Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2022 – 10:12 am BST

PDB ID	:	7O3L
Title	:	Crystal Structure of AcrB Double Mutant
Authors	:	Ababou, A.
Deposited on	:	2021-04-02
Resolution	:	3.53 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:

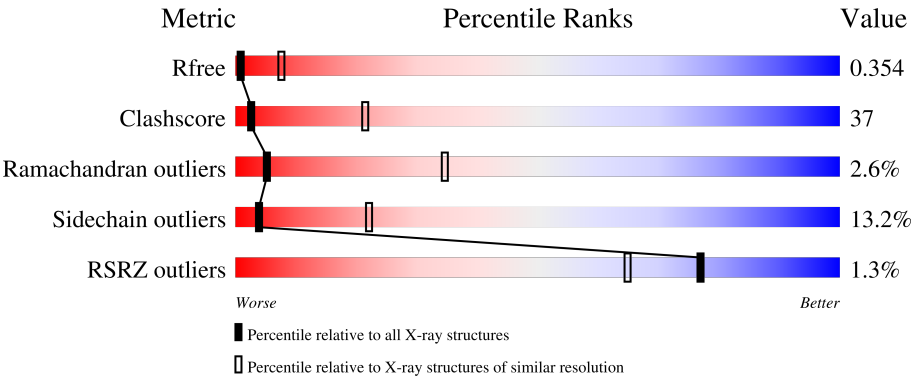
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.53 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	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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	35% 52% 10%
1	B	1069	3% 36% 51% 10%
1	C	1069	3% 32% 55% 10%
1	D	1069	42% 48% 7%
1	E	1069	44% 46% 8%

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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 47722 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
			7930	5093	1315	1479	43			
1	B	1042	Total	C	N	O	S	0	0	0
			7913	5083	1311	1476	43			
1	C	1042	Total	C	N	O	S	0	0	0
			7913	5083	1311	1476	43			
1	D	1044	Total	C	N	O	S	0	0	0
			7930	5093	1315	1479	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7913	5083	1311	1476	43			
1	F	1042	Total	C	N	O	S	0	0	0
			7913	5083	1311	1476	43			

There are 132 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	615	ALA	PHE	engineered mutation	UNP E2QH56
A	617	ALA	PHE	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	615	ALA	PHE	engineered mutation	UNP E2QH56
B	617	ALA	PHE	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP E2QH56
C	-3	ARG	-	expression tag	UNP E2QH56
C	-2	GLY	-	expression tag	UNP E2QH56
C	-1	SER	-	expression tag	UNP E2QH56
C	0	HIS	-	expression tag	UNP E2QH56
C	615	ALA	PHE	engineered mutation	UNP E2QH56
C	617	ALA	PHE	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	615	ALA	PHE	engineered mutation	UNP E2QH56
D	617	ALA	PHE	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

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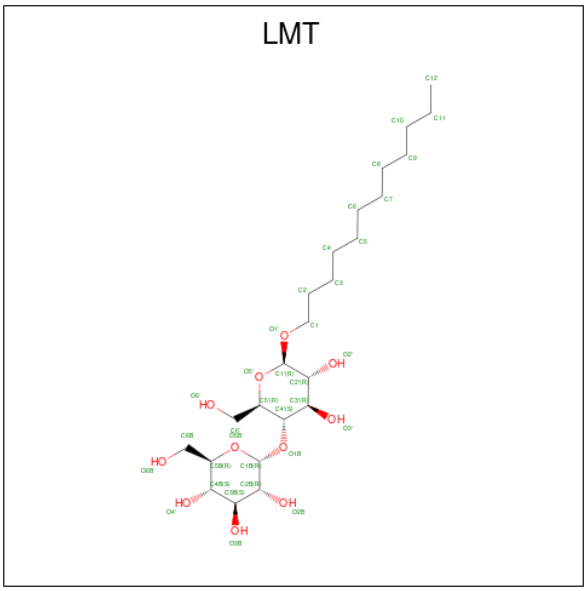
Chain	Residue	Modelled	Actual	Comment	Reference
E	-6	LEU	-	expression tag	UNP E2QH56
E	-5	VAL	-	expression tag	UNP E2QH56
E	-4	PRO	-	expression tag	UNP E2QH56
E	-3	ARG	-	expression tag	UNP E2QH56
E	-2	GLY	-	expression tag	UNP E2QH56
E	-1	SER	-	expression tag	UNP E2QH56
E	0	HIS	-	expression tag	UNP E2QH56
E	615	ALA	PHE	engineered mutation	UNP E2QH56
E	617	ALA	PHE	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	615	ALA	PHE	engineered mutation	UNP E2QH56
F	617	ALA	PHE	engineered mutation	UNP E2QH56

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



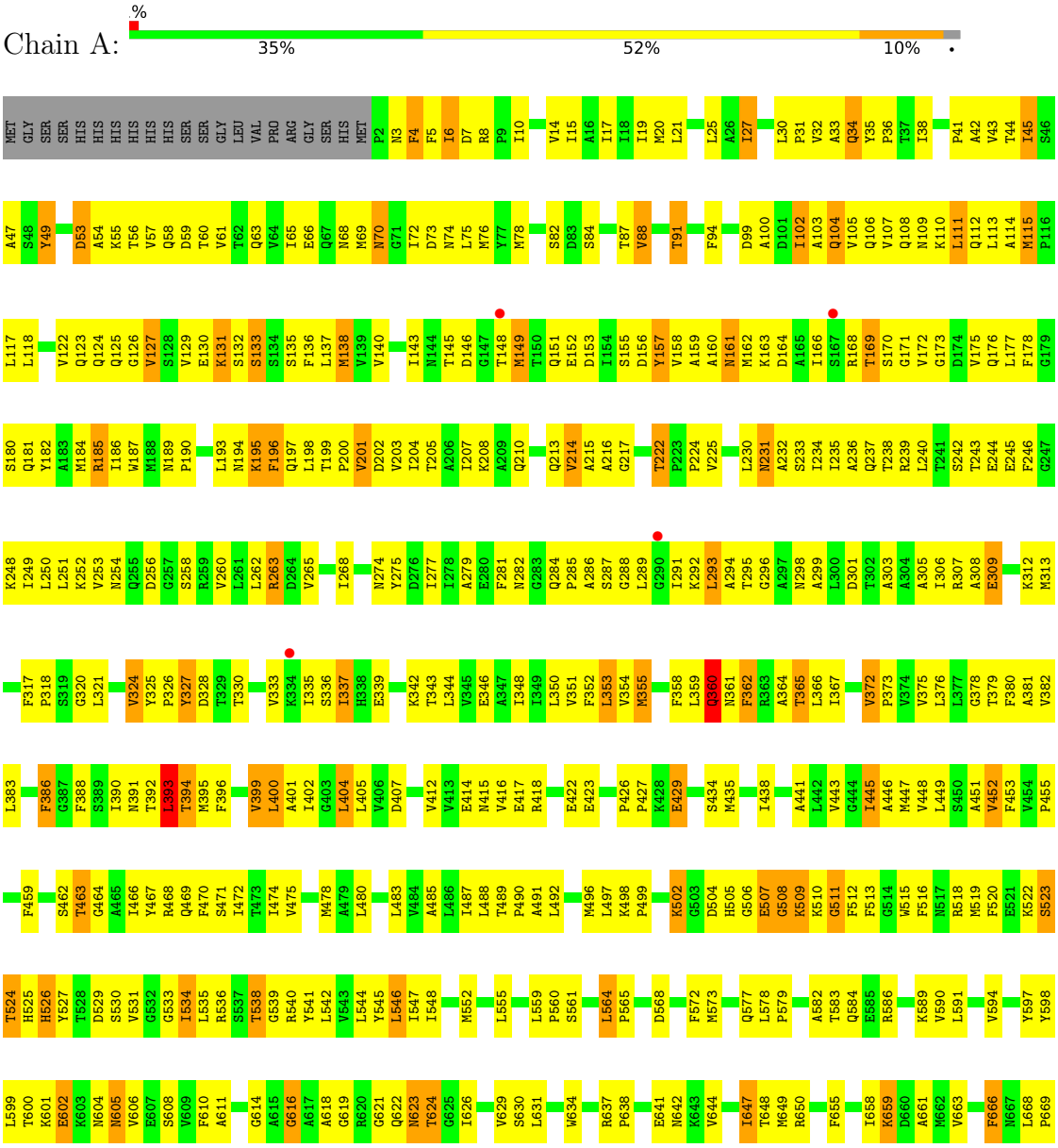
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			35	24	11		
2	B	1	Total	C	O	0	0
			35	24	11		
2	C	1	Total	C	O	0	0
			35	24	11		
2	D	1	Total	C	O	0	0
			35	24	11		
2	E	1	Total	C	O	0	0
			35	24	11		
2	F	1	Total	C	O	0	0
			35	24	11		

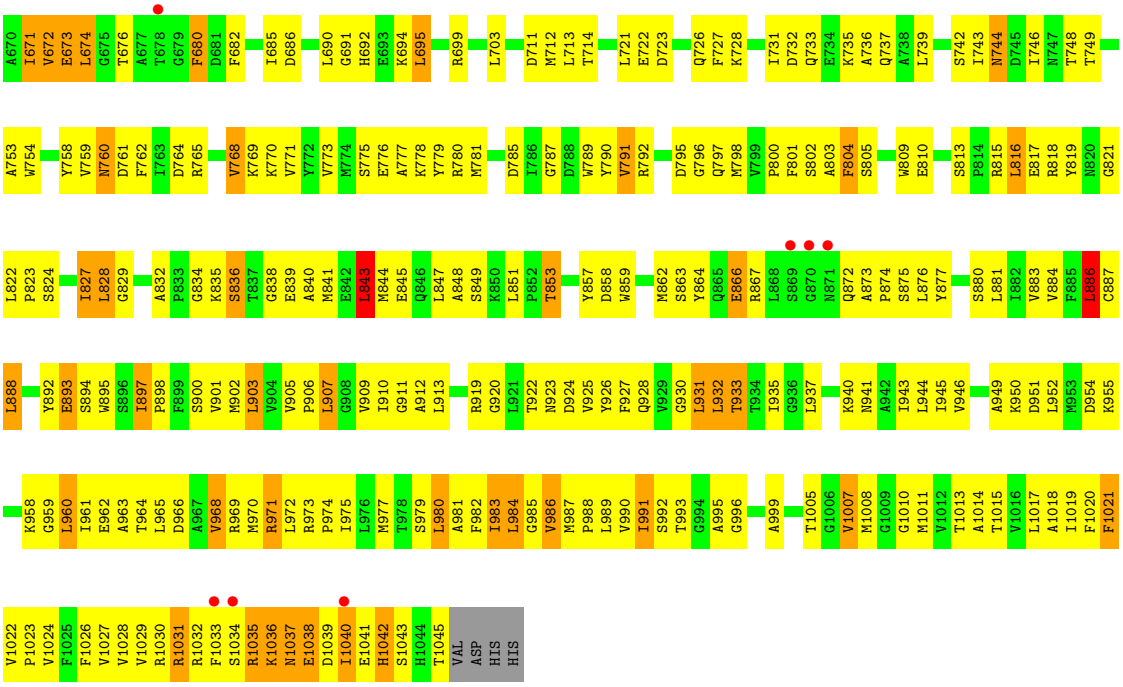
3 Residue-property plots (i)

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.

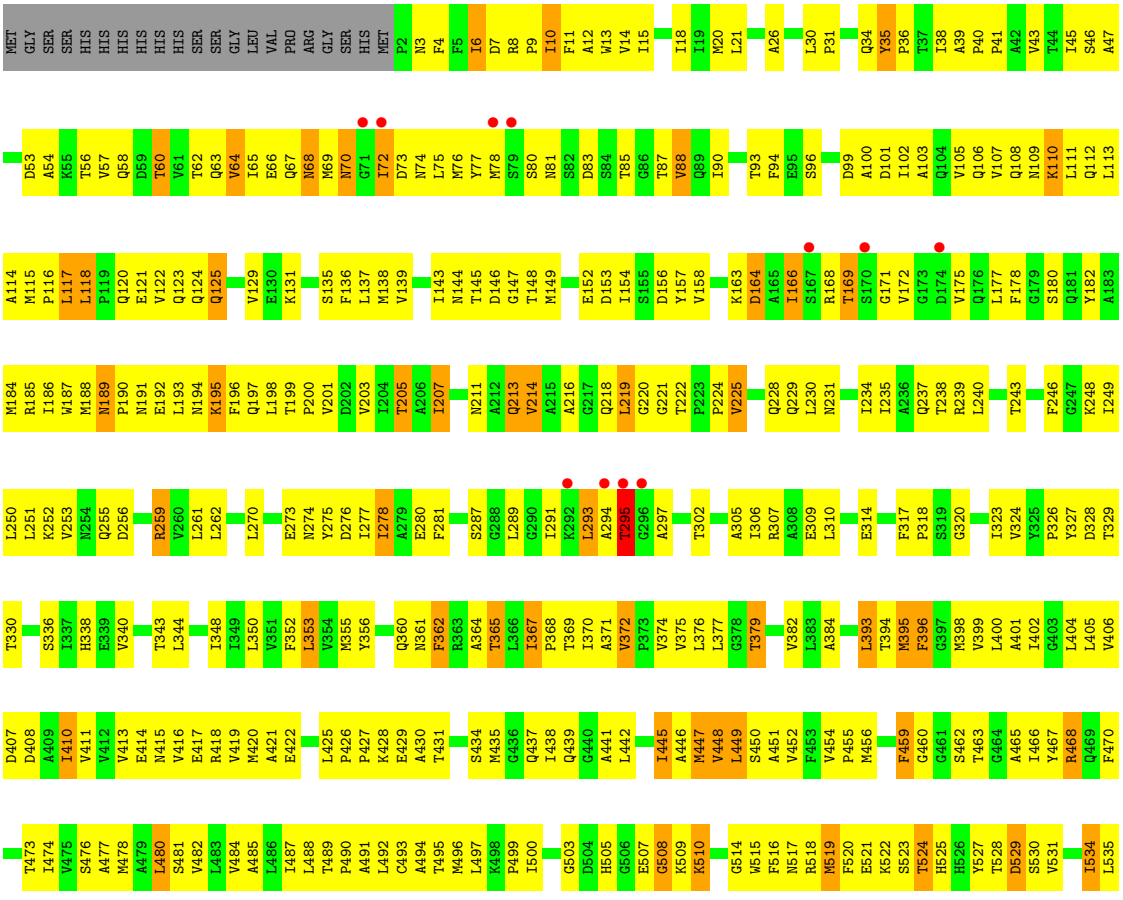
- Molecule 1: Efflux pump membrane transporter

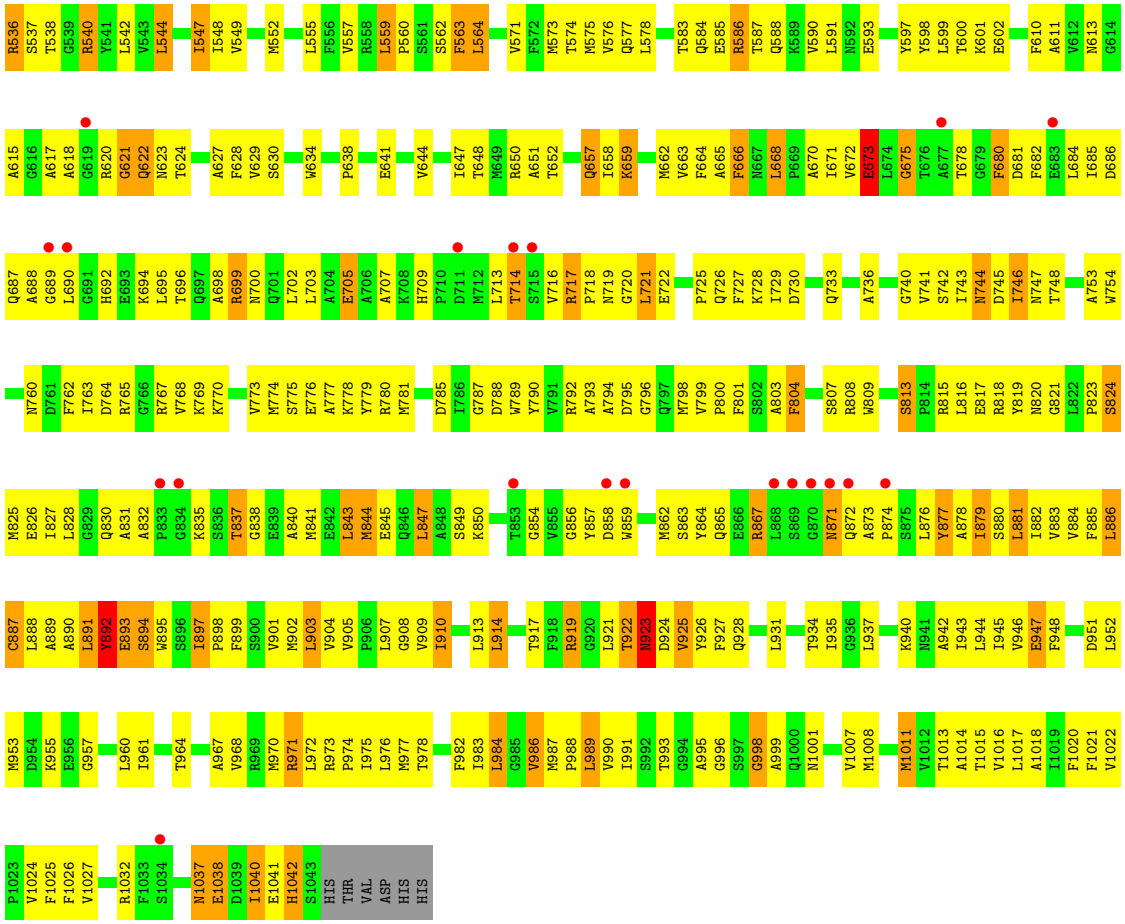
Chain A:





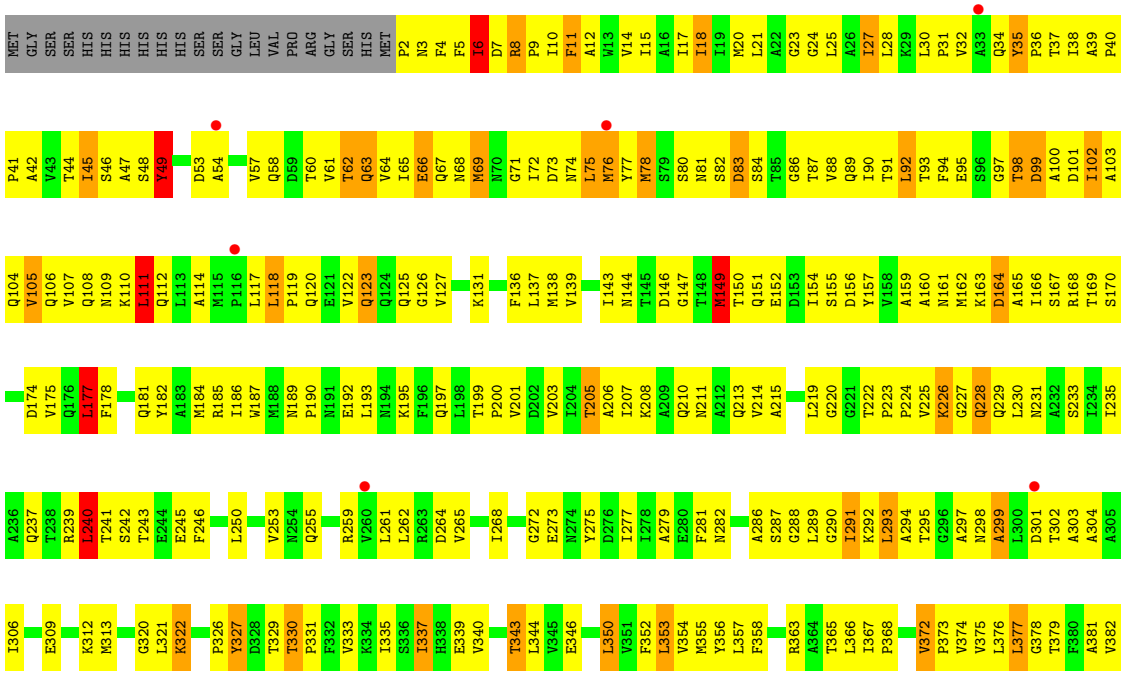
• Molecule 1: Efflux pump membrane transporter

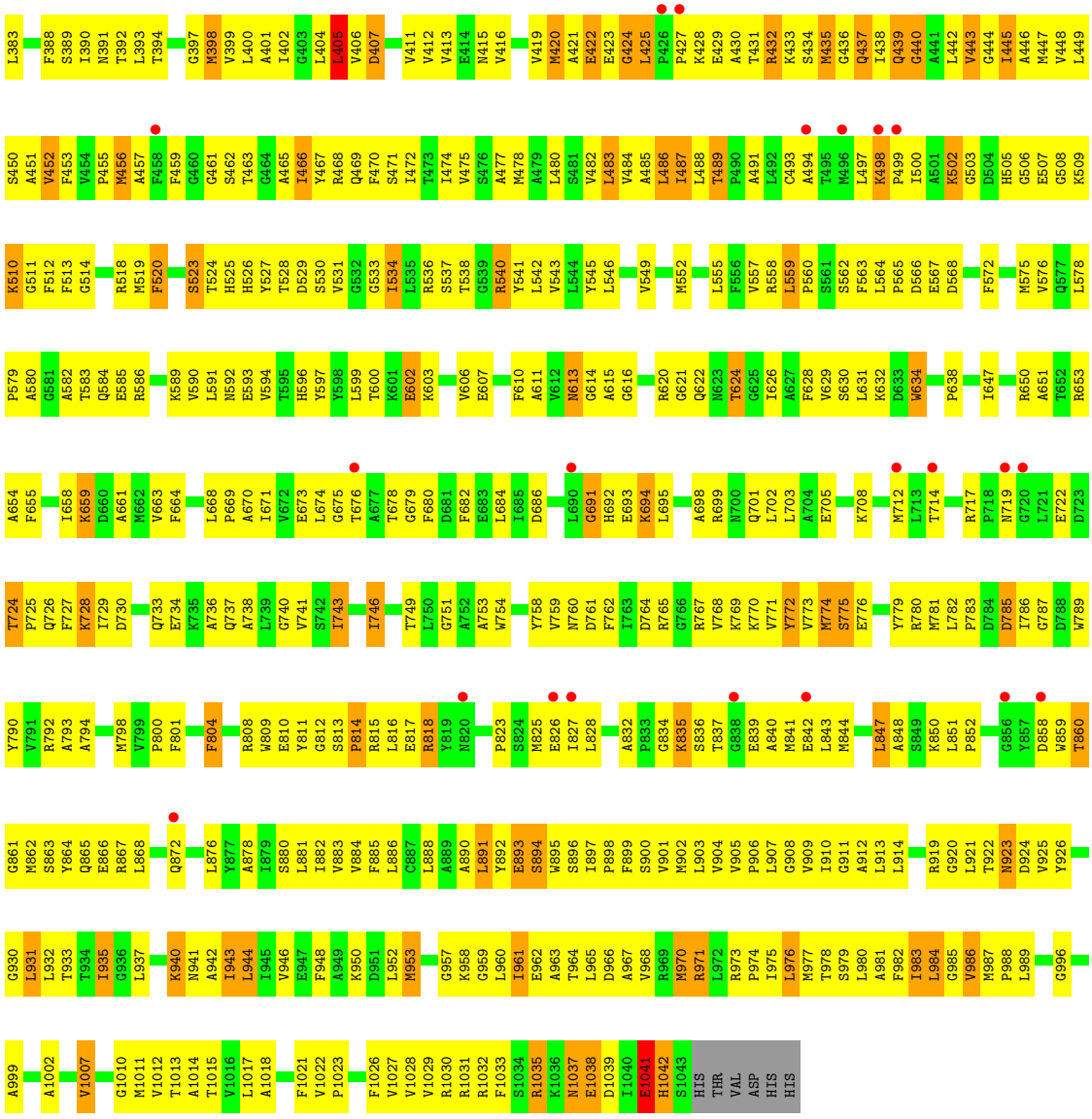




• Molecule 1: Efflux pump membrane transporter

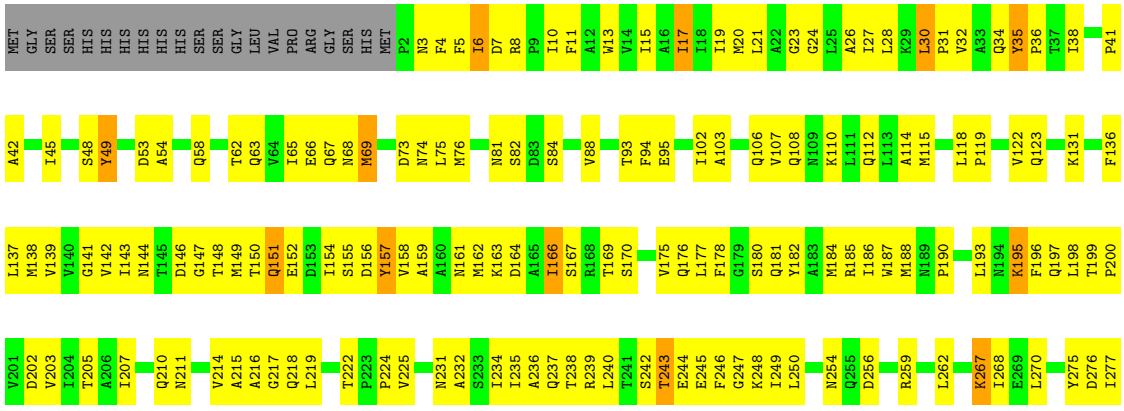
Chain C:

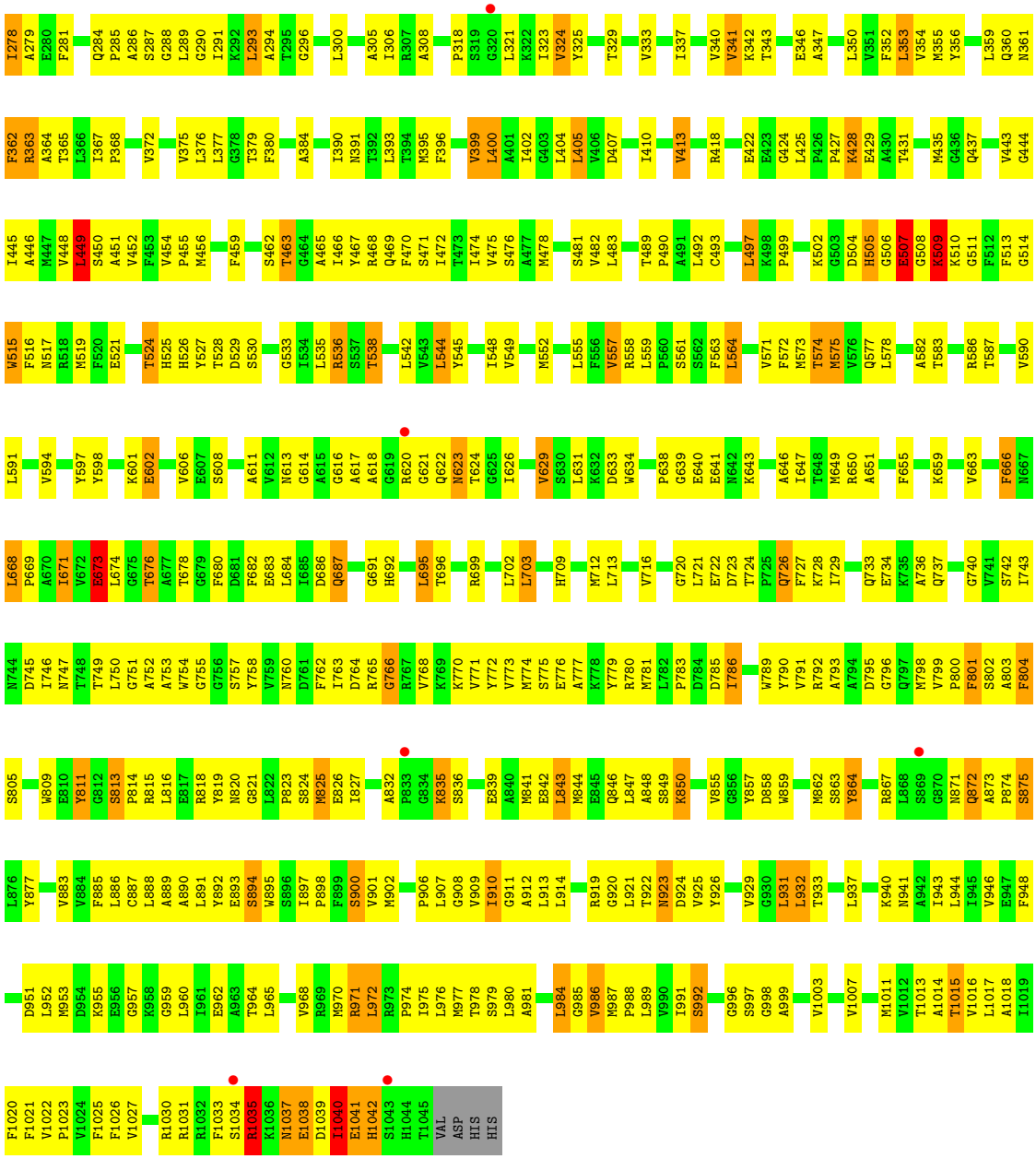




• Molecule 1: Efflux pump membrane transporter

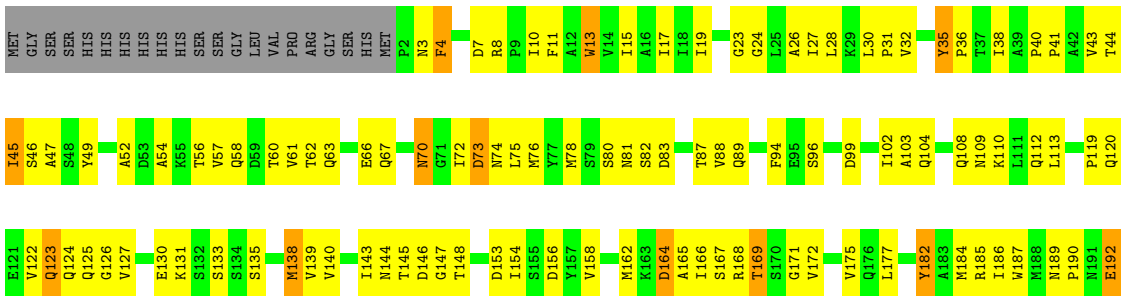
Chain D:

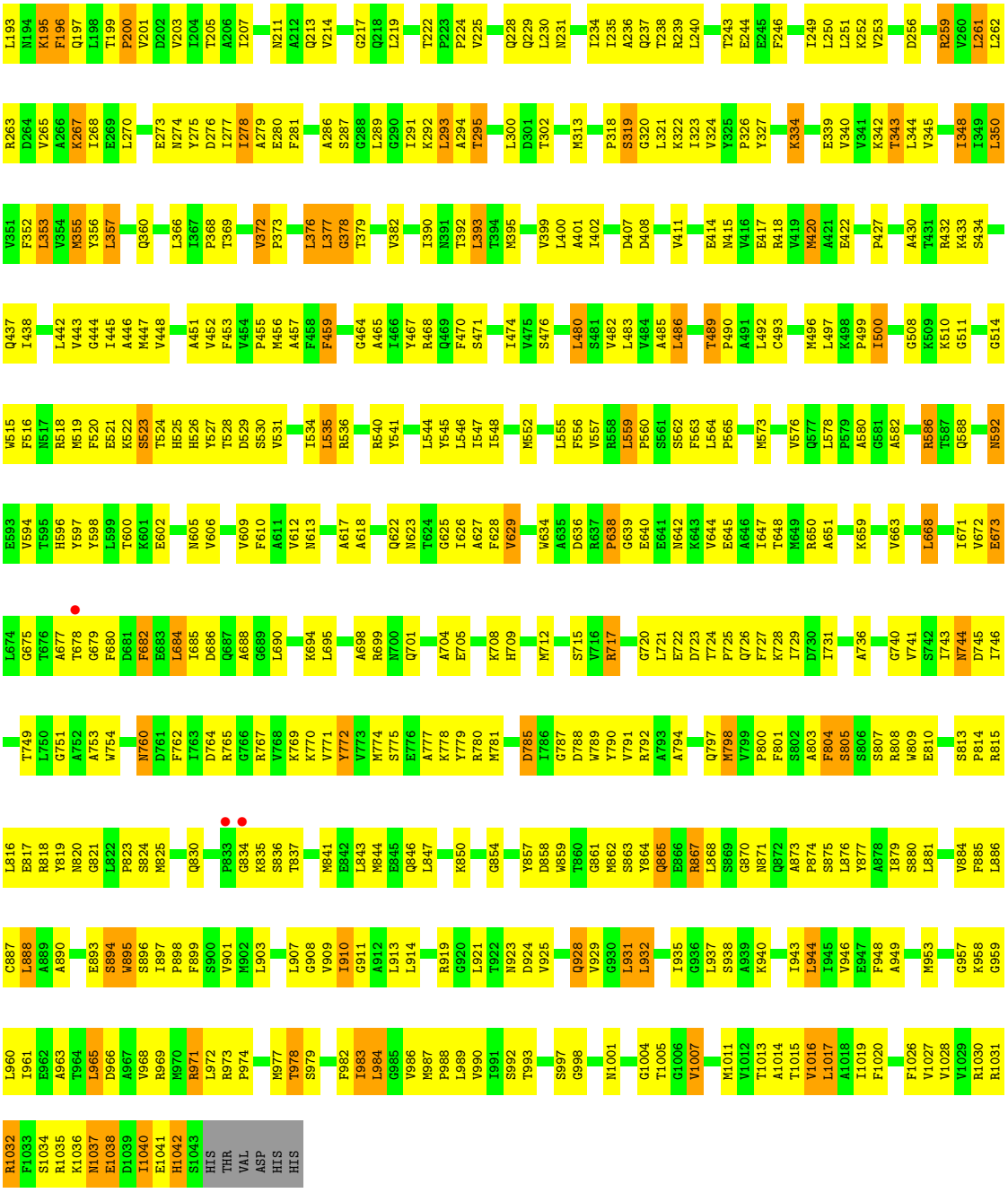




• Molecule 1: Efflux pump membrane transporter

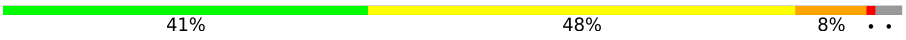
Chain E:

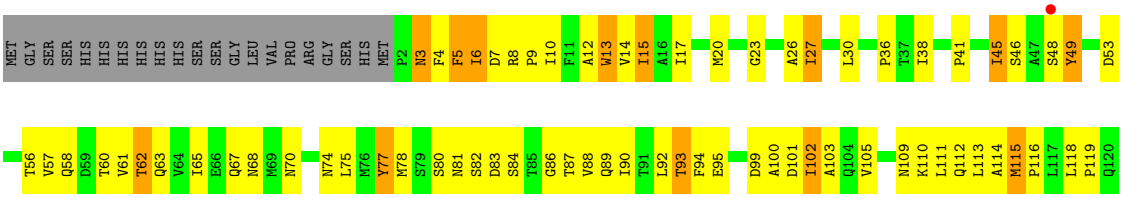


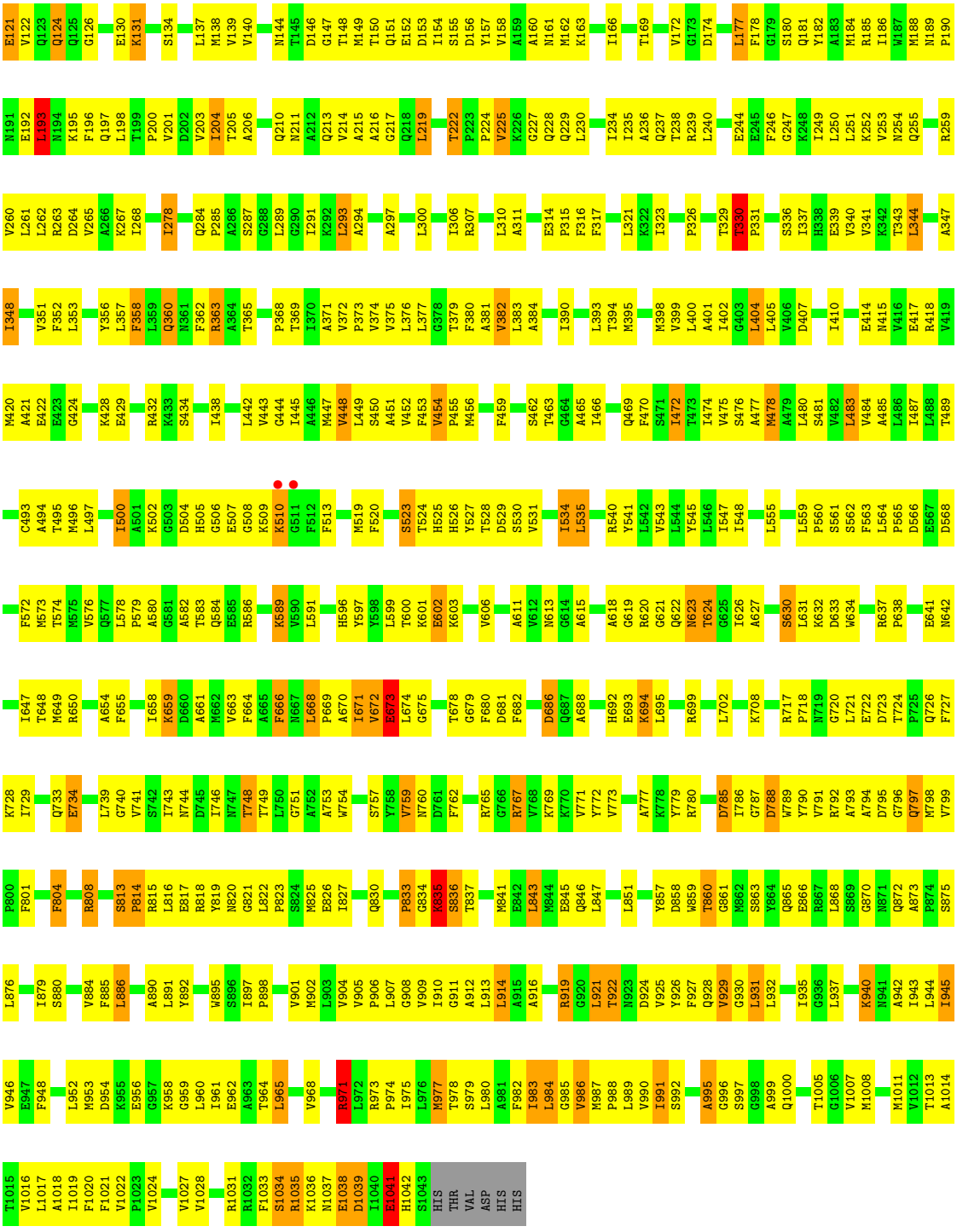


• Molecule 1: Efflux pump membrane transporter

Chain F:



