Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 01:18 pm BST

PDB ID	:	7O3M
Title	:	Crystal Structure of AcrB Single Mutant - 1
Authors	:	Ababou, A.
Deposited on	:	2021-04-02
Resolution	:	3.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

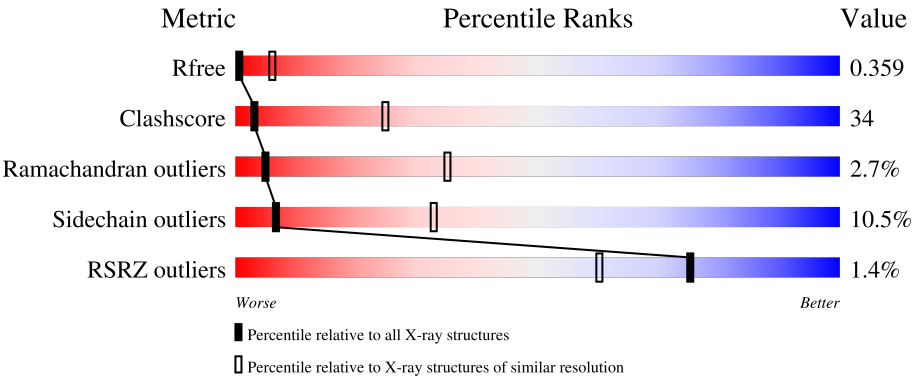
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 3.55 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	1020 (3.62-3.50)
Clashscore	141614	1100 (3.62-3.50)
Ramachandran outliers	138981	1065 (3.62-3.50)
Sidechain outliers	138945	1066 (3.62-3.50)
RSRZ outliers	127900	1009 (3.64-3.48)

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	1069	41% 51% 6%
1	B	1069	44% 45% 7%
1	C	1069	41% 49% 7%
1	D	1069	42% 48% 8%
1	E	1069	3% 38% 52% 7%

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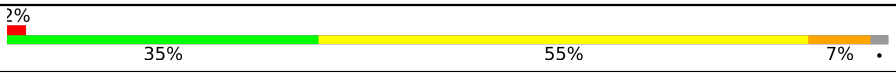
Mol	Chain	Length	Quality of chain
1	F	1069	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	A	2000	X	-	-	-
2	LMT	B	2000	X	-	-	-
2	LMT	C	2000	X	-	-	-
2	LMT	D	2000	X	-	-	-
2	LMT	E	2000	X	-	-	-
2	LMT	F	2000	X	-	-	-

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 47792 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 Efflux pump membrane transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	C	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	D	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7919	5092	1308	1476	43			
1	F	1044	Total	C	N	O	S	0	0	0
			7936	5102	1312	1479	43			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP E2QH56
A	-18	GLY	-	expression tag	UNP E2QH56
A	-17	SER	-	expression tag	UNP E2QH56
A	-16	SER	-	expression tag	UNP E2QH56
A	-15	HIS	-	expression tag	UNP E2QH56
A	-14	HIS	-	expression tag	UNP E2QH56
A	-13	HIS	-	expression tag	UNP E2QH56
A	-12	HIS	-	expression tag	UNP E2QH56
A	-11	HIS	-	expression tag	UNP E2QH56
A	-10	HIS	-	expression tag	UNP E2QH56
A	-9	SER	-	expression tag	UNP E2QH56
A	-8	SER	-	expression tag	UNP E2QH56
A	-7	GLY	-	expression tag	UNP E2QH56
A	-6	LEU	-	expression tag	UNP E2QH56
A	-5	VAL	-	expression tag	UNP E2QH56
A	-4	PRO	-	expression tag	UNP E2QH56
A	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP E2QH56
A	-1	SER	-	expression tag	UNP E2QH56
A	0	HIS	-	expression tag	UNP E2QH56
A	620	ALA	ARG	engineered mutation	UNP E2QH56
B	-19	MET	-	initiating methionine	UNP E2QH56
B	-18	GLY	-	expression tag	UNP E2QH56
B	-17	SER	-	expression tag	UNP E2QH56
B	-16	SER	-	expression tag	UNP E2QH56
B	-15	HIS	-	expression tag	UNP E2QH56
B	-14	HIS	-	expression tag	UNP E2QH56
B	-13	HIS	-	expression tag	UNP E2QH56
B	-12	HIS	-	expression tag	UNP E2QH56
B	-11	HIS	-	expression tag	UNP E2QH56
B	-10	HIS	-	expression tag	UNP E2QH56
B	-9	SER	-	expression tag	UNP E2QH56
B	-8	SER	-	expression tag	UNP E2QH56
B	-7	GLY	-	expression tag	UNP E2QH56
B	-6	LEU	-	expression tag	UNP E2QH56
B	-5	VAL	-	expression tag	UNP E2QH56
B	-4	PRO	-	expression tag	UNP E2QH56
B	-3	ARG	-	expression tag	UNP E2QH56
B	-2	GLY	-	expression tag	UNP E2QH56
B	-1	SER	-	expression tag	UNP E2QH56
B	0	HIS	-	expression tag	UNP E2QH56
B	620	ALA	ARG	engineered mutation	UNP E2QH56
C	-19	MET	-	initiating methionine	UNP E2QH56
C	-18	GLY	-	expression tag	UNP E2QH56
C	-17	SER	-	expression tag	UNP E2QH56
C	-16	SER	-	expression tag	UNP E2QH56
C	-15	HIS	-	expression tag	UNP E2QH56
C	-14	HIS	-	expression tag	UNP E2QH56
C	-13	HIS	-	expression tag	UNP E2QH56
C	-12	HIS	-	expression tag	UNP E2QH56
C	-11	HIS	-	expression tag	UNP E2QH56
C	-10	HIS	-	expression tag	UNP E2QH56
C	-9	SER	-	expression tag	UNP E2QH56
C	-8	SER	-	expression tag	UNP E2QH56
C	-7	GLY	-	expression tag	UNP E2QH56
C	-6	LEU	-	expression tag	UNP E2QH56
C	-5	VAL	-	expression tag	UNP E2QH56
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	620	ALA	ARG	engineered mutation	UNP E2QH56
D	-19	MET	-	initiating methionine	UNP E2QH56
D	-18	GLY	-	expression tag	UNP E2QH56
D	-17	SER	-	expression tag	UNP E2QH56
D	-16	SER	-	expression tag	UNP E2QH56
D	-15	HIS	-	expression tag	UNP E2QH56
D	-14	HIS	-	expression tag	UNP E2QH56
D	-13	HIS	-	expression tag	UNP E2QH56
D	-12	HIS	-	expression tag	UNP E2QH56
D	-11	HIS	-	expression tag	UNP E2QH56
D	-10	HIS	-	expression tag	UNP E2QH56
D	-9	SER	-	expression tag	UNP E2QH56
D	-8	SER	-	expression tag	UNP E2QH56
D	-7	GLY	-	expression tag	UNP E2QH56
D	-6	LEU	-	expression tag	UNP E2QH56
D	-5	VAL	-	expression tag	UNP E2QH56
D	-4	PRO	-	expression tag	UNP E2QH56
D	-3	ARG	-	expression tag	UNP E2QH56
D	-2	GLY	-	expression tag	UNP E2QH56
D	-1	SER	-	expression tag	UNP E2QH56
D	0	HIS	-	expression tag	UNP E2QH56
D	620	ALA	ARG	engineered mutation	UNP E2QH56
E	-19	MET	-	initiating methionine	UNP E2QH56
E	-18	GLY	-	expression tag	UNP E2QH56
E	-17	SER	-	expression tag	UNP E2QH56
E	-16	SER	-	expression tag	UNP E2QH56
E	-15	HIS	-	expression tag	UNP E2QH56
E	-14	HIS	-	expression tag	UNP E2QH56
E	-13	HIS	-	expression tag	UNP E2QH56
E	-12	HIS	-	expression tag	UNP E2QH56
E	-11	HIS	-	expression tag	UNP E2QH56
E	-10	HIS	-	expression tag	UNP E2QH56
E	-9	SER	-	expression tag	UNP E2QH56
E	-8	SER	-	expression tag	UNP E2QH56
E	-7	GLY	-	expression tag	UNP E2QH56
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56

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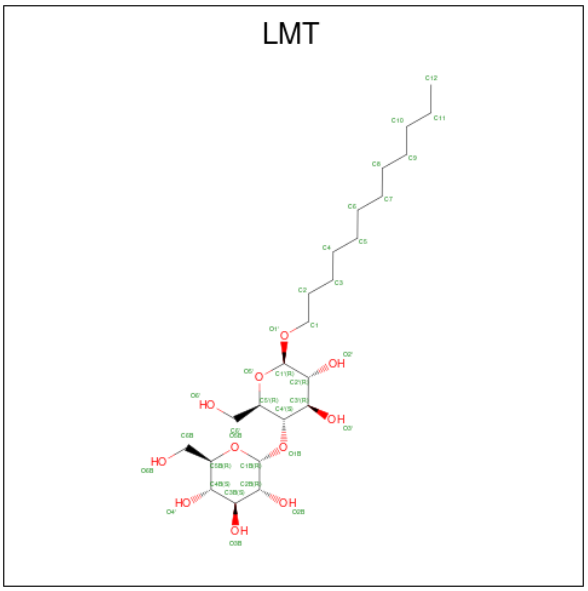
Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	620	ALA	ARG	engineered mutation	UNP E2QH56
F	-19	MET	-	initiating methionine	UNP E2QH56
F	-18	GLY	-	expression tag	UNP E2QH56
F	-17	SER	-	expression tag	UNP E2QH56
F	-16	SER	-	expression tag	UNP E2QH56
F	-15	HIS	-	expression tag	UNP E2QH56
F	-14	HIS	-	expression tag	UNP E2QH56
F	-13	HIS	-	expression tag	UNP E2QH56
F	-12	HIS	-	expression tag	UNP E2QH56
F	-11	HIS	-	expression tag	UNP E2QH56
F	-10	HIS	-	expression tag	UNP E2QH56
F	-9	SER	-	expression tag	UNP E2QH56
F	-8	SER	-	expression tag	UNP E2QH56
F	-7	GLY	-	expression tag	UNP E2QH56
F	-6	LEU	-	expression tag	UNP E2QH56
F	-5	VAL	-	expression tag	UNP E2QH56
F	-4	PRO	-	expression tag	UNP E2QH56
F	-3	ARG	-	expression tag	UNP E2QH56
F	-2	GLY	-	expression tag	UNP E2QH56
F	-1	SER	-	expression tag	UNP E2QH56
F	0	HIS	-	expression tag	UNP E2QH56
F	620	ALA	ARG	engineered mutation	UNP E2QH56

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



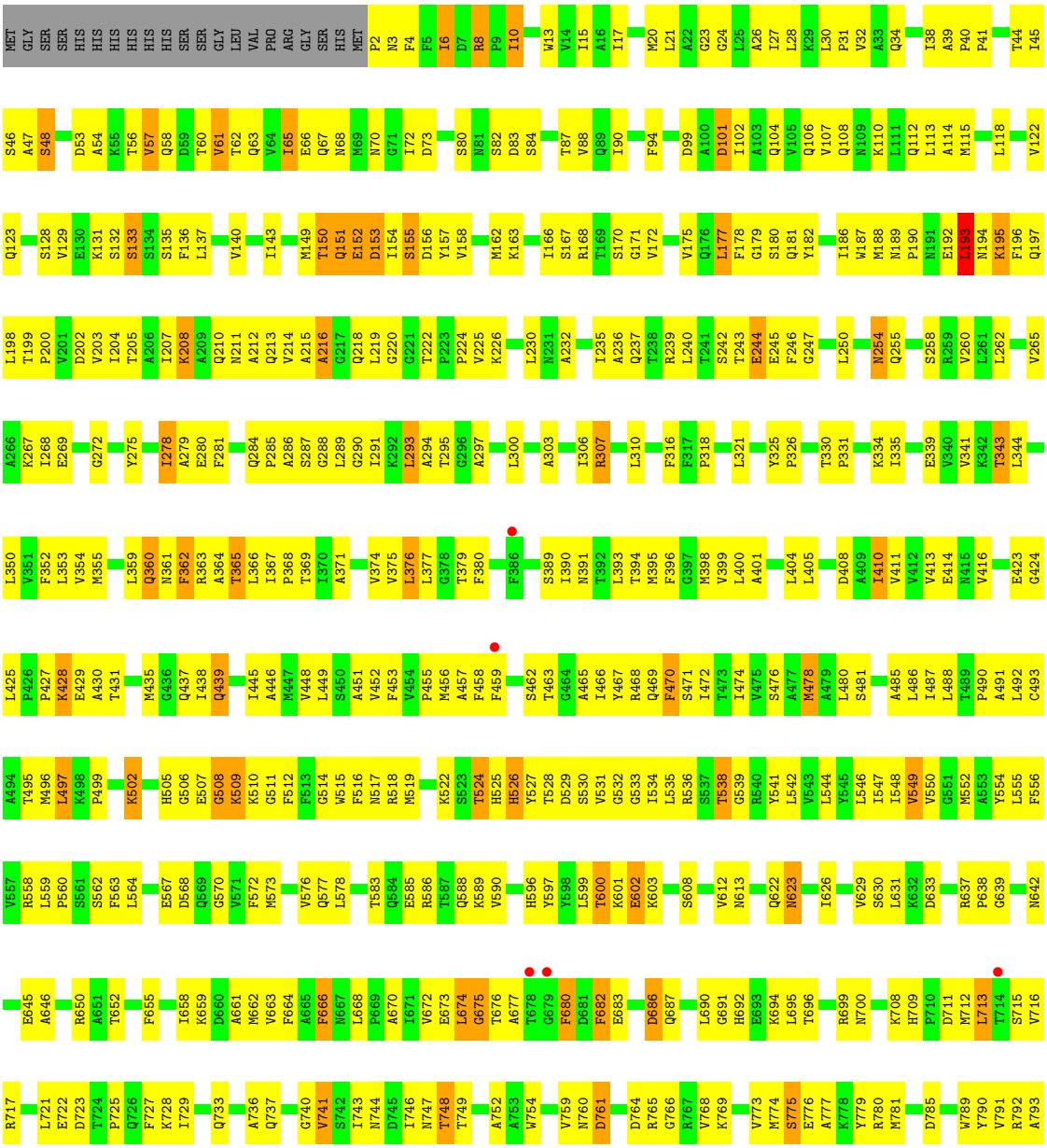
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

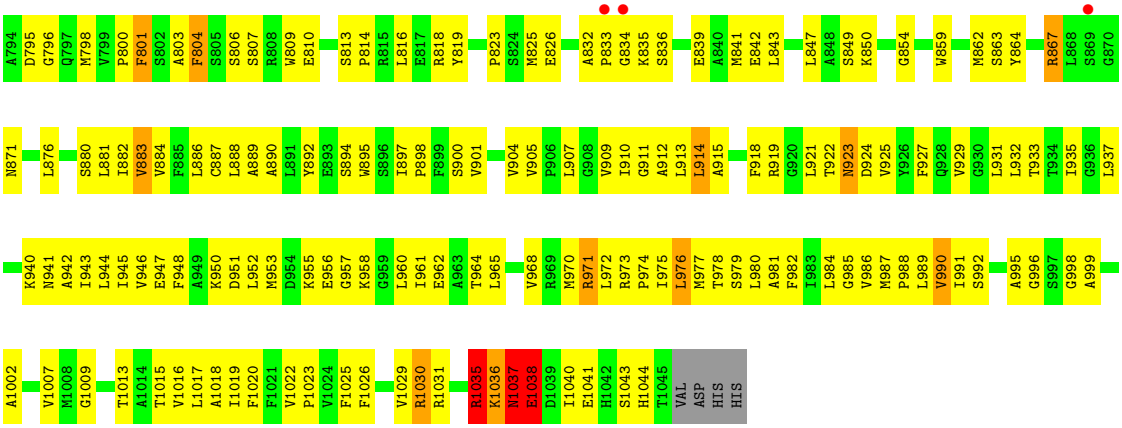
3 Residue-property plots (i)

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: Efflux pump membrane transporter

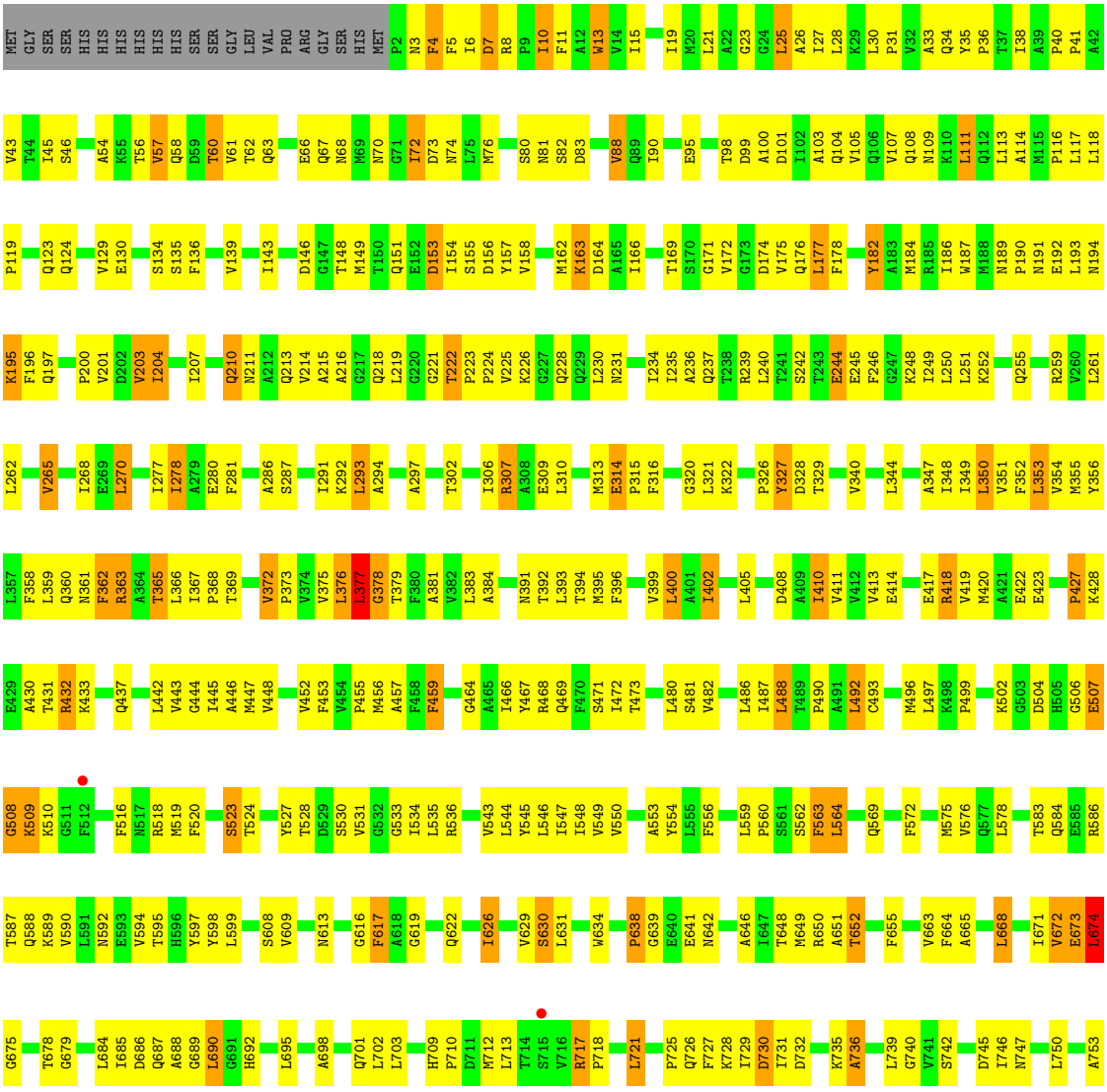
Chain A:

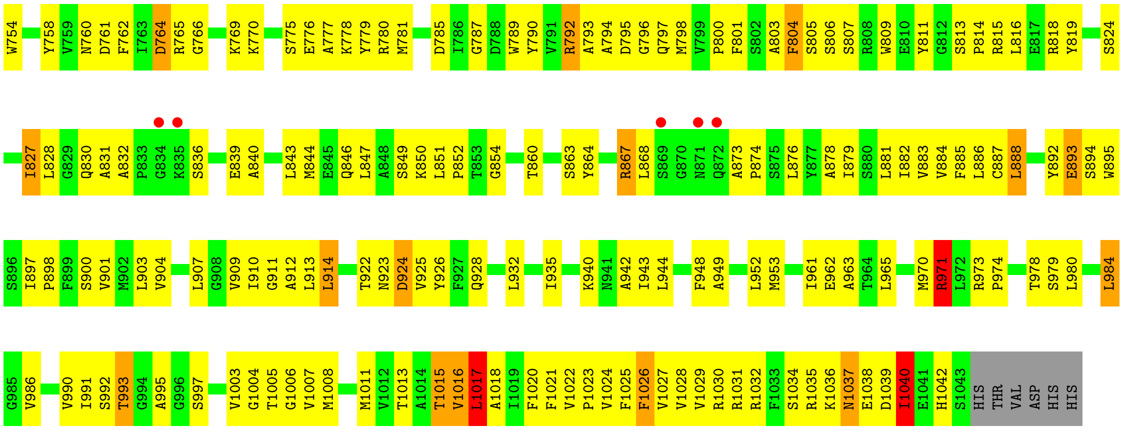




• Molecule 1: Efflux pump membrane transporter

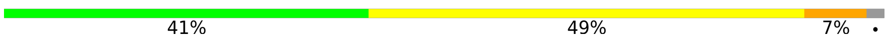
Chain B:

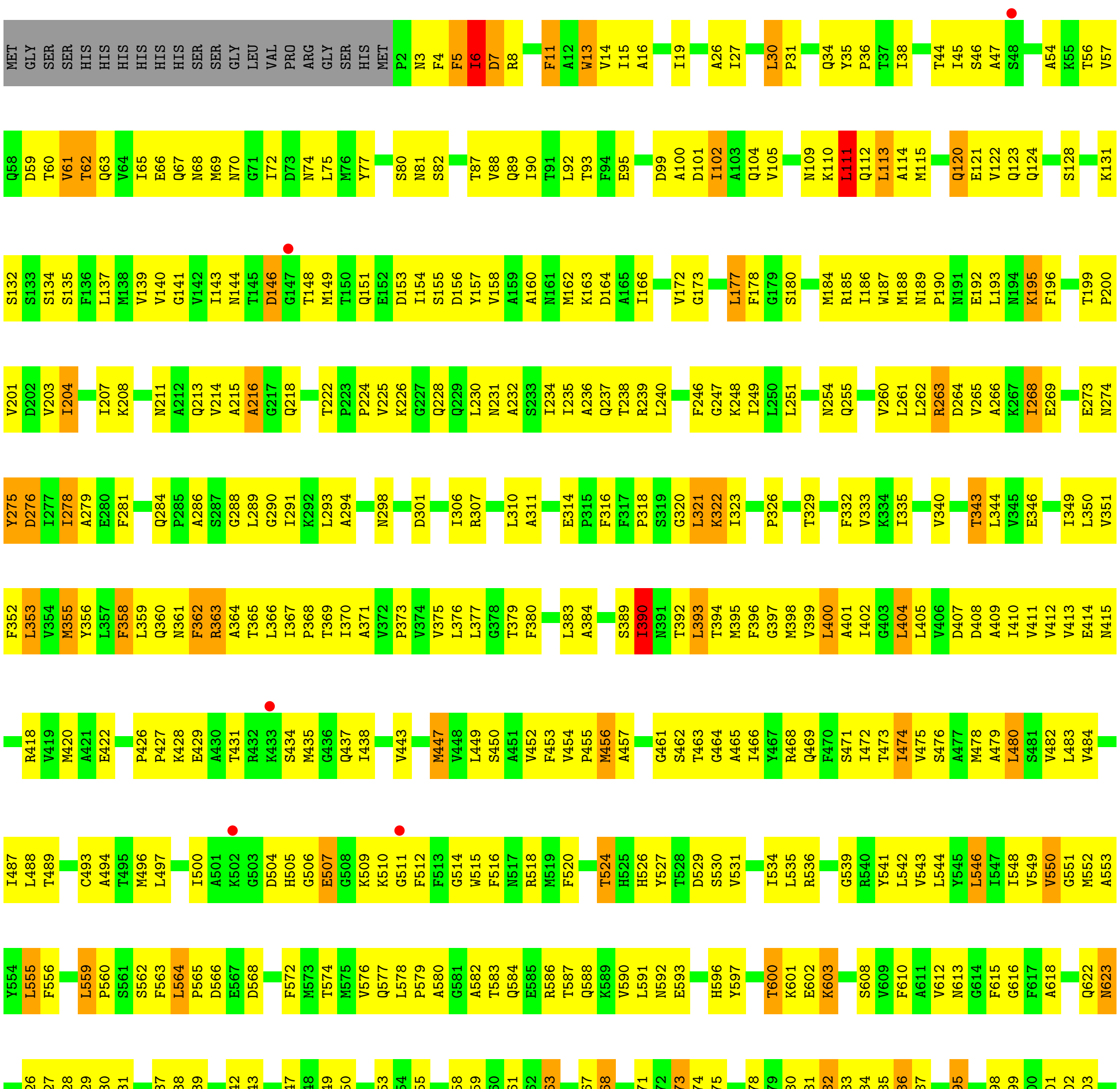


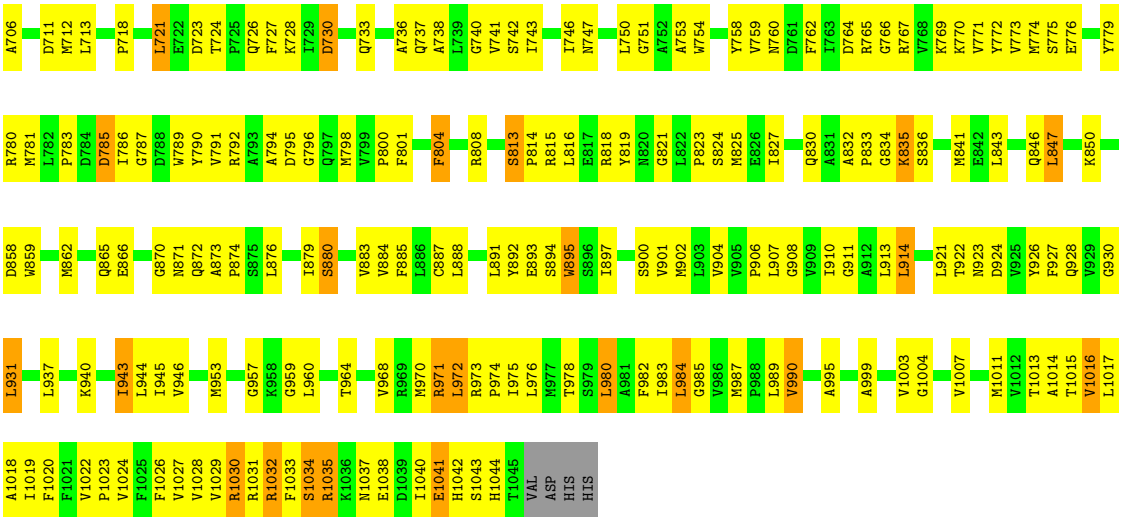


- Molecule 1: Efflux pump membrane transporter

Chain C:

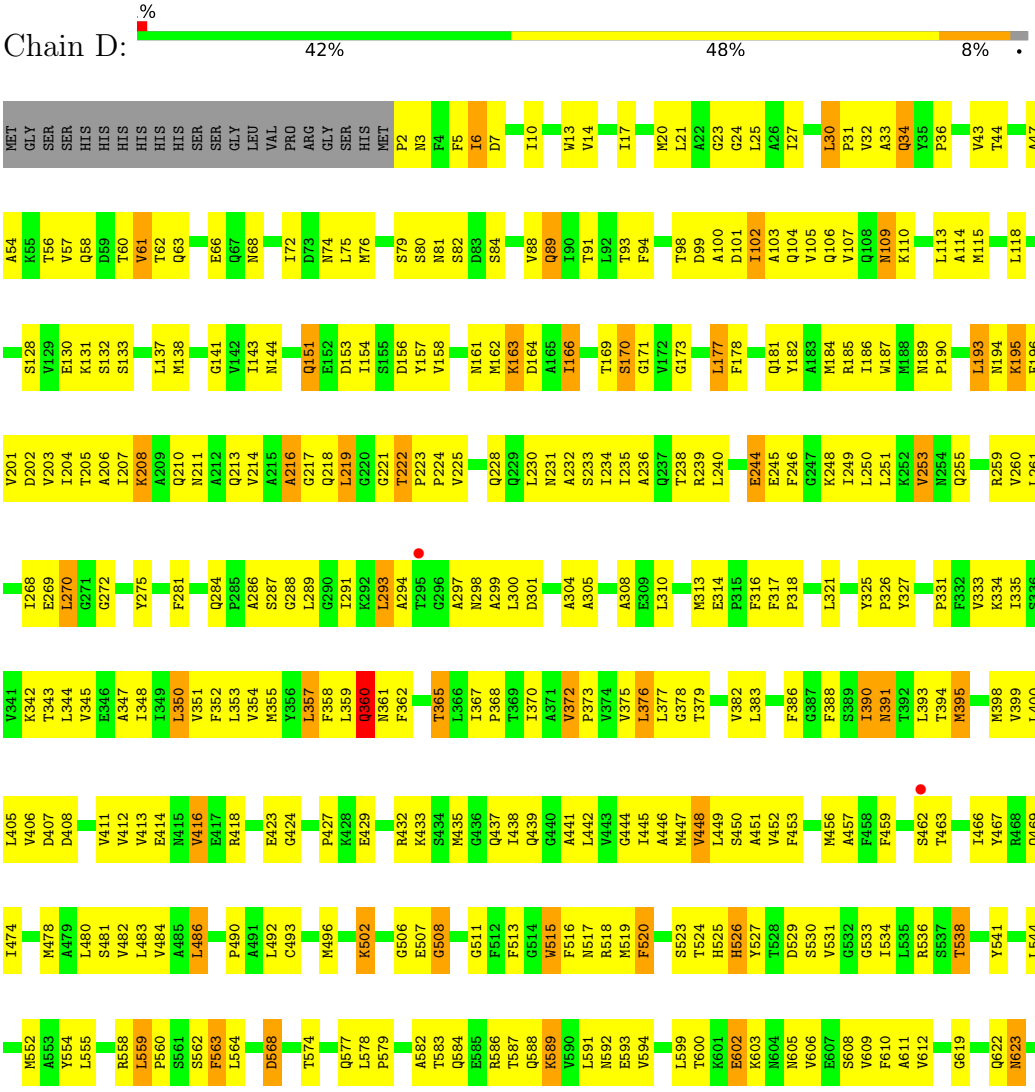


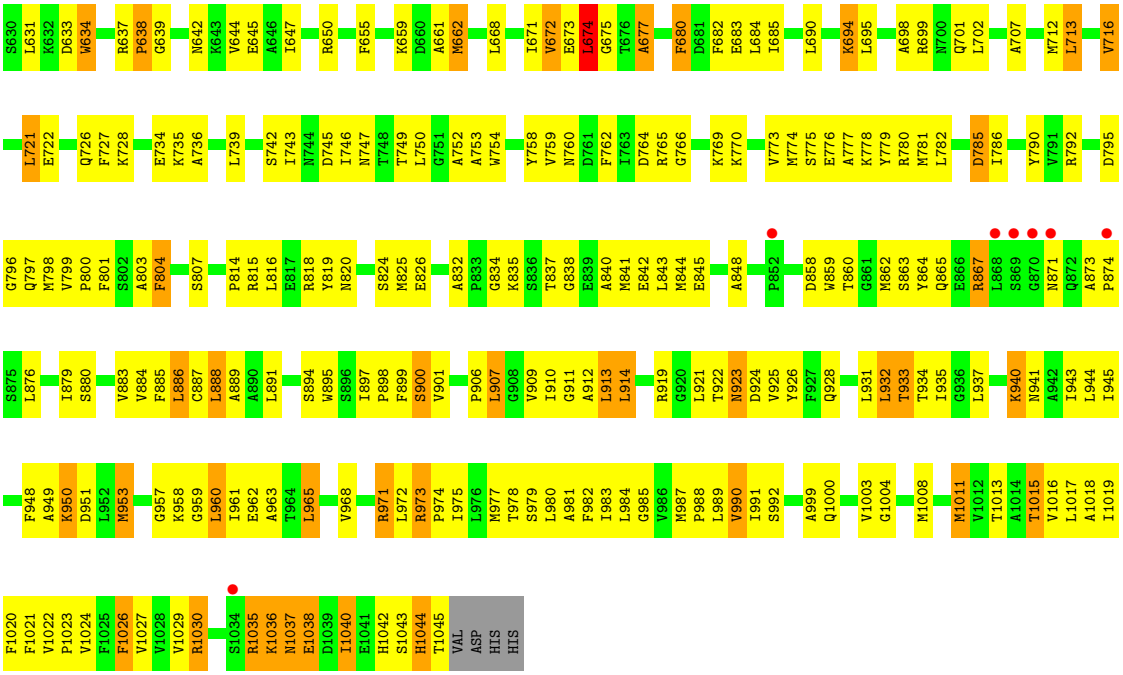




• Molecule 1: Efflux pump membrane transporter

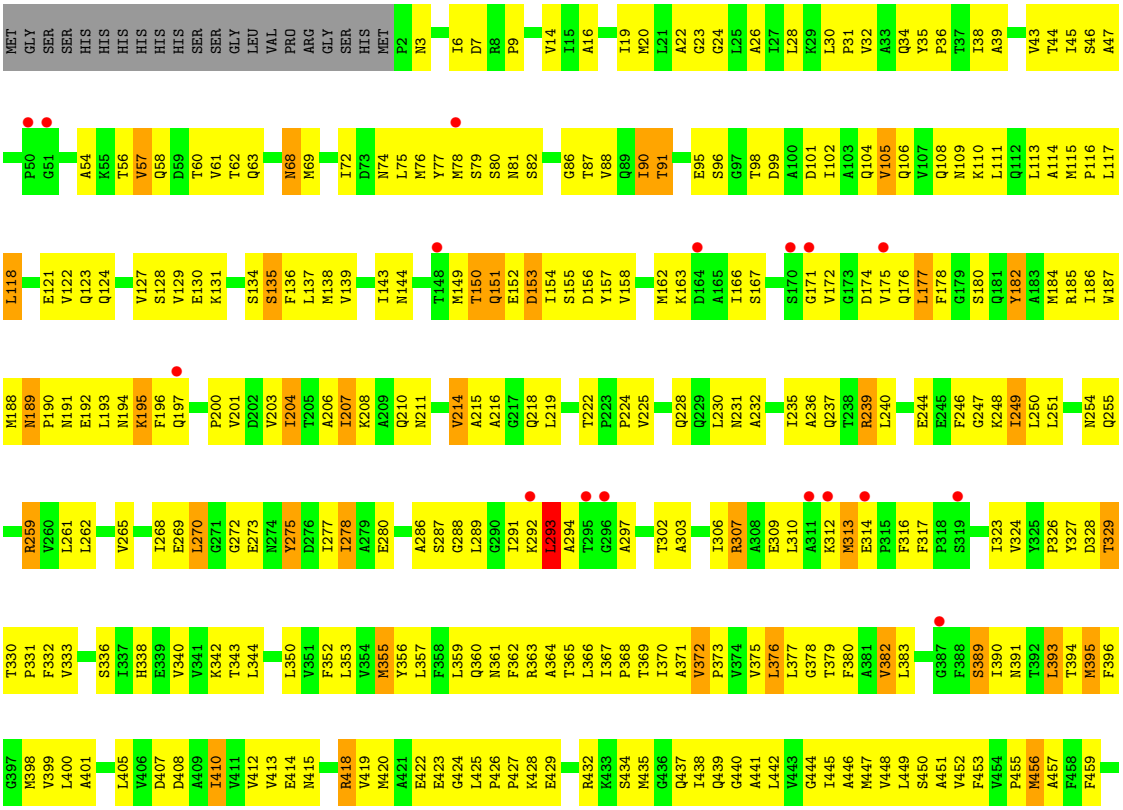
Chain D:

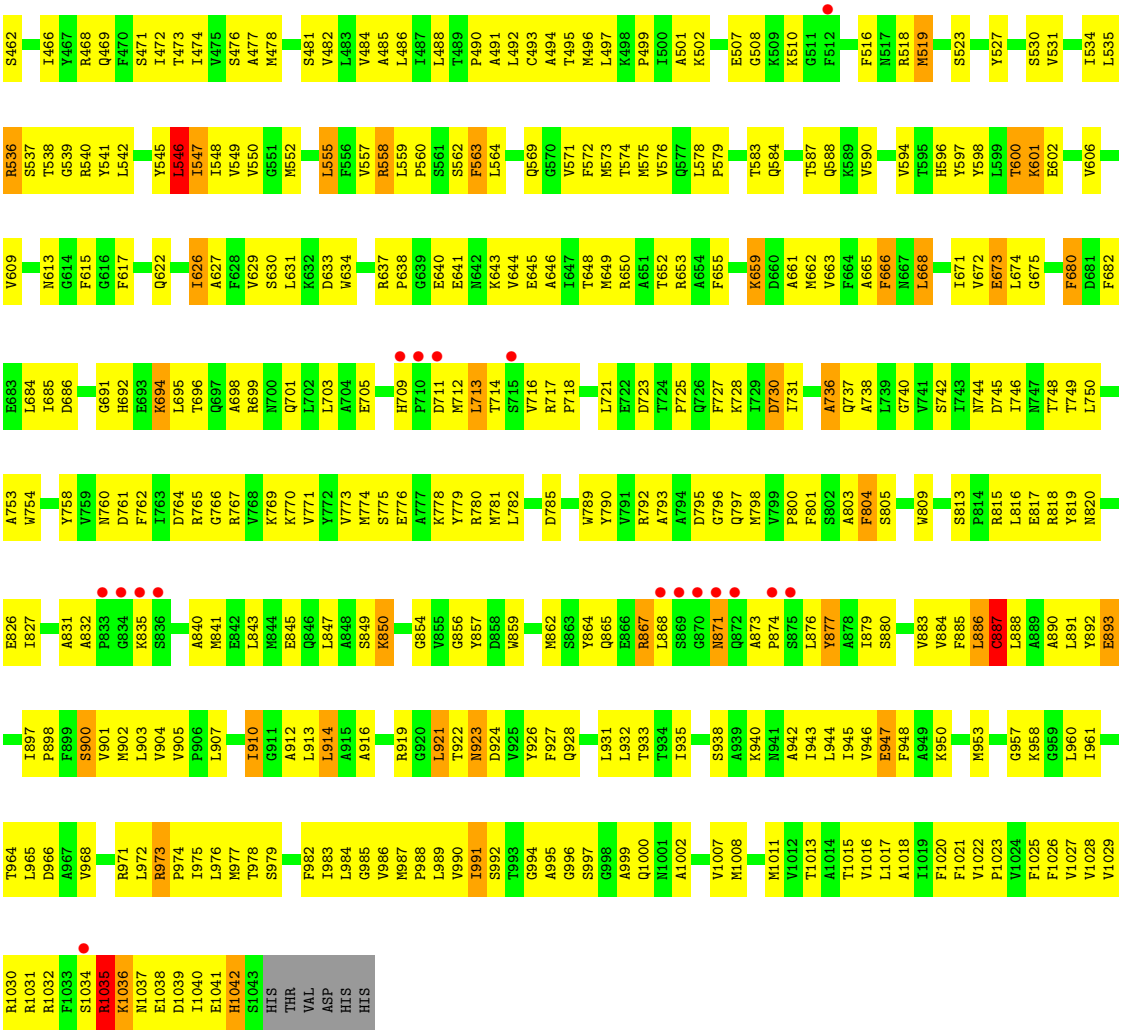




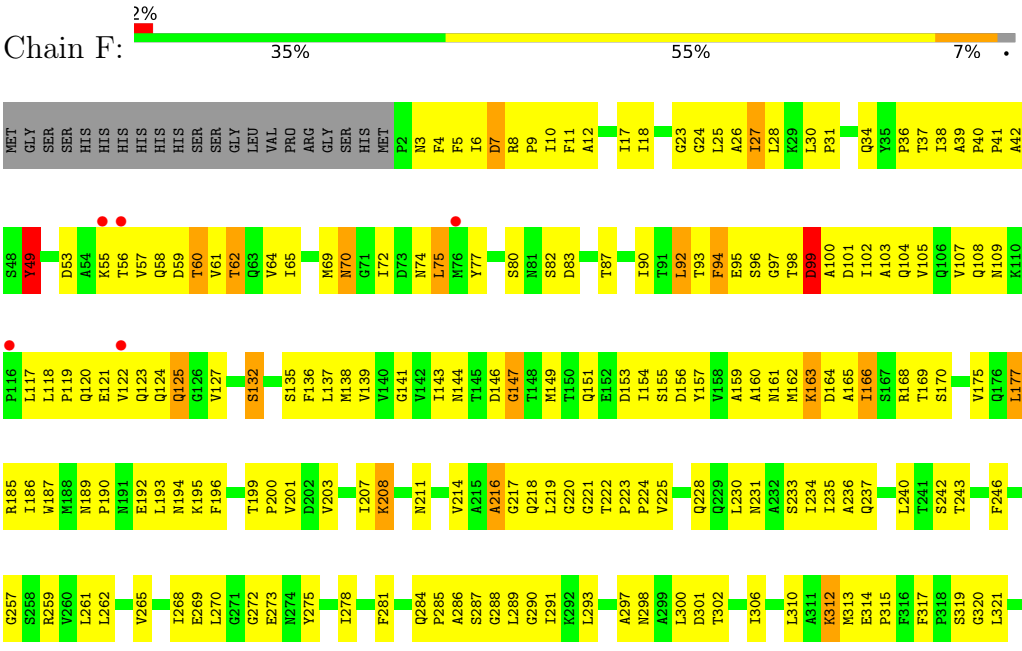
• Molecule 1: Efflux pump membrane transporter

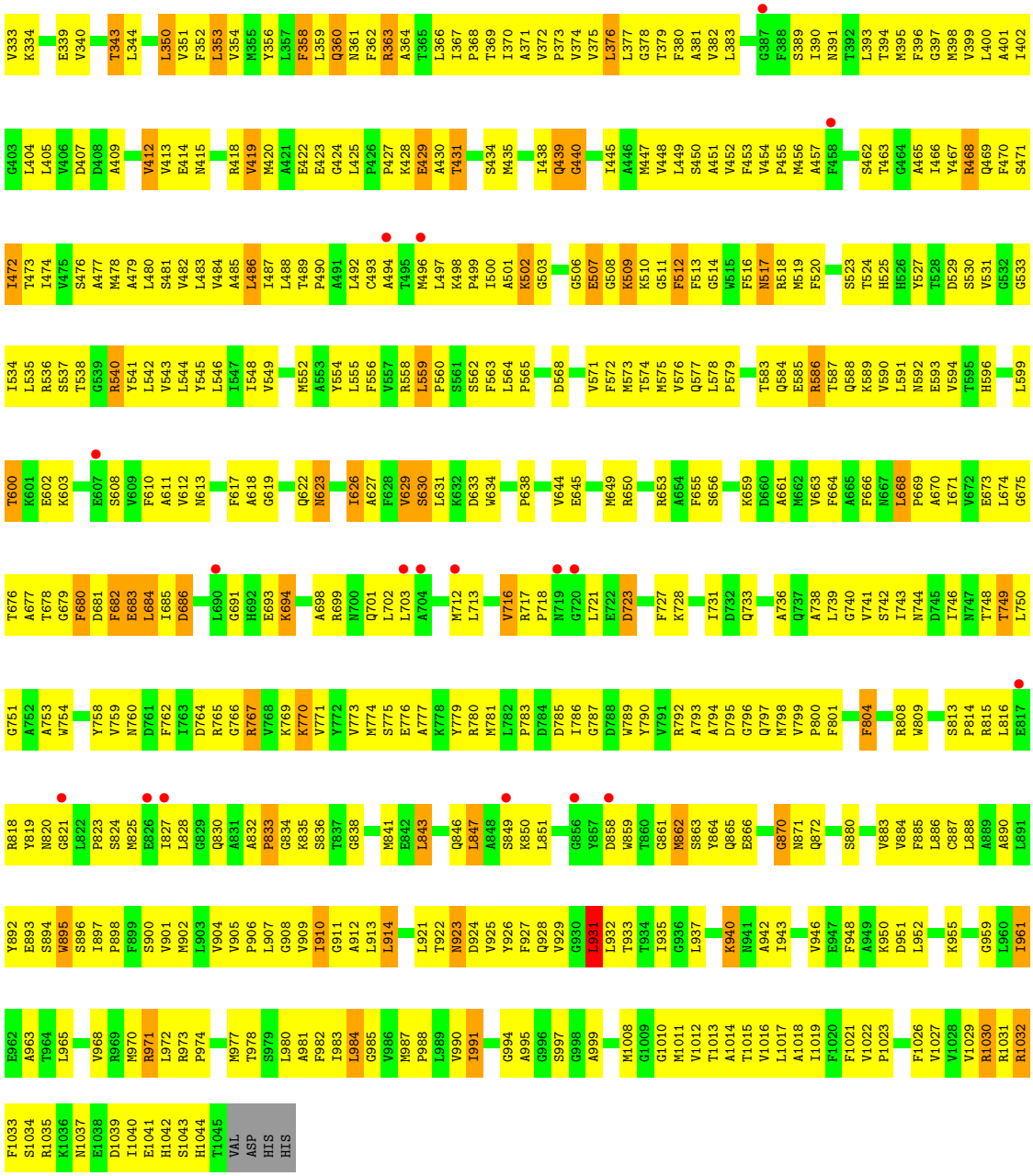
Chain E:





