47	0.44
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.48	0.44
1:B:539:GLY:C	1:B:541:TYR:N	2.71	0.44
1:C:57:VAL:HG12	1:C:88:VAL:HG22	1.99	0.44
1:C:952:LEU:HG	1:C:952:LEU:O	2.18	0.44
1:A:190:PRO:HB3	1:A:789:TRP:CD2	2.52	0.44
1:A:367:ILE:HG22	1:A:496:MET:HE3	1.99	0.44
1:A:540:ARG:HD2	1:A:541:TYR:HE2	1.81	0.44
1:B:309:GLU:O	1:B:312:LYS:HB2	2.17	0.44
1:B:942:ALA:O	1:B:945:ILE:HG13	2.17	0.44
1:C:203:VAL:O	1:C:207:ILE:HG13	2.18	0.44
1:C:254:ASN:O	1:C:256:ASP:N	2.51	0.44
1:C:576:VAL:HG13	1:C:590:VAL:HG11	2.00	0.44
1:C:782:LEU:HB3	1:C:783:PRO:HD2	1.98	0.44
1:A:355:MET:CG	1:A:365:THR:HG22	2.48	0.44
1:A:877:TYR:OH	1:A:932:LEU:HD11	2.17	0.44
1:B:231:ASN:C	1:B:231:ASN:ND2	2.68	0.44
1:B:298:ASN:CB	1:B:301:ASP:HB2	2.47	0.44
1:B:563:PHE:HB2	1:B:866:GLU:HG3	1.98	0.44
1:C:390:ILE:HA	1:C:394:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:657:GLN:O	1:C:659:LYS:N	2.51	0.44
1:A:346:GLU:C	1:A:348:ILE:N	2.71	0.44
1:A:591:LEU:CD1	1:A:613:ASN:HB2	2.48	0.44
1:A:724:THR:HG22	1:A:725:PRO:N	2.33	0.44
1:A:956:GLU:HB3	1:A:958:LYS:HG3	2.00	0.44
1:B:448:VAL:O	1:B:452:VAL:HG22	2.17	0.44
1:B:624:THR:O	1:B:624:THR:HG23	2.17	0.44
1:B:901:VAL:O	1:B:904:VAL:HG23	2.17	0.44
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.44
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.87	0.44
1:C:928:GLN:HA	1:C:931:LEU:HB3	1.98	0.44
1:A:46:SER:HA	1:A:88:VAL:O	2.17	0.44
1:A:252:LYS:HE3	1:A:254:ASN:HB3	2.00	0.44
1:A:959:GLY:HA3	1:A:962:GLU:HB3	2.00	0.44
1:B:450:SER:O	1:B:452:VAL:O	2.36	0.44
1:B:560:PRO:HB2	1:B:836:SER:CB	2.41	0.44
1:C:520:PHE:C	1:C:522:LYS:H	2.22	0.44
1:C:574:THR:HG23	1:C:665:ALA:HB2	1.98	0.44
1:C:931:LEU:O	1:C:935:ILE:HG13	2.18	0.44
1:A:63:GLN:HG2	1:C:768:VAL:HG12	2.00	0.43
1:A:74:ASN:H	1:C:170:SER:HB2	1.83	0.43
1:A:579:PRO:O	1:A:580:ALA:C	2.55	0.43
1:A:733:GLN:HE22	1:A:743:ILE:HD12	1.83	0.43
1:A:780:ARG:NH2	1:C:222:THR:H	2.15	0.43
1:A:866:GLU:HG3	1:A:867:ARG:N	2.33	0.43
1:B:162:MET:HB3	1:B:313:MET:SD	2.58	0.43
1:B:367:ILE:HG22	1:B:489:THR:HG23	1.98	0.43
1:B:749:THR:O	1:B:750:LEU:C	2.56	0.43
1:C:222:THR:CG2	1:C:223:PRO:HD3	2.47	0.43
1:C:541:TYR:C	1:C:543:VAL:H	2.21	0.43
1:C:963:ALA:O	1:C:965:LEU:N	2.51	0.43
1:B:358:PHE:CD1	1:B:977:MET:HB3	2.54	0.43
1:B:894:SER:OG	1:B:897:ILE:HG23	2.18	0.43
1:C:3:ASN:C	1:C:5:PHE:N	2.71	0.43
1:C:65:ILE:HD13	1:C:111:LEU:CD2	2.47	0.43
1:C:779:TYR:N	1:C:779:TYR:CD2	2.85	0.43
1:C:901:VAL:O	1:C:904:VAL:CG2	2.60	0.43
1:C:963:ALA:C	1:C:965:LEU:N	2.71	0.43
1:A:221:GLY:H	1:B:622:GLN:NE2	2.16	0.43
1:B:25:LEU:HD11	1:C:879:ILE:HG12	1.99	0.43
1:B:129:VAL:HG23	1:C:109:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:PRO:HG3	1:C:469:GLN:HG3	2.01	0.43
1:C:194:ASN:O	1:C:195:LYS:C	2.57	0.43
1:C:230:LEU:C	1:C:230:LEU:HD13	2.39	0.43
1:C:418:ARG:NH1	1:C:970:MET:HG2	2.20	0.43
1:C:707:ALA:O	1:C:710:PRO:HD3	2.18	0.43
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.83	0.43
1:A:138:MET:HB2	1:A:327:TYR:O	2.19	0.43
1:A:216:ALA:HA	1:B:751:GLY:HA2	2.00	0.43
1:A:547:ILE:HD13	1:A:547:ILE:HA	1.95	0.43
1:C:393:LEU:CD1	1:C:466:ILE:HG23	2.48	0.43
1:C:456:MET:O	1:C:459:PHE:HD2	2.00	0.43
1:C:591:LEU:HD12	1:C:611:ALA:HB1	2.00	0.43
1:C:609:VAL:HG22	1:C:629:VAL:HG22	2.01	0.43
1:C:687:GLN:HE21	1:C:687:GLN:HB3	1.52	0.43
1:A:80:SER:HG	1:A:818:ARG:HG3	1.81	0.43
1:A:431:THR:O	1:A:435:MET:HB2	2.18	0.43
1:A:451:ALA:C	1:A:453:PHE:H	2.20	0.43
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.19	0.43
1:B:119:PRO:HG2	1:B:122:VAL:HG21	2.00	0.43
1:B:190:PRO:HD3	1:B:779:TYR:CD2	2.53	0.43
1:B:307:ARG:HH11	1:B:307:ARG:HB2	1.83	0.43
1:C:672:VAL:HG13	1:C:675:GLY:N	2.33	0.43
1:C:742:SER:OG	1:C:745:ASP:HB2	2.18	0.43
1:A:254:ASN:CG	1:A:258:SER:OG	2.57	0.43
1:A:568:ASP:OD2	1:A:637:ARG:NH1	2.52	0.43
1:A:584:GLN:N	1:A:622:GLN:HB3	2.33	0.43
1:A:685:ILE:HB	1:A:687:GLN:HE22	1.83	0.43
1:A:979:SER:O	1:A:983:ILE:HG12	2.17	0.43
1:B:166:ILE:HD11	1:B:310:LEU:CD2	2.48	0.43
1:B:921:LEU:HD21	1:B:1002:ALA:HA	2.00	0.43
1:C:115:MET:HA	1:C:118:LEU:CD2	2.49	0.43
1:A:293:LEU:HB3	1:A:294:ALA:H	1.68	0.43
1:A:449:LEU:O	1:A:453:PHE:CD1	2.70	0.43
1:A:566:ASP:HB3	1:A:667:ASN:HD22	1.82	0.43
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.53	0.43
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.54	0.43
1:B:200:PRO:CD	1:B:749:THR:HG23	2.49	0.43
1:B:463:THR:OG1	1:B:464:GLY:N	2.52	0.43
1:B:564:LEU:HD22	1:B:926:TYR:CE2	2.53	0.43
1:B:674:LEU:O	1:B:676:THR:N	2.51	0.43
1:B:705:GLU:HG3	1:B:847:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ILE:HA	1:A:128:SER:O	2.19	0.43
1:A:346:GLU:C	1:A:348:ILE:H	2.22	0.43
1:B:235:ILE:O	1:C:728:LYS:HD2	2.19	0.43
1:B:338:HIS:CE1	1:B:342:LYS:HE3	2.54	0.43
1:C:520:PHE:O	1:C:522:LYS:N	2.52	0.43
1:C:741:VAL:HG11	1:C:746:ILE:HD11	2.01	0.43
1:C:888:LEU:HD13	1:C:901:VAL:HG23	2.00	0.43
1:B:32:VAL:O	1:B:33:ALA:HB2	2.18	0.43
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.84	0.43
1:B:327:TYR:HB2	1:B:628:PHE:HB3	2.01	0.43
1:B:404:LEU:HD21	1:B:937:LEU:CD2	2.49	0.43
1:B:470:PHE:O	1:B:473:THR:N	2.52	0.43
1:B:692:HIS:HE1	1:B:723:ASP:CG	2.22	0.43
1:C:83:ASP:HB2	1:C:87:THR:HB	2.01	0.43
1:C:400:LEU:HD12	1:C:933:THR:HG21	1.99	0.43
1:C:940:LYS:HA	1:C:943:ILE:HD12	2.01	0.43
1:B:852:PRO:O	1:B:853:THR:OG1	2.24	0.43
1:B:947:GLU:HA	1:B:947:GLU:OE2	2.18	0.43
1:B:1013:THR:O	1:B:1017:LEU:HB3	2.18	0.43
1:C:61:VAL:HA	1:C:118:LEU:HD12	2.00	0.43
1:C:658:ILE:O	1:C:659:LYS:HD2	2.18	0.43
1:C:672:VAL:HG12	1:C:672:VAL:O	2.18	0.43
1:C:953:MET:SD	1:C:963:ALA:CB	3.07	0.43
1:C:983:ILE:HD13	1:C:1008:MET:HA	2.00	0.43
1:C:1022:VAL:HA	1:C:1025:PHE:CE2	2.54	0.43
1:B:154:ILE:O	1:B:157:TYR:N	2.52	0.42
1:B:192:GLU:O	1:B:196:PHE:CD2	2.71	0.42
1:C:18:ILE:O	1:C:19:ILE:C	2.58	0.42
1:C:192:GLU:HG2	1:C:264:ASP:O	2.19	0.42
1:C:355:MET:SD	1:C:410:ILE:HD11	2.59	0.42
1:C:690:LEU:HD11	1:C:854:GLY:HA3	2.00	0.42
1:C:983:ILE:HG23	1:C:1008:MET:HG3	2.01	0.42
1:A:476:SER:O	1:A:480:LEU:HB2	2.19	0.42
1:A:736:ALA:HA	1:A:741:VAL:HG12	2.02	0.42
1:B:111:LEU:HD21	1:B:127:VAL:CG1	2.50	0.42
1:B:349:ILE:HG22	1:B:350:LEU:HD23	2.01	0.42
1:B:547:ILE:HD13	1:B:547:ILE:HA	1.85	0.42
1:C:139:VAL:CG1	1:C:326:PRO:HG2	2.49	0.42
1:C:189:ASN:HD21	1:C:191:ASN:HB2	1.84	0.42
1:C:655:PHE:O	1:C:656:SER:C	2.56	0.42
1:C:687:GLN:OE1	1:C:856:GLY:HA3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:MET:HG3	1:A:92:LEU:HD21	2.00	0.42
1:A:317:PHE:HA	1:A:318:PRO:HD2	1.73	0.42
1:A:566:ASP:HB3	1:A:667:ASN:ND2	2.34	0.42
1:A:680:PHE:CZ	1:A:844:MET:CE	3.03	0.42
1:A:733:GLN:O	1:A:736:ALA:HB3	2.20	0.42
1:B:16:ALA:HB2	1:B:488:LEU:HG	2.01	0.42
1:B:87:THR:HG21	1:B:620:ARG:HH12	1.79	0.42
1:B:140:VAL:HG22	1:B:140:VAL:O	2.18	0.42
1:B:155:SER:OG	1:B:179:GLY:HA3	2.20	0.42
1:B:303:ALA:HA	1:B:306:ILE:HD13	2.00	0.42
1:B:391:ASN:O	1:B:395:MET:HG2	2.20	0.42
1:B:721:LEU:HB3	1:B:814:PRO:HG2	2.01	0.42
1:C:395:MET:O	1:C:398:MET:N	2.43	0.42
1:C:597:TYR:CD1	1:C:601:LYS:HG3	2.54	0.42
1:C:952:LEU:HA	1:C:956:GLU:HG2	1.99	0.42
1:A:180:SER:O	1:A:181:GLN:CB	2.67	0.42
1:A:568:ASP:CG	1:A:637:ARG:HH12	2.22	0.42
1:B:24:GLY:CA	1:B:27:ILE:HG23	2.49	0.42
1:B:96:SER:HB3	1:B:461:GLY:HA2	2.00	0.42
1:B:190:PRO:CD	1:B:779:TYR:CE2	3.01	0.42
1:B:216:ALA:O	1:B:234:ILE:HB	2.20	0.42
1:B:327:TYR:HD1	1:B:327:TYR:O	2.03	0.42
1:B:335:ILE:HG13	1:B:634:TRP:HD1	1.82	0.42
1:B:830:GLN:HB2	1:B:831:ALA:H	1.62	0.42
1:B:1012:VAL:CG2	1:B:1013:THR:H	2.32	0.42
1:C:406:VAL:CG1	1:C:407:ASP:N	2.82	0.42
1:C:554:TYR:HD1	1:C:558:ARG:NE	2.17	0.42
1:A:240:LEU:HD12	1:A:240:LEU:N	2.35	0.42
1:A:959:GLY:O	1:A:961:ILE:N	2.53	0.42
1:A:988:PRO:HB2	1:A:989:LEU:H	1.66	0.42
1:B:190:PRO:HG3	1:B:789:TRP:CZ2	2.55	0.42
1:B:327:TYR:CD1	1:B:327:TYR:C	2.92	0.42
1:C:251:LEU:HB2	1:C:260:VAL:O	2.19	0.42
1:C:489:THR:N	1:C:490:PRO:HD2	2.34	0.42
1:A:34:GLN:HG2	1:A:35:TYR:CE1	2.55	0.42
1:A:211:ASN:HA	1:A:240:LEU:HD13	2.02	0.42
1:A:993:THR:HB	1:A:994:GLY:H	1.74	0.42
1:B:185:ARG:HA	1:B:185:ARG:HD3	1.82	0.42
1:B:858:ASP:OD1	1:B:859:TRP:N	2.48	0.42
1:C:325:TYR:N	1:C:325:TYR:HD1	2.14	0.42
1:C:343:THR:CG2	1:C:989:LEU:HD13	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:HE21	1:A:577:GLN:HB2	1.62	0.42
1:A:590:VAL:O	1:A:591:LEU:C	2.56	0.42
1:B:262:LEU:HD23	1:B:262:LEU:HA	1.89	0.42
1:B:401:ALA:HA	1:B:404:LEU:HB2	2.02	0.42
1:B:682:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.42
1:B:819:TYR:OH	1:B:860:THR:HB	2.20	0.42
1:B:833:PRO:O	1:B:834:GLY:O	2.37	0.42