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N191 E192 L193 N194 K195 F196 Q197 L198 T199 P200 V201 D202 V203 I204 T205 A206 Q210 N211 A212 Q213 V214 A215 A216 G217 Q218 L219 T222 P223 P224 V225 K226 G227 Q228 Q229 L230 I234 I235 A236 Q237 T238 R239 L240 E244 E245 F246 G247 K248 I249 L250 L251 K252 V253 N254 Q255 R259
V260 L261 L262 R263 D264 V265 A266 K267 I268 I278 Q284 P285 A286 S287 G288 L289 G290 I291 K292 L293 A294 A297 L300 I306 R307 L310 A311 E314 P315 F316 F317 L321 K322 I323 P326 T329 T330 P331 S336 I337 H338 E339 V340 V341 K342 T343 L344 A347
I348 V351 F352 L353 Y356 L357 F358 L359 Q360 N361 F362 R363 A364 T365 P368 T369 I370 A371 V372 P373 V374 V375 L376 L377 G378 T379 F380 A381 V382 L383 A384 I390 L393 T394 M395 M398 V399 L400 A401 I402 G403 L404 L405 V406 D407 I410 E414 N415 V416 E417 R418 V419
M420 A421 E422 E423 G424 K428 E429 R432 K433 S434 I438 L442 V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454 P455 M456 F459 S462 T463 G464 A465 I466 Q469 F470 S471 I472 T473 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489
C493 A494 T495 M496 L497 I500 A501 K502 G503 D504 H505 G506 E507 G508 K509 K510 G511 F512 F513 M519 F520 S523 T524 H525 H526 Y527 T528 D529 S530 V531 I534 L535 R540 Y541 L542 V543 L544 Y545 L546 I547 I548 L555 L559 P560 S561 S562 F563 L564 P565 D566 E567 D568
F572 M573 T574 M575 V576 Q577 L578 P579 A580 G581 A582 T583 Q584 E585 R586 K589 V590 L591 H596 Y597 Y598 L599 T600 K601 E602 K603 V606 A611 V612 M613 G614 A615 A618 G619 R620 G621 Q622 N623 T624 G625 I626 A627 S630 L631 K632 D633 W634 R637 P638 E641 N642
I647 T648 M649 R650 A654 F655 I658 K659 D660 A661 M662 V663 F664 A665 F666 N667 L668 P669 A670 I671 V672 E673 L674 G675 T678 G679 F680 D681 F682 D686 Q687 A688 H692 E693 K694 L695 R699 L702 K708 R717 P718 N719 G720 L721 E722 D723 T724 P725 Q726 F727
K728 I729 Q733 E734 L739 G740 V741 S742 I743 N744 D745 I746 N747 T748 T749 L750 G751 A752 A753 W754 S757 Y758 V759 N760 D761 F762 R765 G766 R767 V768 K769 K770 V771 Y772 V773 A777 K778 Y779 R780 D785 I786 G787 D788 W789 Y790 V791 R792 A793 A794 D795 G796 Q797 M798 V799
P800 F801 F804 R808 S813 P814 R815 L816 E817 R818 Y819 N820 G821 L822 P823 S824 M825 E826 I827 Q830 P833 G834 R835 S836 T837 M841 E842 L843 M844 E845 Q846 L847 L851 Y857 D858 W859 T860 G861 M862 S863 Y864 Q865 E866 R867 L868 S869 G870 N871 Q872 A873 P874 S875
L876 I879 S880 V884 F885 L886 A890 L891 Y892 W895 S896 I897 P898 V901 M902 L903 V904 V905 P906 L907 G908 V909 I910 G911 A912 L913 L914 A915 A916 R919 G920 L921 T922 N923 D924 V925 Y926 F927 Q928 V929 G930 L931 L932 I935 G936 L937 K940 N941 A942 I943 L944 I945
V946 E947 F948 L952 M953 D954 K955 E956 G957 K958 G959 L960 I961 E962 A963 T964 L965 V968 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 S992 A995 G996 S997 G998 A999 Q1000 T1005 G1006 V1007 M1008 M1011 V1012 T1013 A1014
T1015 V1016 L1017 A1018 I1019 F1020 F1021 V1022 P1023 V1024 V1027 V1028 R1031 R1032 F1033 S1034 R1035 K1036 N1037 E1038 D1039 I1040 E1041 H1042 S1043 HIS THR 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	152.15Å 156.72Å 218.75Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	19.93 – 3.53 19.93 – 3.53	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-3.53) 99.8 (19.93-3.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.264 , 0.354 0.264 , 0.354	Depositor DCC
R_{free} test set	6240 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	104.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.060 for -k,-h,-l 0.074 for k,h,-l 0.074 for h,-k,-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	47722	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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 36.61 % 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 4.8693e-04.*

[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	0.67	1/8080 (0.0%)	0.92	10/10972 (0.1%)
1	B	0.67	1/8062 (0.0%)	0.93	14/10947 (0.1%)
1	C	0.68	0/8062	0.96	20/10947 (0.2%)
1	D	0.69	1/8080 (0.0%)	0.93	11/10972 (0.1%)
1	E	0.72	1/8062 (0.0%)	0.93	8/10947 (0.1%)
1	F	0.71	0/8062	0.95	11/10947 (0.1%)
All	All	0.69	4/48408 (0.0%)	0.94	74/65732 (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	C	0	1
1	F	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	8.43	1.65	1.50
1	E	895	TRP	CB-CG	7.59	1.64	1.50
1	B	13	TRP	CB-CG	-5.38	1.40	1.50
1	A	309	GLU	CB-CG	-5.29	1.42	1.52

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	483	LEU	CA-CB-CG	-10.27	91.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	LEU	CA-CB-CG	9.16	136.36	115.30
1	A	886	LEU	CA-CB-CG	9.03	136.07	115.30
1	C	483	LEU	CA-CB-CG	-8.58	95.56	115.30
1	A	393	LEU	CA-CB-CG	8.36	134.53	115.30
1	C	49	TYR	CA-CB-CG	8.25	129.08	113.40
1	F	111	LEU	CA-CB-CG	7.96	133.61	115.30
1	C	486	LEU	CA-CB-CG	7.00	131.40	115.30
1	F	971	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	497	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	977	MET	CB-CG-SD	-6.65	92.45	112.40
1	C	976	LEU	CA-CB-CG	-6.62	100.07	115.30
1	A	400	LEU	CA-CB-CG	6.62	130.53	115.30
1	D	544	LEU	CA-CB-CG	-6.60	100.12	115.30
1	E	932	LEU	CB-CG-CD1	-6.53	99.91	111.00
1	B	877	TYR	CA-CB-CG	-6.51	101.03	113.40
1	B	118	LEU	CA-CB-CG	6.49	130.22	115.30
1	C	424	GLY	N-CA-C	6.47	129.27	113.10
1	E	357	LEU	CA-CB-CG	6.46	130.17	115.30
1	C	75	LEU	CA-CB-CG	6.45	130.13	115.30
1	D	405	LEU	CB-CG-CD2	-6.28	100.33	111.00
1	A	546	LEU	CA-CB-CG	6.27	129.73	115.30
1	A	843	LEU	CA-CB-CG	6.13	129.40	115.30
1	C	111	LEU	CA-CB-CG	6.04	129.20	115.30
1	F	921	LEU	CA-CB-CG	6.04	129.18	115.30
1	C	177	LEU	CA-CB-CG	5.96	129.01	115.30
1	B	892	TYR	CA-CB-CG	5.90	124.62	113.40
1	B	891	LEU	CA-CB-CG	-5.87	101.79	115.30
1	E	888	LEU	CA-CB-CG	-5.81	101.94	115.30
1	D	673	GLU	N-CA-C	5.79	126.65	111.00
1	B	989	LEU	CA-CB-CG	5.77	128.58	115.30
1	C	440	GLY	N-CA-C	5.77	127.53	113.10
1	D	536	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	D	932	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	932	LEU	CA-CB-CG	-5.64	102.32	115.30
1	D	449	LEU	CA-CB-CG	5.53	128.02	115.30
1	F	193	LEU	CA-CB-CG	5.50	127.95	115.30
1	B	219	LEU	CA-CB-CG	5.47	127.89	115.30
1	E	1037	ASN	C-N-CA	5.45	135.33	121.70
1	E	486	LEU	CA-CB-CG	-5.42	102.83	115.30
1	C	49	TYR	CB-CG-CD1	5.42	124.25	121.00
1	D	535	LEU	CB-CG-CD2	-5.41	101.80	111.00
1	B	998	GLY	N-CA-C	-5.41	99.58	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	355	MET	CB-CG-SD	-5.40	96.19	112.40
1	F	1038	GLU	C-N-CA	5.38	135.16	121.70
1	B	68	ASN	N-CA-C	5.37	125.51	111.00
1	C	118	LEU	CA-CB-CG	5.36	127.63	115.30
1	C	149	MET	N-CA-C	-5.33	96.60	111.00
1	C	405	LEU	CA-CB-CG	5.32	127.53	115.30
1	D	35	TYR	C-N-CD	5.31	139.55	128.40
1	B	989	LEU	CB-CG-CD1	-5.30	102.00	111.00
1	B	847	LEU	CA-CB-CG	5.27	127.43	115.30
1	F	348	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	C	439	GLN	N-CA-C	5.24	125.15	111.00
1	C	240	LEU	CA-CB-CG	5.24	127.35	115.30
1	E	350	LEU	CA-CB-CG	-5.24	103.26	115.30
1	D	755	GLY	N-CA-C	-5.21	100.07	113.10
1	C	691	GLY	N-CA-C	5.20	126.10	113.10
1	C	944	LEU	CA-CB-CG	5.20	127.25	115.30
1	D	30	LEU	CA-CB-CG	5.19	127.23	115.30
1	E	937	LEU	CA-CB-CG	-5.16	103.42	115.30
1	F	886	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	1037	ASN	C-N-CA	5.14	134.55	121.70
1	B	529	ASP	CB-CG-OD1	5.13	122.92	118.30
1	F	344	LEU	CA-CB-CG	5.12	127.08	115.30
1	E	684	LEU	CA-CB-CG	-5.12	103.53	115.30
1	C	241	THR	N-CA-C	5.12	124.81	111.00
1	F	965	LEU	CA-CB-CG	-5.11	103.54	115.30
1	B	675	GLY	N-CA-C	-5.09	100.36	113.10
1	F	971	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	118	LEU	CB-CG-CD2	-5.06	102.39	111.00
1	C	847	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	907	LEU	CA-CB-CG	5.05	126.91	115.30
1	A	828	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1041	GLU	Peptide
1	F	1041	GLU	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	7930	0	8072	634	1
1	B	7913	0	8058	686	1
1	C	7913	0	8058	747	0
1	D	7930	0	8072	547	0
1	E	7913	0	8058	494	0
1	F	7913	0	8058	571	0
2	A	35	0	46	7	0
2	B	35	0	46	3	0
2	C	35	0	46	5	0
2	D	35	0	46	4	0
2	E	35	0	46	17	0
2	F	35	0	46	2	0
All	All	47722	0	48652	3527	1

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 37.