• Molecule 1: Efflux pump membrane transporter




V333 K334 E339 V340 T343 L344 L350 V351 F352 L353 V354 M355 Y356 L357 F358 L359 Q360 N361 F362 R363 A364 T365 L366 I367 P368 T369 I370 A371 V372 P373 V374 V375 L376 L377 G378 T379 F380 A381 V382 L383 G387 F388 S389 I390 N391 T392 L393 T394 M395 F396 G397 M398 V399 L400 A401 I402
G403 L404 L405 V406 D407 D408 A409 V412 V413 E414 N415 R418 V419 M420 A421 E422 E423 G424 L425 P426 P427 K428 E429 A430 T431 S434 M435 I438 Q439 G440 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454 P455 M456 A457 F458 S462 T463 G464 A465 I466 Y467 R468 Q469 F470 S471
I472 T473 I474 V476 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492 C493 A494 T495 M496 L497 K498 P499 I500 A501 K502 G503 G506 E507 G508 K509 K510 G511 F512 F513 G514 W515 F516 N517 R518 M519 F520 S523 T524 H525 H526 Y527 T528 D529 S530 V531 G532 G533
I534 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547 I548 V549 M552 A553 Y554 L555 F556 V557 R558 L559 P560 S561 S562 F563 L564 P565 D568 V571 F572 M573 T574 M575 V576 Q577 L578 P579 T583 Q584 E585 R586 T587 Q588 K589 V590 L591 N592 E593 V594 T595 H596 L599
T600 K601 E602 K603 E607 S608 V609 F610 A611 V612 N613 F617 A618 G619 Q622 N623 I626 A627 F628 V629 S630 L631 K632 D633 W634 P638 V644 E645 M649 R650 R653 A654 F655 S656 K659 D660 A661 M662 V663 F664 A665 F666 N667 L668 P669 A670 I671 V672 E673 L674 G675
T676 A677 T678 G679 F680 D681 F682 E683 L684 I685 D686 L690 G691 H692 E693 K694 A698 R699 N700 Q701 L702 L703 A704 M712 L713 V716 R717 P718 N719 G720 L721 E722 D723 F727 K728 I731 D732 Q733 A736 Q737 A738 L739 G740 V741 S742 I743 N744 D745 I746 N747 T748 T749 L750
G751 A752 A753 W754 Y758 V759 N760 D761 F762 I763 D764 R765 G766 R767 V768 K769 K770 V771 Y772 V773 M774 S775 E776 A777 K778 Y779 R780 M781 L782 P783 D784 D785 I786 G787 D788 W789 Y790 V791 R792 A793 A794 D795 G796 Q797 M798 V799 P800 F801 F804 R808 W809 S813 P814 R815 L816 E817
R818 Y819 N820 G821 L822 P823 S824 M825 E826 I827 L828 G829 Q830 A831 A832 P833 G834 K835 S836 T837 G838 M841 E842 L843 Q846 L847 A848 S849 K850 L851 G856 Y857 D858 W859 T860 G861 M862 S863 Y864 Q865 E866 G870 N871 Q872 S880 V883 V884 F885 L886 C887 L888 A889 A890 L891
Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 G911 A912 L913 L914 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 T933 T934 I935 G936 L937 K940 N941 A942 I943 V946 E947 F948 A949 K950 D951 L952 K955 G959 L960 I961
E962 A963 T964 L965 V968 R969 M970 R971 L972 R973 P974 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 G994 A995 G996 S997 G998 A999 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 F1026 V1027 V1028 V1029 R1030 R1031 R1032
F1033 S1034 R1035 K1036 N1037 E1038 D1039 I1040 E1041 H1042 S1043 H1044 T1045 VAL ASP HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	152.37Å 156.80Å 218.65Å 90.00° 92.48° 90.00°	Depositor
Resolution (Å)	19.95 – 3.55 19.95 – 3.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.95-3.55) 99.6 (19.95-3.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.277 , 0.359 0.277 , 0.359	Depositor DCC
R_{free} test set	6134 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	101.9	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.074 for -k,-h,-l 0.095 for k,h,-l 0.089 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4003e-05.*

[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: LMT

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	0.66	0/8088	0.88	6/10983 (0.1%)
1	B	0.69	0/8070	0.90	11/10958 (0.1%)
1	C	0.67	0/8088	0.90	12/10983 (0.1%)
1	D	0.61	1/8088 (0.0%)	0.85	7/10983 (0.1%)
1	E	0.64	0/8070	0.87	6/10958 (0.1%)
1	F	0.63	0/8088	0.88	8/10983 (0.1%)
All	All	0.65	1/48492 (0.0%)	0.88	50/65848 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	5.94	1.60	1.50

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	971	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	400	LEU	CA-CB-CG	8.33	134.46	115.30
1	F	486	LEU	CA-CB-CG	7.42	132.38	115.30
1	E	357	LEU	CA-CB-CG	7.28	132.05	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	30	LEU	CA-CB-CG	7.08	131.58	115.30
1	B	1017	LEU	CA-CB-CG	7.00	131.40	115.30
1	B	25	LEU	CA-CB-CG	6.86	131.07	115.30
1	F	49	TYR	CA-CB-CG	6.69	126.11	113.40
1	F	75	LEU	CA-CB-CG	6.46	130.16	115.30
1	B	377	LEU	CA-CB-CG	6.43	130.10	115.30
1	C	404	LEU	CB-CG-CD2	-6.27	100.34	111.00
1	E	877	TYR	CA-CB-CG	-6.07	101.88	113.40
1	B	293	LEU	CA-CB-CG	5.98	129.06	115.30
1	D	486	LEU	CA-CB-CG	5.93	128.95	115.30
1	A	497	LEU	CA-CB-CG	5.84	128.73	115.30
1	D	886	LEU	CA-CB-CG	5.74	128.50	115.30
1	C	393	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	1038	GLU	N-CA-C	-5.71	95.59	111.00
1	E	887	CYS	CA-CB-SG	-5.67	103.80	114.00
1	B	350	LEU	CA-CB-CG	-5.63	102.35	115.30
1	E	486	LEU	CA-CB-CG	5.59	128.16	115.30
1	F	684	LEU	CA-CB-CG	5.59	128.16	115.30
1	D	674	LEU	CA-CB-CG	5.55	128.06	115.30
1	F	965	LEU	CA-CB-CG	-5.53	102.59	115.30
1	D	219	LEU	CA-CB-CG	5.49	127.92	115.30
1	D	953	MET	CB-CG-SD	-5.46	96.01	112.40
1	C	390	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	A	219	LEU	CA-CB-CG	5.40	127.73	115.30
1	B	971	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	E	546	LEU	CA-CB-CG	5.37	127.64	115.30
1	B	679	GLY	N-CA-C	5.36	126.50	113.10
1	C	474	ILE	CG1-CB-CG2	-5.35	99.62	111.40
1	C	111	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	250	LEU	CA-CB-CG	5.29	127.48	115.30
1	B	488	LEU	CA-CB-CG	-5.28	103.15	115.30
1	F	931	LEU	CA-CB-CG	5.26	127.40	115.30
1	F	49	TYR	CB-CG-CD2	5.21	124.13	121.00
1	D	965	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	D	674	LEU	CB-CG-CD2	5.18	119.81	111.00
1	B	674	LEU	CA-CB-CG	5.16	127.17	115.30
1	F	838	GLY	N-CA-C	5.16	125.99	113.10
1	C	480	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	616	GLY	N-CA-C	-5.13	100.26	113.10
1	C	529	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	972	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	193	LEU	CA-CB-CG	5.08	127.00	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	293	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	515	TRP	CA-CB-CG	5.04	123.27	113.70
1	A	113	LEU	CA-CB-CG	5.03	126.86	115.30
1	B	410	ILE	CG1-CB-CG2	-5.00	100.40	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	F	7	ASP	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7936	0	8072	516	0
1	B	7919	0	8058	500	0
1	C	7936	0	8072	533	0
1	D	7936	0	8072	541	0
1	E	7919	0	8058	610	0
1	F	7936	0	8072	669	0
2	A	35	0	46	1	0
2	B	35	0	46	12	0
2	C	35	0	46	6	0
2	D	35	0	46	3	0
2	E	35	0	46	6	0
2	F	35	0	46	2	0
All	All	47792	0	48680	3253	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 34.