1:B:946:VAL:HG21	1:B:1026:PHE:CE2	2.55	0.42
1:C:186:ILE:HG13	1:C:268:ILE:HD13	2.00	0.42
1:C:295:THR:HG23	1:C:295:THR:O	2.20	0.42
1:C:395:MET:HA	1:C:395:MET:CE	2.50	0.42
1:A:99:ASP:OD1	1:A:101:ASP:N	2.52	0.42
1:A:330:THR:O	1:A:331:PRO:C	2.58	0.42
1:A:713:LEU:CD2	1:A:714:THR:H	2.27	0.42
1:A:830:GLN:HE21	1:A:831:ALA:H	1.68	0.42
1:B:154:ILE:C	1:B:156:ASP:H	2.23	0.42
1:B:210:GLN:HE22	1:B:249:ILE:HA	1.85	0.42
1:B:699:ARG:CG	1:B:700:ASN:H	2.28	0.42
1:B:911:GLY:HA3	1:B:1013:THR:HG21	2.02	0.42
1:C:445:ILE:O	1:C:448:VAL:N	2.53	0.42
1:C:446:ALA:HB2	1:C:482:VAL:HG21	2.02	0.42
1:C:575:MET:SD	1:C:575:MET:N	2.92	0.42
1:C:905:VAL:CB	1:C:906:PRO:HD3	2.47	0.42
1:C:942:ALA:HB1	1:C:1022:VAL:HG21	2.01	0.42
1:A:780:ARG:HH22	1:C:223:PRO:CD	2.32	0.42
1:A:828:LEU:HA	1:A:828:LEU:HD23	1.83	0.42
1:A:1015:THR:C	1:A:1017:LEU:N	2.73	0.42
1:B:293:LEU:CD1	1:B:297:ALA:HB3	2.50	0.42
1:B:700:ASN:O	1:B:704:ALA:CB	2.68	0.42
1:B:941:ASN:ND2	1:B:1014:ALA:O	2.50	0.42
1:C:425:LEU:H	1:C:426:PRO:CD	2.33	0.42
1:C:538:THR:HG22	1:C:539:GLY:N	2.30	0.42
1:A:52:ALA:HB3	1:A:86:GLY:CA	2.44	0.42
1:A:341:VAL:O	1:A:345:VAL:HG23	2.20	0.42
1:A:445:ILE:HD12	1:A:445:ILE:C	2.40	0.42
1:A:552:MET:HB3	1:A:910:ILE:HG23	2.01	0.42
1:A:923:ASN:C	1:A:923:ASN:HD22	2.22	0.42
1:B:137:LEU:HD13	1:B:293:LEU:HG	2.02	0.42
1:B:409:ALA:HB2	1:B:485:ALA:HB2	2.01	0.42
1:B:556:PHE:HB2	1:B:913:LEU:HD21	2.01	0.42
1:B:686:ASP:HB3	1:B:823:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:PHE:CD2	1:B:771:VAL:HG22	2.55	0.42
1:A:822:LEU:HD12	1:A:822:LEU:HA	1.81	0.41
1:A:882:ILE:O	1:A:886:LEU:HB2	2.19	0.41
1:B:11:PHE:CD1	1:C:890:ALA:HB1	2.55	0.41
1:B:166:ILE:O	1:B:168:ARG:N	2.53	0.41
1:B:251:LEU:HD12	1:B:251:LEU:HA	1.82	0.41
1:B:799:VAL:CG2	1:B:804:PHE:CE2	3.03	0.41
1:B:866:GLU:O	1:B:869:SER:HB3	2.20	0.41
1:B:908:GLY:C	1:B:910:ILE:H	2.23	0.41
1:C:57:VAL:CG2	1:C:86:GLY:HA2	2.48	0.41
1:C:210:GLN:NE2	1:C:249:ILE:HG23	2.35	0.41
1:C:451:ALA:HB1	1:C:883:VAL:HG12	2.02	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CE2	2.55	0.41
1:A:282:ASN:ND2	1:A:609:VAL:H	2.18	0.41
1:A:454:VAL:O	1:A:456:MET:O	2.38	0.41
1:A:582:ALA:HB3	1:A:623:ASN:HB2	2.02	0.41
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.55	0.41
1:A:686:ASP:OD2	1:A:690:LEU:HB2	2.20	0.41
1:B:53:ASP:O	1:B:54:ALA:C	2.59	0.41
1:B:68:ASN:ND2	1:B:114:ALA:HB2	2.34	0.41
1:B:306:ILE:O	1:B:310:LEU:HG	2.20	0.41
1:B:552:MET:SD	1:B:909:VAL:CG2	3.08	0.41
1:B:568:ASP:OD2	1:B:634:TRP:CH2	2.72	0.41
1:C:100:ALA:HB1	1:C:295:THR:HG21	2.01	0.41
1:C:220:GLY:CA	1:C:231:ASN:HD22	2.32	0.41
1:C:577:GLN:O	1:C:577:GLN:HG3	2.20	0.41
1:C:930:GLY:HA3	1:C:1007:VAL:CG2	2.50	0.41
1:A:478:MET:O	1:A:481:SER:HB3	2.19	0.41
1:A:527:TYR:OH	1:A:968:VAL:CG1	2.68	0.41
1:A:754:TRP:HZ2	1:A:786:ILE:HA	1.85	0.41
1:B:743:ILE:N	1:B:743:ILE:CD1	2.69	0.41
1:C:393:LEU:HD11	1:C:466:ILE:HG23	2.02	0.41
1:C:896:SER:OG	1:C:1033:PHE:HD1	2.03	0.41
1:C:904:VAL:O	1:C:906:PRO:N	2.54	0.41
1:A:368:PRO:HB3	1:A:409:ALA:HB1	2.02	0.41
1:A:574:THR:HG21	1:A:594:VAL:HG11	2.01	0.41
1:A:598:TYR:O	1:A:602:GLU:HB2	2.20	0.41
1:A:994:GLY:H	1:A:997:SER:HB3	1.85	0.41
1:A:995:ALA:O	1:A:996:GLY:C	2.59	0.41
1:B:314:GLU:H	1:B:315:PRO:HD3	1.86	0.41
1:B:493:CYS:O	1:B:497:LEU:HB3	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:THR:O	1:B:602:GLU:N	2.50	0.41
1:B:650:ARG:O	1:B:654:ALA:N	2.44	0.41
1:C:601:LYS:C	1:C:603:LYS:N	2.74	0.41
1:A:781:MET:HE2	1:C:225:VAL:N	2.32	0.41
1:B:46:SER:HA	1:B:88:VAL:O	2.21	0.41
1:B:445:ILE:HG13	1:B:940:LYS:CG	2.50	0.41
1:C:189:ASN:HD22	1:C:190:PRO:N	2.18	0.41
1:A:111:LEU:O	1:A:113:LEU:N	2.53	0.41
1:A:551:GLY:O	1:A:555:LEU:HD23	2.21	0.41
1:B:20:MET:CG	1:B:374:VAL:HA	2.51	0.41
1:B:72:ILE:HD11	1:B:75:LEU:HD22	2.01	0.41
1:B:485:ALA:HA	1:B:489:THR:HB	2.02	0.41
1:C:425:LEU:H	1:C:426:PRO:HD3	1.85	0.41
1:A:53:ASP:O	1:A:54:ALA:C	2.58	0.41
1:A:69:MET:CE	1:A:107:VAL:HG13	2.51	0.41
1:A:534:ILE:HB	1:A:541:TYR:CE2	2.56	0.41
1:A:568:ASP:OD1	1:A:634:TRP:CZ3	2.74	0.41
1:A:617:PHE:CE1	1:A:626:ILE:HD11	2.55	0.41
1:A:681:ASP:H	1:A:863:SER:HB3	1.86	0.41
1:B:254:ASN:HD22	1:B:254:ASN:HA	1.58	0.41
1:C:13:TRP:O	1:C:17:ILE:HG13	2.20	0.41
1:C:119:PRO:HG2	1:C:122:VAL:CG2	2.51	0.41
1:C:350:LEU:HD21	1:C:984:LEU:HD22	2.03	0.41
1:C:569:GLN:C	1:C:634:TRP:HZ2	2.24	0.41
1:C:1022:VAL:N	1:C:1023:PRO:CD	2.82	0.41
1:A:706:ALA:HB1	1:A:716:VAL:HG11	2.02	0.41
1:B:535:LEU:HD11	1:B:1023:PRO:O	2.20	0.41
1:B:704:ALA:O	1:B:705:GLU:CB	2.64	0.41
1:C:735:LYS:O	1:C:739:LEU:HD13	2.20	0.41
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.56	0.41
1:A:133:SER:C	1:A:135:SER:H	2.23	0.41
1:A:316:PHE:O	1:A:317:PHE:C	2.60	0.41
1:A:414:GLU:C	1:A:416:VAL:H	2.23	0.41
1:A:451:ALA:C	1:A:453:PHE:N	2.74	0.41
1:A:516:PHE:CE2	1:A:520:PHE:HB2	2.56	0.41
1:A:724:THR:HG22	1:A:725:PRO:O	2.21	0.41
1:B:157:TYR:HA	1:B:161:ASN:HD22	1.86	0.41
1:B:181:GLN:HE21	1:B:181:GLN:HB3	1.52	0.41
1:B:280:GLU:CB	1:B:284:GLN:O	2.63	0.41
1:B:369:THR:O	1:B:372:VAL:HG13	2.21	0.41
1:B:439:GLN:HA	1:B:442:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:TYR:O	1:B:543:VAL:N	2.54	0.41
1:B:578:LEU:HD23	1:B:578:LEU:N	2.36	0.41
1:B:764:ASP:C	1:B:766:GLY:H	2.24	0.41
1:B:1004:GLY:O	1:B:1006:GLY:N	2.54	0.41
1:B:1012:VAL:HG23	1:B:1013:THR:H	1.83	0.41
1:C:158:VAL:HG11	1:C:177:LEU:CD2	2.49	0.41
1:C:189:ASN:ND2	1:C:191:ASN:N	2.66	0.41
1:C:648:THR:OG1	1:C:649:MET:N	2.53	0.41
1:C:648:THR:O	1:C:649:MET:C	2.59	0.41
1:C:712:MET:SD	1:C:843:LEU:HD22	2.61	0.41
1:C:836:SER:HB3	1:C:839:GLU:HG3	2.03	0.41
1:C:919:ARG:HB3	1:C:921:LEU:HD23	2.03	0.41
1:C:950:LYS:HA	1:C:953:MET:HE1	1.99	0.41
1:C:997:SER:OG	1:C:998:GLY:N	2.54	0.41
1:A:38:ILE:HD13	1:A:38:ILE:H	1.86	0.41
1:A:873:ALA:HB3	1:A:874:PRO:CD	2.48	0.41
1:A:886:LEU:HD12	1:A:886:LEU:HA	1.94	0.41
1:A:1029:VAL:O	1:A:1030:ARG:CB	2.66	0.41
1:B:370:ILE:HD13	1:B:370:ILE:HA	1.93	0.41
1:B:415:ASN:HD21	1:B:971:ARG:HG2	1.86	0.41
1:B:1033:PHE:O	1:B:1034:SER:CB	2.68	0.41
1:A:20:MET:HG2	1:A:377:LEU:HD22	2.01	0.40
1:A:113:LEU:HD23	1:C:127:VAL:O	2.21	0.40
1:A:213:GLN:HE21	1:A:213:GLN:HB2	1.74	0.40
1:A:409:ALA:O	1:A:410:ILE:C	2.59	0.40
1:B:40:PRO:HB2	1:B:94:PHE:O	2.21	0.40
1:B:265:VAL:HG22	1:B:265:VAL:O	2.20	0.40
1:B:761:ASP:HB3	1:B:768:VAL:HG13	2.04	0.40
1:B:986:VAL:HG12	1:B:990:VAL:HG22	2.01	0.40
1:C:223:PRO:HA	1:C:224:PRO:HD3	1.92	0.40
1:C:323:ILE:HG22	1:C:325:TYR:CE1	2.56	0.40
1:C:930:GLY:HA3	1:C:1007:VAL:HG22	2.03	0.40
1:A:742:SER:O	1:A:744:ASN:N	2.55	0.40
1:A:758:TYR:CE1	1:A:770:LYS:HB3	2.56	0.40
1:A:911:GLY:CA	1:A:914:LEU:HB2	2.49	0.40
1:B:115:MET:SD	1:B:127:VAL:HG11	2.61	0.40
1:B:909:VAL:O	1:B:913:LEU:HD22	2.21	0.40
1:C:693:GLU:O	1:C:694:LYS:C	2.60	0.40
1:C:815:ARG:CZ	3:C:2002:RFP:H302	2.50	0.40
1:C:965:LEU:HB3	1:C:966:ASP:H	1.61	0.40
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:VAL:O	1:A:337:ILE:HB	2.22	0.40
1:A:578:LEU:CD2	1:A:587:THR:HG23	2.52	0.40
1:A:701:GLN:O	1:A:702:LEU:C	2.60	0.40
1:A:961:ILE:HD12	1:A:1031:ARG:HH22	1.86	0.40
1:B:63:GLN:O	1:B:64:VAL:C	2.60	0.40
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.56	0.40
1:B:327:TYR:CD2	1:B:628:PHE:HB3	2.57	0.40
1:C:210:GLN:HE22	1:C:250:LEU:H	1.69	0.40
1:C:631:LEU:HB2	1:C:637:ARG:NH2	2.36	0.40
1:C:1015:THR:O	1:C:1019:ILE:HB	2.22	0.40
1:A:126:GLY:CA	1:B:116:PRO:HB3	2.43	0.40
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.96	0.40
1:A:959:GLY:C	1:A:961:ILE:N	2.74	0.40
1:B:5:PHE:HB3	1:B:12:ALA:HB2	2.03	0.40
1:B:223:PRO:HA	1:B:224:PRO:HD3	1.83	0.40
1:B:289:LEU:CD1	1:B:289:LEU:N	2.84	0.40
1:B:613:ASN:O	1:B:615:PHE:N	2.49	0.40
1:B:754:TRP:CH2	1:B:785:ASP:HB2	2.54	0.40
1:C:686:ASP:OD2	1:C:690:LEU:N	2.54	0.40
1:C:717:ARG:NH2	3:C:2002:RFP:O8	2.53	0.40
3:C:2002:RFP:H311	3:C:2002:RFP:H323	2.03	0.40
1:A:12:ALA:O	1:A:488:LEU:HD13	2.21	0.40
1:A:883:VAL:O	1:A:883:VAL:HG12	2.20	0.40
1:A:923:ASN:C	1:A:923:ASN:ND2	2.75	0.40
1:B:4:PHE:O	1:B:5:PHE:CB	2.69	0.40
1:B:262:LEU:HA	1:B:265:VAL:HG12	2.04	0.40
1:B:541:TYR:C	1:B:543:VAL:N	2.75	0.40
1:B:910:ILE:C	1:B:912:ALA:H	2.25	0.40
1:C:34:GLN:HB2	1:C:35:TYR:CZ	2.56	0.40
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.56	0.40
1:C:832:ALA:CB	1:C:833:PRO:CD	2.99	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%)	752 (74%)	173 (17%)	93 (9%)	1 4
1	B	1018/1053 (97%)	730 (72%)	201 (20%)	87 (8%)	1 5
1	C	1018/1053 (97%)	760 (75%)	178 (18%)	80 (8%)	1 6
All	All	3054/3159 (97%)	2242 (73%)	552 (18%)	260 (8%)	1 5