All (3527) 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:E:536:ARG:HH21	2:E:2000:LMT:C3B	1.42	1.33
1:E:536:ARG:NE	2:E:2000:LMT:H4B	1.48	1.26
1:E:536:ARG:HE	2:E:2000:LMT:C4B	1.56	1.19
1:A:541:TYR:OH	2:A:2000:LMT:H6E	1.41	1.18
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.34	1.10
1:E:536:ARG:HH21	2:E:2000:LMT:H3B	1.14	1.09
1:B:166:ILE:HA	1:B:309:GLU:HG2	1.37	1.07
1:E:536:ARG:NH2	2:E:2000:LMT:H3B	1.71	1.05
1:E:536:ARG:HH21	2:E:2000:LMT:C2B	1.70	1.05
1:E:4:PHE:HE1	1:E:8:ARG:HD2	1.23	1.04
1:E:156:ASP:OD1	1:E:765:ARG:NH2	1.92	1.02
1:C:452:VAL:HG12	1:C:884:VAL:HG21	1.40	1.01
1:E:536:ARG:NH2	2:E:2000:LMT:C3B	2.24	1.01
1:A:45:ILE:HG23	1:A:129:VAL:HG22	1.43	1.00
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:ASN:HD21	1:A:393:LEU:HD22	1.26	1.00
1:C:905:VAL:HG23	1:C:906:PRO:HD3	1.42	0.99
1:E:376:LEU:O	1:E:378:GLY:N	1.95	0.99
1:F:352:PHE:HD1	1:F:369:THR:HG1	1.00	0.99
1:E:536:ARG:NH2	2:E:2000:LMT:O2B	1.95	0.99
1:C:63:GLN:HB2	1:C:818:ARG:HH22	1.29	0.98
1:C:525:HIS:NE2	1:C:529:ASP:OD2	1.97	0.97
1:D:781:MET:HE1	1:F:225:VAL:H	1.26	0.97
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.41	0.97
1:E:559:LEU:HD22	1:E:560:PRO:HD2	1.44	0.96
1:B:944:LEU:HD22	1:B:971:ARG:HH22	1.30	0.96
1:C:428:LYS:HG3	1:C:494:ALA:HB1	1.46	0.96
1:C:185:ARG:HD2	1:C:187:TRP:HE1	1.32	0.95
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.48	0.95
1:F:228:GLN:HE21	1:F:230:LEU:H	1.10	0.95
1:C:354:VAL:HG21	1:C:981:ALA:HA	1.51	0.93
1:C:74:ASN:O	1:C:95:GLU:N	2.01	0.93
1:A:541:TYR:HH	2:A:2000:LMT:H6E	1.34	0.92
1:B:108:GLN:HB2	1:B:129:VAL:HG11	1.52	0.92
1:E:536:ARG:HE	2:E:2000:LMT:H4B	0.76	0.91
1:E:699:ARG:HD3	1:E:825:MET:HE2	1.50	0.91
1:E:4:PHE:CE1	1:E:8:ARG:HD2	2.04	0.91
1:D:1038:GLU:HB3	1:D:1040:ILE:HA	1.51	0.91
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.52	0.90
1:B:753:ALA:O	1:B:775:SER:OG	1.86	0.90
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.50	0.90
1:B:278:ILE:HG23	1:B:613:ASN:HB3	1.51	0.90
1:D:424:GLY:HA3	1:D:502:LYS:HG2	1.54	0.90
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.03	0.90
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.51	0.90
1:B:685:ILE:HD11	1:B:819:TYR:HB3	1.53	0.89
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.53	0.89
1:C:45:ILE:HD12	1:C:90:ILE:HB	1.52	0.89
1:D:514:GLY:HA2	1:D:517:ASN:HD22	1.37	0.89
1:C:30:LEU:HD12	1:C:31:PRO:HD2	1.54	0.88
1:E:519:MET:O	1:E:523:SER:OG	1.91	0.88
1:C:350:LEU:HD23	1:C:985:GLY:HA2	1.55	0.88
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.55	0.87
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.54	0.87
1:C:228:GLN:OE1	1:C:230:LEU:N	2.07	0.87
1:C:75:LEU:HA	1:C:94:PHE:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:GLN:HE22	1:D:517:ASN:HD21	1.17	0.87
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.55	0.87
1:A:541:TYR:OH	2:A:2000:LMT:C6'	2.23	0.86
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.10	0.86
1:A:519:MET:O	1:A:523:SER:OG	1.93	0.86
1:F:578:LEU:HD12	1:F:579:PRO:HD2	1.56	0.86
1:A:968:VAL:HA	1:A:971:ARG:HH22	1.40	0.86
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	1.57	0.86
1:E:895:TRP:O	1:E:897:ILE:N	2.08	0.86
1:F:6:ILE:HG21	1:F:487:ILE:HG23	1.55	0.86
1:D:360:GLN:HE21	1:D:513:PHE:HB3	1.41	0.86
1:C:400:LEU:HD21	1:C:933:THR:HG21	1.57	0.86
1:F:38:ILE:HG23	1:F:462:SER:HB3	1.58	0.86
1:F:728:LYS:HG2	1:F:808:ARG:HH21	1.39	0.86
1:A:555:LEU:HD22	1:A:913:LEU:HB3	1.56	0.85
1:B:768:VAL:HG11	1:C:60:THR:HG23	1.57	0.85
1:A:170:SER:OG	1:B:75:LEU:N	2.09	0.85
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.58	0.85
1:C:719:ASN:ND2	1:C:817:GLU:OE1	2.10	0.85
1:F:184:MET:HB3	1:F:771:VAL:HG23	1.58	0.85
1:B:621:GLY:O	1:B:623:ASN:N	2.10	0.85
1:B:108:GLN:NE2	1:C:109:ASN:OD1	2.10	0.85
1:B:231:ASN:OD1	1:C:622:GLN:NE2	2.08	0.85
1:B:445:ILE:HG21	1:B:940:LYS:HZ2	1.40	0.85
1:F:263:ARG:NH1	1:F:264:ASP:OD1	2.10	0.85
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.10	0.84
1:C:679:GLY:HA3	1:C:837:THR:HG21	1.59	0.84
1:F:421:ALA:HB2	1:F:500:ILE:HD11	1.57	0.84
1:A:988:PRO:HA	1:A:991:ILE:HD12	1.57	0.84
1:F:65:ILE:HD11	1:F:90:ILE:HD13	1.60	0.84
1:F:692:HIS:NE2	1:F:723:ASP:OD2	2.10	0.84
1:B:115:MET:HA	1:B:118:LEU:HD13	1.60	0.84
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.60	0.83
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.60	0.83
1:F:219:LEU:H	1:F:219:LEU:HD23	1.40	0.83
1:B:376:LEU:O	1:B:379:THR:N	2.11	0.83
1:C:184:MET:HB3	1:C:771:VAL:HG23	1.60	0.83
1:A:236:ALA:O	1:B:728:LYS:NZ	2.10	0.83
1:A:293:LEU:HD22	1:A:294:ALA:H	1.42	0.83
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.61	0.82
1:A:545:TYR:OH	1:A:903:LEU:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:ILE:N	1:A:1039:ASP:OD1	2.11	0.82
1:D:73:ASP:OD2	1:D:106:GLN:NE2	2.13	0.82
1:C:792:ARG:NH1	1:C:793:ALA:O	2.12	0.82
1:B:259:ARG:H	1:B:259:ARG:HD3	1.44	0.82
1:F:455:PRO:HG2	1:F:880:SER:HA	1.61	0.82
1:A:511:GLY:O	1:A:513:PHE:N	2.12	0.82
1:B:69:MET:HA	1:B:110:LYS:HB3	1.61	0.82
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.61	0.82
1:B:404:LEU:HD22	1:B:449:LEU:HD21	1.60	0.82
1:C:58:GLN:HE21	1:C:818:ARG:HH11	1.25	0.82
1:B:934:THR:HA	1:B:937:LEU:HD12	1.61	0.81
1:C:253:VAL:HA	1:C:259:ARG:HG2	1.60	0.81
1:F:343:THR:HG21	1:F:989:LEU:HD21	1.61	0.81
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.60	0.81
1:C:424:GLY:HA3	1:C:502:LYS:HG2	1.60	0.81
1:C:94:PHE:CZ	1:C:107:VAL:HG21	2.16	0.81
1:F:740:GLY:O	1:F:794:ALA:N	2.13	0.81
1:D:671:ILE:HD13	1:D:674:LEU:H	1.46	0.81
1:A:445:ILE:HD13	1:A:940:LYS:HE2	1.62	0.81
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.62	0.81
1:B:379:THR:HA	1:B:382:VAL:HG23	1.63	0.81
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.44	0.81
1:C:391:ASN:ND2	1:C:469:GLN:OE1	2.13	0.80
1:C:693:GLU:H	1:C:694:LYS:HZ3	1.29	0.80
1:D:971:ARG:HE	1:D:974:PRO:HG2	1.46	0.80
1:F:519:MET:O	1:F:523:SER:OG	1.99	0.80
1:B:15:ILE:HD12	1:B:487:ILE:HG21	1.64	0.80
1:B:418:ARG:NH1	1:B:422:GLU:OE2	2.14	0.80
1:D:801:PHE:HA	1:D:804:PHE:HE2	1.46	0.80
1:E:668:LEU:HD23	1:E:668:LEU:H	1.45	0.80
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.63	0.80
1:B:171:GLY:O	1:B:302:THR:OG1	1.99	0.80
1:A:17:ILE:HA	1:A:20:MET:HE2	1.64	0.80
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.64	0.80
1:F:632:LYS:O	1:F:637:ARG:NH1	2.15	0.79
1:A:713:LEU:HD21	1:A:843:LEU:HD11	1.63	0.79
1:C:239:ARG:NH1	1:C:761:ASP:O	2.15	0.79
1:F:455:PRO:HB3	1:F:879:ILE:HG22	1.63	0.79
1:A:544:LEU:HA	1:A:547:ILE:HD12	1.63	0.79
1:E:193:LEU:HD23	1:E:265:VAL:HB	1.65	0.79
1:A:959:GLY:HA3	1:A:1039:ASP:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:ALA:HB3	1:D:835:LYS:HG2	1.64	0.79
1:D:888:LEU:HD22	1:D:892:TYR:HE2	1.47	0.79
1:C:760:ASN:O	1:C:771:VAL:HG12	1.82	0.78
1:F:919:ARG:HH11	1:F:919:ARG:HG3	1.47	0.78
1:A:166:ILE:HG22	1:A:175:VAL:HG21	1.64	0.78
1:A:376:LEU:O	1:A:379:THR:N	2.16	0.78
1:A:552:MET:HB2	1:A:910:ILE:HB	1.65	0.78
1:B:686:ASP:HB3	1:B:823:PRO:HB2	1.65	0.78
1:C:102:ILE:O	1:C:105:VAL:HB	1.84	0.78
1:A:427:PRO:HD3	1:A:499:PRO:HB3	1.64	0.78
1:D:203:VAL:O	1:D:207:ILE:HG12	1.84	0.78
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.17	0.78
1:C:484:VAL:HA	1:C:487:ILE:HB	1.64	0.78
1:C:564:LEU:HD12	1:C:565:PRO:HD2	1.64	0.78
1:C:584:GLN:HB2	1:C:622:GLN:HG2	1.64	0.77
1:D:508:GLY:O	1:D:510:LYS:N	2.16	0.77
1:A:30:LEU:HD23	1:A:31:PRO:HD2	1.65	0.77
1:A:163:LYS:HE3	1:A:177:LEU:HB2	1.66	0.77
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.66	0.77
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.66	0.77
1:F:428:LYS:HG3	1:F:494:ALA:HB1	1.66	0.77
1:C:615:ALA:HB2	1:C:620:ARG:HG2	1.65	0.77
1:B:68:ASN:HB2	1:B:114:ALA:HB2	1.67	0.77
1:B:907:LEU:HD23	1:B:1017:LEU:HB3	1.67	0.77
1:F:596:HIS:O	1:F:600:THR:OG1	2.03	0.77
1:A:897:ILE:O	1:A:900:SER:OG	2.01	0.77
1:B:790:TYR:HB3	1:B:798:MET:HB3	1.67	0.77
1:C:437:GLN:HG3	1:C:438:ILE:HG23	1.67	0.77
1:D:27:ILE:HG12	1:D:380:PHE:CD2	2.20	0.77
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.67	0.77
1:C:440:GLY:O	1:C:892:TYR:OH	2.02	0.77
1:E:278:ILE:HG23	1:E:613:ASN:HB3	1.67	0.77
1:F:393:LEU:HD11	1:F:466:ILE:HG12	1.67	0.77
1:A:372:VAL:HG13	1:A:373:PRO:HD3	1.66	0.77
1:C:210:GLN:NE2	1:C:250:LEU:O	2.17	0.76
1:D:623:ASN:OD1	1:D:623:ASN:N	2.10	0.76
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.20	0.76
1:A:151:GLN:HE22	1:A:279:ALA:H	1.32	0.76
1:B:445:ILE:HG21	1:B:940:LYS:NZ	2.00	0.76
1:F:375:VAL:HG22	1:F:480:LEU:HB3	1.68	0.76
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.65	0.76
1:A:1041:GLU:HG3	1:A:1042:HIS:HA	1.66	0.76
1:D:428:LYS:HZ2	1:D:428:LYS:H	1.30	0.76
1:E:1040:ILE:HG23	1:E:1042:HIS:HB2	1.66	0.76
1:F:200:PRO:HG2	1:F:749:THR:HG23	1.65	0.76
1:D:222:THR:HG22	1:E:622:GLN:NE2	2.01	0.76
1:E:231:ASN:OD1	1:F:622:GLN:NE2	2.18	0.76
1:E:536:ARG:NH2	2:E:2000:LMT:C2B	2.42	0.76
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.66	0.76
1:B:419:VAL:HA	1:B:422:GLU:HG2	1.67	0.76
1:D:197:GLN:O	1:D:792:ARG:HD3	1.86	0.76
1:D:926:TYR:HE1	1:D:999:ALA:HB1	1.51	0.76
1:F:525:HIS:NE2	1:F:529:ASP:OD2	2.18	0.76
1:B:518:ARG:O	1:B:522:LYS:N	2.14	0.76
1:B:687:GLN:HE22	1:B:856:GLY:HA3	1.49	0.76
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.65	0.76
1:F:228:GLN:NE2	1:F:230:LEU:H	1.83	0.76
1:D:776:GLU:HB3	1:D:779:TYR:HD1	1.51	0.76
1:E:94:PHE:CE2	1:E:103:ALA:HB1	2.21	0.76
1:C:186:ILE:HG12	1:C:268:ILE:HD13	1.68	0.75
1:F:360:GLN:NE2	1:F:513:PHE:O	2.19	0.75
1:A:949:ALA:HB3	1:A:1026:PHE:HE1	1.52	0.75
1:B:405:LEU:HD21	1:B:477:ALA:HB1	1.66	0.75
1:C:211:ASN:ND2	1:C:760:ASN:HD21	1.85	0.75
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.50	0.75
1:C:536:ARG:NH1	2:C:2000:LMT:H3B	2.01	0.75
1:E:139:VAL:HB	1:E:327:TYR:HB3	1.69	0.75
1:B:519:MET:N	1:B:519:MET:SD	2.55	0.75
1:B:66:GLU:HG3	1:B:818:ARG:NH2	2.01	0.75
1:B:641:GLU:HB2	1:B:650:ARG:HH22	1.51	0.75
1:C:368:PRO:HG3	1:C:413:VAL:HG21	1.69	0.75
1:E:944:LEU:HD12	1:E:971:ARG:HH21	1.50	0.75
1:B:80:SER:HB3	1:B:818:ARG:HB2	1.68	0.75
1:B:885:PHE:HB2	1:B:902:MET:SD	2.26	0.75
1:B:703:LEU:HG	1:B:716:VAL:HG12	1.68	0.75
1:C:572:PHE:HD2	1:C:631:LEU:HD11	1.52	0.74
1:D:425:LEU:HB3	1:D:429:GLU:HG3	1.69	0.74
1:F:156:ASP:OD2	1:F:769:LYS:NZ	2.19	0.74
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.03	0.74
1:E:536:ARG:CZ	2:E:2000:LMT:H4B	2.17	0.74
1:A:105:VAL:HG11	1:B:105:VAL:HG12	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ALA:HB1	1:A:883:VAL:HG13	1.68	0.74
1:F:144:ASN:O	1:F:284:GLN:NE2	2.20	0.74
1:A:110:LYS:HE3	1:A:113:LEU:HD12	1.67	0.74
1:B:400:LEU:HD11	1:B:1007:VAL:HG21	1.68	0.74
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.17	0.74
1:D:428:LYS:H	1:D:428:LYS:NZ	1.85	0.74
1:D:736:ALA:HB2	1:D:804:PHE:HD1	1.52	0.74
1:E:81:ASN:OD1	1:E:815:ARG:NH2	2.20	0.74
1:E:83:ASP:OD1	1:E:815:ARG:NH1	2.21	0.74
1:D:67:GLN:OE1	1:F:767:ARG:NH2	2.20	0.74
1:D:734:GLU:OE1	1:F:259:ARG:NH2	2.20	0.74
1:A:776:GLU:HB3	1:A:779:TYR:HD1	1.51	0.74
1:A:886:LEU:HD23	1:C:14:VAL:HG13	1.69	0.74
1:F:948:PHE:CE2	1:F:971:ARG:HG3	2.22	0.74
1:E:717:ARG:HG2	1:E:717:ARG:HH11	1.53	0.74
1:E:671:ILE:HG22	1:E:673:GLU:H	1.52	0.74
1:F:211:ASN:O	1:F:760:ASN:ND2	2.20	0.74
1:A:1013:THR:O	1:A:1017:LEU:HB2	1.88	0.74
1:A:391:ASN:ND2	1:A:393:LEU:HD22	2.03	0.73
1:D:1037:ASN:HA	1:D:1038:GLU:HB2	1.69	0.73
1:D:1039:ASP:N	1:D:1040:ILE:HB	2.03	0.73
1:E:146:ASP:O	1:E:148:THR:N	2.22	0.73
1:A:776:GLU:HB3	1:A:779:TYR:CD1	2.24	0.73
1:B:482:VAL:O	1:B:485:ALA:HB3	1.89	0.73
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.68	0.73
1:E:924:ASP:O	1:E:928:GLN:NE2	2.19	0.73
1:D:157:TYR:HE1	1:D:318:PRO:HD3	1.51	0.73
1:B:228:GLN:HE21	1:B:230:LEU:H	1.34	0.73
1:A:445:ILE:HG13	1:A:446:ALA:N	2.03	0.73
1:C:754:TRP:CH2	1:C:780:ARG:HA	2.23	0.73
1:D:846:GLN:O	1:D:849:SER:OG	2.07	0.73
1:E:153:ASP:OD2	1:E:182:TYR:OH	2.05	0.73
1:F:222:THR:HA	1:F:224:PRO:HD3	1.71	0.73
1:C:108:GLN:O	1:C:112:GLN:NE2	2.22	0.73
1:E:234:ILE:HG23	1:F:729:ILE:HD13	1.69	0.73
1:F:576:VAL:HG23	1:F:663:VAL:HG22	1.70	0.73
1:A:68:ASN:HB2	1:A:114:ALA:HB2	1.70	0.72
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.70	0.72
1:D:170:SER:OG	1:E:74:ASN:N	2.21	0.72
1:F:450:SER:HB2	1:F:475:VAL:HG13	1.70	0.72
1:B:83:ASP:HB3	1:B:85:THR:HG22	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:ILE:O	1:B:947:GLU:HB3	1.89	0.72
1:C:910:ILE:O	1:C:914:LEU:HB2	1.89	0.72
1:E:7:ASP:OD2	1:E:432:ARG:NH2	2.21	0.72
1:F:858:ASP:OD2	1:F:859:TRP:N	2.23	0.72
1:C:527:TYR:O	1:C:531:VAL:HG23	1.89	0.72
1:D:222:THR:HG22	1:E:622:GLN:HE21	1.54	0.72
1:F:792:ARG:NH1	1:F:793:ALA:O	2.23	0.72
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.71	0.72
1:B:153:ASP:OD2	1:B:182:TYR:OH	2.05	0.72
1:D:5:PHE:HA	1:D:8:ARG:HB2	1.71	0.72
1:E:907:LEU:HD23	1:E:1017:LEU:HB3	1.71	0.72
1:F:680:PHE:HB2	1:F:859:TRP:HZ3	1.55	0.72
1:D:971:ARG:HG3	1:D:971:ARG:HH11	1.54	0.72
1:F:151:GLN:O	1:F:155:SER:OG	2.02	0.72
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.71	0.71
1:B:83:ASP:OD1	1:B:815:ARG:NH1	2.22	0.71
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.20	0.71
1:C:72:ILE:HD12	1:C:75:LEU:HD22	1.71	0.71
1:B:67:GLN:O	1:B:70:ASN:ND2	2.22	0.71
1:E:417:GLU:OE2	1:E:497:LEU:HD11	1.90	0.71
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.72	0.71
1:A:375:VAL:O	1:A:379:THR:OG1	2.07	0.71
1:D:152:GLU:HB3	1:D:182:TYR:HE1	1.54	0.71
1:D:267:LYS:NZ	1:D:268:ILE:H	1.88	0.71
1:E:563:PHE:O	1:E:564:LEU:HD12	1.90	0.71
2:E:2000:LMT:O4'	2:E:2000:LMT:O6B	2.03	0.71
1:F:672:VAL:O	1:F:674:LEU:N	2.15	0.71
1:F:910:ILE:O	1:F:914:LEU:HB2	1.90	0.71
1:C:190:PRO:HG3	1:C:779:TYR:CG	2.26	0.71
1:C:463:THR:HA	1:C:466:ILE:HG12	1.73	0.71
1:D:216:ALA:HB1	1:D:234:ILE:HG22	1.72	0.71
1:E:339:GLU:O	1:E:343:THR:HG22	1.90	0.71
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.71	0.71
1:D:427:PRO:HB2	1:D:428:LYS:HE3	1.72	0.71
1:D:959:GLY:HA2	1:D:1040:ILE:HG12	1.72	0.71
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.25	0.71
1:A:435:MET:SD	1:A:490:PRO:HB3	2.30	0.71
1:A:605:ASN:HD22	1:A:647:ILE:HD11	1.54	0.71
1:B:66:GLU:HG3	1:B:818:ARG:HH21	1.54	0.71
1:B:525:HIS:HA	1:B:528:THR:HG22	1.72	0.71
1:C:65:ILE:HD11	1:C:118:LEU:HD21	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:922:THR:O	1:B:924:ASP:N	2.22	0.71
1:C:226:LYS:HD3	1:C:226:LYS:H	1.55	0.71
1:F:584:GLN:HB2	1:F:622:GLN:HG2	1.72	0.71
1:E:445:ILE:HD13	1:E:940:LYS:HE3	1.73	0.71
1:B:536:ARG:HG3	1:B:536:ARG:HH21	1.56	0.70
1:B:937:LEU:HD13	1:B:1011:MET:HG2	1.73	0.70
1:C:53:ASP:OD1	1:C:53:ASP:N	2.22	0.70
1:E:239:ARG:NH2	1:F:49:TYR:OH	2.23	0.70
1:F:531:VAL:O	1:F:534:ILE:HG13	1.90	0.70
1:F:791:VAL:HG23	1:F:801:PHE:HE1	1.54	0.70
1:A:619:GLY:H	1:A:815:ARG:NH2	1.89	0.70
1:A:944:LEU:HB3	1:A:971:ARG:HD2	1.72	0.70
1:B:767:ARG:HH21	1:C:117:LEU:HD11	1.56	0.70
1:E:76:MET:SD	1:E:864:TYR:HE2	2.13	0.70
1:A:753:ALA:O	1:A:775:SER:OG	2.01	0.70
1:A:743:ILE:O	1:A:746:ILE:HG12	1.91	0.70
1:E:447:MET:HB3	1:E:887:CYS:SG	2.31	0.70
1:A:884:VAL:O	1:A:888:LEU:HD22	1.90	0.70
1:C:144:ASN:HA	1:C:320:GLY:O	1.91	0.70
1:F:5:PHE:O	1:F:7:ASP:N	2.24	0.70
1:F:658:ILE:O	1:F:659:LYS:NZ	2.16	0.70
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.74	0.70
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.72	0.70
1:F:375:VAL:O	1:F:379:THR:N	2.23	0.70
1:A:880:SER:O	1:A:884:VAL:HG12	1.91	0.70
1:B:775:SER:OG	1:B:780:ARG:HG2	1.91	0.70
1:C:69:MET:SD	1:C:92:LEU:HG	2.32	0.70
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.73	0.70
1:D:110:LYS:NZ	1:F:130:GLU:OE1	2.21	0.70
1:E:598:TYR:HB3	1:E:606:VAL:HG21	1.74	0.70
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.72	0.70
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.57	0.70
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.24	0.70
1:C:38:ILE:HG12	1:C:462:SER:HB3	1.74	0.70
1:C:536:ARG:HD2	2:C:2000:LMT:O4'	1.92	0.70
1:B:43:VAL:HG22	1:B:131:LYS:HA	1.74	0.69
1:B:451:ALA:O	1:B:883:VAL:HG11	1.92	0.69
1:D:768:VAL:HG12	1:E:63:GLN:HG2	1.71	0.69
1:F:373:PRO:O	1:F:377:LEU:N	2.23	0.69
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.07	0.69
1:C:222:THR:HA	1:C:224:PRO:HD3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:596:HIS:O	1:C:600:THR:OG1	2.06	0.69
1:A:840:ALA:HA	1:A:843:LEU:HD12	1.73	0.69
1:A:986:VAL:HG21	1:A:1007:VAL:HG11	1.72	0.69
1:C:376:LEU:O	1:C:379:THR:N	2.24	0.69
1:C:493:CYS:O	1:C:497:LEU:HB3	1.92	0.69
1:C:593:GLU:OE1	1:C:659:LYS:NZ	2.25	0.69
1:D:354:VAL:HG21	1:D:981:ALA:HA	1.74	0.69
1:F:75:LEU:HA	1:F:94:PHE:HD1	1.57	0.69
1:B:445:ILE:HG13	1:B:446:ALA:N	2.08	0.69
1:B:680:PHE:HB2	1:B:859:TRP:HZ3	1.57	0.69
1:C:20:MET:HG2	1:C:374:VAL:HA	1.73	0.69
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.74	0.69
1:C:576:VAL:HG23	1:C:663:VAL:HG22	1.74	0.69
1:C:81:ASN:HB2	1:C:89:GLN:HB2	1.75	0.69
1:C:545:TYR:HB2	1:C:1021:PHE:HE2	1.57	0.69
1:A:407:ASP:OD2	1:A:940:LYS:HE3	1.92	0.69
1:C:401:ALA:HA	1:C:474:ILE:HG23	1.73	0.69
1:E:175:VAL:HG22	1:F:70:ASN:ND2	2.08	0.69
1:F:348:ILE:HG12	1:F:402:ILE:HD13	1.73	0.69
1:B:120:GLN:HA	1:B:123:GLN:HB2	1.73	0.69
1:B:583:THR:HG23	1:B:585:GLU:H	1.58	0.69
1:A:125:GLN:OE1	1:A:770:LYS:NZ	2.26	0.69
1:A:726:GLN:HB3	1:C:235:ILE:HD11	1.73	0.69
1:B:996:GLY:O	1:B:999:ALA:N	2.26	0.69
1:C:156:ASP:OD1	1:C:765:ARG:NH2	2.26	0.69
1:C:375:VAL:HG22	1:C:480:LEU:HB3	1.72	0.69
1:C:393:LEU:HB3	1:C:466:ILE:HG23	1.75	0.69
1:E:293:LEU:HD22	1:E:294:ALA:H	1.58	0.69
1:A:160:ALA:C	1:A:161:ASN:HD22	1.96	0.69
1:B:740:GLY:O	1:B:794:ALA:N	2.23	0.69
1:C:47:ALA:HB2	1:C:127:VAL:HG13	1.74	0.69
1:C:971:ARG:HB3	1:C:971:ARG:HH11	1.58	0.69
1:D:158:VAL:HG22	1:D:162:MET:HE3	1.75	0.69
1:D:513:PHE:O	1:D:516:PHE:HB3	1.92	0.69
1:E:211:ASN:O	1:E:760:ASN:ND2	2.26	0.69
1:F:795:ASP:OD2	1:F:797:GLN:HG3	1.93	0.69
1:E:112:GLN:NE2	1:F:112:GLN:OE1	2.26	0.69
1:B:420:MET:HE1	1:B:499:PRO:HA	1.74	0.68
1:D:910:ILE:HG23	1:D:1013:THR:HG21	1.74	0.68
1:F:534:ILE:HG22	1:F:541:TYR:CE2	2.28	0.68
1:B:727:PHE:HB2	1:B:809:TRP:CZ3	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:GLY:HA3	1:C:378:GLY:HA2	1.73	0.68
1:D:743:ILE:HG23	1:D:746:ILE:HD12	1.75	0.68
1:D:979:SER:OG	1:D:1015:THR:HG21	1.93	0.68
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.76	0.68
1:F:555:LEU:HD22	1:F:913:LEU:HB3	1.73	0.68
1:A:367:ILE:HG12	1:A:496:MET:SD	2.34	0.68
1:F:261:LEU:N	1:F:264:ASP:OD2	2.25	0.68
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.08	0.68
1:A:350:LEU:HD11	1:A:984:LEU:HB3	1.75	0.68
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.22	0.68
1:B:441:ALA:O	1:B:445:ILE:HG23	1.93	0.68
1:F:591:LEU:HD13	1:F:611:ALA:HB1	1.76	0.68
1:B:421:ALA:O	1:B:503:GLY:N	2.26	0.68
1:D:781:MET:HB3	1:F:228:GLN:OE1	1.93	0.68
1:E:139:VAL:O	1:E:326:PRO:HD2	1.93	0.68
1:F:344:LEU:HA	1:F:399:VAL:HG22	1.74	0.68
1:A:614:GLY:O	1:A:621:GLY:N	2.25	0.68
1:D:445:ILE:O	1:D:449:LEU:HB2	1.93	0.68
1:B:919:ARG:NH2	1:B:1001:ASN:OD1	2.24	0.68
1:F:449:LEU:HD21	1:F:937:LEU:HD23	1.75	0.68
1:B:280:GLU:OE1	1:B:588:GLN:NE2	2.27	0.68
1:C:698:ALA:O	1:C:701:GLN:HB3	1.93	0.68
1:D:139:VAL:HG22	1:D:290:GLY:HA2	1.76	0.68
1:E:47:ALA:HB2	1:E:127:VAL:HG13	1.75	0.68
1:E:740:GLY:O	1:E:794:ALA:N	2.25	0.68
1:E:971:ARG:NH1	1:E:974:PRO:HG3	2.09	0.68
1:C:885:PHE:HD2	1:C:886:LEU:HD22	1.57	0.68
1:A:225:VAL:H	1:B:781:MET:HE1	1.58	0.68
1:A:895:TRP:CZ2	1:C:10:ILE:HG13	2.29	0.68
1:E:588:GLN:HB2	1:E:613:ASN:ND2	2.09	0.68
1:A:225:VAL:HG22	1:B:781:MET:HE1	1.76	0.67
1:B:447:MET:HB3	1:B:887:CYS:SG	2.33	0.67
1:C:393:LEU:HD22	1:C:393:LEU:H	1.60	0.67
1:C:101:ASP:O	1:C:105:VAL:HG23	1.93	0.67
1:D:445:ILE:HG22	1:D:943:ILE:HG21	1.74	0.67
1:E:171:GLY:O	1:E:302:THR:OG1	2.10	0.67
1:F:94:PHE:CE2	1:F:103:ALA:HB1	2.29	0.67
1:F:760:ASN:O	1:F:771:VAL:HG12	1.94	0.67
1:A:668:LEU:HD23	1:A:668:LEU:H	1.58	0.67
1:C:405:LEU:HD22	1:C:477:ALA:HB1	1.75	0.67
1:D:362:PHE:HB2	1:D:363:ARG:NH1	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:O	1:A:530:SER:OG	2.12	0.67
1:D:428:LYS:H	1:D:428:LYS:CE	2.08	0.67
1:D:960:LEU:HD21	1:D:1027:VAL:HG13	1.76	0.67
1:E:846:GLN:O	1:E:850:LYS:NZ	2.22	0.67
1:E:858:ASP:OD1	1:E:859:TRP:N	2.27	0.67
1:A:186:ILE:HG12	1:A:268:ILE:HD13	1.76	0.67
1:C:686:ASP:OD2	1:C:823:PRO:HD2	1.95	0.67
1:C:758:TYR:CD1	1:C:770:LYS:HD3	2.30	0.67
1:C:971:ARG:HB3	1:C:971:ARG:NH1	2.10	0.67
1:D:6:ILE:HG12	1:D:7:ASP:N	2.10	0.67
1:E:743:ILE:HA	1:E:746:ILE:HG12	1.75	0.67
1:A:200:PRO:HB2	1:A:749:THR:HG22	1.76	0.67
1:C:451:ALA:HB3	1:C:884:VAL:HG22	1.77	0.67
1:D:157:TYR:CE1	1:D:318:PRO:HD3	2.29	0.67
1:D:277:ILE:HG13	1:D:614:GLY:HA3	1.76	0.67
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.75	0.67
1:E:800:PRO:HG2	1:E:803:ALA:HB2	1.77	0.67
1:A:112:GLN:HA	1:A:115:MET:HB2	1.77	0.67
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.77	0.67
1:D:713:LEU:HD11	1:D:843:LEU:HD12	1.76	0.67
1:D:890:ALA:HB2	1:F:14:VAL:HG11	1.76	0.67
1:F:520:PHE:O	1:F:524:THR:HG22	1.95	0.67
1:F:995:ALA:O	1:F:997:SER:N	2.28	0.67
1:C:250:LEU:HA	1:C:261:LEU:HD22	1.77	0.67
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.76	0.67
1:A:858:ASP:OD2	1:A:859:TRP:N	2.28	0.66
1:A:919:ARG:NH1	1:A:990:VAL:O	2.21	0.66
1:C:693:GLU:H	1:C:694:LYS:NZ	1.92	0.66
1:C:948:PHE:O	1:C:952:LEU:HG	1.94	0.66
1:E:267:LYS:N	1:E:267:LYS:HD2	2.10	0.66
1:F:83:ASP:HB3	1:F:87:THR:O	1.95	0.66
1:A:182:TYR:HB2	1:A:769:LYS:NZ	2.10	0.66
1:A:508:GLY:H	1:A:518:ARG:HG3	1.61	0.66
1:B:166:ILE:HG12	1:B:310:LEU:HD22	1.76	0.66
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.77	0.66
1:D:727:PHE:HB2	1:D:809:TRP:CZ3	2.30	0.66
1:A:122:VAL:O	1:A:125:GLN:N	2.29	0.66
1:B:197:GLN:NE2	1:B:796:GLY:O	2.27	0.66
1:F:414:GLU:HG2	1:F:973:ARG:HH21	1.60	0.66
1:F:699:ARG:HE	1:F:718:PRO:HB3	1.60	0.66
1:A:401:ALA:HB2	1:A:474:ILE:HG23	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:LEU:HG	1:C:466:ILE:HD12	1.76	0.66
1:C:453:PHE:HE2	1:C:474:ILE:HB	1.58	0.66
1:D:801:PHE:HA	1:D:804:PHE:CE2	2.30	0.66
1:E:238:THR:OG1	1:F:728:LYS:NZ	2.29	0.66
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.77	0.66
1:E:997:SER:O	1:E:1001:ASN:ND2	2.27	0.66
1:B:222:THR:HA	1:B:224:PRO:HD3	1.77	0.66
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.77	0.66
1:D:277:ILE:HD13	1:D:620:ARG:HH21	1.60	0.66
1:D:724:THR:O	1:D:726:GLN:NE2	2.29	0.66
1:C:58:GLN:HE21	1:C:818:ARG:NH1	1.94	0.66
1:E:420:MET:HE1	1:E:499:PRO:HA	1.76	0.66
1:F:733:GLN:HE22	1:F:743:ILE:HD13	1.61	0.66
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.78	0.66
1:D:1035:ARG:NE	1:D:1035:ARG:HA	2.11	0.66
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.76	0.66
1:A:203:VAL:O	1:A:207:ILE:HG13	1.94	0.66
1:A:447:MET:HB3	1:A:887:CYS:SG	2.36	0.66
1:B:894:SER:HB2	1:B:897:ILE:HD11	1.78	0.66
1:D:960:LEU:HD23	1:D:1031:ARG:HH21	1.61	0.66
1:E:863:SER:O	1:E:867:ARG:HB2	1.95	0.66
1:A:952:LEU:HB2	1:A:963:ALA:HB1	1.77	0.65
2:A:2000:LMT:O6B	2:A:2000:LMT:O4'	2.12	0.65
1:F:81:ASN:OD1	1:F:815:ARG:NH1	2.28	0.65
1:B:507:GLU:HB3	1:B:518:ARG:HG2	1.78	0.65
1:C:201:VAL:O	1:C:205:THR:OG1	2.13	0.65
1:C:400:LEU:O	1:C:400:LEU:HD13	1.97	0.65
1:C:519:MET:O	1:C:523:SER:OG	2.13	0.65
1:C:905:VAL:CG2	1:C:906:PRO:HD3	2.24	0.65
1:B:485:ALA:HA	1:B:489:THR:OG1	1.96	0.65
1:D:953:MET:SD	1:D:1037:ASN:ND2	2.69	0.65
1:F:23:GLY:HA3	1:F:377:LEU:O	1.95	0.65
1:A:156:ASP:OD1	1:A:765:ARG:NH2	2.29	0.65
1:B:492:LEU:O	1:B:496:MET:HG2	1.96	0.65
1:D:418:ARG:NH1	1:D:422:GLU:OE2	2.30	0.65
1:F:680:PHE:HB2	1:F:859:TRP:CZ3	2.30	0.65
1:C:262:LEU:HA	1:C:265:VAL:HG22	1.77	0.65
1:D:176:GLN:NE2	1:D:177:LEU:O	2.29	0.65
1:D:971:ARG:NE	1:D:974:PRO:HG2	2.10	0.65
1:A:230:LEU:O	1:A:231:ASN:ND2	2.25	0.65
1:C:415:ASN:HB3	1:C:438:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:217:GLY:O	1:D:234:ILE:HB	1.96	0.65
1:D:506:GLY:O	1:D:509:LYS:HB2	1.97	0.65
1:E:527:TYR:O	1:E:530:SER:OG	2.14	0.65
1:F:20:MET:HG2	1:F:374:VAL:HA	1.79	0.65
1:C:6:ILE:HG22	1:C:487:ILE:HG12	1.79	0.65
1:C:181:GLN:OE1	1:C:767:ARG:NH2	2.26	0.65
1:D:525:HIS:NE2	1:D:529:ASP:OD2	2.29	0.65
1:A:886:LEU:HD21	1:C:18:ILE:HG12	1.79	0.65
1:A:1028:VAL:HG13	1:A:1032:ARG:HH12	1.62	0.65
1:C:691:GLY:O	1:C:694:LYS:HG2	1.97	0.65
1:C:968:VAL:HA	1:C:971:ARG:HH12	1.62	0.65
1:D:63:GLN:HE22	1:F:767:ARG:HA	1.62	0.65
1:D:702:LEU:HD22	1:D:848:ALA:HB2	1.79	0.65
1:E:408:ASP:OD1	1:E:940:LYS:NZ	2.20	0.65
1:E:805:SER:O	1:E:805:SER:OG	2.10	0.65
1:F:62:THR:OG1	1:F:63:GLN:N	2.29	0.65
1:C:509:LYS:HB3	1:C:514:GLY:HA3	1.79	0.65
1:D:699:ARG:HG3	1:D:827:ILE:HD11	1.78	0.65
1:E:728:LYS:HD3	1:E:810:GLU:OE2	1.96	0.65
1:A:1037:ASN:HA	1:A:1038:GLU:O	1.97	0.64
1:B:343:THR:HG21	1:B:989:LEU:HD23	1.79	0.64
1:B:668:LEU:HD23	1:B:668:LEU:H	1.62	0.64
1:C:736:ALA:HB2	1:C:804:PHE:CD1	2.32	0.64
1:E:453:PHE:O	1:E:471:SER:OG	2.10	0.64
1:F:1033:PHE:O	1:F:1035:ARG:N	2.30	0.64
1:A:170:SER:HB3	1:B:74:ASN:H	1.62	0.64
1:A:690:LEU:HB3	1:A:694:LYS:HG3	1.79	0.64
1:C:298:ASN:OD1	1:C:299:ALA:N	2.30	0.64
1:C:908:GLY:HA2	1:C:1014:ALA:HB2	1.78	0.64
1:E:448:VAL:HG13	1:E:884:VAL:HG13	1.79	0.64
1:A:895:TRP:O	1:A:898:PRO:HD2	1.97	0.64
1:D:745:ASP:O	1:D:749:THR:OG1	2.11	0.64
1:D:907:LEU:HD23	1:D:1017:LEU:HB3	1.78	0.64
1:D:959:GLY:HA2	1:D:1040:ILE:CG1	2.27	0.64
1:E:295:THR:O	1:E:295:THR:OG1	2.13	0.64
1:F:144:ASN:O	1:F:148:THR:OG1	2.10	0.64
1:F:155:SER:HB3	1:F:180:SER:H	1.61	0.64
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.78	0.64
1:B:195:LYS:HG2	1:B:196:PHE:CE1	2.33	0.64
1:C:754:TRP:CZ2	1:C:780:ARG:HA	2.31	0.64
1:D:743:ILE:O	1:D:746:ILE:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:908:GLY:HA2	1:D:1014:ALA:HB2	1.78	0.64