All (3253) 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:235:ILE:HD11	1:B:726:GLN:HB2	1.41	1.03
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.40	1.00
1:A:352:PHE:HD1	1:A:369:THR:HG1	1.09	0.99
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.41	0.99
1:D:971:ARG:HG2	1:D:974:PRO:HG2	1.47	0.96
1:C:559:LEU:HD22	1:C:560:PRO:HD2	1.47	0.95
1:B:376:LEU:O	1:B:378:GLY:N	1.99	0.95
1:D:23:GLY:HA3	1:D:377:LEU:HB3	1.48	0.94
1:A:359:LEU:O	1:A:361:ASN:N	2.00	0.94
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.49	0.94
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.50	0.93
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.49	0.93
1:D:214:VAL:HG21	1:D:236:ALA:HB3	1.48	0.93
1:D:236:ALA:O	1:E:728:LYS:NZ	2.02	0.93
1:F:586:ARG:HA	1:F:589:LYS:HD2	1.50	0.93
1:A:511:GLY:HA2	1:A:515:TRP:HE1	1.33	0.92
1:D:359:LEU:O	1:D:361:ASN:N	2.02	0.92
1:D:832:ALA:HB3	1:D:835:LYS:HD2	1.51	0.92
1:A:236:ALA:O	1:B:728:LYS:NZ	2.03	0.92
1:C:945:ILE:HG13	1:C:971:ARG:HH22	1.35	0.92
1:B:236:ALA:O	1:C:728:LYS:NZ	2.02	0.92
1:F:38:ILE:HG23	1:F:462:SER:HB3	1.51	0.92
1:B:519:MET:O	1:B:523:SER:OG	1.89	0.91
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.33	0.91
1:A:832:ALA:HB3	1:A:835:LYS:HD2	1.50	0.90
1:A:60:THR:HG22	1:C:239:ARG:HH21	1.33	0.90
1:F:359:LEU:O	1:F:361:ASN:N	2.04	0.90
1:B:703:LEU:HD11	1:B:718:PRO:HD3	1.54	0.90
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.06	0.89
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.05	0.89
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.05	0.89
1:D:559:LEU:HD22	1:D:560:PRO:HD2	1.55	0.89
1:E:541:TYR:HH	2:E:2000:LMT:H6'	1.08	0.88
1:F:576:VAL:HG23	1:F:663:VAL:HG22	1.55	0.88
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.54	0.88
1:F:104:GLN:NE2	1:F:108:GLN:OE1	2.07	0.88
1:E:359:LEU:O	1:E:361:ASN:N	2.07	0.87
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.39	0.87
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.55	0.87
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.56	0.87
1:B:350:LEU:HD13	1:B:984:LEU:HB3	1.57	0.87
1:E:197:GLN:NE2	1:E:796:GLY:O	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:ALA:O	1:C:767:ARG:NH1	2.09	0.86
1:A:945:ILE:HG13	1:A:971:ARG:HH12	1.41	0.85
1:F:74:ASN:O	1:F:95:GLU:N	2.07	0.85
1:C:618:ALA:O	1:C:815:ARG:NH2	2.10	0.85
1:E:444:GLY:HA3	1:E:891:LEU:HD22	1.58	0.85
1:B:924:ASP:O	1:B:928:GLN:HG3	1.77	0.85
1:D:451:ALA:HB1	1:D:883:VAL:HG23	1.59	0.85
1:F:49:TYR:CE1	1:F:60:THR:HG21	2.11	0.85
1:C:151:GLN:NE2	1:C:279:ALA:O	2.09	0.84
1:A:414:GLU:OE1	1:A:973:ARG:NH1	2.10	0.84
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.59	0.84
1:B:583:THR:HG22	1:B:586:ARG:HE	1.43	0.84
1:D:182:TYR:HB2	1:D:769:LYS:HZ3	1.40	0.84
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.59	0.84
1:D:262:LEU:HD12	1:D:268:ILE:HD11	1.57	0.84
1:D:945:ILE:HG13	1:D:971:ARG:HH22	1.43	0.84
1:F:453:PHE:HE2	1:F:474:ILE:HG21	1.42	0.84
1:D:960:LEU:HD21	1:D:1027:VAL:HG22	1.59	0.84
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.09	0.83
1:A:318:PRO:HD2	1:A:321:LEU:HD12	1.60	0.83
1:E:174:ASP:OD2	1:E:176:GLN:NE2	2.11	0.83
1:E:960:LEU:H	1:E:1039:ASP:HB3	1.43	0.83
1:F:375:VAL:O	1:F:379:THR:OG1	1.95	0.83
1:F:728:LYS:HB3	1:F:808:ARG:HG3	1.58	0.83
1:D:400:LEU:HD11	1:D:933:THR:HG21	1.60	0.83
1:C:144:ASN:O	1:C:284:GLN:NE2	2.12	0.82
1:D:671:ILE:HG22	1:D:673:GLU:H	1.44	0.82
1:D:435:MET:SD	1:D:490:PRO:HB3	2.19	0.82
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.60	0.82
1:B:422:GLU:O	1:B:502:LYS:NZ	2.12	0.82
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.62	0.82
1:B:1040:ILE:HG22	1:B:1042:HIS:H	1.45	0.82
1:C:151:GLN:HG2	1:C:278:ILE:HG22	1.62	0.82
1:A:108:GLN:NE2	1:B:109:ASN:O	2.13	0.82
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.59	0.82
1:E:907:LEU:HD23	1:E:1017:LEU:HB3	1.62	0.82
1:F:587:THR:OG1	1:F:622:GLN:O	1.97	0.82
1:D:959:GLY:HA2	1:D:1040:ILE:HG23	1.63	0.81
1:E:3:ASN:HA	1:E:6:ILE:HD13	1.62	0.81
1:C:587:THR:OG1	1:C:622:GLN:O	1.97	0.81
1:E:764:ASP:OD2	1:E:765:ARG:NH2	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:ALA:HB1	1:B:816:LEU:HG	1.63	0.81
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.63	0.81
1:D:399:VAL:HG11	1:D:989:LEU:HD11	1.62	0.81
1:F:713:LEU:HD11	1:F:843:LEU:HD12	1.63	0.81
1:E:171:GLY:O	1:E:302:THR:OG1	1.96	0.81
1:C:649:MET:SD	1:C:653:ARG:NH2	2.54	0.80
1:D:414:GLU:OE1	1:D:973:ARG:NH1	2.14	0.80
1:C:940:LYS:HZ3	1:C:978:THR:HG21	1.46	0.80
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.62	0.80
1:C:1043:SER:OG	1:C:1044:HIS:N	2.14	0.80
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.64	0.80
1:D:612:VAL:HB	1:D:626:ILE:HG22	1.64	0.80
1:B:508:GLY:O	1:B:510:LYS:N	2.13	0.80
1:C:186:ILE:HB	1:C:773:VAL:HG22	1.63	0.79
1:C:393:LEU:HD22	1:C:469:GLN:HB2	1.64	0.79
1:C:428:LYS:HG2	1:C:494:ALA:HB1	1.62	0.79
1:D:859:TRP:HB3	1:D:863:SER:HB3	1.64	0.79
1:B:211:ASN:O	1:B:760:ASN:ND2	2.15	0.79
1:C:15:ILE:O	1:C:19:ILE:HG13	1.81	0.79
1:F:527:TYR:CE2	1:F:972:LEU:HD13	2.16	0.79
1:A:555:LEU:HD11	1:A:914:LEU:HD12	1.63	0.79
1:C:62:THR:HA	1:C:90:ILE:HD11	1.64	0.79
1:B:457:ALA:HB2	1:B:471:SER:HB3	1.65	0.79
1:E:453:PHE:O	1:E:471:SER:OG	2.01	0.79
1:B:534:ILE:HG22	2:B:2000:LMT:H3'	1.64	0.78
1:F:486:LEU:HD12	1:F:487:ILE:HG13	1.62	0.78
1:A:623:ASN:OD1	1:A:623:ASN:N	2.16	0.78
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.64	0.78
1:B:507:GLU:HG2	1:B:518:ARG:HG2	1.66	0.78
1:A:211:ASN:O	1:A:760:ASN:ND2	2.15	0.78
1:A:599:LEU:O	1:A:603:LYS:NZ	2.14	0.78
1:C:359:LEU:O	1:C:361:ASN:N	2.17	0.78
1:C:740:GLY:O	1:C:794:ALA:N	2.15	0.78
1:E:924:ASP:O	1:E:928:GLN:HG3	1.83	0.78
1:F:790:TYR:HB3	1:F:798:MET:HB3	1.64	0.78
1:E:641:GLU:O	1:E:650:ARG:NH2	2.15	0.78
1:F:344:LEU:HD23	1:F:399:VAL:HG22	1.64	0.78
1:D:754:TRP:NE1	1:D:780:ARG:HB3	1.98	0.78
1:B:907:LEU:HB3	1:B:1017:LEU:HD11	1.65	0.78
1:C:713:LEU:HD11	1:C:843:LEU:HD12	1.64	0.78
1:D:144:ASN:O	1:D:284:GLN:NE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:484:VAL:HG13	1:E:488:LEU:HD22	1.65	0.78
1:F:376:LEU:O	1:F:379:THR:N	2.15	0.78
1:A:367:ILE:HD11	1:A:496:MET:HG3	1.64	0.78
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.14	0.77
1:C:455:PRO:HG2	1:C:880:SER:HA	1.66	0.77
1:D:376:LEU:O	1:D:379:THR:N	2.18	0.77
1:E:228:GLN:NE2	1:E:230:LEU:O	2.16	0.77
1:D:372:VAL:HG23	1:D:373:PRO:HD3	1.66	0.77
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.66	0.77
1:A:213:GLN:HG2	1:A:239:ARG:HG3	1.66	0.77
1:B:1013:THR:O	1:B:1017:LEU:HD12	1.85	0.77
1:E:115:MET:HA	1:E:118:LEU:HD22	1.66	0.77
1:A:62:THR:OG1	1:A:88:VAL:HG21	1.83	0.77
1:D:182:TYR:HB2	1:D:769:LYS:NZ	1.99	0.77
1:C:680:PHE:HB2	1:C:859:TRP:HZ3	1.48	0.77
1:C:1033:PHE:O	1:C:1035:ARG:N	2.18	0.77
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.14	0.77
1:D:137:LEU:HD13	1:D:293:LEU:HD13	1.66	0.77
1:E:507:GLU:HA	1:E:518:ARG:HG3	1.67	0.77
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.65	0.76
1:A:459:PHE:O	1:A:468:ARG:NH2	2.18	0.76
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.65	0.76
1:D:141:GLY:HA2	1:D:288:GLY:HA2	1.67	0.76
1:A:293:LEU:HD22	1:A:294:ALA:H	1.49	0.76
1:D:584:GLN:HG2	1:D:622:GLN:HG2	1.68	0.76
1:D:743:ILE:HA	1:D:746:ILE:HD12	1.67	0.76
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.68	0.76
1:A:945:ILE:HA	1:A:971:ARG:HH22	1.51	0.76
1:B:907:LEU:HG	1:B:1017:LEU:HD21	1.67	0.76
1:D:375:VAL:O	1:D:379:THR:OG1	2.03	0.76
1:C:195:LYS:HB3	1:C:196:PHE:CD2	2.19	0.76
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.67	0.76
1:B:652:THR:HG23	1:B:665:ALA:H	1.50	0.76
1:C:982:PHE:O	1:C:985:GLY:N	2.18	0.76
1:E:453:PHE:HE1	1:E:474:ILE:HG21	1.51	0.76
1:E:54:ALA:HB1	1:E:816:LEU:HG	1.66	0.76
1:F:514:GLY:O	1:F:517:ASN:ND2	2.19	0.76
1:F:870:GLY:O	1:F:872:GLN:N	2.19	0.76
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.68	0.75
1:B:223:PRO:HG3	1:C:275:TYR:CD2	2.20	0.75
1:C:801:PHE:HA	1:C:804:PHE:HE2	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:99:ASP:O	1:F:103:ALA:N	2.18	0.75
1:E:248:LYS:HA	1:E:261:LEU:HD13	1.66	0.75
1:E:944:LEU:HB3	1:E:971:ARG:HD3	1.67	0.75
1:F:95:GLU:O	1:F:98:THR:OG1	2.04	0.75
1:F:141:GLY:HA2	1:F:288:GLY:HA2	1.69	0.75
1:A:34:GLN:NE2	1:A:670:ALA:O	2.19	0.75
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.69	0.75
1:C:588:GLN:HG3	1:C:592:ASN:HD21	1.51	0.75
1:D:945:ILE:HA	1:D:971:ARG:HH12	1.51	0.75
1:A:65:ILE:HD13	1:A:90:ILE:HD12	1.68	0.75
1:B:139:VAL:O	1:B:326:PRO:HD2	1.86	0.75
1:C:38:ILE:HG23	1:C:462:SER:HB3	1.69	0.75
1:A:23:GLY:HA3	1:A:377:LEU:HB3	1.68	0.74
1:E:200:PRO:HG2	1:E:749:THR:HG23	1.68	0.74
1:F:77:TYR:O	1:F:93:THR:HB	1.87	0.74
1:F:959:GLY:HA2	1:F:1041:GLU:H	1.49	0.74
1:A:754:TRP:NE1	1:A:780:ARG:HB3	2.01	0.74
1:B:118:LEU:O	1:B:123:GLN:NE2	2.20	0.74
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.69	0.74
1:B:61:VAL:HG11	1:B:88:VAL:HG21	1.69	0.74
1:C:393:LEU:HD11	1:C:466:ILE:HA	1.69	0.74
1:F:394:THR:HG23	1:F:469:GLN:HB3	1.69	0.74
1:B:867:ARG:HH21	1:B:868:LEU:HD23	1.50	0.74
1:E:412:VAL:HG22	1:E:438:ILE:HD11	1.70	0.74
1:A:207:ILE:HG13	1:A:759:VAL:HG11	1.68	0.74
1:B:764:ASP:OD2	1:B:765:ARG:NH2	2.20	0.74
1:F:186:ILE:HG12	1:F:268:ILE:HG12	1.69	0.74
1:F:792:ARG:NH1	1:F:793:ALA:O	2.20	0.74
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.19	0.74
1:A:511:GLY:HA2	1:A:515:TRP:NE1	2.03	0.73
1:C:281:PHE:HD1	1:C:610:PHE:HD1	1.35	0.73
1:E:372:VAL:O	1:E:375:VAL:N	2.21	0.73
1:A:115:MET:O	1:A:123:GLN:NE2	2.21	0.73
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.70	0.73
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.69	0.73
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.21	0.73
1:C:520:PHE:O	1:C:524:THR:OG1	2.05	0.73
1:F:64:VAL:HG11	1:F:118:LEU:HG	1.67	0.73
1:E:730:ASP:OD1	1:E:730:ASP:N	2.15	0.73
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.70	0.73
1:B:527:TYR:O	1:B:530:SER:OG	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:LEU:HB3	1:C:971:ARG:CZ	2.19	0.73
1:D:577:GLN:HE22	1:D:721:LEU:HD21	1.53	0.73
1:F:195:LYS:HD2	1:F:196:PHE:CE1	2.23	0.73
1:F:649:MET:SD	1:F:653:ARG:NH2	2.57	0.73
1:A:244:GLU:HG3	1:A:245:GLU:N	2.02	0.73
1:D:171:GLY:O	1:D:294:ALA:HB2	1.89	0.73
1:E:703:LEU:HG	1:E:716:VAL:HG12	1.71	0.73
1:E:139:VAL:O	1:E:326:PRO:HD2	1.88	0.73
1:E:559:LEU:HD23	1:E:923:ASN:HB2	1.69	0.73
1:F:493:CYS:O	1:F:497:LEU:HB3	1.89	0.73
1:D:345:VAL:HA	1:D:348:ILE:HD12	1.71	0.73
1:E:157:TYR:OH	1:E:316:PHE:O	2.07	0.73
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.68	0.72
1:B:250:LEU:HD13	1:B:261:LEU:HD23	1.71	0.72
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.22	0.72
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.69	0.72
1:B:231:ASN:OD1	1:C:622:GLN:NE2	2.22	0.72
1:E:576:VAL:HG12	1:E:663:VAL:HG13	1.71	0.72
1:B:362:PHE:O	1:B:365:THR:HG22	1.90	0.72
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.23	0.72
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.70	0.72
1:A:583:THR:HA	1:A:622:GLN:OE1	1.90	0.72
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.71	0.72
1:F:684:LEU:HB3	1:F:825:MET:O	1.90	0.72
1:B:762:PHE:CE1	1:B:764:ASP:HB3	2.25	0.72
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.71	0.72
1:F:562:SER:OG	1:F:563:PHE:N	2.22	0.72
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.71	0.72
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.70	0.72
1:C:141:GLY:HA2	1:C:288:GLY:HA2	1.72	0.72
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.72	0.72
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.71	0.71
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.71	0.71
1:E:971:ARG:O	1:E:975:ILE:HG12	1.89	0.71
1:C:63:GLN:O	1:C:67:GLN:NE2	2.22	0.71
1:F:686:ASP:HB3	1:F:823:PRO:O	1.89	0.71
1:B:45:ILE:HG12	1:B:129:VAL:HG22	1.72	0.71
1:B:375:VAL:O	1:B:379:THR:OG1	2.06	0.71
1:C:455:PRO:HB3	1:C:879:ILE:HG22	1.72	0.71
1:B:4:PHE:HE2	1:B:8:ARG:HH11	1.37	0.71
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:ARG:HA	1:D:642:ASN:HD22	1.55	0.71
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.73	0.71
1:A:728:LYS:NZ	1:C:236:ALA:O	2.19	0.71
1:B:457:ALA:HB2	1:B:471:SER:CB	2.20	0.71
1:D:272:GLY:N	1:D:275:TYR:OH	2.22	0.71
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.26	0.71
1:E:600:THR:HB	1:E:601:LYS:HD2	1.71	0.71
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.21	0.71
1:D:61:VAL:HG12	1:D:118:LEU:HD22	1.72	0.71
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.72	0.71
1:F:366:LEU:O	1:F:370:ILE:HG12	1.90	0.71
1:E:867:ARG:HH11	1:E:868:LEU:HA	1.55	0.71
1:F:101:ASP:O	1:F:105:VAL:HG23	1.91	0.71
1:B:641:GLU:O	1:B:650:ARG:NH2	2.24	0.71
1:D:21:LEU:O	1:D:25:LEU:HB2	1.90	0.71
1:B:196:PHE:O	1:B:252:LYS:NZ	2.21	0.71
1:D:3:ASN:O	1:D:6:ILE:HG23	1.90	0.71
1:A:922:THR:O	1:A:924:ASP:N	2.24	0.70
1:E:352:PHE:HD2	1:E:353:LEU:HD23	1.55	0.70
1:B:193:LEU:HD22	1:B:265:VAL:HG22	1.73	0.70
1:C:971:ARG:CZ	1:C:971:ARG:HB3	2.20	0.70
1:D:447:MET:HB3	1:D:887:CYS:SG	2.31	0.70
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.72	0.70
1:B:228:GLN:NE2	1:B:230:LEU:O	2.24	0.70
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.73	0.70
1:E:225:VAL:H	1:F:781:MET:HE3	1.55	0.70
1:E:982:PHE:HD2	1:E:1011:MET:HG3	1.54	0.70
1:C:151:GLN:O	1:C:155:SER:OG	2.05	0.70
1:A:352:PHE:HD2	1:A:353:LEU:HD23	1.56	0.70
1:C:363:ARG:CZ	1:C:363:ARG:H	2.04	0.70
1:D:33:ALA:HA	1:D:299:ALA:HB3	1.72	0.70
1:D:344:LEU:HD21	1:D:399:VAL:HA	1.73	0.70
1:B:3:ASN:HA	1:B:6:ILE:HD13	1.72	0.70
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.57	0.70
1:C:1034:SER:HB3	1:C:1037:ASN:HB3	1.74	0.70
1:E:135:SER:OG	1:E:673:GLU:OE1	2.08	0.70
1:C:437:GLN:HG3	1:C:438:ILE:HG23	1.74	0.70
1:E:867:ARG:NH1	1:E:868:LEU:HA	2.06	0.70
1:E:82:SER:HB3	1:E:816:LEU:HB2	1.74	0.69
1:A:696:THR:O	1:A:700:ASN:ND2	2.24	0.69
1:F:758:TYR:CE1	1:F:770:LYS:HG3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:LEU:HG	1:D:357:LEU:O	1.90	0.69
1:F:12:ALA:HB1	1:F:487:ILE:HG23	1.74	0.69
1:F:455:PRO:HG2	1:F:880:SER:HB2	1.74	0.69
1:B:354:VAL:HG22	1:B:980:LEU:HD23	1.75	0.69
1:F:676:THR:HG22	1:F:681:ASP:HB3	1.74	0.69
1:A:781:MET:HB3	1:C:228:GLN:OE1	1.93	0.69
1:C:375:VAL:O	1:C:379:THR:OG1	2.06	0.69
1:D:513:PHE:O	1:D:516:PHE:HB3	1.91	0.69
1:F:400:LEU:HD21	1:F:933:THR:OG1	1.93	0.69
1:A:193:LEU:HD22	1:A:265:VAL:HB	1.75	0.69
1:A:453:PHE:O	1:A:471:SER:OG	2.08	0.69
1:A:951:ASP:O	1:A:955:LYS:N	2.25	0.69
1:D:372:VAL:HA	1:D:375:VAL:HG12	1.74	0.69
1:F:159:ALA:HA	1:F:163:LYS:HB3	1.75	0.69
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.58	0.69
1:A:988:PRO:O	1:A:992:SER:OG	2.09	0.69
1:B:648:THR:O	1:B:652:THR:OG1	2.10	0.69
1:E:368:PRO:HG3	1:E:413:VAL:HG21	1.73	0.69
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.74	0.69
1:F:401:ALA:HB2	1:F:474:ILE:HG12	1.73	0.69
1:A:953:MET:HB3	1:A:1040:ILE:HG21	1.75	0.69
1:B:778:LYS:HE3	1:B:779:TYR:CZ	2.29	0.68
1:C:36:PRO:O	1:C:38:ILE:HG13	1.94	0.68
1:C:185:ARG:HB3	1:C:187:TRP:HE1	1.57	0.68
1:D:923:ASN:OD1	1:D:928:GLN:NE2	2.27	0.68
1:E:343:THR:HG21	1:E:989:LEU:HD21	1.73	0.68
1:F:30:LEU:HD12	1:F:31:PRO:HD2	1.75	0.68
1:F:137:LEU:HD13	1:F:293:LEU:HD13	1.73	0.68
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.75	0.68
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.76	0.68
1:E:832:ALA:HB3	1:E:835:LYS:HD3	1.76	0.68
1:A:961:ILE:HD11	1:A:1031:ARG:HH22	1.58	0.68
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.75	0.68
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.56	0.68
1:E:974:PRO:O	1:E:977:MET:N	2.26	0.68
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.76	0.68
1:C:588:GLN:O	1:C:592:ASN:ND2	2.26	0.68
1:F:698:ALA:O	1:F:701:GLN:HB3	1.94	0.68
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.75	0.68
1:B:218:GLN:HG3	1:B:221:GLY:HA2	1.75	0.68
1:C:196:PHE:HD1	1:C:260:VAL:HG13	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1025:PHE:O	1:A:1029:VAL:HG13	1.92	0.68
1:B:174:ASP:OD2	1:B:176:GLN:NE2	2.26	0.68
1:B:203:VAL:O	1:B:207:ILE:HG13	1.94	0.68
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.28	0.68
1:E:536:ARG:NH1	2:E:2000:LMT:O3B	2.25	0.68
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.24	0.68
1:A:507:GLU:O	1:A:509:LYS:N	2.27	0.68
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.76	0.68
1:D:680:PHE:HD1	1:D:859:TRP:HZ3	1.42	0.68
1:E:950:LYS:HA	1:E:953:MET:HE2	1.76	0.68
1:C:222:THR:HA	1:C:224:PRO:HD3	1.76	0.68
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.74	0.68
1:F:452:VAL:HG23	1:F:453:PHE:CD1	2.28	0.68
1:D:781:MET:HE2	1:F:225:VAL:HG22	1.76	0.67
1:E:418:ARG:HH21	1:E:419:VAL:HG23	1.60	0.67
1:F:405:LEU:HB2	1:F:481:SER:HB3	1.76	0.67
1:A:163:LYS:HD2	1:A:177:LEU:HD23	1.74	0.67
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.76	0.67
1:F:60:THR:HG23	1:F:61:VAL:HG23	1.76	0.67
1:F:623:ASN:N	1:F:623:ASN:OD1	2.23	0.67
1:F:1043:SER:OG	1:F:1044:HIS:N	2.25	0.67
1:B:175:VAL:HG22	1:C:70:ASN:HD22	1.60	0.67
1:E:114:ALA:HA	1:E:117:LEU:HD13	1.74	0.67
1:E:356:TYR:HD1	1:E:365:THR:HG21	1.59	0.67
1:E:596:HIS:O	1:E:600:THR:OG1	2.12	0.67
1:C:185:ARG:HB3	1:C:187:TRP:NE1	2.10	0.67
1:D:444:GLY:HA3	1:D:891:LEU:HD22	1.77	0.67
1:E:609:VAL:HG13	1:E:629:VAL:HG22	1.75	0.67
1:F:218:GLN:HG3	1:F:221:GLY:HA2	1.74	0.67
1:B:535:LEU:HD22	1:B:1027:VAL:HG11	1.76	0.67
1:C:340:VAL:HG21	1:C:392:THR:HG23	1.77	0.67
1:A:20:MET:HG2	1:A:374:VAL:HG13	1.77	0.67
1:A:150:THR:OG1	1:A:151:GLN:N	2.26	0.67
1:B:533:GLY:HA3	2:B:2000:LMT:H6E	1.75	0.67
1:B:888:LEU:HD11	1:B:943:ILE:HD11	1.75	0.67
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.76	0.67
1:D:453:PHE:O	1:D:471:SER:OG	2.11	0.67
1:F:186:ILE:HB	1:F:773:VAL:HG12	1.75	0.67
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.77	0.67
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.27	0.67
1:D:354:VAL:HG22	1:D:980:LEU:HD23	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:LEU:HD22	1:D:481:SER:HB2	1.75	0.67
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.30	0.67
1:E:108:GLN:NE2	1:F:112:GLN:HE21	1.91	0.67
1:E:108:GLN:HE21	1:F:112:GLN:NE2	1.92	0.67
1:E:425:LEU:HD13	1:E:429:GLU:HG2	1.76	0.67
1:C:398:MET:HG2	1:C:473:THR:HG21	1.77	0.67
1:D:441:ALA:HA	1:D:891:LEU:HD21	1.77	0.67
1:E:382:VAL:HG21	1:E:476:SER:HB3	1.77	0.67
1:E:435:MET:O	1:E:439:GLN:HB2	1.95	0.67
1:D:196:PHE:HD1	1:D:260:VAL:HG13	1.60	0.67
1:E:579:PRO:HD3	1:E:661:ALA:HB2	1.75	0.67
1:E:885:PHE:CD1	1:E:886:LEU:HD22	2.30	0.67
1:C:959:GLY:HA2	1:C:1041:GLU:H	1.59	0.66
1:E:162:MET:HG2	1:E:317:PHE:HZ	1.60	0.66
1:E:905:VAL:HG22	1:E:935:ILE:HD12	1.77	0.66
1:B:146:ASP:OD2	1:B:148:THR:OG1	2.12	0.66
1:C:411:VAL:O	1:C:415:ASN:ND2	2.26	0.66
1:D:907:LEU:HG	1:D:1017:LEU:HB3	1.77	0.66
1:E:239:ARG:NH1	1:E:761:ASP:O	2.25	0.66
1:F:42:ALA:O	1:F:132:SER:OG	2.14	0.66
1:A:612:VAL:HB	1:A:626:ILE:HG22	1.78	0.66
1:B:393:LEU:HD13	1:B:466:ILE:HG23	1.78	0.66
1:D:187:TRP:NE1	1:D:269:GLU:OE2	2.29	0.66
1:A:343:THR:HG21	1:A:989:LEU:HD21	1.77	0.66
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.61	0.66
1:E:817:GLU:OE1	1:E:826:GLU:N	2.26	0.66
1:A:573:MET:HG3	1:A:666:PHE:HE1	1.60	0.66
1:D:44:THR:HG22	1:D:91:THR:HG22	1.77	0.66
1:F:391:ASN:ND2	1:F:469:GLN:OE1	2.29	0.66
1:B:197:GLN:O	1:B:792:ARG:HD3	1.96	0.66
1:C:13:TRP:HH2	1:C:370:ILE:HG21	1.59	0.66
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.77	0.66
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.76	0.66
1:A:2:PRO:HA	1:A:486:LEU:HD23	1.77	0.66
1:A:841:MET:HE1	1:A:867:ARG:HG3	1.77	0.66
1:A:895:TRP:O	1:A:898:PRO:HD2	1.96	0.66
1:C:393:LEU:HD13	1:C:469:GLN:HG3	1.77	0.66
1:F:94:PHE:CZ	1:F:107:VAL:HG21	2.31	0.66
1:B:926:TYR:HB3	1:B:1003:VAL:HG22	1.77	0.65
1:C:1019:ILE:HG13	1:C:1020:PHE:CD1	2.31	0.65
1:D:563:PHE:HB2	1:D:677:ALA:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:PHE:HA	1:E:292:LYS:HG2	1.78	0.65
1:E:400:LEU:HD11	1:E:1007:VAL:HG21	1.77	0.65
1:E:441:ALA:O	1:E:445:ILE:HG23	1.96	0.65
1:B:792:ARG:NH1	1:B:793:ALA:O	2.30	0.65
1:C:733:GLN:HE22	1:C:743:ILE:HD13	1.61	0.65
1:E:547:ILE:HG13	1:E:548:ILE:N	2.10	0.65
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.28	0.65
1:B:200:PRO:HA	1:B:203:VAL:HG23	1.79	0.65
1:F:904:VAL:HG21	1:F:942:ALA:HB2	1.77	0.65
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.79	0.65
1:B:712:MET:O	1:B:832:ALA:N	2.25	0.65
1:B:903:LEU:HB3	1:B:1025:PHE:CZ	2.32	0.65
1:F:599:LEU:O	1:F:603:LYS:HG2	1.97	0.65
1:F:686:ASP:OD2	1:F:823:PRO:HD2	1.97	0.65
1:F:961:ILE:HD12	1:F:961:ILE:H	1.61	0.65
1:A:56:THR:O	1:A:60:THR:OG1	2.15	0.65
1:A:680:PHE:HB2	1:A:863:SER:OG	1.95	0.65
1:A:696:THR:OG1	1:A:825:MET:SD	2.49	0.65
1:E:684:LEU:HD12	1:E:856:GLY:O	1.96	0.65
1:A:743:ILE:O	1:A:746:ILE:HG12	1.97	0.65
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.78	0.65
1:F:1026:PHE:CZ	1:F:1030:ARG:HG3	2.31	0.65
1:B:114:ALA:HA	1:B:117:LEU:HD13	1.78	0.65
1:B:163:LYS:HD2	1:B:177:LEU:HD22	1.77	0.65
1:C:376:LEU:O	1:C:379:THR:N	2.29	0.65
1:E:108:GLN:HE21	1:F:112:GLN:HE21	1.42	0.65
1:F:4:PHE:HA	1:F:7:ASP:HB2	1.77	0.65
1:F:482:VAL:HG22	1:F:483:LEU:HD23	1.77	0.65
1:B:536:ARG:HH11	2:B:2000:LMT:H5B	1.61	0.65
1:C:310:LEU:HD23	1:C:323:ILE:HD13	1.77	0.65
1:D:582:ALA:HA	1:D:586:ARG:NH2	2.11	0.65
1:F:900:SER:HB2	1:F:1029:VAL:HG11	1.78	0.65
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.79	0.64
1:A:168:ARG:HG2	1:B:70:ASN:HA	1.80	0.64
1:F:56:THR:O	1:F:60:THR:HB	1.98	0.64
1:F:228:GLN:NE2	1:F:230:LEU:O	2.30	0.64
1:F:393:LEU:HD22	1:F:393:LEU:H	1.62	0.64
1:A:744:ASN:O	1:A:748:THR:HG22	1.97	0.64
1:B:246:PHE:HB3	1:B:268:ILE:HD13	1.79	0.64
1:B:469:GLN:O	1:B:473:THR:OG1	2.11	0.64
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:795:ASP:OD2	1:D:796:GLY:N	2.29	0.64
1:F:372:VAL:O	1:F:375:VAL:N	2.29	0.64
1:F:676:THR:HG21	1:F:828:LEU:HD22	1.78	0.64
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.80	0.64
1:C:913:LEU:HD23	1:C:927:PHE:HZ	1.61	0.64
1:D:351:VAL:HG22	1:D:981:ALA:HB1	1.77	0.64
1:E:393:LEU:HD13	1:E:466:ILE:HG23	1.80	0.64
1:F:65:ILE:HD11	1:F:111:LEU:HG	1.79	0.64
1:F:75:LEU:HD12	1:F:93:THR:O	1.97	0.64
1:B:195:LYS:HD3	1:B:196:PHE:CE1	2.33	0.64
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.78	0.64
1:C:945:ILE:HA	1:C:971:ARG:HH12	1.63	0.64
1:E:138:MET:HG2	1:E:291:ILE:HB	1.80	0.64
1:E:375:VAL:O	1:E:379:THR:OG1	2.13	0.64
1:F:453:PHE:O	1:F:471:SER:OG	2.16	0.64
1:F:1026:PHE:CE2	1:F:1030:ARG:HG3	2.31	0.64
1:B:418:ARG:HH21	1:B:419:VAL:HG23	1.63	0.64
1:B:456:MET:O	1:B:467:TYR:HB3	1.98	0.64
1:D:14:VAL:HG22	1:E:886:LEU:HD12	1.78	0.64
1:D:115:MET:O	1:D:123:GLN:NE2	2.30	0.64
1:D:199:THR:HG23	1:D:792:ARG:H	1.61	0.64
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.79	0.64
1:E:26:ALA:O	1:E:30:LEU:HD22	1.98	0.64
1:E:294:ALA:HB3	1:E:297:ALA:HB3	1.80	0.64
1:E:535:LEU:HD22	1:E:1027:VAL:HG11	1.78	0.64
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.78	0.64
1:F:801:PHE:HA	1:F:804:PHE:HE2	1.61	0.64
1:A:456:MET:HG3	1:A:932:LEU:HD21	1.80	0.64
1:A:562:SER:OG	1:A:563:PHE:N	2.29	0.64
1:C:363:ARG:HG3	1:C:496:MET:HG2	1.79	0.64
1:C:465:ALA:O	1:C:469:GLN:HG2	1.98	0.64
1:C:682:PHE:HD1	1:C:683:GLU:N	1.96	0.64
1:D:563:PHE:HZ	1:D:865:GLN:HE21	1.44	0.64
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.78	0.64
1:D:13:TRP:NE1	1:D:492:LEU:HD21	2.12	0.64
1:D:195:LYS:HB3	1:D:196:PHE:CD2	2.33	0.64
1:D:441:ALA:O	1:D:445:ILE:HG23	1.98	0.64
1:F:409:ALA:HA	1:F:485:ALA:HB2	1.80	0.64
1:A:3:ASN:O	1:A:6:ILE:HG23	1.96	0.64
1:C:945:ILE:HG13	1:C:971:ARG:NH2	2.10	0.64
1:D:562:SER:OG	1:D:563:PHE:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ILE:HG22	1:E:773:VAL:HG23	1.80	0.64
1:E:448:VAL:HG21	1:E:888:LEU:HG	1.80	0.64
1:F:908:GLY:HA2	1:F:1014:ALA:HB2	1.78	0.64
1:A:225:VAL:HG22	1:B:781:MET:SD	2.38	0.64
1:A:913:LEU:HD23	1:A:927:PHE:CZ	2.33	0.64
1:B:108:GLN:NE2	1:C:112:GLN:HB2	2.11	0.64
1:B:344:LEU:HD22	1:B:402:ILE:HD11	1.78	0.64
1:B:1020:PHE:HZ	2:B:2000:LMT:H42	1.61	0.64
1:C:393:LEU:O	1:C:396:PHE:HB2	1.98	0.64
1:E:222:THR:HA	1:E:224:PRO:HD3	1.79	0.64
1:E:246:PHE:HB3	1:E:268:ILE:HD13	1.80	0.64
1:F:250:LEU:HD13	1:F:261:LEU:HD23	1.79	0.64
1:A:491:ALA:O	1:A:495:THR:OG1	2.15	0.64
1:D:400:LEU:HD21	1:D:933:THR:OG1	1.98	0.64
1:E:259:ARG:H	1:E:259:ARG:HD3	1.63	0.64
1:E:885:PHE:HD1	1:E:886:LEU:HD22	1.63	0.64
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.80	0.63
1:B:668:LEU:HD23	1:B:668:LEU:H	1.63	0.63
1:B:992:SER:O	1:B:997:SER:OG	2.11	0.63
1:C:507:GLU:HG2	1:C:518:ARG:HG3	1.80	0.63
1:C:1003:VAL:HG13	1:C:1004:GLY:H	1.62	0.63
1:E:795:ASP:OD2	1:E:797:GLN:HG2	1.98	0.63
1:F:94:PHE:CE2	1:F:107:VAL:HG21	2.32	0.63
1:A:532:GLY:O	1:A:536:ARG:HG2	1.97	0.63
1:A:562:SER:HB3	1:A:924:ASP:HB3	1.80	0.63
1:D:452:VAL:HG23	1:D:453:PHE:CD1	2.33	0.63
1:E:3:ASN:O	1:E:6:ILE:HB	1.98	0.63
1:E:598:TYR:CE2	1:E:629:VAL:HG21	2.34	0.63
1:E:776:GLU:HB3	1:E:779:TYR:CE1	2.32	0.63
1:A:905:VAL:HG22	1:A:935:ILE:HD11	1.80	0.63
1:B:13:TRP:HA	1:B:13:TRP:CE3	2.32	0.63
1:B:907:LEU:CB	1:B:1017:LEU:HD11	2.28	0.63
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.79	0.63
1:C:971:ARG:HG2	1:C:974:PRO:HG3	1.80	0.63
1:E:201:VAL:HA	1:E:204:ILE:HD12	1.80	0.63
1:E:393:LEU:HD23	1:E:393:LEU:H	1.62	0.63
1:F:506:GLY:C	1:F:508:GLY:H	2.00	0.63
1:B:1026:PHE:HD2	1:B:1026:PHE:O	1.82	0.63
1:E:982:PHE:CD2	1:E:1011:MET:HG3	2.32	0.63
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.79	0.63
1:C:527:TYR:O	1:C:530:SER:OG	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:GLN:O	1:C:661:ALA:HB1	1.99	0.63
1:F:284:GLN:NE2	1:F:285:PRO:O	2.32	0.63
1:A:61:VAL:O	1:A:65:ILE:HG22	1.99	0.63
1:A:175:VAL:HG11	1:A:289:LEU:HD22	1.80	0.63
1:A:1035:ARG:HE	1:A:1036:LYS:HG2	1.63	0.63
1:B:447:MET:HB3	1:B:887:CYS:SG	2.37	0.63
1:F:612:VAL:HB	1:F:626:ILE:HG22	1.81	0.63
1:A:172:VAL:HG22	1:A:306:ILE:HD11	1.81	0.63
1:A:577:GLN:O	1:A:661:ALA:HB1	1.99	0.63
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.80	0.63
1:F:75:LEU:HA	1:F:94:PHE:HA	1.81	0.63
1:A:114:ALA:O	1:A:118:LEU:HG	1.99	0.63
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.34	0.63
1:C:602:GLU:OE1	1:C:650:ARG:HD2	1.99	0.63
1:C:982:PHE:HD2	1:C:1011:MET:HG2	1.63	0.63
1:D:886:LEU:HD21	1:F:17:ILE:HG23	1.81	0.63
1:E:214:VAL:HG21	1:E:236:ALA:HB3	1.80	0.63
1:F:47:ALA:HB1	1:F:122:VAL:HG13	1.80	0.63
1:F:102:ILE:O	1:F:105:VAL:HB	1.97	0.63
1:F:185:ARG:HB3	1:F:187:TRP:HE1	1.64	0.63
1:F:527:TYR:O	1:F:531:VAL:HG23	1.98	0.63
1:B:598:TYR:HE2	1:B:629:VAL:HG11	1.64	0.63
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.81	0.63
1:E:379:THR:HA	1:E:382:VAL:HG13	1.80	0.63
1:F:795:ASP:OD2	1:F:796:GLY:N	2.32	0.63
1:A:84:SER:HB3	1:A:814:PRO:HA	1.80	0.62
1:C:38:ILE:CG2	1:C:462:SER:HB3	2.28	0.62
1:C:833:PRO:C	1:C:835:LYS:H	2.01	0.62
1:D:531:VAL:O	1:D:534:ILE:HG12	1.99	0.62
1:F:350:LEU:HG	1:F:984:LEU:HD12	1.81	0.62
1:F:847:LEU:HA	1:F:850:LYS:HE3	1.79	0.62
1:A:428:LYS:CD	1:A:428:LYS:H	2.08	0.62
1:B:1015:THR:O	1:B:1017:LEU:N	2.32	0.62
1:C:507:GLU:HG2	1:C:518:ARG:CG	2.28	0.62
1:C:623:ASN:OD1	1:C:623:ASN:N	2.24	0.62
1:E:214:VAL:HG11	1:E:237:GLN:HB3	1.80	0.62
1:A:187:TRP:NE1	1:A:269:GLU:OE2	2.32	0.62
1:E:790:TYR:CD1	1:E:800:PRO:HA	2.34	0.62
1:F:554:TYR:CE1	1:F:558:ARG:HG3	2.34	0.62
1:C:443:VAL:HG12	1:C:891:LEU:HD21	1.82	0.62
1:C:658:ILE:O	1:C:659:LYS:NZ	2.19	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:366:LEU:HA	1:E:369:THR:HB	1.82	0.62
1:F:157:TYR:O	1:F:161:ASN:ND2	2.28	0.62
1:F:1033:PHE:O	1:F:1035:ARG:N	2.30	0.62
1:C:434:SER:O	1:C:437:GLN:HG2	1.99	0.62
1:D:351:VAL:HG21	1:D:406:VAL:HG11	1.81	0.62
1:E:130:GLU:HG2	1:F:113:LEU:HD21	1.80	0.62
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.81	0.62
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.34	0.62
1:D:62:THR:OG1	1:D:88:VAL:HG21	1.99	0.62
1:D:1019:ILE:HG13	1:D:1020:PHE:HD1	1.64	0.62
1:E:405:LEU:HD11	1:E:477:ALA:HB1	1.80	0.62
1:F:905:VAL:HG22	1:F:935:ILE:HG13	1.81	0.62
1:A:23:GLY:HA2	1:A:377:LEU:O	2.00	0.62
1:A:364:ALA:HA	1:A:367:ILE:HD13	1.80	0.62
1:C:363:ARG:HA	1:C:366:LEU:HG	1.80	0.62
1:D:203:VAL:O	1:D:207:ILE:HG13	1.99	0.62
1:D:208:LYS:HG3	1:D:759:VAL:HG13	1.80	0.62
1:D:978:THR:O	1:D:982:PHE:N	2.29	0.62
1:E:58:GLN:O	1:E:63:GLN:HG3	1.99	0.62
1:E:943:ILE:O	1:E:947:GLU:HB3	1.99	0.62
1:F:375:VAL:HG13	1:F:480:LEU:HB2	1.81	0.62
1:F:429:GLU:OE1	1:F:430:ALA:N	2.32	0.62
1:A:135:SER:HB3	1:A:672:VAL:HG12	1.80	0.62
1:A:776:GLU:HB3	1:A:779:TYR:CE1	2.34	0.62
1:B:309:GLU:HG2	1:B:313:MET:HE3	1.82	0.62
1:B:559:LEU:HD22	1:B:923:ASN:HB2	1.82	0.62
1:D:707:ALA:HB2	1:D:716:VAL:HG21	1.81	0.62
1:F:211:ASN:ND2	1:F:760:ASN:HD21	1.97	0.62
1:F:462:SER:N	1:F:865:GLN:OE1	2.32	0.62
1:F:509:LYS:HB3	1:F:514:GLY:HA3	1.81	0.62
1:E:231:ASN:OD1	1:F:622:GLN:NE2	2.32	0.62
1:F:372:VAL:HG12	1:F:405:LEU:HD11	1.82	0.62
1:A:300:LEU:HD23	1:A:334:LYS:HE3	1.81	0.62
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.35	0.62
1:B:182:TYR:HB2	1:B:769:LYS:NZ	2.15	0.62
1:C:5:PHE:HE1	1:C:8:ARG:HH11	1.46	0.62
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.81	0.62
1:F:540:ARG:HD3	1:F:541:TYR:CE1	2.34	0.62
1:B:616:GLY:HA2	1:B:626:ILE:HB	1.82	0.61
1:D:2:PRO:HB3	1:D:486:LEU:HD23	1.82	0.61
1:D:211:ASN:O	1:D:760:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:LEU:H	1:D:668:LEU:HD23	1.65	0.61
1:F:564:LEU:HD23	1:F:565:PRO:HD2	1.81	0.61
1:F:600:THR:O	1:F:603:LYS:HG3	2.00	0.61
1:A:404:LEU:HD12	1:A:937:LEU:HD21	1.82	0.61
1:B:58:GLN:HA	1:B:62:THR:HB	1.82	0.61
1:B:214:VAL:CG2	1:B:237:GLN:HB3	2.30	0.61
1:D:408:ASP:OD1	1:D:481:SER:OG	2.16	0.61
1:D:577:GLN:O	1:D:661:ALA:HB1	2.00	0.61
1:E:356:TYR:HA	1:E:365:THR:HG21	1.82	0.61
1:E:418:ARG:CZ	1:E:418:ARG:HB3	2.31	0.61
1:A:508:GLY:HA2	1:A:514:GLY:HA3	1.82	0.61
1:A:945:ILE:HA	1:A:971:ARG:NH2	2.15	0.61
1:B:1020:PHE:CZ	2:B:2000:LMT:H42	2.35	0.61
1:F:49:TYR:HE1	1:F:60:THR:HG21	1.63	0.61
1:F:184:MET:HG2	1:F:246:PHE:CE2	2.35	0.61
1:A:508:GLY:O	1:A:510:LYS:N	2.28	0.61
1:C:61:VAL:HB	1:C:88:VAL:HG11	1.81	0.61
1:D:101:ASP:OD2	1:D:101:ASP:N	2.32	0.61
1:D:776:GLU:OE1	1:D:778:LYS:NZ	2.32	0.61
1:E:110:LYS:HD3	1:E:113:LEU:HD12	1.81	0.61
1:E:407:ASP:OD1	1:E:978:THR:HG21	2.00	0.61
1:F:676:THR:HG23	1:F:677:ALA:H	1.64	0.61
1:F:703:LEU:HD21	1:F:827:ILE:HG23	1.83	0.61
1:A:70:ASN:O	1:A:110:LYS:NZ	2.31	0.61
1:B:359:LEU:O	1:B:361:ASN:N	2.33	0.61
1:B:1027:VAL:HG22	1:B:1031:ARG:HD2	1.82	0.61
1:C:870:GLY:O	1:C:872:GLN:N	2.33	0.61
1:D:622:GLN:NE2	1:F:231:ASN:OD1	2.34	0.61
1:E:344:LEU:HD21	1:E:399:VAL:HA	1.81	0.61
1:F:45:ILE:HD13	1:F:111:LEU:HD12	1.82	0.61
1:F:218:GLN:HA	1:F:234:ILE:HD13	1.81	0.61
1:F:801:PHE:HA	1:F:804:PHE:CE2	2.36	0.61
1:A:971:ARG:CG	1:A:974:PRO:HG2	2.31	0.61
1:C:352:PHE:HD1	1:C:369:THR:HG1	1.49	0.61
1:C:493:CYS:O	1:C:497:LEU:HB3	2.00	0.61
1:E:376:LEU:O	1:E:379:THR:N	2.33	0.61
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.66	0.61
1:B:418:ARG:HD2	1:B:422:GLU:OE1	2.01	0.61
1:C:186:ILE:HD13	1:C:262:LEU:HD21	1.82	0.61
1:D:922:THR:O	1:D:924:ASP:N	2.33	0.61
1:E:380:PHE:HD2	1:E:383:LEU:HD12	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:447:MET:HB3	1:E:887:CYS:SG	2.40	0.61
1:E:493:CYS:O	1:E:497:LEU:HB3	2.01	0.61
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.83	0.61
1:F:450:SER:O	1:F:454:VAL:HG23	2.01	0.61
1:F:476:SER:O	1:F:480:LEU:HG	1.99	0.61
1:F:846:GLN:O	1:F:849:SER:OG	2.18	0.61
1:C:366:LEU:HA	1:C:369:THR:HB	1.83	0.61
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.00	0.61
1:E:69:MET:HG2	1:E:110:LYS:HB3	1.83	0.61
1:F:137:LEU:HD22	1:F:293:LEU:HD13	1.83	0.61
1:F:200:PRO:HA	1:F:203:VAL:HG23	1.83	0.61
1:B:222:THR:HA	1:B:224:PRO:HD3	1.83	0.61
1:B:792:ARG:NH1	1:B:792:ARG:O	2.34	0.61
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.36	0.61
1:D:990:VAL:HG22	1:D:1004:GLY:HA3	1.83	0.61
1:A:362:PHE:O	1:A:365:THR:HG22	2.01	0.60
1:E:457:ALA:HB1	1:E:468:ARG:HG3	1.82	0.60
1:E:775:SER:OG	1:E:780:ARG:HG2	2.00	0.60
1:E:801:PHE:HA	1:E:804:PHE:HE2	1.66	0.60
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.81	0.60
1:F:453:PHE:CE2	1:F:474:ILE:HG21	2.29	0.60
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.82	0.60
1:B:727:PHE:HB2	1:B:809:TRP:HE1	1.66	0.60
1:C:30:LEU:HD13	1:C:384:ALA:HB2	1.83	0.60
1:D:452:VAL:HA	1:D:880:SER:OG	2.00	0.60
1:D:884:VAL:O	1:D:888:LEU:HD22	2.01	0.60
1:E:104:GLN:HE22	1:F:109:ASN:HB3	1.65	0.60
1:E:562:SER:OG	1:E:563:PHE:N	2.34	0.60
1:F:583:THR:HA	1:F:622:GLN:OE1	2.00	0.60
1:F:795:ASP:OD2	1:F:797:GLN:HG2	2.01	0.60
1:A:897:ILE:HD11	1:A:1030:ARG:HH21	1.66	0.60
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.82	0.60
1:C:910:ILE:O	1:C:914:LEU:HB2	2.01	0.60
1:D:587:THR:OG1	1:D:622:GLN:O	2.18	0.60
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.83	0.60
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.66	0.60
1:A:790:TYR:CD1	1:A:800:PRO:HA	2.36	0.60
1:C:186:ILE:HG12	1:C:268:ILE:HG22	1.84	0.60
1:C:971:ARG:O	1:C:975:ILE:HG12	2.01	0.60
1:E:193:LEU:HD22	1:E:265:VAL:HB	1.83	0.60
1:F:352:PHE:HD2	1:F:353:LEU:HD23	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:758:TYR:HE1	1:F:770:LYS:HG3	1.65	0.60
1:A:971:ARG:O	1:A:975:ILE:HG12	2.01	0.60
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.34	0.60
1:B:536:ARG:HD2	2:B:2000:LMT:H5B	1.84	0.60
1:C:5:PHE:C	1:C:7:ASP:H	2.04	0.60
1:C:527:TYR:O	1:C:531:VAL:HG23	2.01	0.60
1:E:996:GLY:O	1:E:999:ALA:N	2.34	0.60
1:F:680:PHE:CE2	1:F:682:PHE:HB2	2.36	0.60
1:E:744:ASN:O	1:E:748:THR:HG23	2.02	0.60
1:E:867:ARG:NH1	1:E:867:ARG:O	2.34	0.60
1:F:819:TYR:C	1:F:821:GLY:H	2.05	0.60
1:A:524:THR:O	1:A:528:THR:HG23	2.02	0.60
1:B:702:LEU:HD22	1:B:851:LEU:HD11	1.83	0.60
1:B:904:VAL:O	1:B:907:LEU:HB2	2.02	0.60
1:D:102:ILE:O	1:D:106:GLN:HG2	2.02	0.60
1:D:623:ASN:OD1	1:D:623:ASN:N	2.34	0.60
1:E:225:VAL:N	1:F:781:MET:HE3	2.16	0.60
1:F:45:ILE:HD12	1:F:90:ILE:HG23	1.84	0.60
1:F:207:ILE:HG22	1:F:249:ILE:HD13	1.82	0.60
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.82	0.60
1:E:901:VAL:HG22	1:E:946:VAL:HG21	1.82	0.60
1:F:669:PRO:HD3	1:F:676:THR:O	2.01	0.60
1:F:684:LEU:O	1:F:824:SER:HB2	2.01	0.60
1:F:982:PHE:O	1:F:985:GLY:N	2.34	0.60
1:C:326:PRO:O	1:C:630:SER:HB2	2.01	0.60
1:E:415:ASN:CG	1:E:418:ARG:HH22	2.04	0.60
1:E:519:MET:O	1:E:523:SER:OG	2.17	0.60
1:E:685:ILE:HD11	1:E:819:TYR:CD1	2.36	0.60
1:E:944:LEU:HD13	1:E:971:ARG:HH11	1.67	0.60
1:F:533:GLY:HA2	1:F:536:ARG:NH1	2.17	0.60
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.83	0.60
1:B:80:SER:HB2	1:B:818:ARG:HB2	1.84	0.60
1:D:559:LEU:HD12	1:D:923:ASN:HB2	1.82	0.60
1:F:922:THR:O	1:F:924:ASP:N	2.35	0.60
1:A:467:TYR:CE2	1:A:925:VAL:HG23	2.37	0.59
1:B:195:LYS:HD3	1:B:196:PHE:CZ	2.36	0.59
1:B:576:VAL:HG22	1:B:663:VAL:HG13	1.84	0.59
1:B:598:TYR:CE2	1:B:629:VAL:HG11	2.37	0.59
1:C:65:ILE:HG13	1:C:111:LEU:HD23	1.82	0.59
1:D:390:ILE:O	1:D:394:THR:OG1	2.19	0.59
1:E:428:LYS:HG2	1:E:494:ALA:HB1	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:958:LYS:NZ	1:E:966:ASP:OD2	2.35	0.59
1:E:1041:GLU:O	1:E:1042:HIS:HB2	2.00	0.59
1:B:894:SER:HB2	1:B:897:ILE:HG13	1.84	0.59
1:C:99:ASP:OD2	1:C:102:ILE:HB	2.02	0.59
1:C:380:PHE:HD2	1:C:383:LEU:HD12	1.66	0.59
1:D:34:GLN:HG2	1:D:333:VAL:HG22	1.83	0.59
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.02	0.59
1:B:293:LEU:HD21	1:B:297:ALA:O	2.02	0.59
1:C:892:TYR:HD1	1:C:897:ILE:HG21	1.67	0.59
1:F:404:LEU:HD11	1:F:449:LEU:HD22	1.84	0.59
1:A:687:GLN:N	1:A:854:GLY:O	2.33	0.59
1:B:119:PRO:O	1:B:123:GLN:HG3	2.03	0.59
1:C:363:ARG:HB3	1:C:363:ARG:NH1	2.17	0.59
1:C:572:PHE:HD1	1:C:631:LEU:HD11	1.67	0.59
1:D:75:LEU:HB3	1:F:169:THR:O	2.02	0.59
1:D:754:TRP:CE2	1:D:780:ARG:HB3	2.37	0.59
1:D:945:ILE:HG13	1:D:971:ARG:NH2	2.15	0.59
1:F:418:ARG:O	1:F:422:GLU:HB2	2.02	0.59
1:B:344:LEU:HD23	1:B:399:VAL:HG22	1.85	0.59
1:D:394:THR:HB	1:D:473:THR:HG21	1.83	0.59
1:E:197:GLN:O	1:E:792:ARG:HD3	2.03	0.59
1:F:187:TRP:HA	1:F:774:MET:O	2.03	0.59
1:F:465:ALA:O	1:F:469:GLN:HG2	2.02	0.59
1:A:795:ASP:OD2	1:A:796:GLY:N	2.36	0.59
1:C:590:VAL:O	1:C:593:GLU:HB2	2.02	0.59
1:D:395:MET:HE2	1:D:398:MET:HG3	1.84	0.59
1:D:416:VAL:HG11	1:D:493:CYS:SG	2.43	0.59
1:D:1019:ILE:HG13	1:D:1020:PHE:CD1	2.38	0.59
1:E:102:ILE:HA	1:E:105:VAL:HG23	1.84	0.59
1:F:64:VAL:HG21	1:F:118:LEU:HD23	1.83	0.59
1:A:428:LYS:H	1:A:428:LYS:HD2	1.67	0.59
1:B:414:GLU:OE1	1:B:973:ARG:NH1	2.36	0.59
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.83	0.59
1:C:596:HIS:O	1:C:600:THR:OG1	2.21	0.59
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.37	0.59
1:E:365:THR:O	1:E:368:PRO:HD2	2.03	0.59
1:B:520:PHE:HE1	1:B:973:ARG:HD2	1.67	0.59
1:E:162:MET:HG2	1:E:317:PHE:CZ	2.37	0.59
1:F:163:LYS:NZ	1:F:177:LEU:HB2	2.17	0.59
1:A:709:HIS:CE1	1:A:847:LEU:HD11	2.37	0.59
1:A:1018:ALA:O	1:A:1022:VAL:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:HA	1:B:13:TRP:HE3	1.68	0.59
1:B:453:PHE:O	1:B:471:SER:OG	2.13	0.59
1:C:187:TRP:HA	1:C:774:MET:O	2.01	0.59
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.84	0.59
1:E:905:VAL:HG22	1:E:935:ILE:HG23	1.84	0.59
1:A:518:ARG:O	1:A:522:LYS:HG3	2.03	0.59
1:B:910:ILE:O	1:B:914:LEU:HB2	2.03	0.59
1:D:637:ARG:NH1	1:D:642:ASN:O	2.35	0.59
1:E:102:ILE:CG2	1:E:106:GLN:HE22	2.16	0.59
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.18	0.59
1:A:181:GLN:HG2	1:A:769:LYS:HZ2	1.68	0.58
1:B:730:ASP:OD1	1:B:730:ASP:N	2.24	0.58
1:C:99:ASP:O	1:C:102:ILE:HG22	2.02	0.58
1:C:944:LEU:HB3	1:C:971:ARG:NE	2.16	0.58
1:D:367:ILE:HG23	1:D:496:MET:HE3	1.85	0.58
1:F:588:GLN:HG3	1:F:592:ASN:HD21	1.68	0.58
1:A:163:LYS:O	1:A:163:LYS:HG2	2.02	0.58
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.38	0.58
1:A:974:PRO:HA	1:A:977:MET:HG2	1.85	0.58
1:A:1036:LYS:HB3	1:A:1040:ILE:HD13	1.85	0.58
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.85	0.58
1:D:983:ILE:HD11	1:D:1011:MET:HB3	1.85	0.58
1:F:358:PHE:CD1	1:F:977:MET:HG2	2.38	0.58
1:A:715:SER:HB3	1:A:717:ARG:HD2	1.85	0.58
1:B:182:TYR:HB2	1:B:769:LYS:HZ2	1.67	0.58
1:C:240:LEU:HB2	1:C:246:PHE:CZ	2.38	0.58
1:E:24:GLY:N	1:E:377:LEU:HD12	2.18	0.58
1:E:947:GLU:HG3	1:E:948:PHE:CD2	2.38	0.58
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.67	0.58
1:A:58:GLN:O	1:A:63:GLN:HG3	2.03	0.58
1:B:280:GLU:OE1	1:B:588:GLN:NE2	2.35	0.58
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.84	0.58
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.67	0.58
1:C:379:THR:HG23	1:C:476:SER:OG	2.02	0.58
1:D:511:GLY:HA2	1:D:515:TRP:HD1	1.68	0.58
1:F:57:VAL:HA	1:F:60:THR:HG22	1.85	0.58
1:F:166:ILE:HG21	1:F:289:LEU:HD13	1.86	0.58
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.39	0.58
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.85	0.58
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.04	0.58
1:B:108:GLN:HE21	1:C:112:GLN:NE2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:LEU:HD12	1:B:265:VAL:HG12	1.85	0.58
1:C:100:ALA:HB1	1:C:131:LYS:HE3	1.85	0.58
1:C:298:ASN:HD22	1:C:301:ASP:CG	2.06	0.58
1:C:924:ASP:O	1:C:928:GLN:HG3	2.04	0.58
1:D:442:LEU:O	1:D:445:ILE:HG13	2.03	0.58
1:D:538:THR:HG22	1:D:1024:VAL:HG13	1.85	0.58
1:E:203:VAL:O	1:E:207:ILE:HG13	2.03	0.58
1:A:452:VAL:HA	1:A:880:SER:OG	2.04	0.58
1:A:467:TYR:HE2	1:A:925:VAL:HG23	1.69	0.58
1:A:1043:SER:OG	1:A:1044:HIS:N	2.35	0.58
1:D:335:ILE:O	1:D:339:GLU:HG2	2.04	0.58
1:E:982:PHE:CE2	1:E:1007:VAL:HG13	2.39	0.58
1:F:6:ILE:HG21	1:F:487:ILE:HG12	1.85	0.58
1:F:668:LEU:H	1:F:668:LEU:HD22	1.69	0.58
1:F:790:TYR:CE1	1:F:800:PRO:HA	2.39	0.58
1:A:262:LEU:HA	1:A:265:VAL:HG22	1.86	0.58
1:A:781:MET:HE2	1:C:225:VAL:HG22	1.86	0.58
1:B:201:VAL:HA	1:B:204:ILE:HD12	1.86	0.58
1:C:414:GLU:HA	1:C:973:ARG:HH22	1.67	0.58
1:D:199:THR:CG2	1:D:792:ARG:H	2.17	0.58
1:D:860:THR:H	1:D:863:SER:HB2	1.67	0.58
1:D:940:LYS:O	1:D:943:ILE:N	2.36	0.58
1:D:1003:VAL:HG13	1:D:1004:GLY:H	1.68	0.58
1:E:81:ASN:O	1:E:88:VAL:HA	2.04	0.58
1:B:36:PRO:O	1:B:38:ILE:HG13	2.04	0.58
1:C:578:LEU:CD2	1:C:579:PRO:HD2	2.34	0.58
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.86	0.58
1:D:982:PHE:O	1:D:985:GLY:N	2.34	0.58
1:D:1026:PHE:O	1:D:1026:PHE:HD2	1.87	0.58
1:F:160:ALA:O	1:F:767:ARG:NH1	2.37	0.58
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.86	0.58
1:F:272:GLY:N	1:F:275:TYR:OH	2.36	0.58
1:A:544:LEU:O	1:A:548:ILE:HG13	2.04	0.58
1:B:376:LEU:C	1:B:378:GLY:H	1.98	0.58
1:B:795:ASP:OD2	1:B:796:GLY:N	2.37	0.58
1:D:47:ALA:HB3	1:D:88:VAL:HG13	1.86	0.58
1:D:178:PHE:HB2	1:D:288:GLY:H	1.69	0.58
1:F:214:VAL:HG11	1:F:236:ALA:HB3	1.85	0.58
1:F:350:LEU:HD23	1:F:984:LEU:O	2.03	0.58
1:C:193:LEU:HD22	1:C:265:VAL:HB	1.85	0.57
1:E:987:MET:O	1:E:990:VAL:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:691:GLY:O	1:F:694:LYS:HG2	2.03	0.57
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.86	0.57
1:A:622:GLN:CD	1:C:231:ASN:HD22	2.07	0.57
1:A:1035:ARG:O	1:A:1037:ASN:N	2.37	0.57
1:D:3:ASN:OD1	1:D:6:ILE:HD12	2.03	0.57
1:D:30:LEU:HD22	1:D:31:PRO:HD2	1.87	0.57
1:D:75:LEU:O	1:F:170:SER:OG	2.23	0.57
1:D:408:ASP:O	1:D:411:VAL:HG12	2.04	0.57
1:E:587:THR:OG1	1:E:622:GLN:O	2.14	0.57
1:E:790:TYR:HB3	1:E:798:MET:HB3	1.85	0.57
1:B:239:ARG:NH1	1:B:761:ASP:O	2.37	0.57
1:B:433:LYS:O	1:B:437:GLN:HG3	2.03	0.57
1:C:394:THR:HG22	1:C:469:GLN:HB3	1.85	0.57
1:C:944:LEU:HD13	1:C:971:ARG:HE	1.69	0.57
1:D:350:LEU:HD23	1:D:985:GLY:HA2	1.85	0.57
1:D:600:THR:O	1:D:603:LYS:HG3	2.04	0.57
1:D:734:GLU:O	1:D:736:ALA:N	2.36	0.57
1:E:344:LEU:HG	1:E:399:VAL:HG22	1.86	0.57
1:A:723:ASP:OD2	1:A:813:SER:OG	2.21	0.57
1:B:909:VAL:O	1:B:912:ALA:N	2.37	0.57
1:C:5:PHE:O	1:C:7:ASP:N	2.37	0.57
1:C:414:GLU:HG2	1:C:973:ARG:NH1	2.18	0.57
1:C:484:VAL:O	1:C:488:LEU:N	2.32	0.57
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.85	0.57
1:D:619:GLY:HA3	1:D:815:ARG:HH12	1.69	0.57
1:F:462:SER:HB2	1:F:865:GLN:HG2	1.86	0.57
1:F:527:TYR:CD2	1:F:972:LEU:HD22	2.39	0.57
1:A:235:ILE:HD11	1:B:726:GLN:CB	2.26	0.57
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.04	0.57
1:C:149:MET:HG3	1:C:154:ILE:HD11	1.87	0.57
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.86	0.57
1:D:202:ASP:O	1:D:206:ALA:HB2	2.04	0.57
1:D:932:LEU:O	1:D:935:ILE:HB	2.05	0.57
1:E:293:LEU:HD13	1:E:294:ALA:O	2.04	0.57
1:F:4:PHE:O	1:F:7:ASP:HB2	2.05	0.57
1:A:278:ILE:HG23	1:A:613:ASN:HB3	1.86	0.57
1:B:843:LEU:O	1:B:847:LEU:HG	2.05	0.57
1:C:45:ILE:HA	1:C:128:SER:O	2.05	0.57
1:C:203:VAL:O	1:C:207:ILE:HG12	2.05	0.57
1:C:335:ILE:HG23	1:C:995:ALA:HB1	1.87	0.57
1:C:465:ALA:HA	1:C:468:ARG:NH1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:926:TYR:HE2	1:C:999:ALA:HB1	1.69	0.57
1:D:594:VAL:HG22	1:D:655:PHE:CE2	2.39	0.57
1:D:698:ALA:O	1:D:701:GLN:HB3	2.03	0.57
1:E:195:LYS:HD2	1:E:196:PHE:CE1	2.39	0.57
1:F:682:PHE:HB3	1:F:827:ILE:O	2.05	0.57
1:F:691:GLY:HA3	1:F:694:LYS:HE2	1.87	0.57
1:A:189:ASN:HB3	1:A:192:GLU:HG2	1.87	0.57
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.86	0.57
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.87	0.57
1:B:76:MET:HG2	1:B:864:TYR:HE2	1.68	0.57
1:C:366:LEU:O	1:C:370:ILE:HG13	2.04	0.57
1:D:10:ILE:HB	1:E:893:GLU:HG3	1.87	0.57
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.39	0.57
1:E:294:ALA:HB3	1:E:297:ALA:CB	2.34	0.57
1:F:379:THR:O	1:F:383:LEU:HG	2.04	0.57
1:A:527:TYR:CE2	1:A:972:LEU:HD13	2.39	0.57
1:D:919:ARG:HH12	1:D:990:VAL:HG12	1.70	0.57
1:E:790:TYR:HD1	1:E:800:PRO:HA	1.70	0.57
1:D:186:ILE:HB	1:D:773:VAL:HG12	1.85	0.57
1:D:924:ASP:O	1:D:928:GLN:HG2	2.04	0.57
1:D:931:LEU:O	1:D:935:ILE:HG13	2.04	0.57
1:A:400:LEU:HD23	1:A:474:ILE:HD11	1.85	0.57
1:B:671:ILE:HB	1:B:674:LEU:HB2	1.87	0.57
1:C:375:VAL:HG13	1:C:480:LEU:HB2	1.85	0.57
1:D:841:MET:O	1:D:845:GLU:HG3	2.04	0.57
1:E:153:ASP:OD1	1:E:153:ASP:N	2.37	0.57
1:E:356:TYR:HE1	1:E:362:PHE:HA	1.70	0.57
1:F:572:PHE:HD2	1:F:631:LEU:HD11	1.69	0.57
1:B:100:ALA:O	1:B:103:ALA:N	2.38	0.56
1:E:572:PHE:HD2	1:E:631:LEU:HD21	1.70	0.56
1:B:26:ALA:O	1:B:30:LEU:HB2	2.05	0.56
1:B:671:ILE:HD12	1:B:674:LEU:HG	1.87	0.56
1:C:746:ILE:HG22	1:C:791:VAL:HG11	1.87	0.56
1:C:900:SER:HB3	1:C:1029:VAL:HG21	1.86	0.56
1:E:214:VAL:CG1	1:E:237:GLN:HB3	2.34	0.56
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.70	0.56
1:F:948:PHE:O	1:F:952:LEU:HG	2.06	0.56
1:B:175:VAL:HG22	1:C:70:ASN:ND2	2.20	0.56
1:B:559:LEU:HD23	1:B:560:PRO:HD2	1.86	0.56
1:C:352:PHE:HD2	1:C:353:LEU:HD23	1.70	0.56
1:C:702:LEU:HD22	1:C:827:ILE:HD13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:VAL:HG13	1:D:88:VAL:HB	1.86	0.56
1:D:100:ALA:O	1:D:103:ALA:N	2.37	0.56
1:D:157:TYR:O	1:D:161:ASN:ND2	2.27	0.56
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.87	0.56
1:D:414:GLU:CD	1:D:974:PRO:HG3	2.25	0.56
1:D:459:PHE:CE2	1:D:876:LEU:HD12	2.40	0.56
1:F:372:VAL:HG23	1:F:373:PRO:HD3	1.88	0.56
1:F:407:ASP:OD2	1:F:940:LYS:HD2	2.05	0.56
1:F:723:ASP:HA	1:F:813:SER:HA	1.86	0.56
1:F:974:PRO:O	1:F:978:THR:HG22	2.06	0.56
1:C:743:ILE:HA	1:C:746:ILE:HG12	1.87	0.56
1:D:838:GLY:O	1:D:841:MET:HB2	2.05	0.56
1:E:236:ALA:O	1:F:728:LYS:NZ	2.30	0.56
1:F:985:GLY:O	1:F:988:PRO:HD2	2.06	0.56
1:A:190:PRO:HB3	1:A:789:TRP:CZ2	2.40	0.56
1:A:596:HIS:O	1:A:600:THR:HG22	2.05	0.56
1:A:690:LEU:O	1:A:694:LYS:HB2	2.05	0.56
1:A:895:TRP:C	1:A:898:PRO:HD2	2.25	0.56
1:A:979:SER:OG	1:A:1015:THR:HG21	2.06	0.56
1:B:151:GLN:OE1	1:B:278:ILE:HG22	2.05	0.56
1:B:575:MET:CE	1:B:617:PHE:HB2	2.36	0.56
1:C:983:ILE:HD11	1:C:1011:MET:HG3	1.88	0.56
1:D:781:MET:HB2	1:D:782:LEU:HD12	1.88	0.56
1:F:727:PHE:HD1	1:F:809:TRP:CD1	2.23	0.56
1:A:131:LYS:NZ	1:B:73:ASP:OD1	2.22	0.56
1:B:961:ILE:HG13	1:B:962:GLU:H	1.70	0.56
1:D:58:GLN:HG3	1:D:818:ARG:HD2	1.88	0.56
1:D:526:HIS:CD2	2:D:2000:LMT:H41	2.40	0.56
1:F:273:GLU:OE2	1:F:770:LYS:HD3	2.05	0.56
1:F:897:ILE:CG2	1:F:946:VAL:HG11	2.36	0.56
1:B:344:LEU:HD22	1:B:402:ILE:CD1	2.35	0.56
1:B:530:SER:HA	2:B:2000:LMT:H6D	1.87	0.56
1:D:170:SER:OG	1:E:75:LEU:N	2.39	0.56
1:D:776:GLU:HG2	1:D:777:ALA:H	1.71	0.56
1:E:36:PRO:O	1:E:38:ILE:HG13	2.05	0.56
1:E:47:ALA:O	1:E:87:THR:HA	2.05	0.56
1:E:987:MET:HG3	1:E:1008:MET:SD	2.46	0.56
1:F:3:ASN:O	1:F:7:ASP:N	2.38	0.56
1:A:272:GLY:N	1:A:275:TYR:OH	2.38	0.56
1:D:578:LEU:HD12	1:D:579:PRO:HD2	1.88	0.56
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:PHE:O	1:E:249:ILE:HG23	2.06	0.56
1:E:435:MET:SD	1:E:490:PRO:HB3	2.46	0.56
1:E:831:ALA:HB2	1:E:840:ALA:HB2	1.88	0.56
1:F:594:VAL:HG22	1:F:655:PHE:CE2	2.40	0.56
1:A:230:LEU:HD11	1:B:809:TRP:HH2	1.71	0.56
1:B:21:LEU:O	1:B:25:LEU:HB2	2.06	0.56
1:D:526:HIS:HD2	2:D:2000:LMT:H41	1.70	0.56
1:D:894:SER:OG	1:D:897:ILE:HG12	2.06	0.56
1:E:555:LEU:HD11	1:E:914:LEU:HD12	1.88	0.56
1:F:404:LEU:HD12	1:F:937:LEU:HD23	1.88	0.56
1:F:423:GLU:O	1:F:502:LYS:HB2	2.06	0.56
1:F:564:LEU:CD2	1:F:565:PRO:HD2	2.35	0.56
1:F:792:ARG:HG2	1:F:792:ARG:HH11	1.71	0.56
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.87	0.56
1:A:586:ARG:O	1:A:589:LYS:HB3	2.07	0.55
1:A:696:THR:HG23	1:A:699:ARG:NH1	2.21	0.55
1:C:565:PRO:HG3	1:C:999:ALA:HA	1.87	0.55
1:D:244:GLU:HG3	1:D:245:GLU:N	2.20	0.55
1:E:423:GLU:O	1:E:502:LYS:HB2	2.05	0.55
1:E:426:PRO:HG2	1:E:429:GLU:HB2	1.87	0.55
1:E:584:GLN:HB2	1:E:622:GLN:HG2	1.87	0.55
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.41	0.55
1:F:833:PRO:C	1:F:835:LYS:H	2.10	0.55
1:A:189:ASN:O	1:A:193:LEU:HB2	2.07	0.55
1:A:712:MET:O	1:A:832:ALA:N	2.39	0.55
1:A:953:MET:SD	1:A:960:LEU:HA	2.45	0.55
1:B:372:VAL:O	1:B:375:VAL:N	2.38	0.55
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.41	0.55
1:D:344:LEU:HD11	1:D:398:MET:HB3	1.87	0.55
1:D:435:MET:O	1:D:439:GLN:HB2	2.07	0.55
1:E:379:THR:O	1:E:382:VAL:HG22	2.06	0.55
1:E:703:LEU:HD11	1:E:718:PRO:HD3	1.88	0.55
1:F:358:PHE:HB3	1:F:977:MET:HE1	1.88	0.55
1:F:420:MET:SD	1:F:500:ILE:HB	2.46	0.55
1:C:404:LEU:O	1:C:407:ASP:HB2	2.07	0.55
1:C:959:GLY:CA	1:C:1041:GLU:H	2.19	0.55
1:C:1026:PHE:CE1	1:C:1030:ARG:HG2	2.41	0.55
1:D:36:PRO:HG3	1:D:469:GLN:HG3	1.89	0.55
1:D:105:VAL:HG21	1:E:105:VAL:HB	1.88	0.55
1:D:605:ASN:HD22	1:D:647:ILE:HD11	1.70	0.55
1:E:96:SER:OG	1:E:865:GLN:NE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PRO:HB2	1:F:122:VAL:HB	1.88	0.55
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.88	0.55
1:A:682:PHE:HD2	1:A:683:GLU:N	2.04	0.55
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.40	0.55
1:C:190:PRO:HG3	1:C:779:TYR:HB3	1.89	0.55
1:C:572:PHE:HA	1:C:668:LEU:HD21	1.89	0.55
1:E:682:PHE:HE2	1:E:684:LEU:HB2	1.71	0.55
1:F:555:LEU:HD11	1:F:914:LEU:HD12	1.88	0.55
1:F:983:ILE:HD13	1:F:1012:VAL:HG22	1.88	0.55
1:A:740:GLY:O	1:A:793:ALA:HB1	2.06	0.55
1:B:904:VAL:HG21	1:B:942:ALA:CB	2.36	0.55
1:C:362:PHE:HB2	1:C:363:ARG:HH22	1.70	0.55
1:D:143:ILE:HG22	1:D:286:ALA:CB	2.36	0.55
1:D:945:ILE:HA	1:D:971:ARG:NH1	2.20	0.55
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.89	0.55
1:F:535:LEU:HD22	1:F:1027:VAL:HG21	1.89	0.55
1:A:198:LEU:N	1:A:798:MET:HE1	2.21	0.55
1:B:844:MET:HE1	1:B:847:LEU:HD12	1.89	0.55
1:B:979:SER:OG	1:B:1015:THR:HG21	2.06	0.55
1:C:139:VAL:O	1:C:326:PRO:HD2	2.05	0.55
1:C:320:GLY:O	1:C:322:LYS:N	2.39	0.55
1:C:414:GLU:HG2	1:C:973:ARG:CZ	2.37	0.55
1:C:562:SER:OG	1:C:924:ASP:HB3	2.05	0.55
1:D:728:LYS:HD2	1:F:235:ILE:O	2.07	0.55
1:D:826:GLU:HG3	1:D:826:GLU:O	2.06	0.55
1:E:76:MET:HG2	1:E:864:TYR:OH	2.07	0.55
1:E:557:VAL:C	1:E:559:LEU:H	2.10	0.55
1:E:598:TYR:HB3	1:E:606:VAL:HG21	1.89	0.55
1:E:1015:THR:O	1:E:1017:LEU:N	2.40	0.55
1:F:64:VAL:HG13	1:F:117:LEU:HB2	1.88	0.55
1:F:144:ASN:CG	1:F:320:GLY:HA3	2.26	0.55
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.89	0.55
1:D:619:GLY:N	1:D:815:ARG:HH22	2.05	0.55
1:E:167:SER:HB3	1:F:70:ASN:HD22	1.72	0.55