All (260) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	181	GLN
1	A	182	TYR
1	A	282	ASN
1	A	293	LEU
1	A	294	ALA
1	A	319	SER
1	A	388	PHE
1	A	392	THR
1	A	439	GLN
1	A	580	ALA
1	A	601	LYS
1	A	659	LYS
1	A	661	ALA
1	A	677	ALA
1	A	678	THR
1	A	713	LEU
1	A	715	SER
1	A	746	ILE
1	A	831	ALA
1	A	893	GLU
1	A	960	LEU
1	A	992	SER
1	A	1016	VAL
1	B	2	PRO
1	B	22	ALA
1	B	54	ALA
1	B	124	GLN
1	B	147	GLY
1	B	228	GLN
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	326	PRO
1	B	358	PHE
1	B	583	THR
1	B	601	LYS
1	B	633	ASP
1	B	638	PRO
1	B	640	GLU
1	B	656	SER
1	B	669	PRO
1	B	671	ILE
1	B	675	GLY
1	B	676	THR
1	B	733	GLN
1	B	775	SER
1	B	806	SER
1	B	918	PHE
1	B	1016	VAL
1	B	1021	PHE
1	B	1034	SER
1	C	226	LYS
1	C	266	ALA
1	C	326	PRO
1	C	463	THR
1	C	464	GLY
1	C	520	PHE
1	C	553	ALA
1	C	580	ALA
1	C	602	GLU
1	C	678	THR
1	C	720	GLY
1	C	806	SER
1	C	832	ALA
1	C	869	SER
1	C	872	GLN
1	C	905	VAL
1	C	921	LEU
1	C	960	LEU
1	C	965	LEU
1	C	993	THR
1	C	998	GLY
1	A	19	ILE
1	A	52	ALA