1:F:415:ASN:OD1	1:F:438:ILE:HG21	1.97	0.64
1:F:813:SER:HB2	1:F:816:LEU:HD21	1.78	0.64
1:D:186:ILE:HB	1:D:773:VAL:HG12	1.79	0.64
1:D:795:ASP:OD2	1:D:796:GLY:N	2.26	0.64
1:F:453:PHE:HD2	1:F:456:MET:HE2	1.62	0.64
1:A:960:LEU:O	1:A:964:THR:HG23	1.98	0.64
1:E:26:ALA:O	1:E:30:LEU:HB2	1.98	0.64
1:E:274:ASN:OD1	1:E:276:ASP:N	2.30	0.64
1:E:352:PHE:HD2	1:E:353:LEU:HD23	1.61	0.64
1:A:186:ILE:HB	1:A:773:VAL:HG12	1.79	0.64
1:A:913:LEU:HD23	1:A:927:PHE:HZ	1.61	0.64
1:B:590:VAL:O	1:B:593:GLU:HG2	1.98	0.64
1:B:685:ILE:HG22	1:B:687:GLN:HG3	1.79	0.64
1:B:971:ARG:O	1:B:975:ILE:HG13	1.98	0.64
1:C:930:GLY:HA2	1:C:1007:VAL:HG23	1.79	0.64
1:E:727:PHE:CD2	1:E:729:ILE:HD11	2.33	0.64
1:A:10:ILE:HG12	1:B:894:SER:HA	1.79	0.64
1:A:57:VAL:HG23	1:A:82:SER:HB3	1.78	0.64
1:A:305:ALA:O	1:A:308:ALA:HB3	1.98	0.64
1:B:216:ALA:HB1	1:B:234:ILE:HG22	1.80	0.64
1:C:42:ALA:HB2	1:C:93:THR:HG23	1.79	0.64
1:E:320:GLY:O	1:E:322:LYS:HG2	1.98	0.64
1:F:930:GLY:HA2	1:F:1007:VAL:HG23	1.78	0.64
1:F:983:ILE:HG22	1:F:984:LEU:HD23	1.78	0.64
1:C:261:LEU:N	1:C:264:ASP:OD2	2.29	0.64
1:C:344:LEU:HG	1:C:398:MET:SD	2.38	0.64
1:D:530:SER:HA	2:D:2000:LMT:O2'	1.98	0.64
1:A:199:THR:HG21	1:A:791:VAL:HA	1.80	0.63
1:A:682:PHE:HB3	1:A:827:ILE:HG23	1.80	0.63
1:A:744:ASN:O	1:A:748:THR:HG23	1.98	0.63
1:C:61:VAL:HG11	1:C:88:VAL:HG11	1.81	0.63
1:D:722:GLU:HG3	1:D:723:ASP:H	1.63	0.63
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.79	0.63
1:C:63:GLN:HB2	1:C:818:ARG:NH2	2.07	0.63
1:C:545:TYR:HD1	1:C:546:LEU:HD12	1.63	0.63
1:D:900:SER:HB3	1:D:1026:PHE:HA	1.80	0.63
1:E:801:PHE:HA	1:E:804:PHE:HE2	1.64	0.63
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.80	0.63
1:D:944:LEU:HB3	1:D:971:ARG:NH1	2.13	0.63
1:F:669:PRO:HG2	1:F:671:ILE:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HD21	1:A:922:THR:HA	1.80	0.63
1:A:582:ALA:HB1	1:A:586:ARG:HE	1.63	0.63
1:A:55:LYS:HG2	1:A:59:ASP:OD2	1.97	0.63
1:A:623:ASN:OD1	1:A:623:ASN:N	2.22	0.63
1:B:490:PRO:O	1:B:493:CYS:HB2	1.99	0.63
1:C:450:SER:OG	1:C:478:MET:SD	2.50	0.63
1:C:982:PHE:O	1:C:985:GLY:N	2.31	0.63
1:D:407:ASP:OD1	1:D:940:LYS:HG2	1.99	0.63
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.80	0.63
1:F:908:GLY:HA2	1:F:1014:ALA:HB2	1.79	0.63
1:A:155:SER:HB3	1:A:180:SER:H	1.63	0.63
1:A:217:GLY:O	1:A:234:ILE:HB	1.98	0.63
1:B:407:ASP:OD1	1:B:978:THR:HG21	1.98	0.63
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.79	0.63
1:B:703:LEU:HD11	1:B:718:PRO:HD3	1.80	0.63
1:A:105:VAL:CG1	1:B:105:VAL:HG12	2.27	0.63
1:A:281:PHE:HD1	1:A:610:PHE:HD1	1.44	0.63
1:B:591:LEU:HD13	1:B:611:ALA:HB1	1.80	0.63
1:D:17:ILE:CG2	1:E:886:LEU:HD21	2.29	0.63
1:D:777:ALA:HB1	1:F:225:VAL:HG22	1.80	0.63
1:F:307:ARG:NH1	1:F:311:ALA:HB2	2.13	0.63
1:A:452:VAL:HA	1:A:880:SER:OG	1.99	0.63
1:C:498:LYS:HG3	1:C:499:PRO:HD2	1.81	0.63
1:F:525:HIS:HA	1:F:528:THR:HG22	1.81	0.63
1:A:163:LYS:HD2	1:A:289:LEU:HD11	1.80	0.62
1:A:393:LEU:CD2	1:A:469:GLN:HG2	2.29	0.62
1:B:982:PHE:CE2	1:B:1007:VAL:HG13	2.34	0.62
1:C:27:ILE:HA	1:C:30:LEU:HB2	1.81	0.62
1:C:790:TYR:HE1	1:C:800:PRO:HB3	1.64	0.62
1:C:840:ALA:O	1:C:844:MET:HG2	1.98	0.62
1:F:1024:VAL:HA	1:F:1027:VAL:HG12	1.81	0.62
1:A:544:LEU:O	1:A:547:ILE:HB	1.99	0.62
1:B:445:ILE:HD13	1:B:940:LYS:HE2	1.80	0.62
1:C:38:ILE:HG23	1:C:462:SER:OG	1.99	0.62
1:C:65:ILE:HG21	1:C:111:LEU:HG	1.81	0.62
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.81	0.62
1:F:898:PRO:HA	1:F:901:VAL:HG12	1.80	0.62
1:A:111:LEU:HD21	1:A:127:VAL:HG21	1.82	0.62
1:C:58:GLN:HB2	1:C:82:SER:OG	1.98	0.62
1:B:184:MET:HB2	1:B:762:PHE:CE2	2.34	0.62
1:B:451:ALA:HB1	1:B:883:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:MET:C	1:C:164:ASP:H	2.02	0.62
1:C:597:TYR:OH	1:C:651:ALA:HA	1.99	0.62
1:F:160:ALA:HA	1:F:767:ARG:NH1	2.15	0.62
1:F:307:ARG:HH12	1:F:311:ALA:HB2	1.62	0.62
1:A:70:ASN:HD22	1:A:70:ASN:H	1.46	0.62
1:B:817:GLU:OE1	1:B:826:GLU:N	2.32	0.62
1:C:187:TRP:HA	1:C:774:MET:O	2.00	0.62
1:A:680:PHE:CB	1:A:859:TRP:HZ3	2.11	0.62
1:A:971:ARG:HB3	1:A:971:ARG:NH1	2.13	0.62
1:B:379:THR:O	1:B:382:VAL:N	2.33	0.62
1:C:24:GLY:O	1:C:28:LEU:HG	1.99	0.62
1:E:122:VAL:O	1:E:125:GLN:N	2.28	0.62
1:F:158:VAL:HG22	1:F:162:MET:HE3	1.80	0.62
1:F:244:GLU:O	1:F:247:GLY:N	2.32	0.62
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.82	0.62
1:B:534:ILE:HG22	2:B:2000:LMT:H3'	1.80	0.62
1:B:537:SER:HB2	1:B:540:ARG:CZ	2.30	0.62
1:B:944:LEU:HD13	1:B:971:ARG:HH12	1.63	0.62
1:C:699:ARG:HD3	1:C:825:MET:SD	2.40	0.62
1:C:961:ILE:HG22	1:C:965:LEU:HD12	1.82	0.62
1:D:948:PHE:O	1:D:952:LEU:HG	1.99	0.62
1:E:446:ALA:HB2	1:E:482:VAL:HG21	1.82	0.62
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.98	0.62
1:A:33:ALA:HA	1:A:299:ALA:H	1.64	0.62
1:A:197:GLN:O	1:A:792:ARG:HD3	1.99	0.62
1:B:190:PRO:HG3	1:B:779:TYR:HB3	1.82	0.62
1:B:910:ILE:O	1:B:914:LEU:HB2	2.00	0.62
1:C:397:GLY:HA2	1:C:470:PHE:CD2	2.35	0.62
1:C:427:PRO:HD3	1:C:499:PRO:HB3	1.80	0.62
1:D:573:MET:HA	1:D:629:VAL:HG13	1.82	0.62
1:F:80:SER:OG	1:F:818:ARG:HB2	2.00	0.62
1:A:195:LYS:HB3	1:A:196:PHE:HD2	1.65	0.62
1:B:420:MET:HB3	1:B:500:ILE:HB	1.81	0.62
1:C:440:GLY:O	1:C:443:VAL:HG13	2.00	0.62
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.82	0.62
1:E:1011:MET:O	1:E:1015:THR:HG23	1.98	0.62
1:F:278:ILE:HG23	1:F:613:ASN:HB3	1.82	0.62
1:A:591:LEU:HD13	1:A:611:ALA:HB1	1.81	0.62
1:B:219:LEU:HD23	1:C:754:TRP:CZ3	2.35	0.62
1:B:940:LYS:O	1:B:943:ILE:HB	1.99	0.62
1:E:910:ILE:O	1:E:914:LEU:HB2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.82	0.62
1:A:14:VAL:HG21	1:B:890:ALA:HB2	1.82	0.61
1:A:618:ALA:HB3	1:A:815:ARG:NH1	2.15	0.61
1:B:62:THR:HG21	1:B:818:ARG:HD2	1.80	0.61
1:C:671:ILE:HB	1:C:862:MET:SD	2.40	0.61
1:D:1038:GLU:CB	1:D:1040:ILE:HA	2.28	0.61
1:A:1038:GLU:HA	1:A:1039:ASP:HB2	1.81	0.61
1:B:426:PRO:HG2	1:B:429:GLU:HB3	1.81	0.61
1:B:687:GLN:NE2	1:B:856:GLY:HA3	2.15	0.61
1:B:960:LEU:O	1:B:964:THR:HG23	2.00	0.61
1:C:679:GLY:HA3	1:C:837:THR:CG2	2.30	0.61
1:D:909:VAL:HG22	1:D:931:LEU:HD11	1.82	0.61
1:A:445:ILE:HD13	1:A:940:LYS:CE	2.30	0.61
1:A:445:ILE:HG21	1:A:940:LYS:NZ	2.16	0.61
1:C:953:MET:N	1:C:953:MET:SD	2.73	0.61
1:D:360:GLN:HG2	1:D:513:PHE:HD2	1.65	0.61
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.65	0.61
1:A:277:ILE:HD13	1:A:614:GLY:HA3	1.83	0.61
1:A:746:ILE:O	1:A:749:THR:OG1	2.16	0.61
1:B:531:VAL:O	1:B:534:ILE:HG12	2.00	0.61
1:C:119:PRO:HB2	1:C:122:VAL:HG23	1.82	0.61
1:C:242:SER:O	1:C:246:PHE:CD1	2.53	0.61
1:D:375:VAL:HG21	1:D:481:SER:HA	1.81	0.61
1:E:536:ARG:HH21	2:E:2000:LMT:C4B	2.10	0.61
1:C:75:LEU:HD12	1:C:93:THR:O	2.01	0.61
1:C:563:PHE:HB2	1:C:866:GLU:HG3	1.83	0.61
1:F:945:ILE:HG12	1:F:971:ARG:CZ	2.31	0.61
1:D:926:TYR:CE1	1:D:999:ALA:HB1	2.34	0.61
1:E:705:GLU:HA	1:E:708:LYS:HD2	1.81	0.61
1:A:36:PRO:O	1:A:38:ILE:HG13	2.00	0.61
1:B:686:ASP:HA	1:B:854:GLY:O	2.00	0.61
1:C:367:ILE:HG21	1:C:489:THR:OG1	2.00	0.61
1:C:669:PRO:HG3	1:C:675:GLY:HA3	1.81	0.61
1:D:986:VAL:HG21	1:D:1007:VAL:HG11	1.82	0.61
1:E:355:MET:SD	1:E:368:PRO:HG2	2.40	0.61
1:F:112:GLN:HA	1:F:115:MET:HB3	1.83	0.61
1:B:924:ASP:OD1	1:B:925:VAL:N	2.33	0.61
1:C:12:ALA:HB1	1:C:487:ILE:CG2	2.31	0.61
1:B:3:ASN:O	1:B:6:ILE:HG13	2.00	0.61
1:B:555:LEU:HD22	1:B:913:LEU:HB3	1.82	0.61
1:B:801:PHE:HA	1:B:804:PHE:HE2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:24:GLY:O	1:E:28:LEU:HD22	2.00	0.61
1:E:418:ARG:O	1:E:422:GLU:HG3	2.00	0.61
1:F:352:PHE:HD1	1:F:369:THR:OG1	1.77	0.61
1:F:885:PHE:HB2	1:F:902:MET:SD	2.40	0.61
1:A:343:THR:HG21	1:A:989:LEU:HD11	1.82	0.61
1:A:396:PHE:O	1:A:400:LEU:HB2	2.00	0.61
1:B:46:SER:HA	1:B:88:VAL:O	2.01	0.61
1:B:72:ILE:HB	1:B:110:LYS:HZ1	1.65	0.61
1:C:225:VAL:O	1:C:228:GLN:HB3	2.00	0.61
1:B:675:GLY:HA2	1:B:862:MET:SD	2.41	0.60
1:B:871:ASN:OD1	1:B:871:ASN:N	2.34	0.60
1:D:971:ARG:C	1:D:974:PRO:HD2	2.20	0.60
1:E:420:MET:HG3	1:E:500:ILE:HB	1.81	0.60
1:A:249:ILE:O	1:A:262:LEU:N	2.34	0.60
1:A:728:LYS:HA	1:C:235:ILE:HB	1.83	0.60
1:C:227:GLY:O	1:C:229:GLN:HG2	2.01	0.60
1:D:972:LEU:HD13	1:D:976:LEU:HD13	1.83	0.60
1:E:559:LEU:HD12	1:E:923:ASN:HB2	1.83	0.60
1:F:140:VAL:HG11	1:F:310:LEU:HD21	1.84	0.60
1:B:225:VAL:N	1:C:781:MET:HE1	2.16	0.60
1:D:276:ASP:HB3	1:D:277:ILE:HD12	1.82	0.60
1:D:960:LEU:O	1:D:964:THR:HG23	2.02	0.60
1:E:203:VAL:O	1:E:207:ILE:HG13	2.02	0.60
1:F:637:ARG:HB3	1:F:642:ASN:HB3	1.83	0.60
1:A:618:ALA:HB3	1:A:815:ARG:HH12	1.65	0.60
1:B:38:ILE:HG21	1:B:671:ILE:HD13	1.84	0.60
1:B:163:LYS:NZ	1:B:163:LYS:HB3	2.16	0.60
1:C:699:ARG:HD2	1:C:827:ILE:HD11	1.83	0.60
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.36	0.60
1:A:441:ALA:O	1:A:445:ILE:HG23	2.00	0.60
1:B:139:VAL:HB	1:B:327:TYR:HB3	1.84	0.60
1:B:618:ALA:HB1	1:B:720:GLY:HA2	1.82	0.60
1:C:65:ILE:HA	1:C:114:ALA:HB1	1.82	0.60
1:C:240:LEU:HD23	1:C:246:PHE:CE2	2.37	0.60
1:C:255:GLN:H	1:C:255:GLN:CD	2.05	0.60
1:D:428:LYS:HZ2	1:D:428:LYS:N	1.97	0.60
1:A:233:SER:HB2	1:B:726:GLN:HB3	1.83	0.60
1:A:1030:ARG:C	1:A:1032:ARG:H	2.04	0.60
1:C:758:TYR:CE1	1:C:770:LYS:HD3	2.37	0.60
1:F:13:TRP:CE3	1:F:13:TRP:HA	2.37	0.60
1:F:340:VAL:HG12	1:F:395:MET:HE3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HA	1:A:224:PRO:HD3	1.83	0.60
1:B:832:ALA:HB3	1:B:835:LYS:HD3	1.83	0.60
1:C:525:HIS:HA	1:C:528:THR:HG22	1.83	0.60
1:C:693:GLU:N	1:C:694:LYS:HZ3	1.98	0.60
1:C:961:ILE:HD12	1:C:961:ILE:H	1.67	0.60
1:D:356:TYR:HD1	1:D:365:THR:HG21	1.65	0.60
1:E:197:GLN:O	1:E:792:ARG:HD3	2.02	0.60
1:E:801:PHE:HA	1:E:804:PHE:CE2	2.36	0.60
1:F:562:SER:OG	1:F:924:ASP:HB3	2.02	0.60
1:F:672:VAL:HG23	1:F:673:GLU:HG2	1.83	0.60
1:D:23:GLY:O	1:D:27:ILE:HG13	2.02	0.60
1:D:686:ASP:HB2	1:D:695:LEU:HG	1.84	0.60
1:D:895:TRP:O	1:D:898:PRO:HD2	2.01	0.60
1:D:1018:ALA:O	1:D:1022:VAL:HG23	2.02	0.60
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.37	0.60
1:B:139:VAL:O	1:B:326:PRO:HD2	2.00	0.60
1:B:905:VAL:HG22	1:B:935:ILE:HD12	1.84	0.60
1:C:693:GLU:HB3	1:C:694:LYS:HD3	1.83	0.60
1:C:923:ASN:O	1:C:923:ASN:ND2	2.28	0.60
1:D:112:GLN:NE2	1:E:112:GLN:HB3	2.16	0.60
1:D:1040:ILE:HG13	1:D:1041:GLU:N	2.17	0.60
1:A:274:ASN:OD1	1:A:275:TYR:N	2.35	0.59
1:B:218:GLN:HG3	1:B:221:GLY:HA2	1.84	0.59
1:C:137:LEU:HB2	1:C:293:LEU:HD23	1.83	0.59
1:D:4:PHE:HB3	1:D:8:ARG:NH1	2.16	0.59
1:D:195:LYS:HG2	1:D:196:PHE:CE2	2.37	0.59
1:E:196:PHE:O	1:E:252:LYS:NZ	2.35	0.59
1:E:236:ALA:O	1:F:728:LYS:NZ	2.23	0.59
1:E:898:PRO:O	1:E:901:VAL:HG12	2.02	0.59
1:F:189:ASN:O	1:F:193:LEU:HD23	2.02	0.59
1:A:414:GLU:HG3	1:A:974:PRO:HG3	1.82	0.59
1:A:524:THR:O	1:A:527:TYR:HB3	2.03	0.59
1:C:242:SER:O	1:C:246:PHE:HD1	1.85	0.59
1:D:211:ASN:ND2	1:D:760:ASN:HD22	2.00	0.59
1:D:284:GLN:HG3	1:D:285:PRO:HD2	1.84	0.59
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.83	0.59
1:F:615:ALA:HB2	1:F:620:ARG:HG2	1.84	0.59
1:A:367:ILE:HG12	1:A:496:MET:CE	2.33	0.59
1:B:38:ILE:HG23	1:B:462:SER:HB3	1.83	0.59
1:B:58:GLN:O	1:B:63:GLN:HG3	2.02	0.59
1:C:5:PHE:C	1:C:7:ASP:H	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLN:OE1	1:C:229:GLN:N	2.35	0.59
1:D:525:HIS:HA	1:D:528:THR:HG22	1.84	0.59
1:D:971:ARG:O	1:D:974:PRO:HD2	2.02	0.59
1:E:373:PRO:O	1:E:377:LEU:N	2.35	0.59
1:F:876:LEU:HD21	1:F:932:LEU:HD11	1.82	0.59
1:A:161:ASN:HD22	1:A:161:ASN:N	2.00	0.59
1:A:189:ASN:O	1:A:193:LEU:HD23	2.02	0.59
1:A:836:SER:OG	1:A:839:GLU:HG3	2.01	0.59
1:A:945:ILE:HG13	1:A:971:ARG:CZ	2.32	0.59
1:B:185:ARG:HB3	1:B:187:TRP:NE1	2.17	0.59
1:C:186:ILE:HB	1:C:773:VAL:HG12	1.83	0.59
1:C:888:LEU:HD13	1:C:901:VAL:HG11	1.84	0.59
1:D:17:ILE:HG21	1:E:886:LEU:HD21	1.85	0.59
1:D:872:GLN:O	1:D:875:SER:OG	2.19	0.59
1:E:417:GLU:HG2	1:E:497:LEU:HD21	1.83	0.59
1:F:62:THR:O	1:F:65:ILE:HG12	2.03	0.59
1:F:808:ARG:HD3	1:F:808:ARG:N	2.18	0.59
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.84	0.59
1:B:714:THR:HG22	1:B:830:GLN:HB2	1.83	0.59
1:D:143:ILE:O	1:D:321:LEU:HD22	2.01	0.59
1:D:445:ILE:HD13	1:D:940:LYS:HD2	1.83	0.59
1:E:685:ILE:HD11	1:E:819:TYR:HB3	1.84	0.59
1:E:762:PHE:CE1	1:E:764:ASP:HB2	2.38	0.59
1:A:108:GLN:NE2	1:B:113:LEU:HD11	2.17	0.59
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.84	0.59
1:B:944:LEU:HB3	1:B:971:ARG:NH1	2.18	0.59
1:F:453:PHE:CD2	1:F:456:MET:HE2	2.38	0.59
1:A:76:MET:SD	1:A:864:TYR:HE2	2.25	0.59
1:A:844:MET:HE2	1:A:847:LEU:HD12	1.85	0.59
1:B:408:ASP:OD1	1:B:940:LYS:NZ	2.35	0.59
1:C:303:ALA:HA	1:C:306:ILE:HG22	1.84	0.59
1:C:337:ILE:HA	1:C:340:VAL:HG22	1.84	0.59
1:D:58:GLN:HA	1:D:62:THR:HB	1.84	0.59
1:F:965:LEU:HA	1:F:968:VAL:HG22	1.85	0.59
1:B:220:GLY:H	1:C:781:MET:HA	1.68	0.59
1:B:480:LEU:O	1:B:484:VAL:HG13	2.03	0.59
1:B:889:ALA:HB2	1:B:898:PRO:HG3	1.84	0.59
1:C:740:GLY:O	1:C:794:ALA:N	2.31	0.59
1:F:151:GLN:OE1	1:F:151:GLN:N	2.25	0.59
1:F:210:GLN:NE2	1:F:250:LEU:O	2.36	0.59
1:F:597:TYR:CD2	1:F:655:PHE:HZ	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:ALA:O	1:B:781:MET:HG3	2.03	0.59
1:B:831:ALA:HB2	1:B:837:THR:HA	1.84	0.59
1:C:578:LEU:HD13	1:C:661:ALA:HB2	1.83	0.59
1:E:120:GLN:HA	1:E:123:GLN:HB2	1.83	0.59
1:E:146:ASP:OD2	1:E:320:GLY:HA3	2.03	0.59
1:F:578:LEU:CD1	1:F:579:PRO:HD2	2.32	0.59
1:A:108:GLN:HG2	1:B:113:LEU:HD21	1.84	0.59
1:B:250:LEU:HD22	1:C:734:GLU:HG2	1.85	0.59
1:D:684:LEU:O	1:D:824:SER:OG	2.16	0.59
1:D:1030:ARG:NE	1:D:1033:PHE:HD2	2.00	0.59
1:F:101:ASP:O	1:F:105:VAL:HG23	2.02	0.59
1:F:728:LYS:HG2	1:F:808:ARG:NH2	2.14	0.59
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.85	0.58
1:B:459:PHE:HD2	1:B:460:GLY:H	1.49	0.58
1:C:466:ILE:O	1:C:470:PHE:HD1	1.85	0.58
1:B:455:PRO:HG2	1:B:880:SER:HA	1.85	0.58
1:B:1037:ASN:HA	1:B:1038:GLU:HB2	1.86	0.58
1:C:958:LYS:HA	1:C:1041:GLU:OE2	2.03	0.58
1:D:68:ASN:O	1:D:110:LYS:HD2	2.03	0.58
1:D:573:MET:HG3	1:D:666:PHE:CE1	2.38	0.58
1:E:3:ASN:OD1	1:E:4:PHE:N	2.34	0.58
1:F:146:ASP:O	1:F:148:THR:N	2.37	0.58
1:F:201:VAL:HA	1:F:204:ILE:HD12	1.84	0.58
1:B:203:VAL:O	1:B:207:ILE:HG12	2.03	0.58
1:B:228:GLN:NE2	1:B:230:LEU:O	2.37	0.58
1:B:344:LEU:HD12	1:B:399:VAL:HG22	1.85	0.58
1:B:944:LEU:HD12	1:B:975:ILE:HG12	1.85	0.58
1:E:259:ARG:H	1:E:259:ARG:HD3	1.68	0.58
1:E:685:ILE:HD13	1:E:824:SER:HB3	1.84	0.58
1:A:108:GLN:NE2	1:A:129:VAL:HB	2.18	0.58
1:A:350:LEU:O	1:A:353:LEU:HB2	2.03	0.58
1:A:393:LEU:HD23	1:A:469:GLN:HG2	1.85	0.58
1:A:485:ALA:HA	1:A:489:THR:HB	1.84	0.58
1:B:880:SER:O	1:B:884:VAL:HG23	2.02	0.58
1:B:947:GLU:HG3	1:B:948:PHE:CD1	2.38	0.58
1:E:222:THR:HA	1:E:224:PRO:HD3	1.83	0.58
1:E:438:ILE:O	1:E:442:LEU:HG	2.03	0.58
1:E:944:LEU:HD12	1:E:971:ARG:NH2	2.18	0.58
1:C:25:LEU:HD23	1:C:28:LEU:HD12	1.85	0.58
1:C:790:TYR:CE1	1:C:800:PRO:HB3	2.38	0.58
1:E:877:TYR:O	1:E:881:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:GLN:HB2	1:E:613:ASN:HD21	1.69	0.58
1:B:564:LEU:HD22	1:B:671:ILE:HG13	1.85	0.58
1:D:166:ILE:O	1:D:169:THR:HG22	2.03	0.58
1:D:1021:PHE:HB3	1:D:1025:PHE:CE1	2.39	0.58
1:F:252:LYS:NZ	1:F:254:ASN:OD1	2.36	0.58
1:A:138:MET:HG2	1:A:291:ILE:HD12	1.85	0.58
1:C:206:ALA:O	1:C:210:GLN:HG3	2.04	0.58
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	1.84	0.58
1:D:164:ASP:OD2	1:E:67:GLN:HG2	2.04	0.58
1:D:188:MET:HE1	1:D:200:PRO:HG3	1.85	0.58
1:E:780:ARG:HD2	1:E:780:ARG:O	2.03	0.58
1:E:957:GLY:CA	1:E:1042:HIS:HB3	2.34	0.58
1:F:227:GLY:O	1:F:229:GLN:HG2	2.04	0.58
1:F:307:ARG:HH11	1:F:307:ARG:HG3	1.68	0.58
1:A:3:ASN:O	1:A:6:ILE:HG23	2.04	0.58
1:A:760:ASN:O	1:A:771:VAL:HB	2.04	0.58
1:A:1028:VAL:HG13	1:A:1032:ARG:NH1	2.19	0.58
1:B:178:PHE:O	1:B:287:SER:OG	2.17	0.58
1:B:727:PHE:HB2	1:B:809:TRP:HZ3	1.67	0.58
1:C:98:THR:HG22	1:C:98:THR:O	2.04	0.58
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.37	0.58
1:C:682:PHE:O	1:C:826:GLU:HA	2.04	0.58
1:D:54:ALA:HB2	1:D:84:SER:HB3	1.85	0.58
1:F:940:LYS:O	1:F:943:ILE:HB	2.04	0.58
1:A:5:PHE:CE1	1:A:487:ILE:HG12	2.39	0.58
1:A:169:THR:HG22	1:A:172:VAL:HG23	1.86	0.58
1:A:795:ASP:OD2	1:A:796:GLY:N	2.34	0.58
1:B:923:ASN:O	1:B:923:ASN:ND2	2.37	0.58
1:C:12:ALA:HB1	1:C:487:ILE:HG23	1.86	0.58
1:C:578:LEU:HD13	1:C:579:PRO:HD2	1.84	0.58
1:C:859:TRP:HE3	1:C:863:SER:HG	1.50	0.58
1:E:119:PRO:O	1:E:123:GLN:HG3	2.04	0.58
1:F:921:LEU:HD11	1:F:1005:THR:HB	1.86	0.58
1:B:982:PHE:CD2	1:B:1011:MET:HG3	2.39	0.57
1:C:445:ILE:HD11	1:C:940:LYS:HG3	1.85	0.57
1:C:1035:ARG:NE	1:C:1035:ARG:HA	2.19	0.57
1:D:555:LEU:HD22	1:D:913:LEU:HB3	1.85	0.57
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.86	0.57
1:A:961:ILE:HG13	1:A:1039:ASP:OD2	2.03	0.57
1:B:77:TYR:CZ	1:B:93:THR:HB	2.40	0.57
1:B:146:ASP:O	1:B:148:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:THR:O	1:B:295:THR:OG1	2.18	0.57
1:B:343:THR:HG21	1:B:989:LEU:CD2	2.34	0.57
1:B:352:PHE:HD1	1:B:369:THR:HG1	1.51	0.57
1:B:361:ASN:HB3	1:B:364:ALA:HB3	1.86	0.57
1:B:508:GLY:H	1:B:518:ARG:HG3	1.69	0.57
1:C:74:ASN:HB2	1:C:98:THR:HG21	1.85	0.57
1:C:157:TYR:HE2	1:C:161:ASN:CG	2.06	0.57
1:C:714:THR:HB	1:C:832:ALA:HA	1.86	0.57
1:D:218:GLN:OE1	1:D:231:ASN:ND2	2.35	0.57
1:D:350:LEU:HD13	1:D:985:GLY:HA2	1.86	0.57
1:D:668:LEU:H	1:D:668:LEU:HD23	1.70	0.57
1:E:556:PHE:HD1	1:E:913:LEU:HD21	1.69	0.57
1:F:190:PRO:HG3	1:F:779:TYR:CG	2.39	0.57
1:F:836:SER:HB2	1:F:922:THR:HG21	1.86	0.57
1:A:359:LEU:C	1:A:360:GLN:HG2	2.23	0.57
1:A:616:GLY:HA2	1:A:626:ILE:CD1	2.35	0.57
1:B:448:VAL:O	1:B:452:VAL:HG13	2.05	0.57
1:B:520:PHE:HZ	1:B:973:ARG:HA	1.68	0.57
1:B:717:ARG:NE	1:B:828:LEU:HB2	2.17	0.57
1:D:278:ILE:HG23	1:D:613:ASN:HB3	1.86	0.57
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.86	0.57
1:D:591:LEU:HD13	1:D:611:ALA:HB1	1.85	0.57
1:D:841:MET:HG2	1:D:859:TRP:CH2	2.39	0.57
1:F:682:PHE:CE1	1:F:857:TYR:HB2	2.39	0.57
1:F:801:PHE:HA	1:F:804:PHE:HE2	1.69	0.57
1:A:982:PHE:O	1:A:985:GLY:N	2.34	0.57
1:C:200:PRO:HB2	1:C:749:THR:HG22	1.87	0.57
1:C:559:LEU:HD22	1:C:560:PRO:HD2	1.87	0.57
1:F:870:GLY:C	1:F:872:GLN:H	2.08	0.57
1:B:356:TYR:HA	1:B:365:THR:OG1	2.05	0.57
1:B:634:TRP:CD1	1:B:634:TRP:N	2.70	0.57
1:B:717:ARG:HE	1:B:828:LEU:CB	2.14	0.57
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.85	0.57
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.87	0.57
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.39	0.57
1:A:909:VAL:O	1:A:912:ALA:N	2.38	0.57
1:C:64:VAL:HG13	1:C:117:LEU:HB2	1.86	0.57
1:C:419:VAL:HG21	1:C:434:SER:HB2	1.87	0.57
1:C:470:PHE:O	1:C:474:ILE:HG13	2.05	0.57
1:C:699:ARG:HG3	1:C:827:ILE:HD11	1.86	0.57
1:D:524:THR:O	1:D:527:TYR:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:SER:HB2	1:F:814:PRO:O	2.05	0.57
1:C:510:LYS:HD2	1:C:511:GLY:H	1.69	0.57
1:C:940:LYS:HD3	1:C:941:ASN:N	2.20	0.57
1:D:602:GLU:OE2	1:D:647:ILE:HG12	2.04	0.57
1:E:399:VAL:HA	1:E:402:ILE:HG13	1.87	0.57
1:E:442:LEU:HA	1:E:445:ILE:HG12	1.86	0.57
1:F:186:ILE:HB	1:F:773:VAL:HG12	1.86	0.57
1:F:351:VAL:HG21	1:F:402:ILE:HG22	1.86	0.57
1:B:58:GLN:O	1:B:62:THR:HB	2.04	0.57
1:B:394:THR:HG22	1:B:473:THR:OG1	2.04	0.57
1:B:484:VAL:HB	1:B:488:LEU:HB3	1.86	0.57
1:B:576:VAL:HA	1:B:663:VAL:HG13	1.87	0.57
1:C:53:ASP:O	1:C:57:VAL:HG22	2.05	0.57
1:C:407:ASP:OD2	1:C:940:LYS:NZ	2.24	0.57
1:C:422:GLU:OE2	1:C:423:GLU:HB3	2.04	0.57
1:C:674:LEU:HD22	1:C:861:GLY:HA2	1.87	0.57
1:D:533:GLY:HA2	1:D:536:ARG:HD2	1.87	0.57
1:D:944:LEU:HB3	1:D:971:ARG:HH12	1.68	0.57
1:E:545:TYR:HD1	1:E:546:LEU:HD23	1.70	0.57
1:E:777:ALA:O	1:E:781:MET:HG3	2.05	0.57
1:F:394:THR:O	1:F:398:MET:HG3	2.04	0.57
1:C:81:ASN:ND2	1:C:89:GLN:OE1	2.21	0.57
1:C:572:PHE:CD2	1:C:631:LEU:HD11	2.38	0.57
1:D:30:LEU:HG	1:D:390:ILE:HG12	1.86	0.57
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.53	0.57
1:E:775:SER:OG	1:E:780:ARG:HG2	2.04	0.57
1:A:15:ILE:HD12	1:A:487:ILE:HD13	1.86	0.57
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.87	0.57
1:A:463:THR:O	1:A:467:TYR:HD1	1.88	0.57
1:B:166:ILE:O	1:B:169:THR:HB	2.04	0.57
1:B:801:PHE:HA	1:B:804:PHE:CE2	2.39	0.57
1:C:483:LEU:HD23	1:C:486:LEU:HD21	1.86	0.57
1:C:880:SER:O	1:C:883:VAL:HG12	2.05	0.57
1:D:74:ASN:HB3	1:D:95:GLU:HB2	1.87	0.57
1:E:201:VAL:HG23	1:E:749:THR:HG23	1.87	0.57
1:E:324:VAL:O	1:E:326:PRO:HD3	2.05	0.57
1:A:58:GLN:OE1	1:A:816:LEU:HB3	2.05	0.56
1:A:637:ARG:NH1	1:A:642:ASN:O	2.38	0.56
1:A:818:ARG:NH1	1:A:823:PRO:HG3	2.19	0.56
1:B:18:ILE:HD11	1:C:886:LEU:HB3	1.87	0.56
1:B:274:ASN:OD1	1:B:276:ASP:N	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ASN:OD1	1:B:275:TYR:N	2.38	0.56
1:B:356:TYR:O	1:B:360:GLN:HG3	2.05	0.56
1:C:240:LEU:HB2	1:C:246:PHE:CZ	2.40	0.56
1:C:743:ILE:O	1:C:746:ILE:HG23	2.04	0.56
1:C:841:MET:HG3	1:C:859:TRP:CZ2	2.40	0.56
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.04	0.56
1:A:181:GLN:HG2	1:A:182:TYR:N	2.19	0.56
1:B:111:LEU:HD22	1:B:114:ALA:HB3	1.87	0.56
1:B:293:LEU:HD22	1:B:294:ALA:H	1.71	0.56
1:C:62:THR:HG21	1:C:80:SER:HB2	1.86	0.56
1:C:444:GLY:O	1:C:448:VAL:HG13	2.04	0.56
1:D:948:PHE:CE2	1:D:971:ARG:HD3	2.41	0.56
1:E:46:SER:OG	1:E:89:GLN:HG2	2.06	0.56
1:E:250:LEU:HD21	1:F:734:GLU:HG3	1.87	0.56
1:F:336:SER:O	1:F:340:VAL:HG23	2.05	0.56
1:A:911:GLY:HA3	1:A:1013:THR:HG21	1.87	0.56
1:A:954:ASP:HB3	1:A:955:LYS:HD3	1.87	0.56
1:A:1019:ILE:HG13	1:A:1020:PHE:CD1	2.40	0.56
1:B:240:LEU:HB2	1:B:246:PHE:CE1	2.39	0.56
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.88	0.56
1:C:453:PHE:CD2	1:C:471:SER:HA	2.41	0.56
1:D:69:MET:CE	1:D:107:VAL:HG13	2.35	0.56
1:D:170:SER:HB2	1:E:75:LEU:H	1.69	0.56
1:D:544:LEU:HD23	1:D:548:ILE:HD11	1.86	0.56
1:D:909:VAL:O	1:D:912:ALA:N	2.36	0.56
1:E:73:ASP:OD2	1:E:73:ASP:N	2.32	0.56
1:E:108:GLN:NE2	1:F:109:ASN:OD1	2.38	0.56
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.86	0.56
1:E:420:MET:CG	1:E:500:ILE:HB	2.35	0.56
1:E:727:PHE:CZ	1:E:807:SER:HB2	2.41	0.56
1:F:155:SER:CB	1:F:180:SER:H	2.18	0.56
1:B:14:VAL:HG13	1:B:18:ILE:HD12	1.88	0.56
1:B:578:LEU:HD11	1:B:586:ARG:HB2	1.87	0.56
1:C:506:GLY:C	1:C:508:GLY:H	2.09	0.56
1:C:699:ARG:HH11	1:C:825:MET:HB3	1.69	0.56
1:D:343:THR:HG22	1:D:399:VAL:HG21	1.86	0.56
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.88	0.56
1:E:135:SER:HB2	1:E:673:GLU:OE2	2.05	0.56
1:F:139:VAL:O	1:F:326:PRO:HD2	2.06	0.56
1:A:438:ILE:O	1:A:441:ALA:HB3	2.04	0.56
1:B:108:GLN:CB	1:B:129:VAL:HG11	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ALA:HB1	1:B:883:VAL:HG22	1.88	0.56
1:B:702:LEU:HD12	1:B:705:GLU:HB3	1.87	0.56
1:C:445:ILE:HG23	1:C:449:LEU:HD12	1.88	0.56
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.40	0.56
1:A:488:LEU:O	1:A:492:LEU:N	2.39	0.56
1:B:213:GLN:HG2	1:B:239:ARG:HG3	1.87	0.56
1:B:696:THR:HG22	1:B:699:ARG:HH12	1.70	0.56
1:D:169:THR:HG21	1:D:306:ILE:HG12	1.88	0.56
1:F:6:ILE:HG22	1:F:12:ALA:HB2	1.87	0.56
1:A:108:GLN:HB2	1:B:109:ASN:HB3	1.87	0.56
1:A:190:PRO:HG3	1:A:779:TYR:HB3	1.87	0.56
1:A:513:PHE:O	1:A:516:PHE:HB3	2.04	0.56
1:B:375:VAL:HG13	1:B:480:LEU:HD21	1.86	0.56
1:B:946:VAL:HG13	1:B:1026:PHE:CD2	2.41	0.56
1:C:107:VAL:HA	1:C:110:LYS:HB2	1.88	0.56
1:C:1027:VAL:HG13	1:C:1028:VAL:N	2.21	0.56
1:D:190:PRO:HB3	1:D:789:TRP:CZ3	2.41	0.56
1:D:293:LEU:HD13	1:D:294:ALA:H	1.71	0.56
1:D:922:THR:O	1:D:924:ASP:N	2.38	0.56
1:E:544:LEU:O	1:E:547:ILE:HB	2.04	0.56
1:F:379:THR:O	1:F:382:VAL:HG12	2.04	0.56
1:F:1033:PHE:C	1:F:1035:ARG:H	2.08	0.56
1:A:65:ILE:HG22	1:A:69:MET:HB2	1.87	0.56
1:B:54:ALA:HB1	1:B:816:LEU:HG	1.87	0.56
1:B:336:SER:O	1:B:340:VAL:HG23	2.05	0.56
1:B:382:VAL:HG11	1:B:476:SER:OG	2.06	0.56
1:B:455:PRO:HB3	1:B:879:ILE:HG22	1.88	0.56
1:C:394:THR:HA	1:C:469:GLN:HB3	1.88	0.56
1:D:236:ALA:O	1:E:728:LYS:NZ	2.39	0.56
1:D:1037:ASN:CA	1:D:1038:GLU:HB2	2.35	0.56
1:E:17:ILE:HG21	1:F:886:LEU:HD21	1.88	0.56
1:E:420:MET:HE2	1:E:500:ILE:H	1.71	0.56
1:F:166:ILE:HD12	1:F:306:ILE:HD12	1.88	0.56
1:F:293:LEU:HD13	1:F:294:ALA:H	1.70	0.56
1:F:578:LEU:HD12	1:F:661:ALA:HB2	1.85	0.56
1:A:578:LEU:HD13	1:A:579:PRO:HD2	1.87	0.56
1:A:680:PHE:CE2	1:A:829:GLY:HA3	2.40	0.56
1:B:350:LEU:HD22	1:B:984:LEU:HD12	1.88	0.56
1:B:367:ILE:HG23	1:B:368:PRO:HD3	1.87	0.56
1:B:398:MET:HG2	1:B:473:THR:CG2	2.36	0.56
1:C:545:TYR:CE1	1:C:903:LEU:HD23	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:728:LYS:HG2	1:C:808:ARG:CZ	2.35	0.56
1:D:362:PHE:HB2	1:D:363:ARG:HH11	1.69	0.56
1:F:193:LEU:HD22	1:F:265:VAL:HB	1.88	0.56
1:B:72:ILE:HD13	1:B:107:VAL:HG23	1.88	0.56
1:B:164:ASP:OD1	1:C:67:GLN:HA	2.06	0.56
1:B:844:MET:HG3	1:B:845:GLU:N	2.20	0.56
1:D:764:ASP:O	1:D:766:GLY:N	2.35	0.56
1:F:172:VAL:HG13	1:F:291:ILE:HG23	1.86	0.56
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.87	0.56
1:F:841:MET:HG3	1:F:859:TRP:CZ2	2.41	0.56
1:A:162:MET:HA	1:A:313:MET:SD	2.46	0.55
1:A:898:PRO:HA	1:A:901:VAL:HG12	1.88	0.55
1:B:435:MET:CE	1:B:490:PRO:HB3	2.37	0.55
1:B:449:LEU:HD23	1:B:478:MET:HG3	1.87	0.55
1:B:790:TYR:CD1	1:B:800:PRO:HA	2.41	0.55
1:D:641:GLU:H	1:D:641:GLU:CD	2.08	0.55
1:D:743:ILE:HA	1:D:746:ILE:HG13	1.88	0.55
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.88	0.55
1:E:165:ALA:HB3	1:E:313:MET:HE2	1.88	0.55
1:E:520:PHE:HE2	1:E:973:ARG:HG3	1.68	0.55
1:F:678:THR:O	1:F:830:GLN:HG2	2.06	0.55
1:A:527:TYR:CE2	1:A:972:LEU:HG	2.40	0.55
1:A:1038:GLU:CA	1:A:1039:ASP:HB2	2.36	0.55
1:C:272:GLY:N	1:C:275:TYR:OH	2.39	0.55
1:C:465:ALA:O	1:C:469:GLN:HG2	2.05	0.55
1:D:527:TYR:O	1:D:530:SER:HB3	2.07	0.55
1:D:549:VAL:HG22	1:D:906:PRO:HG2	1.88	0.55
1:D:801:PHE:CD1	1:D:805:SER:HB3	2.40	0.55
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.39	0.55
1:F:77:TYR:CD1	1:F:93:THR:HB	2.41	0.55
1:F:186:ILE:HG13	1:F:268:ILE:HG13	1.87	0.55
1:A:508:GLY:N	1:A:518:ARG:HG3	2.20	0.55
1:A:979:SER:OG	1:A:1015:THR:HG21	2.06	0.55
1:B:369:THR:O	1:B:372:VAL:HG23	2.07	0.55
1:B:602:GLU:OE2	1:B:647:ILE:HG12	2.06	0.55