1:E:912:ALA:HB3	1:E:931:LEU:HD21	1.89	0.55
1:E:944:LEU:HD13	1:E:971:ARG:NH1	2.21	0.55
1:A:38:ILE:HG23	1:A:462:SER:HB3	1.89	0.55
1:A:555:LEU:HD12	1:A:910:ILE:HD12	1.89	0.55
1:A:942:ALA:O	1:A:946:VAL:HG12	2.06	0.55
1:C:684:LEU:HD22	1:C:695:LEU:HD11	1.88	0.55
1:D:261:LEU:HD13	1:D:263:ARG:HH21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:PHE:HD1	1:D:677:ALA:HA	1.72	0.55
1:F:593:GLU:OE2	1:F:659:LYS:HE3	2.07	0.55
1:F:596:HIS:O	1:F:600:THR:OG1	2.25	0.55
1:A:646:ALA:O	1:A:650:ARG:HG2	2.06	0.55
1:C:163:LYS:O	1:C:163:LYS:HG2	2.06	0.55
1:C:461:GLY:O	1:C:464:GLY:N	2.40	0.55
1:C:588:GLN:HG3	1:C:592:ASN:ND2	2.21	0.55
1:D:47:ALA:HB3	1:D:88:VAL:CG1	2.37	0.55
1:D:57:VAL:HG12	1:D:82:SER:HB3	1.89	0.55
1:D:261:LEU:CD1	1:D:263:ARG:HH21	2.20	0.55
1:D:407:ASP:OD1	1:D:978:THR:HG21	2.07	0.55
1:D:552:MET:HB2	1:D:910:ILE:HB	1.88	0.55
1:E:892:TYR:O	1:E:893:GLU:HB2	2.06	0.55
1:F:448:VAL:CG2	1:F:884:VAL:HG13	2.37	0.55
1:A:897:ILE:HD11	1:A:1030:ARG:HE	1.70	0.55
1:B:214:VAL:HG21	1:B:237:GLN:HB3	1.88	0.55
1:B:732:ASP:N	1:B:804:PHE:O	2.38	0.55
1:D:958:LYS:NZ	1:D:962:GLU:OE1	2.34	0.55
1:D:1026:PHE:HE2	1:D:1030:ARG:HE	1.54	0.55
1:E:675:GLY:HA2	1:E:862:MET:SD	2.46	0.55
1:F:343:THR:HG22	1:F:399:VAL:HG11	1.89	0.55
1:B:171:GLY:O	1:B:302:THR:OG1	2.17	0.54
1:C:563:PHE:HB2	1:C:866:GLU:HB2	1.89	0.54
1:D:530:SER:O	1:D:533:GLY:N	2.40	0.54
1:D:583:THR:HA	1:D:622:GLN:OE1	2.08	0.54
1:E:167:SER:HB3	1:F:70:ASN:HB3	1.89	0.54
1:E:637:ARG:NH1	1:E:643:LYS:HA	2.22	0.54
1:A:280:GLU:OE2	1:A:588:GLN:NE2	2.40	0.54
1:B:775:SER:OG	1:B:776:GLU:N	2.40	0.54
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.88	0.54
1:C:172:VAL:HG12	1:C:173:GLY:O	2.07	0.54
1:D:481:SER:O	1:D:484:VAL:HG12	2.07	0.54
1:D:945:ILE:CA	1:D:971:ARG:HH12	2.18	0.54
1:E:871:ASN:OD1	1:E:871:ASN:N	2.40	0.54
1:F:147:GLY:O	1:F:149:MET:HG3	2.07	0.54
1:F:163:LYS:HD2	1:F:289:LEU:HD21	1.87	0.54
1:F:520:PHE:O	1:F:523:SER:OG	2.25	0.54
1:B:294:ALA:HB3	1:B:297:ALA:HB2	1.88	0.54
1:C:207:ILE:HG22	1:C:249:ILE:HD13	1.88	0.54
1:D:402:ILE:O	1:D:406:VAL:HG22	2.06	0.54
1:E:767:ARG:HG2	1:E:767:ARG:HH11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:THR:HG21	1:F:818:ARG:HD3	1.88	0.54
1:F:281:PHE:HD1	1:F:610:PHE:HD1	1.55	0.54
1:F:364:ALA:HA	1:F:367:ILE:HD13	1.88	0.54
1:A:203:VAL:O	1:A:207:ILE:HG12	2.07	0.54
1:A:355:MET:SD	1:A:410:ILE:HD11	2.48	0.54
1:A:929:VAL:O	1:A:932:LEU:HB2	2.07	0.54
1:C:273:GLU:OE2	1:C:770:LYS:HD2	2.07	0.54
1:C:1031:ARG:HH22	1:C:1040:ILE:HD11	1.72	0.54
1:D:886:LEU:HD23	1:F:18:ILE:HG13	1.89	0.54
1:E:576:VAL:HG12	1:E:663:VAL:CG1	2.38	0.54
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.90	0.54
1:F:608:SER:OG	1:F:630:SER:OG	2.12	0.54
1:F:897:ILE:HB	1:F:898:PRO:HD3	1.89	0.54
1:A:335:ILE:O	1:A:339:GLU:HG2	2.07	0.54
1:B:686:ASP:HB2	1:B:695:LEU:HD13	1.89	0.54
1:B:692:HIS:NE2	1:B:813:SER:OG	2.23	0.54
1:D:84:SER:HB3	1:D:814:PRO:HA	1.89	0.54
1:D:968:VAL:HG11	1:D:1023:PRO:HG3	1.90	0.54
1:E:452:VAL:HA	1:E:880:SER:OG	2.07	0.54
1:E:714:THR:OG1	1:E:832:ALA:HA	2.07	0.54
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.43	0.54
1:E:778:LYS:HE3	1:E:779:TYR:CZ	2.42	0.54
1:F:149:MET:HB3	1:F:153:ASP:OD1	2.07	0.54
1:F:858:ASP:OD2	1:F:859:TRP:N	2.36	0.54
1:A:465:ALA:O	1:A:469:GLN:HG2	2.08	0.54
1:A:530:SER:O	1:A:533:GLY:N	2.40	0.54
1:A:948:PHE:O	1:A:952:LEU:HG	2.08	0.54
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.89	0.54
1:E:62:THR:OG1	1:E:88:VAL:HG21	2.08	0.54
1:E:545:TYR:HB2	1:E:1021:PHE:HE2	1.72	0.54
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.90	0.54
1:F:465:ALA:HA	1:F:468:ARG:HD2	1.90	0.54
1:F:479:ALA:O	1:F:483:LEU:HG	2.07	0.54
1:F:841:MET:HG3	1:F:859:TRP:CZ2	2.42	0.54
1:B:383:LEU:CD2	1:B:472:ILE:HG22	2.36	0.54
1:C:412:VAL:HG13	1:C:435:MET:CE	2.38	0.54
1:D:24:GLY:N	1:D:377:LEU:HD22	2.23	0.54
1:D:124:GLN:CD	1:D:758:TYR:HD2	2.11	0.54
1:D:211:ASN:ND2	1:D:240:LEU:HG	2.23	0.54
1:A:3:ASN:HA	1:A:6:ILE:HG23	1.89	0.54
1:A:806:SER:O	1:A:807:SER:OG	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:THR:O	1:B:473:THR:HG21	2.08	0.54
1:B:961:ILE:HG12	1:B:1039:ASP:OD2	2.08	0.54
1:C:373:PRO:O	1:C:377:LEU:N	2.41	0.54
1:C:420:MET:SD	1:C:500:ILE:HB	2.47	0.54
1:E:31:PRO:HB2	1:E:389:SER:HB3	1.90	0.54
1:F:378:GLY:O	1:F:382:VAL:HG23	2.07	0.54
1:F:462:SER:O	1:F:466:ILE:HG12	2.07	0.54
1:A:46:SER:HB2	1:A:128:SER:OG	2.07	0.54
1:C:530:SER:OG	1:C:531:VAL:N	2.39	0.54
1:C:743:ILE:O	1:C:746:ILE:HG12	2.08	0.54
1:D:979:SER:OG	1:D:1011:MET:SD	2.58	0.54
1:E:78:MET:HG3	1:E:90:ILE:HD11	1.89	0.54
1:E:910:ILE:O	1:E:914:LEU:HB2	2.07	0.54
1:E:972:LEU:HD22	1:E:976:LEU:HD13	1.90	0.54
1:A:210:GLN:O	1:A:237:GLN:NE2	2.40	0.54
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.43	0.54
1:C:776:GLU:HB2	1:C:779:TYR:CD1	2.43	0.54
1:D:375:VAL:HG23	1:D:480:LEU:CB	2.37	0.54
1:E:46:SER:HA	1:E:88:VAL:O	2.07	0.54
1:E:187:TRP:HA	1:E:774:MET:O	2.09	0.54
1:E:452:VAL:O	1:E:455:PRO:HD2	2.08	0.54
1:E:698:ALA:HA	1:E:701:GLN:HE21	1.72	0.54
1:F:97:GLY:C	1:F:99:ASP:H	2.09	0.54
1:F:530:SER:O	1:F:533:GLY:N	2.41	0.54
1:B:418:ARG:NH1	1:B:970:MET:HE2	2.23	0.53
1:B:903:LEU:HB3	1:B:1025:PHE:CE2	2.42	0.53
1:C:208:LYS:HG3	1:C:759:VAL:CG1	2.38	0.53
1:C:531:VAL:O	1:C:534:ILE:HG12	2.08	0.53
1:C:801:PHE:HA	1:C:804:PHE:CE2	2.38	0.53
1:D:331:PRO:HA	1:D:334:LYS:HD2	1.89	0.53
1:F:163:LYS:HZ2	1:F:177:LEU:H	1.55	0.53
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.21	0.53
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.90	0.53
1:E:597:TYR:CD1	1:E:655:PHE:HZ	2.26	0.53
1:E:754:TRP:CZ2	1:E:780:ARG:HA	2.43	0.53
1:F:602:GLU:OE1	1:F:650:ARG:HD2	2.08	0.53
1:A:13:TRP:HE1	1:A:492:LEU:HD21	1.74	0.53
1:A:375:VAL:HG21	1:A:481:SER:HA	1.89	0.53
1:C:957:GLY:HA3	1:C:1043:SER:HB2	1.91	0.53
1:D:189:ASN:OD1	1:D:190:PRO:HD2	2.09	0.53
1:D:362:PHE:O	1:D:365:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:ARG:C	1:D:974:PRO:HD2	2.28	0.53
1:E:44:THR:OG1	1:E:91:THR:OG1	2.11	0.53
1:E:519:MET:SD	1:E:519:MET:N	2.80	0.53
1:F:571:VAL:O	1:F:668:LEU:HD21	2.08	0.53
1:A:890:ALA:HB2	1:C:14:VAL:HG11	1.89	0.53
1:A:945:ILE:HG13	1:A:971:ARG:NH1	2.19	0.53
1:A:957:GLY:O	1:A:1041:GLU:HA	2.08	0.53
1:C:401:ALA:HA	1:C:404:LEU:HD22	1.91	0.53
1:C:686:ASP:OD2	1:C:823:PRO:HD2	2.09	0.53
1:D:456:MET:O	1:D:467:TYR:HB3	2.08	0.53
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.89	0.53
1:F:144:ASN:OD1	1:F:320:GLY:HA3	2.08	0.53
1:F:190:PRO:HG3	1:F:779:TYR:HB3	1.90	0.53
1:F:352:PHE:CD2	1:F:353:LEU:HD23	2.43	0.53
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.89	0.53
1:B:13:TRP:CZ3	1:B:488:LEU:HD11	2.43	0.53
1:B:46:SER:HA	1:B:88:VAL:O	2.08	0.53
1:B:157:TYR:OH	1:B:316:PHE:O	2.27	0.53
1:C:68:ASN:HB3	1:C:110:LYS:O	2.09	0.53
1:C:960:LEU:H	1:C:1040:ILE:HG23	1.73	0.53
1:D:1003:VAL:HG13	1:D:1004:GLY:N	2.23	0.53
1:E:139:VAL:HG23	1:E:327:TYR:HD1	1.73	0.53
1:E:211:ASN:HB2	1:E:240:LEU:HD11	1.91	0.53
1:E:602:GLU:HB3	1:E:606:VAL:HG23	1.91	0.53
1:E:885:PHE:HB2	1:E:902:MET:SD	2.49	0.53
1:B:63:GLN:HE21	1:B:818:ARG:NH1	2.06	0.53
1:B:162:MET:HE2	1:B:310:LEU:HD11	1.90	0.53
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.90	0.53
1:D:222:THR:HA	1:D:224:PRO:HD3	1.91	0.53
1:D:250:LEU:HD23	1:E:737:GLN:OE1	2.09	0.53
1:D:781:MET:HB3	1:F:228:GLN:OE1	2.09	0.53
1:E:214:VAL:HG22	1:E:237:GLN:O	2.09	0.53
1:E:293:LEU:HD22	1:E:294:ALA:H	1.74	0.53
1:F:363:ARG:HB3	1:F:496:MET:HG2	1.91	0.53
1:F:509:LYS:HG3	1:F:513:PHE:HB2	1.90	0.53
1:A:958:LYS:HG2	1:A:962:GLU:OE1	2.09	0.53
1:E:800:PRO:HG2	1:E:803:ALA:HB2	1.89	0.53
1:F:783:PRO:O	1:F:786:ILE:HG12	2.08	0.53
1:A:889:ALA:HA	1:A:894:SER:O	2.09	0.53
1:C:858:ASP:OD2	1:C:859:TRP:N	2.41	0.53
1:D:382:VAL:HG12	1:D:386:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.90	0.53
1:E:214:VAL:HG21	1:E:237:GLN:N	2.24	0.53
1:F:203:VAL:O	1:F:207:ILE:HG12	2.09	0.53
1:F:452:VAL:CG1	1:F:884:VAL:HG21	2.39	0.53
1:F:586:ARG:O	1:F:589:LYS:HB2	2.08	0.53
1:F:1015:THR:O	1:F:1017:LEU:N	2.42	0.53
1:A:151:GLN:HG3	1:A:152:GLU:N	2.24	0.53
1:A:946:VAL:HG23	1:A:1026:PHE:CD2	2.43	0.53
1:B:61:VAL:CG1	1:B:88:VAL:HG21	2.39	0.53
1:B:949:ALA:HB3	1:B:1026:PHE:CE1	2.44	0.53
1:C:139:VAL:HA	1:C:289:LEU:O	2.09	0.53
1:C:157:TYR:OH	1:C:316:PHE:O	2.16	0.53
1:D:588:GLN:HE21	1:D:592:ASN:ND2	2.06	0.53
1:D:747:ASN:ND2	1:F:237:GLN:OE1	2.40	0.53
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.90	0.53
1:E:452:VAL:C	1:E:455:PRO:HD2	2.28	0.53
1:E:698:ALA:O	1:E:701:GLN:HB3	2.09	0.53
1:F:165:ALA:HA	1:F:168:ARG:HB2	1.89	0.53
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.90	0.53
1:A:597:TYR:HE1	1:A:601:LYS:HD2	1.73	0.53
1:A:674:LEU:HD22	1:A:675:GLY:N	2.24	0.53
1:C:56:THR:O	1:C:60:THR:OG1	2.15	0.53
1:D:231:ASN:HD22	1:E:622:GLN:CD	2.13	0.53
1:F:297:ALA:HB1	1:F:302:THR:OG1	2.09	0.53
1:F:655:PHE:HB3	1:F:663:VAL:HB	1.91	0.53
1:B:66:GLU:CD	1:B:818:ARG:HE	2.12	0.52
1:B:543:VAL:O	1:B:547:ILE:HD13	2.09	0.52
1:E:531:VAL:HG11	1:E:968:VAL:HG21	1.91	0.52
1:F:23:GLY:CA	1:F:381:ALA:HB2	2.35	0.52
1:C:582:ALA:HA	1:C:586:ARG:NH2	2.24	0.52
1:D:68:ASN:HB2	1:D:114:ALA:HB2	1.91	0.52
1:D:1035:ARG:O	1:D:1037:ASN:N	2.43	0.52
1:A:725:PRO:O	1:C:232:ALA:HB1	2.09	0.52
1:A:729:ILE:HD13	1:C:234:ILE:HG23	1.90	0.52
1:A:804:PHE:CD2	1:A:804:PHE:N	2.75	0.52
1:A:971:ARG:C	1:A:974:PRO:HD2	2.30	0.52
1:C:449:LEU:HD21	1:C:937:LEU:HD23	1.92	0.52
1:F:540:ARG:HD3	1:F:541:TYR:HE1	1.73	0.52
1:A:888:LEU:HB2	1:A:898:PRO:HB3	1.91	0.52
1:B:418:ARG:O	1:B:422:GLU:HG3	2.10	0.52
1:C:11:PHE:O	1:C:11:PHE:HD2	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.90	0.52
1:D:412:VAL:HG22	1:D:438:ILE:HD11	1.91	0.52
1:D:992:SER:OG	1:D:1000:GLN:OE1	2.22	0.52
1:E:302:THR:O	1:E:306:ILE:HB	2.09	0.52
1:E:485:ALA:O	1:E:490:PRO:HD3	2.09	0.52
1:F:682:PHE:HD1	1:F:683:GLU:N	2.08	0.52
1:A:400:LEU:HD21	1:A:933:THR:OG1	2.09	0.52
1:A:919:ARG:NH1	1:A:990:VAL:HG12	2.24	0.52
1:B:860:THR:HA	1:B:864:TYR:HB2	1.91	0.52
1:E:211:ASN:OD1	1:E:240:LEU:HG	2.10	0.52
1:F:69:MET:HB3	1:F:72:ILE:HD11	1.91	0.52
1:F:586:ARG:O	1:F:590:VAL:HG23	2.10	0.52
1:F:676:THR:HG23	1:F:677:ALA:N	2.25	0.52
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.91	0.52
1:F:994:GLY:O	1:F:997:SER:OG	2.28	0.52
1:B:66:GLU:OE2	1:B:80:SER:OG	2.24	0.52
1:B:486:LEU:O	1:B:490:PRO:HG3	2.10	0.52
2:B:2000:LMT:O6'	2:B:2000:LMT:O2B	2.25	0.52
1:C:72:ILE:HD12	1:C:75:LEU:HD13	1.91	0.52
1:C:562:SER:OG	1:C:563:PHE:N	2.41	0.52
1:C:1003:VAL:HG13	1:C:1004:GLY:N	2.24	0.52
1:E:155:SER:O	1:E:158:VAL:HB	2.10	0.52
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.91	0.52
1:F:506:GLY:O	1:F:508:GLY:N	2.42	0.52
1:F:549:VAL:O	1:F:552:MET:HB3	2.08	0.52
1:A:196:PHE:HD1	1:A:260:VAL:HG13	1.75	0.52
1:A:414:GLU:HG3	1:A:974:PRO:HG3	1.92	0.52
1:B:35:TYR:CE2	1:B:671:ILE:HG12	2.44	0.52
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.90	0.52
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.91	0.52
1:E:338:HIS:CE1	1:E:342:LYS:HE3	2.44	0.52
1:F:452:VAL:HA	1:F:880:SER:OG	2.09	0.52
1:F:924:ASP:O	1:F:928:GLN:HG3	2.09	0.52
1:B:191:ASN:O	1:B:194:ASN:HB3	2.10	0.52
1:C:792:ARG:HG2	1:C:792:ARG:HH11	1.74	0.52
1:D:527:TYR:O	1:D:531:VAL:HG23	2.10	0.52
1:D:563:PHE:CZ	1:D:674:LEU:HD11	2.45	0.52
1:F:112:GLN:HA	1:F:115:MET:HG3	1.92	0.52
1:F:196:PHE:O	1:F:252:LYS:NZ	2.31	0.52
1:F:379:THR:HG23	1:F:476:SER:OG	2.09	0.52
1:F:543:VAL:O	1:F:546:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:VAL:HA	1:A:1025:PHE:CD1	2.45	0.52
1:B:314:GLU:N	1:B:315:PRO:HD2	2.25	0.52
1:B:533:GLY:HA2	1:B:536:ARG:NH1	2.24	0.52
1:C:414:GLU:OE1	1:C:974:PRO:HD3	2.10	0.52
1:D:712:MET:HB3	1:D:713:LEU:HD22	1.92	0.52
1:D:758:TYR:CE1	1:D:770:LYS:HD3	2.45	0.52
1:E:764:ASP:OD1	1:E:765:ARG:NE	2.25	0.52
1:E:1023:PRO:O	1:E:1027:VAL:HG12	2.10	0.52
1:F:394:THR:CG2	1:F:469:GLN:HB3	2.36	0.52
1:F:588:GLN:HG3	1:F:592:ASN:ND2	2.25	0.52
1:A:278:ILE:HG13	1:A:279:ALA:N	2.19	0.52
1:A:368:PRO:HA	1:A:371:ALA:HB2	1.92	0.52
1:A:572:PHE:HB2	1:A:666:PHE:O	2.09	0.52
1:A:790:TYR:HD1	1:A:800:PRO:HA	1.74	0.52
1:A:971:ARG:O	1:A:974:PRO:HD2	2.10	0.52
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.39	0.52
1:B:249:ILE:HD12	1:B:262:LEU:HD23	1.92	0.52
1:C:685:ILE:HD11	1:C:819:TYR:HB3	1.92	0.52
1:C:976:LEU:O	1:C:980:LEU:HB2	2.10	0.52
1:E:492:LEU:O	1:E:496:MET:HG2	2.10	0.52
1:E:776:GLU:HB3	1:E:779:TYR:CD1	2.44	0.52
1:F:354:VAL:HG12	1:F:980:LEU:HD23	1.91	0.52
1:F:415:ASN:O	1:F:419:VAL:HG13	2.10	0.52
1:A:157:TYR:OH	1:A:316:PHE:O	2.28	0.51
1:C:47:ALA:HB1	1:C:122:VAL:HG13	1.92	0.51
1:C:610:PHE:HB3	1:C:628:PHE:HB2	1.92	0.51
1:D:448:VAL:HB	1:D:884:VAL:HG13	1.92	0.51
1:D:900:SER:HA	1:D:1029:VAL:HG21	1.91	0.51
1:F:163:LYS:HZ3	1:F:177:LEU:HB2	1.74	0.51
1:F:448:VAL:HA	1:F:451:ALA:HB3	1.92	0.51
1:F:971:ARG:HG2	1:F:974:PRO:HG3	1.92	0.51
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.09	0.51
1:A:57:VAL:HG21	1:A:83:ASP:O	2.11	0.51
1:A:449:LEU:O	1:A:453:PHE:HD1	1.94	0.51
1:A:451:ALA:HB1	1:A:883:VAL:CG1	2.40	0.51
1:A:964:THR:O	1:A:968:VAL:HG13	2.09	0.51
1:B:177:LEU:HD12	1:B:178:PHE:N	2.25	0.51
1:B:553:ALA:O	1:B:556:PHE:HB3	2.10	0.51
1:B:652:THR:HG22	1:B:664:PHE:CD2	2.45	0.51
1:E:850:LYS:HD3	1:E:850:LYS:N	2.24	0.51
1:F:6:ILE:HG23	1:F:12:ALA:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:925:VAL:HG12	1:F:926:TYR:CD2	2.46	0.51
1:A:826:GLU:O	1:A:826:GLU:HG3	2.10	0.51
1:C:47:ALA:O	1:C:87:THR:HA	2.10	0.51
1:D:170:SER:HB3	1:E:74:ASN:H	1.74	0.51
1:D:683:GLU:HG3	1:D:824:SER:OG	2.11	0.51
1:F:34:GLN:OE1	1:F:332:PHE:HD2	1.92	0.51
1:F:243:THR:OG1	1:F:268:ILE:HG22	2.10	0.51
1:F:892:TYR:HB3	1:F:897:ILE:HD12	1.92	0.51
1:F:912:ALA:N	1:F:1010:GLY:HA2	2.25	0.51
1:A:516:PHE:O	1:A:519:MET:N	2.43	0.51
1:A:563:PHE:O	1:A:564:LEU:HG	2.10	0.51
1:A:733:GLN:HE22	1:A:743:ILE:HG23	1.74	0.51
1:A:971:ARG:CZ	1:A:971:ARG:CB	2.83	0.51
1:B:108:GLN:OE1	1:B:129:VAL:HB	2.10	0.51
1:C:600:THR:O	1:C:603:LYS:HG2	2.09	0.51
1:C:746:ILE:HG13	1:C:747:ASN:N	2.26	0.51
1:C:804:PHE:CD2	1:C:804:PHE:N	2.79	0.51
1:D:452:VAL:HG13	1:D:884:VAL:HG21	1.92	0.51
1:D:568:ASP:CG	1:D:637:ARG:HH22	2.14	0.51
1:A:1037:ASN:O	1:A:1037:ASN:ND2	2.39	0.51
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.93	0.51
1:B:638:PRO:HD2	1:B:642:ASN:HD22	1.75	0.51
1:C:479:ALA:O	1:C:483:LEU:HG	2.09	0.51
1:D:281:PHE:HB2	1:D:610:PHE:CD1	2.46	0.51
1:D:310:LEU:O	1:D:314:GLU:HG3	2.10	0.51
1:D:894:SER:CB	1:D:897:ILE:HG12	2.40	0.51
1:E:14:VAL:HG11	1:F:890:ALA:HB2	1.91	0.51
1:A:775:SER:OG	1:A:780:ARG:HG2	2.10	0.51
1:B:423:GLU:O	1:B:502:LYS:HB2	2.10	0.51
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.45	0.51
1:B:507:GLU:O	1:B:509:LYS:N	2.44	0.51
1:B:754:TRP:CZ2	1:B:780:ARG:HA	2.46	0.51
1:B:961:ILE:HG13	1:B:962:GLU:N	2.26	0.51
1:C:158:VAL:HG22	1:C:162:MET:HE3	1.91	0.51
1:C:412:VAL:HG13	1:C:435:MET:HE1	1.92	0.51
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.11	0.51
1:C:982:PHE:CD2	1:C:1011:MET:HG2	2.44	0.51
1:D:138:MET:HG3	1:D:291:ILE:HD12	1.93	0.51
1:D:400:LEU:HD11	1:D:933:THR:CG2	2.35	0.51
1:D:423:GLU:O	1:D:502:LYS:HB3	2.11	0.51
1:E:537:SER:HB3	1:E:540:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:546:LEU:HD13	1:E:547:ILE:N	2.25	0.51
1:F:36:PRO:HG2	1:F:38:ILE:CG1	2.41	0.51
1:F:351:VAL:HG22	1:F:981:ALA:HB1	1.92	0.51
1:A:535:LEU:HD21	1:A:1023:PRO:HB2	1.91	0.51
1:A:608:SER:OG	1:A:630:SER:HB3	2.10	0.51
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.93	0.51
1:C:764:ASP:O	1:C:766:GLY:N	2.44	0.51
1:C:1015:THR:O	1:C:1017:LEU:N	2.44	0.51
1:D:313:MET:HB3	1:D:317:PHE:CE1	2.46	0.51
1:E:415:ASN:O	1:E:419:VAL:HG23	2.11	0.51
1:E:572:PHE:CD2	1:E:631:LEU:HD21	2.46	0.51
1:E:671:ILE:HB	1:E:674:LEU:HG	1.93	0.51
1:E:742:SER:O	1:E:746:ILE:HG13	2.10	0.51
1:F:45:ILE:HD13	1:F:111:LEU:CD1	2.41	0.51
1:F:393:LEU:HG	1:F:466:ILE:HG23	1.93	0.51
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.92	0.51
1:B:863:SER:O	1:B:867:ARG:HB2	2.11	0.51
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.91	0.51
1:D:988:PRO:HA	1:D:991:ILE:HD12	1.93	0.51
1:E:250:LEU:HD12	1:E:251:LEU:H	1.74	0.51
1:E:350:LEU:HD12	1:E:984:LEU:HD12	1.93	0.51
1:E:453:PHE:CE1	1:E:474:ILE:HG21	2.40	0.51
1:A:597:TYR:O	1:A:600:THR:HG23	2.11	0.51
1:A:971:ARG:HG3	1:A:974:PRO:HG2	1.93	0.51
1:B:235:ILE:O	1:C:728:LYS:HG3	2.11	0.51
1:B:892:TYR:O	1:B:893:GLU:HB2	2.10	0.51
1:C:457:ALA:HB2	1:C:471:SER:CB	2.41	0.51
1:C:612:VAL:HG11	1:C:615:PHE:HD1	1.76	0.51
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.26	0.51
1:D:300:LEU:O	1:D:304:ALA:HB2	2.11	0.51
1:E:240:LEU:HD12	1:E:246:PHE:CZ	2.46	0.51
1:E:988:PRO:HA	1:E:991:ILE:HB	1.91	0.51
1:F:62:THR:OG1	1:F:80:SER:HB3	2.11	0.51
1:F:685:ILE:HD13	1:F:824:SER:HB3	1.92	0.51
1:A:72:ILE:HD13	1:A:107:VAL:CG2	2.39	0.51
1:C:355:MET:O	1:C:359:LEU:HG	2.11	0.51
1:C:960:LEU:N	1:C:1040:ILE:HG23	2.26	0.51
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.46	0.51
1:D:375:VAL:HG23	1:D:480:LEU:HB2	1.92	0.51
1:E:185:ARG:HD2	1:E:187:TRP:CZ2	2.46	0.51
1:E:408:ASP:OD1	1:E:940:LYS:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:VAL:O	1:E:552:MET:HB3	2.11	0.51
1:E:922:THR:HG23	1:E:924:ASP:OD2	2.10	0.51
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.92	0.51
1:F:358:PHE:CE1	1:F:977:MET:HG2	2.46	0.51
1:F:693:GLU:H	1:F:694:LYS:NZ	2.09	0.51
1:A:155:SER:OG	1:A:180:SER:O	2.28	0.50
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.93	0.50
1:A:944:LEU:O	1:A:947:GLU:HB3	2.11	0.50
1:B:62:THR:HG21	1:B:818:ARG:HD3	1.93	0.50
1:B:108:GLN:HE21	1:C:112:GLN:HE21	1.58	0.50
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.47	0.50
1:B:468:ARG:HB2	1:B:468:ARG:CZ	2.40	0.50
1:B:575:MET:HA	1:B:626:ILE:HG13	1.91	0.50
1:B:944:LEU:HB3	1:B:971:ARG:NH1	2.26	0.50
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.94	0.50
1:C:730:ASP:OD1	1:C:808:ARG:NH1	2.43	0.50
1:C:926:TYR:CE2	1:C:999:ALA:HB1	2.46	0.50
1:D:932:LEU:O	1:D:935:ILE:N	2.44	0.50
1:E:211:ASN:O	1:E:760:ASN:ND2	2.44	0.50
1:E:239:ARG:HH12	1:E:762:PHE:HA	1.76	0.50
1:E:901:VAL:HG13	1:E:942:ALA:HB3	1.93	0.50
1:F:242:SER:O	1:F:246:PHE:CD1	2.64	0.50
1:F:885:PHE:HB2	1:F:902:MET:HE1	1.93	0.50
1:A:108:GLN:O	1:A:112:GLN:HG2	2.12	0.50
1:A:247:GLY:HA2	1:A:268:ILE:HD12	1.93	0.50
1:A:672:VAL:O	1:A:673:GLU:HG2	2.11	0.50
1:B:34:GLN:O	1:B:392:THR:HG22	2.10	0.50
1:B:578:LEU:HD11	1:B:587:THR:N	2.26	0.50
1:B:668:LEU:HD12	1:B:672:VAL:HG13	1.93	0.50
1:C:238:THR:HG22	1:C:239:ARG:O	2.11	0.50
1:D:181:GLN:HG2	1:D:182:TYR:N	2.26	0.50
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.11	0.50
1:E:731:ILE:HA	1:E:805:SER:HA	1.93	0.50
1:F:151:GLN:OE1	1:F:151:GLN:N	2.37	0.50
1:F:360:GLN:NE2	1:F:513:PHE:O	2.45	0.50
1:F:380:PHE:O	1:F:383:LEU:HB2	2.12	0.50
1:F:445:ILE:HG13	1:F:943:ILE:HG21	1.93	0.50
1:F:473:THR:HG23	1:F:474:ILE:HG13	1.93	0.50
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.93	0.50
1:A:158:VAL:HG12	1:A:177:LEU:HD21	1.93	0.50
1:B:493:CYS:O	1:B:497:LEU:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:PHE:O	1:C:7:ASP:HB2	2.12	0.50
1:C:655:PHE:HB3	1:C:663:VAL:HG13	1.91	0.50
1:C:1020:PHE:CE2	2:C:2000:LMT:H32	2.46	0.50
1:D:200:PRO:HA	1:D:203:VAL:HG23	1.92	0.50
1:F:242:SER:O	1:F:246:PHE:HD1	1.94	0.50
1:F:375:VAL:HG13	1:F:480:LEU:CB	2.42	0.50
1:F:405:LEU:CD2	1:F:477:ALA:HB1	2.41	0.50
1:F:424:GLY:HA2	1:F:502:LYS:N	2.26	0.50
1:B:250:LEU:HD12	1:B:251:LEU:H	1.76	0.50
1:C:843:LEU:HD22	1:C:846:GLN:HB2	1.92	0.50
1:D:197:GLN:HA	1:D:798:MET:HE2	1.93	0.50
1:D:355:MET:HE1	1:D:977:MET:HG2	1.93	0.50
1:D:378:GLY:O	1:D:382:VAL:HG23	2.12	0.50
1:D:483:LEU:HA	1:D:486:LEU:HD13	1.94	0.50
1:D:726:GLN:HG2	1:F:233:SER:HB2	1.93	0.50
1:E:451:ALA:CB	1:E:883:VAL:HG12	2.41	0.50
1:F:359:LEU:HD21	1:F:977:MET:CE	2.41	0.50
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.94	0.50
1:A:242:SER:O	1:A:246:PHE:HD1	1.95	0.50
1:A:999:ALA:O	1:A:1002:ALA:HB3	2.11	0.50
1:B:63:GLN:HE21	1:B:818:ARG:HH12	1.60	0.50
1:B:320:GLY:O	1:B:322:LYS:HG2	2.11	0.50
1:B:572:PHE:CD2	1:B:631:LEU:HD11	2.46	0.50
1:B:792:ARG:HB3	1:B:798:MET:SD	2.51	0.50
1:E:940:LYS:O	1:E:943:ILE:HB	2.12	0.50
1:F:452:VAL:HG13	1:F:884:VAL:HG21	1.93	0.50
1:A:17:ILE:HG13	1:A:20:MET:HE2	1.92	0.50
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.43	0.50
1:B:72:ILE:CD1	1:B:107:VAL:HG23	2.42	0.50
1:B:166:ILE:O	1:B:169:THR:OG1	2.28	0.50
1:B:340:VAL:HG22	1:B:396:PHE:CE2	2.47	0.50
1:C:121:GLU:O	1:C:124:GLN:HG2	2.12	0.50
1:C:841:MET:HG3	1:C:859:TRP:CZ2	2.47	0.50
1:D:350:LEU:HG	1:D:984:LEU:HB3	1.93	0.50
1:D:832:ALA:O	1:D:835:LYS:HB2	2.12	0.50
1:D:888:LEU:HD11	1:D:943:ILE:HD11	1.93	0.50
1:E:34:GLN:HB2	1:E:333:VAL:HG22	1.92	0.50
1:E:355:MET:CE	1:E:410:ILE:HG13	2.41	0.50
1:F:537:SER:OG	1:F:540:ARG:HD2	2.11	0.50
1:F:544:LEU:O	1:F:548:ILE:HG12	2.12	0.50
1:A:404:LEU:HD12	1:A:937:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLY:HA2	1:A:517:ASN:OD1	2.12	0.50
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.46	0.50
1:B:559:LEU:HD23	1:B:560:PRO:CD	2.41	0.50
1:B:688:ALA:O	1:B:690:LEU:N	2.44	0.50
1:B:898:PRO:O	1:B:901:VAL:HG12	2.12	0.50
1:C:5:PHE:O	1:C:8:ARG:HG3	2.12	0.50
1:C:455:PRO:HB3	1:C:879:ILE:CG2	2.40	0.50
1:C:457:ALA:HB1	1:C:468:ARG:HG3	1.94	0.50
1:C:552:MET:HB2	1:C:910:ILE:HB	1.93	0.50
1:C:790:TYR:HB3	1:C:798:MET:HB3	1.93	0.50
1:C:1034:SER:HB2	1:C:1038:GLU:HB2	1.92	0.50
1:D:845:GLU:OE1	1:D:867:ARG:NH1	2.44	0.50
1:F:1027:VAL:O	1:F:1031:ARG:HG3	2.11	0.50
1:A:531:VAL:HA	1:A:534:ILE:HG12	1.93	0.50
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.94	0.50
1:C:542:LEU:O	1:C:546:LEU:HD23	2.12	0.50
1:C:678:THR:O	1:C:830:GLN:HG2	2.12	0.50
1:C:974:PRO:O	1:C:978:THR:HG22	2.12	0.50
1:D:382:VAL:HG21	1:D:480:LEU:HD11	1.92	0.50
1:E:394:THR:HG22	1:E:469:GLN:HB3	1.94	0.50
1:E:424:GLY:HA2	1:E:501:ALA:HA	1.92	0.50
1:E:843:LEU:O	1:E:847:LEU:HG	2.12	0.50
1:F:144:ASN:ND2	1:F:319:SER:O	2.44	0.50
1:A:61:VAL:HG11	1:A:122:VAL:HG21	1.94	0.50
1:A:600:THR:OG1	1:A:601:LYS:N	2.43	0.50
1:B:383:LEU:HD11	1:B:473:THR:HA	1.93	0.50
1:B:762:PHE:HE1	1:B:764:ASP:HB3	1.74	0.50
1:D:104:GLN:HE21	1:D:131:LYS:HG2	1.77	0.50
1:D:181:GLN:OE1	1:D:769:LYS:HE2	2.11	0.50
1:D:222:THR:HG23	1:E:622:GLN:HE21	1.76	0.50
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.93	0.50
1:D:781:MET:HE3	1:F:220:GLY:HA2	1.94	0.50
1:D:801:PHE:HA	1:D:804:PHE:HE2	1.76	0.50
1:E:80:SER:HB2	1:E:818:ARG:HD3	1.94	0.50
1:E:484:VAL:HG22	1:E:488:LEU:HD13	1.93	0.50
1:E:916:ALA:O	1:E:919:ARG:N	2.45	0.50
1:F:80:SER:HB2	1:F:818:ARG:HB2	1.94	0.50
1:F:405:LEU:HD22	1:F:477:ALA:HB1	1.94	0.50
1:F:427:PRO:HD3	1:F:499:PRO:HA	1.94	0.50
1:A:692:HIS:HD2	1:A:816:LEU:HD11	1.77	0.49
1:B:572:PHE:HD2	1:B:631:LEU:HD11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:VAL:HG13	1:B:629:VAL:HG12	1.93	0.49
1:D:675:GLY:HA3	1:D:862:MET:SD	2.51	0.49
1:E:578:LEU:HD11	1:E:587:THR:N	2.26	0.49
1:E:841:MET:O	1:E:845:GLU:HG3	2.12	0.49
1:F:832:ALA:O	1:F:834:GLY:N	2.44	0.49
1:A:600:THR:HA	1:A:603:LYS:HE2	1.93	0.49
1:B:533:GLY:HA3	2:B:2000:LMT:C6'	2.42	0.49
1:C:356:TYR:HB2	1:C:365:THR:HG21	1.94	0.49
1:C:435:MET:HE1	1:C:438:ILE:HD11	1.93	0.49
1:C:456:MET:HB3	1:C:876:LEU:HD21	1.93	0.49
1:E:80:SER:HB2	1:E:818:ARG:HB2	1.94	0.49
1:E:557:VAL:O	1:E:559:LEU:N	2.45	0.49
1:F:72:ILE:HD12	1:F:75:LEU:HD22	1.94	0.49
1:A:47:ALA:O	1:A:87:THR:HA	2.12	0.49
1:A:909:VAL:HA	1:A:931:LEU:CD1	2.40	0.49
1:B:111:LEU:C	1:B:113:LEU:H	2.16	0.49
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.46	0.49
1:B:878:ALA:O	1:B:882:ILE:HB	2.12	0.49
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.94	0.49
1:C:1023:PRO:O	1:C:1027:VAL:HG22	2.12	0.49
1:D:781:MET:CE	1:F:225:VAL:HG22	2.41	0.49
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.28	0.49
1:E:150:THR:OG1	1:E:151:GLN:N	2.44	0.49
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.94	0.49
1:F:183:ALA:HA	1:F:770:LYS:O	2.12	0.49
1:F:257:GLY:O	1:F:259:ARG:NH1	2.46	0.49
1:F:404:LEU:HA	1:F:937:LEU:HD21	1.94	0.49
1:A:686:ASP:HB3	1:A:695:LEU:HD13	1.94	0.49
1:A:696:THR:O	1:A:699:ARG:HB3	2.13	0.49
1:A:904:VAL:HG22	1:A:1025:PHE:CE1	2.47	0.49
1:B:1018:ALA:O	1:B:1022:VAL:HG23	2.12	0.49
1:C:409:ALA:O	1:C:413:VAL:HG23	2.13	0.49
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.95	0.49
1:C:1024:VAL:HA	1:C:1027:VAL:HG22	1.94	0.49
1:D:450:SER:N	1:D:478:MET:HE1	2.28	0.49
1:D:944:LEU:HB3	1:D:971:ARG:CZ	2.42	0.49
1:A:31:PRO:HB2	1:A:389:SER:CB	2.43	0.49
1:A:881:LEU:HD23	1:A:882:ILE:HD13	1.94	0.49
1:B:23:GLY:HA2	1:B:381:ALA:HB2	1.95	0.49
1:B:536:ARG:NH1	2:B:2000:LMT:H3B	2.27	0.49
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:586:ARG:O	1:D:589:LYS:HB3	2.12	0.49
1:D:1036:LYS:O	1:D:1038:GLU:N	2.45	0.49
1:E:19:ILE:HG22	1:E:378:GLY:HA2	1.95	0.49
1:E:375:VAL:HG11	1:E:405:LEU:HD13	1.93	0.49
1:E:459:PHE:CD1	1:E:876:LEU:HD12	2.47	0.49
1:F:40:PRO:HB2	1:F:94:PHE:O	2.12	0.49
1:F:60:THR:CG2	1:F:61:VAL:HG23	2.41	0.49
1:F:65:ILE:HG21	1:F:92:LEU:HD21	1.95	0.49
1:F:562:SER:HB3	1:F:924:ASP:HB3	1.94	0.49
1:F:602:GLU:OE2	1:F:650:ARG:NH1	2.46	0.49
1:A:727:PHE:HB2	1:A:809:TRP:NE1	2.27	0.49
1:B:361:ASN:OD1	1:B:363:ARG:HG3	2.13	0.49
1:B:1016:VAL:CG2	2:B:2000:LMT:H82	2.43	0.49
1:B:1024:VAL:HA	1:B:1027:VAL:HG12	1.95	0.49
1:C:101:ASP:O	1:C:105:VAL:HG23	2.13	0.49
1:C:344:LEU:HA	1:C:399:VAL:HG22	1.95	0.49
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.95	0.49
1:D:895:TRP:O	1:D:898:PRO:HD2	2.13	0.49
1:E:104:GLN:NE2	1:F:109:ASN:HB3	2.27	0.49
1:E:310:LEU:HD23	1:E:323:ILE:HG21	1.93	0.49
1:E:455:PRO:HG2	1:E:880:SER:HA	1.93	0.49
1:E:537:SER:HB3	1:E:540:ARG:NH2	2.27	0.49
1:F:159:ALA:HB2	1:F:177:LEU:HD12	1.94	0.49
1:F:201:VAL:HG23	1:F:749:THR:HG23	1.93	0.49
1:F:396:PHE:HE1	1:F:999:ALA:HB1	1.78	0.49
1:F:677:ALA:HB1	1:F:830:GLN:HG2	1.94	0.49
1:F:932:LEU:O	1:F:935:ILE:HG22	2.13	0.49
1:A:428:LYS:HD2	1:A:428:LYS:N	2.28	0.49
1:B:13:TRP:CH2	1:B:492:LEU:HD21	2.48	0.49
1:B:155:SER:O	1:B:158:VAL:HB	2.13	0.49
1:B:455:PRO:O	1:B:876:LEU:HD11	2.13	0.49
1:B:867:ARG:NH2	1:B:868:LEU:HD23	2.22	0.49
1:C:187:TRP:HE3	1:C:775:SER:O	1.96	0.49
1:C:261:LEU:N	1:C:264:ASP:OD2	2.42	0.49
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.27	0.49
1:D:200:PRO:HB2	1:D:749:THR:HG22	1.94	0.49
1:D:538:THR:HG22	1:D:1024:VAL:CG1	2.42	0.49
1:F:240:LEU:HD12	1:F:246:PHE:CE2	2.48	0.49
1:F:699:ARG:HH22	1:F:718:PRO:HB2	1.77	0.49
1:F:790:TYR:CD1	1:F:800:PRO:HA	2.48	0.49
1:B:143:ILE:HG22	1:B:286:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:686:ASP:HB3	1:C:823:PRO:O	2.13	0.49
1:C:699:ARG:HD3	1:C:825:MET:SD	2.53	0.49
1:D:251:LEU:HD12	1:D:260:VAL:HG12	1.93	0.49
1:D:305:ALA:O	1:D:308:ALA:HB3	2.13	0.49
1:D:734:GLU:C	1:D:736:ALA:H	2.14	0.49
1:D:858:ASP:OD1	1:D:859:TRP:N	2.42	0.49
1:F:240:LEU:HD12	1:F:246:PHE:CZ	2.48	0.49
1:F:819:TYR:O	1:F:821:GLY:N	2.46	0.49
1:F:913:LEU:HD23	1:F:927:PHE:CZ	2.47	0.49
1:A:199:THR:HG23	1:A:792:ARG:H	1.77	0.49
1:B:153:ASP:O	1:B:156:ASP:HB3	2.13	0.49
1:B:1015:THR:O	1:B:1018:ALA:N	2.46	0.49
1:C:362:PHE:HB2	1:C:363:ARG:NH2	2.27	0.49
1:D:554:TYR:CE2	1:D:558:ARG:HG3	2.48	0.49
1:D:682:PHE:HE2	1:D:684:LEU:HB2	1.77	0.49
1:E:184:MET:HG2	1:E:246:PHE:CZ	2.47	0.49
1:E:398:MET:HG2	1:E:473:THR:CG2	2.43	0.49
1:F:368:PRO:HA	1:F:371:ALA:HB2	1.94	0.49
1:F:693:GLU:N	1:F:694:LYS:HZ3	2.11	0.49
1:A:222:THR:HA	1:A:224:PRO:HD3	1.94	0.49
1:A:235:ILE:H	1:A:235:ILE:HD12	1.78	0.49
1:A:728:LYS:HD2	1:C:235:ILE:O	2.13	0.49
1:A:733:GLN:O	1:A:737:GLN:HB2	2.13	0.49
1:B:327:TYR:C	1:B:327:TYR:CD2	2.87	0.49
1:B:352:PHE:CE1	1:B:365:THR:HG23	2.48	0.49
1:B:776:GLU:HB3	1:B:779:TYR:CD1	2.48	0.49
1:C:368:PRO:O	1:C:371:ALA:HB3	2.13	0.49
1:D:214:VAL:O	1:D:216:ALA:N	2.45	0.49
1:D:244:GLU:O	1:D:248:LYS:HG2	2.12	0.49
1:D:690:LEU:HG	1:D:694:LYS:HE3	1.95	0.49
1:D:785:ASP:OD2	1:D:785:ASP:N	2.44	0.49
1:D:925:VAL:O	1:D:928:GLN:N	2.44	0.49
1:E:364:ALA:O	1:E:368:PRO:HD3	2.13	0.49
1:E:792:ARG:NH1	1:E:793:ALA:O	2.45	0.49
1:F:64:VAL:O	1:F:114:ALA:HB1	2.12	0.49
1:A:135:SER:HB3	1:A:672:VAL:CG1	2.43	0.48
1:A:785:ASP:OD1	1:A:785:ASP:N	2.46	0.48
1:B:235:ILE:HD11	1:C:726:GLN:HB3	1.94	0.48
1:B:684:LEU:HB2	1:B:827:ILE:HD11	1.95	0.48
1:B:1005:THR:HG23	1:B:1006:GLY:N	2.28	0.48
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:NE2	1:C:230:LEU:O	2.41	0.48
1:C:804:PHE:H	1:C:804:PHE:HD2	1.59	0.48
1:D:230:LEU:HG	1:D:231:ASN:N	2.28	0.48
1:D:889:ALA:HB1	1:D:895:TRP:CE3	2.48	0.48
1:D:900:SER:CA	1:D:1029:VAL:HG21	2.43	0.48
1:D:919:ARG:HD3	1:D:921:LEU:HD13	1.95	0.48
1:E:108:GLN:NE2	1:F:112:GLN:HB2	2.28	0.48
1:E:121:GLU:N	1:E:121:GLU:OE2	2.44	0.48
1:E:691:GLY:H	1:E:694:LYS:HD3	1.78	0.48
1:F:175:VAL:CG1	1:F:289:LEU:HD22	2.42	0.48
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.47	0.48
1:A:53:ASP:OD1	1:A:56:THR:OG1	2.22	0.48
1:D:457:ALA:HB2	1:D:471:SER:HB3	1.95	0.48
1:D:752:ALA:O	1:D:774:MET:HA	2.13	0.48
1:E:259:ARG:HD3	1:E:259:ARG:N	2.27	0.48
1:E:356:TYR:CD1	1:E:365:THR:HG21	2.43	0.48
1:E:527:TYR:CD2	1:E:972:LEU:HG	2.47	0.48
1:E:944:LEU:HD12	1:E:975:ILE:HD13	1.95	0.48
1:E:1007:VAL:HG12	1:E:1008:MET:N	2.28	0.48
1:F:281:PHE:CD1	1:F:610:PHE:HD1	2.31	0.48
1:F:676:THR:CG2	1:F:681:ASP:HB3	2.42	0.48
1:A:21:LEU:HD13	1:A:21:LEU:HA	1.75	0.48
1:A:132:SER:OG	1:A:133:SER:N	2.47	0.48
1:B:184:MET:HG2	1:B:246:PHE:CZ	2.48	0.48
1:B:578:LEU:HD11	1:B:586:ARG:HB2	1.95	0.48
1:C:560:PRO:O	1:C:922:THR:OG1	2.17	0.48
1:C:913:LEU:HD23	1:C:927:PHE:CZ	2.47	0.48
1:D:925:VAL:HA	1:D:928:GLN:HG2	1.95	0.48
1:E:767:ARG:NH2	1:F:117:LEU:HD11	2.29	0.48
1:F:4:PHE:CA	1:F:7:ASP:HB2	2.42	0.48
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.14	0.48
1:A:525:HIS:CE1	1:A:529:ASP:OD2	2.67	0.48
1:B:327:TYR:C	1:B:327:TYR:HD2	2.16	0.48
1:B:546:LEU:HA	1:B:549:VAL:HG12	1.95	0.48
1:C:68:ASN:O	1:C:110:LYS:HD2	2.14	0.48
1:C:736:ALA:HB2	1:C:804:PHE:HD1	1.77	0.48
1:D:463:THR:HA	1:D:466:ILE:HD12	1.95	0.48
1:D:897:ILE:HB	1:D:898:PRO:HD3	1.94	0.48
1:E:362:PHE:CE2	1:E:366:LEU:HD21	2.48	0.48
1:E:423:GLU:C	1:E:502:LYS:HB2	2.34	0.48
1:F:488:LEU:HD21	1:F:492:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:683:GLU:OE1	1:F:685:ILE:HG12	2.13	0.48
1:A:54:ALA:HB1	1:A:816:LEU:HD23	1.93	0.48
1:A:366:LEU:HA	1:A:369:THR:HB	1.96	0.48
1:A:1036:LYS:O	1:A:1038:GLU:N	2.45	0.48
1:B:237:GLN:OE1	1:C:747:ASN:ND2	2.41	0.48
1:B:379:THR:HA	1:B:480:LEU:HD12	1.95	0.48
1:B:846:GLN:O	1:B:850:LYS:NZ	2.28	0.48
1:C:211:ASN:ND2	1:C:760:ASN:HD21	2.11	0.48
1:D:74:ASN:HA	1:F:170:SER:HB3	1.94	0.48
1:D:602:GLU:OE2	1:D:650:ARG:HD2	2.13	0.48
1:E:167:SER:CB	1:F:70:ASN:HD22	2.26	0.48
1:E:960:LEU:O	1:E:964:THR:HG23	2.13	0.48
1:F:101:ASP:OD1	1:F:101:ASP:N	2.45	0.48
1:F:542:LEU:O	1:F:546:LEU:HD23	2.13	0.48
1:F:565:PRO:O	1:F:670:ALA:HB2	2.13	0.48
1:A:408:ASP:OD2	1:A:940:LYS:NZ	2.38	0.48
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.34	0.48
1:B:234:ILE:HD11	1:C:754:TRP:CE3	2.48	0.48
1:B:545:TYR:O	1:B:548:ILE:N	2.46	0.48
1:B:595:THR:O	1:B:599:LEU:HG	2.13	0.48
1:B:736:ALA:HB2	1:B:804:PHE:HB3	1.94	0.48
1:D:158:VAL:HA	1:D:162:MET:CE	2.44	0.48
1:E:536:ARG:HD2	2:E:2000:LMT:C3B	2.43	0.48
1:E:537:SER:OG	1:E:540:ARG:NH1	2.47	0.48
1:F:447:MET:HB3	1:F:887:CYS:SG	2.54	0.48
1:A:154:ILE:HG22	1:A:287:SER:HB3	1.96	0.48
1:B:182:TYR:O	1:B:769:LYS:HD3	2.12	0.48
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.94	0.48
1:B:617:PHE:O	1:B:619:GLY:N	2.45	0.48
1:B:678:THR:O	1:B:830:GLN:HB2	2.13	0.48
1:C:5:PHE:HE1	1:C:8:ARG:NH1	2.09	0.48
1:C:81:ASN:O	1:C:88:VAL:HG23	2.14	0.48
1:C:904:VAL:HG23	1:C:907:LEU:HD22	1.95	0.48
1:D:684:LEU:O	1:D:824:SER:OG	2.23	0.48
1:E:352:PHE:HD1	1:E:369:THR:OG1	1.96	0.48
1:E:382:VAL:HG21	1:E:476:SER:CB	2.44	0.48
1:E:408:ASP:OD2	1:E:445:ILE:HD11	2.14	0.48
1:E:888:LEU:HD11	1:E:943:ILE:HD11	1.95	0.48
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.96	0.48
1:A:3:ASN:O	1:A:6:ILE:N	2.45	0.48
1:A:187:TRP:HA	1:A:774:MET:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:HA	1:A:798:MET:HE1	1.96	0.48
1:B:23:GLY:HA3	1:B:377:LEU:O	2.14	0.48
1:B:776:GLU:HG2	1:B:777:ALA:H	1.78	0.48
1:C:427:PRO:O	1:C:431:THR:HG23	2.13	0.48
1:D:43:VAL:HG23	1:D:94:PHE:HE1	1.79	0.48
1:D:444:GLY:O	1:D:447:MET:HB2	2.14	0.48
1:D:900:SER:OG	1:D:1029:VAL:HG11	2.14	0.48
1:D:1035:ARG:HA	1:D:1035:ARG:HD2	1.68	0.48
1:E:182:TYR:HD2	1:E:765:ARG:HH22	1.61	0.48
1:E:1022:VAL:HA	1:E:1025:PHE:CD1	2.49	0.48
1:E:1035:ARG:HB3	1:E:1036:LYS:H	1.53	0.48
1:F:208:LYS:HG3	1:F:759:VAL:HG13	1.95	0.48
1:F:431:THR:HG21	1:F:490:PRO:HA	1.96	0.48
1:F:740:GLY:O	1:F:794:ALA:N	2.47	0.48
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.95	0.48
1:A:182:TYR:O	1:A:769:LYS:HD3	2.13	0.48
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.14	0.48
1:A:832:ALA:CB	1:A:835:LYS:HD2	2.35	0.48
1:D:137:LEU:HD22	1:D:293:LEU:HD13	1.95	0.48
1:D:736:ALA:HA	1:D:739:LEU:HD13	1.96	0.48
1:E:57:VAL:HG21	1:E:86:GLY:HA2	1.95	0.48
1:E:230:LEU:HG	1:E:231:ASN:N	2.27	0.48
1:E:571:VAL:O	1:E:668:LEU:HD21	2.14	0.48
1:E:957:GLY:O	1:E:1041:GLU:HA	2.13	0.48
1:A:736:ALA:HB2	1:A:804:PHE:HB3	1.95	0.48
1:A:974:PRO:O	1:A:977:MET:HG2	2.14	0.48
1:A:982:PHE:O	1:A:985:GLY:N	2.47	0.48
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.48
1:B:1023:PRO:O	1:B:1027:VAL:HG12	2.14	0.48
1:C:465:ALA:HA	1:C:468:ARG:HH12	1.78	0.48
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.48	0.48
1:D:394:THR:HG22	1:D:469:GLN:HB3	1.96	0.48
1:D:584:GLN:NE2	1:F:222:THR:HG22	2.28	0.48
1:D:837:THR:O	1:D:840:ALA:HB3	2.14	0.48
1:D:1038:GLU:CD	1:D:1038:GLU:H	2.16	0.48
1:F:74:ASN:HB3	1:F:95:GLU:CB	2.29	0.48
1:F:545:TYR:HB2	1:F:1021:PHE:HE2	1.79	0.48
1:F:703:LEU:HD13	1:F:718:PRO:HB3	1.95	0.48
1:F:754:TRP:CZ2	1:F:780:ARG:HA	2.49	0.48
1:F:987:MET:HG2	1:F:1008:MET:HE1	1.96	0.48
1:A:541:TYR:N	1:A:541:TYR:CD1	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:GLU:HG3	1:A:646:ALA:N	2.29	0.47
1:A:754:TRP:CE2	1:A:780:ARG:HB3	2.48	0.47
1:A:888:LEU:HD11	1:A:901:VAL:HB	1.96	0.47
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.96	0.47
1:B:366:LEU:O	1:B:369:THR:HB	2.14	0.47
1:B:530:SER:HG	1:B:531:VAL:H	1.62	0.47
1:C:398:MET:HG2	1:C:473:THR:CG2	2.44	0.47
1:C:750:LEU:O	1:C:753:ALA:HB3	2.13	0.47
1:D:68:ASN:CB	1:D:114:ALA:HB2	2.44	0.47
1:D:196:PHE:CD2	1:D:196:PHE:N	2.80	0.47
1:D:438:ILE:O	1:D:441:ALA:HB3	2.14	0.47
1:D:492:LEU:HB3	1:D:496:MET:CE	2.43	0.47
1:E:95:GLU:HB2	1:E:98:THR:OG1	2.14	0.47
1:E:219:LEU:HA	1:F:754:TRP:HZ3	1.79	0.47
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.33	0.47
1:F:36:PRO:HG2	1:F:38:ILE:HG13	1.95	0.47
1:F:312:LYS:O	1:F:312:LYS:HE3	2.14	0.47
1:F:467:TYR:HE1	1:F:925:VAL:HG22	1.78	0.47
1:A:462:SER:O	1:A:466:ILE:HG12	2.14	0.47
1:A:674:LEU:HD22	1:A:675:GLY:H	1.79	0.47
1:B:971:ARG:CG	1:B:971:ARG:HH11	2.27	0.47
1:C:66:GLU:OE2	1:C:821:GLY:HA2	2.14	0.47
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.14	0.47
1:D:235:ILE:O	1:E:728:LYS:HD2	2.14	0.47
1:D:423:GLU:OE1	1:D:433:LYS:HE2	2.14	0.47
1:D:926:TYR:HE1	1:D:999:ALA:CB	2.27	0.47
1:E:166:ILE:HD13	1:E:310:LEU:HD13	1.95	0.47
1:F:4:PHE:C	1:F:7:ASP:HB2	2.35	0.47
1:F:250:LEU:HD12	1:F:251:LEU:H	1.79	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.48	0.47
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.14	0.47
1:A:414:GLU:CG	1:A:974:PRO:HG3	2.44	0.47
1:A:602:GLU:OE2	1:A:650:ARG:NH2	2.47	0.47
1:A:736:ALA:O	1:A:741:VAL:HG12	2.13	0.47
1:B:352:PHE:C	1:B:352:PHE:CD2	2.87	0.47
1:B:368:PRO:HG3	1:B:413:VAL:HG21	1.96	0.47
1:C:452:VAL:O	1:C:455:PRO:HD2	2.15	0.47
1:C:608:SER:OG	1:C:630:SER:HB3	2.15	0.47
1:D:162:MET:HG2	1:D:313:MET:SD	2.54	0.47
1:D:360:GLN:NE2	1:D:517:ASN:HD21	2.11	0.47
1:D:776:GLU:HG2	1:D:777:ALA:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:950:LYS:HE2	1:D:950:LYS:HB2	1.62	0.47
1:E:31:PRO:O	1:E:390:ILE:HG12	2.13	0.47
1:E:206:ALA:HB1	1:E:249:ILE:HD11	1.95	0.47
1:E:244:GLU:OE1	1:E:248:LYS:NZ	2.29	0.47
1:E:641:GLU:OE1	1:E:641:GLU:N	2.39	0.47
1:F:24:GLY:O	1:F:27:ILE:HG12	2.13	0.47
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.14	0.47
1:F:211:ASN:CG	1:F:240:LEU:HG	2.35	0.47
1:A:242:SER:OG	1:A:245:GLU:HG3	2.14	0.47
1:B:166:ILE:HD12	1:B:166:ILE:HA	1.82	0.47
1:B:1011:MET:O	1:B:1015:THR:HG23	2.14	0.47
1:C:120:GLN:O	1:C:124:GLN:HB3	2.13	0.47
1:C:135:SER:HB3	1:C:673:GLU:HA	1.95	0.47
1:C:358:PHE:HB3	1:C:359:LEU:HD23	1.96	0.47
1:C:785:ASP:N	1:C:785:ASP:OD1	2.47	0.47
1:D:151:GLN:H	1:D:151:GLN:HG3	1.28	0.47
1:D:462:SER:O	1:D:466:ILE:HG13	2.15	0.47
1:E:219:LEU:HD23	1:F:754:TRP:CZ3	2.49	0.47
1:E:235:ILE:O	1:F:728:LYS:HD2	2.15	0.47
1:E:559:LEU:HD12	1:E:560:PRO:HD2	1.96	0.47
1:E:648:THR:HG23	1:E:665:ALA:O	2.13	0.47
1:E:971:ARG:C	1:E:974:PRO:HD2	2.34	0.47
1:E:986:VAL:HG11	1:E:1007:VAL:CG1	2.45	0.47
1:F:420:MET:CE	1:F:427:PRO:HG3	2.44	0.47
1:A:996:GLY:C	1:A:998:GLY:H	2.17	0.47
1:C:6:ILE:C	1:C:8:ARG:H	2.17	0.47
1:C:34:GLN:HG3	1:C:333:VAL:HG22	1.96	0.47
1:C:190:PRO:HG3	1:C:779:TYR:CG	2.49	0.47
1:C:742:SER:O	1:C:746:ILE:HG23	2.14	0.47
1:D:515:TRP:O	1:D:519:MET:HG3	2.14	0.47
1:D:520:PHE:O	1:D:523:SER:OG	2.23	0.47
1:D:873:ALA:N	1:D:874:PRO:HD2	2.29	0.47
1:E:219:LEU:HD11	1:F:727:PHE:CD2	2.50	0.47
1:E:379:THR:O	1:E:382:VAL:N	2.47	0.47
1:E:536:ARG:HD2	2:E:2000:LMT:H4B	1.97	0.47
1:E:873:ALA:N	1:E:874:PRO:HD2	2.29	0.47
1:F:326:PRO:HA	1:F:630:SER:OG	2.15	0.47
1:F:414:GLU:OE2	1:F:973:ARG:NH1	2.48	0.47
1:F:618:ALA:O	1:F:815:ARG:NH2	2.48	0.47
1:F:885:PHE:CE2	1:F:886:LEU:HD23	2.50	0.47
1:F:983:ILE:CD1	1:F:1012:VAL:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1026:PHE:O	1:F:1030:ARG:HB2	2.15	0.47
1:F:1030:ARG:C	1:F:1032:ARG:H	2.16	0.47
1:A:294:ALA:HB3	1:A:297:ALA:HB3	1.97	0.47
1:B:201:VAL:HG21	1:B:745:ASP:OD2	2.14	0.47
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.40	0.47
1:B:726:GLN:NE2	1:B:811:TYR:O	2.47	0.47
1:B:971:ARG:HH11	1:B:971:ARG:HG3	1.79	0.47
1:C:1031:ARG:NH2	1:C:1040:ILE:HD11	2.29	0.47
1:D:72:ILE:HG21	1:D:107:VAL:HG23	1.96	0.47
1:D:214:VAL:HG22	1:D:216:ALA:N	2.30	0.47
1:E:166:ILE:HD12	1:E:166:ILE:HA	1.65	0.47
1:E:185:ARG:HB3	1:E:187:TRP:NE1	2.30	0.47
1:E:222:THR:HA	1:E:224:PRO:CD	2.44	0.47
1:E:451:ALA:HB1	1:E:883:VAL:HG12	1.96	0.47
1:F:62:THR:O	1:F:90:ILE:HD12	2.14	0.47
1:F:143:ILE:HG22	1:F:286:ALA:CB	2.45	0.47
1:F:162:MET:HG2	1:F:313:MET:SD	2.54	0.47
1:F:281:PHE:CE1	1:F:608:SER:HB2	2.50	0.47
1:F:563:PHE:CE2	1:F:564:LEU:HD12	2.49	0.47
1:A:293:LEU:HD22	1:A:294:ALA:N	2.23	0.47
1:A:360:GLN:OE1	1:A:517:ASN:ND2	2.44	0.47
1:A:525:HIS:O	1:A:526:HIS:C	2.53	0.47
1:A:576:VAL:HA	1:A:663:VAL:HG22	1.97	0.47
1:A:658:ILE:O	1:A:659:LYS:NZ	2.25	0.47
1:A:764:ASP:C	1:A:766:GLY:H	2.18	0.47
1:A:888:LEU:CB	1:A:898:PRO:HB3	2.45	0.47
1:A:909:VAL:O	1:A:912:ALA:N	2.43	0.47
1:A:965:LEU:O	1:A:968:VAL:HG22	2.15	0.47
1:B:363:ARG:NH1	1:B:496:MET:O	2.48	0.47
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.96	0.47
1:B:742:SER:O	1:B:746:ILE:HG13	2.15	0.47
1:B:909:VAL:HG23	1:B:935:ILE:HD11	1.97	0.47
1:C:184:MET:HB2	1:C:762:PHE:CD2	2.50	0.47
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.96	0.47
1:C:536:ARG:HD2	2:C:2000:LMT:O4'	2.14	0.47
1:C:833:PRO:C	1:C:835:LYS:N	2.68	0.47
2:C:2000:LMT:O4'	2:C:2000:LMT:O6B	2.25	0.47
1:D:355:MET:CE	1:D:977:MET:HG2	2.45	0.47
1:D:895:TRP:CZ2	1:F:10:ILE:HD12	2.49	0.47
1:D:926:TYR:CE1	1:D:999:ALA:HB1	2.50	0.47
1:D:949:ALA:HB3	1:D:1026:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:GLY:HA2	1:E:377:LEU:O	2.14	0.47
1:E:139:VAL:HA	1:E:289:LEU:O	2.15	0.47
1:E:172:VAL:HG22	1:E:302:THR:HG23	1.97	0.47
1:E:185:ARG:HB3	1:E:187:TRP:CZ2	2.50	0.47
1:E:420:MET:SD	1:E:427:PRO:HA	2.55	0.47
1:E:536:ARG:HH11	2:E:2000:LMT:C3B	2.28	0.47
1:E:652:THR:HG22	1:E:665:ALA:H	1.79	0.47
1:E:750:LEU:O	1:E:753:ALA:HB3	2.14	0.47
1:E:926:TYR:HE1	1:E:999:ALA:HB1	1.78	0.47
1:E:961:ILE:HG22	1:E:965:LEU:HD12	1.97	0.47
1:E:1015:THR:OG1	1:E:1016:VAL:N	2.48	0.47
1:A:66:GLU:OE2	1:A:80:SER:OG	2.23	0.47
1:A:996:GLY:C	1:A:998:GLY:N	2.67	0.47
1:B:54:ALA:O	1:B:57:VAL:HG23	2.14	0.47
1:B:444:GLY:O	1:B:447:MET:HB2	2.15	0.47
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.95	0.47
1:C:507:GLU:HG2	1:C:518:ARG:HG2	1.95	0.47
1:C:524:THR:HG23	1:C:972:LEU:HD12	1.97	0.47
1:D:281:PHE:HD1	1:D:610:PHE:HD1	1.62	0.47
1:E:313:MET:HB3	1:E:317:PHE:CE1	2.49	0.47
1:E:904:VAL:HA	1:E:907:LEU:HD13	1.96	0.47
1:F:163:LYS:O	1:F:163:LYS:HG2	2.15	0.47
1:F:776:GLU:HB2	1:F:779:TYR:CD1	2.50	0.47
1:F:911:GLY:HA3	1:F:1013:THR:OG1	2.15	0.47
1:A:84:SER:N	1:A:814:PRO:O	2.48	0.47
1:A:158:VAL:CG1	1:A:177:LEU:HD21	2.45	0.47
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.97	0.47
1:A:746:ILE:HG22	1:A:791:VAL:HG21	1.95	0.47
1:B:13:TRP:CE3	1:B:488:LEU:HD11	2.50	0.47
1:B:81:ASN:O	1:B:88:VAL:HA	2.14	0.47
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.75	0.47
1:B:805:SER:OG	1:B:806:SER:N	2.48	0.47
1:C:101:ASP:OD1	1:C:101:ASP:N	2.47	0.47
1:C:712:MET:O	1:C:832:ALA:N	2.36	0.47
1:D:58:GLN:OE1	1:D:816:LEU:HB3	2.15	0.47
1:D:736:ALA:HB2	1:D:804:PHE:HB3	1.96	0.47
1:D:987:MET:HA	1:D:990:VAL:HG23	1.96	0.47
1:E:359:LEU:C	1:E:361:ASN:H	2.15	0.47
1:E:450:SER:N	1:E:478:MET:HE1	2.30	0.47
1:E:785:ASP:N	1:E:785:ASP:OD1	2.48	0.47
1:E:897:ILE:HD13	1:E:950:LYS:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:925:VAL:HA	1:F:928:GLN:OE1	2.15	0.47
1:A:166:ILE:HD12	1:A:166:ILE:HA	1.78	0.47
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.55	0.47
1:A:909:VAL:HG22	1:A:931:LEU:HD11	1.95	0.47
1:A:914:LEU:O	1:A:918:PHE:HB2	2.15	0.47
1:B:105:VAL:HG22	1:C:109:ASN:OD1	2.15	0.47
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.97	0.47
1:B:1005:THR:HG23	1:B:1006:GLY:H	1.80	0.47
1:C:435:MET:CE	1:C:438:ILE:HD11	2.45	0.47
1:C:565:PRO:HG3	1:C:999:ALA:CA	2.45	0.47
1:C:698:ALA:O	1:C:701:GLN:HB3	2.14	0.47
1:C:758:TYR:CE1	1:C:770:LYS:HD3	2.50	0.47
1:D:166:ILE:HD12	1:D:166:ILE:HA	1.70	0.47
1:D:228:GLN:NE2	1:D:230:LEU:O	2.42	0.47
1:D:337:ILE:HA	1:D:337:ILE:HD12	1.70	0.47
1:D:404:LEU:HD12	1:D:937:LEU:HD21	1.97	0.47
1:D:909:VAL:O	1:D:912:ALA:N	2.46	0.47
1:E:56:THR:O	1:E:60:THR:OG1	2.32	0.47
1:E:356:TYR:CE1	1:E:362:PHE:HA	2.50	0.47
1:E:376:LEU:O	1:E:377:LEU:C	2.54	0.47
1:E:462:SER:O	1:E:466:ILE:HG13	2.15	0.47
1:F:42:ALA:HB2	1:F:93:THR:HG23	1.97	0.47
1:F:121:GLU:O	1:F:124:GLN:HG2	2.15	0.47
1:F:588:GLN:O	1:F:592:ASN:ND2	2.48	0.47
1:F:750:LEU:O	1:F:753:ALA:HB3	2.15	0.47
1:B:778:LYS:HE3	1:B:779:TYR:CE2	2.49	0.46
1:C:26:ALA:HB1	1:C:384:ALA:HB3	1.97	0.46
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.98	0.46
1:C:408:ASP:O	1:C:412:VAL:HG23	2.15	0.46
1:C:453:PHE:O	1:C:456:MET:HG3	2.15	0.46
1:C:684:LEU:HD12	1:C:827:ILE:HD11	1.97	0.46
1:C:987:MET:O	1:C:990:VAL:HG22	2.15	0.46
1:D:128:SER:HB3	1:D:130:GLU:OE2	2.15	0.46
1:D:218:GLN:HG2	1:D:233:SER:HA	1.95	0.46
1:D:933:THR:HG22	1:D:934:THR:N	2.30	0.46
1:E:115:MET:O	1:E:123:GLN:NE2	2.48	0.46
1:E:590:VAL:HG11	1:E:663:VAL:HG21	1.97	0.46
1:F:137:LEU:N	1:F:291:ILE:O	2.48	0.46
1:F:467:TYR:O	1:F:470:PHE:HB2	2.15	0.46
1:A:355:MET:HE2	1:A:368:PRO:HG2	1.97	0.46
1:A:425:LEU:HD22	1:A:429:GLU:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:O	1:A:466:ILE:HB	2.15	0.46
1:A:800:PRO:O	1:A:803:ALA:HB3	2.16	0.46
1:B:135:SER:OG	1:B:673:GLU:OE1	2.33	0.46
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.97	0.46
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.97	0.46
1:B:608:SER:O	1:B:630:SER:N	2.44	0.46
1:C:54:ALA:HB1	1:C:816:LEU:HG	1.97	0.46
1:C:298:ASN:HB3	1:C:301:ASP:CB	2.33	0.46
1:C:355:MET:HB3	1:C:365:THR:HG23	1.98	0.46
1:C:414:GLU:HG3	1:C:974:PRO:HB3	1.97	0.46
1:C:758:TYR:HB2	1:C:772:TYR:CE2	2.51	0.46
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.97	0.46
1:D:690:LEU:O	1:D:694:LYS:HD3	2.14	0.46
1:D:727:PHE:HE1	1:D:807:SER:OG	1.98	0.46
1:D:889:ALA:HB1	1:D:895:TRP:CZ3	2.50	0.46
1:D:910:ILE:O	1:D:914:LEU:HB2	2.15	0.46
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.97	0.46
1:E:288:GLY:C	1:E:289:LEU:HD22	2.35	0.46
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.96	0.46
1:E:422:GLU:C	1:E:502:LYS:HG3	2.36	0.46
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.50	0.46
1:F:397:GLY:HA3	1:F:470:PHE:HD2	1.79	0.46
1:F:577:GLN:NE2	1:F:721:LEU:HD11	2.29	0.46
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.98	0.46
1:A:904:VAL:HG22	1:A:1025:PHE:CD1	2.50	0.46
1:B:327:TYR:HE2	1:B:329:THR:HG23	1.80	0.46
1:B:405:LEU:HD22	1:B:481:SER:HB2	1.97	0.46
1:B:801:PHE:HA	1:B:804:PHE:HE2	1.76	0.46
1:D:182:TYR:O	1:D:769:LYS:HD3	2.15	0.46
1:D:194:ASN:HA	1:D:798:MET:HE3	1.97	0.46
1:D:224:PRO:CB	1:E:781:MET:HE1	2.45	0.46
1:D:345:VAL:O	1:D:348:ILE:HB	2.15	0.46
1:E:150:THR:HG23	1:E:153:ASP:OD1	2.15	0.46
1:E:167:SER:OG	1:E:175:VAL:HG11	2.15	0.46
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.95	0.46
1:F:372:VAL:HG23	1:F:373:PRO:CD	2.45	0.46
1:F:850:LYS:O	1:F:851:LEU:HD23	2.16	0.46
1:A:549:VAL:O	1:A:552:MET:HB3	2.14	0.46
1:B:456:MET:HA	1:B:876:LEU:HD21	1.98	0.46
1:B:594:VAL:HG22	1:B:655:PHE:CZ	2.51	0.46
1:B:721:LEU:HB3	1:B:814:PRO:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ILE:HD13	1:C:487:ILE:HD13	1.96	0.46
1:C:922:THR:O	1:C:924:ASP:N	2.47	0.46
1:D:17:ILE:O	1:D:20:MET:HB2	2.16	0.46
1:D:445:ILE:HG21	1:D:940:LYS:CD	2.45	0.46
1:D:695:LEU:HD23	1:D:825:MET:HG3	1.96	0.46
1:E:188:MET:SD	1:E:203:VAL:HG21	2.55	0.46
1:E:280:GLU:OE2	1:E:588:GLN:NE2	2.49	0.46
1:E:641:GLU:H	1:E:641:GLU:CD	2.16	0.46
1:E:686:ASP:HA	1:E:854:GLY:O	2.16	0.46
1:E:992:SER:HB3	1:E:1000:GLN:OE1	2.15	0.46
1:F:58:GLN:OE1	1:F:818:ARG:HD2	2.15	0.46
1:F:509:LYS:CG	1:F:513:PHE:HB2	2.45	0.46
1:F:535:LEU:HD23	1:F:535:LEU:HA	1.66	0.46
1:F:717:ARG:HG3	1:F:828:LEU:HB2	1.97	0.46
1:F:744:ASN:O	1:F:748:THR:HG23	2.15	0.46
1:F:982:PHE:O	1:F:983:ILE:C	2.54	0.46
1:B:688:ALA:HB3	1:B:690:LEU:HD22	1.97	0.46
1:C:222:THR:HA	1:C:224:PRO:CD	2.44	0.46
1:C:576:VAL:HG21	1:C:591:LEU:HD21	1.97	0.46
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.97	0.46
1:D:400:LEU:HD23	1:D:474:ILE:HD13	1.98	0.46
1:E:340:VAL:HG11	1:E:395:MET:CB	2.39	0.46
1:E:575:MET:HB2	1:E:626:ILE:HD11	1.98	0.46
1:E:680:PHE:CG	1:E:859:TRP:CZ3	3.04	0.46
1:F:352:PHE:HE1	1:F:366:LEU:HD23	1.79	0.46
1:F:904:VAL:HG21	1:F:942:ALA:CB	2.43	0.46
1:F:961:ILE:H	1:F:961:ILE:CD1	2.21	0.46
1:A:472:ILE:O	1:A:476:SER:HB3	2.15	0.46
1:A:637:ARG:HA	1:A:642:ASN:HD22	1.80	0.46
1:A:686:ASP:OD2	1:A:823:PRO:HB2	2.15	0.46
1:A:752:ALA:O	1:A:774:MET:HA	2.14	0.46
1:B:544:LEU:O	1:B:548:ILE:HG13	2.16	0.46
1:B:609:VAL:HG13	1:B:629:VAL:CG1	2.46	0.46
1:C:888:LEU:HD23	1:C:888:LEU:HA	1.67	0.46
1:C:926:TYR:HE2	1:C:999:ALA:CB	2.29	0.46
1:D:62:THR:O	1:D:66:GLU:HG3	2.15	0.46
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.62	0.46
1:D:525:HIS:CE1	1:D:529:ASP:OD1	2.68	0.46
1:D:680:PHE:CD1	1:D:859:TRP:HZ3	2.29	0.46
1:D:702:LEU:HD11	1:D:848:ALA:HB2	1.97	0.46
1:E:45:ILE:HG12	1:E:129:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:ARG:HB3	1:E:187:TRP:CE2	2.51	0.46
1:E:219:LEU:N	1:E:232:ALA:O	2.45	0.46
1:E:558:ARG:HE	1:E:558:ARG:HB3	1.52	0.46
1:F:465:ALA:O	1:F:468:ARG:HG2	2.16	0.46
1:F:506:GLY:C	1:F:508:GLY:N	2.68	0.46
1:F:764:ASP:O	1:F:766:GLY:N	2.49	0.46
1:A:62:THR:O	1:A:66:GLU:HG3	2.16	0.46
1:A:198:LEU:HD22	1:A:202:ASP:HB2	1.97	0.46
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.97	0.46
1:A:455:PRO:O	1:A:458:PHE:HB2	2.16	0.46
2:A:2000:LMT:H11	2:A:2000:LMT:H2'	1.64	0.46
1:B:33:ALA:O	1:B:391:ASN:HA	2.16	0.46
1:B:588:GLN:HB2	1:B:613:ASN:ND2	2.30	0.46
1:B:894:SER:CB	1:B:897:ILE:HG13	2.46	0.46
1:C:960:LEU:O	1:C:964:THR:HG23	2.16	0.46
1:D:109:ASN:HD22	1:E:109:ASN:HD21	1.64	0.46
1:D:253:VAL:HG12	1:D:259:ARG:HG2	1.96	0.46
1:E:539:GLY:O	1:E:542:LEU:HB2	2.14	0.46
1:F:36:PRO:O	1:F:38:ILE:HG13	2.14	0.46
1:F:125:GLN:NE2	1:F:125:GLN:O	2.48	0.46
1:F:164:ASP:HB2	1:F:767:ARG:HH21	1.80	0.46
1:F:208:LYS:HG3	1:F:759:VAL:CG1	2.46	0.46
1:F:371:ALA:O	1:F:375:VAL:HG23	2.16	0.46
1:F:577:GLN:O	1:F:661:ALA:HB1	2.15	0.46
1:F:785:ASP:N	1:F:785:ASP:OD1	2.48	0.46
1:A:212:ALA:C	1:A:239:ARG:HG2	2.36	0.46
1:A:393:LEU:HD13	1:A:466:ILE:HA	1.97	0.46
1:A:712:MET:HG3	1:A:713:LEU:HD13	1.97	0.46
1:B:721:LEU:HA	1:B:721:LEU:HD13	1.64	0.46
1:C:543:VAL:O	1:C:546:LEU:HB2	2.16	0.46
1:D:367:ILE:HA	1:D:496:MET:HE3	1.98	0.46
1:D:376:LEU:O	1:D:377:LEU:C	2.53	0.46
1:D:672:VAL:HG23	1:D:673:GLU:OE2	2.16	0.46
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.97	0.46
1:F:144:ASN:HA	1:F:320:GLY:O	2.14	0.46
1:F:331:PRO:O	1:F:334:LYS:HB2	2.15	0.46
1:F:372:VAL:O	1:F:376:LEU:N	2.33	0.46
1:F:738:ALA:O	1:F:740:GLY:N	2.48	0.46
1:F:775:SER:OG	1:F:780:ARG:HG2	2.16	0.46
1:F:940:LYS:O	1:F:943:ILE:HB	2.15	0.46
1:A:239:ARG:NH1	1:A:761:ASP:H	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:OD1	1:A:393:LEU:HB2	2.16	0.46
1:B:242:SER:OG	1:B:245:GLU:HG3	2.16	0.46
1:B:359:LEU:C	1:B:361:ASN:H	2.19	0.46
1:C:26:ALA:HB1	1:C:384:ALA:CB	2.46	0.46
1:C:699:ARG:HE	1:C:718:PRO:HB3	1.81	0.46
1:E:39:ALA:HB2	1:E:673:GLU:HG3	1.97	0.46
1:E:79:SER:O	1:E:90:ILE:HA	2.16	0.46
1:F:182:TYR:O	1:F:769:LYS:HB3	2.15	0.46
1:F:219:LEU:HG	1:F:234:ILE:HD11	1.97	0.46
1:F:354:VAL:HG21	1:F:981:ALA:HA	1.97	0.46
1:F:888:LEU:HD12	1:F:901:VAL:HG11	1.97	0.46
1:A:186:ILE:HB	1:A:773:VAL:HG12	1.98	0.46
1:A:243:THR:OG1	1:A:268:ILE:HG22	2.16	0.46
1:B:235:ILE:CD1	1:C:726:GLN:HB3	2.46	0.46
1:B:758:TYR:CD1	1:B:770:LYS:HD3	2.51	0.46
1:B:1036:LYS:O	1:B:1037:ASN:ND2	2.49	0.46
1:C:57:VAL:HG13	1:C:88:VAL:HB	1.98	0.46
1:D:124:GLN:NE2	1:D:758:TYR:HB3	2.31	0.46
1:D:157:TYR:OH	1:D:316:PHE:O	2.34	0.46
1:E:200:PRO:HA	1:E:203:VAL:HG23	1.98	0.46
1:E:343:THR:CG2	1:E:399:VAL:HG11	2.46	0.46
1:E:434:SER:O	1:E:437:GLN:HG2	2.15	0.46
1:E:442:LEU:O	1:E:445:ILE:HG13	2.16	0.46