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Mol	Chain	Res	Type
1	A	64	VAL
1	A	95	GLU
1	A	134	SER
1	A	170	SER
1	A	221	GLY
1	A	256	ASP
1	A	354	VAL
1	A	358	PHE
1	A	362	PHE
1	A	424	GLY
1	A	428	LYS
1	A	460	GLY
1	A	534	ILE
1	A	638	PRO
1	A	675	GLY
1	A	743	ILE
1	A	870	GLY
1	A	903	LEU
1	A	958	LYS
1	A	975	ILE
1	A	988	PRO
1	A	998	GLY
1	A	1017	LEU
1	A	1034	SER
1	B	140	VAL
1	B	216	ALA
1	B	227	GLY
1	B	243	THR
1	B	361	ASN
1	B	486	LEU
1	B	542	LEU
1	B	580	ALA
1	B	613	ASN
1	B	654	ALA
1	B	666	PHE
1	B	672	VAL
1	B	690	LEU
1	B	705	GLU
1	B	834	GLY
1	B	852	PRO
1	B	899	PHE
1	B	953	MET

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Mol	Chain	Res	Type
1	B	1005	THR
1	C	86	GLY
1	C	255	GLN
1	C	438	ILE
1	C	521	GLU
1	C	601	LYS
1	C	656	SER
1	C	674	LEU
1	C	711	ASP
1	C	713	LEU
1	C	952	LEU
1	C	953	MET
1	C	997	SER
1	C	1027	VAL
1	A	53	ASP
1	A	112	GLN
1	A	167	SER
1	A	174	ASP
1	A	236	ALA
1	A	436	GLY
1	A	452	VAL
1	A	618	ALA
1	B	167	SER
1	B	222	THR
1	B	319	SER
1	B	360	GLN
1	B	439	GLN
1	B	517	ASN
1	B	540	ARG
1	B	553	ALA
1	B	585	GLU
1	B	618	ALA
1	B	655	PHE
1	B	677	ALA
1	B	723	ASP
1	B	765	ARG
1	B	794	ALA
1	B	889	ALA
1	B	968	VAL
1	C	285	PRO
1	C	328	ASP
1	C	336	SER