1:C:680:PHE:CD2	1:C:859:TRP:HZ3	2.24	0.55
1:D:167:SER:OG	1:E:70:ASN:HB2	2.07	0.55
1:D:781:MET:HE1	1:F:225:VAL:N	2.10	0.55
1:F:155:SER:HB3	1:F:180:SER:N	2.21	0.55
1:F:744:ASN:O	1:F:748:THR:HG23	2.06	0.55
1:A:622:GLN:NE2	1:C:231:ASN:OD1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:HD12	1:B:323:ILE:HG13	1.88	0.55
1:D:30:LEU:HD13	1:D:384:ALA:HB2	1.88	0.55
1:D:225:VAL:HG13	1:E:781:MET:SD	2.47	0.55
1:D:514:GLY:HA2	1:D:517:ASN:ND2	2.15	0.55
1:A:359:LEU:HD13	1:A:417:GLU:HG3	1.89	0.55
1:A:515:TRP:HB3	1:A:519:MET:CE	2.37	0.55
1:B:1011:MET:O	1:B:1015:THR:HG23	2.07	0.55
1:C:151:GLN:O	1:C:155:SER:OG	2.17	0.55
1:C:346:GLU:O	1:C:350:LEU:HD22	2.07	0.55
1:C:876:LEU:HD21	1:C:932:LEU:HD11	1.89	0.55
1:E:961:ILE:O	1:E:965:LEU:HD22	2.07	0.55
1:F:9:PRO:HG3	1:F:495:THR:HG21	1.88	0.55
1:B:682:PHE:HE2	1:B:857:TYR:HA	1.72	0.55
1:C:83:ASP:HB3	1:C:87:THR:O	2.07	0.55
1:D:764:ASP:C	1:D:766:GLY:H	2.09	0.55
1:E:767:ARG:HH22	1:F:67:GLN:CD	2.09	0.55
1:F:149:MET:HB2	1:F:153:ASP:HB3	1.87	0.55
1:F:504:ASP:O	1:F:506:GLY:N	2.40	0.55
1:B:35:TYR:OH	1:B:670:ALA:HB1	2.06	0.55
1:B:867:ARG:O	1:B:867:ARG:NE	2.22	0.55
1:C:728:LYS:HG2	1:C:808:ARG:NH2	2.22	0.55
1:D:671:ILE:HD13	1:D:674:LEU:N	2.19	0.55
1:E:133:SER:OG	1:E:292:LYS:NZ	2.38	0.55
1:E:894:SER:HB3	1:E:897:ILE:HG12	1.88	0.55
1:F:679:GLY:HA2	1:F:837:THR:HG23	1.88	0.55
1:F:924:ASP:OD1	1:F:926:TYR:N	2.40	0.55
1:A:239:ARG:HD3	1:A:761:ASP:O	2.07	0.55
1:A:582:ALA:CB	1:A:586:ARG:HE	2.20	0.55
1:A:602:GLU:HB3	1:A:606:VAL:HG23	1.89	0.55
1:D:909:VAL:HG13	1:D:931:LEU:HD21	1.88	0.55
1:E:10:ILE:HG13	1:F:895:TRP:CZ2	2.42	0.55
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.88	0.55
1:E:790:TYR:HB3	1:E:798:MET:HB3	1.89	0.55
1:F:699:ARG:HD3	1:F:825:MET:SD	2.47	0.55
1:A:136:PHE:HA	1:A:292:LYS:HA	1.88	0.55
1:B:239:ARG:HD2	1:B:763:ILE:HD11	1.87	0.55
1:C:84:SER:HB2	1:C:814:PRO:HA	1.89	0.55
1:D:38:ILE:HB	1:D:462:SER:OG	2.07	0.55
1:D:641:GLU:OE1	1:D:641:GLU:N	2.40	0.55
1:F:520:PHE:HE2	1:F:973:ARG:HG3	1.71	0.55
1:F:906:PRO:O	1:F:910:ILE:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:990:VAL:HG21	1:F:1008:MET:SD	2.47	0.55
1:A:344:LEU:HG	1:A:399:VAL:HG23	1.88	0.55
1:A:905:VAL:HG23	1:A:906:PRO:HD3	1.89	0.55
1:C:213:GLN:HA	1:C:237:GLN:O	2.07	0.55
1:C:557:VAL:C	1:C:559:LEU:H	2.10	0.55
1:C:960:LEU:HD23	1:C:1031:ARG:HH21	1.72	0.55
1:D:136:PHE:CE2	1:D:290:GLY:HA3	2.42	0.55
1:D:728:LYS:HD2	1:F:235:ILE:HB	1.89	0.55
1:D:850:LYS:NZ	1:D:850:LYS:HB2	2.22	0.55
1:E:60:THR:HG22	1:E:119:PRO:HD3	1.87	0.55
1:E:130:GLU:HG2	1:F:113:LEU:HD21	1.89	0.55
1:E:888:LEU:HD13	1:E:901:VAL:HG11	1.89	0.55
1:B:880:SER:O	1:B:883:VAL:HG12	2.07	0.54
1:C:402:ILE:O	1:C:406:VAL:HG22	2.07	0.54
1:D:343:THR:HA	1:D:346:GLU:OE1	2.07	0.54
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.89	0.54
1:F:356:TYR:HA	1:F:365:THR:HG21	1.89	0.54
1:A:108:GLN:HE21	1:A:129:VAL:HB	1.72	0.54
1:A:817:GLU:HG3	1:A:824:SER:O	2.06	0.54
1:B:727:PHE:CZ	1:B:807:SER:HB2	2.42	0.54
1:C:279:ALA:HB3	1:C:286:ALA:O	2.08	0.54
1:C:419:VAL:CG2	1:C:434:SER:HB2	2.36	0.54
1:D:75:LEU:HA	1:D:94:PHE:HD2	1.72	0.54
1:E:143:ILE:HG22	1:E:286:ALA:CB	2.37	0.54
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.89	0.54
1:E:350:LEU:HD22	1:E:984:LEU:HD12	1.90	0.54
1:F:184:MET:HB2	1:F:762:PHE:CE2	2.43	0.54
1:F:573:MET:HG3	1:F:666:PHE:HE2	1.70	0.54
1:F:1038:GLU:HA	1:F:1039:ASP:CG	2.27	0.54
1:A:109:ASN:ND2	1:B:109:ASN:HD21	2.06	0.54
1:A:383:LEU:O	1:A:386:PHE:N	2.36	0.54
1:A:584:GLN:N	1:A:622:GLN:OE1	2.24	0.54
1:C:5:PHE:C	1:C:7:ASP:N	2.61	0.54
1:C:465:ALA:O	1:C:468:ARG:HB3	2.08	0.54
1:C:466:ILE:HD13	1:C:466:ILE:N	2.22	0.54
1:D:294:ALA:O	1:D:296:GLY:N	2.40	0.54
1:E:680:PHE:HB2	1:E:859:TRP:HZ3	1.72	0.54
1:E:907:LEU:HG	1:E:1017:LEU:HD22	1.89	0.54
1:F:534:ILE:HG22	1:F:541:TYR:CZ	2.42	0.54
1:F:757:SER:O	1:F:772:TYR:HA	2.06	0.54
1:F:919:ARG:HG3	1:F:919:ARG:NH1	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:ILE:HD11	1:A:1024:VAL:CG2	2.38	0.54
1:B:974:PRO:O	1:B:977:MET:N	2.39	0.54
1:C:671:ILE:HG21	1:C:674:LEU:HB2	1.89	0.54
1:D:267:LYS:HZ1	1:D:268:ILE:H	1.53	0.54
1:D:959:GLY:HA3	1:D:1040:ILE:HG21	1.89	0.54
1:E:743:ILE:HG23	1:E:746:ILE:HD11	1.88	0.54
1:F:443:VAL:HG12	1:F:891:LEU:HD21	1.89	0.54
1:B:437:GLN:HG3	1:B:438:ILE:HG23	1.89	0.54
1:B:878:ALA:O	1:B:882:ILE:HG13	2.07	0.54
1:B:919:ARG:NH2	1:B:990:VAL:O	2.40	0.54
1:C:435:MET:HA	1:C:438:ILE:HG12	1.88	0.54
1:D:81:ASN:O	1:D:88:VAL:HA	2.08	0.54
1:D:754:TRP:NE1	1:D:780:ARG:HB3	2.22	0.54
1:E:801:PHE:HD1	1:E:804:PHE:HE2	1.54	0.54
1:F:56:THR:O	1:F:60:THR:OG1	2.13	0.54
1:A:605:ASN:N	1:A:605:ASN:OD1	2.40	0.54
1:A:924:ASP:OD1	1:A:926:TYR:N	2.41	0.54
1:B:684:LEU:HD12	1:B:856:GLY:O	2.07	0.54
1:C:74:ASN:HB2	1:C:98:THR:CG2	2.37	0.54
1:C:509:LYS:HZ2	1:C:513:PHE:HB2	1.73	0.54
1:D:737:GLN:HE22	1:F:250:LEU:HD23	1.73	0.54
1:E:686:ASP:HB3	1:E:823:PRO:HB2	1.88	0.54
1:E:925:VAL:HA	1:E:928:GLN:HG2	1.90	0.54
1:E:957:GLY:HA2	1:E:1042:HIS:HB3	1.88	0.54
1:F:584:GLN:N	1:F:622:GLN:OE1	2.30	0.54
1:F:621:GLY:O	1:F:624:THR:OG1	2.24	0.54
1:F:909:VAL:HG13	1:F:931:LEU:HD11	1.89	0.54
1:A:170:SER:HB3	1:B:74:ASN:N	2.21	0.54
1:C:430:ALA:O	1:C:434:SER:HB3	2.08	0.54
1:C:926:TYR:HE1	1:C:999:ALA:HB1	1.71	0.54
1:F:121:GLU:HA	1:F:124:GLN:HG2	1.90	0.54
1:F:693:GLU:HB3	1:F:694:LYS:HE3	1.88	0.54
1:A:70:ASN:OD1	1:C:167:SER:OG	2.20	0.54
1:A:674:LEU:HD22	1:A:862:MET:HB3	1.90	0.54
1:A:1041:GLU:CG	1:A:1042:HIS:HA	2.37	0.54
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.88	0.54
1:E:199:THR:HB	1:E:749:THR:HG21	1.90	0.54
1:A:281:PHE:CE2	1:A:324:VAL:HG21	2.42	0.54
1:B:185:ARG:HB3	1:B:187:TRP:HE1	1.73	0.54
1:C:49:TYR:CE2	1:C:119:PRO:HG2	2.43	0.54
1:C:97:GLY:C	1:C:99:ASP:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:860:THR:HA	1:C:864:TYR:HB2	1.90	0.54
1:D:364:ALA:HB2	1:D:497:LEU:HD13	1.89	0.54
1:E:690:LEU:HD22	1:E:694:LYS:HD2	1.90	0.54
1:A:308:ALA:O	1:A:312:LYS:HG3	2.08	0.54
1:A:354:VAL:HG22	1:A:980:LEU:HD23	1.90	0.54
1:A:834:GLY:C	1:A:835:LYS:HD2	2.28	0.54
1:A:900:SER:HA	1:A:1029:VAL:HG21	1.90	0.54
1:B:278:ILE:HD11	1:B:280:GLU:OE1	2.07	0.54
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.72	0.54
1:E:138:MET:O	1:E:291:ILE:N	2.39	0.54
1:E:445:ILE:HG21	1:E:940:LYS:HD2	1.89	0.54
1:E:597:TYR:HE2	1:E:651:ALA:HA	1.73	0.54
1:F:414:GLU:OE2	1:F:415:ASN:ND2	2.41	0.54
1:A:149:MET:SD	1:A:153:ASP:HB3	2.48	0.53
1:A:1030:ARG:O	1:A:1032:ARG:N	2.42	0.53
1:C:468:ARG:O	1:C:472:ILE:HG22	2.08	0.53
1:D:94:PHE:CE1	1:D:103:ALA:HB1	2.43	0.53
1:D:142:VAL:HG21	1:D:158:VAL:HG22	1.90	0.53
1:D:190:PRO:HB3	1:D:789:TRP:CH2	2.43	0.53
1:D:836:SER:HB3	1:D:839:GLU:HG3	1.90	0.53
1:E:790:TYR:HD1	1:E:800:PRO:HA	1.73	0.53
1:F:348:ILE:HD11	1:F:372:VAL:HG11	1.89	0.53
1:F:940:LYS:HZ3	1:F:978:THR:HG21	1.71	0.53
1:C:508:GLY:O	1:C:509:LYS:HB2	2.09	0.53
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.29	0.53
1:D:746:ILE:O	1:D:749:THR:OG1	2.26	0.53
1:D:992:SER:O	1:D:997:SER:OG	2.24	0.53
1:E:62:THR:HG21	1:E:818:ARG:HD3	1.89	0.53
1:E:527:TYR:CE1	1:E:968:VAL:HG13	2.43	0.53
1:F:178:PHE:O	1:F:287:SER:OG	2.12	0.53
1:F:919:ARG:HH11	1:F:919:ARG:CG	2.20	0.53
1:A:214:VAL:HG23	1:A:236:ALA:HB1	1.90	0.53
1:A:530:SER:HB2	2:A:2000:LMT:H1'	1.91	0.53
1:A:685:ILE:HD11	1:A:819:TYR:HD2	1.73	0.53
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.08	0.53
1:C:4:PHE:CE2	1:C:436:GLY:HA3	2.43	0.53
1:C:68:ASN:HB3	1:C:114:ALA:HB2	1.90	0.53
1:C:291:ILE:HD13	1:C:306:ILE:HD12	1.91	0.53
1:C:762:PHE:HE1	1:C:764:ASP:HB2	1.73	0.53
1:F:922:THR:O	1:F:924:ASP:N	2.41	0.53
1:B:597:TYR:HE1	1:B:651:ALA:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:HD12	1:D:789:TRP:HZ3	1.73	0.53
1:D:359:LEU:C	1:D:361:ASN:H	2.12	0.53
1:E:7:ASP:O	1:E:8:ARG:HG3	2.09	0.53
1:E:445:ILE:HD13	1:E:940:LYS:CE	2.38	0.53
1:E:457:ALA:HB2	1:E:471:SER:CB	2.39	0.53
1:F:565:PRO:O	1:F:670:ALA:HB2	2.07	0.53
1:F:674:LEU:HD22	1:F:861:GLY:HA2	1.91	0.53
1:B:682:PHE:CE2	1:B:857:TYR:HA	2.43	0.53
1:B:971:ARG:HB3	1:B:971:ARG:HH11	1.74	0.53
1:C:456:MET:HA	1:C:459:PHE:HD1	1.73	0.53
1:C:952:LEU:HB2	1:C:963:ALA:HB1	1.91	0.53
1:D:578:LEU:HD21	1:D:587:THR:HA	1.90	0.53
1:E:709:HIS:ND1	1:E:843:LEU:HD21	2.24	0.53
1:F:45:ILE:HD11	1:F:92:LEU:HD21	1.90	0.53
1:F:62:THR:HG22	1:F:88:VAL:HG21	1.91	0.53
1:F:566:ASP:OD1	1:F:678:THR:HG23	2.09	0.53
1:A:488:LEU:HG	1:A:492:LEU:HG	1.90	0.53
1:A:932:LEU:O	1:A:935:ILE:HB	2.09	0.53
1:B:189:ASN:ND2	1:B:190:PRO:HD2	2.24	0.53
1:B:597:TYR:CE1	1:B:651:ALA:HA	2.43	0.53
1:B:889:ALA:CB	1:B:898:PRO:HG3	2.38	0.53
1:B:953:MET:SD	1:B:1040:ILE:HD13	2.49	0.53
1:C:120:GLN:HA	1:C:123:GLN:HB2	1.89	0.53
1:C:836:SER:OG	1:C:837:THR:N	2.40	0.53
1:D:859:TRP:CE3	1:D:863:SER:HB3	2.42	0.53
1:D:886:LEU:HD11	1:F:17:ILE:HG22	1.90	0.53
1:D:901:VAL:HG21	1:D:943:ILE:HG12	1.91	0.53
1:A:109:ASN:HD22	1:B:109:ASN:HD21	1.57	0.53
1:A:214:VAL:HG23	1:A:236:ALA:CB	2.38	0.53
1:A:790:TYR:HE2	1:A:800:PRO:HB3	1.74	0.53
1:B:719:ASN:HB2	1:B:828:LEU:HG	1.91	0.53
1:B:818:ARG:NH2	1:B:821:GLY:O	2.42	0.53
1:C:48:SER:HA	1:C:86:GLY:O	2.09	0.53
1:C:330:THR:H	1:C:331:PRO:HD2	1.74	0.53
1:D:119:PRO:HB2	1:D:122:VAL:HG23	1.90	0.53
1:D:142:VAL:HG13	1:D:321:LEU:HD11	1.91	0.53
1:D:341:VAL:HG23	1:D:395:MET:HE1	1.91	0.53
1:D:456:MET:SD	1:D:877:TYR:OH	2.53	0.53
1:E:99:ASP:HB3	1:E:102:ILE:HB	1.91	0.53
1:E:573:MET:HB3	1:E:628:PHE:HA	1.91	0.53
1:F:944:LEU:HB3	1:F:971:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.90	0.53
1:B:69:MET:HG2	1:B:110:LYS:C	2.29	0.53
1:B:420:MET:SD	1:B:430:ALA:HB3	2.49	0.53
1:B:435:MET:O	1:B:439:GLN:HG3	2.09	0.53
1:B:584:GLN:HB2	1:B:622:GLN:HG2	1.90	0.53
1:B:1021:PHE:O	1:B:1025:PHE:N	2.38	0.53
1:C:5:PHE:O	1:C:7:ASP:N	2.42	0.53
1:C:424:GLY:HA3	1:C:502:LYS:N	2.24	0.53
1:C:467:TYR:HE1	1:C:872:GLN:HE22	1.57	0.53
1:E:744:ASN:N	1:E:744:ASN:OD1	2.40	0.53
1:F:17:ILE:HA	1:F:20:MET:HE2	1.90	0.53
1:F:911:GLY:HA3	1:F:1013:THR:OG1	2.08	0.53
1:A:199:THR:HG21	1:A:792:ARG:H	1.74	0.53
1:A:216:ALA:HB1	1:A:234:ILE:HG22	1.90	0.53
1:B:559:LEU:HD11	1:B:922:THR:HA	1.91	0.53
1:B:883:VAL:O	1:B:887:CYS:HB3	2.09	0.53
1:C:27:ILE:HA	1:C:30:LEU:HD22	1.91	0.53
1:C:455:PRO:HG2	1:C:880:SER:HB2	1.90	0.53
1:C:585:GLU:O	1:C:589:LYS:HG3	2.09	0.53
1:D:143:ILE:HG21	1:D:281:PHE:CD2	2.44	0.53
1:E:420:MET:CE	1:E:500:ILE:H	2.22	0.53
1:F:393:LEU:CD1	1:F:466:ILE:HA	2.39	0.53
1:F:647:ILE:HG22	1:F:648:THR:N	2.24	0.53
1:F:654:ALA:O	1:F:658:ILE:HG12	2.09	0.53
1:A:244:GLU:HG2	1:A:248:LYS:HE2	1.91	0.53
1:A:877:TYR:O	1:A:881:LEU:HB2	2.09	0.53
1:B:225:VAL:H	1:C:781:MET:HE1	1.74	0.53
1:B:1018:ALA:O	1:B:1022:VAL:HG23	2.09	0.53
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.91	0.53
1:C:429:GLU:O	1:C:433:LYS:HG2	2.09	0.53
1:E:214:VAL:HG23	1:E:237:GLN:HB3	1.91	0.53
1:E:698:ALA:O	1:E:701:GLN:HG2	2.09	0.53
1:F:5:PHE:C	1:F:7:ASP:H	2.10	0.53
1:F:795:ASP:OD2	1:F:796:GLY:N	2.42	0.53
1:A:44:THR:HG22	1:A:91:THR:OG1	2.09	0.52
1:B:186:ILE:HD13	1:B:262:LEU:HD21	1.91	0.52
1:B:214:VAL:CG2	1:B:237:GLN:HB3	2.39	0.52
1:B:681:ASP:HA	1:B:828:LEU:HA	1.91	0.52
1:B:899:PHE:HD1	1:B:902:MET:HE1	1.73	0.52
1:C:138:MET:O	1:C:291:ILE:HG13	2.09	0.52
1:C:503:GLY:HA2	1:C:505:HIS:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:896:SER:HB2	1:C:1029:VAL:CG1	2.39	0.52
1:F:137:LEU:HD22	1:F:293:LEU:HD23	1.91	0.52
1:A:768:VAL:HG12	1:B:63:GLN:OE1	2.09	0.52
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.44	0.52
1:C:57:VAL:HA	1:C:61:VAL:HG23	1.91	0.52
1:C:81:ASN:OD1	1:C:815:ARG:NH1	2.41	0.52
1:C:966:ASP:O	1:C:970:MET:SD	2.68	0.52
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.08	0.52
1:D:549:VAL:O	1:D:552:MET:HB3	2.08	0.52
1:D:695:LEU:HD13	1:D:825:MET:SD	2.50	0.52
1:F:348:ILE:HG12	1:F:402:ILE:CD1	2.39	0.52
1:A:45:ILE:HG23	1:A:129:VAL:CG2	2.28	0.52
1:A:133:SER:OG	1:A:135:SER:O	2.22	0.52
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.45	0.52
1:B:45:ILE:HD11	1:B:107:VAL:HG11	1.91	0.52
1:B:696:THR:O	1:B:700:ASN:ND2	2.41	0.52
1:C:6:ILE:HG22	1:C:12:ALA:HB2	1.91	0.52
1:C:35:TYR:HB3	1:C:36:PRO:HD2	1.92	0.52
1:C:65:ILE:HA	1:C:114:ALA:CB	2.38	0.52
1:D:24:GLY:O	1:D:28:LEU:HG	2.09	0.52
1:D:785:ASP:OD1	1:D:785:ASP:N	2.43	0.52
1:E:508:GLY:H	1:E:518:ARG:HE	1.57	0.52
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.91	0.52
1:A:343:THR:OG1	1:A:989:LEU:HD21	2.09	0.52
1:A:359:LEU:O	1:A:361:ASN:N	2.42	0.52
1:B:152:GLU:HB3	1:B:182:TYR:HE1	1.74	0.52
1:B:180:SER:OG	1:B:274:ASN:O	2.22	0.52
1:B:618:ALA:O	1:B:815:ARG:NE	2.42	0.52
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.92	0.52
1:D:112:GLN:HE21	1:E:112:GLN:HB3	1.74	0.52
1:D:801:PHE:HD1	1:D:805:SER:HB3	1.74	0.52
1:E:30:LEU:HB3	1:E:390:ILE:HD11	1.92	0.52
1:E:143:ILE:HD13	1:E:281:PHE:HD2	1.74	0.52
1:E:986:VAL:HG21	1:E:1007:VAL:HG11	1.91	0.52
1:F:383:LEU:HD23	1:F:472:ILE:HD12	1.92	0.52
1:A:515:TRP:O	1:A:519:MET:HG3	2.10	0.52
1:B:219:LEU:HA	1:C:754:TRP:HZ3	1.75	0.52
1:D:340:VAL:HG12	1:D:395:MET:HE3	1.92	0.52
1:E:552:MET:HB2	1:E:910:ILE:HG12	1.91	0.52
1:F:219:LEU:H	1:F:219:LEU:CD2	2.16	0.52
1:B:754:TRP:CD2	1:B:780:ARG:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:PHE:HD2	1:C:610:PHE:CE1	2.28	0.52
1:D:13:TRP:HE1	1:D:492:LEU:HD21	1.74	0.52
1:D:293:LEU:HD13	1:D:294:ALA:N	2.24	0.52
1:E:158:VAL:HG11	1:E:177:LEU:HD13	1.92	0.52
1:E:274:ASN:OD1	1:E:275:TYR:N	2.42	0.52
1:E:456:MET:O	1:E:467:TYR:HB3	2.10	0.52
1:E:1015:THR:OG1	1:E:1016:VAL:N	2.43	0.52
1:F:188:MET:HE1	1:F:200:PRO:HG3	1.90	0.52
1:F:785:ASP:N	1:F:785:ASP:OD1	2.41	0.52
1:F:833:PRO:C	1:F:835:LYS:H	2.11	0.52
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.91	0.52
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.90	0.52
1:A:422:GLU:HG3	1:A:423:GLU:HG3	1.91	0.52
1:A:520:PHE:HE2	1:A:973:ARG:HG3	1.75	0.52
1:A:960:LEU:HD11	1:A:1027:VAL:HA	1.92	0.52
1:A:961:ILE:HG13	1:A:1039:ASP:CG	2.30	0.52
1:B:235:ILE:HD11	1:C:726:GLN:OE1	2.09	0.52
1:C:136:PHE:HA	1:C:292:LYS:HA	1.92	0.52
1:C:146:ASP:CG	1:C:147:GLY:H	2.12	0.52
1:D:347:ALA:HA	1:D:350:LEU:HD12	1.91	0.52
1:E:787:GLY:O	1:E:789:TRP:N	2.43	0.52
1:F:15:ILE:HG21	1:F:487:ILE:HG21	1.92	0.52
1:F:240:LEU:HB2	1:F:246:PHE:HE1	1.72	0.52
1:F:597:TYR:CD1	1:F:601:LYS:HD2	2.45	0.52
1:F:870:GLY:O	1:F:872:GLN:N	2.42	0.52
1:F:901:VAL:O	1:F:904:VAL:HG23	2.09	0.52
1:A:109:ASN:HD22	1:B:109:ASN:ND2	2.07	0.52
1:B:34:GLN:C	1:B:35:TYR:HD1	2.13	0.52
1:B:158:VAL:HG13	1:B:289:LEU:HD11	1.91	0.52
1:C:73:ASP:O	1:C:98:THR:HG21	2.10	0.52
1:C:394:THR:HB	1:C:469:GLN:OE1	2.09	0.52
1:C:509:LYS:NZ	1:C:513:PHE:HB2	2.25	0.52
1:D:20:MET:HE3	1:D:377:LEU:HD22	1.92	0.52
1:D:193:LEU:CD1	1:D:200:PRO:HD3	2.39	0.52
1:D:544:LEU:HG	1:D:544:LEU:O	2.10	0.52
1:E:480:LEU:HA	1:E:483:LEU:HD12	1.91	0.52
1:E:986:VAL:HG11	1:E:1007:VAL:HG12	1.92	0.52
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.16	0.52
1:F:190:PRO:HB3	1:F:789:TRP:CH2	2.45	0.52
1:A:214:VAL:HG11	1:B:747:ASN:ND2	2.25	0.52
1:B:76:MET:HE3	1:B:864:TYR:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HA	1:B:451:ALA:HB3	1.91	0.52
1:C:858:ASP:OD2	1:C:859:TRP:N	2.43	0.52
1:D:222:THR:HA	1:D:224:PRO:HD3	1.92	0.52
1:E:366:LEU:O	1:E:369:THR:HB	2.10	0.52
1:F:177:LEU:HD22	1:F:178:PHE:N	2.25	0.52
1:F:453:PHE:O	1:F:456:MET:HG2	2.10	0.52
1:A:68:ASN:C	1:A:70:ASN:H	2.13	0.52
1:B:36:PRO:O	1:B:38:ILE:HG13	2.10	0.52
1:B:108:GLN:OE1	1:C:112:GLN:HB3	2.10	0.52
1:C:163:LYS:HD2	1:C:289:LEU:CD2	2.39	0.52
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.91	0.52
1:D:451:ALA:HB1	1:D:883:VAL:HG12	1.92	0.52
1:D:804:PHE:CD2	1:D:804:PHE:N	2.78	0.52
1:D:1011:MET:O	1:D:1015:THR:HG23	2.09	0.52
1:E:514:GLY:C	1:E:516:PHE:H	2.12	0.52
1:F:99:ASP:O	1:F:102:ILE:HG22	2.10	0.52
1:F:294:ALA:HB3	1:F:297:ALA:HB2	1.92	0.52
1:F:310:LEU:HD23	1:F:323:ILE:HD13	1.91	0.52
1:F:310:LEU:HD23	1:F:323:ILE:HG21	1.91	0.52
1:F:330:THR:H	1:F:331:PRO:HD2	1.75	0.52
1:F:420:MET:SD	1:F:500:ILE:HG23	2.49	0.52
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.91	0.52
1:F:1038:GLU:HA	1:F:1039:ASP:CB	2.40	0.52
1:A:388:PHE:HE1	1:A:472:ILE:HG12	1.75	0.51
1:A:468:ARG:HG3	1:A:472:ILE:HD13	1.91	0.51
1:A:507:GLU:CG	1:A:518:ARG:HG2	2.39	0.51
1:A:540:ARG:HB3	1:A:541:TYR:CD2	2.45	0.51
1:A:559:LEU:HD23	1:A:560:PRO:CD	2.40	0.51
1:A:990:VAL:HG21	1:A:1008:MET:SD	2.50	0.51
1:B:156:ASP:CG	1:B:765:ARG:HH22	2.13	0.51
1:B:407:ASP:CG	1:B:940:LYS:HE3	2.30	0.51
1:C:77:TYR:O	1:C:93:THR:HB	2.10	0.51
1:C:435:MET:HE1	1:C:439:GLN:HA	1.92	0.51
1:C:686:ASP:HB3	1:C:823:PRO:O	2.09	0.51
1:C:738:ALA:O	1:C:740:GLY:N	2.43	0.51
1:C:940:LYS:O	1:C:943:ILE:HB	2.10	0.51
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.92	0.51
1:D:597:TYR:HE2	1:D:651:ALA:HA	1.76	0.51
1:E:434:SER:O	1:E:437:GLN:N	2.40	0.51
1:E:790:TYR:CD1	1:E:800:PRO:HA	2.44	0.51
1:E:949:ALA:HB3	1:E:1026:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:TYR:CD2	1:F:819:TYR:OH	2.62	0.51
1:A:1039:ASP:N	1:A:1040:ILE:HA	2.25	0.51
1:B:38:ILE:CG2	1:B:462:SER:HB3	2.40	0.51
1:C:185:ARG:HD2	1:C:187:TRP:NE1	2.12	0.51
1:D:157:TYR:HE2	1:D:161:ASN:CG	2.12	0.51
1:D:583:THR:HA	1:D:622:GLN:OE1	2.10	0.51
1:D:897:ILE:HG12	1:D:1030:ARG:HD3	1.92	0.51
1:D:980:LEU:O	1:D:984:LEU:HB2	2.11	0.51
1:E:459:PHE:CE2	1:E:876:LEU:HD12	2.45	0.51
1:E:605:ASN:ND2	1:E:647:ILE:HD11	2.25	0.51
1:F:41:PRO:O	1:F:94:PHE:HB2	2.10	0.51
1:F:356:TYR:C	1:F:358:PHE:H	2.12	0.51
1:F:401:ALA:HA	1:F:404:LEU:HD22	1.91	0.51
1:F:459:PHE:HE2	1:F:876:LEU:HA	1.76	0.51
1:A:375:VAL:HG23	1:A:480:LEU:HB3	1.92	0.51
1:B:899:PHE:HA	1:B:902:MET:HE3	1.93	0.51
1:C:358:PHE:CD1	1:C:977:MET:HG2	2.45	0.51
1:C:591:LEU:HD13	1:C:611:ALA:HB1	1.92	0.51
1:D:545:TYR:HA	1:D:548:ILE:HD12	1.91	0.51
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.93	0.51
1:D:712:MET:O	1:D:832:ALA:N	2.43	0.51
1:E:219:LEU:HD23	1:F:754:TRP:CZ3	2.45	0.51
1:E:527:TYR:OH	1:E:1019:ILE:O	2.21	0.51
1:E:885:PHE:CE1	1:E:899:PHE:CE1	2.99	0.51
1:E:909:VAL:O	1:E:911:GLY:N	2.43	0.51
1:F:77:TYR:CE1	1:F:93:THR:HB	2.46	0.51
1:F:873:ALA:HB2	1:F:928:GLN:HE21	1.73	0.51
1:A:4:PHE:O	1:A:8:ARG:HD2	2.10	0.51
1:A:281:PHE:HB2	1:A:610:PHE:CE1	2.44	0.51
1:B:368:PRO:O	1:B:371:ALA:HB3	2.10	0.51
1:B:448:VAL:O	1:B:451:ALA:HB3	2.10	0.51
1:B:925:VAL:O	1:B:928:GLN:N	2.44	0.51
1:B:1016:VAL:O	1:B:1017:LEU:HD12	2.11	0.51
1:C:412:VAL:HG11	1:C:485:ALA:O	2.10	0.51
1:C:540:ARG:HD3	1:C:541:TYR:HE1	1.76	0.51
1:C:702:LEU:HB2	1:C:851:LEU:HD11	1.91	0.51
1:C:909:VAL:O	1:C:912:ALA:N	2.44	0.51
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.91	0.51
1:E:594:VAL:O	1:E:597:TYR:N	2.44	0.51
1:E:645:GLU:O	1:E:648:THR:OG1	2.25	0.51
1:F:163:LYS:O	1:F:163:LYS:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:417:GLU:OE2	1:F:500:ILE:HG21	2.11	0.51
1:A:117:LEU:HD11	1:C:125:GLN:OE1	2.10	0.51
1:A:182:TYR:HB2	1:A:769:LYS:HZ2	1.74	0.51
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.92	0.51
1:B:524:THR:O	1:B:528:THR:N	2.39	0.51
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.92	0.51
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.91	0.51
1:C:563:PHE:HB2	1:C:866:GLU:CG	2.40	0.51
1:D:246:PHE:O	1:D:262:LEU:HD23	2.10	0.51
1:E:465:ALA:HA	1:E:468:ARG:NH1	2.25	0.51
1:E:722:GLU:HG3	1:E:723:ASP:H	1.76	0.51
1:F:240:LEU:HD11	1:F:249:ILE:HD11	1.92	0.51
1:A:35:TYR:HA	1:A:391:ASN:ND2	2.25	0.51
1:A:38:ILE:HG22	1:A:462:SER:OG	2.09	0.51
1:A:117:LEU:HD11	1:C:125:GLN:HE22	1.76	0.51
1:A:157:TYR:HE1	1:A:318:PRO:HD2	1.75	0.51
1:A:178:PHE:HB2	1:A:288:GLY:H	1.76	0.51
1:A:195:LYS:HB3	1:A:196:PHE:CD2	2.46	0.51
1:B:253:VAL:HG13	1:B:259:ARG:HB3	1.91	0.51
1:B:402:ILE:O	1:B:406:VAL:HG22	2.11	0.51
1:D:573:MET:HG3	1:D:666:PHE:HE1	1.74	0.51
1:D:737:GLN:NE2	1:F:250:LEU:HD23	2.24	0.51
1:D:760:ASN:H	1:D:771:VAL:HB	1.75	0.51
1:D:858:ASP:OD2	1:D:859:TRP:N	2.42	0.51
1:E:717:ARG:O	1:E:717:ARG:HD3	2.11	0.51
1:F:182:TYR:HB2	1:F:769:LYS:NZ	2.25	0.51
1:F:249:ILE:HB	1:F:262:LEU:HB2	1.93	0.51
1:F:393:LEU:CD1	1:F:466:ILE:HG12	2.40	0.51
1:F:452:VAL:HG12	1:F:884:VAL:CG2	2.41	0.51
1:F:1033:PHE:C	1:F:1035:ARG:N	2.64	0.51
1:A:43:VAL:O	1:A:91:THR:HA	2.11	0.51
1:A:240:LEU:HD12	1:A:246:PHE:CE2	2.46	0.51
1:A:372:VAL:HA	1:A:375:VAL:HG12	1.93	0.51
1:A:507:GLU:HG3	1:A:518:ARG:HG2	1.92	0.51
1:A:990:VAL:HG13	1:A:1005:THR:OG1	2.10	0.51
1:B:986:VAL:HG21	1:B:1007:VAL:CG1	2.37	0.51
1:C:108:GLN:HG3	1:C:112:GLN:HE22	1.76	0.51
1:C:138:MET:HG3	1:C:327:TYR:O	2.11	0.51
1:C:607:GLU:HB2	1:C:632:LYS:HG3	1.93	0.51
1:C:864:TYR:HE1	1:C:867:ARG:NH2	2.09	0.51
1:D:210:GLN:HE22	1:D:250:LEU:HB3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:VAL:HG11	1:D:405:LEU:HD21	1.92	0.51
1:E:66:GLU:OE1	1:E:821:GLY:HA2	2.11	0.51
1:E:634:TRP:CD1	1:E:634:TRP:N	2.76	0.51
1:F:940:LYS:CE	1:F:978:THR:HG21	2.41	0.51
1:A:388:PHE:CE1	1:A:472:ILE:HG21	2.46	0.51
1:B:164:ASP:O	1:B:168:ARG:HG3	2.11	0.51
1:B:393:LEU:HD12	1:B:466:ILE:HG23	1.92	0.51
1:B:573:MET:SD	1:B:628:PHE:HE2	2.34	0.51
1:D:281:PHE:CE2	1:D:324:VAL:HG21	2.46	0.51
1:E:13:TRP:HA	1:E:13:TRP:CE3	2.46	0.51
1:E:167:SER:OG	1:F:70:ASN:ND2	2.44	0.51
1:E:190:PRO:HG3	1:E:779:TYR:HB3	1.93	0.51
1:F:5:PHE:CE1	1:F:8:ARG:HD2	2.45	0.51
1:F:573:MET:HG3	1:F:666:PHE:CE2	2.46	0.51
1:A:1031:ARG:C	1:A:1032:ARG:HD2	2.31	0.51
1:B:648:THR:O	1:B:652:THR:HG22	2.11	0.51
1:B:1021:PHE:HB3	1:B:1025:PHE:CE1	2.46	0.51
1:C:95:GLU:O	1:C:98:THR:OG1	2.06	0.51
1:C:181:GLN:HG2	1:C:182:TYR:N	2.24	0.51
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.45	0.51
1:C:404:LEU:HG	1:C:449:LEU:HD13	1.91	0.51
1:C:452:VAL:HG12	1:C:884:VAL:CG2	2.28	0.51
1:C:896:SER:HB2	1:C:1029:VAL:HG12	1.92	0.51
1:D:465:ALA:O	1:D:469:GLN:HG2	2.11	0.51
1:D:470:PHE:CE2	1:D:929:VAL:HG11	2.46	0.51
1:D:555:LEU:HD11	1:D:914:LEU:HD12	1.91	0.51
1:D:702:LEU:CD2	1:D:848:ALA:HB2	2.40	0.51
1:D:753:ALA:O	1:D:774:MET:HG2	2.11	0.51
1:F:1027:VAL:HG13	1:F:1028:VAL:N	2.25	0.51
1:A:658:ILE:O	1:A:659:LYS:NZ	2.33	0.51
1:B:682:PHE:HB3	1:B:827:ILE:HB	1.93	0.51
1:C:125:GLN:OE1	1:C:125:GLN:HA	2.10	0.51
1:C:154:ILE:O	1:C:157:TYR:N	2.43	0.51
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.93	0.51
1:C:416:VAL:HG23	1:C:438:ILE:HD11	1.92	0.51
1:C:895:TRP:O	1:C:898:PRO:HD2	2.10	0.51
1:C:931:LEU:O	1:C:935:ILE:HG22	2.11	0.51
1:E:1037:ASN:HB3	1:E:1040:ILE:HG13	1.93	0.51
1:F:382:VAL:HG11	1:F:476:SER:CB	2.41	0.51
1:F:545:TYR:HB2	1:F:1021:PHE:HE2	1.75	0.51
1:F:843:LEU:O	1:F:843:LEU:HD22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:ARG:HD2	1:B:763:ILE:CD1	2.41	0.50
1:C:586:ARG:HA	1:C:589:LYS:HE2	1.92	0.50
1:C:698:ALA:HB2	1:C:852:PRO:HG2	1.92	0.50
1:C:900:SER:HB3	1:C:1029:VAL:HG11	1.92	0.50
1:C:902:MET:O	1:C:905:VAL:HG22	2.10	0.50
1:D:108:GLN:NE2	1:E:109:ASN:O	2.41	0.50
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.92	0.50
1:D:404:LEU:HD23	1:D:449:LEU:HD11	1.92	0.50
1:E:736:ALA:HB1	1:E:741:VAL:CG2	2.41	0.50
1:F:493:CYS:O	1:F:497:LEU:HB3	2.11	0.50
1:A:838:GLY:HA2	1:A:841:MET:HB2	1.93	0.50
1:A:909:VAL:HG12	1:A:913:LEU:HG	1.94	0.50
1:A:986:VAL:HG21	1:A:1007:VAL:CG1	2.41	0.50
1:B:199:THR:O	1:B:203:VAL:HG23	2.11	0.50
1:C:5:PHE:CD1	1:C:6:ILE:HG12	2.47	0.50
1:C:393:LEU:HD22	1:C:393:LEU:N	2.26	0.50
1:D:249:ILE:O	1:D:262:LEU:N	2.43	0.50
1:E:144:ASN:ND2	1:E:319:SER:O	2.40	0.50
1:E:492:LEU:O	1:E:496:MET:HG2	2.09	0.50
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.92	0.50
1:F:720:GLY:HA2	1:F:815:ARG:HH21	1.75	0.50
1:A:559:LEU:HD22	1:A:923:ASN:H	1.77	0.50
1:B:14:VAL:HG22	1:C:886:LEU:HD12	1.93	0.50
1:C:423:GLU:OE2	1:C:430:ALA:HA	2.12	0.50
1:C:575:MET:HA	1:C:626:ILE:HG13	1.93	0.50
1:C:621:GLY:O	1:C:624:THR:HG23	2.12	0.50
1:D:641:GLU:HB2	1:D:650:ARG:HH22	1.76	0.50
1:D:1020:PHE:CE1	2:D:2000:LMT:H31	2.46	0.50
1:E:990:VAL:HG13	1:E:1005:THR:OG1	2.11	0.50
1:F:75:LEU:HA	1:F:94:PHE:CD1	2.42	0.50
1:F:434:SER:O	1:F:438:ILE:HG12	2.10	0.50
1:F:817:GLU:OE2	1:F:825:MET:HA	2.12	0.50
1:A:166:ILE:CD1	1:A:309:GLU:HG2	2.42	0.50
1:A:680:PHE:HA	1:A:863:SER:OG	2.10	0.50
1:A:735:LYS:O	1:A:739:LEU:HB2	2.11	0.50
1:B:1037:ASN:CA	1:B:1038:GLU:HB2	2.41	0.50
1:C:104:GLN:HE21	1:C:131:LYS:HG3	1.74	0.50
1:C:1027:VAL:HG13	1:C:1028:VAL:HG23	1.93	0.50
1:D:959:GLY:H	1:D:962:GLU:HB3	1.76	0.50
1:E:4:PHE:CD1	1:E:4:PHE:C	2.85	0.50
1:F:959:GLY:HA2	1:F:1041:GLU:H	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:979:SER:HB2	1:F:1011:MET:HE3	1.93	0.50
1:A:112:GLN:NE2	1:B:112:GLN:HB3	2.26	0.50
1:A:239:ARG:NH2	1:B:60:THR:HG23	2.26	0.50
1:A:872:GLN:O	1:A:875:SER:N	2.44	0.50
1:B:76:MET:CE	1:B:864:TYR:HE2	2.24	0.50
1:B:78:MET:O	1:B:819:TYR:HA	2.12	0.50
1:B:149:MET:CE	1:B:153:ASP:HB3	2.40	0.50
1:B:509:LYS:O	1:B:510:LYS:HG2	2.11	0.50
1:C:185:ARG:CD	1:C:187:TRP:HE1	2.16	0.50
1:C:582:ALA:HB1	1:C:586:ARG:HE	1.75	0.50
1:C:897:ILE:HB	1:C:898:PRO:HD3	1.94	0.50
1:F:414:GLU:HG2	1:F:973:ARG:HE	1.77	0.50
1:F:658:ILE:HG13	1:F:659:LYS:NZ	2.27	0.50
1:A:138:MET:HB2	1:A:328:ASP:OD1	2.11	0.50
1:A:186:ILE:HD13	1:A:262:LEU:HD21	1.93	0.50
1:A:193:LEU:HD22	1:A:265:VAL:HB	1.92	0.50
1:A:239:ARG:HH22	1:B:60:THR:HG23	1.76	0.50
1:A:924:ASP:O	1:A:928:GLN:HB2	2.12	0.50
1:C:367:ILE:HD12	1:C:488:LEU:HD21	1.92	0.50
1:E:143:ILE:HD13	1:E:281:PHE:CD2	2.47	0.50
1:E:277:ILE:HD12	1:E:277:ILE:O	2.12	0.50
1:A:113:LEU:HG	1:C:127:VAL:O	2.11	0.50
1:A:545:TYR:O	1:A:548:ILE:N	2.44	0.50
1:B:76:MET:HE3	1:B:864:TYR:CE2	2.47	0.50
1:B:730:ASP:OD1	1:B:808:ARG:NH2	2.45	0.50
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.94	0.50
1:C:456:MET:HB3	1:C:876:LEU:CD2	2.42	0.50
1:C:493:CYS:HA	1:C:497:LEU:HB2	1.93	0.50
1:E:169:THR:HG22	1:E:172:VAL:HG23	1.93	0.50