1:E:953:MET:HE2	1:E:953:MET:HB2	1.69	0.46
1:E:960:LEU:HD23	1:E:961:ILE:N	2.31	0.46
1:E:979:SER:CB	1:E:1015:THR:HG21	2.45	0.46
1:F:27:ILE:HA	1:F:30:LEU:HB2	1.97	0.46
1:F:136:PHE:HB2	1:F:327:TYR:CE2	2.51	0.46
1:F:214:VAL:HG12	1:F:216:ALA:N	2.31	0.46
1:F:439:GLN:CG	1:F:440:GLY:H	2.28	0.46
1:F:470:PHE:CD1	1:F:929:VAL:HG21	2.51	0.46
1:F:885:PHE:CD1	1:F:898:PRO:HB2	2.51	0.46
1:F:984:LEU:HD22	1:F:984:LEU:HA	1.69	0.46
1:A:24:GLY:O	1:A:28:LEU:HD13	2.16	0.45
1:A:396:PHE:HE1	1:A:999:ALA:HB1	1.80	0.45
1:A:922:THR:HG23	1:A:924:ASP:OD2	2.16	0.45
1:B:100:ALA:O	1:B:101:ASP:C	2.54	0.45
1:B:192:GLU:HA	1:B:195:LYS:HD2	1.98	0.45
1:B:210:GLN:NE2	1:B:250:LEU:H	2.14	0.45
1:C:401:ALA:HB2	1:C:474:ILE:HD13	1.97	0.45
1:C:944:LEU:HB3	1:C:971:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:982:PHE:O	1:C:983:ILE:C	2.55	0.45
1:D:7:ASP:CG	1:D:432:ARG:HH21	2.20	0.45
1:E:447:MET:HB3	1:E:887:CYS:HB3	1.98	0.45
1:E:527:TYR:O	1:E:530:SER:HB3	2.16	0.45
1:E:546:LEU:HD13	1:E:547:ILE:HG22	1.98	0.45
1:F:359:LEU:HD21	1:F:977:MET:HE1	1.98	0.45
1:F:428:LYS:CG	1:F:494:ALA:HB1	2.45	0.45
1:F:431:THR:CG2	1:F:490:PRO:HA	2.46	0.45
1:F:787:GLY:C	1:F:789:TRP:H	2.20	0.45
1:F:991:ILE:HD12	1:F:991:ILE:HA	1.70	0.45
1:A:284:GLN:HG3	1:A:285:PRO:HD2	1.98	0.45
1:B:58:GLN:O	1:B:63:GLN:HG3	2.16	0.45
1:B:685:ILE:HG12	1:B:824:SER:HB2	1.97	0.45
1:C:44:THR:N	1:C:132:SER:OG	2.44	0.45
1:C:68:ASN:HB2	1:C:114:ALA:HB2	1.98	0.45
1:C:146:ASP:O	1:C:148:THR:N	2.49	0.45
1:D:214:VAL:CG2	1:D:236:ALA:HB3	2.32	0.45
1:D:445:ILE:HD13	1:D:940:LYS:HE2	1.97	0.45
1:E:116:PRO:HD2	1:E:117:LEU:HD12	1.98	0.45
1:E:907:LEU:HD23	1:E:1017:LEU:CB	2.41	0.45
1:F:354:VAL:CG1	1:F:980:LEU:HD23	2.47	0.45
1:B:294:ALA:HB3	1:B:297:ALA:CB	2.46	0.45
1:B:344:LEU:CD2	1:B:399:VAL:HG22	2.47	0.45
1:C:46:SER:HA	1:C:88:VAL:O	2.17	0.45
1:C:549:VAL:O	1:C:552:MET:HB3	2.15	0.45
1:C:885:PHE:HB2	1:C:902:MET:SD	2.57	0.45
1:D:98:THR:O	1:D:99:ASP:C	2.54	0.45
1:E:3:ASN:O	1:E:6:ILE:N	2.45	0.45
1:E:225:VAL:HB	1:F:777:ALA:HB1	1.99	0.45
1:F:23:GLY:HA3	1:F:377:LEU:O	2.17	0.45
1:F:310:LEU:O	1:F:314:GLU:HG3	2.16	0.45
1:F:952:LEU:HD11	1:F:970:MET:CE	2.47	0.45
1:A:61:VAL:CG1	1:A:122:VAL:HG21	2.46	0.45
1:A:401:ALA:O	1:A:405:LEU:HG	2.17	0.45
1:A:416:VAL:HG22	1:A:431:THR:HA	1.99	0.45
1:A:505:HIS:O	1:A:507:GLU:HG2	2.15	0.45
1:A:578:LEU:HD23	1:A:661:ALA:HB2	1.98	0.45
1:B:5:PHE:CE1	1:B:487:ILE:HG13	2.51	0.45
1:B:225:VAL:HG22	1:C:781:MET:CE	2.47	0.45
1:B:888:LEU:HG	1:B:901:VAL:HG11	1.98	0.45
1:C:792:ARG:HG3	1:C:798:MET:SD	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:PHE:CD1	1:D:610:PHE:HD1	2.34	0.45
1:D:776:GLU:HB3	1:D:779:TYR:HD1	1.78	0.45
1:E:309:GLU:HA	1:E:312:LYS:HE3	1.98	0.45
1:F:434:SER:O	1:F:438:ILE:HG12	2.17	0.45
1:A:177:LEU:HA	1:A:177:LEU:HD22	1.63	0.45
1:A:393:LEU:CD1	1:A:466:ILE:HA	2.47	0.45
1:A:455:PRO:HG2	1:A:880:SER:HB2	1.99	0.45
1:C:352:PHE:HD1	1:C:369:THR:OG1	1.98	0.45
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.98	0.45
1:C:1030:ARG:HD3	1:C:1030:ARG:HA	1.81	0.45
1:D:609:VAL:HG22	1:D:629:VAL:HG13	1.98	0.45
1:D:631:LEU:HD21	1:D:647:ILE:HD12	1.99	0.45
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.51	0.45
1:E:72:ILE:HG23	1:E:106:GLN:CB	2.46	0.45
1:E:1018:ALA:O	1:E:1022:VAL:HG23	2.16	0.45
1:F:415:ASN:ND2	1:F:948:PHE:HZ	2.14	0.45
1:B:10:ILE:HB	1:C:893:GLU:OE1	2.16	0.45
1:B:203:VAL:HG12	1:B:207:ILE:HD11	1.98	0.45
1:C:390:ILE:HG23	1:C:395:MET:SD	2.57	0.45
1:C:655:PHE:HB3	1:C:663:VAL:CG1	2.47	0.45
1:C:738:ALA:O	1:C:740:GLY:N	2.50	0.45
1:D:44:THR:CG2	1:D:91:THR:HG22	2.45	0.45
1:D:462:SER:OG	1:D:674:LEU:HD12	2.17	0.45
1:D:584:GLN:HG2	1:D:622:GLN:CG	2.43	0.45
1:D:685:ILE:HD11	1:D:819:TYR:CD2	2.52	0.45
1:E:24:GLY:O	1:E:28:LEU:HD13	2.16	0.45
1:E:344:LEU:HD23	1:E:344:LEU:HA	1.65	0.45
1:E:398:MET:HE3	1:E:398:MET:HB3	1.80	0.45
1:E:594:VAL:HG22	1:E:655:PHE:CE2	2.52	0.45
1:E:947:GLU:HG3	1:E:948:PHE:N	2.30	0.45
1:F:394:THR:HG22	1:F:469:GLN:O	2.16	0.45
1:F:577:GLN:HE22	1:F:721:LEU:HD11	1.80	0.45
1:A:668:LEU:HD23	1:A:668:LEU:H	1.81	0.45
1:B:105:VAL:HG21	1:C:105:VAL:HG13	1.97	0.45
1:B:116:PRO:C	1:B:118:LEU:H	2.19	0.45
1:B:184:MET:HG2	1:B:246:PHE:CE2	2.52	0.45
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.73	0.45
1:B:646:ALA:O	1:B:649:MET:HB3	2.17	0.45
1:B:836:SER:OG	1:B:839:GLU:HG3	2.17	0.45
1:B:1031:ARG:O	1:B:1032:ARG:HG3	2.16	0.45
1:C:80:SER:HB2	1:C:818:ARG:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:HD22	1:C:178:PHE:N	2.32	0.45
1:C:945:ILE:HD13	1:C:968:VAL:HG22	1.97	0.45
1:D:198:LEU:H	1:D:798:MET:HE1	1.81	0.45
1:E:77:TYR:HE2	1:E:864:TYR:CD2	2.35	0.45
1:E:398:MET:HG2	1:E:473:THR:HG21	1.98	0.45
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.99	0.45
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.66	0.45
1:E:900:SER:HB3	1:E:1026:PHE:HA	1.99	0.45
1:F:312:LYS:O	1:F:315:PRO:HD2	2.17	0.45
1:F:363:ARG:HB3	1:F:496:MET:CG	2.47	0.45
1:F:428:LYS:HG2	1:F:494:ALA:CB	2.46	0.45
1:F:452:VAL:O	1:F:455:PRO:HD2	2.16	0.45
1:A:167:SER:OG	1:B:70:ASN:HB2	2.16	0.45
1:A:485:ALA:O	1:A:490:PRO:HD3	2.17	0.45
1:A:790:TYR:CE1	1:A:800:PRO:HA	2.52	0.45
1:A:960:LEU:HD23	1:A:1031:ARG:CZ	2.47	0.45
1:A:1036:LYS:HE3	1:A:1040:ILE:CD1	2.46	0.45
1:B:114:ALA:O	1:B:118:LEU:HG	2.16	0.45
1:B:559:LEU:HD12	1:B:913:LEU:HD22	1.98	0.45
1:B:684:LEU:HD12	1:B:684:LEU:HA	1.86	0.45
1:B:690:LEU:HD21	1:B:854:GLY:HA3	1.99	0.45
1:B:970:MET:HE2	1:B:970:MET:HB2	1.72	0.45
1:C:13:TRP:CH2	1:C:370:ILE:HG21	2.47	0.45
1:C:158:VAL:HA	1:C:162:MET:HE2	1.98	0.45
1:C:551:GLY:O	1:C:555:LEU:HB2	2.17	0.45
1:D:58:GLN:O	1:D:63:GLN:HG3	2.17	0.45
1:D:347:ALA:HB1	1:D:402:ILE:HG21	1.99	0.45
1:E:448:VAL:HA	1:E:451:ALA:HB3	1.98	0.45
1:F:47:ALA:O	1:F:87:THR:HA	2.17	0.45
1:F:372:VAL:C	1:F:374:VAL:N	2.69	0.45
1:F:448:VAL:HG23	1:F:884:VAL:HG13	1.98	0.45
1:F:721:LEU:HB3	1:F:814:PRO:HG2	1.97	0.45
1:B:452:VAL:HG13	1:B:884:VAL:HG21	1.98	0.45
1:B:528:THR:HG23	1:B:965:LEU:HD22	1.98	0.45
1:B:583:THR:HG22	1:B:586:ARG:NE	2.22	0.45
1:B:685:ILE:HD11	1:B:819:TYR:HB3	1.97	0.45
1:B:764:ASP:O	1:B:766:GLY:N	2.50	0.45
1:B:944:LEU:HG	1:B:971:ARG:NH2	2.32	0.45
1:C:213:GLN:HG2	1:C:239:ARG:HG3	1.98	0.45
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.98	0.45
1:D:79:SER:OG	1:D:91:THR:OG1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:GLY:HA3	1:D:518:ARG:HD3	1.98	0.45
1:E:680:PHE:CG	1:E:859:TRP:HZ3	2.34	0.45
1:F:363:ARG:HB3	1:F:496:MET:SD	2.57	0.45
1:F:462:SER:HB2	1:F:865:GLN:CG	2.47	0.45
1:F:540:ARG:HD3	1:F:541:TYR:CD1	2.51	0.45
1:A:131:LYS:H	1:A:131:LYS:HG2	1.52	0.45
1:A:597:TYR:CD2	1:A:655:PHE:CZ	3.05	0.45
1:B:226:LYS:NZ	1:B:226:LYS:HB3	2.32	0.45
1:B:488:LEU:HD12	1:B:488:LEU:HA	1.81	0.45
1:B:1024:VAL:HA	1:B:1027:VAL:CG1	2.47	0.45
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.99	0.45
1:E:189:ASN:ND2	1:E:190:PRO:HD2	2.32	0.45
1:E:778:LYS:HE3	1:E:779:TYR:OH	2.17	0.45
1:E:792:ARG:HG2	1:E:792:ARG:HH11	1.82	0.45
1:F:58:GLN:O	1:F:58:GLN:HG2	2.16	0.45
1:F:65:ILE:HG13	1:F:111:LEU:HA	1.98	0.45
1:F:83:ASP:HB3	1:F:87:THR:O	2.17	0.45
1:F:157:TYR:HE2	1:F:317:PHE:CE1	2.35	0.45
1:F:228:GLN:NE2	1:F:230:LEU:H	2.15	0.45
1:F:424:GLY:HA2	1:F:501:ALA:C	2.37	0.45
1:A:151:GLN:HE22	1:A:179:GLY:HA2	1.81	0.44
1:A:972:LEU:HG	1:A:976:LEU:CD1	2.47	0.44
1:B:193:LEU:HD13	1:B:265:VAL:HG21	1.99	0.44
1:B:718:PRO:HA	1:B:827:ILE:HA	1.99	0.44
1:B:789:TRP:O	1:B:801:PHE:HD2	2.00	0.44
1:B:844:MET:CE	1:B:847:LEU:HD12	2.47	0.44
1:B:1017:LEU:HD13	1:B:1018:ALA:N	2.32	0.44
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.44
1:C:563:PHE:CG	1:C:866:GLU:HB2	2.51	0.44
1:C:930:GLY:HA2	1:C:1007:VAL:HG23	1.99	0.44
1:D:158:VAL:HG11	1:D:177:LEU:HD21	1.99	0.44
1:D:213:GLN:HG2	1:D:239:ARG:HG3	1.98	0.44
1:D:931:LEU:HD12	1:D:932:LEU:N	2.32	0.44
1:E:105:VAL:HG11	1:F:108:GLN:NE2	2.32	0.44
1:E:250:LEU:HD13	1:E:261:LEU:HD23	2.00	0.44
1:E:649:MET:CE	1:E:653:ARG:HH11	2.31	0.44
1:E:736:ALA:HB2	1:E:804:PHE:HB3	1.99	0.44
1:E:905:VAL:HG13	1:E:935:ILE:HD11	1.98	0.44
1:E:913:LEU:HD23	1:E:927:PHE:HZ	1.81	0.44
1:F:356:TYR:C	1:F:358:PHE:H	2.20	0.44
1:F:723:ASP:OD1	1:F:723:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:733:GLN:OE1	1:F:743:ILE:HG23	2.17	0.44
1:B:392:THR:HG23	1:B:393:LEU:N	2.32	0.44
1:C:483:LEU:O	1:C:487:ILE:HB	2.18	0.44
1:C:541:TYR:OH	2:C:2000:LMT:H2'	2.16	0.44
1:C:564:LEU:HD23	1:C:565:PRO:HD2	1.99	0.44
1:C:706:ALA:HA	1:C:847:LEU:HD21	1.99	0.44
1:C:790:TYR:CE2	1:C:800:PRO:HB3	2.53	0.44
1:D:764:ASP:C	1:D:766:GLY:H	2.21	0.44
1:E:101:ASP:O	1:E:104:GLN:HB3	2.17	0.44
1:E:482:VAL:O	1:E:485:ALA:HB3	2.17	0.44
1:F:578:LEU:CD2	1:F:579:PRO:HD2	2.47	0.44
1:F:656:SER:HB3	1:F:664:PHE:HE1	1.82	0.44
1:F:762:PHE:CD2	1:F:771:VAL:HG22	2.52	0.44
1:B:225:VAL:H	1:C:781:MET:HE3	1.82	0.44
1:B:459:PHE:HD2	1:B:459:PHE:HA	1.69	0.44
1:C:402:ILE:O	1:C:405:LEU:HG	2.17	0.44
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.52	0.44
1:D:466:ILE:HG22	1:D:470:PHE:CE2	2.51	0.44
1:D:549:VAL:HG22	1:D:906:PRO:CG	2.47	0.44
1:D:913:LEU:N	1:D:913:LEU:HD23	2.32	0.44
1:D:945:ILE:CG1	1:D:971:ARG:HH12	2.30	0.44
1:D:1026:PHE:HE2	1:D:1030:ARG:NE	2.16	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.99	0.44
1:E:668:LEU:HD23	1:E:668:LEU:H	1.82	0.44
1:F:702:LEU:HD22	1:F:827:ILE:HD12	1.99	0.44
1:A:150:THR:HG23	1:A:152:GLU:HG2	1.99	0.44
1:A:214:VAL:O	1:A:216:ALA:N	2.50	0.44
1:A:600:THR:O	1:A:603:LYS:HB2	2.18	0.44
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.99	0.44
1:A:971:ARG:HA	1:A:974:PRO:HD2	1.99	0.44
1:B:362:PHE:CD2	1:B:366:LEU:HD21	2.52	0.44
1:B:376:LEU:C	1:B:378:GLY:N	2.63	0.44
1:B:873:ALA:N	1:B:874:PRO:HD2	2.32	0.44
1:C:3:ASN:C	1:C:5:PHE:N	2.69	0.44
1:C:397:GLY:O	1:C:400:LEU:HB3	2.17	0.44
1:C:597:TYR:CD2	1:C:655:PHE:HZ	2.34	0.44
1:C:673:GLU:H	1:C:673:GLU:HG2	1.35	0.44
1:C:1015:THR:OG1	1:C:1016:VAL:N	2.50	0.44
1:D:30:LEU:HD13	1:D:31:PRO:HD2	1.98	0.44
1:D:162:MET:O	1:D:164:ASP:N	2.50	0.44
1:D:362:PHE:O	1:D:365:THR:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1016:VAL:O	1:D:1016:VAL:HG12	2.18	0.44
1:E:43:VAL:HG13	1:E:130:GLU:O	2.16	0.44
1:E:57:VAL:HG11	1:E:86:GLY:O	2.17	0.44
1:E:189:ASN:O	1:E:193:LEU:HB2	2.18	0.44
1:E:491:ALA:O	1:E:495:THR:OG1	2.28	0.44
1:F:53:ASP:N	1:F:53:ASP:OD1	2.49	0.44
1:F:61:VAL:HA	1:F:118:LEU:CD2	2.47	0.44
1:F:154:ILE:HG22	1:F:287:SER:HB2	2.00	0.44
1:F:193:LEU:HD22	1:F:265:VAL:HB	1.99	0.44
1:F:195:LYS:HG3	1:F:196:PHE:N	2.32	0.44
1:F:393:LEU:HG	1:F:466:ILE:HA	1.99	0.44
1:A:84:SER:HB3	1:A:814:PRO:CA	2.46	0.44
1:A:102:ILE:HG21	1:C:101:ASP:OD2	2.17	0.44
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.70	0.44
1:A:538:THR:O	1:A:542:LEU:HD13	2.17	0.44
1:A:1022:VAL:HG22	1:A:1023:PRO:HD3	1.99	0.44
1:B:575:MET:HE1	1:B:617:PHE:HB2	1.98	0.44
1:C:647:ILE:HA	1:C:650:ARG:HG2	1.99	0.44
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.85	0.44
1:C:667:ASN:ND2	1:C:668:LEU:O	2.51	0.44
2:C:2000:LMT:O4'	2:C:2000:LMT:O2B	2.35	0.44
1:D:742:SER:O	1:D:746:ILE:HG13	2.18	0.44
1:E:201:VAL:HG21	1:E:745:ASP:OD2	2.16	0.44
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.99	0.44
1:E:414:GLU:HG2	1:E:973:ARG:NH2	2.32	0.44
1:E:527:TYR:CD1	1:E:1020:PHE:HE2	2.35	0.44
1:E:563:PHE:O	1:E:564:LEU:HG	2.18	0.44
1:E:597:TYR:CD1	1:E:655:PHE:CZ	3.05	0.44
1:E:703:LEU:HG	1:E:716:VAL:CG1	2.45	0.44
1:E:921:LEU:HA	1:E:921:LEU:HD13	1.68	0.44
1:F:376:LEU:O	1:F:377:LEU:C	2.56	0.44
1:F:952:LEU:HB2	1:F:963:ALA:HB1	1.99	0.44
1:A:190:PRO:HB3	1:A:789:TRP:CH2	2.53	0.44
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.18	0.44
1:B:26:ALA:HB1	1:B:384:ALA:CB	2.48	0.44
1:B:408:ASP:O	1:B:411:VAL:HG12	2.18	0.44
1:B:1007:VAL:HG12	1:B:1008:MET:N	2.32	0.44
1:C:276:ASP:OD2	1:C:276:ASP:N	2.50	0.44
1:C:363:ARG:HB2	1:C:496:MET:SD	2.58	0.44
1:E:68:ASN:HB2	1:E:114:ALA:HB2	1.99	0.44
1:E:184:MET:HB3	1:E:771:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:TRP:HE1	1:E:269:GLU:HG2	1.81	0.44
1:E:764:ASP:C	1:E:766:GLY:H	2.21	0.44
1:F:27:ILE:HG22	1:F:380:PHE:HB3	2.00	0.44
1:F:273:GLU:OE1	1:F:770:LYS:NZ	2.30	0.44
1:F:352:PHE:HD1	1:F:369:THR:HG21	1.83	0.44
1:F:573:MET:HG3	1:F:666:PHE:CE1	2.52	0.44
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.48	0.44
1:B:43:VAL:HG13	1:B:130:GLU:O	2.18	0.44
1:B:68:ASN:HD22	1:B:68:ASN:HA	1.67	0.44
1:B:347:ALA:O	1:B:351:VAL:HG23	2.17	0.44
1:B:717:ARG:HE	1:B:828:LEU:CB	2.27	0.44
1:D:645:GLU:HA	1:D:645:GLU:OE2	2.18	0.44
1:D:898:PRO:O	1:D:901:VAL:HG12	2.18	0.44
1:E:104:GLN:NE2	1:F:109:ASN:HD22	2.16	0.44
1:E:139:VAL:H	1:E:327:TYR:HB3	1.82	0.44
1:E:367:ILE:HB	1:E:368:PRO:HD3	2.00	0.44
1:E:982:PHE:O	1:E:983:ILE:C	2.56	0.44
1:A:197:GLN:HA	1:A:798:MET:CE	2.47	0.44
1:A:391:ASN:O	1:A:395:MET:HG2	2.17	0.44
1:A:559:LEU:HD22	1:A:923:ASN:H	1.82	0.44
1:B:244:GLU:HG3	1:B:248:LYS:HD3	2.00	0.44
1:C:6:ILE:HD12	1:C:487:ILE:HG12	2.00	0.44
1:C:843:LEU:HD13	1:C:847:LEU:HD22	2.00	0.44
1:C:847:LEU:HD12	1:C:847:LEU:HA	1.69	0.44
1:D:960:LEU:HD23	1:D:961:ILE:N	2.33	0.44
1:E:531:VAL:O	1:E:534:ILE:HG12	2.18	0.44
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.53	0.44
1:E:867:ARG:HH11	1:E:867:ARG:C	2.21	0.44
1:F:572:PHE:CE2	1:F:629:VAL:HB	2.53	0.44
2:F:2000:LMT:H121	2:F:2000:LMT:H91	1.86	0.44
1:A:188:MET:HE1	1:A:200:PRO:HG3	2.00	0.44
1:A:267:LYS:HD2	1:A:268:ILE:H	1.83	0.44
1:A:683:GLU:HG2	1:A:819:TYR:CB	2.48	0.44
1:A:932:LEU:O	1:A:935:ILE:HG22	2.18	0.44
1:B:95:GLU:O	1:B:98:THR:OG1	2.22	0.44
1:B:124:GLN:NE2	1:B:758:TYR:HD2	2.16	0.44
1:B:944:LEU:HB3	1:B:971:ARG:HH12	1.82	0.44
1:C:62:THR:HG21	1:C:818:ARG:HD3	2.00	0.44
1:C:350:LEU:HB3	1:C:984:LEU:HB3	2.00	0.44
1:C:504:ASP:O	1:C:506:GLY:N	2.51	0.44
1:D:294:ALA:HB3	1:D:297:ALA:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:HIS:O	1:D:526:HIS:C	2.56	0.44
1:D:957:GLY:HA2	1:D:1040:ILE:HD11	1.99	0.44
1:E:3:ASN:HA	1:E:6:ILE:CD1	2.41	0.44
1:E:111:LEU:C	1:E:113:LEU:H	2.21	0.44
1:F:49:TYR:CE1	1:F:57:VAL:HG12	2.52	0.44
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.99	0.44
1:F:143:ILE:HG22	1:F:286:ALA:HB2	2.00	0.44
1:F:594:VAL:HG22	1:F:655:PHE:CZ	2.52	0.44
1:A:240:LEU:HD12	1:A:246:PHE:CZ	2.53	0.43
1:A:567:GLU:OE1	1:A:996:GLY:HA2	2.18	0.43
1:A:978:THR:HG23	1:A:979:SER:N	2.33	0.43
1:B:136:PHE:CE1	1:B:292:LYS:HE2	2.53	0.43
1:B:250:LEU:HD12	1:B:251:LEU:N	2.33	0.43
1:B:750:LEU:O	1:B:753:ALA:HB3	2.18	0.43
1:D:250:LEU:HD12	1:D:251:LEU:H	1.83	0.43
1:D:492:LEU:HB3	1:D:496:MET:HE1	1.99	0.43
1:E:484:VAL:O	1:E:488:LEU:HB3	2.17	0.43
1:E:703:LEU:O	1:E:703:LEU:HD23	2.18	0.43
1:F:159:ALA:HB2	1:F:177:LEU:CD1	2.46	0.43
1:F:413:VAL:HG22	1:F:489:THR:OG1	2.17	0.43
1:F:452:VAL:HG23	1:F:453:PHE:HD1	1.81	0.43
1:F:671:ILE:H	1:F:862:MET:HE2	1.83	0.43
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.33	0.43
1:A:237:GLN:OE1	1:B:747:ASN:ND2	2.44	0.43
1:B:4:PHE:HE2	1:B:8:ARG:HD3	1.83	0.43
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.74	0.43
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.53	0.43
1:B:560:PRO:O	1:B:922:THR:OG1	2.34	0.43
1:B:710:PRO:C	1:B:712:MET:H	2.20	0.43
1:B:787:GLY:C	1:B:789:TRP:H	2.20	0.43
1:C:34:GLN:HG2	1:C:35:TYR:CD1	2.53	0.43
1:C:77:TYR:CE1	1:C:93:THR:HG21	2.53	0.43
1:C:246:PHE:O	1:C:262:LEU:HD23	2.17	0.43
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.84	0.43
1:C:776:GLU:HB2	1:C:779:TYR:HD1	1.83	0.43
1:D:359:LEU:C	1:D:361:ASN:H	2.12	0.43
1:D:891:LEU:HA	1:D:891:LEU:HD12	1.66	0.43
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.52	0.43
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.98	0.43
1:E:696:THR:HG23	1:E:699:ARG:NH1	2.32	0.43
1:F:119:PRO:O	1:F:123:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:ASN:CG	1:F:790:TYR:HD2	2.22	0.43
1:F:572:PHE:CD2	1:F:631:LEU:HD11	2.51	0.43
1:F:574:THR:CG2	1:F:627:ALA:HB3	2.48	0.43
1:F:951:ASP:O	1:F:955:LYS:N	2.51	0.43
1:A:232:ALA:HB1	1:B:725:PRO:O	2.18	0.43
1:A:435:MET:O	1:A:439:GLN:HB2	2.19	0.43
1:A:448:VAL:HG13	1:A:884:VAL:HG22	2.00	0.43
1:A:448:VAL:HG22	1:A:887:CYS:HB3	2.00	0.43
1:A:957:GLY:CA	1:A:1041:GLU:HA	2.48	0.43
1:B:104:GLN:CD	1:C:109:ASN:HD22	2.21	0.43
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.82	0.43
1:B:586:ARG:O	1:B:589:LYS:HB3	2.17	0.43
1:B:709:HIS:ND1	1:B:847:LEU:HD11	2.32	0.43
1:B:727:PHE:CB	1:B:809:TRP:HE1	2.31	0.43
1:C:46:SER:OG	1:C:89:GLN:HG2	2.18	0.43
1:C:188:MET:HA	1:C:266:ALA:HB2	2.01	0.43
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.19	0.43
1:D:331:PRO:O	1:D:334:LYS:HB2	2.18	0.43
1:D:347:ALA:HB3	1:D:402:ILE:HD12	2.00	0.43
1:D:987:MET:O	1:D:990:VAL:HG23	2.18	0.43
1:E:69:MET:CG	1:E:110:LYS:HB3	2.48	0.43
1:E:452:VAL:HG23	1:E:453:PHE:CD2	2.54	0.43
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.42	0.43
1:E:641:GLU:HA	1:E:646:ALA:CB	2.48	0.43
1:E:900:SER:OG	1:E:1029:VAL:HG11	2.18	0.43
1:E:926:TYR:HE1	1:E:999:ALA:CB	2.31	0.43
1:F:467:TYR:CE1	1:F:925:VAL:HG22	2.53	0.43
1:F:804:PHE:CD2	1:F:804:PHE:N	2.87	0.43
1:A:136:PHE:HE2	1:A:290:GLY:HA3	1.83	0.43
1:A:178:PHE:HB2	1:A:288:GLY:H	1.83	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.54	0.43
1:A:941:ASN:OD1	1:A:941:ASN:N	2.50	0.43
1:B:909:VAL:O	1:B:911:GLY:N	2.51	0.43
1:C:16:ALA:O	1:C:19:ILE:N	2.51	0.43
1:C:31:PRO:HB2	1:C:389:SER:OG	2.18	0.43
1:C:293:LEU:HD13	1:C:294:ALA:N	2.33	0.43
1:C:723:ASP:HA	1:C:813:SER:HA	2.00	0.43
1:C:983:ILE:HD13	1:C:983:ILE:HA	1.77	0.43
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.99	0.43
1:D:210:GLN:OE1	1:D:249:ILE:HG23	2.18	0.43
1:D:568:ASP:O	1:D:634:TRP:HZ3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:680:PHE:HE1	1:D:844:MET:HG3	1.83	0.43
1:D:690:LEU:HG	1:D:694:LYS:HG2	2.00	0.43
1:D:919:ARG:NH1	1:D:990:VAL:HG12	2.32	0.43
1:E:191:ASN:O	1:E:194:ASN:HB3	2.18	0.43
1:E:211:ASN:CG	1:E:240:LEU:HG	2.39	0.43
1:E:609:VAL:HG13	1:E:629:VAL:CG2	2.44	0.43
1:F:147:GLY:O	1:F:149:MET:N	2.51	0.43
1:F:242:SER:OG	1:F:243:THR:N	2.50	0.43
1:F:243:THR:O	1:F:246:PHE:HB2	2.19	0.43
1:F:694:LYS:CD	1:F:694:LYS:H	2.31	0.43
1:F:736:ALA:HB1	1:F:741:VAL:CG2	2.48	0.43
1:F:909:VAL:HG22	1:F:931:LEU:HD21	1.99	0.43
1:A:15:ILE:HD13	1:A:487:ILE:HD13	2.00	0.43
1:A:39:ALA:HA	1:A:40:PRO:HD2	1.68	0.43
1:A:776:GLU:HB3	1:A:779:TYR:HE1	1.83	0.43
1:B:76:MET:HG2	1:B:864:TYR:CE2	2.51	0.43
1:B:98:THR:O	1:B:99:ASP:C	2.57	0.43
1:C:111:LEU:C	1:C:113:LEU:H	2.21	0.43
1:C:247:GLY:CA	1:C:263:ARG:HB2	2.48	0.43
1:C:870:GLY:C	1:C:872:GLN:H	2.21	0.43
1:C:873:ALA:N	1:C:874:PRO:HD2	2.33	0.43
1:D:184:MET:HG2	1:D:246:PHE:CE2	2.54	0.43
1:D:219:LEU:HA	1:E:754:TRP:HZ3	1.83	0.43
1:D:680:PHE:HB2	1:D:863:SER:OG	2.18	0.43
1:E:137:LEU:HD12	1:E:329:THR:HB	2.00	0.43
1:E:425:LEU:HD13	1:E:429:GLU:CG	2.47	0.43
1:E:682:PHE:HD2	1:E:827:ILE:HD12	1.84	0.43
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.70	0.43
1:F:412:VAL:HG12	1:F:413:VAL:N	2.34	0.43
1:F:455:PRO:HG2	1:F:880:SER:CB	2.43	0.43
1:A:242:SER:O	1:A:246:PHE:CD1	2.71	0.43
1:A:554:TYR:CE1	1:A:558:ARG:HG3	2.53	0.43
1:A:674:LEU:HD13	1:A:675:GLY:O	2.19	0.43
1:A:692:HIS:HE2	1:A:813:SER:CB	2.31	0.43
1:B:291:ILE:HD13	1:B:306:ILE:HD13	2.01	0.43
1:B:576:VAL:HG13	1:B:663:VAL:HG22	2.00	0.43
1:B:688:ALA:HB3	1:B:690:LEU:CD2	2.48	0.43
1:B:903:LEU:HD23	1:B:903:LEU:HA	1.49	0.43
1:C:13:TRP:CE3	1:C:13:TRP:HA	2.54	0.43
1:C:214:VAL:O	1:C:216:ALA:N	2.51	0.43
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ASP:OD1	1:D:56:THR:OG1	2.13	0.43
1:F:25:LEU:HD12	1:F:28:LEU:HD12	1.99	0.43
1:F:144:ASN:ND2	1:F:320:GLY:HA3	2.33	0.43
1:F:182:TYR:HD1	1:F:182:TYR:HA	1.69	0.43
1:F:184:MET:HB2	1:F:762:PHE:CD2	2.53	0.43
1:F:289:LEU:HD23	1:F:289:LEU:HA	1.82	0.43
1:F:375:VAL:HG11	1:F:405:LEU:HD22	2.00	0.43
1:F:507:GLU:HA	1:F:518:ARG:HG3	2.01	0.43
1:F:682:PHE:HA	1:F:859:TRP:CZ3	2.54	0.43
1:A:394:THR:O	1:A:398:MET:HG2	2.18	0.43
1:A:474:ILE:O	1:A:478:MET:HB3	2.19	0.43
1:B:193:LEU:HD21	1:B:265:VAL:HG13	2.01	0.43
1:B:831:ALA:HB2	1:B:840:ALA:HB2	2.01	0.43
1:C:185:ARG:HA	1:C:185:ARG:HD3	1.78	0.43
1:C:418:ARG:O	1:C:422:GLU:HB2	2.19	0.43
1:C:550:VAL:O	1:C:553:ALA:HB3	2.19	0.43
1:D:33:ALA:O	1:D:391:ASN:HB2	2.19	0.43
1:D:207:ILE:HG23	1:D:249:ILE:HD13	2.00	0.43
1:D:563:PHE:CE2	1:D:674:LEU:HD11	2.54	0.43
1:D:879:ILE:O	1:D:883:VAL:HG22	2.19	0.43
1:E:250:LEU:HD12	1:E:251:LEU:N	2.33	0.43
1:E:390:ILE:O	1:E:390:ILE:HG13	2.18	0.43
1:E:713:LEU:HD21	1:E:843:LEU:HD12	2.01	0.43
1:F:135:SER:HB3	1:F:673:GLU:HA	2.01	0.43
1:F:425:LEU:HB3	1:F:429:GLU:OE1	2.19	0.43
1:A:527:TYR:CZ	1:A:531:VAL:HG21	2.53	0.43
1:A:570:GLY:O	1:A:631:LEU:HD23	2.19	0.43
1:A:996:GLY:O	1:A:998:GLY:N	2.52	0.43
1:C:34:GLN:CG	1:C:333:VAL:HG22	2.48	0.43
1:C:751:GLY:O	1:C:753:ALA:N	2.52	0.43
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.63	0.43
1:D:197:GLN:HA	1:D:798:MET:CE	2.49	0.43
1:D:662:MET:HA	1:D:662:MET:CE	2.49	0.43
1:D:886:LEU:HD23	1:F:18:ILE:CG1	2.49	0.43
1:E:195:LYS:HD2	1:E:196:PHE:CZ	2.53	0.43
1:E:270:LEU:HD13	1:E:270:LEU:HA	1.60	0.43
1:F:222:THR:HA	1:F:224:PRO:HD3	2.00	0.43
1:F:438:ILE:HG21	1:F:438:ILE:HD13	1.78	0.43
1:F:905:VAL:HB	1:F:906:PRO:HD3	2.01	0.43
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.33	0.43
1:A:188:MET:CE	1:A:200:PRO:HG3	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.66	0.43
1:A:950:LYS:HA	1:A:953:MET:HE2	2.01	0.43
1:B:442:LEU:O	1:B:445:ILE:HG13	2.19	0.43
1:B:764:ASP:C	1:B:766:GLY:H	2.21	0.43
1:B:867:ARG:HH21	1:B:868:LEU:HA	1.84	0.43
1:B:971:ARG:HD2	1:B:974:PRO:HG3	2.01	0.43
1:C:137:LEU:HD12	1:C:329:THR:OG1	2.19	0.43
1:C:248:LYS:HD3	1:C:263:ARG:NH2	2.34	0.43
1:C:412:VAL:HG11	1:C:489:THR:HG21	2.00	0.43
1:C:906:PRO:O	1:C:910:ILE:HG22	2.19	0.43
1:D:2:PRO:O	1:D:5:PHE:HD1	2.02	0.43
1:D:177:LEU:HD13	1:D:178:PHE:C	2.39	0.43
1:D:193:LEU:HD22	1:D:265:VAL:HB	2.01	0.43
1:D:1015:THR:O	1:D:1017:LEU:N	2.52	0.43
1:E:214:VAL:CG2	1:E:236:ALA:HB3	2.47	0.43
1:E:273:GLU:CD	1:E:770:LYS:HD2	2.39	0.43
1:E:508:GLY:C	1:E:510:LYS:H	2.22	0.43
1:E:652:THR:CG2	1:E:665:ALA:H	2.32	0.43
1:E:659:LYS:HE2	1:E:659:LYS:HA	2.01	0.43
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.53	0.43
1:E:1015:THR:O	1:E:1018:ALA:N	2.52	0.43
1:F:23:GLY:O	1:F:26:ALA:N	2.51	0.43
1:F:199:THR:CG2	1:F:792:ARG:H	2.32	0.43
1:F:457:ALA:CB	1:F:468:ARG:HA	2.48	0.43
1:F:575:MET:HB2	1:F:626:ILE:HD11	2.01	0.43
1:F:693:GLU:H	1:F:694:LYS:HZ3	1.66	0.43
1:F:971:ARG:C	1:F:974:PRO:HD2	2.38	0.43
1:A:101:ASP:OD1	1:A:101:ASP:N	2.51	0.43
1:A:376:LEU:O	1:A:379:THR:N	2.51	0.43
1:A:777:ALA:HB1	1:C:225:VAL:HG12	2.01	0.43
1:A:944:LEU:HA	1:A:944:LEU:HD23	1.66	0.43
1:A:971:ARG:CA	1:A:974:PRO:HD2	2.48	0.43
1:C:11:PHE:O	1:C:15:ILE:HG13	2.18	0.43
1:C:189:ASN:HB3	1:C:192:GLU:HB2	2.01	0.43
1:C:450:SER:HB2	1:C:475:VAL:HG13	1.99	0.43
1:D:10:ILE:HG21	1:E:893:GLU:C	2.39	0.43
1:D:57:VAL:O	1:D:61:VAL:HG23	2.19	0.43
1:D:109:ASN:HD22	1:E:109:ASN:ND2	2.16	0.43
1:D:289:LEU:HD13	1:D:289:LEU:HA	1.73	0.43
1:D:602:GLU:HB3	1:D:606:VAL:CG2	2.48	0.43
1:D:795:ASP:OD2	1:D:797:GLN:N	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:MET:HG2	1:E:110:LYS:CB	2.49	0.43
1:E:175:VAL:HG22	1:F:70:ASN:CG	2.39	0.43
1:E:456:MET:SD	1:E:471:SER:OG	2.77	0.43
1:E:496:MET:HG2	1:E:496:MET:H	1.54	0.43
1:E:712:MET:HB3	1:E:713:LEU:HD22	2.00	0.43
1:E:922:THR:O	1:E:924:ASP:N	2.44	0.43
1:F:382:VAL:HG21	1:F:476:SER:HB2	2.00	0.43
1:F:952:LEU:HD11	1:F:970:MET:HE3	2.00	0.43
1:A:48:SER:O	1:A:122:VAL:HA	2.19	0.42
1:A:195:LYS:HG2	1:A:196:PHE:CE2	2.54	0.42
1:A:888:LEU:CD1	1:A:901:VAL:HB	2.49	0.42
1:B:56:THR:O	1:B:60:THR:OG1	2.34	0.42
1:B:901:VAL:O	1:B:904:VAL:HG23	2.19	0.42
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.54	0.42
1:C:764:ASP:C	1:C:766:GLY:H	2.22	0.42
1:C:894:SER:O	1:C:895:TRP:HE3	2.02	0.42
1:C:944:LEU:HD12	1:C:975:ILE:HD13	2.01	0.42
1:D:250:LEU:HD13	1:D:261:LEU:HD23	2.00	0.42
1:D:376:LEU:O	1:D:378:GLY:N	2.51	0.42
1:D:593:GLU:OE1	1:D:659:LYS:HE3	2.19	0.42
1:D:987:MET:HB2	1:D:1008:MET:HE1	2.01	0.42
1:E:371:ALA:O	1:E:375:VAL:HG23	2.19	0.42
1:E:376:LEU:HD22	1:E:398:MET:HE3	2.01	0.42
1:E:555:LEU:CD1	1:E:914:LEU:HD12	2.49	0.42
1:E:705:GLU:OE2	1:E:847:LEU:HB3	2.19	0.42
1:F:100:ALA:O	1:F:101:ASP:C	2.57	0.42
1:F:165:ALA:HB3	1:F:313:MET:HE1	2.00	0.42
1:F:177:LEU:HD23	1:F:178:PHE:N	2.34	0.42
1:F:502:LYS:O	1:F:503:GLY:C	2.57	0.42
1:F:588:GLN:N	1:F:613:ASN:ND2	2.67	0.42
1:F:591:LEU:HD13	1:F:611:ALA:HB1	2.00	0.42
1:A:423:GLU:O	1:A:502:LYS:HB3	2.19	0.42
1:B:8:ARG:HB3	1:C:893:GLU:CD	2.39	0.42
1:B:851:LEU:HA	1:B:852:PRO:HD3	1.87	0.42
1:B:953:MET:HE2	1:B:963:ALA:HB3	2.00	0.42
1:D:113:LEU:HG	1:F:127:VAL:O	2.19	0.42
1:D:413:VAL:O	1:D:416:VAL:HG13	2.20	0.42
1:D:451:ALA:HB3	1:D:884:VAL:HG22	2.01	0.42
1:D:602:GLU:HB3	1:D:606:VAL:HG23	2.01	0.42
1:D:885:PHE:CE1	1:D:899:PHE:HE2	2.37	0.42
1:D:960:LEU:O	1:D:963:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:ALA:O	1:E:307:ARG:HB2	2.19	0.42
1:E:355:MET:SD	1:E:368:PRO:HG2	2.59	0.42
1:E:764:ASP:O	1:E:766:GLY:N	2.51	0.42
1:E:905:VAL:HG13	1:E:935:ILE:CD1	2.49	0.42
1:F:634:TRP:CD1	1:F:634:TRP:N	2.86	0.42
1:F:717:ARG:HA	1:F:718:PRO:HD3	1.89	0.42
1:F:790:TYR:HE1	1:F:800:PRO:HA	1.82	0.42
1:B:731:ILE:HA	1:B:805:SER:HA	2.01	0.42
1:B:900:SER:HB2	1:B:1029:VAL:HG21	2.01	0.42
1:C:447:MET:HE3	1:C:447:MET:HB2	1.91	0.42
1:C:637:ARG:NH1	1:C:642:ASN:O	2.51	0.42
1:C:1027:VAL:O	1:C:1031:ARG:HG3	2.20	0.42
1:D:185:ARG:HD3	1:D:185:ARG:HA	1.91	0.42
1:D:404:LEU:HD11	1:D:449:LEU:CD2	2.49	0.42
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.51	0.42
1:E:440:GLY:O	1:E:891:LEU:HD11	2.19	0.42
1:E:531:VAL:HG21	1:E:968:VAL:HG11	2.01	0.42
1:E:926:TYR:HD1	1:E:1002:ALA:HB3	1.83	0.42
1:F:5:PHE:HE2	1:F:8:ARG:HH11	1.68	0.42
1:F:24:GLY:CA	1:F:377:LEU:HD22	2.49	0.42
1:F:31:PRO:HB2	1:F:389:SER:OG	2.18	0.42
1:F:55:LYS:HA	1:F:816:LEU:HD12	2.00	0.42
1:F:111:LEU:C	1:F:113:LEU:H	2.23	0.42
1:F:469:GLN:O	1:F:472:ILE:HG23	2.19	0.42
1:A:53:ASP:O	1:A:56:THR:HB	2.20	0.42
1:A:61:VAL:HG12	1:A:118:LEU:HD22	1.99	0.42
1:A:428:LYS:CD	1:A:428:LYS:N	2.79	0.42
1:A:493:CYS:O	1:A:497:LEU:HB3	2.19	0.42
1:B:211:ASN:CG	1:B:240:LEU:HG	2.39	0.42
1:C:153:ASP:O	1:C:156:ASP:HB3	2.19	0.42
1:C:396:PHE:O	1:C:400:LEU:HB2	2.19	0.42
1:D:294:ALA:HB3	1:D:297:ALA:HB2	2.01	0.42
1:D:527:TYR:HE1	1:D:972:LEU:HB2	1.84	0.42
1:D:552:MET:HG3	1:D:909:VAL:HG12	2.01	0.42
1:D:911:GLY:HA3	1:D:1013:THR:OG1	2.19	0.42
1:E:166:ILE:HG13	1:E:306:ILE:HG23	2.00	0.42
1:E:228:GLN:NE2	1:E:230:LEU:H	2.18	0.42
1:E:682:PHE:CE2	1:E:684:LEU:HB2	2.53	0.42
1:E:781:MET:HB2	1:E:782:LEU:HD22	2.00	0.42
1:E:994:GLY:O	1:E:997:SER:HB2	2.20	0.42
1:F:656:SER:HB3	1:F:664:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:733:GLN:HE22	1:F:743:ILE:CG2	2.32	0.42
1:F:888:LEU:HD23	1:F:888:LEU:HA	1.68	0.42
1:F:1015:THR:OG1	1:F:1016:VAL:N	2.50	0.42
1:A:262:LEU:O	1:A:265:VAL:HG22	2.19	0.42
1:A:508:GLY:HA2	1:A:514:GLY:CA	2.49	0.42
1:B:15:ILE:O	1:B:19:ILE:HG13	2.19	0.42
1:B:214:VAL:HG23	1:B:237:GLN:HB3	2.00	0.42
1:B:420:MET:HG2	1:B:430:ALA:CB	2.49	0.42
1:B:531:VAL:O	1:B:534:ILE:HG12	2.19	0.42
1:B:533:GLY:HA2	1:B:536:ARG:CZ	2.50	0.42
1:B:563:PHE:O	1:B:564:LEU:HD12	2.19	0.42
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.02	0.42
1:C:356:TYR:C	1:C:358:PHE:N	2.73	0.42
1:C:390:ILE:O	1:C:390:ILE:HG22	2.19	0.42
1:C:544:LEU:O	1:C:548:ILE:HG13	2.19	0.42
1:C:577:GLN:HE22	1:C:721:LEU:HD11	1.85	0.42
1:C:733:GLN:OE1	1:C:743:ILE:HG23	2.20	0.42
1:D:68:ASN:HD22	1:D:68:ASN:HA	1.58	0.42
1:D:80:SER:HB2	1:D:818:ARG:HB2	2.01	0.42
1:D:538:THR:O	1:D:541:TYR:N	2.44	0.42
1:D:549:VAL:O	1:D:552:MET:HB3	2.19	0.42
1:E:201:VAL:O	1:E:204:ILE:HB	2.19	0.42
1:E:727:PHE:HD1	1:E:809:TRP:NE1	2.18	0.42
1:E:904:VAL:HG13	1:E:938:SER:HB2	2.01	0.42
1:A:27:ILE:HD11	1:A:380:PHE:CD2	2.54	0.42
1:A:208:LYS:HG3	1:A:759:VAL:HG13	2.01	0.42
1:A:220:GLY:HA2	1:B:781:MET:HG2	2.02	0.42
1:A:463:THR:HA	1:A:466:ILE:HG12	2.02	0.42
1:A:563:PHE:HB2	1:A:677:ALA:HB2	2.01	0.42
1:A:859:TRP:HB3	1:A:863:SER:HB3	2.02	0.42
1:B:562:SER:OG	1:B:563:PHE:N	2.51	0.42
1:B:907:LEU:HB3	1:B:1017:LEU:CD1	2.44	0.42
1:C:201:VAL:O	1:C:204:ILE:HB	2.20	0.42
1:C:602:GLU:OE2	1:C:650:ARG:NH1	2.53	0.42
1:C:884:VAL:HG12	1:C:902:MET:HE1	2.01	0.42
1:D:418:ARG:HD2	1:D:418:ARG:C	2.39	0.42
1:D:541:TYR:N	1:D:541:TYR:CD2	2.88	0.42
1:E:843:LEU:HD13	1:E:847:LEU:HG	2.01	0.42
1:E:903:LEU:HD23	1:E:903:LEU:HA	1.85	0.42
1:F:368:PRO:O	1:F:371:ALA:HB3	2.19	0.42
1:F:457:ALA:HB2	1:F:471:SER:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:556:PHE:HE1	1:F:923:ASN:ND2	2.17	0.42
1:F:1040:ILE:HG22	1:F:1041:GLU:HG3	2.00	0.42
1:A:140:VAL:HG11	1:A:310:LEU:HD21	2.01	0.42
1:B:8:ARG:HB3	1:C:893:GLU:OE2	2.20	0.42
1:B:111:LEU:O	1:B:111:LEU:HD22	2.20	0.42
1:B:795:ASP:OD2	1:B:797:GLN:HG2	2.19	0.42
1:C:34:GLN:HE21	1:C:332:PHE:HD2	1.67	0.42
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.47	0.42
1:C:185:ARG:NH2	1:C:772:TYR:HD1	2.18	0.42
1:C:535:LEU:HD22	1:C:1027:VAL:HG21	2.00	0.42
1:D:132:SER:OG	1:D:173:GLY:HA3	2.20	0.42
1:D:344:LEU:CD2	1:D:399:VAL:HA	2.46	0.42
1:D:544:LEU:O	1:D:548:ILE:HG13	2.20	0.42
1:D:638:PRO:HB2	1:D:639:GLY:H	1.61	0.42
1:E:43:VAL:HG22	1:E:131:LYS:HA	2.01	0.42
1:E:709:HIS:HB2	1:E:713:LEU:CD2	2.50	0.42
1:F:26:ALA:O	1:F:30:LEU:HB2	2.20	0.42
1:F:422:GLU:OE1	1:F:423:GLU:HG3	2.19	0.42
1:F:453:PHE:CE2	1:F:474:ILE:HD13	2.55	0.42
1:F:536:ARG:HD2	2:F:2000:LMT:H5B	2.01	0.42
1:F:619:GLY:HA2	1:F:815:ARG:HH12	1.85	0.42
1:F:674:LEU:HD23	1:F:674:LEU:HA	1.84	0.42
1:F:680:PHE:CD2	1:F:859:TRP:CZ3	3.07	0.42
1:F:762:PHE:HD2	1:F:771:VAL:HG22	1.85	0.42
1:A:330:THR:HB	1:A:331:PRO:HD3	2.01	0.42
1:A:728:LYS:HB2	1:A:810:GLU:OE2	2.20	0.42
1:A:743:ILE:HA	1:A:746:ILE:HG12	2.01	0.42
1:B:162:MET:O	1:B:164:ASP:N	2.53	0.42
1:B:189:ASN:O	1:B:193:LEU:HD23	2.20	0.42
1:C:355:MET:HE2	1:C:355:MET:HB2	1.86	0.42
1:C:566:ASP:OD2	1:C:678:THR:HG23	2.19	0.42
1:C:989:LEU:HD23	1:C:989:LEU:HA	1.46	0.42
1:C:1035:ARG:HD2	1:C:1035:ARG:HA	1.61	0.42
1:D:352:PHE:HD2	1:D:353:LEU:HD23	1.85	0.42
1:E:154:ILE:HG22	1:E:287:SER:HB3	2.02	0.42
1:E:424:GLY:HA2	1:E:502:LYS:N	2.34	0.42
1:E:442:LEU:HD23	1:E:442:LEU:HA	1.64	0.42
1:E:601:LYS:HD2	1:E:601:LYS:H	1.85	0.42
1:E:946:VAL:HG22	1:E:1026:PHE:HD1	1.85	0.42
1:E:947:GLU:HG3	1:E:948:PHE:HD2	1.83	0.42
1:E:971:ARG:CZ	1:E:971:ARG:CB	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:OG	1:B:74:ASN:HA	2.20	0.42
1:A:462:SER:O	1:A:465:ALA:HB3	2.19	0.42
1:B:578:LEU:CD1	1:B:586:ARG:HB2	2.50	0.42
1:B:727:PHE:HB2	1:B:809:TRP:NE1	2.32	0.42
1:C:971:ARG:C	1:C:974:PRO:HD2	2.39	0.42
1:D:169:THR:C	1:D:170:SER:HG	2.20	0.42
1:D:217:GLY:O	1:D:234:ILE:HB	2.20	0.42
1:D:223:PRO:HG3	1:E:275:TYR:CD2	2.54	0.42
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.68	0.42
1:D:275:TYR:HB2	1:F:223:PRO:HD3	2.01	0.42
1:D:370:ILE:O	1:D:373:PRO:HD2	2.19	0.42
1:D:372:VAL:HA	1:D:375:VAL:CG1	2.47	0.42
1:E:34:GLN:OE1	1:E:332:PHE:HE2	2.02	0.42
1:E:177:LEU:HG	1:E:289:LEU:HD11	2.00	0.42
1:E:190:PRO:O	1:E:194:ASN:HB2	2.20	0.42
1:E:444:GLY:O	1:E:447:MET:HB2	2.19	0.42
1:E:535:LEU:CD2	1:E:1027:VAL:HG11	2.49	0.42
1:F:39:ALA:HA	1:F:40:PRO:HD2	1.91	0.42
1:F:364:ALA:O	1:F:367:ILE:HD13	2.20	0.42
1:F:578:LEU:HD22	1:F:579:PRO:HD2	2.02	0.42
1:F:886:LEU:HD23	1:F:886:LEU:HA	1.87	0.42
1:F:959:GLY:CA	1:F:1041:GLU:H	2.25	0.42
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.33	0.42
1:A:112:GLN:OE1	1:A:115:MET:HG3	2.20	0.42
1:A:254:ASN:HB2	1:A:258:SER:O	2.20	0.42
1:A:559:LEU:HD22	1:A:923:ASN:HB2	2.02	0.42
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.78	0.42
1:B:270:LEU:HD12	1:B:270:LEU:HA	1.75	0.42
1:B:417:GLU:HG2	1:B:497:LEU:HD21	2.02	0.42
1:B:907:LEU:HG	1:B:1017:LEU:CD2	2.45	0.42
1:B:993:THR:HA	1:B:997:SER:OG	2.20	0.42
1:C:26:ALA:O	1:C:30:LEU:HD13	2.18	0.42
1:C:364:ALA:HA	1:C:367:ILE:HG13	2.01	0.42
1:C:404:LEU:HB3	1:C:478:MET:SD	2.60	0.42
1:C:563:PHE:HE2	1:C:671:ILE:HD11	1.84	0.42
1:D:404:LEU:HD12	1:D:937:LEU:CD2	2.50	0.42
1:E:189:ASN:HB3	1:E:192:GLU:HB2	2.02	0.42
1:E:352:PHE:CD2	1:E:353:LEU:HD23	2.45	0.42
1:F:397:GLY:CA	1:F:470:PHE:HD2	2.33	0.42
1:F:463:THR:O	1:F:466:ILE:HB	2.20	0.42
1:F:885:PHE:HB2	1:F:902:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:PRO:O	1:A:630:SER:HB2	2.20	0.41
1:A:652:THR:HG23	1:A:664:PHE:CD1	2.56	0.41
1:B:19:ILE:HG22	1:B:378:GLY:HA3	2.01	0.41
1:B:28:LEU:HD23	1:B:28:LEU:HA	1.90	0.41
1:B:736:ALA:HA	1:B:739:LEU:HD12	2.01	0.41
1:B:885:PHE:CD1	1:B:898:PRO:HB2	2.55	0.41
1:B:1028:VAL:HA	1:B:1031:ARG:HG2	2.02	0.41
1:C:189:ASN:O	1:C:193:LEU:N	2.52	0.41
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.20	0.41
1:D:673:GLU:O	1:D:674:LEU:HB3	2.19	0.41
1:D:690:LEU:HG	1:D:694:LYS:CE	2.50	0.41
1:E:277:ILE:HG21	1:E:615:PHE:HB2	2.01	0.41
1:E:366:LEU:O	1:E:370:ILE:HG12	2.19	0.41
1:E:723:ASP:OD1	1:E:813:SER:OG	2.30	0.41
1:E:982:PHE:HE2	1:E:1007:VAL:HG13	1.85	0.41
1:E:1026:PHE:O	1:E:1030:ARG:HB2	2.20	0.41
1:F:399:VAL:HA	1:F:402:ILE:HG13	2.02	0.41
1:F:514:GLY:CA	1:F:517:ASN:HD21	2.32	0.41
1:A:194:ASN:ND2	1:A:798:MET:HG3	2.35	0.41
1:A:427:PRO:HD2	1:A:428:LYS:NZ	2.35	0.41
1:A:818:ARG:HH12	1:A:823:PRO:HG3	1.86	0.41
1:A:892:TYR:OH	1:A:943:ILE:HG12	2.20	0.41
1:A:901:VAL:O	1:A:904:VAL:HG23	2.19	0.41
1:B:740:GLY:O	1:B:794:ALA:N	2.53	0.41
1:B:778:LYS:HE3	1:B:779:TYR:OH	2.19	0.41
1:B:952:LEU:HB2	1:B:963:ALA:HB1	2.01	0.41
1:C:38:ILE:HD13	1:C:38:ILE:HG21	1.71	0.41
1:C:358:PHE:C	1:C:359:LEU:HD23	2.40	0.41
1:C:380:PHE:CZ	1:C:398:MET:HE1	2.54	0.41
1:C:527:TYR:CE1	1:C:972:LEU:HD23	2.55	0.41
1:C:536:ARG:NH1	2:C:2000:LMT:O6B	2.53	0.41
1:C:783:PRO:O	1:C:786:ILE:HB	2.20	0.41
1:C:888:LEU:HD13	1:C:901:VAL:HG11	2.01	0.41
1:D:774:MET:HG2	1:D:775:SER:H	1.85	0.41
1:E:152:GLU:HB3	1:E:182:TYR:HE1	1.86	0.41
1:E:344:LEU:CD2	1:E:399:VAL:HA	2.47	0.41
1:E:559:LEU:HD12	1:E:559:LEU:HA	1.79	0.41
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.86	0.41
1:F:3:ASN:HD22	1:F:435:MET:HG3	1.84	0.41
1:F:34:GLN:CG	1:F:333:VAL:HG22	2.50	0.41
1:F:525:HIS:ND1	1:F:529:ASP:OD2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:527:TYR:OH	1:F:1019:ILE:HB	2.21	0.41
1:F:659:LYS:HD3	1:F:659:LYS:HA	1.90	0.41
1:A:363:ARG:H	1:A:363:ARG:HG2	1.64	0.41
1:A:455:PRO:O	1:A:876:LEU:HD13	2.20	0.41
1:A:740:GLY:C	1:A:793:ALA:HB1	2.40	0.41
1:A:836:SER:OG	1:A:839:GLU:HG3	2.19	0.41
1:B:58:GLN:HG3	1:B:818:ARG:HD2	2.01	0.41
1:B:187:TRP:HB3	1:B:776:GLU:HA	2.03	0.41
1:B:400:LEU:HD12	1:B:400:LEU:O	2.20	0.41
1:B:617:PHE:N	1:B:626:ILE:HD12	2.36	0.41
1:B:641:GLU:HB2	1:B:650:ARG:HH22	1.85	0.41
1:B:844:MET:CE	1:B:844:MET:HA	2.50	0.41
1:C:555:LEU:HD22	1:C:555:LEU:HA	1.89	0.41
1:C:556:PHE:HE1	1:C:923:ASN:ND2	2.17	0.41
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.50	0.41
1:C:795:ASP:OD2	1:C:796:GLY:N	2.53	0.41
1:D:13:TRP:HE1	1:D:492:LEU:HD21	1.84	0.41
1:D:76:MET:HB2	1:D:93:THR:O	2.21	0.41
1:D:81:ASN:HB2	1:D:89:GLN:HB3	2.02	0.41
1:D:398:MET:O	1:D:401:ALA:N	2.53	0.41
1:D:754:TRP:CE2	1:D:780:ARG:CB	3.04	0.41
1:D:932:LEU:HA	1:D:935:ILE:HD12	2.01	0.41
1:E:76:MET:HE3	1:E:864:TYR:CE2	2.55	0.41
1:E:555:LEU:HD23	1:E:555:LEU:HA	1.79	0.41
1:E:867:ARG:HH11	1:E:868:LEU:CA	2.30	0.41
1:E:985:GLY:O	1:E:988:PRO:HD2	2.19	0.41
1:F:65:ILE:HA	1:F:114:ALA:CB	2.50	0.41
1:F:136:PHE:HB2	1:F:327:TYR:HE2	1.86	0.41
1:F:228:GLN:HE21	1:F:230:LEU:H	1.66	0.41
1:F:699:ARG:NH2	1:F:718:PRO:HB2	2.34	0.41
1:F:712:MET:SD	1:F:843:LEU:HG	2.60	0.41
1:F:888:LEU:CD1	1:F:901:VAL:HG11	2.51	0.41
1:A:158:VAL:HG22	1:A:162:MET:HE1	2.02	0.41
1:A:303:ALA:O	1:A:307:ARG:HB2	2.21	0.41
1:A:683:GLU:HG2	1:A:819:TYR:HB2	2.02	0.41
1:A:897:ILE:HD11	1:A:1030:ARG:NH2	2.32	0.41
1:B:727:PHE:CE2	1:B:729:ILE:HD11	2.55	0.41
1:C:112:GLN:HA	1:C:115:MET:HB2	2.02	0.41
1:C:214:VAL:CG2	1:C:237:GLN:HB2	2.51	0.41
1:C:344:LEU:CA	1:C:399:VAL:HG22	2.50	0.41
1:C:539:GLY:O	1:C:542:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:THR:HG22	1:C:622:GLN:OE1	2.19	0.41
1:C:787:GLY:C	1:C:789:TRP:H	2.22	0.41
1:D:17:ILE:CG2	1:E:886:LEU:HG	2.51	0.41
1:D:262:LEU:O	1:D:265:VAL:HG22	2.20	0.41
1:D:342:LYS:O	1:D:345:VAL:HB	2.20	0.41
1:D:414:GLU:HG3	1:D:974:PRO:HG3	2.03	0.41
1:D:445:ILE:HG21	1:D:940:LYS:HD2	2.03	0.41
1:E:19:ILE:HA	1:E:22:ALA:HB3	2.02	0.41
1:E:144:ASN:HD22	1:E:149:MET:HG2	1.85	0.41
1:E:203:VAL:HG12	1:E:207:ILE:HD11	2.03	0.41
1:E:293:LEU:HD11	1:E:297:ALA:O	2.20	0.41
1:F:27:ILE:HA	1:F:30:LEU:HD22	2.02	0.41
1:F:72:ILE:HD12	1:F:75:LEU:CD2	2.50	0.41
1:F:184:MET:HE3	1:F:269:GLU:O	2.20	0.41
1:F:362:PHE:CE2	1:F:366:LEU:HD21	2.55	0.41
1:F:535:LEU:HD13	1:F:1027:VAL:HG21	2.02	0.41
1:F:674:LEU:HD22	1:F:861:GLY:HA2	2.03	0.41
1:A:26:ALA:O	1:A:30:LEU:HB2	2.20	0.41
1:A:151:GLN:O	1:A:155:SER:HB3	2.21	0.41
1:A:171:GLY:O	1:A:294:ALA:HB2	2.21	0.41
1:A:723:ASP:HA	1:A:813:SER:HA	2.02	0.41
1:B:350:LEU:HA	1:B:350:LEU:HD23	1.59	0.41
1:B:594:VAL:O	1:B:597:TYR:HB3	2.20	0.41
1:C:281:PHE:CD1	1:C:610:PHE:HD1	2.26	0.41
1:C:411:VAL:O	1:C:414:GLU:HB3	2.20	0.41
1:C:776:GLU:HB2	1:C:779:TYR:CE1	2.56	0.41
1:C:972:LEU:O	1:C:975:ILE:HB	2.20	0.41
1:C:1022:VAL:N	1:C:1023:PRO:HD2	2.36	0.41
1:C:1030:ARG:C	1:C:1032:ARG:H	2.21	0.41
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.85	0.41
1:D:195:LYS:HB3	1:D:196:PHE:CE2	2.55	0.41
1:D:412:VAL:O	1:D:416:VAL:HG12	2.20	0.41
1:D:739:LEU:HD23	1:D:799:VAL:HG11	2.02	0.41
1:D:750:LEU:O	1:D:753:ALA:HB3	2.20	0.41
1:E:228:GLN:HE21	1:E:230:LEU:H	1.69	0.41
1:E:247:GLY:O	1:E:261:LEU:HB3	2.21	0.41
1:E:249:ILE:O	1:E:249:ILE:HG13	2.17	0.41
1:E:272:GLY:O	1:E:275:TYR:HE1	2.04	0.41
1:E:330:THR:HB	1:E:331:PRO:HD3	2.02	0.41
1:E:362:PHE:O	1:E:365:THR:OG1	2.27	0.41
1:E:738:ALA:O	1:E:740:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:932:LEU:HD23	1:E:932:LEU:HA	1.92	0.41
1:F:24:GLY:HA2	1:F:27:ILE:HG23	2.02	0.41
1:F:525:HIS:CE1	1:F:529:ASP:OD2	2.73	0.41
1:F:894:SER:O	1:F:895:TRP:HE3	2.03	0.41
1:F:896:SER:HB3	1:F:1029:VAL:HG12	2.02	0.41
1:A:68:ASN:HD22	1:A:68:ASN:HA	1.60	0.41
1:A:331:PRO:O	1:A:335:ILE:HG13	2.20	0.41
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.51	0.41
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.82	0.41
1:A:774:MET:HG2	1:A:775:SER:H	1.86	0.41
1:A:909:VAL:O	1:A:911:GLY:N	2.54	0.41
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.20	0.41
1:B:242:SER:O	1:B:246:PHE:HD1	2.03	0.41
1:B:506:GLY:O	1:B:509:LYS:HE2	2.20	0.41
1:C:373:PRO:HB2	1:C:377:LEU:HD12	2.03	0.41
1:C:1024:VAL:HA	1:C:1027:VAL:CG2	2.50	0.41
1:D:14:VAL:HG11	1:E:890:ALA:HB2	2.02	0.41
1:D:110:LYS:HZ3	1:D:113:LEU:HD13	1.86	0.41
1:D:201:VAL:HG11	1:D:745:ASP:OD2	2.21	0.41
1:D:352:PHE:CE1	1:D:365:THR:HG23	2.56	0.41
1:D:982:PHE:O	1:D:983:ILE:C	2.59	0.41
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.50	0.41
1:E:410:ILE:HD12	1:E:410:ILE:HA	1.85	0.41
1:E:557:VAL:C	1:E:559:LEU:N	2.72	0.41
1:E:641:GLU:HB2	1:E:650:ARG:NH2	2.35	0.41
1:F:8:ARG:HA	1:F:9:PRO:HD3	1.82	0.41
1:A:344:LEU:HG	1:A:399:VAL:HG22	2.03	0.41
1:B:250:LEU:HD23	1:C:737:GLN:OE1	2.21	0.41
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.74	0.41
1:B:775:SER:OG	1:B:780:ARG:HG2	2.20	0.41
1:B:1016:VAL:HG22	2:B:2000:LMT:H82	2.02	0.41
1:B:1026:PHE:CD2	1:B:1026:PHE:C	2.94	0.41
1:C:279:ALA:HB3	1:C:286:ALA:O	2.21	0.41
1:C:721:LEU:HB3	1:C:814:PRO:HG2	2.02	0.41
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.70	0.41
1:D:177:LEU:HD22	1:D:177:LEU:HA	1.74	0.41
1:D:961:ILE:HG22	1:D:965:LEU:HD12	2.02	0.41
1:E:30:LEU:HA	1:E:31:PRO:HD3	1.89	0.41
1:E:72:ILE:HG12	1:E:106:GLN:HB3	2.02	0.41
1:E:445:ILE:HD12	1:E:449:LEU:HD12	2.03	0.41
1:F:105:VAL:O	1:F:109:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:146:ASP:OD2	1:F:147:GLY:N	2.41	0.41
1:F:540:ARG:O	1:F:543:VAL:HB	2.21	0.41
1:F:859:TRP:O	1:F:864:TYR:HD1	2.03	0.41
1:A:108:GLN:HB2	1:A:129:VAL:HG11	2.02	0.41
1:A:368:PRO:HG3	1:A:413:VAL:HG21	2.02	0.41
1:A:413:VAL:HA	1:A:493:CYS:SG	2.61	0.41
1:A:427:PRO:O	1:A:430:ALA:HB3	2.20	0.41
1:A:468:ARG:CZ	1:A:468:ARG:HB2	2.50	0.41
1:A:488:LEU:O	1:A:488:LEU:HD22	2.21	0.41
1:A:552:MET:HG3	1:A:909:VAL:CG1	2.50	0.41
1:A:907:LEU:HD23	1:A:1017:LEU:HB3	2.02	0.41
1:A:1015:THR:OG1	1:A:1016:VAL:N	2.53	0.41
1:B:172:VAL:HG22	1:B:302:THR:HG23	2.01	0.41
1:B:356:TYR:C	1:B:358:PHE:H	2.23	0.41
1:B:549:VAL:HG13	1:B:550:VAL:N	2.35	0.41
1:C:249:ILE:HD12	1:C:262:LEU:HD23	2.03	0.41
1:C:608:SER:O	1:C:629:VAL:HA	2.21	0.41
1:D:232:ALA:HB1	1:E:725:PRO:O	2.21	0.41
1:D:424:GLY:HA3	1:D:502:LYS:HG2	2.02	0.41
1:D:516:PHE:O	1:D:519:MET:N	2.53	0.41
1:D:937:LEU:HA	1:D:937:LEU:HD23	1.70	0.41
1:E:139:VAL:HG22	1:E:178:PHE:HE1	1.86	0.41
1:E:368:PRO:O	1:E:371:ALA:HB3	2.20	0.41
1:E:538:THR:O	1:E:541:TYR:N	2.50	0.41
1:E:845:GLU:O	1:E:849:SER:HB2	2.21	0.41
1:E:867:ARG:HD3	1:E:868:LEU:N	2.35	0.41
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.72	0.41
1:F:352:PHE:HZ	1:F:362:PHE:CZ	2.39	0.41
1:F:531:VAL:O	1:F:534:ILE:HG12	2.20	0.41
1:F:863:SER:HA	1:F:866:GLU:OE2	2.21	0.41
1:A:131:LYS:HB2	1:A:295:THR:OG1	2.21	0.41
1:A:235:ILE:HD12	1:A:235:ILE:N	2.36	0.41
1:A:293:LEU:HD13	1:A:294:ALA:O	2.21	0.41
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.88	0.41
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.94	0.41
1:A:452:VAL:HA	1:A:880:SER:HG	1.86	0.41
1:A:542:LEU:O	1:A:546:LEU:HD23	2.21	0.41
1:A:567:GLU:CD	1:A:996:GLY:HA2	2.40	0.41
1:A:676:THR:HB	1:A:677:ALA:H	1.68	0.41
1:A:708:LYS:HE2	1:A:708:LYS:HB3	1.84	0.41
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:ILE:CD1	1:A:1030:ARG:HE	2.33	0.41
1:A:937:LEU:HA	1:A:937:LEU:HD23	1.65	0.41
1:B:182:TYR:HD2	1:B:765:ARG:HH22	1.69	0.41
1:B:302:THR:O	1:B:306:ILE:HB	2.21	0.41
1:B:362:PHE:O	1:B:366:LEU:HG	2.21	0.41
1:B:428:LYS:O	1:B:431:THR:HB	2.21	0.41
1:B:597:TYR:OH	1:B:651:ALA:HA	2.21	0.41
1:B:698:ALA:O	1:B:701:GLN:HB3	2.21	0.41
1:B:785:ASP:OD1	1:B:785:ASP:N	2.54	0.41
1:C:5:PHE:C	1:C:7:ASP:N	2.70	0.41
1:C:355:MET:SD	1:C:410:ILE:HD11	2.61	0.41
1:C:474:ILE:HG23	1:C:474:ILE:HD12	1.67	0.41
1:C:721:LEU:HA	1:C:721:LEU:HD12	1.87	0.41
1:C:730:ASP:CG	1:C:808:ARG:HH12	2.25	0.41
1:C:751:GLY:O	1:C:754:TRP:N	2.53	0.41
1:D:23:GLY:HA2	1:D:377:LEU:O	2.21	0.41
1:D:178:PHE:O	1:D:287:SER:OG	2.26	0.41
1:D:383:LEU:HD21	1:D:473:THR:HA	2.03	0.41
1:D:536:ARG:HG3	2:D:2000:LMT:C3B	2.51	0.41
1:D:578:LEU:HD21	1:D:587:THR:HA	2.03	0.41
1:D:790:TYR:CE1	1:D:800:PRO:HB3	2.55	0.41
1:D:900:SER:CB	1:D:1029:VAL:HG21	2.51	0.41
1:D:941:ASN:HB3	1:D:975:ILE:HD12	2.03	0.41
1:E:45:ILE:HA	1:E:128:SER:O	2.21	0.41
1:E:207:ILE:O	1:E:211:ASN:HB3	2.21	0.41
1:E:344:LEU:CG	1:E:399:VAL:HG22	2.50	0.41
1:E:400:LEU:HD21	1:E:933:THR:OG1	2.20	0.41
1:E:573:MET:O	1:E:666:PHE:HD2	2.04	0.41
1:E:584:GLN:HB2	1:E:622:GLN:CG	2.51	0.41
1:E:644:VAL:HG12	1:E:645:GLU:N	2.36	0.41
1:E:709:HIS:HE1	1:E:847:LEU:HD21	1.85	0.41
1:E:758:TYR:CE1	1:E:770:LYS:HD3	2.55	0.41
1:E:898:PRO:O	1:E:902:MET:HG3	2.20	0.41
1:E:1027:VAL:HG13	1:E:1028:VAL:N	2.36	0.41
1:E:1031:ARG:O	1:E:1032:ARG:HG3	2.20	0.41
1:F:99:ASP:HB3	1:F:102:ILE:HB	2.03	0.41
1:F:138:MET:HE3	1:F:138:MET:HB2	1.88	0.41
1:F:195:LYS:HG3	1:F:196:PHE:CD1	2.55	0.41
1:F:352:PHE:HE1	1:F:366:LEU:CD2	2.33	0.41
1:F:514:GLY:C	1:F:516:PHE:N	2.73	0.41
1:F:559:LEU:HD22	1:F:559:LEU:HA	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:671:ILE:H	1:F:862:MET:CE	2.33	0.41
1:F:723:ASP:OD1	1:F:813:SER:OG	2.35	0.41
1:F:927:PHE:O	1:F:931:LEU:HB2	2.21	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CE2	2.56	0.41
1:A:196:PHE:CD2	1:A:196:PHE:N	2.89	0.41
1:A:470:PHE:CD1	1:A:929:VAL:HG21	2.56	0.41
1:B:932:LEU:O	1:B:935:ILE:N	2.54	0.41
1:B:1026:PHE:HD2	1:B:1026:PHE:C	2.25	0.41
1:C:514:GLY:C	1:C:516:PHE:N	2.72	0.41
1:C:1027:VAL:HG23	1:C:1028:VAL:N	2.36	0.41
1:D:457:ALA:HB2	1:D:471:SER:CB	2.51	0.41
1:D:886:LEU:HD21	1:F:17:ILE:CG2	2.49	0.41
1:D:1044:HIS:O	1:D:1045:THR:HB	2.20	0.41
1:E:364:ALA:HA	1:E:367:ILE:HD12	2.02	0.41
1:E:598:TYR:CD2	1:E:629:VAL:HG21	2.56	0.41
1:E:901:VAL:HG13	1:E:942:ALA:CB	2.51	0.41
1:F:139:VAL:HB	1:F:327:TYR:HB3	2.02	0.41
1:F:321:LEU:HD23	1:F:321:LEU:HA	1.88	0.41
1:F:361:ASN:O	1:F:364:ALA:HB3	2.21	0.41
1:A:539:GLY:O	1:A:542:LEU:HB2	2.21	0.40
1:A:675:GLY:HA2	1:A:862:MET:HE2	2.03	0.40
1:A:729:ILE:HD12	1:A:729:ILE:N	2.35	0.40
1:B:443:VAL:O	1:B:447:MET:HG2	2.21	0.40
1:C:888:LEU:HD11	1:C:943:ILE:HD11	2.03	0.40
1:C:953:MET:HE1	1:C:960:LEU:HA	2.02	0.40
1:D:33:ALA:HB2	1:D:299:ALA:H	1.86	0.40
1:D:122:VAL:O	1:D:125:GLN:N	2.52	0.40
1:D:496:MET:H	1:D:496:MET:HG2	1.75	0.40
1:D:545:TYR:O	1:D:548:ILE:N	2.54	0.40
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.51	0.40
1:D:949:ALA:O	1:D:953:MET:HE3	2.22	0.40
1:E:536:ARG:CD	2:E:2000:LMT:H4B	2.51	0.40
1:E:692:HIS:HD2	1:E:816:LEU:HD22	1.86	0.40
1:F:65:ILE:HG23	1:F:69:MET:HE2	2.02	0.40
1:F:175:VAL:HG12	1:F:289:LEU:HD22	2.02	0.40
1:F:498:LYS:HB2	1:F:498:LYS:HE3	1.83	0.40
1:F:703:LEU:HD23	1:F:716:VAL:HG13	2.04	0.40
1:F:843:LEU:HD22	1:F:846:GLN:HB3	2.03	0.40
1:A:82:SER:HB2	1:A:816:LEU:HB2	2.03	0.40
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.84	0.40
1:A:194:ASN:HD21	1:A:798:MET:HG3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HA	1:A:203:VAL:HG23	2.03	0.40
1:A:952:LEU:O	1:A:956:GLU:HB2	2.21	0.40
1:B:149:MET:H	1:B:149:MET:HG2	1.54	0.40
1:B:348:ILE:O	1:B:351:VAL:HB	2.22	0.40
1:B:457:ALA:HB1	1:B:468:ARG:HG3	2.03	0.40
1:B:879:ILE:O	1:B:883:VAL:HG23	2.22	0.40
1:B:990:VAL:HG22	1:B:1004:GLY:HA3	2.04	0.40
1:C:190:PRO:HG3	1:C:779:TYR:CB	2.49	0.40
1:C:195:LYS:HB3	1:C:196:PHE:HD2	1.81	0.40
1:C:453:PHE:HB3	1:C:471:SER:HA	2.04	0.40
1:C:588:GLN:N	1:C:613:ASN:ND2	2.70	0.40
1:C:681:ASP:OD2	1:C:681:ASP:N	2.54	0.40
1:C:1027:VAL:HG23	1:C:1028:VAL:HG23	2.02	0.40
1:D:344:LEU:HD11	1:D:398:MET:CB	2.51	0.40
1:D:527:TYR:CD1	1:D:972:LEU:HG	2.56	0.40
1:E:166:ILE:HD11	1:E:310:LEU:N	2.36	0.40
1:E:530:SER:O	1:E:534:ILE:HG23	2.21	0.40
1:E:695:LEU:HD23	1:E:695:LEU:HA	1.88	0.40
1:E:892:TYR:HE2	1:E:897:ILE:CG2	2.34	0.40
1:E:1011:MET:O	1:E:1015:THR:HG23	2.22	0.40
1:F:151:GLN:O	1:F:155:SER:HB3	2.22	0.40
1:F:175:VAL:HG11	1:F:289:LEU:HD22	2.03	0.40
1:F:534:ILE:C	1:F:536:ARG:N	2.74	0.40
1:F:568:ASP:OD1	1:F:644:VAL:HG23	2.21	0.40
1:F:1016:VAL:HG23	1:F:1017:LEU:HD12	2.03	0.40
1:A:27:ILE:HD11	1:A:380:PHE:HD2	1.86	0.40
1:A:149:MET:HB2	1:A:153:ASP:HB2	2.02	0.40
1:A:396:PHE:O	1:A:400:LEU:HB2	2.20	0.40
1:A:437:GLN:OE1	1:A:438:ILE:HG22	2.21	0.40
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.85	0.40
1:A:910:ILE:O	1:A:910:ILE:HG13	2.19	0.40
1:B:62:THR:HG23	1:B:90:ILE:HD11	2.02	0.40
1:B:195:LYS:H	1:B:195:LYS:HG3	1.68	0.40
1:B:219:LEU:HD11	1:C:727:PHE:CD2	2.57	0.40
1:B:703:LEU:CD1	1:B:718:PRO:HD3	2.39	0.40
1:B:948:PHE:CD2	1:B:971:ARG:HG3	2.57	0.40
1:C:149:MET:HG3	1:C:154:ILE:CD1	2.50	0.40
1:C:426:PRO:HD2	1:C:429:GLU:HB3	2.03	0.40
1:C:578:LEU:HD22	1:C:579:PRO:HD2	2.02	0.40
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.56	0.40
1:C:953:MET:HE3	1:C:953:MET:HB2	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:ASP:HB3	1:E:102:ILE:HG21	2.03	0.40
1:D:163:LYS:HG2	1:D:163:LYS:O	2.21	0.40
1:D:393:LEU:O	1:D:470:PHE:HE1	2.05	0.40
1:D:437:GLN:HG3	1:D:948:PHE:CE1	2.56	0.40
1:E:124:GLN:NE2	1:E:758:TYR:HD2	2.20	0.40
1:E:444:GLY:HA2	1:E:447:MET:HB2	2.03	0.40
1:E:692:HIS:CD2	1:E:816:LEU:HD22	2.56	0.40
1:F:457:ALA:HB2	1:F:471:SER:HB2	2.02	0.40
1:F:509:LYS:HA	1:F:509:LYS:HD2	1.71	0.40
1:F:590:VAL:O	1:F:593:GLU:N	2.54	0.40
1:F:751:GLY:C	1:F:753:ALA:N	2.73	0.40
1:A:211:ASN:HB2	1:A:240:LEU:HD11	2.04	0.40
1:A:446:ALA:O	1:A:478:MET:HE3	2.21	0.40
1:A:886:LEU:HD22	1:C:14:VAL:HG22	2.03	0.40
1:A:941:ASN:HB3	1:A:975:ILE:HD12	2.03	0.40
1:A:960:LEU:HD23	1:A:1031:ARG:NH2	2.36	0.40
1:B:222:THR:HA	1:B:224:PRO:CD	2.50	0.40
1:B:530:SER:HG	1:B:531:VAL:N	2.20	0.40
1:C:343:THR:O	1:C:346:GLU:HB2	2.22	0.40
1:C:409:ALA:O	1:C:412:VAL:HB	2.20	0.40
1:D:235:ILE:O	1:E:728:LYS:HA	2.21	0.40
1:D:325:TYR:HA	1:D:326:PRO:HD2	2.00	0.40
1:D:712:MET:HG3	1:D:713:LEU:HD13	2.03	0.40
1:D:713:LEU:HD21	1:D:843:LEU:HD12	2.03	0.40
1:D:979:SER:O	1:D:983:ILE:N	2.54	0.40
1:E:34:GLN:HE21	1:E:333:VAL:HG22	1.85	0.40
1:E:35:TYR:HD2	1:E:38:ILE:CD1	2.34	0.40
1:E:680:PHE:CD1	1:E:859:TRP:CZ3	3.10	0.40
1:E:945:ILE:HD13	1:E:945:ILE:HA	1.78	0.40
1:F:36:PRO:HG2	1:F:38:ILE:HD11	2.04	0.40
1:F:217:GLY:O	1:F:234:ILE:HD13	2.21	0.40
1:F:645:GLU:OE2	1:F:645:GLU:HA	2.21	0.40
1:F:742:SER:O	1:F:746:ILE:HG22	2.21	0.40
1:A:10:ILE:HG13	1:B:895:TRP:CZ2	2.56	0.40
1:A:721:LEU:HD23	1:A:721:LEU:HA	1.77	0.40
1:A:945:ILE:CG1	1:A:971:ARG:HH22	2.35	0.40
1:B:638:PRO:HB2	1:B:639:GLY:H	1.68	0.40
1:C:214:VAL:HG23	1:C:237:GLN:HB2	2.03	0.40
1:C:249:ILE:HD12	1:C:262:LEU:CD2	2.52	0.40
1:C:685:ILE:HD13	1:C:824:SER:HB3	2.03	0.40
1:C:1019:ILE:HG13	1:C:1020:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.51	0.40
1:D:445:ILE:HG21	1:D:940:LYS:HD3	2.04	0.40
1:D:531:VAL:HG11	1:D:968:VAL:HG21	2.03	0.40
1:E:9:PRO:HD2	1:F:893:GLU:OE1	2.22	0.40
1:E:215:ALA:O	1:F:751:GLY:HA2	2.21	0.40
1:E:740:GLY:HA3	1:E:793:ALA:HB1	2.03	0.40
1:E:789:TRP:O	1:E:801:PHE:HD2	2.04	0.40
1:F:41:PRO:HD3	1:F:96:SER:HA	2.04	0.40
1:F:47:ALA:CB	1:F:122:VAL:HG13	2.48	0.40
1:F:371:ALA:HB1	1:F:484:VAL:HG11	2.02	0.40
1:F:675:GLY:HA3	1:F:862:MET:HG3	2.04	0.40
1:F:678:THR:O	1:F:680:PHE:HB3	2.21	0.40
1:F:910:ILE:O	1:F:914:LEU:HB2	2.22	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	1042/1069 (98%)	880 (84%)	133 (13%)	29 (3%)	5	34
1	B	1040/1069 (97%)	894 (86%)	116 (11%)	30 (3%)	4	34
1	C	1042/1069 (98%)	901 (86%)	114 (11%)	27 (3%)	5	35
1	D	1042/1069 (98%)	888 (85%)	126 (12%)	28 (3%)	5	35
1	E	1040/1069 (97%)	895 (86%)	119 (11%)	26 (2%)	5	36
1	F	1042/1069 (98%)	884 (85%)	132 (13%)	26 (2%)	5	36
All	All	6248/6414 (97%)	5342 (86%)	740 (12%)	166 (3%)	5	35