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Mol	Chain	Res	Type
1	C	427	PRO
1	C	468	ARG
1	C	554	TYR
1	C	555	LEU
1	C	620	ARG
1	C	636	ASP
1	C	658	ILE
1	C	712	MET
1	C	721	LEU
1	C	722	GLU
1	C	756	GLY
1	C	873	ALA
1	C	994	GLY
1	A	317	PHE
1	A	376	LEU
1	A	427	PRO
1	A	517	ASN
1	A	539	GLY
1	A	953	MET
1	A	987	MET
1	B	120	GLN
1	B	127	VAL
1	B	453	PHE
1	B	796	GLY
1	B	820	ASN
1	B	909	VAL
1	C	377	LEU
1	C	425	LEU
1	C	497	LEU
1	C	541	TYR
1	C	675	GLY
1	C	802	SER
1	C	885	PHE
1	C	974	PRO
1	C	983	ILE
1	A	133	SER
1	A	180	SER
1	A	334	LYS
1	A	347	ALA
1	A	421	ALA
1	A	456	MET
1	A	689	GLY

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Mol	Chain	Res	Type
1	A	1030	ARG
1	B	440	GLY
1	B	442	LEU
1	B	515	TRP
1	B	614	GLY
1	B	851	LEU
1	B	974	PRO
1	B	1017	LEU
1	C	62	THR
1	C	477	ALA
1	C	552	MET
1	C	825	MET
1	C	964	THR
1	C	967	ALA
1	A	9	PRO
1	A	18	ILE
1	A	220	GLY
1	A	268	ILE
1	A	318	PRO
1	A	330	THR
1	A	360	GLN
1	A	496	MET
1	A	687	GLN
1	B	125	GLN
1	B	283	GLY
1	B	602	GLU
1	B	921	LEU
1	C	332	PHE
1	C	343	THR
1	C	751	GLY
1	C	784	ASP
1	C	1005	THR
1	C	1035	ARG
1	A	105	VAL
1	A	351	VAL
1	B	86	GLY
1	C	1028	VAL
1	A	38	ILE
1	A	335	ILE
1	B	975	ILE
1	C	935	ILE
1	C	1006	GLY

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Mol	Chain	Res	Type
1	A	15	ILE
1	A	139	VAL
1	A	320	GLY
1	A	410	ILE
1	A	787	GLY
1	B	201	VAL
1	B	306	ILE
1	C	15	ILE
1	A	461	GLY
1	B	223	PRO
1	B	647	ILE
1	B	874	PRO
1	B	961	ILE
1	C	222	THR
1	C	224	PRO
1	C	671	ILE
1	C	975	ILE
1	C	1016	VAL
1	A	340	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	833/859 (97%)	707 (85%)	126 (15%)	3	13
1	B	833/859 (97%)	708 (85%)	125 (15%)	3	13
1	C	833/859 (97%)	715 (86%)	118 (14%)	3	15
All	All	2499/2577 (97%)	2130 (85%)	369 (15%)	3	13

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	13	TRP
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	38	ILE
1	A	44	THR
1	A	49	TYR
1	A	58	GLN
1	A	60	THR
1	A	63	GLN
1	A	65	ILE
1	A	69	MET
1	A	70	ASN
1	A	76	MET
1	A	96	SER
1	A	105	VAL
1	A	108	GLN
1	A	109	ASN
1	A	110	LYS
1	A	117	LEU
1	A	120	GLN
1	A	164	ASP
1	A	181	GLN
1	A	193	LEU
1	A	207	ILE
1	A	210	GLN
1	A	213	GLN
1	A	225	VAL
1	A	226	LYS
1	A	234	ILE
1	A	243	THR
1	A	250	LEU
1	A	255	GLN
1	A	277	ILE
1	A	284	GLN
1	A	293	LEU
1	A	298	ASN
1	A	302	THR
1	A	323	ILE
1	A	337	ILE
1	A	341	VAL
1	A	358	PHE
1	A	359	LEU
1	A	361	ASN
1	A	376	LEU
1	A	377	LEU

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Mol	Chain	Res	Type
1	A	382	VAL
1	A	394	THR
1	A	405	LEU
1	A	406	VAL
1	A	414	GLU
1	A	417	GLU
1	A	418	ARG
1	A	422	GLU
1	A	423	GLU
1	A	454	VAL
1	A	462	SER
1	A	473	THR
1	A	475	VAL
1	A	476	SER
1	A	480	LEU
1	A	483	LEU
1	A	489	THR
1	A	496	MET
1	A	516	PHE
1	A	530	SER
1	A	534	ILE
1	A	537	SER
1	A	540	ARG
1	A	544	LEU
1	A	549	VAL
1	A	556	PHE
1	A	563	PHE
1	A	576	VAL
1	A	577	GLN
1	A	578	LEU
1	A	586	ARG
1	A	589	LYS
1	A	597	TYR
1	A	603	LYS
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	636	ASP
1	A	645	GLU
1	A	658	ILE
1	A	659	LYS
1	A	668	LEU

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Mol	Chain	Res	Type
1	A	671	ILE
1	A	680	PHE
1	A	686	ASP
1	A	687	GLN
1	A	713	LEU
1	A	714	THR
1	A	741	VAL
1	A	750	LEU
1	A	768	VAL
1	A	773	VAL
1	A	780	ARG
1	A	801	PHE
1	A	808	ARG
1	A	810	GLU
1	A	815	ARG
1	A	817	GLU
1	A	822	LEU
1	A	843	LEU
1	A	844	MET
1	A	865	GLN
1	A	866	GLU
1	A	867	ARG
1	A	881	LEU
1	A	887	CYS
1	A	899	PHE
1	A	904	VAL
1	A	919	ARG
1	A	923	ASN
1	A	956	GLU
1	A	960	LEU
1	A	976	LEU
1	A	982	PHE
1	A	991	ILE
1	A	993	THR
1	A	1001	ASN
1	A	1008	MET
1	A	1011	MET
1	A	1017	LEU
1	A	1034	SER
1	B	3	ASN
1	B	8	ARG
1	B	13	TRP

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Mol	Chain	Res	Type
1	B	27	ILE
1	B	30	LEU
1	B	56	THR
1	B	60	THR
1	B	67	GLN
1	B	70	ASN
1	B	72	ILE
1	B	85	THR
1	B	88	VAL
1	B	95	GLU
1	B	104	GLN
1	B	120	GLN
1	B	121	GLU
1	B	129	VAL
1	B	137	LEU
1	B	140	VAL
1	B	145	THR
1	B	146	ASP
1	B	149	MET
1	B	150	THR
1	B	153	ASP
1	B	155	SER
1	B	156	ASP
1	B	169	THR
1	B	170	SER
1	B	176	GLN
1	B	181	GLN
1	B	189	ASN
1	B	190	PRO
1	B	194	ASN
1	B	199	THR
1	B	225	VAL
1	B	230	LEU
1	B	238	THR
1	B	243	THR
1	B	244	GLU
1	B	253	VAL
1	B	254	ASN
1	B	261	LEU
1	B	280	GLU
1	B	289	LEU
1	B	291	ILE

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Mol	Chain	Res	Type
1	B	292	LYS
1	B	293	LEU
1	B	314	GLU
1	B	324	VAL
1	B	327	TYR
1	B	330	THR
1	B	337	ILE
1	B	343	THR
1	B	359	LEU
1	B	372	VAL
1	B	406	VAL
1	B	408	ASP
1	B	410	ILE
1	B	411	VAL
1	B	414	GLU
1	B	415	ASN
1	B	435	MET
1	B	438	ILE
1	B	448	VAL
1	B	449	LEU
1	B	452	VAL
1	B	459	PHE
1	B	473	THR
1	B	480	LEU
1	B	488	LEU
1	B	497	LEU
1	B	515	TRP
1	B	516	PHE
1	B	520	PHE
1	B	536	ARG
1	B	540	ARG
1	B	547	ILE
1	B	559	LEU
1	B	571	VAL
1	B	589	LYS
1	B	601	LYS
1	B	606	VAL
1	B	607	GLU
1	B	620	ARG
1	B	629	VAL
1	B	649	MET
1	B	653	ARG

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Mol	Chain	Res	Type
1	B	655	PHE
1	B	668	LEU
1	B	669	PRO
1	B	674	LEU
1	B	690	LEU
1	B	693	GLU
1	B	696	THR
1	B	702	LEU
1	B	712	MET
1	B	741	VAL
1	B	743	ILE
1	B	750	LEU
1	B	758	TYR
1	B	770	LYS
1	B	774	MET
1	B	779	TYR
1	B	782	LEU
1	B	788	ASP
1	B	795	ASP
1	B	813	SER
1	B	842	GLU
1	B	851	LEU
1	B	879	ILE
1	B	891	LEU
1	B	900	SER
1	B	913	LEU
1	B	952	LEU
1	B	954	ASP
1	B	956	GLU
1	B	960	LEU
1	B	966	ASP
1	B	978	THR
1	B	989	LEU
1	B	1007	VAL
1	B	1020	PHE
1	B	1022	VAL
1	B	1027	VAL
1	B	1034	SER
1	C	8	ARG
1	C	13	TRP
1	C	32	VAL
1	C	35	TYR