1:E:278:ILE:HD11	1:E:280:GLU:OE1	2.12	0.50
1:F:217:GLY:O	1:F:234:ILE:HB	2.11	0.50
1:F:393:LEU:HD13	1:F:466:ILE:HA	1.93	0.50
1:F:450:SER:HA	1:F:475:VAL:HG22	1.94	0.50
1:F:583:THR:H	1:F:586:ARG:HG3	1.77	0.50
1:A:143:ILE:O	1:A:321:LEU:HD22	2.11	0.50
1:A:208:LYS:HG3	1:A:759:VAL:HG13	1.93	0.50
1:A:351:VAL:HG22	1:A:981:ALA:HB1	1.93	0.50
1:B:415:ASN:O	1:B:419:VAL:HG22	2.12	0.50
1:B:442:LEU:HD13	1:B:485:ALA:HB1	1.92	0.50
1:B:446:ALA:HB2	1:B:482:VAL:HG11	1.93	0.50
1:B:578:LEU:CD1	1:B:586:ARG:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.94	0.50
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.94	0.50
1:D:141:GLY:O	1:D:323:ILE:HG23	2.12	0.50
1:D:144:ASN:ND2	1:D:148:THR:OG1	2.44	0.50
1:D:187:TRP:HB2	1:D:267:LYS:HB2	1.94	0.50
1:D:267:LYS:HZ2	1:D:268:ILE:H	1.57	0.50
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.42	0.50
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.12	0.50
1:F:787:GLY:C	1:F:789:TRP:H	2.15	0.50
1:F:790:TYR:HB3	1:F:798:MET:HB3	1.93	0.50
1:A:641:GLU:HB2	1:A:650:ARG:HH22	1.77	0.50
1:A:986:VAL:O	1:A:990:VAL:HG23	2.12	0.50
1:A:1024:VAL:O	1:A:1028:VAL:HB	2.12	0.50
1:B:137:LEU:HD12	1:B:329:THR:HG22	1.94	0.50
1:B:187:TRP:HB3	1:B:776:GLU:CG	2.42	0.50
1:B:905:VAL:HG13	1:B:935:ILE:HD12	1.92	0.50
1:B:953:MET:O	1:B:957:GLY:HA2	2.12	0.50
1:C:277:ILE:HG12	1:C:614:GLY:HA3	1.92	0.50
1:C:602:GLU:OE1	1:C:650:ARG:NE	2.31	0.50
1:C:787:GLY:C	1:C:789:TRP:H	2.13	0.50
1:D:1015:THR:OG1	1:D:1016:VAL:N	2.45	0.50
1:E:43:VAL:HG22	1:E:131:LYS:HA	1.94	0.50
1:E:433:LYS:O	1:E:437:GLN:HG3	2.12	0.50
1:E:909:VAL:HG22	1:E:931:LEU:HD21	1.94	0.50
1:F:444:GLY:HA3	1:F:892:TYR:OH	2.12	0.50
1:F:535:LEU:HD21	1:F:1027:VAL:HG21	1.94	0.50
1:A:155:SER:CB	1:A:180:SER:H	2.25	0.49
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.33	0.49
1:A:466:ILE:HD12	1:A:925:VAL:HG21	1.94	0.49
1:A:949:ALA:HB3	1:A:1026:PHE:CE1	2.40	0.49
1:C:3:ASN:O	1:C:7:ASP:N	2.45	0.49
1:C:962:GLU:O	1:C:966:ASP:HB2	2.12	0.49
1:D:75:LEU:HA	1:D:94:PHE:CD2	2.47	0.49
1:D:536:ARG:HD3	2:D:2000:LMT:H4B	1.92	0.49
1:E:175:VAL:HG22	1:F:70:ASN:HD21	1.73	0.49
1:E:476:SER:O	1:E:480:LEU:HB2	2.11	0.49
1:E:729:ILE:HG22	1:E:731:ILE:HD12	1.93	0.49
1:A:5:PHE:CD1	1:A:487:ILE:HG12	2.47	0.49
1:A:47:ALA:O	1:A:87:THR:HA	2.12	0.49
1:B:64:VAL:HG11	1:B:117:LEU:HB3	1.94	0.49
1:B:198:LEU:HD21	1:B:252:LYS:HE3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:ILE:HD11	1:E:726:GLN:HB2	1.93	0.49
1:D:472:ILE:O	1:D:476:SER:HB3	2.13	0.49
1:D:515:TRP:O	1:D:519:MET:HG3	2.12	0.49
1:E:489:THR:HG22	1:E:490:PRO:HD3	1.93	0.49
1:F:151:GLN:HG2	1:F:278:ILE:HG13	1.93	0.49
1:F:459:PHE:CE2	1:F:876:LEU:HA	2.47	0.49
1:F:560:PRO:HG2	1:F:922:THR:HG22	1.93	0.49
1:F:905:VAL:HG22	1:F:935:ILE:HD12	1.92	0.49
1:A:60:THR:HG23	1:A:61:VAL:HG23	1.94	0.49
1:B:11:PHE:CE1	1:C:891:LEU:HG	2.47	0.49
1:B:573:MET:HG3	1:B:666:PHE:CE2	2.47	0.49
1:B:727:PHE:CE2	1:B:729:ILE:HD11	2.46	0.49
1:B:780:ARG:HD2	1:B:780:ARG:O	2.12	0.49
1:B:951:ASP:OD1	1:B:955:LYS:NZ	2.30	0.49
1:C:393:LEU:HG	1:C:466:ILE:CD1	2.42	0.49
1:D:41:PRO:O	1:D:94:PHE:HB2	2.12	0.49
1:D:450:SER:O	1:D:454:VAL:HG23	2.12	0.49
1:D:909:VAL:HG12	1:D:913:LEU:HG	1.94	0.49
1:E:13:TRP:HA	1:E:13:TRP:HE3	1.76	0.49
1:E:52:ALA:HB1	1:E:56:THR:HB	1.93	0.49
1:E:189:ASN:OD1	1:E:190:PRO:HD2	2.12	0.49
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.94	0.49
1:F:785:ASP:O	1:F:789:TRP:HD1	1.94	0.49
1:B:139:VAL:HA	1:B:289:LEU:O	2.12	0.49
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.48	0.49
1:B:923:ASN:HD22	1:B:923:ASN:C	2.14	0.49
1:C:65:ILE:HG12	1:C:118:LEU:HD11	1.95	0.49
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.94	0.49
1:D:175:VAL:HG11	1:D:289:LEU:HD22	1.93	0.49
1:E:225:VAL:CG1	1:F:777:ALA:HB1	2.43	0.49
1:E:352:PHE:C	1:E:352:PHE:CD2	2.86	0.49
1:E:576:VAL:HG13	1:E:663:VAL:HG22	1.94	0.49
1:B:53:ASP:OD1	1:B:56:THR:OG1	2.31	0.49
1:B:66:GLU:OE1	1:B:818:ARG:NE	2.45	0.49
1:B:398:MET:HG2	1:B:473:THR:HG21	1.95	0.49
1:B:688:ALA:O	1:B:690:LEU:N	2.43	0.49
1:B:987:MET:O	1:B:990:VAL:N	2.44	0.49
1:C:226:LYS:H	1:C:226:LYS:CD	2.23	0.49
1:C:726:GLN:NE2	1:C:812:GLY:HA3	2.26	0.49
1:D:722:GLU:O	1:D:814:PRO:HD2	2.12	0.49
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:293:LEU:HD13	1:F:294:ALA:N	2.27	0.49
1:F:759:VAL:HG23	1:F:771:VAL:HG13	1.94	0.49
1:F:821:GLY:O	1:F:822:LEU:HD23	2.11	0.49
1:A:401:ALA:O	1:A:404:LEU:HD12	2.13	0.49
1:B:295:THR:OG1	1:C:73:ASP:OD1	2.18	0.49
1:B:845:GLU:O	1:B:849:SER:HB2	2.12	0.49
1:C:383:LEU:HD22	1:C:388:PHE:HD1	1.77	0.49
1:D:53:ASP:OD1	1:D:53:ASP:N	2.38	0.49
1:D:376:LEU:O	1:D:379:THR:N	2.44	0.49
1:E:459:PHE:O	1:E:464:GLY:HA3	2.12	0.49
1:E:753:ALA:O	1:E:775:SER:OG	2.15	0.49
1:F:190:PRO:HB3	1:F:789:TRP:CZ3	2.48	0.49
1:A:163:LYS:O	1:A:163:LYS:HG2	2.13	0.49
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.78	0.49
1:A:534:ILE:HD11	1:A:1024:VAL:HG21	1.93	0.49
1:A:941:ASN:ND2	1:A:975:ILE:HG23	2.28	0.49
1:B:982:PHE:HE2	1:B:1007:VAL:HG13	1.75	0.49
1:C:346:GLU:C	1:C:350:LEU:HD22	2.32	0.49
1:C:457:ALA:HB2	1:C:471:SER:OG	2.12	0.49
1:C:964:THR:O	1:C:968:VAL:HG23	2.12	0.49
1:D:24:GLY:HA2	1:D:27:ILE:HD12	1.95	0.49
1:D:413:VAL:HG23	1:D:493:CYS:SG	2.53	0.49
1:D:909:VAL:HG22	1:D:931:LEU:CD1	2.42	0.49
1:E:445:ILE:HG13	1:E:446:ALA:N	2.28	0.49
1:A:105:VAL:HG22	1:B:106:GLN:HA	1.94	0.49
1:A:145:THR:N	1:A:320:GLY:O	2.41	0.49
1:A:184:MET:HB2	1:A:762:PHE:CE2	2.47	0.49
1:A:335:ILE:O	1:A:339:GLU:HG2	2.13	0.49
1:A:568:ASP:CG	1:A:637:ARG:HH22	2.16	0.49
1:B:197:GLN:O	1:B:792:ARG:HD3	2.12	0.49
1:B:246:PHE:O	1:B:249:ILE:HG12	2.13	0.49
1:B:484:VAL:O	1:B:489:THR:N	2.41	0.49
1:B:573:MET:HG3	1:B:666:PHE:HE2	1.77	0.49
1:B:743:ILE:HA	1:B:746:ILE:HG13	1.95	0.49
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.93	0.49
1:C:497:LEU:HG	1:C:498:LYS:O	2.13	0.49
1:D:293:LEU:HD22	1:D:294:ALA:H	1.78	0.49
1:D:343:THR:HG21	1:D:989:LEU:HD21	1.95	0.49
1:D:360:GLN:HG2	1:D:513:PHE:CD2	2.47	0.49
1:E:83:ASP:HB2	1:E:87:THR:OG1	2.13	0.49
1:F:150:THR:O	1:F:153:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:465:ALA:O	1:F:469:GLN:HG2	2.12	0.49
1:F:971:ARG:CZ	1:F:971:ARG:HB3	2.28	0.49
1:A:27:ILE:HD11	1:A:380:PHE:CD1	2.48	0.49
1:A:196:PHE:CD2	1:A:196:PHE:N	2.81	0.49
1:B:78:MET:HE3	1:B:820:ASN:C	2.33	0.49
1:B:294:ALA:HB3	1:B:297:ALA:CB	2.43	0.49
1:B:690:LEU:HD22	1:B:694:LYS:HD2	1.95	0.49
1:C:582:ALA:HB2	1:C:586:ARG:HH21	1.77	0.49
1:E:40:PRO:HG3	1:E:865:GLN:OE1	2.13	0.49
1:E:217:GLY:O	1:E:234:ILE:HB	2.13	0.49
1:F:68:ASN:O	1:F:110:LYS:HB3	2.13	0.49
1:F:961:ILE:HG22	1:F:965:LEU:HD12	1.95	0.49
1:A:99:ASP:OD1	1:A:102:ILE:HB	2.13	0.49
1:A:115:MET:SD	1:A:118:LEU:HD12	2.53	0.49
1:A:336:SER:O	1:A:339:GLU:HB2	2.12	0.49
1:B:53:ASP:OD1	1:B:53:ASP:N	2.41	0.49
1:B:201:VAL:O	1:B:205:THR:OG1	2.26	0.49
1:B:415:ASN:OD1	1:B:418:ARG:NH2	2.46	0.49
1:B:714:THR:HB	1:B:831:ALA:C	2.34	0.49
1:B:779:TYR:O	1:B:789:TRP:NE1	2.42	0.49
1:B:792:ARG:HG2	1:B:792:ARG:HH11	1.78	0.49
1:C:428:LYS:O	1:C:432:ARG:HB2	2.13	0.49
1:C:878:ALA:O	1:C:882:ILE:HG12	2.13	0.49
1:D:597:TYR:CE1	1:D:601:LYS:HB2	2.48	0.49
1:D:742:SER:O	1:D:745:ASP:HB2	2.13	0.49
1:E:43:VAL:HG21	1:E:104:GLN:HG3	1.94	0.49
1:F:65:ILE:HD11	1:F:90:ILE:CD1	2.37	0.49
1:F:525:HIS:CD2	1:F:529:ASP:OD2	2.64	0.49
1:A:711:ASP:O	1:A:712:MET:HG3	2.12	0.48
1:B:525:HIS:CD2	1:B:529:ASP:OD2	2.65	0.48
1:B:919:ARG:HB3	1:B:921:LEU:CD2	2.43	0.48
1:C:979:SER:HB2	1:C:1015:THR:HG21	1.94	0.48
1:D:709:HIS:HB2	1:D:713:LEU:CD2	2.43	0.48
1:D:953:MET:HE1	1:D:960:LEU:HD12	1.95	0.48
1:E:536:ARG:NH2	2:E:2000:LMT:H4B	2.28	0.48
1:E:679:GLY:HA2	1:E:830:GLN:HA	1.93	0.48
1:E:801:PHE:O	1:E:805:SER:HB3	2.13	0.48
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.96	0.48
1:F:235:ILE:HG22	1:F:236:ALA:N	2.28	0.48
1:F:455:PRO:HB3	1:F:879:ILE:CG2	2.39	0.48
1:F:964:THR:O	1:F:968:VAL:HG13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASN:OD1	1:A:190:PRO:HD2	2.14	0.48
1:A:414:GLU:CG	1:A:974:PRO:HG3	2.42	0.48
1:A:504:ASP:O	1:A:506:GLY:N	2.46	0.48
1:A:764:ASP:OD2	1:A:769:LYS:HE3	2.13	0.48
1:B:393:LEU:O	1:B:396:PHE:HB2	2.13	0.48
1:B:416:VAL:HA	1:B:419:VAL:HG22	1.95	0.48
1:B:819:TYR:OH	1:B:859:TRP:O	2.20	0.48
1:C:66:GLU:HB3	1:C:78:MET:HE1	1.95	0.48
1:C:71:GLY:O	1:C:106:GLN:NE2	2.36	0.48
1:C:483:LEU:HD23	1:C:486:LEU:HD11	1.95	0.48
1:C:669:PRO:HG3	1:C:862:MET:HG3	1.94	0.48
1:C:968:VAL:CA	1:C:971:ARG:HH12	2.27	0.48
1:C:971:ARG:NE	1:C:971:ARG:O	2.46	0.48
1:C:1041:GLU:O	1:C:1042:HIS:HB2	2.12	0.48
1:D:193:LEU:HD13	1:D:200:PRO:HD3	1.94	0.48
1:E:13:TRP:CH2	1:E:492:LEU:HD21	2.48	0.48
1:E:345:VAL:O	1:E:348:ILE:HG22	2.12	0.48
1:E:678:THR:HA	1:E:837:THR:OG1	2.12	0.48
1:F:314:GLU:HG2	1:F:315:PRO:HD3	1.94	0.48
1:F:948:PHE:HE2	1:F:971:ARG:HG3	1.71	0.48
1:A:583:THR:H	1:A:586:ARG:HG3	1.78	0.48
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.48	0.48
1:B:143:ILE:HG21	1:B:281:PHE:CD2	2.48	0.48
1:B:235:ILE:HD12	1:C:810:GLU:OE2	2.13	0.48
1:B:451:ALA:HB1	1:B:883:VAL:CG1	2.42	0.48
1:C:970:MET:SD	1:C:970:MET:N	2.86	0.48
1:D:478:MET:O	1:D:481:SER:OG	2.20	0.48
1:D:571:VAL:HA	1:D:631:LEU:HD13	1.95	0.48
1:D:752:ALA:O	1:D:774:MET:HA	2.13	0.48
1:D:910:ILE:O	1:D:914:LEU:HB2	2.13	0.48
1:F:827:ILE:N	1:F:827:ILE:HD12	2.28	0.48
1:A:75:LEU:H	1:C:170:SER:HB2	1.79	0.48
1:B:72:ILE:CD1	1:B:107:VAL:HG23	2.43	0.48
1:B:172:VAL:C	1:B:294:ALA:HB2	2.34	0.48
1:B:259:ARG:HD3	1:B:259:ARG:N	2.22	0.48
1:B:375:VAL:O	1:B:379:THR:OG1	2.29	0.48
1:C:984:LEU:HD22	1:C:984:LEU:HA	1.47	0.48
1:D:5:PHE:HE2	1:D:11:PHE:CD1	2.31	0.48
1:F:36:PRO:HG3	1:F:469:GLN:CD	2.34	0.48
1:F:600:THR:HB	1:F:601:LYS:HG3	1.94	0.48
1:A:151:GLN:HE22	1:A:279:ALA:N	2.04	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:THR:HB	1:A:200:PRO:HD2	1.96	0.48
1:B:652:THR:HG1	1:B:664:PHE:HD2	1.59	0.48
1:B:680:PHE:HB2	1:B:859:TRP:CZ3	2.45	0.48
1:B:685:ILE:CD1	1:B:819:TYR:HB3	2.35	0.48
1:C:594:VAL:O	1:C:597:TYR:HB3	2.14	0.48
1:C:860:THR:CA	1:C:864:TYR:HB2	2.44	0.48
1:C:893:GLU:HG3	1:C:894:SER:N	2.28	0.48
1:D:11:PHE:O	1:D:15:ILE:HG13	2.13	0.48
1:D:146:ASP:O	1:D:148:THR:N	2.47	0.48
1:D:188:MET:CE	1:D:200:PRO:HG3	2.43	0.48
1:D:425:LEU:HD22	1:D:429:GLU:OE1	2.13	0.48
1:D:467:TYR:HE2	1:D:925:VAL:HG22	1.78	0.48
1:D:960:LEU:HD23	1:D:1031:ARG:NH2	2.27	0.48
1:E:925:VAL:O	1:E:928:GLN:HB2	2.13	0.48
1:F:344:LEU:CA	1:F:399:VAL:HG22	2.43	0.48
1:F:602:GLU:CD	1:F:650:ARG:HD2	2.33	0.48
1:A:298:ASN:ND2	1:A:301:ASP:OD2	2.46	0.48
1:B:149:MET:HE2	1:B:153:ASP:HB3	1.95	0.48
1:B:228:GLN:HE21	1:B:230:LEU:N	2.08	0.48
1:B:376:LEU:HA	1:B:379:THR:OG1	2.14	0.48
1:B:577:GLN:HE22	1:B:721:LEU:HD11	1.77	0.48
1:B:699:ARG:NE	1:B:722:GLU:OE1	2.46	0.48
1:C:6:ILE:CG2	1:C:487:ILE:HG12	2.44	0.48
1:C:222:THR:HA	1:C:224:PRO:CD	2.42	0.48
1:C:301:ASP:HA	1:C:304:ALA:CB	2.44	0.48
1:C:401:ALA:HB2	1:C:474:ILE:HG12	1.96	0.48
1:C:616:GLY:HA2	1:C:626:ILE:HB	1.95	0.48
1:C:654:ALA:O	1:C:658:ILE:HG12	2.14	0.48
1:C:864:TYR:HD2	1:C:865:GLN:HE21	1.61	0.48
1:C:900:SER:HA	1:C:1029:VAL:HG21	1.96	0.48
1:D:24:GLY:O	1:D:27:ILE:HB	2.13	0.48
1:D:35:TYR:HE2	1:D:564:LEU:HD11	1.78	0.48
1:D:210:GLN:NE2	1:D:250:LEU:O	2.47	0.48
1:D:249:ILE:HB	1:D:262:LEU:HB2	1.96	0.48
1:D:692:HIS:NE2	1:D:813:SER:HB2	2.28	0.48
1:E:885:PHE:HD2	1:E:886:LEU:HD12	1.78	0.48
1:F:139:VAL:HA	1:F:289:LEU:O	2.12	0.48
1:F:448:VAL:O	1:F:452:VAL:HG13	2.13	0.48
1:F:945:ILE:HD13	1:F:971:ARG:HH22	1.76	0.48
1:A:568:ASP:O	1:A:634:TRP:CZ3	2.67	0.48
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.59	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:HA	1:B:405:LEU:HD12	1.94	0.48
1:B:508:GLY:N	1:B:518:ARG:HG3	2.29	0.48
1:B:544:LEU:O	1:B:547:ILE:HB	2.14	0.48
1:B:719:ASN:CB	1:B:828:LEU:HG	2.43	0.48
1:C:64:VAL:HG11	1:C:117:LEU:C	2.34	0.48
1:C:358:PHE:HB3	1:C:977:MET:HE2	1.96	0.48
1:C:376:LEU:HD13	1:C:398:MET:HG3	1.95	0.48
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.95	0.48
1:C:880:SER:HA	1:C:883:VAL:HG12	1.94	0.48
1:D:137:LEU:HD22	1:D:293:LEU:HD23	1.95	0.48
1:D:155:SER:HB3	1:D:180:SER:H	1.77	0.48
1:D:475:VAL:HG13	1:D:478:MET:HE1	1.94	0.48
1:F:13:TRP:HA	1:F:13:TRP:HE3	1.79	0.48
1:F:255:GLN:H	1:F:255:GLN:CD	2.17	0.48
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.95	0.48
1:A:100:ALA:HB1	1:A:295:THR:HG21	1.96	0.48
1:A:197:GLN:HB2	1:A:252:LYS:NZ	2.29	0.48
1:A:944:LEU:HB3	1:A:971:ARG:CD	2.40	0.48
1:A:971:ARG:C	1:A:974:PRO:HD2	2.34	0.48
1:B:481:SER:HA	1:B:484:VAL:HG22	1.95	0.48
1:B:827:ILE:HD12	1:B:827:ILE:N	2.29	0.48
1:B:894:SER:CB	1:B:897:ILE:HD11	2.43	0.48
1:C:165:ALA:HB3	1:C:313:MET:HE1	1.95	0.48
1:C:393:LEU:CG	1:C:466:ILE:HD12	2.44	0.48
1:C:456:MET:HB3	1:C:876:LEU:HD22	1.95	0.48
1:D:279:ALA:HB3	1:D:286:ALA:O	2.14	0.48
1:D:355:MET:HE2	1:D:368:PRO:HG2	1.95	0.48
1:D:359:LEU:O	1:D:361:ASN:N	2.47	0.48
1:D:888:LEU:HD22	1:D:892:TYR:CE2	2.37	0.48
1:E:213:GLN:HA	1:E:237:GLN:O	2.13	0.48
1:E:453:PHE:O	1:E:456:MET:HG2	2.14	0.48
1:F:169:THR:HG21	1:F:306:ILE:HD13	1.96	0.48
1:F:410:ILE:HD13	1:F:977:MET:HG2	1.95	0.48
1:F:960:LEU:CD2	1:F:1031:ARG:HE	2.27	0.48
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.78	0.48
1:A:659:LYS:NZ	1:A:659:LYS:HB2	2.29	0.48
1:A:801:PHE:HA	1:A:804:PHE:CE2	2.48	0.48
1:B:8:ARG:HB3	1:B:11:PHE:HB3	1.96	0.48
1:B:26:ALA:O	1:B:30:LEU:HD22	2.14	0.48
1:B:885:PHE:CD2	1:B:886:LEU:HD22	2.48	0.48
1:C:76:MET:HE1	1:C:864:TYR:HE2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HG22	1:C:446:ALA:N	2.29	0.48
1:C:559:LEU:HD11	1:C:922:THR:HA	1.95	0.48
1:D:350:LEU:HD13	1:D:984:LEU:O	2.13	0.48
1:D:684:LEU:HD11	1:D:855:VAL:HG13	1.95	0.48
1:D:687:GLN:HG2	1:F:316:PHE:CD1	2.49	0.48
1:D:757:SER:O	1:D:772:TYR:HA	2.14	0.48
1:D:885:PHE:HA	1:D:902:MET:HE1	1.96	0.48
1:D:959:GLY:CA	1:D:1040:ILE:HG21	2.42	0.48
1:D:971:ARG:HH11	1:D:971:ARG:CG	2.25	0.48
1:A:559:LEU:CD2	1:A:922:THR:HA	2.43	0.48
1:C:162:MET:C	1:C:164:ASP:N	2.67	0.48
1:C:400:LEU:HD13	1:C:400:LEU:C	2.35	0.48
1:C:530:SER:O	1:C:533:GLY:N	2.47	0.48
1:C:727:PHE:CD2	1:C:729:ILE:HD11	2.49	0.48
1:C:727:PHE:HB2	1:C:809:TRP:HZ3	1.78	0.48
1:D:242:SER:O	1:D:246:PHE:HD1	1.97	0.48
1:D:360:GLN:NE2	1:D:513:PHE:HB3	2.19	0.48
1:D:393:LEU:HD13	1:D:466:ILE:HG23	1.94	0.48
1:E:24:GLY:O	1:E:27:ILE:HB	2.14	0.48
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.94	0.48
1:E:444:GLY:O	1:E:447:MET:HB2	2.13	0.48
1:E:451:ALA:HB3	1:E:884:VAL:HG22	1.96	0.48
1:F:5:PHE:HE1	1:F:8:ARG:HD2	1.77	0.48
1:F:206:ALA:O	1:F:210:GLN:HG3	2.14	0.48
1:F:348:ILE:HD12	1:F:348:ILE:HG23	1.60	0.48
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.95	0.48
1:F:785:ASP:O	1:F:789:TRP:CD1	2.67	0.48
1:F:904:VAL:HG21	1:F:942:ALA:HB2	1.95	0.48
1:F:960:LEU:HD21	1:F:1031:ARG:HE	1.79	0.48
1:A:232:ALA:HB1	1:B:725:PRO:O	2.14	0.47
1:A:497:LEU:HD12	1:A:498:LYS:H	1.79	0.47
1:A:525:HIS:O	1:A:526:HIS:C	2.49	0.47
1:A:531:VAL:HA	1:A:534:ILE:HG23	1.97	0.47
1:A:573:MET:O	1:A:666:PHE:HD1	1.96	0.47
1:A:911:GLY:HA3	1:A:1013:THR:CG2	2.43	0.47
1:B:376:LEU:HD21	1:B:405:LEU:HD11	1.96	0.47
1:B:434:SER:O	1:B:437:GLN:HG2	2.14	0.47
1:C:293:LEU:HD21	1:C:297:ALA:HB3	1.96	0.47
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.49	0.47
1:D:169:THR:HG21	1:D:306:ILE:CG1	2.44	0.47
1:D:926:TYR:HB3	1:D:1003:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:ILE:HG22	1:F:886:LEU:HD11	1.96	0.47
1:E:356:TYR:O	1:E:360:GLN:N	2.36	0.47
1:F:641:GLU:HB2	1:F:650:ARG:NH2	2.29	0.47
1:F:641:GLU:HB2	1:F:650:ARG:HH22	1.79	0.47
1:A:176:GLN:NE2	1:A:177:LEU:O	2.45	0.47
1:A:181:GLN:HG2	1:A:769:LYS:NZ	2.29	0.47
1:A:242:SER:OG	1:A:245:GLU:HG3	2.14	0.47
1:A:893:GLU:OE2	1:C:9:PRO:HD2	2.14	0.47
1:B:548:ILE:HG23	1:B:910:ILE:HG13	1.96	0.47
1:C:31:PRO:HB2	1:C:389:SER:OG	2.15	0.47
1:C:455:PRO:HG2	1:C:880:SER:CA	2.44	0.47
1:C:727:PHE:CZ	1:C:783:PRO:HB3	2.49	0.47
1:D:42:ALA:HB2	1:D:93:THR:HG23	1.96	0.47
1:D:247:GLY:HA2	1:D:268:ILE:HD12	1.95	0.47
1:D:721:LEU:HD13	1:D:721:LEU:HA	1.44	0.47
1:E:35:TYR:HB3	1:E:36:PRO:HD2	1.96	0.47
1:F:451:ALA:O	1:F:454:VAL:HG23	2.14	0.47
1:A:70:ASN:HB2	1:C:167:SER:O	2.14	0.47
1:A:545:TYR:CE1	1:A:903:LEU:HD13	2.49	0.47
1:A:686:ASP:HB2	1:A:695:LEU:HG	1.97	0.47
1:B:889:ALA:HA	1:B:898:PRO:HG3	1.95	0.47
1:B:899:PHE:CD1	1:B:902:MET:HE1	2.49	0.47
1:C:181:GLN:HG2	1:C:769:LYS:HZ2	1.80	0.47
1:C:220:GLY:HA2	1:C:228:GLN:NE2	2.30	0.47
1:C:761:ASP:OD1	1:C:770:LYS:HA	2.14	0.47
1:D:76:MET:HB2	1:D:93:THR:O	2.13	0.47
1:D:683:GLU:OE2	1:D:826:GLU:HB3	2.14	0.47
1:D:971:ARG:O	1:D:975:ILE:HG12	2.14	0.47
1:E:75:LEU:HA	1:E:94:PHE:HD1	1.79	0.47
1:F:193:LEU:HD12	1:F:200:PRO:HD3	1.96	0.47
1:F:602:GLU:O	1:F:606:VAL:HG22	2.14	0.47
1:F:786:ILE:HG23	1:F:801:PHE:HD2	1.80	0.47
1:A:193:LEU:CD2	1:A:265:VAL:HB	2.45	0.47
1:A:303:ALA:O	1:A:307:ARG:HB2	2.14	0.47
1:A:364:ALA:HA	1:A:367:ILE:HD11	1.95	0.47
1:A:393:LEU:HD21	1:A:469:GLN:HG2	1.97	0.47
1:A:721:LEU:HA	1:A:721:LEU:HD13	1.62	0.47
1:B:819:TYR:N	1:B:824:SER:OG	2.47	0.47
1:B:971:ARG:C	1:B:974:PRO:HD2	2.34	0.47
1:C:634:TRP:H	1:C:634:TRP:HD1	1.57	0.47
1:C:790:TYR:HB3	1:C:798:MET:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:946:VAL:HG13	1:C:1026:PHE:CD1	2.49	0.47
1:C:968:VAL:HG21	1:C:1023:PRO:HB3	1.96	0.47
1:D:152:GLU:HB3	1:D:182:TYR:CE1	2.41	0.47
1:D:709:HIS:HB2	1:D:713:LEU:HD23	1.96	0.47
1:D:783:PRO:O	1:D:786:ILE:HB	2.14	0.47
1:D:941:ASN:HB3	1:D:975:ILE:HD12	1.96	0.47
1:E:58:GLN:HA	1:E:62:THR:HB	1.97	0.47
1:E:61:VAL:HG11	1:E:88:VAL:HG11	1.96	0.47
1:E:525:HIS:O	1:E:526:HIS:C	2.53	0.47
1:E:592:ASN:O	1:E:592:ASN:ND2	2.39	0.47
1:E:778:LYS:HA	1:E:781:MET:HE2	1.95	0.47
1:E:979:SER:OG	1:E:1015:THR:HG21	2.15	0.47
1:F:779:TYR:HB2	1:F:789:TRP:HZ2	1.79	0.47
1:F:843:LEU:HD22	1:F:846:GLN:HB3	1.96	0.47
1:A:210:GLN:O	1:A:237:GLN:NE2	2.48	0.47
1:A:254:ASN:HB2	1:A:258:SER:O	2.15	0.47
1:A:671:ILE:HG12	1:A:673:GLU:O	2.14	0.47
1:B:85:THR:HG21	1:B:620:ARG:HD3	1.96	0.47
1:B:110:LYS:HB2	1:B:110:LYS:HZ2	1.80	0.47
1:B:135:SER:OG	1:B:673:GLU:OE1	2.33	0.47
1:B:338:HIS:ND1	1:B:338:HIS:C	2.68	0.47
1:B:634:TRP:HD1	1:B:634:TRP:H	1.52	0.47
1:C:108:GLN:O	1:C:112:GLN:HB2	2.13	0.47
1:C:367:ILE:HD12	1:C:488:LEU:CD2	2.44	0.47
1:C:394:THR:CA	1:C:469:GLN:HB3	2.44	0.47
1:C:446:ALA:HA	1:C:478:MET:HB2	1.95	0.47
1:C:534:ILE:HG12	2:C:2000:LMT:H12	1.95	0.47
1:C:864:TYR:CE1	1:C:867:ARG:NH2	2.82	0.47
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.96	0.47
1:C:937:LEU:O	1:C:940:LYS:HB3	2.14	0.47
1:D:17:ILE:HG22	1:E:886:LEU:HD21	1.96	0.47
1:D:521:GLU:O	1:D:524:THR:HG23	2.13	0.47
1:E:196:PHE:N	1:E:196:PHE:CD1	2.81	0.47
1:E:686:ASP:HB2	1:E:695:LEU:HD13	1.97	0.47
1:E:688:ALA:HB3	1:E:690:LEU:HG	1.96	0.47
1:F:58:GLN:HA	1:F:62:THR:HG23	1.96	0.47
1:F:424:GLY:HA3	1:F:502:LYS:HG3	1.96	0.47
1:F:527:TYR:O	1:F:530:SER:HB3	2.14	0.47
1:F:681:ASP:OD2	1:F:681:ASP:N	2.47	0.47
1:B:195:LYS:HZ1	1:B:196:PHE:HE1	1.63	0.47
1:B:250:LEU:HA	1:B:261:LEU:HD23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:THR:HG23	1:B:988:PRO:HB2	1.97	0.47
1:B:559:LEU:CD1	1:B:922:THR:HA	2.43	0.47
1:B:621:GLY:O	1:B:624:THR:HG22	2.14	0.47
1:B:873:ALA:N	1:B:874:PRO:HD2	2.30	0.47
1:C:41:PRO:HD2	1:C:95:GLU:C	2.34	0.47
1:C:72:ILE:HG21	1:C:94:PHE:CE2	2.50	0.47
1:C:353:LEU:HD22	1:C:353:LEU:HA	1.71	0.47
1:C:540:ARG:O	1:C:543:VAL:HB	2.15	0.47
1:C:676:THR:HG21	1:C:828:LEU:HD22	1.97	0.47
1:E:108:GLN:OE1	1:F:112:GLN:HB3	2.15	0.47
1:E:727:PHE:HB2	1:E:809:TRP:HZ3	1.79	0.47
1:F:48:SER:HA	1:F:86:GLY:O	2.15	0.47
1:F:804:PHE:CD2	1:F:804:PHE:N	2.82	0.47
1:F:971:ARG:NH1	1:F:971:ARG:O	2.48	0.47
1:A:36:PRO:HD3	1:A:391:ASN:OD1	2.15	0.47
1:A:109:ASN:HB2	1:B:109:ASN:OD1	2.14	0.47
1:A:111:LEU:HD13	1:A:115:MET:HG2	1.96	0.47
1:A:388:PHE:HE1	1:A:472:ILE:HG21	1.79	0.47
1:A:394:THR:OG1	1:A:469:GLN:HG3	2.14	0.47
1:A:754:TRP:CZ2	1:A:780:ARG:HA	2.50	0.47
1:A:790:TYR:CE2	1:A:800:PRO:HB3	2.48	0.47
1:A:843:LEU:HD13	1:A:844:MET:N	2.29	0.47
1:A:961:ILE:H	1:A:1039:ASP:CG	2.13	0.47
1:A:969:ARG:NH1	1:A:970:MET:HB3	2.27	0.47
1:B:47:ALA:O	1:B:87:THR:HA	2.14	0.47
1:B:177:LEU:HA	1:B:289:LEU:HD23	1.96	0.47
1:B:459:PHE:CD1	1:B:876:LEU:HD12	2.50	0.47
1:B:493:CYS:O	1:B:497:LEU:HB3	2.15	0.47
1:B:564:LEU:HD12	1:B:925:VAL:HG11	1.96	0.47
1:B:714:THR:OG1	1:B:832:ALA:HA	2.14	0.47
1:B:742:SER:O	1:B:745:ASP:HB2	2.15	0.47
1:C:11:PHE:HE2	1:C:15:ILE:HD11	1.78	0.47
1:C:120:GLN:NE2	1:C:123:GLN:OE1	2.48	0.47
1:C:138:MET:HB3	1:C:291:ILE:HD11	1.97	0.47
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.95	0.47
1:C:166:ILE:HG22	1:C:175:VAL:HG21	1.97	0.47
1:C:367:ILE:HG23	1:C:488:LEU:HD22	1.96	0.47
1:C:423:GLU:OE2	1:C:425:LEU:HD23	2.14	0.47
1:C:931:LEU:HD22	1:C:931:LEU:HA	1.50	0.47
1:D:13:TRP:NE1	1:D:492:LEU:HD21	2.30	0.47
1:D:114:ALA:O	1:D:118:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:ASN:HB3	1:D:256:ASP:OD1	2.14	0.47
1:D:350:LEU:HD22	1:D:984:LEU:HD12	1.96	0.47
1:D:1030:ARG:CZ	1:D:1033:PHE:HD2	2.28	0.47
1:E:35:TYR:CD2	1:E:671:ILE:HG12	2.50	0.47
1:E:722:GLU:O	1:E:814:PRO:HD2	2.15	0.47
1:E:834:GLY:O	1:E:835:LYS:HD2	2.15	0.47
1:E:888:LEU:HD21	1:E:943:ILE:HD11	1.97	0.47
1:E:1037:ASN:HA	1:E:1038:GLU:CB	2.45	0.47
1:F:363:ARG:HB3	1:F:363:ARG:NH1	2.30	0.47
1:F:597:TYR:CD2	1:F:655:PHE:CZ	3.01	0.47
1:F:602:GLU:OE1	1:F:650:ARG:HD2	2.14	0.47
1:F:1034:SER:O	1:F:1036:LYS:N	2.47	0.47
1:A:263:ARG:HE	1:A:263:ARG:HB3	1.46	0.47
1:A:578:LEU:CD1	1:A:579:PRO:HD2	2.44	0.47
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.95	0.47
1:B:573:MET:O	1:B:666:PHE:HD2	1.97	0.47
1:B:578:LEU:HD11	1:B:587:THR:N	2.30	0.47
1:B:744:ASN:OD1	1:B:744:ASN:N	2.48	0.47
1:B:785:ASP:OD1	1:B:785:ASP:N	2.48	0.47
1:C:420:MET:SD	1:C:500:ILE:HB	2.55	0.47
1:C:451:ALA:CB	1:C:884:VAL:HG22	2.43	0.47
1:D:974:PRO:HA	1:D:977:MET:CE	2.44	0.47
1:E:110:LYS:O	1:E:113:LEU:HB2	2.15	0.47
1:E:888:LEU:HA	1:E:888:LEU:HD23	1.54	0.47
1:A:552:MET:SD	1:A:909:VAL:HB	2.54	0.47
1:B:10:ILE:HA	1:B:10:ILE:HD13	1.64	0.47
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.55	0.47
1:B:100:ALA:CB	1:B:131:LYS:HD3	2.45	0.47
1:B:277:ILE:HD12	1:B:277:ILE:O	2.15	0.47
1:B:944:LEU:HB3	1:B:971:ARG:HH12	1.80	0.47
1:C:78:MET:SD	1:C:92:LEU:HD12	2.55	0.47
1:C:664:PHE:CE2	1:C:717:ARG:HB3	2.49	0.47
1:D:151:GLN:HG3	1:D:152:GLU:N	2.30	0.47
1:D:597:TYR:HD2	1:D:655:PHE:CZ	2.33	0.47
1:E:238:THR:HG22	1:E:239:ARG:O	2.15	0.47
1:F:65:ILE:HA	1:F:114:ALA:CB	2.44	0.47
1:F:470:PHE:CD1	1:F:929:VAL:HG21	2.50	0.47
1:F:559:LEU:HD23	1:F:560:PRO:HD2	1.96	0.47
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.30	0.47
1:A:515:TRP:HB3	1:A:519:MET:HE3	1.96	0.47
1:A:911:GLY:CA	1:A:1013:THR:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:O	1:B:102:ILE:HG12	2.15	0.47
1:B:101:ASP:HB3	1:C:105:VAL:CG1	2.45	0.47
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.80	0.47
1:B:375:VAL:CG1	1:B:405:LEU:HD22	2.44	0.47
1:B:465:ALA:O	1:B:468:ARG:HB2	2.15	0.47
1:B:767:ARG:HH21	1:C:117:LEU:CD1	2.24	0.47
1:C:453:PHE:CE2	1:C:474:ILE:HD12	2.49	0.47
1:C:712:MET:SD	1:C:843:LEU:HG	2.54	0.47
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.50	0.47
1:E:139:VAL:HA	1:E:289:LEU:O	2.15	0.47
1:E:165:ALA:HB3	1:E:313:MET:CE	2.45	0.47
1:E:528:THR:HG21	1:E:969:ARG:HG3	1.96	0.47
1:F:371:ALA:HB1	1:F:484:VAL:HG11	1.97	0.47
1:F:568:ASP:O	1:F:634:TRP:HH2	1.96	0.47
1:A:214:VAL:HG11	1:B:747:ASN:CG	2.36	0.46
1:A:352:PHE:CE1	1:A:365:THR:HB	2.50	0.46
1:A:902:MET:O	1:A:905:VAL:HG22	2.14	0.46
1:B:169:THR:OG1	1:B:305:ALA:O	2.33	0.46
1:B:417:GLU:OE2	1:B:497:LEU:HD11	2.15	0.46
1:B:448:VAL:HG12	1:B:884:VAL:HA	1.96	0.46
1:B:746:ILE:HG22	1:B:801:PHE:HE1	1.80	0.46
1:C:356:TYR:C	1:C:358:PHE:H	2.18	0.46
1:D:463:THR:O	1:D:466:ILE:HB	2.15	0.46
1:D:909:VAL:O	1:D:911:GLY:N	2.48	0.46
1:F:379:THR:O	1:F:382:VAL:N	2.47	0.46
1:F:404:LEU:HG	1:F:449:LEU:CD1	2.45	0.46
1:F:418:ARG:O	1:F:422:GLU:HG3	2.16	0.46
1:F:530:SER:OG	2:F:2000:LMT:H21	2.16	0.46
1:F:686:ASP:OD2	1:F:823:PRO:HB2	2.16	0.46
1:A:54:ALA:HB2	1:A:84:SER:HB3	1.97	0.46
1:A:117:LEU:HD21	1:C:125:GLN:OE1	2.14	0.46
1:A:979:SER:HA	1:A:1011:MET:HE1	1.96	0.46
1:B:527:TYR:OH	1:B:968:VAL:HG13	2.15	0.46
1:B:600:THR:HB	1:B:601:LYS:HD2	1.97	0.46
1:B:657:GLN:HG3	1:B:658:ILE:HG23	1.98	0.46
1:B:787:GLY:O	1:B:789:TRP:N	2.48	0.46
1:C:49:TYR:CD2	1:C:57:VAL:HG12	2.49	0.46
1:C:416:VAL:CG2	1:C:438:ILE:HD11	2.45	0.46
1:C:439:GLN:O	1:C:442:LEU:HG	2.15	0.46
1:C:483:LEU:HA	1:C:486:LEU:HG	1.97	0.46
1:C:650:ARG:HA	1:C:653:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:959:GLY:HA2	1:C:1041:GLU:H	1.80	0.46
1:E:201:VAL:HG21	1:E:745:ASP:HA	1.97	0.46
1:E:251:LEU:HD21	1:E:262:LEU:HB2	1.98	0.46
1:E:467:TYR:OH	1:E:928:GLN:HG3	2.14	0.46
1:E:736:ALA:HB2	1:E:804:PHE:CD1	2.50	0.46
1:E:861:GLY:O	1:E:864:TYR:N	2.45	0.46
1:F:36:PRO:O	1:F:38:ILE:HG13	2.15	0.46
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.15	0.46
1:A:157:TYR:HE1	1:A:318:PRO:CD	2.28	0.46
1:A:168:ARG:O	1:B:75:LEU:HB2	2.15	0.46
1:A:281:PHE:CD1	1:A:610:PHE:HD1	2.27	0.46
1:A:448:VAL:CG1	1:A:884:VAL:HG23	2.45	0.46
1:A:754:TRP:HZ2	1:A:785:ASP:HB2	1.80	0.46
1:B:376:LEU:HA	1:B:376:LEU:HD23	1.72	0.46
1:C:356:TYR:O	1:C:358:PHE:N	2.48	0.46
1:C:520:PHE:HE2	1:C:973:ARG:HG3	1.80	0.46
1:D:391:ASN:ND2	1:D:469:GLN:OE1	2.48	0.46
1:D:792:ARG:HB2	1:D:798:MET:SD	2.55	0.46
1:E:414:GLU:OE1	1:E:973:ARG:HD3	2.14	0.46
1:E:427:PRO:O	1:E:430:ALA:N	2.49	0.46
1:E:486:LEU:O	1:E:490:PRO:HG3	2.15	0.46
1:F:909:VAL:O	1:F:912:ALA:N	2.48	0.46
1:A:65:ILE:O	1:A:69:MET:N	2.47	0.46
1:A:108:GLN:CB	1:B:109:ASN:HB3	2.45	0.46
1:A:166:ILE:CG2	1:A:175:VAL:HG21	2.41	0.46
1:A:246:PHE:O	1:A:262:LEU:HD23	2.15	0.46
1:A:726:GLN:HG2	1:C:233:SER:HB2	1.97	0.46