All (166) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLN
1	A	508	GLY
1	A	638	PRO
1	A	833	PRO
1	A	871	ASN
1	B	216	ALA
1	B	360	GLN
1	B	377	LEU
1	B	507	GLU
1	B	509	LYS
1	B	516	PHE
1	B	638	PRO
1	B	673	GLU
1	B	893	GLU
1	B	1035	ARG
1	B	1040	ILE
1	C	216	ALA
1	C	360	GLN
1	C	836	SER
1	C	871	ASN
1	C	1034	SER
1	D	133	SER
1	D	170	SER
1	D	216	ALA
1	D	360	GLN
1	D	638	PRO
1	D	674	LEU
1	D	820	ASN
1	D	1037	ASN
1	D	1042	HIS
1	E	360	GLN
1	E	516	PHE
1	E	638	PRO
1	E	820	ASN
1	E	893	GLU
1	E	1034	SER
1	F	216	ALA
1	F	360	GLN
1	F	439	GLN
1	F	871	ASN
1	F	1034	SER
1	F	1042	HIS
1	A	216	ALA

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Mol	Chain	Res	Type
1	A	509	LYS
1	A	675	GLY
1	A	1036	LYS
1	A	1037	ASN
1	B	215	ALA
1	B	508	GLY
1	B	675	GLY
1	B	1038	GLU
1	C	6	ILE
1	C	511	GLY
1	C	835	LYS
1	D	390	ILE
1	D	508	GLY
1	D	677	ALA
1	D	871	ASN
1	D	1036	LYS
1	E	99	ASP
1	E	216	ALA
1	E	391	ASN
1	E	673	GLU
1	E	1035	ARG
1	E	1040	ILE
1	E	1042	HIS
1	F	99	ASP
1	F	440	GLY
1	F	507	GLU
1	F	512	PHE
1	F	679	GLY
1	F	820	ASN
1	F	870	GLY
1	A	133	SER
1	A	215	ALA
1	A	674	LEU
1	A	1035	ARG
1	B	376	LEU
1	B	378	GLY
1	B	672	VAL
1	B	689	GLY
1	B	1034	SER
1	C	146	ASP
1	C	195	LYS
1	C	505	HIS