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Mol	Chain	Res	Type
1	C	38	ILE
1	C	44	THR
1	C	48	SER
1	C	49	TYR
1	C	56	THR
1	C	63	GLN
1	C	84	SER
1	C	89	GLN
1	C	91	THR
1	C	96	SER
1	C	112	GLN
1	C	119	PRO
1	C	124	GLN
1	C	125	GLN
1	C	127	VAL
1	C	128	SER
1	C	133	SER
1	C	134	SER
1	C	150	THR
1	C	158	VAL
1	C	177	LEU
1	C	189	ASN
1	C	226	LYS
1	C	230	LEU
1	C	239	ARG
1	C	244	GLU
1	C	253	VAL
1	C	259	ARG
1	C	274	ASN
1	C	306	ILE
1	C	316	PHE
1	C	324	VAL
1	C	325	TYR
1	C	339	GLU
1	C	344	LEU
1	C	349	ILE
1	C	350	LEU
1	C	351	VAL
1	C	355	MET
1	C	356	TYR
1	C	367	ILE
1	C	370	ILE

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Mol	Chain	Res	Type
1	C	379	THR
1	C	394	THR
1	C	400	LEU
1	C	402	ILE
1	C	408	ASP
1	C	416	VAL
1	C	418	ARG
1	C	429	GLU
1	C	432	ARG
1	C	471	SER
1	C	472	ILE
1	C	480	LEU
1	C	492	LEU
1	C	493	CYS
1	C	497	LEU
1	C	521	GLU
1	C	525	HIS
1	C	529	ASP
1	C	542	LEU
1	C	544	LEU
1	C	566	ASP
1	C	571	VAL
1	C	577	GLN
1	C	578	LEU
1	C	588	GLN
1	C	591	LEU
1	C	596	HIS
1	C	605	ASN
1	C	624	THR
1	C	636	ASP
1	C	644	VAL
1	C	659	LYS
1	C	681	ASP
1	C	684	LEU
1	C	685	ILE
1	C	686	ASP
1	C	687	GLN
1	C	695	LEU
1	C	697	GLN
1	C	699	ARG
1	C	713	LEU
1	C	714	THR

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Mol	Chain	Res	Type
1	C	715	SER
1	C	722	GLU
1	C	724	THR
1	C	731	ILE
1	C	745	ASP
1	C	750	LEU
1	C	759	VAL
1	C	760	ASN
1	C	779	TYR
1	C	799	VAL
1	C	808	ARG
1	C	847	LEU
1	C	849	SER
1	C	851	LEU
1	C	868	LEU
1	C	869	SER
1	C	871	ASN
1	C	879	ILE
1	C	900	SER
1	C	901	VAL
1	C	907	LEU
1	C	922	THR
1	C	931	LEU
1	C	941	ASN
1	C	954	ASP
1	C	982	PHE
1	C	1017	LEU
1	C	1029	VAL
1	C	1033	PHE
1	C	1035	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	67	GLN
1	A	89	GLN
1	A	104	GLN
1	A	106	GLN
1	A	108	GLN
1	A	109	ASN
1	A	120	GLN

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Mol	Chain	Res	Type
1	A	181	GLN
1	A	191	ASN
1	A	210	GLN
1	A	213	GLN
1	A	254	ASN
1	A	282	ASN
1	A	298	ASN
1	A	360	GLN
1	A	361	ASN
1	A	577	GLN
1	A	584	GLN
1	A	687	GLN
1	A	709	HIS
1	A	719	ASN
1	A	726	GLN
1	A	830	GLN
1	A	846	GLN
1	A	923	ASN
1	A	928	GLN
1	A	1001	ASN
1	B	34	GLN
1	B	68	ASN
1	B	70	ASN
1	B	74	ASN
1	B	104	GLN
1	B	106	GLN
1	B	108	GLN
1	B	112	GLN
1	B	120	GLN
1	B	124	GLN
1	B	125	GLN
1	B	144	ASN
1	B	161	ASN
1	B	189	ASN
1	B	210	GLN
1	B	213	GLN
1	B	228	GLN
1	B	231	ASN
1	B	254	ASN
1	B	274	ASN
1	B	338	HIS
1	B	415	ASN

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Mol	Chain	Res	Type
1	B	517	ASN
1	B	526	HIS
1	B	569	GLN
1	B	605	ASN
1	B	642	ASN
1	B	692	HIS
1	B	744	ASN
1	B	846	GLN
1	B	865	GLN
1	C	63	GLN
1	C	68	ASN
1	C	89	GLN
1	C	104	GLN
1	C	109	ASN
1	C	123	GLN
1	C	124	GLN
1	C	125	GLN
1	C	144	ASN
1	C	176	GLN
1	C	189	ASN
1	C	197	GLN
1	C	210	GLN
1	C	211	ASN
1	C	213	GLN
1	C	231	ASN
1	C	274	ASN
1	C	577	GLN
1	C	588	GLN
1	C	657	GLN
1	C	726	GLN
1	C	737	GLN
1	C	760	ASN
1	C	871	ASN
1	C	872	GLN
1	C	928	GLN
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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MIY	A	2001	-	35,36,36	1.89	3 (8%)	41,58,58	1.90	12 (29%)
3	RFP	C	2002	-	63,63,63	1.97	3 (4%)	94,94,94	1.86	15 (15%)

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	MIY	A	2001	-	-	7/12/70/70	0/4/4/4
3	RFP	C	2002	-	-	18/60/85/85	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2002	RFP	O4-C11	13.30	1.43	1.21
2	A	2001	MIY	O5-C15	9.81	1.44	1.23
3	C	2002	RFP	O7-C35	5.54	1.47	1.35
3	C	2002	RFP	O5-C29	3.37	1.48	1.39
2	A	2001	MIY	C18-C1	-2.45	1.51	1.55
2	A	2001	MIY	C16-C15	2.15	1.52	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2002	RFP	O4-C11-C5	-8.62	115.37	131.81
3	C	2002	RFP	C41-C42-N4	6.18	117.78	110.80
2	A	2001	MIY	O5-C15-C14	-5.82	110.99	121.99
2	A	2001	MIY	O5-C15-C16	-5.31	112.64	120.78
3	C	2002	RFP	O7-C35-C36	4.62	119.60	111.09
3	C	2002	RFP	O4-C11-C12	-4.29	111.82	120.56
3	C	2002	RFP	C42-N4-C39	4.21	115.42	109.52
3	C	2002	RFP	C12-O5-C29	3.57	126.67	117.84
3	C	2002	RFP	O3-C6-C7	3.56	127.26	121.14
3	C	2002	RFP	C3-C43-N2	3.50	126.62	121.54
3	C	2002	RFP	C30-C16-C17	-3.42	115.14	123.42
3	C	2002	RFP	C2-C3-C43	-3.00	121.12	124.17
2	A	2001	MIY	C15-C16-C17	2.93	121.12	118.80
2	A	2001	MIY	O6-C17-C16	-2.90	119.93	123.90
3	C	2002	RFP	C12-C11-C5	-2.83	101.75	107.30
2	A	2001	MIY	O2-C3-C2	-2.54	118.51	122.96
2	A	2001	MIY	C71-N7-CN7	-2.50	108.08	116.12
3	C	2002	RFP	C4-C3-C43	2.42	119.41	116.52
2	A	2001	MIY	C18-C1-C2	2.38	119.54	115.75
2	A	2001	MIY	O6-C17-C18	2.36	116.79	113.37
3	C	2002	RFP	C40-C39-N4	2.34	113.45	110.80
2	A	2001	MIY	C14-C15-C16	-2.28	114.64	118.53
3	C	2002	RFP	C39-C40-N3	2.18	114.05	110.51
2	A	2001	MIY	C11-C10-N7	-2.10	118.62	121.59
2	A	2001	MIY	C13-C14-C15	-2.10	118.40	121.47
2	A	2001	MIY	C18-C5-C4	2.06	114.45	111.64
3	C	2002	RFP	O7-C25-C24	2.00	112.16	107.50

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	MIY	C1-C2-C21-O8
2	A	2001	MIY	C3-C2-C21-O8
2	A	2001	MIY	C1-C2-C21-N2
2	A	2001	MIY	C3-C2-C21-N2
2	A	2001	MIY	C5-C4-N1-C20
3	C	2002	RFP	C4-C3-C43-N2
3	C	2002	RFP	C26-C27-O6-C37
3	C	2002	RFP	C28-C27-O6-C37
3	C	2002	RFP	C43-N2-N3-C40