1:A:968:VAL:HA	1:A:971:ARG:NH2	2.20	0.46
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.97	0.46
1:B:405:LEU:CD2	1:B:477:ALA:HB1	2.41	0.46
1:B:707:ALA:N	1:B:716:VAL:HG21	2.30	0.46
1:C:5:PHE:O	1:C:8:ARG:HB2	2.16	0.46
1:C:792:ARG:HG2	1:C:792:ARG:HH11	1.80	0.46
1:C:851:LEU:HB3	1:C:852:PRO:HD2	1.96	0.46
1:D:362:PHE:O	1:D:365:THR:HG22	2.15	0.46
1:D:504:ASP:O	1:D:506:GLY:N	2.47	0.46
1:D:897:ILE:HG12	1:D:1030:ARG:CD	2.46	0.46
1:E:23:GLY:O	1:E:26:ALA:N	2.49	0.46
1:E:195:LYS:HB3	1:E:196:PHE:CD1	2.50	0.46
1:E:411:VAL:HG13	1:E:971:ARG:HH22	1.81	0.46
1:E:690:LEU:HD11	1:E:854:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:727:PHE:HB2	1:E:809:TRP:CZ3	2.50	0.46
1:F:119:PRO:O	1:F:122:VAL:HG22	2.15	0.46
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.97	0.46
1:F:960:LEU:O	1:F:964:THR:HG23	2.15	0.46
1:A:82:SER:HB2	1:A:816:LEU:HB2	1.96	0.46
1:A:452:VAL:HG23	1:A:453:PHE:CD2	2.50	0.46
1:B:972:LEU:HD22	1:B:976:LEU:HD13	1.98	0.46
1:C:61:VAL:HB	1:C:88:VAL:HG21	1.97	0.46
1:C:461:GLY:HA3	1:C:868:LEU:HD21	1.97	0.46
1:C:669:PRO:HG2	1:C:671:ILE:O	2.16	0.46
1:C:974:PRO:O	1:C:975:ILE:C	2.53	0.46
1:D:5:PHE:O	1:D:8:ARG:N	2.45	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.16	0.46
1:D:758:TYR:CD1	1:D:770:LYS:HD3	2.51	0.46
1:D:968:VAL:HG22	1:D:1023:PRO:HG3	1.98	0.46
1:E:610:PHE:O	1:E:627:ALA:HA	2.14	0.46
1:E:727:PHE:HD2	1:E:729:ILE:HD11	1.80	0.46
1:E:754:TRP:CD2	1:E:780:ARG:HB2	2.50	0.46
1:E:865:GLN:H	1:E:865:GLN:HG2	1.60	0.46
1:F:197:GLN:O	1:F:792:ARG:HD3	2.15	0.46
1:F:506:GLY:O	1:F:508:GLY:N	2.48	0.46
1:F:940:LYS:HE2	1:F:978:THR:HG21	1.97	0.46
1:A:105:VAL:HG13	1:B:109:ASN:HB2	1.97	0.46
1:A:282:ASN:OD1	1:A:599:LEU:HD11	2.16	0.46
1:A:448:VAL:O	1:A:452:VAL:HG13	2.15	0.46
1:A:455:PRO:O	1:A:876:LEU:HD13	2.16	0.46
1:A:676:THR:O	1:A:676:THR:OG1	2.32	0.46
1:A:731:ILE:CG2	1:A:733:GLN:HE21	2.28	0.46
1:B:401:ALA:CB	1:B:474:ILE:HG23	2.45	0.46
1:B:476:SER:O	1:B:480:LEU:HB3	2.16	0.46
1:B:696:THR:HG22	1:B:699:ARG:NH1	2.31	0.46
1:C:901:VAL:HG21	1:C:943:ILE:HD13	1.97	0.46
1:D:929:VAL:HA	1:D:932:LEU:HD12	1.98	0.46
1:E:104:GLN:HB3	1:F:109:ASN:ND2	2.31	0.46
1:E:445:ILE:HD13	1:E:940:LYS:CD	2.45	0.46
1:E:536:ARG:NE	2:E:2000:LMT:C4B	2.37	0.46
1:E:557:VAL:C	1:E:559:LEU:H	2.18	0.46
1:E:908:GLY:HA2	1:E:1014:ALA:HB2	1.97	0.46
1:E:982:PHE:O	1:E:983:ILE:C	2.51	0.46
1:F:158:VAL:HA	1:F:162:MET:HE3	1.98	0.46
1:F:600:THR:O	1:F:603:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:HB3	1:A:293:LEU:HB3	1.96	0.46
1:A:376:LEU:O	1:A:378:GLY:N	2.49	0.46
1:A:805:SER:O	1:A:805:SER:OG	2.30	0.46
1:B:4:PHE:HZ	1:B:8:ARG:HH11	1.62	0.46
1:B:680:PHE:CB	1:B:859:TRP:HZ3	2.28	0.46
1:B:986:VAL:HG11	1:B:1007:VAL:HG12	1.98	0.46
1:B:1007:VAL:HG12	1:B:1008:MET:N	2.31	0.46
1:C:564:LEU:CD2	1:C:670:ALA:HB3	2.46	0.46
1:C:594:VAL:HG22	1:C:655:PHE:CE2	2.51	0.46
1:D:149:MET:HG3	1:D:154:ILE:HG13	1.97	0.46
1:E:760:ASN:H	1:E:771:VAL:HB	1.81	0.46
1:F:445:ILE:HG12	1:F:940:LYS:HG2	1.98	0.46
1:F:875:SER:O	1:F:879:ILE:HD13	2.16	0.46
1:F:924:ASP:OD1	1:F:925:VAL:N	2.49	0.46
1:A:72:ILE:HD12	1:A:107:VAL:HA	1.98	0.46
1:A:682:PHE:CE2	1:A:857:TYR:HB2	2.51	0.46
1:A:714:THR:OG1	1:A:832:ALA:HA	2.16	0.46
1:A:944:LEU:CB	1:A:971:ARG:HD2	2.45	0.46
1:A:968:VAL:HG21	1:A:1023:PRO:HG3	1.97	0.46
1:B:947:GLU:HG3	1:B:948:PHE:N	2.30	0.46
1:C:46:SER:HA	1:C:88:VAL:O	2.15	0.46
1:C:578:LEU:CD1	1:C:579:PRO:HD2	2.46	0.46
1:C:888:LEU:HD13	1:C:943:ILE:HD11	1.96	0.46
1:D:10:ILE:HB	1:E:893:GLU:OE1	2.16	0.46
1:D:454:VAL:HB	1:D:455:PRO:HD3	1.97	0.46
1:D:751:GLY:O	1:D:754:TRP:N	2.49	0.46
1:A:21:LEU:O	1:A:25:LEU:HB2	2.15	0.46
1:A:140:VAL:HG13	1:A:325:TYR:CE2	2.51	0.46
1:A:600:THR:HG23	1:A:601:LYS:N	2.30	0.46
1:A:762:PHE:HE1	1:A:764:ASP:HB2	1.80	0.46
1:B:362:PHE:O	1:B:365:THR:HG22	2.16	0.46
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.98	0.46
1:B:491:ALA:O	1:B:495:THR:OG1	2.14	0.46
1:B:844:MET:HG3	1:B:845:GLU:H	1.80	0.46
1:C:456:MET:O	1:C:467:TYR:HD1	1.98	0.46
1:C:979:SER:HA	1:C:1011:MET:CE	2.46	0.46
1:D:1034:SER:HB3	1:D:1035:ARG:H	1.43	0.46
1:E:602:GLU:OE2	1:E:650:ARG:HD2	2.15	0.46
1:E:791:VAL:O	1:E:798:MET:HA	2.16	0.46
1:E:1037:ASN:HA	1:E:1038:GLU:CG	2.46	0.46
1:F:263:ARG:HD2	1:F:264:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:LYS:C	1:F:268:ILE:HD12	2.36	0.46
1:F:362:PHE:O	1:F:365:THR:OG1	2.21	0.46
1:F:586:ARG:O	1:F:589:LYS:HB2	2.16	0.46
1:A:200:PRO:O	1:A:203:VAL:N	2.49	0.46
1:B:110:LYS:HB2	1:B:110:LYS:NZ	2.30	0.46
1:C:54:ALA:HB1	1:C:816:LEU:HG	1.98	0.46
1:C:503:GLY:HA2	1:C:505:HIS:ND1	2.30	0.46
1:C:751:GLY:O	1:C:753:ALA:N	2.49	0.46
1:C:786:ILE:O	1:C:789:TRP:HB2	2.16	0.46
1:D:69:MET:HE3	1:D:107:VAL:HG13	1.98	0.46
1:D:733:GLN:HE22	1:D:743:ILE:HG23	1.81	0.46
1:D:740:GLY:O	1:D:793:ALA:HB1	2.16	0.46
1:E:81:ASN:HD21	1:E:817:GLU:HG2	1.81	0.46
1:E:699:ARG:HH11	1:E:825:MET:CE	2.29	0.46
1:E:893:GLU:HG3	1:E:893:GLU:O	2.16	0.46
1:F:578:LEU:CD1	1:F:661:ALA:HB2	2.45	0.46
1:A:35:TYR:CE2	1:A:671:ILE:HG22	2.51	0.45
1:A:364:ALA:HA	1:A:367:ILE:CD1	2.46	0.45
1:B:45:ILE:CD1	1:B:107:VAL:HG11	2.46	0.45
1:B:451:ALA:HB1	1:B:883:VAL:CG2	2.47	0.45
1:B:681:ASP:N	1:B:681:ASP:OD1	2.49	0.45
1:C:363:ARG:HA	1:C:366:LEU:HG	1.98	0.45
1:C:586:ARG:O	1:C:589:LYS:HB2	2.16	0.45
1:C:898:PRO:HA	1:C:901:VAL:HG12	1.97	0.45
1:D:444:GLY:O	1:D:448:VAL:HG23	2.16	0.45
1:E:138:MET:HG2	1:E:140:VAL:HG23	1.98	0.45
1:E:545:TYR:OH	1:E:903:LEU:HD22	2.15	0.45
1:E:873:ALA:N	1:E:874:PRO:HD2	2.30	0.45
1:F:944:LEU:HD12	1:F:975:ILE:HD13	1.98	0.45
1:F:974:PRO:O	1:F:977:MET:N	2.49	0.45
1:A:958:LYS:HG2	1:A:962:GLU:OE1	2.15	0.45
1:B:35:TYR:HB3	1:B:36:PRO:HD2	1.98	0.45
1:B:425:LEU:HB3	1:B:426:PRO:HD2	1.98	0.45
1:C:54:ALA:O	1:C:82:SER:HB3	2.16	0.45
1:C:177:LEU:HD23	1:C:288:GLY:O	2.16	0.45
1:C:199:THR:HG21	1:C:792:ARG:H	1.81	0.45
1:C:909:VAL:HG12	1:C:913:LEU:HG	1.97	0.45
1:C:909:VAL:HG13	1:C:931:LEU:HD11	1.98	0.45
1:D:181:GLN:HG2	1:D:182:TYR:N	2.32	0.45
1:D:944:LEU:CB	1:D:971:ARG:HH12	2.29	0.45
1:D:1038:GLU:HB3	1:D:1040:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:CYS:O	1:E:497:LEU:HB3	2.15	0.45
1:F:46:SER:OG	1:F:89:GLN:HG2	2.17	0.45
1:F:363:ARG:HB2	1:F:496:MET:HE2	1.98	0.45
1:F:368:PRO:O	1:F:371:ALA:HB3	2.16	0.45
1:F:534:ILE:HG23	2:F:2000:LMT:H3'	1.98	0.45
1:F:987:MET:O	1:F:990:VAL:N	2.48	0.45
1:A:672:VAL:O	1:A:673:GLU:HB2	2.17	0.45
1:A:713:LEU:CD2	1:A:843:LEU:HD11	2.39	0.45
1:A:1010:GLY:O	1:A:1014:ALA:HB2	2.16	0.45
1:B:238:THR:HG22	1:B:239:ARG:O	2.16	0.45
1:B:448:VAL:HG13	1:B:888:LEU:HG	1.99	0.45
1:B:467:TYR:CE2	1:B:925:VAL:HG23	2.52	0.45
1:B:744:ASN:O	1:B:748:THR:HG23	2.17	0.45
1:C:34:GLN:CD	1:C:333:VAL:HG22	2.36	0.45
1:C:358:PHE:CE1	1:C:977:MET:HA	2.52	0.45
1:C:420:MET:CE	1:C:427:PRO:HA	2.46	0.45
1:C:506:GLY:C	1:C:508:GLY:N	2.70	0.45
1:C:567:GLU:HG2	1:C:670:ALA:HB2	1.99	0.45
1:C:835:LYS:HA	1:C:835:LYS:NZ	2.31	0.45
1:D:34:GLN:CG	1:D:333:VAL:HG22	2.46	0.45
1:D:139:VAL:HG11	1:D:178:PHE:HE1	1.81	0.45
1:D:232:ALA:HB1	1:E:725:PRO:O	2.16	0.45
1:D:305:ALA:O	1:D:308:ALA:HB3	2.16	0.45
1:D:413:VAL:HA	1:D:493:CYS:SG	2.56	0.45
1:D:574:THR:HG1	1:D:598:TYR:HE2	1.64	0.45
1:D:582:ALA:HB1	1:D:586:ARG:HE	1.80	0.45
1:E:525:HIS:CD2	1:E:529:ASP:OD2	2.69	0.45
1:E:540:ARG:NH2	1:E:541:TYR:OH	2.43	0.45
1:F:77:TYR:HD2	1:F:819:TYR:OH	1.98	0.45
1:F:146:ASP:OD2	1:F:146:ASP:N	2.40	0.45
1:F:182:TYR:HB2	1:F:769:LYS:HZ2	1.81	0.45
1:F:971:ARG:C	1:F:974:PRO:HD2	2.36	0.45
1:A:56:THR:O	1:A:60:THR:HG22	2.17	0.45
1:A:74:ASN:N	1:C:170:SER:OG	2.49	0.45
1:A:448:VAL:O	1:A:451:ALA:HB3	2.17	0.45
1:A:712:MET:HA	1:A:835:LYS:HE3	1.97	0.45
1:A:960:LEU:HB3	1:A:1039:ASP:OD2	2.17	0.45
1:B:187:TRP:HB3	1:B:776:GLU:HG2	1.99	0.45
1:B:905:VAL:O	1:B:909:VAL:HG23	2.17	0.45
1:C:393:LEU:CB	1:C:466:ILE:HG23	2.46	0.45
1:C:394:THR:HB	1:C:469:GLN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:VAL:CA	1:C:487:ILE:HB	2.42	0.45
1:C:537:SER:OG	1:C:540:ARG:HD2	2.17	0.45
1:C:589:LYS:O	1:C:592:ASN:HB2	2.17	0.45
1:C:785:ASP:O	1:C:789:TRP:HD1	1.98	0.45
1:D:284:GLN:HG3	1:D:285:PRO:CD	2.45	0.45
1:E:715:SER:O	1:E:717:ARG:HD2	2.16	0.45
1:E:1031:ARG:O	1:E:1032:ARG:HG3	2.16	0.45
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.16	0.45
1:A:15:ILE:O	1:A:19:ILE:HG13	2.17	0.45
1:A:33:ALA:HA	1:A:299:ALA:HB3	1.98	0.45
1:A:137:LEU:HB2	1:A:293:LEU:CB	2.45	0.45
1:A:240:LEU:HB2	1:A:246:PHE:CE1	2.52	0.45
1:B:7:ASP:O	1:B:8:ARG:HG3	2.17	0.45
1:B:108:GLN:NE2	1:C:112:GLN:OE1	2.50	0.45
1:B:450:SER:O	1:B:454:VAL:HG23	2.16	0.45
1:B:536:ARG:HH21	1:B:536:ARG:CG	2.25	0.45
1:B:841:MET:CE	1:B:863:SER:HB3	2.46	0.45
1:C:11:PHE:O	1:C:11:PHE:HD2	1.99	0.45
1:C:61:VAL:HG22	1:C:119:PRO:CD	2.45	0.45
1:C:350:LEU:HD21	1:C:988:PRO:HG2	1.98	0.45
1:C:358:PHE:CE1	1:C:977:MET:HG2	2.51	0.45
1:C:583:THR:H	1:C:586:ARG:HG3	1.82	0.45
1:C:883:VAL:HG13	1:C:884:VAL:N	2.32	0.45
1:D:747:ASN:OD1	1:F:214:VAL:HG11	2.16	0.45
1:D:850:LYS:HB2	1:D:850:LYS:HZ3	1.80	0.45
1:E:143:ILE:HG22	1:E:286:ALA:HB2	1.98	0.45
1:E:186:ILE:HG12	1:E:268:ILE:CD1	2.45	0.45
1:E:273:GLU:CD	1:E:770:LYS:HD2	2.37	0.45
1:E:407:ASP:OD2	1:E:940:LYS:HG2	2.17	0.45
1:F:157:TYR:HE1	1:F:161:ASN:CG	2.19	0.45
1:A:673:GLU:HG3	1:A:674:LEU:HB2	1.98	0.45
1:B:211:ASN:O	1:B:760:ASN:ND2	2.50	0.45
1:B:459:PHE:CZ	1:B:873:ALA:HA	2.52	0.45
1:B:507:GLU:HB3	1:B:518:ARG:CG	2.46	0.45
1:B:774:MET:SD	1:B:780:ARG:NH2	2.90	0.45
1:B:831:ALA:CB	1:B:837:THR:HA	2.47	0.45
1:B:1037:ASN:CB	1:B:1040:ILE:HG13	2.47	0.45
1:C:456:MET:HA	1:C:459:PHE:CD1	2.52	0.45
1:D:818:ARG:HH12	1:D:823:PRO:HG3	1.82	0.45
1:D:985:GLY:O	1:D:988:PRO:HD2	2.15	0.45
1:E:717:ARG:HG2	1:E:717:ARG:NH1	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:958:LYS:HG2	1:F:962:GLU:OE1	2.17	0.45
1:A:32:VAL:HG22	1:A:390:ILE:HG13	1.97	0.45
1:A:70:ASN:HA	1:C:168:ARG:HG2	1.98	0.45
1:A:73:ASP:HB2	1:A:106:GLN:HE22	1.81	0.45
1:A:112:GLN:HG2	1:B:112:GLN:OE1	2.17	0.45
1:A:344:LEU:HD23	1:A:402:ILE:CD1	2.46	0.45
1:B:355:MET:CE	1:B:410:ILE:HG13	2.47	0.45
1:B:577:GLN:HB3	1:B:662:MET:O	2.17	0.45
1:B:887:CYS:O	1:B:890:ALA:HB3	2.17	0.45
1:B:889:ALA:CA	1:B:898:PRO:HG3	2.46	0.45
1:B:895:TRP:O	1:B:898:PRO:HG2	2.17	0.45
1:C:273:GLU:CD	1:C:770:LYS:HZ3	2.20	0.45
1:C:450:SER:HA	1:C:475:VAL:HG22	1.99	0.45
1:C:468:ARG:O	1:C:471:SER:OG	2.35	0.45
1:C:482:VAL:O	1:C:486:LEU:HG	2.16	0.45
1:C:483:LEU:O	1:C:487:ILE:HD12	2.17	0.45
1:C:536:ARG:HD2	2:C:2000:LMT:H4O1	1.82	0.45
1:C:983:ILE:HD11	1:C:1012:VAL:HG23	1.99	0.45
1:D:26:ALA:O	1:D:30:LEU:HB2	2.15	0.45
1:D:342:LYS:HB2	1:D:342:LYS:HE3	1.62	0.45
1:D:431:THR:O	1:D:435:MET:HB2	2.17	0.45
1:D:614:GLY:O	1:D:621:GLY:N	2.41	0.45
1:E:11:PHE:CE1	1:F:890:ALA:HB1	2.52	0.45
1:E:279:ALA:HB3	1:E:286:ALA:O	2.16	0.45
1:F:78:MET:N	1:F:820:ASN:OD1	2.50	0.45
1:F:584:GLN:N	1:F:622:GLN:HB3	2.32	0.45
1:F:668:LEU:H	1:F:668:LEU:HG	1.30	0.45
1:F:759:VAL:HG23	1:F:760:ASN:H	1.81	0.45
1:F:916:ALA:HA	1:F:921:LEU:HD12	1.98	0.45
1:A:185:ARG:HD2	1:A:187:TRP:CH2	2.52	0.45
1:A:238:THR:HG22	1:A:239:ARG:O	2.17	0.45
1:A:737:GLN:OE1	1:C:250:LEU:HD23	2.17	0.45
1:B:20:MET:HG2	1:B:374:VAL:HA	1.97	0.45
1:B:790:TYR:HD1	1:B:800:PRO:HA	1.79	0.45
1:C:298:ASN:CG	1:C:301:ASP:HB2	2.37	0.45
1:C:335:ILE:O	1:C:339:GLU:HG2	2.16	0.45
1:C:562:SER:OG	1:C:563:PHE:N	2.50	0.45
1:D:847:LEU:C	1:D:849:SER:H	2.20	0.45
1:F:188:MET:CE	1:F:200:PRO:HG3	2.47	0.45
1:F:197:GLN:HA	1:F:798:MET:CE	2.47	0.45
1:F:321:LEU:HD22	1:F:321:LEU:HA	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:634:TRP:CD1	1:F:634:TRP:N	2.84	0.45
1:F:905:VAL:O	1:F:909:VAL:HG23	2.17	0.45
1:A:6:ILE:HG22	1:A:490:PRO:HB2	1.99	0.45
1:A:343:THR:HA	1:A:346:GLU:OE1	2.17	0.45
1:A:594:VAL:HG12	1:A:655:PHE:CE2	2.52	0.45
1:A:605:ASN:O	1:A:631:LEU:HD23	2.17	0.45
1:B:850:LYS:HD3	1:B:850:LYS:N	2.31	0.45
1:B:904:VAL:HG21	1:B:942:ALA:HB2	1.99	0.45
1:B:951:ASP:O	1:B:955:LYS:HG3	2.17	0.45
1:C:104:GLN:HG2	1:C:108:GLN:OE1	2.17	0.45
1:C:178:PHE:O	1:C:287:SER:OG	2.22	0.45
1:C:400:LEU:HD22	1:C:400:LEU:HA	1.43	0.45
1:D:69:MET:HE1	1:D:107:VAL:HG13	1.98	0.45
1:D:154:ILE:HG22	1:D:287:SER:CB	2.47	0.45
1:D:277:ILE:CD1	1:D:620:ARG:HE	2.30	0.45
1:E:41:PRO:O	1:E:94:PHE:HB2	2.17	0.45
1:E:184:MET:CE	1:E:243:THR:HG22	2.47	0.45
1:E:609:VAL:HG13	1:E:629:VAL:HG13	1.99	0.45
1:E:790:TYR:CB	1:E:798:MET:HG2	2.47	0.45
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.99	0.45
1:F:827:ILE:HD12	1:F:827:ILE:H	1.81	0.45
1:A:53:ASP:OD2	1:A:56:THR:OG1	2.34	0.45
1:A:337:ILE:HD11	1:A:392:THR:HA	1.99	0.45
1:A:339:GLU:O	1:A:342:LYS:HB3	2.17	0.45
1:A:355:MET:HB3	1:A:365:THR:HG23	1.99	0.45
1:A:376:LEU:HD23	1:A:376:LEU:HA	1.84	0.45
1:A:378:GLY:O	1:A:381:ALA:N	2.50	0.45
1:A:449:LEU:HB2	1:A:478:MET:SD	2.57	0.45
1:A:548:ILE:HG23	1:A:910:ILE:HD13	1.99	0.45
1:A:692:HIS:NE2	1:A:723:ASP:OD2	2.46	0.45
1:B:990:VAL:O	1:B:991:ILE:HD13	2.17	0.45
1:C:564:LEU:HD21	1:C:670:ALA:HB3	1.99	0.45
1:C:1038:GLU:CA	1:C:1039:ASP:HB2	2.47	0.45
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.83	0.45
1:D:275:TYR:O	1:F:222:THR:OG1	2.33	0.45
1:D:324:VAL:HG12	1:D:325:TYR:H	1.82	0.45
1:F:356:TYR:O	1:F:358:PHE:N	2.50	0.45
1:F:459:PHE:CD2	1:F:876:LEU:HD13	2.52	0.45
1:A:125:GLN:NE2	1:A:125:GLN:HA	2.31	0.44
1:A:960:LEU:HD23	1:A:1031:ARG:HH11	1.82	0.44
1:B:106:GLN:O	1:B:110:LYS:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:PHE:N	1:B:196:PHE:CD1	2.83	0.44
1:B:559:LEU:HD13	1:B:560:PRO:HD2	1.99	0.44
1:B:590:VAL:HA	1:B:593:GLU:OE2	2.17	0.44
1:B:778:LYS:HE3	1:B:779:TYR:OH	2.17	0.44
1:B:901:VAL:HG23	1:B:942:ALA:CB	2.35	0.44
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.99	0.44
1:C:36:PRO:HG2	1:C:38:ILE:HG13	1.97	0.44
1:C:69:MET:HB3	1:C:72:ILE:HD11	1.98	0.44
1:D:65:ILE:HD13	1:D:114:ALA:CB	2.46	0.44
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.99	0.44
1:D:400:LEU:CD1	1:D:933:THR:HG21	2.48	0.44
1:E:300:LEU:HD23	1:E:334:LYS:HE3	1.99	0.44
1:A:42:ALA:HB3	1:A:132:SER:O	2.17	0.44
1:A:505:HIS:O	1:A:507:GLU:N	2.45	0.44
1:A:754:TRP:CZ2	1:A:785:ASP:HB2	2.51	0.44
1:A:959:GLY:CA	1:A:1039:ASP:H	2.24	0.44
1:B:21:LEU:HA	1:B:21:LEU:HD23	1.63	0.44
1:B:527:TYR:O	1:B:530:SER:HB3	2.17	0.44
1:B:549:VAL:O	1:B:552:MET:HB3	2.16	0.44
1:B:702:LEU:HA	1:B:705:GLU:HB2	1.98	0.44
1:B:707:ALA:HB2	1:B:716:VAL:HB	1.99	0.44
1:C:3:ASN:ND2	1:C:435:MET:SD	2.84	0.44
1:C:49:TYR:HD2	1:C:57:VAL:HG12	1.81	0.44
1:C:58:GLN:NE2	1:C:818:ARG:HD2	2.31	0.44
1:C:189:ASN:O	1:C:193:LEU:HB2	2.18	0.44
1:C:542:LEU:O	1:C:546:LEU:HD13	2.16	0.44
1:C:668:LEU:HD23	1:C:668:LEU:H	1.82	0.44
1:D:211:ASN:O	1:D:760:ASN:ND2	2.50	0.44
1:D:747:ASN:O	1:D:750:LEU:N	2.50	0.44
1:D:974:PRO:HA	1:D:977:MET:HE2	1.99	0.44
1:E:699:ARG:HH11	1:E:825:MET:HE1	1.82	0.44
1:E:990:VAL:HG22	1:E:1004:GLY:C	2.37	0.44
1:F:3:ASN:OD1	1:F:3:ASN:N	2.50	0.44
1:F:971:ARG:HG2	1:F:974:PRO:CG	2.47	0.44
1:A:72:ILE:HD11	1:A:110:LYS:HB2	1.99	0.44
1:A:350:LEU:HD21	1:A:984:LEU:HB3	1.98	0.44
1:C:40:PRO:CB	1:C:94:PHE:O	2.66	0.44
1:C:376:LEU:O	1:C:378:GLY:N	2.50	0.44
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.16	0.44
1:C:926:TYR:CE1	1:C:999:ALA:HB1	2.51	0.44
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594:VAL:HG22	1:D:655:PHE:CE2	2.53	0.44
1:E:78:MET:HB3	1:E:820:ASN:HA	1.99	0.44
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.73	0.44
1:E:668:LEU:H	1:E:668:LEU:CD2	2.19	0.44
1:E:875:SER:O	1:E:879:ILE:HD13	2.17	0.44
1:F:131:LYS:HB3	1:F:131:LYS:HE2	1.81	0.44
1:F:203:VAL:O	1:F:206:ALA:HB3	2.17	0.44
1:F:1034:SER:OG	1:F:1037:ASN:HB2	2.16	0.44
1:A:711:ASP:C	1:A:835:LYS:HE3	2.37	0.44
1:A:727:PHE:HB2	1:A:809:TRP:CZ3	2.52	0.44
1:B:122:VAL:O	1:B:125:GLN:N	2.47	0.44
1:B:353:LEU:HD22	1:B:353:LEU:HA	1.64	0.44
1:B:544:LEU:HD22	1:B:547:ILE:HB	1.99	0.44
1:B:571:VAL:O	1:B:668:LEU:HD21	2.18	0.44
1:B:948:PHE:HE1	1:B:971:ARG:HH21	1.65	0.44
1:C:99:ASP:CB	1:C:102:ILE:HB	2.46	0.44
1:C:727:PHE:HB2	1:C:809:TRP:CZ3	2.53	0.44
1:D:559:LEU:HD22	1:D:923:ASN:H	1.82	0.44
1:D:676:THR:H	1:D:862:MET:HE2	1.81	0.44
1:E:792:ARG:HG2	1:E:792:ARG:HH11	1.81	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.67	0.44
1:A:27:ILE:HA	1:A:27:ILE:HD13	1.59	0.44
1:A:115:MET:SD	1:A:123:GLN:HG2	2.58	0.44
1:A:161:ASN:HB2	1:A:162:MET:SD	2.57	0.44
1:A:194:ASN:OD1	1:A:798:MET:HG3	2.18	0.44
1:A:622:GLN:HE21	1:A:622:GLN:HB2	1.57	0.44
1:B:81:ASN:HD22	1:B:815:ARG:HH21	1.65	0.44
1:B:401:ALA:HB2	1:B:474:ILE:HG23	1.99	0.44
1:B:923:ASN:ND2	1:B:923:ASN:C	2.71	0.44
1:C:20:MET:CG	1:C:374:VAL:HA	2.47	0.44
1:C:394:THR:CB	1:C:469:GLN:HB3	2.47	0.44
1:C:555:LEU:HD23	1:C:555:LEU:O	2.18	0.44
1:C:682:PHE:HB2	1:C:859:TRP:CZ3	2.52	0.44
1:D:4:PHE:O	1:D:8:ARG:HD2	2.18	0.44
1:D:156:ASP:HA	1:D:181:GLN:HA	2.00	0.44
1:D:163:LYS:HG3	1:D:177:LEU:HB2	1.99	0.44
1:D:951:ASP:CG	1:D:955:LYS:HZ1	2.19	0.44
1:E:675:GLY:HA2	1:E:862:MET:SD	2.57	0.44
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.98	0.44
1:F:30:LEU:HD13	1:F:384:ALA:HB2	1.99	0.44
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:ASN:HD22	1:A:975:ILE:HG23	1.83	0.44
1:B:76:MET:HE1	1:B:865:GLN:HE21	1.82	0.44
1:B:105:VAL:HG13	1:C:108:GLN:HE21	1.83	0.44
1:B:420:MET:CE	1:B:427:PRO:HA	2.48	0.44
1:B:467:TYR:HE2	1:B:925:VAL:HG23	1.83	0.44
1:B:492:LEU:HD22	1:B:496:MET:SD	2.58	0.44
1:B:527:TYR:CD2	1:B:972:LEU:HG	2.52	0.44
1:B:695:LEU:O	1:B:698:ALA:HB3	2.18	0.44
1:C:25:LEU:HD23	1:C:28:LEU:CD1	2.47	0.44
1:C:25:LEU:HA	1:C:28:LEU:HD12	2.00	0.44
1:C:262:LEU:CG	1:C:268:ILE:HD11	2.47	0.44
1:D:538:THR:HG23	1:D:542:LEU:HD13	2.00	0.44
1:E:545:TYR:HE2	1:E:907:LEU:CD1	2.30	0.44
1:E:565:PRO:HG2	1:E:998:GLY:C	2.38	0.44
1:E:586:ARG:HE	1:E:586:ARG:HB2	1.58	0.44
1:E:787:GLY:C	1:E:789:TRP:H	2.21	0.44
1:E:992:SER:C	1:E:997:SER:HG	2.21	0.44
1:E:1036:LYS:HA	1:E:1038:GLU:HG2	2.00	0.44
1:F:38:ILE:CG2	1:F:462:SER:HB3	2.39	0.44
1:F:483:LEU:HA	1:F:483:LEU:HD23	1.61	0.44
1:F:623:ASN:OD1	1:F:623:ASN:N	2.42	0.44
1:F:773:VAL:HG23	1:F:773:VAL:O	2.18	0.44
1:F:792:ARG:HG2	1:F:792:ARG:HH11	1.82	0.44
1:A:445:ILE:HG21	1:A:940:LYS:HZ3	1.83	0.44
1:A:781:MET:HB3	1:C:228:GLN:HE21	1.82	0.44
1:A:1035:ARG:HG3	1:A:1036:LYS:H	1.83	0.44
1:B:62:THR:O	1:B:66:GLU:HG2	2.18	0.44
1:B:105:VAL:CG2	1:C:105:VAL:HG13	2.48	0.44
1:B:163:LYS:NZ	1:B:163:LYS:CB	2.80	0.44
1:B:447:MET:HB3	1:B:887:CYS:HG	1.81	0.44
1:C:157:TYR:CE2	1:C:161:ASN:CG	2.88	0.44
1:C:253:VAL:HG13	1:C:259:ARG:HD3	2.00	0.44
1:C:912:ALA:HB2	1:C:1010:GLY:HA3	2.00	0.44
1:D:199:THR:HB	1:D:749:THR:HG21	1.98	0.44
1:D:418:ARG:CZ	1:D:970:MET:HE2	2.48	0.44
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.34	0.44
1:D:819:TYR:O	1:D:820:ASN:HB2	2.17	0.44
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.47	0.44
1:E:948:PHE:CE2	1:E:971:ARG:HD3	2.52	0.44
1:E:958:LYS:O	1:E:1040:ILE:HG21	2.18	0.44
1:E:987:MET:HB3	1:E:988:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:945:ILE:HG12	1:F:971:ARG:NH2	2.33	0.44
1:A:6:ILE:HG13	1:A:7:ASP:N	2.32	0.44
1:A:240:LEU:HD11	1:A:249:ILE:HD11	1.99	0.44
1:A:502:LYS:H	1:A:502:LYS:HG3	1.60	0.44
1:A:572:PHE:CE1	1:A:648:THR:HG22	2.53	0.44
1:A:787:GLY:O	1:A:789:TRP:N	2.51	0.44
1:A:945:ILE:HG13	1:A:971:ARG:NH2	2.32	0.44
1:B:115:MET:SD	1:B:123:GLN:HG2	2.58	0.44
1:B:361:ASN:O	1:B:365:THR:N	2.39	0.44
1:B:398:MET:HE3	1:B:398:MET:HB3	1.82	0.44
1:B:692:HIS:CD2	1:B:816:LEU:HD22	2.53	0.44
1:B:754:TRP:CZ2	1:B:780:ARG:HA	2.53	0.44
1:B:996:GLY:O	1:B:998:GLY:N	2.50	0.44
1:B:1015:THR:O	1:B:1017:LEU:N	2.51	0.44
1:C:534:ILE:HG22	1:C:541:TYR:CZ	2.53	0.44
1:C:727:PHE:CD1	1:C:809:TRP:CZ3	3.05	0.44
1:C:774:MET:HB3	1:C:774:MET:HE2	1.48	0.44
1:C:924:ASP:N	1:C:924:ASP:OD2	2.45	0.44
1:D:244:GLU:OE1	1:D:248:LYS:HE2	2.18	0.44
1:D:937:LEU:O	1:D:940:LYS:HB3	2.18	0.44
1:D:968:VAL:CG2	1:D:1023:PRO:HG3	2.47	0.44
1:D:1041:GLU:CB	1:D:1042:HIS:HA	2.48	0.44
1:E:15:ILE:O	1:E:19:ILE:HG13	2.17	0.44
1:E:352:PHE:CD2	1:E:353:LEU:HD23	2.48	0.44
1:F:101:ASP:OD1	1:F:131:LYS:HE3	2.18	0.44
1:F:235:ILE:HG22	1:F:236:ALA:O	2.16	0.44
1:F:658:ILE:O	1:F:658:ILE:HG13	2.17	0.44
1:A:63:GLN:OE1	1:C:768:VAL:HG23	2.17	0.44
1:B:11:PHE:O	1:B:15:ILE:HG13	2.18	0.44
1:B:14:VAL:O	1:B:18:ILE:HB	2.18	0.44
1:B:364:ALA:O	1:B:368:PRO:HD3	2.18	0.44
1:C:4:PHE:CZ	1:C:436:GLY:HA3	2.53	0.44
1:C:373:PRO:O	1:C:377:LEU:HB2	2.18	0.44
1:C:375:VAL:CG1	1:C:477:ALA:HA	2.48	0.44
1:C:415:ASN:O	1:C:419:VAL:HG22	2.18	0.44
1:D:112:GLN:HA	1:D:115:MET:HB2	1.99	0.44
1:D:591:LEU:CD1	1:D:613:ASN:HB2	2.48	0.44
1:D:775:SER:OG	1:D:780:ARG:HD3	2.17	0.44
1:D:873:ALA:N	1:D:874:PRO:HD2	2.33	0.44
1:E:415:ASN:OD1	1:E:434:SER:HB2	2.17	0.44
1:E:443:VAL:O	1:E:447:MET:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:LEU:HD22	1:E:559:LEU:HA	1.80	0.44
1:F:185:ARG:HD3	1:F:185:ARG:HA	1.79	0.44
1:F:400:LEU:O	1:F:404:LEU:HD22	2.18	0.44
1:F:982:PHE:O	1:F:985:GLY:N	2.51	0.44
1:A:53:ASP:O	1:A:56:THR:HB	2.17	0.43
1:A:58:GLN:O	1:A:63:GLN:HG3	2.18	0.43
1:A:169:THR:HG21	1:A:306:ILE:HD11	1.99	0.43
1:A:358:PHE:C	1:A:360:GLN:HE21	2.20	0.43
1:A:417:GLU:OE1	1:A:497:LEU:HD21	2.18	0.43
1:A:509:LYS:O	1:A:510:LYS:HB2	2.17	0.43
1:B:438:ILE:HD12	1:B:442:LEU:HG	2.00	0.43
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.51	0.43
1:C:136:PHE:CE2	1:C:292:LYS:HG3	2.53	0.43
1:C:160:ALA:HA	1:C:767:ARG:CZ	2.47	0.43
1:C:478:MET:O	1:C:482:VAL:HG23	2.18	0.43
1:C:520:PHE:CE2	1:C:973:ARG:HG3	2.53	0.43
1:C:775:SER:OG	1:C:776:GLU:O	2.36	0.43
1:C:941:ASN:ND2	1:C:975:ILE:HG23	2.33	0.43
1:D:23:GLY:CA	1:D:377:LEU:O	2.66	0.43
1:D:102:ILE:HD13	1:D:102:ILE:HA	1.88	0.43
1:D:178:PHE:HB2	1:D:288:GLY:H	1.82	0.43
1:D:277:ILE:HD13	1:D:620:ARG:HE	1.83	0.43
1:D:793:ALA:HB3	1:D:795:ASP:OD2	2.18	0.43
1:E:146:ASP:OD2	1:E:146:ASP:N	2.45	0.43
1:E:182:TYR:HB2	1:E:769:LYS:NZ	2.33	0.43
1:E:520:PHE:CE2	1:E:973:ARG:HG3	2.51	0.43
1:E:523:SER:O	1:E:526:HIS:HB2	2.18	0.43
1:E:552:MET:HB2	1:E:910:ILE:CG1	2.48	0.43
1:E:1026:PHE:CD2	1:E:1026:PHE:C	2.92	0.43
1:F:4:PHE:HB3	1:F:432:ARG:HH22	1.82	0.43
1:A:123:GLN:O	1:B:116:PRO:HB2	2.17	0.43
1:A:354:VAL:HG21	1:A:981:ALA:HA	2.00	0.43
1:A:443:VAL:O	1:A:447:MET:HG2	2.18	0.43
1:A:459:PHE:CB	1:A:464:GLY:HA2	2.48	0.43
1:A:515:TRP:HB3	1:A:519:MET:HE1	2.00	0.43
1:A:776:GLU:HG2	1:A:777:ALA:H	1.81	0.43
1:A:845:GLU:O	1:A:849:SER:HB2	2.18	0.43
1:A:1011:MET:O	1:A:1015:THR:HG23	2.18	0.43
1:B:188:MET:HE1	1:B:200:PRO:HG3	2.00	0.43
1:B:340:VAL:HG12	1:B:395:MET:SD	2.57	0.43
1:B:411:VAL:HG21	1:B:944:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LEU:HD23	1:B:670:ALA:HB3	2.01	0.43
1:B:574:THR:HA	1:B:665:ALA:HA	2.00	0.43
1:B:575:MET:HE2	1:B:575:MET:HB2	1.79	0.43
1:B:792:ARG:NH1	1:B:793:ALA:O	2.52	0.43
1:B:891:LEU:HD12	1:B:891:LEU:HA	1.61	0.43
1:C:162:MET:O	1:C:164:ASP:N	2.51	0.43
1:C:230:LEU:HG	1:C:231:ASN:N	2.32	0.43
1:D:34:GLN:HG3	1:D:333:VAL:HG22	1.99	0.43
1:D:36:PRO:O	1:D:38:ILE:HG23	2.19	0.43
1:D:157:TYR:CE2	1:D:161:ASN:CG	2.91	0.43
1:D:641:GLU:HA	1:D:646:ALA:HB3	2.00	0.43
1:D:957:GLY:HA2	1:D:1042:HIS:CG	2.53	0.43
1:E:75:LEU:HA	1:E:94:PHE:CD1	2.52	0.43
1:E:382:VAL:HG11	1:E:476:SER:OG	2.18	0.43
1:E:704:ALA:O	1:E:708:LYS:HG3	2.17	0.43
1:A:598:TYR:CE2	1:A:629:VAL:HG21	2.53	0.43
1:A:888:LEU:HB3	1:A:898:PRO:HG3	1.99	0.43
1:B:194:ASN:OD1	1:B:790:TYR:HD2	2.01	0.43
1:B:531:VAL:HG21	1:B:968:VAL:HG11	2.00	0.43
1:B:680:PHE:CD1	1:B:859:TRP:CH2	3.06	0.43
1:B:702:LEU:O	1:B:705:GLU:N	2.51	0.43
1:C:34:GLN:HG3	1:C:333:VAL:HG13	2.00	0.43
1:C:679:GLY:CA	1:C:837:THR:HG21	2.38	0.43
1:C:705:GLU:OE2	1:C:851:LEU:HD21	2.18	0.43
1:D:137:LEU:O	1:D:329:THR:HG23	2.18	0.43
1:D:470:PHE:O	1:D:474:ILE:HG13	2.19	0.43
1:E:953:MET:HE2	1:E:963:ALA:HB3	2.00	0.43
1:F:156:ASP:OD1	1:F:765:ARG:NH2	2.51	0.43
1:A:577:GLN:OE1	1:A:624:THR:HG23	2.19	0.43
1:A:742:SER:O	1:A:746:ILE:HG23	2.19	0.43
1:B:190:PRO:HB3	1:B:789:TRP:CZ3	2.53	0.43
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.55	0.43
1:B:680:PHE:CD1	1:B:859:TRP:HH2	2.37	0.43
1:B:948:PHE:O	1:B:952:LEU:HG	2.17	0.43
1:C:372:VAL:O	1:C:373:PRO:C	2.56	0.43
1:D:11:PHE:CD2	1:E:890:ALA:HB1	2.53	0.43
1:D:720:GLY:C	1:D:721:LEU:HD22	2.39	0.43
1:E:54:ALA:HB1	1:E:816:LEU:HG	2.00	0.43
1:E:518:ARG:O	1:E:522:LYS:HG3	2.18	0.43
1:E:556:PHE:HB2	1:E:913:LEU:HD11	2.00	0.43
1:F:57:VAL:O	1:F:62:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:ARG:NH1	1:F:307:ARG:HG3	2.31	0.43
1:F:414:GLU:HG2	1:F:973:ARG:NH2	2.32	0.43
1:F:469:GLN:O	1:F:472:ILE:HG22	2.18	0.43
1:F:989:LEU:HD23	1:F:989:LEU:HA	1.58	0.43
1:A:680:PHE:HB2	1:A:859:TRP:CZ3	2.45	0.43
1:A:1038:GLU:HB3	1:A:1041:GLU:HB2	1.99	0.43
1:B:484:VAL:O	1:B:489:THR:HG23	2.17	0.43
1:B:736:ALA:HB1	1:B:741:VAL:HG23	1.99	0.43
1:B:971:ARG:HA	1:B:971:ARG:HD2	1.59	0.43
1:C:65:ILE:HG23	1:C:111:LEU:HA	2.00	0.43
1:C:527:TYR:HE1	1:C:968:VAL:HG12	1.83	0.43
1:C:531:VAL:HA	1:C:534:ILE:HD11	2.00	0.43
1:C:699:ARG:HD2	1:C:827:ILE:CD1	2.47	0.43
1:C:1037:ASN:O	1:C:1038:GLU:HB2	2.17	0.43
1:E:452:VAL:HG12	1:E:884:VAL:HG21	1.99	0.43
1:E:485:ALA:O	1:E:486:LEU:HD23	2.19	0.43
1:F:36:PRO:HG3	1:F:469:GLN:CG	2.49	0.43
1:F:154:ILE:HG22	1:F:287:SER:HB3	2.00	0.43
1:A:157:TYR:HE2	1:A:161:ASN:ND2	2.17	0.43
1:A:185:ARG:HD3	1:A:185:ARG:HA	1.74	0.43
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.99	0.43
1:A:298:ASN:ND2	1:A:301:ASP:HB2	2.34	0.43
1:A:470:PHE:O	1:A:474:ILE:HG13	2.19	0.43
1:A:873:ALA:N	1:A:874:PRO:HD2	2.33	0.43
1:B:68:ASN:OD1	1:B:117:LEU:HD23	2.19	0.43
1:B:80:SER:O	1:B:817:GLU:HA	2.18	0.43
1:B:185:ARG:HD3	1:B:185:ARG:HA	1.75	0.43
1:B:427:PRO:O	1:B:431:THR:OG1	2.22	0.43
1:B:615:ALA:CB	1:B:620:ARG:HA	2.48	0.43
1:B:885:PHE:CE1	1:B:899:PHE:CE1	3.06	0.43
1:B:892:TYR:O	1:B:893:GLU:HB2	2.17	0.43