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Mol	Chain	Res	Type
1	C	507	GLU
1	C	512	PHE
1	C	638	PRO
1	C	765	ARG
1	D	163	LYS
1	D	204	ILE
1	D	208	LYS
1	D	507	GLU
1	D	923	ASN
1	E	1038	GLU
1	F	376	LEU
1	F	638	PRO
1	F	923	ASN
1	A	208	LYS
1	A	226	LYS
1	A	506	GLY
1	A	568	ASP
1	A	775	SER
1	A	923	ASN
1	B	163	LYS
1	C	204	ILE
1	C	215	ALA
1	C	568	ASP
1	C	1042	HIS
1	D	735	LYS
1	D	1043	SER
1	E	16	ALA
1	E	134	SER
1	F	163	LYS
1	F	765	ARG
1	F	833	PRO
1	F	1037	ASN
1	A	765	ARG
1	A	995	ALA
1	B	134	SER
1	B	735	LYS
1	B	736	ALA
1	B	995	ALA
1	B	1037	ASN
1	D	568	ASP
1	D	765	ARG
1	D	834	GLY

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Mol	Chain	Res	Type
1	E	135	SER
1	E	163	LYS
1	E	208	LYS
1	E	376	LEU
1	E	923	ASN
1	E	995	ALA
1	E	1036	LYS
1	F	836	SER
1	F	995	ALA
1	A	99	ASP
1	A	376	LEU
1	A	439	GLN
1	A	639	GLY
1	B	321	LEU
1	B	807	SER
1	C	5	PHE
1	C	134	SER
1	C	226	LYS
1	D	376	LEU
1	D	427	PRO
1	E	736	ALA
1	F	147	GLY
1	F	208	LYS
1	F	390	ILE
1	A	204	ILE
1	A	691	GLY
1	C	834	GLY
1	C	1016	VAL
1	E	672	VAL
1	D	221	GLY
1	E	204	ILE
1	B	204	ILE
1	B	427	PRO
1	C	390	ILE
1	C	639	GLY
1	A	834	GLY
1	C	675	GLY
1	D	506	GLY
1	F	511	GLY

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	849/871 (98%)	766 (90%)	83 (10%)	8	35
1	B	847/871 (97%)	758 (90%)	89 (10%)	7	33
1	C	849/871 (98%)	757 (89%)	92 (11%)	6	32
1	D	849/871 (98%)	757 (89%)	92 (11%)	6	32
1	E	847/871 (97%)	755 (89%)	92 (11%)	6	31
1	F	849/871 (98%)	761 (90%)	88 (10%)	7	33
All	All	5090/5226 (97%)	4554 (90%)	536 (10%)	7	33

All (536) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	8	ARG
1	A	10	ILE
1	A	44	THR
1	A	48	SER
1	A	57	VAL
1	A	61	VAL
1	A	65	ILE
1	A	67	GLN
1	A	101	ASP
1	A	104	GLN
1	A	150	THR
1	A	151	GLN
1	A	152	GLU
1	A	153	ASP
1	A	155	SER
1	A	177	LEU
1	A	193	LEU
1	A	195	LYS
1	A	205	THR
1	A	218	GLN
1	A	244	GLU

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Mol	Chain	Res	Type
1	A	254	ASN
1	A	255	GLN
1	A	278	ILE
1	A	293	LEU
1	A	307	ARG
1	A	341	VAL
1	A	343	THR
1	A	362	PHE
1	A	365	THR
1	A	410	ILE
1	A	411	VAL
1	A	428	LYS
1	A	470	PHE
1	A	478	MET
1	A	502	LYS
1	A	512	PHE
1	A	524	THR
1	A	526	HIS
1	A	538	THR
1	A	547	ILE
1	A	549	VAL
1	A	550	VAL
1	A	585	GLU
1	A	590	VAL
1	A	600	THR
1	A	602	GLU
1	A	623	ASN
1	A	629	VAL
1	A	633	ASP
1	A	662	MET
1	A	666	PHE
1	A	680	PHE
1	A	682	PHE
1	A	686	ASP
1	A	711	ASP
1	A	713	LEU
1	A	716	VAL
1	A	741	VAL
1	A	748	THR
1	A	761	ASP
1	A	801	PHE
1	A	804	PHE

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Mol	Chain	Res	Type
1	A	842	GLU
1	A	849	SER
1	A	850	LYS
1	A	864	TYR
1	A	867	ARG
1	A	883	VAL
1	A	914	LEU
1	A	921	LEU
1	A	970	MET
1	A	971	ARG
1	A	976	LEU
1	A	980	LEU
1	A	984	LEU
1	A	990	VAL
1	A	991	ILE
1	A	1030	ARG
1	A	1035	ARG
1	A	1037	ASN
1	A	1038	GLU
1	B	4	PHE
1	B	7	ASP
1	B	10	ILE
1	B	11	PHE
1	B	13	TRP
1	B	27	ILE
1	B	57	VAL
1	B	60	THR
1	B	67	GLN
1	B	72	ILE
1	B	83	ASP
1	B	88	VAL
1	B	111	LEU
1	B	153	ASP
1	B	177	LEU
1	B	182	TYR
1	B	195	LYS
1	B	203	VAL
1	B	210	GLN
1	B	222	THR
1	B	244	GLU
1	B	255	GLN
1	B	259	ARG

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Mol	Chain	Res	Type
1	B	265	VAL
1	B	270	LEU
1	B	277	ILE
1	B	278	ILE
1	B	307	ARG
1	B	314	GLU
1	B	327	TYR
1	B	349	ILE
1	B	353	LEU
1	B	355	MET
1	B	362	PHE
1	B	363	ARG
1	B	365	THR
1	B	372	VAL
1	B	400	LEU
1	B	402	ILE
1	B	410	ILE
1	B	418	ARG
1	B	432	ARG
1	B	459	PHE
1	B	492	LEU
1	B	504	ASP
1	B	523	SER
1	B	524	THR
1	B	554	TYR
1	B	563	PHE
1	B	564	LEU
1	B	569	GLN
1	B	590	VAL
1	B	592	ASN
1	B	617	PHE
1	B	626	ILE
1	B	630	SER
1	B	634	TRP
1	B	652	THR
1	B	668	LEU
1	B	674	LEU
1	B	687	GLN
1	B	690	LEU
1	B	717	ARG
1	B	721	LEU
1	B	730	ASP

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Mol	Chain	Res	Type
1	B	764	ASP
1	B	792	ARG
1	B	804	PHE
1	B	815	ARG
1	B	827	ILE
1	B	849	SER
1	B	867	ARG
1	B	881	LEU
1	B	886	LEU
1	B	888	LEU
1	B	914	LEU
1	B	924	ASP
1	B	925	VAL
1	B	971	ARG
1	B	978	THR
1	B	984	LEU
1	B	991	ILE
1	B	993	THR
1	B	1015	THR
1	B	1016	VAL
1	B	1017	LEU
1	B	1026	PHE
1	B	1030	ARG
1	B	1040	ILE
1	C	6	ILE
1	C	7	ASP
1	C	11	PHE
1	C	13	TRP
1	C	59	ASP
1	C	61	VAL
1	C	62	THR
1	C	102	ILE
1	C	104	GLN
1	C	111	LEU
1	C	113	LEU
1	C	120	GLN
1	C	164	ASP
1	C	166	ILE
1	C	177	LEU
1	C	180	SER
1	C	199	THR
1	C	218	GLN

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Mol	Chain	Res	Type
1	C	254	ASN
1	C	255	GLN
1	C	263	ARG
1	C	268	ILE
1	C	269	GLU
1	C	274	ASN
1	C	275	TYR
1	C	276	ASP
1	C	278	ILE
1	C	307	ARG
1	C	321	LEU
1	C	322	LYS
1	C	343	THR
1	C	349	ILE
1	C	353	LEU
1	C	355	MET
1	C	358	PHE
1	C	362	PHE
1	C	363	ARG
1	C	447	MET
1	C	456	MET
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	509	LYS
1	C	510	LYS
1	C	524	THR
1	C	526	HIS
1	C	546	LEU
1	C	550	VAL
1	C	555	LEU
1	C	559	LEU
1	C	564	LEU
1	C	600	THR
1	C	603	LYS
1	C	623	ASN
1	C	626	ILE
1	C	643	LYS
1	C	663	VAL
1	C	668	LEU
1	C	673	GLU
1	C	674	LEU

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Mol	Chain	Res	Type
1	C	682	PHE
1	C	686	ASP
1	C	687	GLN
1	C	695	LEU
1	C	711	ASP
1	C	721	LEU
1	C	730	ASP
1	C	741	VAL
1	C	785	ASP
1	C	804	PHE
1	C	813	SER
1	C	847	LEU
1	C	850	LYS
1	C	862	MET
1	C	865	GLN
1	C	880	SER
1	C	883	VAL
1	C	887	CYS
1	C	895	TRP
1	C	914	LEU
1	C	921	LEU
1	C	931	LEU
1	C	943	ILE
1	C	970	MET
1	C	971	ARG
1	C	980	LEU
1	C	984	LEU
1	C	990	VAL
1	C	1030	ARG
1	C	1032	ARG
1	C	1035	ARG
1	C	1041	GLU
1	D	6	ILE
1	D	27	ILE
1	D	30	LEU
1	D	34	GLN
1	D	49	TYR
1	D	61	VAL
1	D	89	GLN
1	D	102	ILE
1	D	109	ASN
1	D	151	GLN

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Mol	Chain	Res	Type
1	D	153	ASP
1	D	166	ILE
1	D	177	LEU
1	D	193	LEU
1	D	195	LYS
1	D	205	THR
1	D	222	THR
1	D	238	THR
1	D	244	GLU
1	D	253	VAL
1	D	255	GLN
1	D	263	ARG
1	D	270	LEU
1	D	293	LEU
1	D	327	TYR
1	D	337	ILE
1	D	343	THR
1	D	350	LEU
1	D	357	LEU
1	D	358	PHE
1	D	360	GLN
1	D	365	THR
1	D	372	VAL
1	D	388	PHE
1	D	391	ASN
1	D	395	MET
1	D	402	ILE
1	D	416	VAL
1	D	429	GLU
1	D	448	VAL
1	D	502	LYS
1	D	520	PHE
1	D	524	THR
1	D	526	HIS
1	D	538	THR
1	D	555	LEU
1	D	559	LEU
1	D	563	PHE
1	D	564	LEU
1	D	589	LYS
1	D	599	LEU
1	D	602	GLU

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Mol	Chain	Res	Type
1	D	623	ASN
1	D	629	VAL
1	D	633	ASP
1	D	634	TRP
1	D	644	VAL
1	D	662	MET
1	D	672	VAL
1	D	680	PHE
1	D	694	LYS
1	D	713	LEU
1	D	716	VAL
1	D	721	LEU
1	D	785	ASP
1	D	786	ILE
1	D	804	PHE
1	D	842	GLU
1	D	864	TYR
1	D	867	ARG
1	D	888	LEU
1	D	900	SER
1	D	907	LEU
1	D	913	LEU
1	D	914	LEU
1	D	932	LEU
1	D	933	THR
1	D	940	LYS
1	D	950	LYS
1	D	951	ASP
1	D	960	LEU
1	D	971	ARG
1	D	973	ARG
1	D	990	VAL
1	D	1011	MET
1	D	1015	THR
1	D	1026	PHE
1	D	1030	ARG
1	D	1035	ARG
1	D	1038	GLU
1	D	1040	ILE
1	D	1044	HIS
1	E	20	MET
1	E	32	VAL