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Mol	Chain	Res	Type	Atoms
3	C	2002	RFP	C43-N2-N3-C41
3	C	2002	RFP	O6-C27-C28-C29
3	C	2002	RFP	C2-C3-C43-N2
3	C	2002	RFP	C32-C22-C23-C24
3	C	2002	RFP	C23-C24-C25-C26
3	C	2002	RFP	C21-C22-C23-C24
3	C	2002	RFP	C34-C26-C27-C28
3	C	2002	RFP	C32-C22-C23-O9
3	C	2002	RFP	C25-C26-C27-C28
2	A	2001	MIY	C3-C4-N1-C19
2	A	2001	MIY	C5-C4-N1-C19
3	C	2002	RFP	C33-C24-C25-C26
3	C	2002	RFP	C23-C24-C25-O7
3	C	2002	RFP	C34-C26-C27-O6
3	C	2002	RFP	C25-C26-C27-O6
3	C	2002	RFP	C16-C17-C18-C19

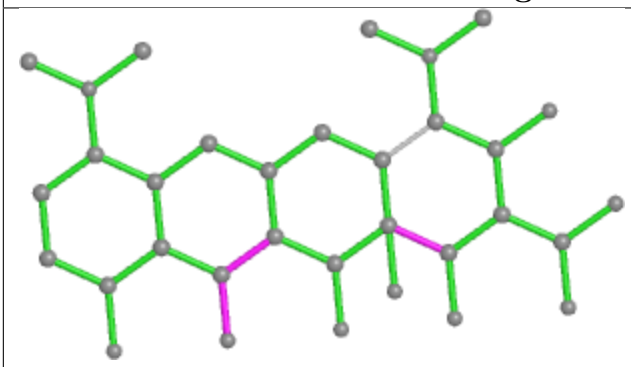
There are no ring outliers.

1 monomer is involved in 4 short contacts:

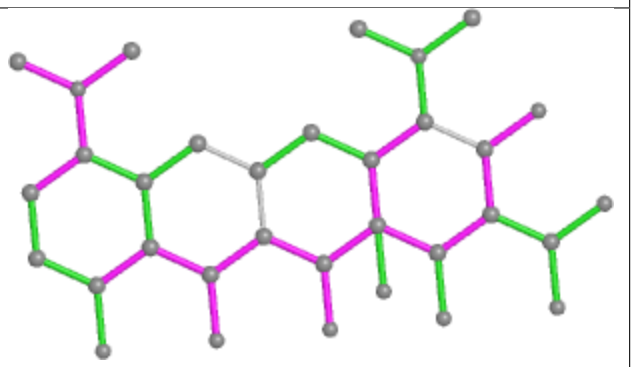
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2002	RFP	4	0

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.

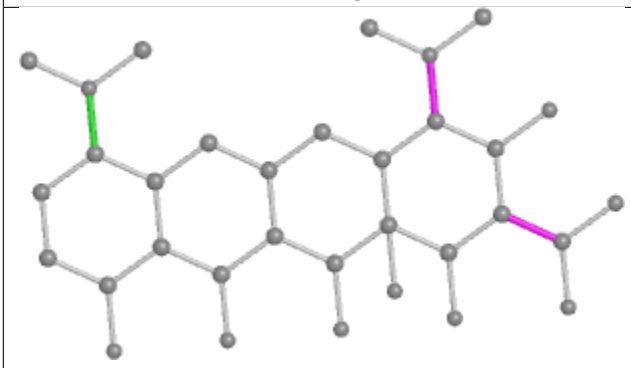
Ligand MIY A 2001



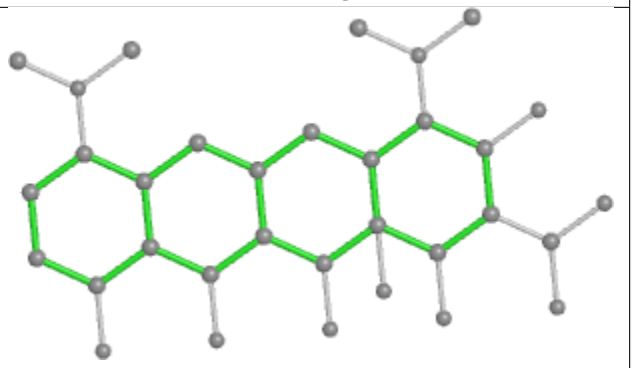
Bond lengths



Bond angles

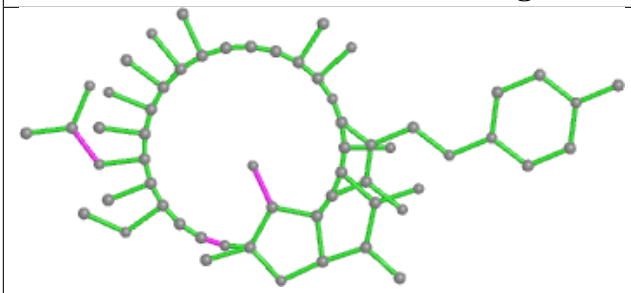


Torsions

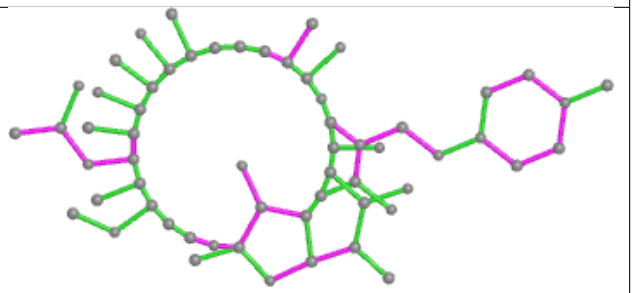


Rings

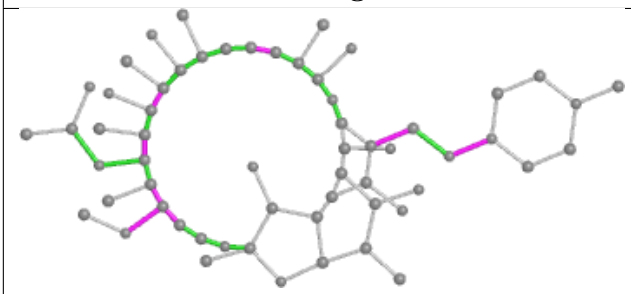
Ligand RFP C 2002



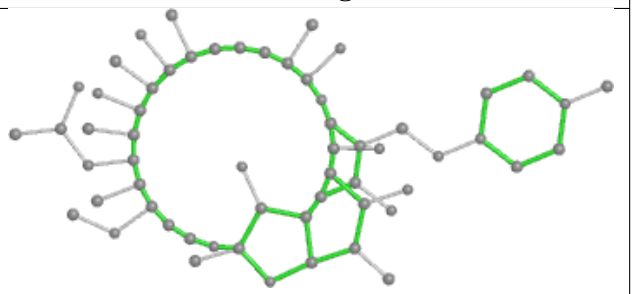
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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%)	0.03	30 (2%)	51	50	52, 102, 136, 167	0
1	B	1022/1053 (97%)	0.10	23 (2%)	60	59	65, 106, 140, 169	0
1	C	1022/1053 (97%)	-0.02	31 (3%)	50	49	49, 100, 148, 183	0
All	All	3066/3159 (97%)	0.04	84 (2%)	54	52	49, 103, 142, 183	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	872	GLN	5.8
1	C	514	GLY	5.3
1	C	515	TRP	5.1
1	A	32	VAL	4.9
1	C	425	LEU	4.8
1	C	538	THR	4.4
1	A	145	THR	4.1
1	B	993	THR	4.0
1	B	675	GLY	3.9
1	C	424	GLY	3.8
1	C	540	ARG	3.7
1	A	198	LEU	3.6
1	A	1036	LYS	3.5
1	C	676	THR	3.4
1	A	1034	SER	3.3
1	C	871	ASN	3.2
1	C	833	PRO	3.2
1	A	515	TRP	3.2
1	C	7	ASP	3.2
1	C	539	GLY	3.1
1	A	871	ASN	3.0
1	C	362	PHE	3.0
1	A	513	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	538	THR	2.9
1	A	957	GLY	2.9
1	C	513	PHE	2.9
1	A	230	LEU	2.9
1	C	497	LEU	2.8
1	B	6	ILE	2.8
1	A	1033	PHE	2.8
1	C	8	ARG	2.8
1	B	1034	SER	2.7
1	A	188	MET	2.7
1	C	537	SER	2.6
1	A	1035	ARG	2.6
1	C	671	ILE	2.6
1	C	870	GLY	2.6
1	C	357	LEU	2.6
1	A	4	PHE	2.6
1	B	424	GLY	2.6
1	B	604	ASN	2.6
1	B	1036	LYS	2.6
1	A	196	PHE	2.6
1	C	962	GLU	2.6
1	A	3	ASN	2.6
1	B	134	SER	2.5
1	C	361	ASN	2.5
1	A	390	ILE	2.5
1	A	917	THR	2.5
1	B	1035	ARG	2.5
1	B	727	PHE	2.4
1	C	1033	PHE	2.4
1	A	259	ARG	2.4
1	C	520	PHE	2.4
1	B	437	GLN	2.4
1	B	655	PHE	2.4
1	C	496	MET	2.3
1	A	958	LYS	2.3
1	B	535	LEU	2.3
1	B	253	VAL	2.3
1	A	714	THR	2.3
1	B	7	ASP	2.3
1	B	513	PHE	2.3
1	B	635	ALA	2.3
1	C	9	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	869	SER	2.2
1	A	962	GLU	2.2
1	C	257	GLY	2.2
1	A	30	LEU	2.2
1	A	427	PRO	2.2
1	A	149	MET	2.2
1	B	426	PRO	2.2
1	B	412	VAL	2.2
1	A	497	LEU	2.2
1	C	541	TYR	2.2
1	B	542	LEU	2.1
1	C	426	PRO	2.1
1	C	360	GLN	2.1
1	A	952	LEU	2.1
1	B	540	ARG	2.1
1	B	135	SER	2.1
1	A	964	THR	2.0
1	A	636	ASP	2.0
1	B	992	SER	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.