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Mol	Chain	Res	Type
1	E	57	VAL
1	E	68	ASN
1	E	90	ILE
1	E	91	THR
1	E	105	VAL
1	E	118	LEU
1	E	150	THR
1	E	151	GLN
1	E	153	ASP
1	E	177	LEU
1	E	180	SER
1	E	182	TYR
1	E	189	ASN
1	E	195	LYS
1	E	207	ILE
1	E	210	GLN
1	E	214	VAL
1	E	218	GLN
1	E	239	ARG
1	E	249	ILE
1	E	254	ASN
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	275	TYR
1	E	278	ILE
1	E	293	LEU
1	E	307	ARG
1	E	313	MET
1	E	314	GLU
1	E	324	VAL
1	E	329	THR
1	E	336	SER
1	E	355	MET
1	E	363	ARG
1	E	372	VAL
1	E	382	VAL
1	E	389	SER
1	E	393	LEU
1	E	395	MET
1	E	410	ILE
1	E	418	ARG

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Mol	Chain	Res	Type
1	E	456	MET
1	E	472	ILE
1	E	519	MET
1	E	536	ARG
1	E	546	LEU
1	E	547	ILE
1	E	550	VAL
1	E	555	LEU
1	E	558	ARG
1	E	563	PHE
1	E	569	GLN
1	E	583	THR
1	E	600	THR
1	E	601	LYS
1	E	617	PHE
1	E	626	ILE
1	E	630	SER
1	E	633	ASP
1	E	634	TRP
1	E	640	GLU
1	E	659	LYS
1	E	662	MET
1	E	666	PHE
1	E	668	LEU
1	E	680	PHE
1	E	694	LYS
1	E	711	ASP
1	E	713	LEU
1	E	717	ARG
1	E	721	LEU
1	E	730	ASP
1	E	804	PHE
1	E	815	ARG
1	E	850	LYS
1	E	867	ARG
1	E	871	ASN
1	E	879	ILE
1	E	886	LEU
1	E	887	CYS
1	E	900	SER
1	E	910	ILE
1	E	914	LEU

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Mol	Chain	Res	Type
1	E	921	LEU
1	E	947	GLU
1	E	973	ARG
1	E	991	ILE
1	E	1035	ARG
1	E	1037	ASN
1	F	11	PHE
1	F	27	ILE
1	F	37	THR
1	F	44	THR
1	F	49	TYR
1	F	59	ASP
1	F	60	THR
1	F	62	THR
1	F	70	ASN
1	F	92	LEU
1	F	94	PHE
1	F	99	ASP
1	F	125	GLN
1	F	132	SER
1	F	166	ILE
1	F	177	LEU
1	F	270	LEU
1	F	278	ILE
1	F	300	LEU
1	F	312	LYS
1	F	339	GLU
1	F	343	THR
1	F	350	LEU
1	F	353	LEU
1	F	358	PHE
1	F	363	ARG
1	F	398	MET
1	F	412	VAL
1	F	419	VAL
1	F	429	GLU
1	F	431	THR
1	F	456	MET
1	F	468	ARG
1	F	472	ILE
1	F	478	MET
1	F	502	LYS

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Mol	Chain	Res	Type
1	F	509	LYS
1	F	510	LYS
1	F	512	PHE
1	F	517	ASN
1	F	519	MET
1	F	524	THR
1	F	538	THR
1	F	540	ARG
1	F	559	LEU
1	F	585	GLU
1	F	586	ARG
1	F	600	THR
1	F	617	PHE
1	F	623	ASN
1	F	626	ILE
1	F	629	VAL
1	F	630	SER
1	F	633	ASP
1	F	668	LEU
1	F	680	PHE
1	F	682	PHE
1	F	683	GLU
1	F	686	ASP
1	F	694	LYS
1	F	716	VAL
1	F	723	ASP
1	F	731	ILE
1	F	749	THR
1	F	767	ARG
1	F	770	LYS
1	F	804	PHE
1	F	843	LEU
1	F	847	LEU
1	F	862	MET
1	F	883	VAL
1	F	895	TRP
1	F	910	ILE
1	F	914	LEU
1	F	921	LEU
1	F	931	LEU
1	F	940	LYS
1	F	950	LYS

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Mol	Chain	Res	Type
1	F	961	ILE
1	F	968	VAL
1	F	971	ARG
1	F	984	LEU
1	F	990	VAL
1	F	991	ILE
1	F	1011	MET
1	F	1030	ARG
1	F	1032	ARG
1	F	1039	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	63	GLN
1	A	123	GLN
1	A	194	ASN
1	A	218	GLN
1	A	592	ASN
1	A	642	ASN
1	B	189	ASN
1	B	1000	GLN
1	B	1037	ASN
1	C	112	GLN
1	C	211	ASN
1	C	588	GLN
1	C	592	ASN
1	D	108	GLN
1	D	109	ASN
1	D	123	GLN
1	D	231	ASN
1	D	284	GLN
1	D	517	ASN
1	D	526	HIS
1	D	577	GLN
1	D	584	GLN
1	D	592	ASN
1	D	642	ASN
1	D	865	GLN
1	E	34	GLN
1	E	104	GLN

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Mol	Chain	Res	Type
1	E	106	GLN
1	E	108	GLN
1	E	123	GLN
1	E	701	GLN
1	F	70	ASN
1	F	211	ASN
1	F	517	ASN
1	F	588	GLN
1	F	592	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

6 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	LMT	E	2000	-	36,36,36	1.86	8 (22%)	47,47,47	1.38	8 (17%)
2	LMT	C	2000	-	36,36,36	1.80	8 (22%)	47,47,47	1.74	10 (21%)
2	LMT	F	2000	-	36,36,36	1.90	9 (25%)	47,47,47	1.50	9 (19%)
2	LMT	A	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.54	12 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	LMT	D	2000	-	36,36,36	2.01	9 (25%)	47,47,47	1.33	5 (10%)
2	LMT	B	2000	-	36,36,36	1.93	9 (25%)	47,47,47	1.27	7 (14%)

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	LMT	E	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	C	2000	-	3/3/10/10	6/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	12/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	14/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	B	2000	-	1/1/10/10	13/21/61/61	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	LMT	O5'-C5'	5.00	1.56	1.44
2	D	2000	LMT	O1'-C1'	4.64	1.48	1.40
2	B	2000	LMT	O1'-C1'	4.59	1.48	1.40
2	E	2000	LMT	O5'-C5'	4.48	1.55	1.44
2	A	2000	LMT	O1'-C1'	4.42	1.47	1.40
2	D	2000	LMT	O5'-C5'	4.39	1.55	1.44
2	F	2000	LMT	O5B-C1B	4.19	1.52	1.41
2	B	2000	LMT	O5B-C1B	4.07	1.52	1.41
2	F	2000	LMT	O5'-C5'	4.06	1.54	1.44
2	E	2000	LMT	O1'-C1'	4.06	1.47	1.40
2	D	2000	LMT	O5'-C1'	4.01	1.52	1.41
2	F	2000	LMT	O1'-C1'	4.00	1.47	1.40
2	C	2000	LMT	O1'-C1'	3.98	1.47	1.40
2	A	2000	LMT	O5'-C1'	3.98	1.52	1.41
2	A	2000	LMT	O5B-C1B	3.95	1.51	1.41
2	C	2000	LMT	C6'-C5'	-3.94	1.38	1.51
2	D	2000	LMT	O5B-C1B	3.76	1.51	1.41
2	B	2000	LMT	O5'-C5'	3.71	1.53	1.44
2	E	2000	LMT	O5'-C1'	3.69	1.51	1.41
2	D	2000	LMT	C6'-C5'	-3.61	1.39	1.51
2	C	2000	LMT	O5B-C1B	3.58	1.51	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	LMT	O3B-C3B	3.52	1.51	1.43
2	B	2000	LMT	C6'-C5'	-3.35	1.40	1.51
2	F	2000	LMT	O5'-C1'	3.33	1.50	1.41
2	F	2000	LMT	C6'-C5'	-3.33	1.40	1.51
2	A	2000	LMT	C6'-C5'	-3.32	1.40	1.51
2	E	2000	LMT	O5B-C1B	3.31	1.50	1.41
2	C	2000	LMT	O5'-C5'	3.30	1.52	1.44
2	E	2000	LMT	C6'-C5'	-3.20	1.41	1.51
2	C	2000	LMT	O2'-C2'	3.13	1.50	1.43
2	D	2000	LMT	O3B-C3B	3.06	1.50	1.43
2	B	2000	LMT	O5'-C1'	3.00	1.49	1.41
2	C	2000	LMT	O3B-C3B	2.95	1.49	1.43
2	E	2000	LMT	O3B-C3B	2.94	1.49	1.43
2	F	2000	LMT	O3B-C3B	2.87	1.49	1.43
2	D	2000	LMT	O2'-C2'	2.86	1.49	1.43
2	F	2000	LMT	C3B-C2B	-2.84	1.45	1.52
2	C	2000	LMT	O5'-C1'	2.68	1.48	1.41
2	E	2000	LMT	C3'-C2'	-2.68	1.45	1.52
2	A	2000	LMT	O3B-C3B	2.47	1.48	1.43
2	F	2000	LMT	O2'-C2'	2.45	1.48	1.43
2	A	2000	LMT	O2'-C2'	2.36	1.48	1.43
2	E	2000	LMT	O2'-C2'	2.35	1.48	1.43
2	F	2000	LMT	C3'-C2'	-2.35	1.46	1.52
2	B	2000	LMT	C3B-C2B	-2.29	1.46	1.52
2	C	2000	LMT	C3B-C2B	-2.29	1.46	1.52
2	D	2000	LMT	C3'-C2'	-2.28	1.46	1.52
2	A	2000	LMT	C3'-C2'	-2.26	1.46	1.52
2	B	2000	LMT	O2'-C2'	2.19	1.48	1.43
2	A	2000	LMT	C5-C4	2.12	1.63	1.51
2	D	2000	LMT	O3'-C3'	2.08	1.47	1.43
2	B	2000	LMT	O3'-C3'	2.05	1.47	1.43

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2000	LMT	C2'-C3'-C4'	5.21	121.58	109.68
2	F	2000	LMT	O1'-C1'-C2'	4.77	115.75	108.30
2	C	2000	LMT	O1'-C1'-C2'	4.04	114.61	108.30
2	D	2000	LMT	C1'-O5'-C5'	3.87	121.28	113.69
2	E	2000	LMT	C1B-O1B-C4'	-3.61	109.02	117.96
2	B	2000	LMT	O1'-C1'-C2'	3.54	113.83	108.30
2	C	2000	LMT	O1B-C1B-C2B	3.53	117.24	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2000	LMT	O5B-C5B-C4B	3.48	116.01	109.69
2	C	2000	LMT	C1'-C2'-C3'	3.45	117.17	110.00
2	F	2000	LMT	O5B-C5B-C4B	3.39	115.85	109.69
2	F	2000	LMT	C1B-O5B-C5B	3.19	119.95	113.69
2	A	2000	LMT	C3B-C4B-C5B	3.10	115.77	110.24
2	C	2000	LMT	C6B-C5B-C4B	-3.01	105.94	113.00
2	A	2000	LMT	O1B-C1B-C2B	2.98	115.83	108.10
2	A	2000	LMT	O5'-C5'-C6'	2.97	113.83	106.44
2	C	2000	LMT	O6'-C6'-C5'	-2.90	101.35	111.29
2	A	2000	LMT	O1B-C4'-C3'	2.87	114.91	107.28
2	D	2000	LMT	O5'-C5'-C4'	2.87	115.80	109.75
2	B	2000	LMT	C4B-C3B-C2B	-2.85	105.84	110.82
2	F	2000	LMT	C1B-O1B-C4'	-2.71	111.26	117.96
2	F	2000	LMT	C4B-C3B-C2B	-2.70	106.10	110.82
2	A	2000	LMT	C6'-C5'-C4'	-2.70	105.47	113.33
2	F	2000	LMT	O2B-C2B-C3B	-2.67	104.18	110.35
2	D	2000	LMT	O5B-C5B-C4B	2.66	114.52	109.69
2	F	2000	LMT	O1B-C1B-C2B	2.56	114.72	108.10
2	A	2000	LMT	O5'-C1'-O1'	2.55	116.02	109.97
2	D	2000	LMT	O4'-C4B-C5B	2.54	115.61	109.30
2	E	2000	LMT	O5'-C5'-C6'	2.53	112.72	106.44
2	B	2000	LMT	C1'-C2'-C3'	2.52	115.24	110.00
2	E	2000	LMT	O1B-C4'-C3'	2.48	113.88	107.28
2	C	2000	LMT	C1B-O5B-C5B	-2.46	108.86	113.69
2	B	2000	LMT	C2'-C3'-C4'	2.40	115.16	109.68
2	A	2000	LMT	C4B-C3B-C2B	2.39	114.99	110.82
2	A	2000	LMT	O3B-C3B-C4B	-2.31	105.00	110.35
2	E	2000	LMT	O5B-C5B-C6B	2.31	112.17	106.44
2	E	2000	LMT	C1B-O5B-C5B	-2.30	109.18	113.69
2	C	2000	LMT	C1'-O5'-C5'	-2.28	109.21	113.69
2	B	2000	LMT	O5B-C1B-C2B	2.24	115.09	110.35
2	C	2000	LMT	O1B-C4'-C5'	-2.17	103.49	109.45
2	B	2000	LMT	O3B-C3B-C2B	2.16	115.35	110.35
2	A	2000	LMT	C1B-O1B-C4'	-2.16	112.62	117.96
2	A	2000	LMT	C1-O1'-C1'	2.13	117.37	113.84
2	C	2000	LMT	O2'-C2'-C3'	-2.13	105.43	110.35
2	F	2000	LMT	O2B-C2B-C1B	2.11	115.18	110.05
2	B	2000	LMT	O5B-C5B-C6B	2.05	111.54	106.44
2	E	2000	LMT	C6'-C5'-C4'	-2.05	107.37	113.33
2	E	2000	LMT	O5B-C5B-C4B	2.03	113.38	109.69
2	F	2000	LMT	O5B-C1B-C2B	2.02	114.63	110.35
2	E	2000	LMT	C2'-C3'-C4'	2.02	114.29	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2000	LMT	C1B-C2B-C3B	2.01	114.18	110.00
2	D	2000	LMT	C6'-C5'-C4'	-2.01	107.48	113.33

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2000	LMT	C3'
2	A	2000	LMT	C4B
2	B	2000	LMT	C3'
2	C	2000	LMT	C2B
2	C	2000	LMT	C1B
2	C	2000	LMT	C4B
2	D	2000	LMT	C3'
2	D	2000	LMT	C4B
2	E	2000	LMT	C3'
2	E	2000	LMT	C4B
2	F	2000	LMT	C3'
2	F	2000	LMT	C2'
2	F	2000	LMT	C4B

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2000	LMT	C2'-C1'-O1'-C1
2	A	2000	LMT	O5'-C1'-O1'-C1
2	D	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	O5'-C1'-O1'-C1
2	E	2000	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	C2'-C1'-O1'-C1
2	F	2000	LMT	O5'-C1'-O1'-C1
2	F	2000	LMT	C2-C1-O1'-C1'
2	B	2000	LMT	O5B-C1B-O1B-C4'
2	C	2000	LMT	C2B-C1B-O1B-C4'
2	A	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	O5'-C5'-C6'-O6'
2	C	2000	LMT	O5'-C5'-C6'-O6'
2	C	2000	LMT	C4'-C5'-C6'-O6'
2	A	2000	LMT	C4B-C5B-C6B-O6B
2	D	2000	LMT	O5'-C5'-C6'-O6'
2	B	2000	LMT	O5B-C5B-C6B-O6B
2	B	2000	LMT	O5'-C5'-C6'-O6'
2	B	2000	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
2	E	2000	LMT	C2'-C1'-O1'-C1
2	D	2000	LMT	C7-C8-C9-C10
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	C4'-C5'-C6'-O6'
2	A	2000	LMT	C4'-C5'-C6'-O6'
2	B	2000	LMT	C4B-C5B-C6B-O6B
2	C	2000	LMT	O5'-C1'-O1'-C1
2	F	2000	LMT	C4'-C5'-C6'-O6'
2	B	2000	LMT	C3-C4-C5-C6
2	F	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C6-C7-C8-C9
2	A	2000	LMT	C11-C10-C9-C8
2	E	2000	LMT	O5B-C5B-C6B-O6B
2	F	2000	LMT	C6-C7-C8-C9
2	A	2000	LMT	C4-C5-C6-C7
2	E	2000	LMT	C4-C5-C6-C7
2	B	2000	LMT	C5-C6-C7-C8
2	F	2000	LMT	O5B-C5B-C6B-O6B
2	D	2000	LMT	C2'-C1'-O1'-C1
2	E	2000	LMT	C1-C2-C3-C4
2	D	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	C9-C10-C11-C12
2	B	2000	LMT	C2B-C1B-O1B-C4'
2	B	2000	LMT	C1-C2-C3-C4
2	E	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	C1-C2-C3-C4
2	A	2000	LMT	C5-C6-C7-C8
2	D	2000	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	O1'-C1-C2-C3
2	A	2000	LMT	C1-C2-C3-C4
2	E	2000	LMT	O1'-C1-C2-C3
2	D	2000	LMT	O1'-C1-C2-C3
2	C	2000	LMT	C1-C2-C3-C4
2	A	2000	LMT	O5B-C1B-O1B-C4'
2	B	2000	LMT	C7-C8-C9-C10
2	A	2000	LMT	C7-C8-C9-C10
2	B	2000	LMT	C9-C10-C11-C12
2	B	2000	LMT	C11-C10-C9-C8
2	F	2000	LMT	C5-C6-C7-C8
2	E	2000	LMT	C7-C8-C9-C10
2	E	2000	LMT	C11-C10-C9-C8
2	A	2000	LMT	O1'-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	D	2000	LMT	O5B-C5B-C6B-O6B
2	A	2000	LMT	C3-C4-C5-C6
2	D	2000	LMT	C3'-C4'-O1B-C1B
2	C	2000	LMT	C5-C6-C7-C8

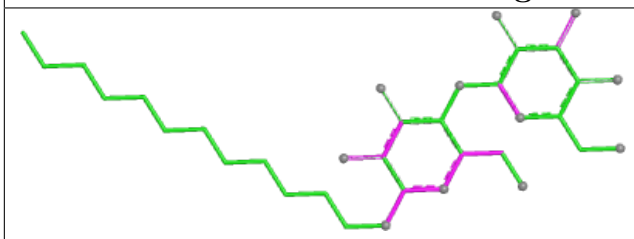
There are no ring outliers.

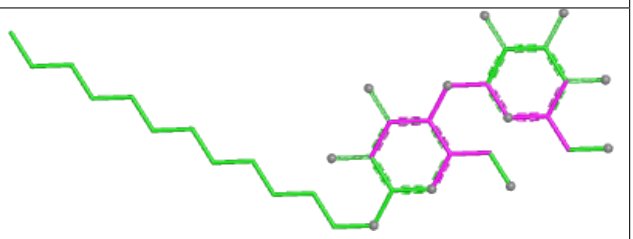
6 monomers are involved in 30 short contacts:

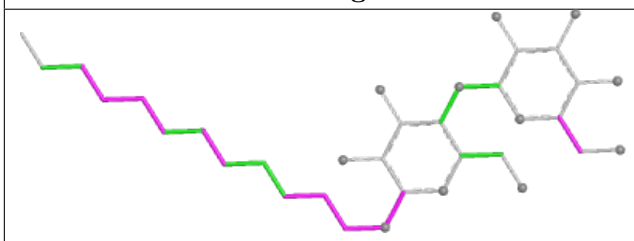
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2000	LMT	6	0
2	C	2000	LMT	6	0
2	F	2000	LMT	2	0
2	A	2000	LMT	1	0
2	D	2000	LMT	3	0
2	B	2000	LMT	12	0

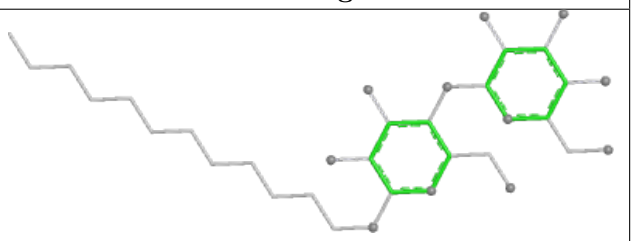
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 LMT E 2000

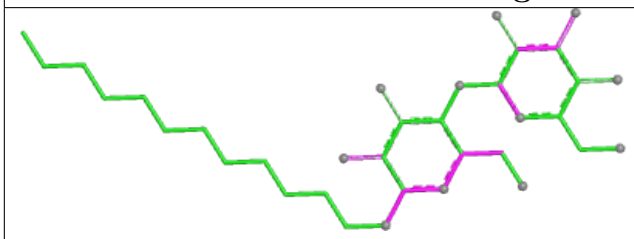

Bond lengths

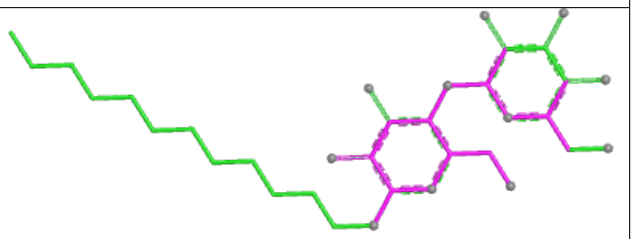

Bond angles

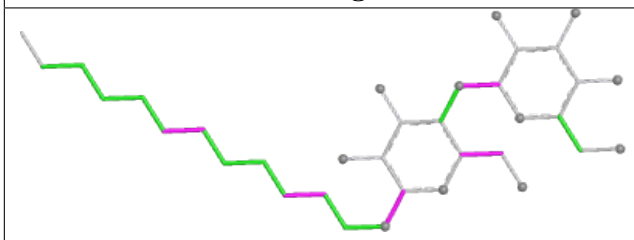

Torsions

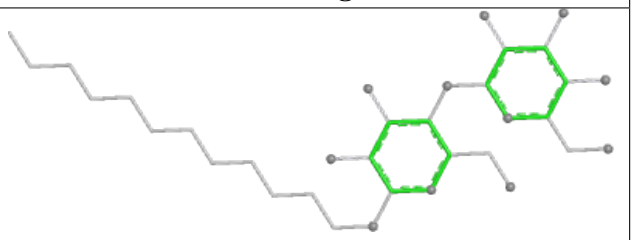

Rings

Ligand LMT C 2000

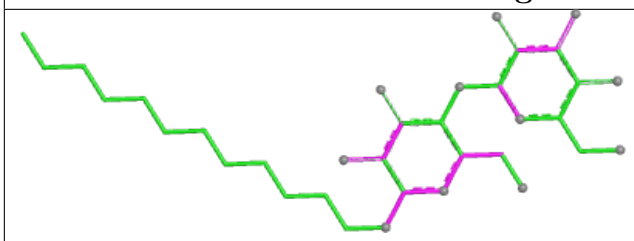

Bond lengths

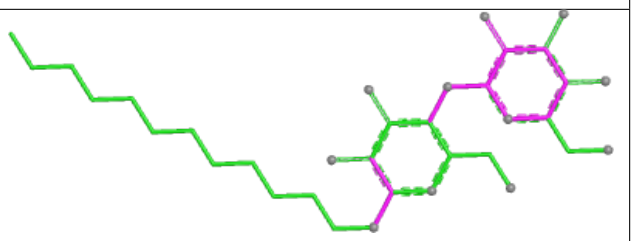

Bond angles

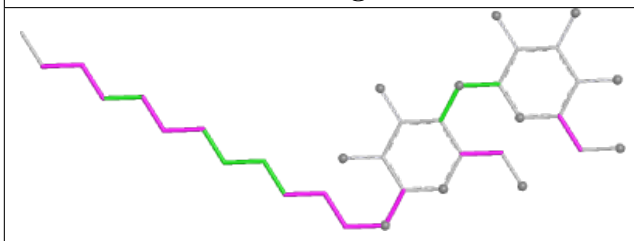

Torsions

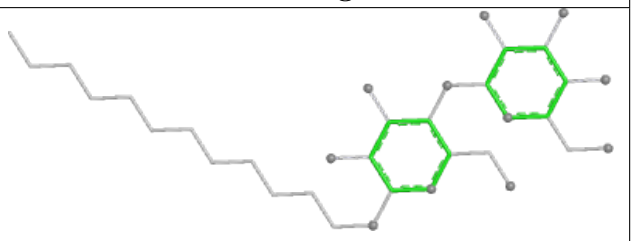

Rings

Ligand LMT F 2000

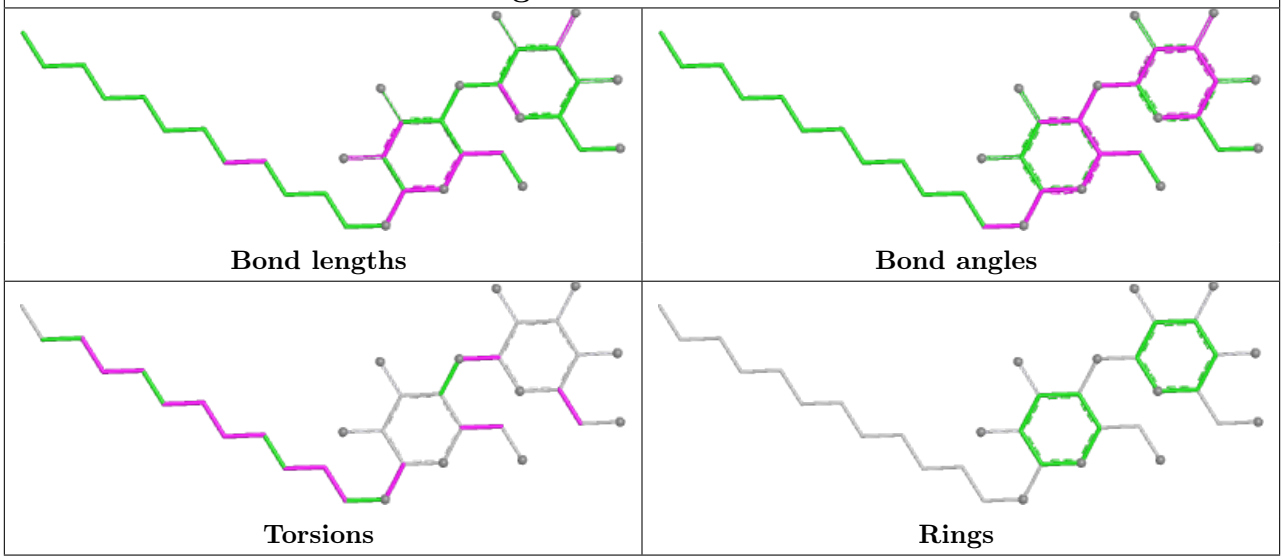

Bond lengths


Bond angles

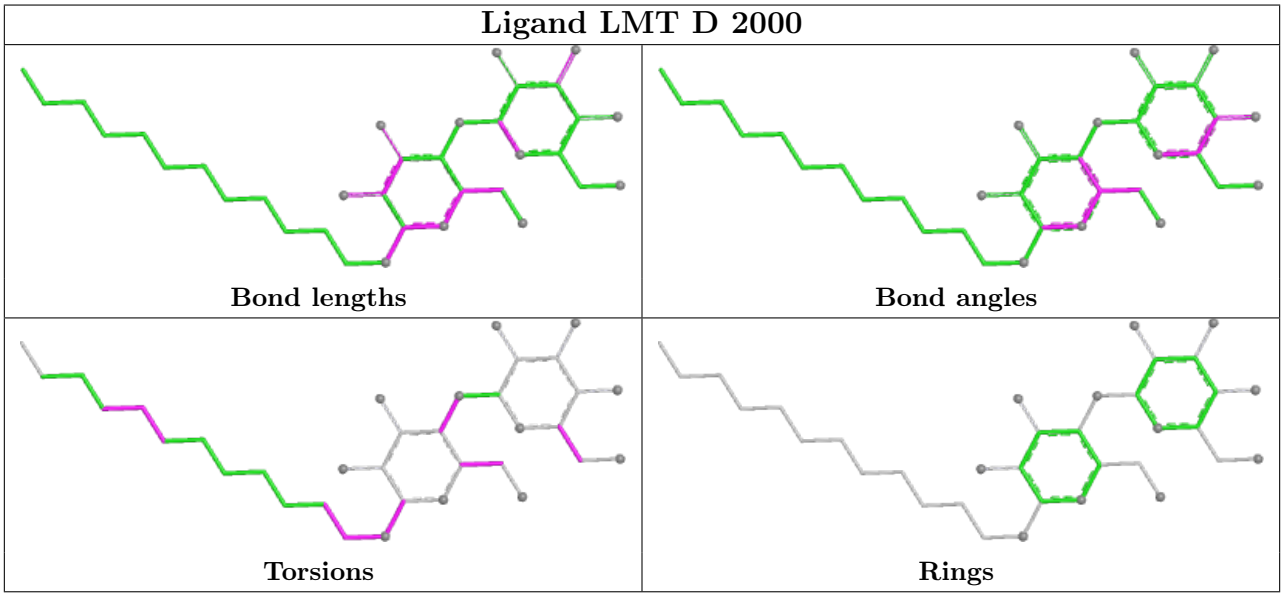

Torsions


Rings

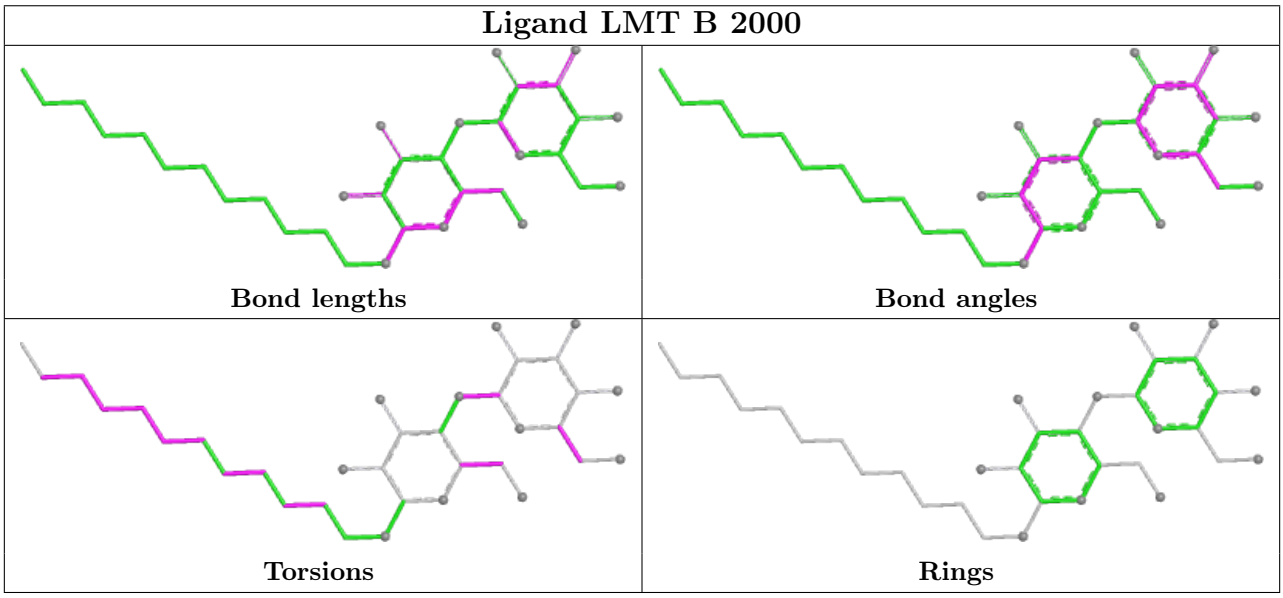
Ligand LMT A 2000



Ligand LMT D 2000



Ligand LMT B 2000



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1044/1069 (97%)	-0.45	8 (0%)	86	74	5, 35, 83, 118	0
1	B	1042/1069 (97%)	-0.55	7 (0%)	87	78	3, 27, 62, 108	0
1	C	1044/1069 (97%)	-0.55	5 (0%)	91	83	4, 29, 60, 88	0
1	D	1044/1069 (97%)	-0.36	9 (0%)	84	72	10, 49, 88, 114	0
1	E	1042/1069 (97%)	-0.26	34 (3%)	46	32	5, 46, 100, 129	0
1	F	1044/1069 (97%)	-0.24	23 (2%)	62	45	5, 54, 104, 142	0
All	All	6260/6414 (97%)	-0.40	86 (1%)	75	60	3, 39, 90, 142	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	715	SER	6.5
1	F	849	SER	6.4
1	E	295	THR	5.2
1	E	834	GLY	4.5
1	E	170	SER	4.5
1	F	720	GLY	4.2
1	D	1034	SER	4.0
1	E	711	ASP	4.0
1	A	714	THR	3.9
1	C	511	GLY	3.8
1	F	116	PRO	3.6
1	E	869	SER	3.5
1	E	296	GLY	3.4
1	B	715	SER	3.3
1	E	710	PRO	3.3
1	E	319	SER	3.2
1	E	311	ALA	3.2
1	E	164	ASP	3.1
1	D	871	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	858	ASP	3.1
1	E	836	SER	3.1
1	E	875	SER	3.1
1	E	292	LYS	3.1
1	E	868	LEU	3.1
1	F	826	GLU	3.1
1	E	148	THR	3.1
1	E	872	GLN	3.0
1	F	387	GLY	2.9
1	F	690	LEU	2.9
1	F	856	GLY	2.8
1	B	871	ASN	2.8
1	D	869	SER	2.7
1	E	709	HIS	2.6
1	B	834	GLY	2.6
1	D	852	PRO	2.6
1	E	512	PHE	2.6
1	A	386	PHE	2.6
1	F	76	MET	2.6
1	E	78	MET	2.5
1	A	678	THR	2.5
1	E	50	PRO	2.5
1	A	869	SER	2.5
1	D	874	PRO	2.5
1	D	868	LEU	2.5
1	F	827	ILE	2.5
1	D	870	GLY	2.5
1	D	295	THR	2.4
1	E	314	GLU	2.4
1	D	462	SER	2.4
1	E	835	LYS	2.4
1	E	1034	SER	2.4
1	E	870	GLY	2.4
1	C	48	SER	2.3
1	F	55	LYS	2.3
1	A	459	PHE	2.3
1	A	834	GLY	2.3
1	F	712	MET	2.3
1	E	874	PRO	2.3
1	B	835	LYS	2.3
1	F	817	GLU	2.2
1	F	494	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	703	LEU	2.2
1	F	458	PHE	2.2
1	F	607	GLU	2.2
1	C	147	GLY	2.2
1	F	56	THR	2.2
1	F	496	MET	2.2
1	C	433	LYS	2.2
1	F	719	ASN	2.2
1	E	51	GLY	2.2
1	E	871	ASN	2.2
1	C	502	LYS	2.2
1	F	704	ALA	2.2
1	B	512	PHE	2.2
1	A	833	PRO	2.1
1	E	387	GLY	2.1
1	A	679	GLY	2.1
1	E	175	VAL	2.1
1	B	872	GLN	2.1
1	E	171	GLY	2.1
1	B	869	SER	2.1
1	E	197	GLN	2.0
1	F	821	GLY	2.0
1	E	833	PRO	2.0
1	F	122	VAL	2.0
1	E	312	LYS	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)

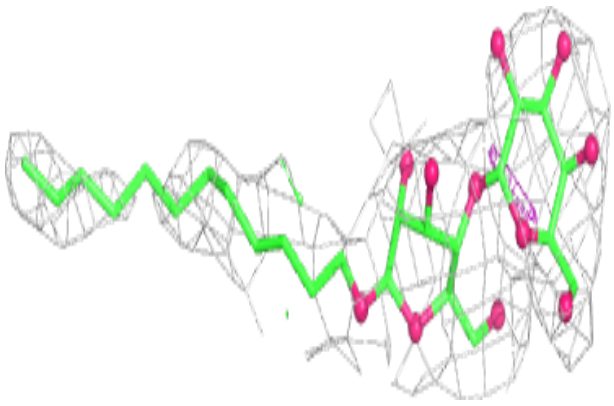
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

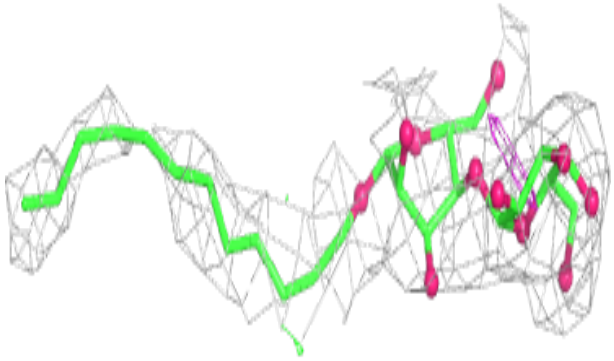
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	A	2000	35/35	0.86	0.37	2,31,49,54	0
2	LMT	F	2000	35/35	0.86	0.34	13,38,54,58	0
2	LMT	D	2000	35/35	0.87	0.26	1,25,38,40	0
2	LMT	C	2000	35/35	0.88	0.25	5,22,46,50	0
2	LMT	B	2000	35/35	0.89	0.29	6,32,47,61	0
2	LMT	E	2000	35/35	0.90	0.34	3,34,48,49	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 LMT A 2000:

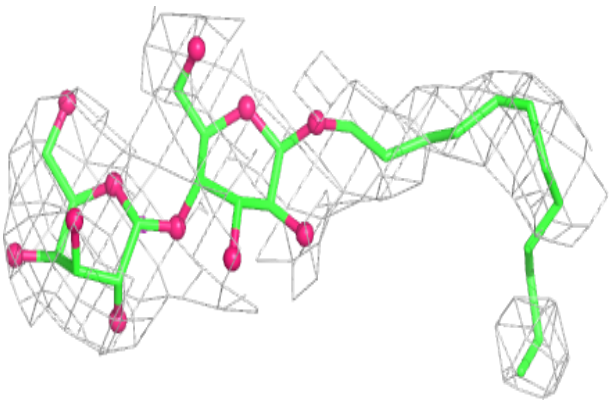
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

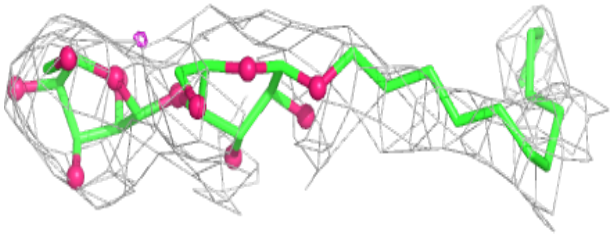


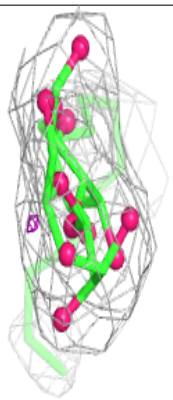


Electron density around LMT F 2000:

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

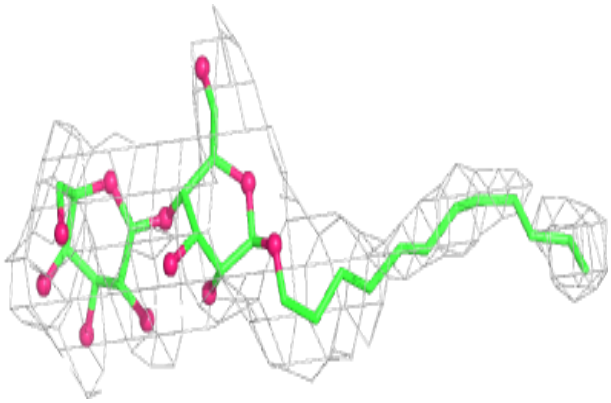


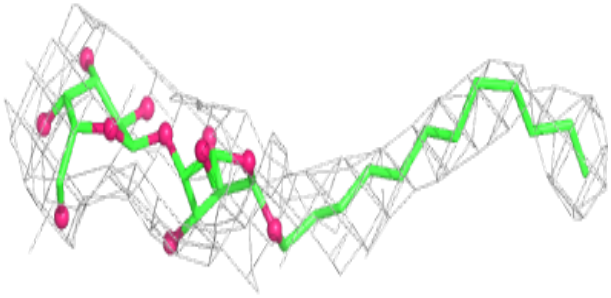




Electron density around LMT D 2000:

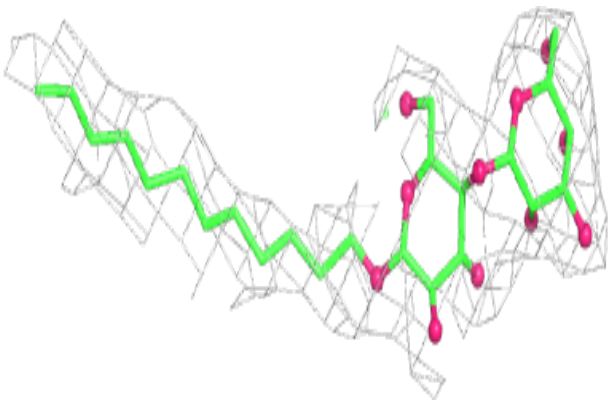
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

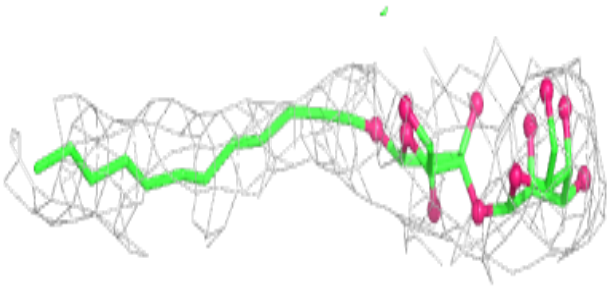


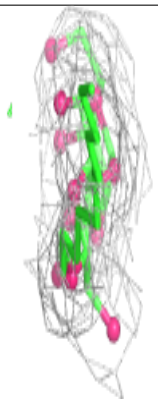


Electron density around LMT C 2000:

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

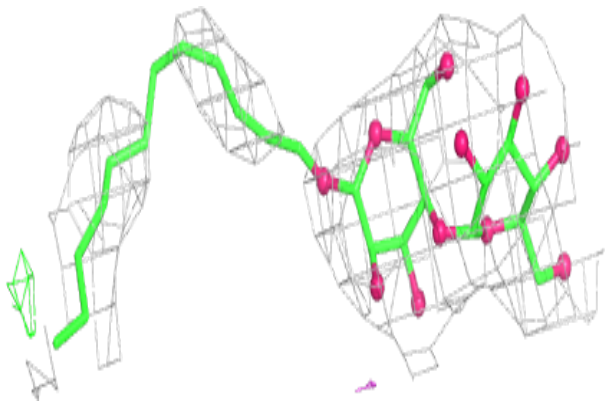


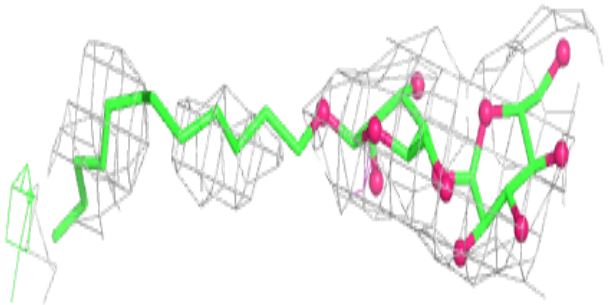


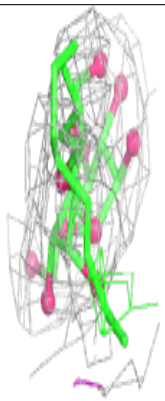


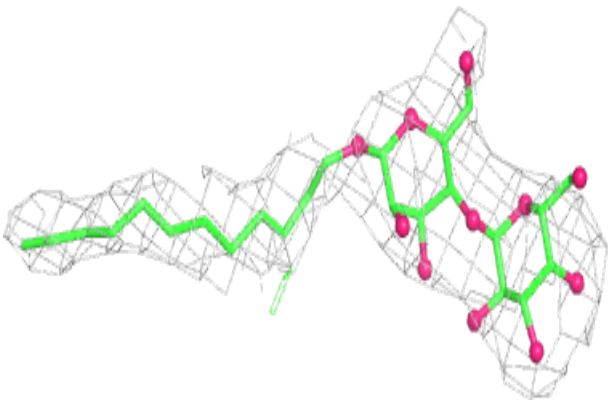
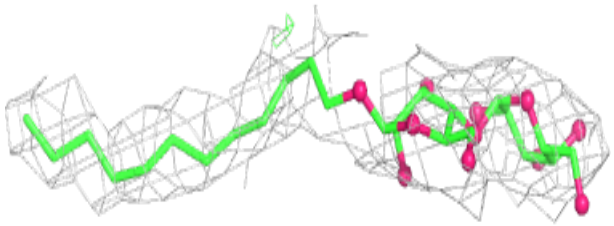
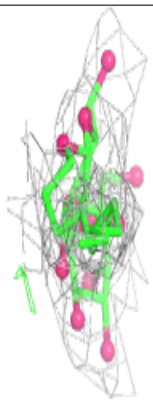
Electron density around LMT B 2000:

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







Electron density around LMT E 2000: $2mF_o$-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.