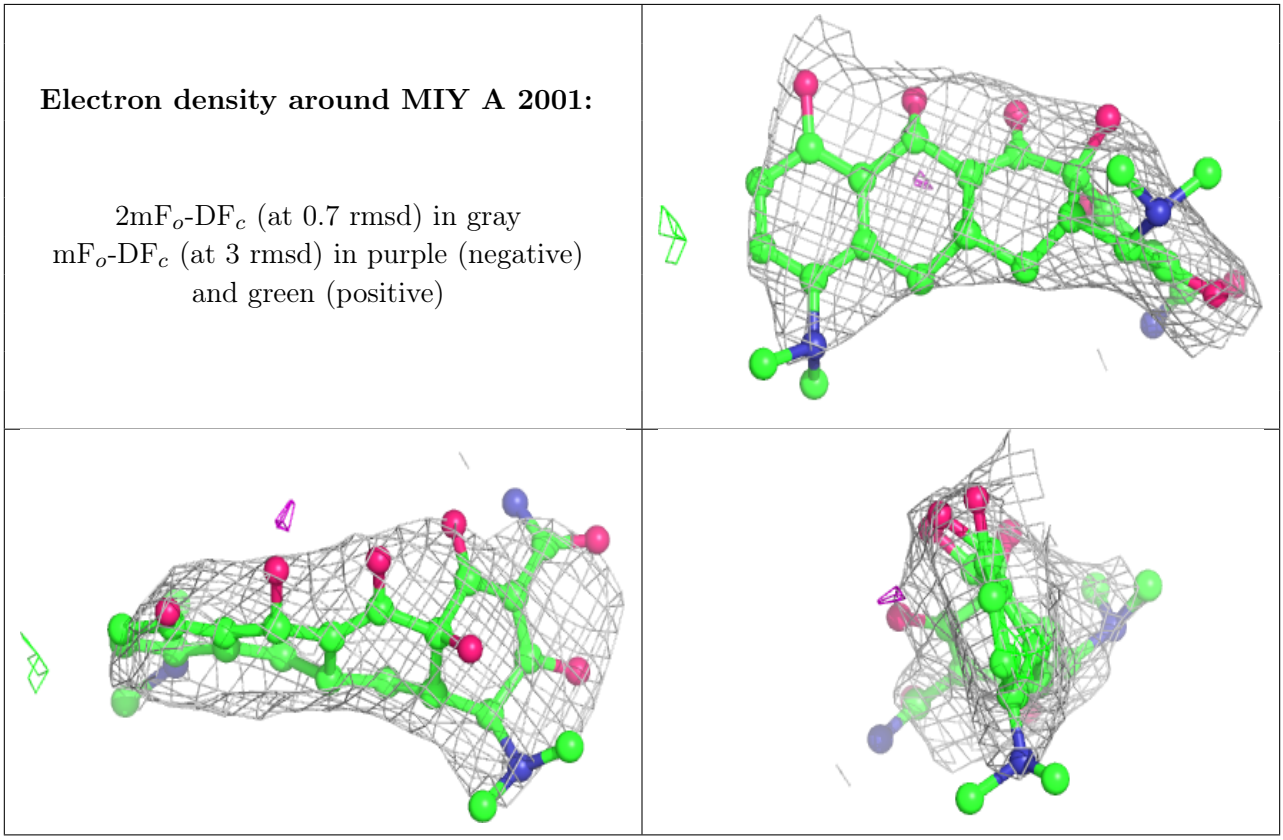
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MIY	A	2001	33/33	0.87	0.25	134,138,142,142	0
3	RFP	C	2002	59/59	0.91	0.26	131,136,139,140	0

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.

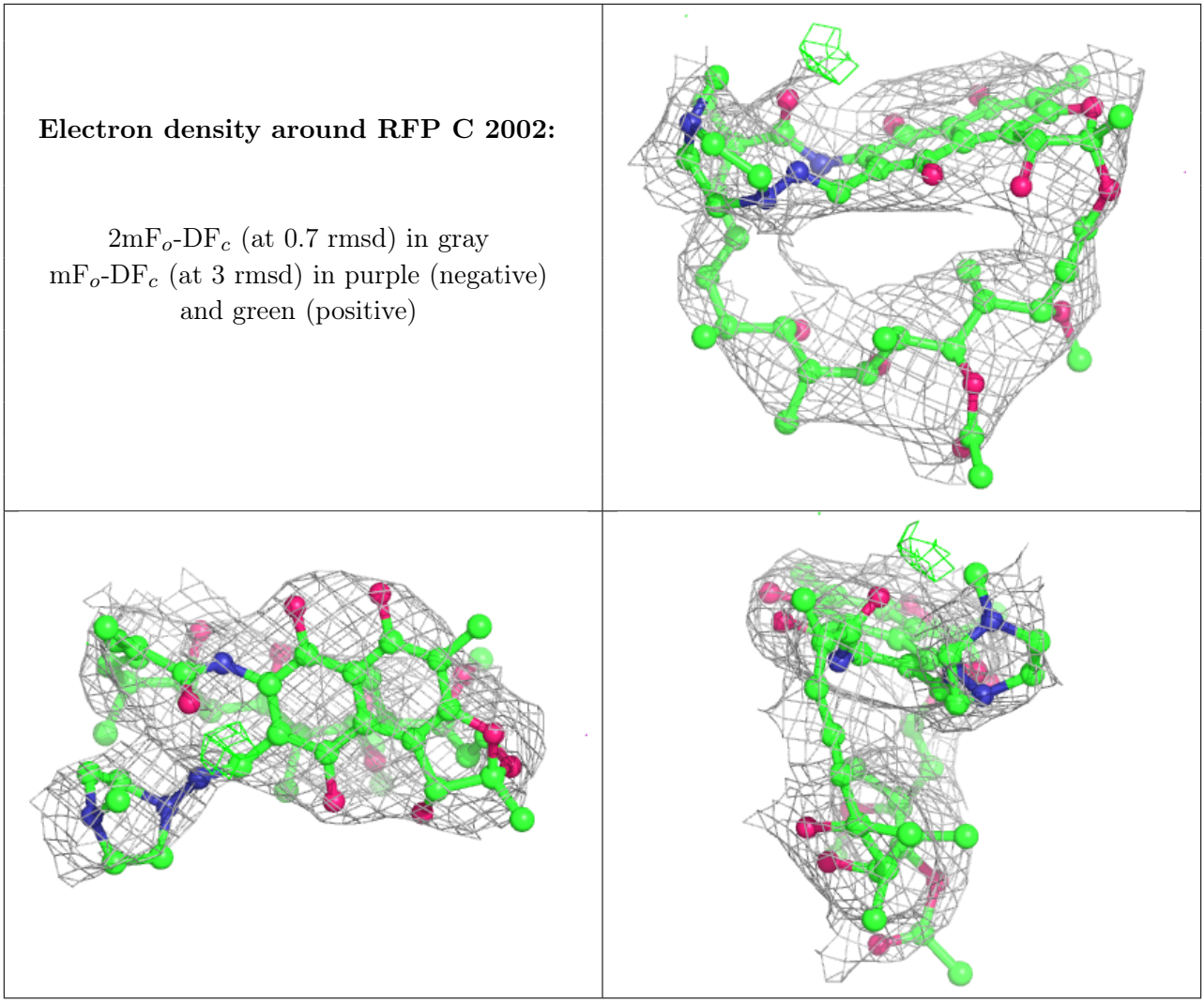
Electron density around MIY A 2001:

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



Electron density around RFP C 2002:

$2mF_o$-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.