1:C:594:VAL:HA	1:C:655:PHE:CE2	2.54	0.43
1:C:600:THR:O	1:C:603:LYS:HG3	2.18	0.43
1:C:691:GLY:C	1:C:694:LYS:HG2	2.38	0.43
1:D:428:LYS:H	1:D:428:LYS:HE3	1.82	0.43
1:D:574:THR:OG1	1:D:598:TYR:HE2	2.02	0.43
1:D:671:ILE:C	1:D:673:GLU:N	2.71	0.43
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.53	0.43
1:F:249:ILE:O	1:F:261:LEU:HA	2.19	0.43
1:F:672:VAL:O	1:F:675:GLY:N	2.50	0.43
1:F:905:VAL:HG13	1:F:935:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ASP:O	1:A:969:ARG:HB3	2.19	0.43
1:A:1028:VAL:O	1:A:1032:ARG:NH1	2.47	0.43
1:B:105:VAL:HA	1:C:109:ASN:HD21	1.83	0.43
1:B:402:ILE:O	1:B:405:LEU:HB2	2.19	0.43
1:B:515:TRP:O	1:B:517:ASN:N	2.52	0.43
1:C:197:GLN:HA	1:C:798:MET:HE2	2.01	0.43
1:C:367:ILE:HD13	1:C:367:ILE:N	2.33	0.43
1:C:932:LEU:O	1:C:935:ILE:HG23	2.19	0.43
1:D:102:ILE:HD12	1:F:101:ASP:HB3	1.99	0.43
1:D:577:GLN:OE1	1:D:624:THR:HG22	2.19	0.43
1:E:187:TRP:HA	1:E:774:MET:O	2.19	0.43
1:E:235:ILE:HG22	1:E:236:ALA:H	1.84	0.43
1:E:240:LEU:HD12	1:E:246:PHE:CD2	2.54	0.43
1:F:181:GLN:HG2	1:F:182:TYR:N	2.33	0.43
1:F:326:PRO:O	1:F:630:SER:HB2	2.18	0.43
1:F:909:VAL:HG12	1:F:913:LEU:HG	2.01	0.43
1:F:968:VAL:HA	1:F:971:ARG:HH22	1.83	0.43
1:A:362:PHE:CD2	1:A:362:PHE:N	2.87	0.43
1:A:471:SER:O	1:A:475:VAL:HG23	2.19	0.43
1:A:699:ARG:HG2	1:A:703:LEU:CD1	2.49	0.43
1:B:255:GLN:CD	1:B:255:GLN:H	2.22	0.43
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.01	0.43
1:B:462:SER:O	1:B:466:ILE:HG13	2.19	0.43
1:B:562:SER:OG	1:B:563:PHE:N	2.52	0.43
1:B:838:GLY:O	1:B:841:MET:HB2	2.19	0.43
1:C:40:PRO:HB2	1:C:94:PHE:O	2.19	0.43
1:C:136:PHE:CD2	1:C:292:LYS:HG3	2.54	0.43
1:C:139:VAL:O	1:C:326:PRO:HD2	2.19	0.43
1:C:154:ILE:CG2	1:C:287:SER:HB3	2.48	0.43
1:C:563:PHE:HB2	1:C:866:GLU:CB	2.48	0.43
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.84	0.43
1:C:743:ILE:HA	1:C:746:ILE:HG23	2.00	0.43
1:C:922:THR:O	1:C:924:ASP:N	2.52	0.43
1:C:961:ILE:H	1:C:961:ILE:CD1	2.25	0.43
1:D:131:LYS:HZ3	1:D:131:LYS:HB2	1.84	0.43
1:D:360:GLN:HE22	1:D:517:ASN:ND2	2.00	0.43
1:D:362:PHE:HD2	1:D:363:ARG:HH12	1.67	0.43
1:E:49:TYR:HB3	1:E:57:VAL:HG12	1.99	0.43
1:E:390:ILE:HG23	1:E:395:MET:SD	2.59	0.43
1:E:448:VAL:HG13	1:E:884:VAL:CG1	2.48	0.43
1:E:544:LEU:HA	1:E:547:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:347:ALA:CB	1:F:402:ILE:HD12	2.46	0.43
1:F:845:GLU:HG2	1:F:857:TYR:CE1	2.54	0.43
1:F:876:LEU:HD12	1:F:876:LEU:O	2.19	0.43
1:A:34:GLN:NE2	1:A:333:VAL:HG22	2.34	0.43
1:A:536:ARG:HD3	2:A:2000:LMT:H4B	2.01	0.43
1:A:713:LEU:HD11	1:A:843:LEU:HD11	2.01	0.43
1:A:1035:ARG:HG3	1:A:1036:LYS:N	2.34	0.43
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.39	0.43
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	1.99	0.43
1:B:849:SER:HB3	1:B:850:LYS:HD3	2.01	0.43
1:C:39:ALA:HA	1:C:40:PRO:HD2	1.76	0.43
1:C:225:VAL:HG22	1:C:226:LYS:HD3	2.00	0.43
1:C:356:TYR:HA	1:C:365:THR:HG21	2.00	0.43
1:D:243:THR:O	1:D:246:PHE:HB2	2.19	0.43
1:D:703:LEU:O	1:D:703:LEU:HD22	2.19	0.43
1:D:931:LEU:HD22	1:D:931:LEU:HA	1.76	0.43
1:E:455:PRO:O	1:E:876:LEU:HD13	2.18	0.43
1:F:27:ILE:HA	1:F:30:LEU:HD22	2.00	0.43
1:F:62:THR:HG21	1:F:82:SER:OG	2.19	0.43
1:F:754:TRP:CZ3	1:F:780:ARG:HA	2.53	0.43
1:A:78:MET:HE2	1:C:168:ARG:NH1	2.34	0.43
1:A:690:LEU:HD22	1:A:694:LYS:NZ	2.34	0.43
1:A:695:LEU:HA	1:A:695:LEU:HD23	1.75	0.43
1:A:768:VAL:HG11	1:B:63:GLN:HB3	2.01	0.43
1:B:899:PHE:O	1:B:903:LEU:HD22	2.19	0.43
1:C:282:ASN:OD1	1:C:599:LEU:HD11	2.19	0.43
1:C:393:LEU:H	1:C:393:LEU:CD2	2.31	0.43
1:C:506:GLY:O	1:C:508:GLY:N	2.51	0.43
1:C:736:ALA:HB1	1:C:741:VAL:CG1	2.48	0.43
1:C:921:LEU:HD13	1:C:1002:ALA:HA	2.01	0.43
1:E:688:ALA:O	1:E:690:LEU:N	2.50	0.43
1:E:971:ARG:HA	1:E:971:ARG:HD2	1.39	0.43
1:F:913:LEU:HD23	1:F:927:PHE:HZ	1.84	0.43
1:F:948:PHE:O	1:F:952:LEU:HG	2.19	0.43
1:A:327:TYR:CD2	1:A:327:TYR:C	2.92	0.42
1:A:1033:PHE:CG	1:A:1034:SER:N	2.87	0.42
1:B:450:SER:N	1:B:478:MET:SD	2.92	0.42
1:B:598:TYR:CE2	1:B:629:VAL:HG21	2.53	0.42
1:B:888:LEU:HD23	1:B:888:LEU:HA	1.66	0.42
1:C:104:GLN:HE21	1:C:131:LYS:CG	2.32	0.42
1:C:190:PRO:HB3	1:C:789:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASN:CB	1:C:301:ASP:HB2	2.49	0.42
1:C:400:LEU:HG	1:C:933:THR:OG1	2.19	0.42
1:C:488:LEU:O	1:C:491:ALA:N	2.52	0.42
1:C:953:MET:O	1:C:957:GLY:HA2	2.18	0.42
1:D:62:THR:O	1:D:66:GLU:HG3	2.19	0.42
1:D:435:MET:HA	1:D:435:MET:CE	2.49	0.42
1:D:618:ALA:HB1	1:D:815:ARG:CZ	2.49	0.42
1:D:674:LEU:HD23	1:D:674:LEU:HA	1.84	0.42
1:D:790:TYR:HA	1:D:799:VAL:O	2.19	0.42
1:E:578:LEU:O	1:E:623:ASN:HB2	2.19	0.42
1:E:978:THR:HG22	1:E:979:SER:N	2.33	0.42
1:F:157:TYR:CE1	1:F:161:ASN:CG	2.92	0.42
1:F:186:ILE:CB	1:F:773:VAL:HG12	2.48	0.42
1:F:228:GLN:NE2	1:F:230:LEU:O	2.52	0.42
1:A:284:GLN:HA	1:A:285:PRO:HD3	1.90	0.42
1:A:538:THR:HG23	1:A:539:GLY:H	1.83	0.42
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.35	0.42
1:A:853:THR:O	1:A:853:THR:OG1	2.36	0.42
1:A:900:SER:CA	1:A:1029:VAL:HG21	2.48	0.42
1:A:984:LEU:HD22	1:A:984:LEU:HA	1.50	0.42
1:B:445:ILE:HD12	1:B:449:LEU:HD22	2.00	0.42
1:B:840:ALA:O	1:B:844:MET:HG2	2.19	0.42
1:B:877:TYR:HD2	1:B:877:TYR:HA	1.38	0.42
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.95	0.42
1:C:293:LEU:HD22	1:C:294:ALA:H	1.84	0.42
1:C:388:PHE:CZ	1:C:468:ARG:HD3	2.53	0.42
1:C:906:PRO:O	1:C:910:ILE:HG22	2.19	0.42
1:C:967:ALA:HA	1:C:970:MET:HE1	2.01	0.42
1:D:364:ALA:CB	1:D:497:LEU:HD13	2.49	0.42
1:D:404:LEU:HD21	1:D:449:LEU:HD21	2.01	0.42
1:E:122:VAL:O	1:E:124:GLN:N	2.52	0.42
1:E:536:ARG:NH2	2:E:2000:LMT:C4B	2.76	0.42
1:E:638:PRO:HB2	1:E:639:GLY:H	1.66	0.42
1:E:932:LEU:O	1:E:935:ILE:HB	2.19	0.42
1:E:1027:VAL:HG23	1:E:1028:VAL:N	2.34	0.42
1:F:452:VAL:HG12	1:F:884:VAL:HG21	2.01	0.42
1:A:198:LEU:HD22	1:A:202:ASP:CB	2.49	0.42
1:A:222:THR:OG1	1:B:275:TYR:O	2.37	0.42
1:A:586:ARG:O	1:A:589:LYS:HB3	2.20	0.42
1:A:778:LYS:HG3	1:A:779:TYR:CE2	2.54	0.42
1:A:800:PRO:HG2	1:A:803:ALA:CB	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:930:GLY:O	1:A:933:THR:HG22	2.19	0.42
1:B:222:THR:HA	1:B:224:PRO:CD	2.46	0.42
1:B:416:VAL:HG23	1:B:431:THR:HA	2.00	0.42
1:B:452:VAL:C	1:B:455:PRO:HD2	2.40	0.42
1:B:560:PRO:O	1:B:922:THR:HG23	2.19	0.42
1:B:913:LEU:HD23	1:B:927:PHE:HZ	1.84	0.42
1:B:926:TYR:CD1	1:B:999:ALA:HA	2.55	0.42
1:C:152:GLU:CD	1:C:152:GLU:H	2.23	0.42
1:C:197:GLN:O	1:C:792:ARG:HD3	2.20	0.42
1:C:214:VAL:HG12	1:C:215:ALA:O	2.19	0.42
1:C:277:ILE:HD12	1:C:620:ARG:NH1	2.34	0.42
1:C:281:PHE:HD2	1:C:610:PHE:HE1	1.65	0.42
1:C:326:PRO:HA	1:C:630:SER:OG	2.18	0.42
1:C:714:THR:CB	1:C:832:ALA:HA	2.49	0.42
1:D:136:PHE:HE2	1:D:290:GLY:HA3	1.85	0.42
1:D:894:SER:OG	1:D:897:ILE:HG13	2.20	0.42
1:E:1037:ASN:HA	1:E:1038:GLU:HB2	2.01	0.42
1:F:99:ASP:HB3	1:F:102:ILE:CG2	2.50	0.42
1:F:307:ARG:NH1	1:F:307:ARG:O	2.52	0.42
1:F:619:GLY:O	1:F:624:THR:HG21	2.19	0.42
1:B:524:THR:HA	1:B:527:TYR:HB3	2.02	0.42
1:B:527:TYR:CD1	1:B:1020:PHE:HE1	2.36	0.42
1:B:709:HIS:HB2	1:B:713:LEU:HD12	2.01	0.42
1:B:778:LYS:HG3	1:B:779:TYR:CE2	2.54	0.42
1:D:65:ILE:C	1:D:67:GLN:H	2.22	0.42
1:D:234:ILE:HG23	1:E:729:ILE:HD13	2.00	0.42
1:D:250:LEU:HD11	1:D:259:ARG:HB3	1.99	0.42
1:D:407:ASP:OD2	1:D:978:THR:HG21	2.20	0.42
1:F:26:ALA:O	1:F:30:LEU:HD13	2.19	0.42
1:F:315:PRO:C	1:F:317:PHE:H	2.22	0.42
1:F:404:LEU:HD11	1:F:937:LEU:HD11	2.01	0.42
1:F:478:MET:O	1:F:481:SER:N	2.53	0.42
1:A:559:LEU:HD23	1:A:560:PRO:N	2.34	0.42
1:B:78:MET:HB3	1:B:820:ASN:HA	2.00	0.42
1:B:507:GLU:O	1:B:508:GLY:C	2.57	0.42
1:B:610:PHE:O	1:B:627:ALA:HA	2.20	0.42
1:B:727:PHE:CE1	1:B:807:SER:HB2	2.55	0.42
1:B:889:ALA:HB1	1:B:894:SER:O	2.20	0.42
1:B:892:TYR:CD2	1:B:897:ILE:HB	2.55	0.42
1:B:1013:THR:O	1:B:1017:LEU:HB2	2.20	0.42
1:C:74:ASN:HB3	1:C:95:GLU:CB	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:LYS:HE2	1:C:511:GLY:N	2.35	0.42
1:C:549:VAL:O	1:C:552:MET:HB3	2.19	0.42
1:C:676:THR:HG21	1:C:828:LEU:HD13	2.02	0.42
1:C:974:PRO:O	1:C:977:MET:N	2.53	0.42
1:D:158:VAL:O	1:D:162:MET:HB2	2.20	0.42
1:D:530:SER:CA	2:D:2000:LMT:O2'	2.68	0.42
1:D:682:PHE:CE2	1:D:857:TYR:HB2	2.55	0.42
1:D:687:GLN:HG2	1:F:316:PHE:HD1	1.83	0.42
1:D:729:ILE:O	1:D:729:ILE:HG22	2.19	0.42
1:D:743:ILE:O	1:D:746:ILE:HB	2.20	0.42
1:D:753:ALA:O	1:D:775:SER:OG	2.11	0.42
1:E:126:GLY:HA3	1:F:116:PRO:HB3	2.02	0.42
1:E:261:LEU:HD23	1:E:263:ARG:NH1	2.35	0.42
1:F:77:TYR:CE2	1:F:860:THR:OG1	2.69	0.42
1:F:835:LYS:HZ2	1:F:836:SER:H	1.68	0.42
1:A:6:ILE:HA	1:A:491:ALA:HA	2.00	0.42
1:A:578:LEU:HD13	1:A:661:ALA:HB2	2.02	0.42
1:A:743:ILE:O	1:A:746:ILE:N	2.52	0.42
1:A:937:LEU:HD23	1:A:937:LEU:HA	1.67	0.42
1:A:1030:ARG:C	1:A:1032:ARG:N	2.72	0.42
1:B:449:LEU:HB2	1:B:478:MET:SD	2.60	0.42
1:B:525:HIS:NE2	1:B:529:ASP:OD2	2.52	0.42
1:B:685:ILE:HD11	1:B:819:TYR:HD2	1.85	0.42
1:C:220:GLY:HA3	1:C:230:LEU:O	2.19	0.42
1:C:375:VAL:HG22	1:C:480:LEU:CB	2.45	0.42
1:C:393:LEU:HG	1:C:466:ILE:CG1	2.49	0.42
1:C:451:ALA:O	1:C:883:VAL:HG11	2.20	0.42
1:C:699:ARG:CG	1:C:827:ILE:HD11	2.48	0.42
1:C:727:PHE:O	1:C:729:ILE:HD12	2.19	0.42
1:C:781:MET:HB2	1:C:782:LEU:HD22	2.02	0.42
1:D:65:ILE:C	1:D:67:GLN:N	2.73	0.42
1:E:343:THR:HB	1:E:989:LEU:HD21	2.01	0.42
1:E:392:THR:HB	1:E:393:LEU:HD23	2.01	0.42
1:F:200:PRO:HA	1:F:203:VAL:HG23	2.02	0.42
1:F:741:VAL:HG21	1:F:804:PHE:HE1	1.85	0.42
1:F:787:GLY:O	1:F:789:TRP:N	2.51	0.42
1:F:953:MET:SD	1:F:960:LEU:HA	2.59	0.42
1:A:196:PHE:HD2	1:A:196:PHE:N	2.17	0.42
1:A:199:THR:OG1	1:A:201:VAL:HG13	2.19	0.42
1:A:535:LEU:HD13	1:A:961:ILE:HG23	2.01	0.42
1:A:895:TRP:CE2	1:C:10:ILE:HG13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:GLN:HA	1:B:115:MET:HB2	2.01	0.42
1:B:352:PHE:HD1	1:B:369:THR:OG1	2.00	0.42
1:B:867:ARG:HE	1:B:867:ARG:C	2.16	0.42
1:C:184:MET:HG2	1:C:246:PHE:CE2	2.55	0.42
1:C:614:GLY:O	1:C:620:ARG:HA	2.19	0.42
1:C:787:GLY:O	1:C:789:TRP:N	2.52	0.42
1:D:267:LYS:HZ1	1:D:268:ILE:N	2.18	0.42
1:D:396:PHE:HD2	1:D:396:PHE:HA	1.71	0.42
1:D:713:LEU:HD21	1:D:843:LEU:CD1	2.49	0.42
1:D:996:GLY:O	1:D:998:GLY:N	2.53	0.42
1:E:948:PHE:HE2	1:E:971:ARG:HD3	1.85	0.42
1:F:341:VAL:CG2	1:F:395:MET:HE1	2.49	0.42
1:F:564:LEU:HG	1:F:565:PRO:HD2	2.00	0.42
1:F:727:PHE:O	1:F:729:ILE:HD12	2.20	0.42
1:F:771:VAL:HG13	1:F:771:VAL:O	2.20	0.42
1:B:420:MET:SD	1:B:427:PRO:HA	2.60	0.42
1:C:203:VAL:O	1:C:207:ILE:HG13	2.20	0.42
1:C:483:LEU:O	1:C:487:ILE:HB	2.20	0.42
1:C:559:LEU:HD22	1:C:559:LEU:HA	1.51	0.42
1:C:985:GLY:O	1:C:988:PRO:HD2	2.20	0.42
1:D:11:PHE:CE1	1:D:15:ILE:HD11	2.54	0.42
1:D:185:ARG:HD3	1:D:185:ARG:HA	1.75	0.42
1:D:239:ARG:HB2	1:D:763:ILE:HD13	2.02	0.42
1:D:359:LEU:C	1:D:361:ASN:N	2.73	0.42
1:D:514:GLY:CA	1:D:517:ASN:HD22	2.21	0.42
1:D:591:LEU:HD11	1:D:613:ASN:HB2	2.01	0.42
1:E:45:ILE:O	1:E:89:GLN:HA	2.20	0.42
1:E:228:GLN:HE21	1:E:230:LEU:H	1.67	0.42
1:E:324:VAL:C	1:E:326:PRO:HD3	2.39	0.42
1:E:612:VAL:O	1:E:612:VAL:HG12	2.20	0.42
1:F:356:TYR:C	1:F:358:PHE:N	2.73	0.42
1:F:722:GLU:HG3	1:F:723:ASP:H	1.84	0.42
1:A:124:GLN:CD	1:A:758:TYR:HD2	2.23	0.42
1:A:235:ILE:HD11	1:B:726:GLN:CD	2.40	0.42
1:A:256:ASP:OD2	1:A:258:SER:HB2	2.19	0.42
1:A:350:LEU:HD11	1:A:984:LEU:C	2.39	0.42
1:A:361:ASN:O	1:A:364:ALA:N	2.48	0.42
1:A:859:TRP:CE3	1:A:863:SER:HB3	2.54	0.42
1:A:1007:VAL:HG12	1:A:1008:MET:N	2.35	0.42
1:B:733:GLN:HE22	1:B:743:ILE:HG23	1.85	0.42
1:C:100:ALA:O	1:C:103:ALA:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HG22	1:C:290:GLY:HA2	2.01	0.42
1:C:208:LYS:HG3	1:C:759:VAL:HG13	2.02	0.42
1:C:321:LEU:HA	1:C:321:LEU:HD22	1.63	0.42
1:C:400:LEU:HD11	1:C:933:THR:HG23	2.02	0.42
1:C:483:LEU:HD23	1:C:483:LEU:HA	1.80	0.42
1:D:443:VAL:O	1:D:446:ALA:HB3	2.20	0.42
1:D:459:PHE:HZ	1:D:873:ALA:HA	1.85	0.42
1:E:80:SER:HB3	1:E:818:ARG:HB2	2.02	0.42
1:E:344:LEU:CD2	1:E:402:ILE:HD11	2.40	0.42
1:E:712:MET:SD	1:E:835:LYS:HG2	2.60	0.42
1:E:960:LEU:N	1:E:1040:ILE:HD13	2.34	0.42
1:F:198:LEU:HD23	1:F:198:LEU:HA	1.89	0.42
1:F:931:LEU:HD22	1:F:931:LEU:HA	1.54	0.42
1:F:974:PRO:O	1:F:975:ILE:C	2.58	0.42
1:A:104:GLN:HE21	1:A:131:LYS:HG2	1.85	0.42
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.74	0.42
1:A:158:VAL:HG11	1:A:177:LEU:HD21	2.01	0.42
1:A:250:LEU:HD12	1:A:260:VAL:O	2.20	0.42
1:A:857:TYR:CD2	1:A:857:TYR:N	2.88	0.42
1:B:169:THR:HG21	1:B:306:ILE:CG1	2.50	0.42
1:B:364:ALA:HA	1:B:367:ILE:HG22	2.01	0.42
1:C:203:VAL:O	1:C:206:ALA:HB3	2.20	0.42
1:C:427:PRO:O	1:C:431:THR:OG1	2.19	0.42
1:C:527:TYR:CE1	1:C:968:VAL:HG12	2.55	0.42
1:C:882:ILE:O	1:C:885:PHE:HB3	2.19	0.42
1:D:242:SER:OG	1:D:245:GLU:HG3	2.20	0.42
1:D:680:PHE:CZ	1:D:844:MET:HG3	2.55	0.42
1:D:695:LEU:HD23	1:D:695:LEU:HA	1.76	0.42
1:E:23:GLY:HA3	1:E:377:LEU:O	2.19	0.42
1:E:36:PRO:O	1:E:38:ILE:HG13	2.20	0.42
1:E:625:GLY:O	1:E:626:ILE:HG13	2.20	0.42
1:F:682:PHE:HE1	1:F:857:TYR:HB2	1.82	0.42
1:F:897:ILE:N	1:F:897:ILE:HD13	2.35	0.42
1:F:988:PRO:O	1:F:992:SER:OG	2.38	0.42
1:A:130:GLU:HB3	1:A:173:GLY:CA	2.50	0.41
1:A:669:PRO:HB2	1:A:671:ILE:HD13	2.01	0.41
1:B:39:ALA:HB2	1:B:673:GLU:HG3	2.01	0.41
1:B:187:TRP:HB3	1:B:776:GLU:HG3	2.02	0.41
1:B:395:MET:HA	1:B:398:MET:HG3	2.01	0.41
1:B:414:GLU:HG2	1:B:973:ARG:HH11	1.83	0.41
1:B:467:TYR:HA	1:B:470:PHE:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:PRO:HG2	1:C:880:SER:CB	2.50	0.41
1:C:510:LYS:CD	1:C:511:GLY:H	2.31	0.41
1:C:616:GLY:CA	1:C:626:ILE:HB	2.50	0.41
1:C:885:PHE:HE1	1:C:899:PHE:CE1	2.38	0.41
1:D:198:LEU:HD22	1:D:202:ASP:HB2	2.02	0.41
1:E:164:ASP:O	1:E:168:ARG:HG3	2.19	0.41
1:E:459:PHE:CB	1:E:464:GLY:HA2	2.50	0.41
1:F:151:GLN:HE22	1:F:285:PRO:HB3	1.85	0.41
1:F:548:ILE:CG2	1:F:910:ILE:HG21	2.50	0.41
1:A:159:ALA:HB3	1:A:181:GLN:HG3	2.02	0.41
1:A:470:PHE:O	1:A:471:SER:C	2.57	0.41
1:B:9:PRO:O	1:B:12:ALA:HB3	2.20	0.41
1:B:78:MET:HE3	1:B:821:GLY:N	2.35	0.41
1:B:459:PHE:HD2	1:B:460:GLY:N	2.17	0.41
1:B:519:MET:O	1:B:523:SER:OG	2.38	0.41
1:B:678:THR:OG1	1:B:831:ALA:HB3	2.20	0.41
1:B:892:TYR:HB3	1:B:893:GLU:H	1.50	0.41
1:C:143:ILE:O	1:C:321:LEU:HA	2.20	0.41
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.56	0.41
1:C:497:LEU:HD12	1:C:498:LYS:H	1.84	0.41
1:C:536:ARG:CD	2:C:2000:LMT:O4'	2.66	0.41
1:C:568:ASP:O	1:C:634:TRP:HH2	2.03	0.41
1:C:703:LEU:HD21	1:C:827:ILE:HG23	2.00	0.41
1:C:741:VAL:HA	1:C:793:ALA:HA	2.02	0.41
1:C:1011:MET:O	1:C:1015:THR:HG23	2.20	0.41
1:D:355:MET:HE1	1:D:410:ILE:HG12	2.00	0.41
1:D:557:VAL:C	1:D:559:LEU:H	2.24	0.41
1:D:684:LEU:HD11	1:D:855:VAL:CG1	2.50	0.41
1:E:47:ALA:O	1:E:87:THR:HA	2.20	0.41
1:E:277:ILE:H	1:E:277:ILE:HG13	1.58	0.41
1:E:486:LEU:HD23	1:E:486:LEU:HA	1.58	0.41
1:E:727:PHE:O	1:E:729:ILE:HD12	2.21	0.41
1:E:903:LEU:HA	1:E:903:LEU:HD23	1.55	0.41
1:E:946:VAL:HG13	1:E:1026:PHE:CD1	2.55	0.41
1:E:982:PHE:CE2	1:E:1011:MET:HG3	2.55	0.41
1:E:1016:VAL:O	1:E:1016:VAL:HG13	2.19	0.41
1:F:186:ILE:CG2	1:F:773:VAL:HG12	2.49	0.41
1:F:597:TYR:HD1	1:F:601:LYS:HD2	1.86	0.41
1:F:664:PHE:HE2	1:F:717:ARG:HB3	1.85	0.41
1:A:213:GLN:OE1	1:B:56:THR:OG1	2.29	0.41
1:A:359:LEU:C	1:A:361:ASN:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:SER:OG	1:A:435:MET:N	2.53	0.41
1:A:453:PHE:HB3	1:A:475:VAL:CG2	2.50	0.41
1:A:547:ILE:HG22	1:A:548:ILE:HD13	2.01	0.41
1:A:781:MET:SD	1:C:225:VAL:HG12	2.61	0.41
1:A:954:ASP:CB	1:A:955:LYS:HD3	2.49	0.41
1:A:1038:GLU:HA	1:A:1039:ASP:CB	2.46	0.41
1:B:26:ALA:HB1	1:B:384:ALA:HB2	2.01	0.41
1:B:94:PHE:HE2	1:B:103:ALA:HB1	1.85	0.41
1:B:521:GLU:HA	1:B:524:THR:HG22	2.01	0.41
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.54	0.41
1:B:864:TYR:CD2	1:B:865:GLN:HG3	2.55	0.41
1:B:892:TYR:CD2	1:B:897:ILE:HD12	2.55	0.41
1:B:924:ASP:OD1	1:B:926:TYR:N	2.53	0.41
1:B:984:LEU:HA	1:B:984:LEU:HD22	1.78	0.41
1:C:150:THR:O	1:C:151:GLN:C	2.59	0.41
1:C:356:TYR:C	1:C:358:PHE:N	2.74	0.41
1:C:528:THR:O	1:C:531:VAL:HB	2.20	0.41
1:C:613:ASN:HD22	1:C:614:GLY:N	2.18	0.41
1:C:719:ASN:ND2	1:C:817:GLU:CD	2.73	0.41
1:C:730:ASP:OD1	1:C:808:ARG:NH2	2.37	0.41
1:D:891:LEU:HD12	1:D:891:LEU:HA	1.85	0.41
1:D:926:TYR:HB3	1:D:1003:VAL:CG2	2.51	0.41
1:E:72:ILE:HG21	1:E:94:PHE:HZ	1.83	0.41
1:E:582:ALA:HA	1:E:586:ARG:NH2	2.35	0.41
1:E:751:GLY:O	1:E:753:ALA:N	2.53	0.41
1:E:841:MET:HG2	1:E:859:TRP:CH2	2.55	0.41
1:F:49:TYR:CE1	1:F:60:THR:HG21	2.56	0.41
1:F:158:VAL:HG11	1:F:177:LEU:HD23	2.02	0.41
1:F:634:TRP:H	1:F:634:TRP:HD1	1.63	0.41
1:A:412:VAL:HG11	1:A:489:THR:HG22	2.02	0.41
1:A:533:GLY:CA	2:A:2000:LMT:H3B	2.50	0.41
1:B:420:MET:O	1:B:500:ILE:HG22	2.19	0.41
1:B:790:TYR:HA	1:B:799:VAL:O	2.21	0.41
1:B:858:ASP:OD1	1:B:859:TRP:N	2.54	0.41
1:C:174:ASP:OD2	1:C:175:VAL:N	2.53	0.41
1:C:193:LEU:HA	1:C:193:LEU:HD23	1.66	0.41
1:C:540:ARG:HD3	1:C:541:TYR:CE1	2.54	0.41
1:C:599:LEU:O	1:C:603:LYS:HG2	2.21	0.41
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.01	0.41
1:C:728:LYS:HE3	1:C:808:ARG:HH22	1.85	0.41
1:D:34:GLN:HB2	1:D:333:VAL:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.55	0.41
1:D:835:LYS:HA	1:D:835:LYS:HD3	1.37	0.41
1:D:889:ALA:HA	1:D:894:SER:O	2.20	0.41
1:D:996:GLY:C	1:D:998:GLY:N	2.73	0.41
1:E:246:PHE:O	1:E:249:ILE:HG12	2.20	0.41
1:E:379:THR:HA	1:E:480:LEU:CD1	2.50	0.41
1:E:448:VAL:O	1:E:452:VAL:HG13	2.21	0.41
1:E:555:LEU:CD1	1:E:914:LEU:HD12	2.50	0.41
1:F:110:LYS:HD3	1:F:110:LYS:HA	1.80	0.41
1:F:597:TYR:CE1	1:F:601:LYS:HD2	2.56	0.41
1:F:991:ILE:O	1:F:991:ILE:HD13	2.20	0.41
1:A:137:LEU:N	1:A:291:ILE:O	2.54	0.41
1:A:162:MET:HG3	1:A:313:MET:SD	2.60	0.41
1:A:177:LEU:HD22	1:A:178:PHE:N	2.36	0.41
1:A:177:LEU:HD23	1:A:289:LEU:CD1	2.49	0.41
1:A:416:VAL:HG11	1:A:497:LEU:HD23	2.01	0.41
1:A:426:PRO:HD2	1:A:429:GLU:HG3	2.01	0.41
1:A:821:GLY:O	1:A:822:LEU:HD23	2.20	0.41
1:A:886:LEU:HD23	1:C:14:VAL:CG1	2.46	0.41
1:A:907:LEU:HD12	1:A:1017:LEU:HB3	2.02	0.41
1:A:982:PHE:O	1:A:983:ILE:C	2.58	0.41
1:B:187:TRP:HA	1:B:774:MET:O	2.21	0.41
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.88	0.41
1:B:671:ILE:HG22	1:B:673:GLU:H	1.85	0.41
1:C:32:VAL:HG22	1:C:390:ILE:HD11	2.01	0.41
1:C:211:ASN:ND2	1:C:240:LEU:HD22	2.36	0.41
1:C:455:PRO:HB2	1:C:876:LEU:CD1	2.50	0.41
1:C:733:GLN:O	1:C:737:GLN:HB2	2.20	0.41
1:D:214:VAL:HG23	1:D:237:GLN:HB3	2.02	0.41
1:D:342:LYS:O	1:D:346:GLU:HG3	2.20	0.41
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.80	0.41
1:D:468:ARG:HB2	1:D:468:ARG:CZ	2.50	0.41
1:D:976:LEU:O	1:D:980:LEU:HG	2.20	0.41
1:E:172:VAL:HG13	1:E:291:ILE:HG23	2.03	0.41
1:E:726:GLN:HG3	1:E:810:GLU:HG3	2.02	0.41
1:E:727:PHE:HA	1:E:808:ARG:O	2.20	0.41
1:E:880:SER:O	1:E:884:VAL:HG23	2.20	0.41
1:F:753:ALA:HB3	1:F:754:TRP:HD1	1.85	0.41
1:A:182:TYR:HD1	1:A:182:TYR:HA	1.71	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CZ2	2.55	0.41
1:A:288:GLY:C	1:A:289:LEU:HD22	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ALA:HA	1:A:478:MET:SD	2.60	0.41
1:B:110:LYS:HA	1:B:113:LEU:HG	2.02	0.41
1:B:138:MET:HE3	1:B:291:ILE:HD12	2.02	0.41
1:B:186:ILE:HG22	1:B:773:VAL:HG23	2.02	0.41
1:B:191:ASN:HB2	1:B:192:GLU:OE1	2.21	0.41
1:B:456:MET:HE3	1:B:467:TYR:O	2.20	0.41
1:B:520:PHE:C	1:B:520:PHE:CD2	2.94	0.41
1:B:713:LEU:HD11	1:B:843:LEU:HD12	2.02	0.41
1:B:754:TRP:HA	1:B:780:ARG:HD3	2.03	0.41
1:C:34:GLN:CG	1:C:333:VAL:HG22	2.51	0.41
1:C:38:ILE:HG23	1:C:462:SER:CB	2.51	0.41
1:C:57:VAL:HA	1:C:61:VAL:CG2	2.51	0.41
1:C:62:THR:HA	1:C:90:ILE:CG1	2.50	0.41
1:C:163:LYS:HD2	1:C:289:LEU:HD21	2.02	0.41
1:C:421:ALA:O	1:C:505:HIS:HE1	2.03	0.41
1:C:560:PRO:HB3	1:C:839:GLU:HG3	2.02	0.41
1:C:566:ASP:OD1	1:C:678:THR:HG23	2.19	0.41
1:C:971:ARG:C	1:C:974:PRO:HD2	2.41	0.41
1:D:219:LEU:HD23	1:D:234:ILE:HD11	2.01	0.41
1:D:470:PHE:O	1:D:471:SER:C	2.59	0.41
1:D:573:MET:O	1:D:666:PHE:HD1	2.03	0.41
1:E:185:ARG:NH2	1:E:772:TYR:CD1	2.89	0.41
1:E:192:GLU:H	1:E:192:GLU:HG2	1.34	0.41
1:E:684:LEU:HD12	1:E:684:LEU:HA	1.91	0.41
1:E:867:ARG:O	1:E:867:ARG:NE	2.53	0.41
1:F:45:ILE:O	1:F:89:GLN:HA	2.21	0.41
1:F:363:ARG:HB3	1:F:363:ARG:HH11	1.85	0.41
1:F:897:ILE:HB	1:F:898:PRO:HD3	2.03	0.41
1:A:17:ILE:HG21	1:B:886:LEU:HG	2.02	0.41
1:A:131:LYS:HE2	1:B:73:ASP:OD2	2.21	0.41
1:A:149:MET:HG2	1:A:153:ASP:HB3	2.03	0.41
1:A:792:ARG:HB2	1:A:798:MET:SD	2.61	0.41
1:A:835:LYS:HD2	1:A:835:LYS:N	2.35	0.41
1:A:964:THR:O	1:A:968:VAL:HB	2.21	0.41
1:B:83:ASP:HB2	1:B:87:THR:O	2.21	0.41
1:B:578:LEU:HB2	1:B:623:ASN:O	2.20	0.41
1:B:905:VAL:HG13	1:B:935:ILE:CD1	2.51	0.41
1:C:166:ILE:HG13	1:C:306:ILE:HG13	2.03	0.41
1:C:222:THR:HA	1:C:223:PRO:HA	1.75	0.41
1:C:293:LEU:HD13	1:C:294:ALA:H	1.85	0.41
1:C:400:LEU:HD11	1:C:933:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:OD1	1:C:438:ILE:HG21	2.21	0.41
1:C:420:MET:HE1	1:C:427:PRO:HA	2.02	0.41
1:C:457:ALA:HB2	1:C:471:SER:CB	2.50	0.41
1:D:159:ALA:HB2	1:D:177:LEU:HG	2.02	0.41
1:D:195:LYS:HZ1	1:D:196:PHE:HE2	1.67	0.41
1:E:470:PHE:CG	1:E:929:VAL:HG21	2.55	0.41
1:E:535:LEU:HG	1:E:1027:VAL:HG21	2.02	0.41
1:F:339:GLU:HB3	1:F:1000:GLN:HE22	1.86	0.41
1:F:633:ASP:N	1:F:633:ASP:OD1	2.54	0.41
1:F:926:TYR:HE1	1:F:999:ALA:CB	2.34	0.41
1:A:907:LEU:HD11	1:A:1021:PHE:CE1	2.56	0.41
1:A:925:VAL:O	1:A:928:GLN:N	2.54	0.41
1:A:971:ARG:O	1:A:974:PRO:HD2	2.21	0.41
1:B:967:ALA:HA	1:B:970:MET:CE	2.51	0.41
1:B:1020:PHE:CD2	2:B:2000:LMT:H52	2.56	0.41
1:C:391:ASN:HD21	1:C:469:GLN:CD	2.17	0.41
1:C:510:LYS:HG2	1:C:518:ARG:NH1	2.36	0.41
1:C:971:ARG:HE	1:C:975:ILE:HG13	1.85	0.41
1:D:492:LEU:HD23	1:D:492:LEU:HA	1.81	0.41
1:E:785:ASP:N	1:E:785:ASP:OD1	2.54	0.41
1:E:1037:ASN:HA	1:E:1038:GLU:HG2	2.02	0.41
1:F:62:THR:HG22	1:F:88:VAL:CG2	2.50	0.41
1:F:897:ILE:O	1:F:901:VAL:HG12	2.20	0.41
1:F:944:LEU:HB3	1:F:971:ARG:CD	2.51	0.41
1:A:162:MET:SD	1:A:317:PHE:CZ	3.13	0.41
1:A:736:ALA:HB2	1:A:804:PHE:CD1	2.56	0.41
1:A:892:TYR:CD2	1:A:897:ILE:HG22	2.56	0.41
1:B:344:LEU:HD23	1:B:348:ILE:HG12	2.02	0.41
1:B:370:ILE:HD12	1:B:370:ILE:HG23	1.75	0.41
1:B:370:ILE:HD13	1:B:370:ILE:HA	1.76	0.41
1:B:531:VAL:HA	1:B:534:ILE:HD13	2.02	0.41
1:B:557:VAL:C	1:B:559:LEU:H	2.24	0.41
1:B:659:LYS:HD2	1:B:659:LYS:HA	1.90	0.41
1:B:787:GLY:C	1:B:789:TRP:H	2.24	0.41
1:B:881:LEU:HD12	1:B:881:LEU:HA	1.72	0.41
1:B:961:ILE:H	1:B:961:ILE:HG13	1.58	0.41
2:B:2000:LMT:H121	2:B:2000:LMT:H91	1.90	0.41
1:C:68:ASN:CB	1:C:114:ALA:HB2	2.50	0.41
1:C:344:LEU:HD22	1:C:344:LEU:HA	1.66	0.41
1:C:352:PHE:CD2	1:C:352:PHE:C	2.94	0.41
1:C:400:LEU:HD12	1:C:474:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:606:VAL:HG13	1:C:629:VAL:CG1	2.51	0.41
1:C:708:LYS:HB3	1:C:708:LYS:HE2	1.91	0.41
1:C:781:MET:O	1:C:782:LEU:HD13	2.21	0.41
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.49	0.41
1:D:19:ILE:HD13	1:D:19:ILE:HG21	1.84	0.41
1:D:250:LEU:CD1	1:D:259:ARG:HB3	2.50	0.41
1:D:352:PHE:CD2	1:D:352:PHE:C	2.95	0.41
1:D:405:LEU:CD2	1:D:481:SER:HB3	2.51	0.41
1:D:505:HIS:O	1:D:507:GLU:N	2.44	0.41
1:D:572:PHE:O	1:D:629:VAL:HG13	2.21	0.41
1:D:597:TYR:CD2	1:D:655:PHE:CZ	3.08	0.41
1:D:640:GLU:O	1:D:643:LYS:HB2	2.21	0.41
1:D:727:PHE:O	1:D:729:ILE:HD12	2.21	0.41
1:D:906:PRO:O	1:D:910:ILE:HG22	2.21	0.41
1:D:1022:VAL:HA	1:D:1025:PHE:HD1	1.85	0.41
1:D:1041:GLU:HB2	1:D:1042:HIS:HA	2.02	0.41
1:E:162:MET:C	1:E:164:ASP:H	2.24	0.41
1:E:186:ILE:CD1	1:E:262:LEU:HD21	2.50	0.41
1:E:417:GLU:CG	1:E:497:LEU:HD21	2.51	0.41
1:E:545:TYR:O	1:E:548:ILE:N	2.54	0.41
1:E:555:LEU:HA	1:E:555:LEU:HD23	1.71	0.41
1:E:596:HIS:O	1:E:600:THR:OG1	2.18	0.41
1:E:736:ALA:HB2	1:E:804:PHE:HD1	1.86	0.41
1:E:877:TYR:HD2	1:E:877:TYR:HA	1.53	0.41
1:F:58:GLN:O	1:F:63:GLN:HB2	2.20	0.41
1:F:148:THR:HG22	1:F:149:MET:O	2.21	0.41
1:F:166:ILE:HD13	1:F:166:ILE:HA	1.79	0.41
1:F:251:LEU:HG	1:F:260:VAL:O	2.21	0.41
1:F:380:PHE:CZ	1:F:398:MET:HE1	2.56	0.41
1:F:682:PHE:O	1:F:826:GLU:HA	2.20	0.41
1:F:859:TRP:CE3	1:F:863:SER:HB2	2.55	0.41
1:F:986:VAL:O	1:F:987:MET:C	2.59	0.41
1:F:1019:ILE:HG13	1:F:1020:PHE:CD1	2.56	0.41
1:A:275:TYR:CG	1:C:223:PRO:HG3	2.56	0.41
1:A:418:ARG:NH1	1:A:422:GLU:OE1	2.43	0.41
1:A:545:TYR:HE1	1:A:903:LEU:HD13	1.84	0.41
1:A:801:PHE:HA	1:A:804:PHE:HE2	1.85	0.41
1:B:154:ILE:CG2	1:B:287:SER:HB3	2.47	0.41
1:B:527:TYR:CZ	1:B:968:VAL:HG13	2.55	0.41
1:C:444:GLY:CA	1:C:892:TYR:HE1	2.34	0.41
1:C:545:TYR:CD1	1:C:546:LEU:HD12	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:C	1:D:49:TYR:CD2	2.94	0.41
1:D:575:MET:O	1:D:663:VAL:HA	2.21	0.41
1:D:696:THR:HG21	1:D:722:GLU:OE1	2.21	0.41
1:E:527:TYR:CE1	1:E:972:LEU:HD23	2.56	0.41
1:E:605:ASN:OD1	1:E:642:ASN:ND2	2.54	0.41
1:E:868:LEU:HD23	1:E:868:LEU:HA	1.68	0.41
1:F:100:ALA:O	1:F:103:ALA:HB3	2.21	0.41
1:F:112:GLN:HG2	1:F:115:MET:SD	2.61	0.41
1:F:186:ILE:O	1:F:773:VAL:HA	2.21	0.41
1:F:216:ALA:HB1	1:F:234:ILE:HG22	2.03	0.41
1:F:442:LEU:HD13	1:F:485:ALA:HB1	2.02	0.41
1:F:669:PRO:HG3	1:F:675:GLY:HA3	2.03	0.41
1:F:985:GLY:O	1:F:988:PRO:HD2	2.21	0.41
1:A:240:LEU:HB2	1:A:246:PHE:CZ	2.56	0.40
1:A:542:LEU:O	1:A:546:LEU:HD13	2.21	0.40
1:A:597:TYR:CD2	1:A:655:PHE:CZ	3.09	0.40
1:A:602:GLU:OE1	1:A:650:ARG:HD2	2.21	0.40
1:A:996:GLY:O	1:A:999:ALA:N	2.54	0.40
1:B:144:ASN:HA	1:B:320:GLY:O	2.21	0.40
1:B:485:ALA:C	1:B:490:PRO:HD3	2.42	0.40
1:B:559:LEU:HD23	1:B:917:THR:OG1	2.21	0.40
1:B:692:HIS:CE1	1:B:813:SER:HB2	2.56	0.40
1:B:926:TYR:HE1	1:B:999:ALA:CB	2.34	0.40
1:C:322:LYS:HB2	1:C:322:LYS:HE2	1.77	0.40
1:C:378:GLY:O	1:C:381:ALA:HB3	2.22	0.40
1:C:751:GLY:C	1:C:753:ALA:N	2.75	0.40
1:C:893:GLU:CG	1:C:894:SER:N	2.84	0.40
1:C:908:GLY:HA2	1:C:1014:ALA:CB	2.47	0.40
1:D:353:LEU:HD22	1:D:353:LEU:HA	1.74	0.40
1:E:108:GLN:HG2	1:F:112:GLN:OE1	2.21	0.40
1:E:235:ILE:HD11	1:F:726:GLN:HB3	2.02	0.40
1:E:528:THR:O	1:E:529:ASP:C	2.59	0.40
1:E:541:TYR:CD1	1:E:541:TYR:N	2.89	0.40
1:E:1030:ARG:HD2	1:E:1030:ARG:HA	1.93	0.40
1:F:190:PRO:HA	1:F:193:LEU:HB2	2.03	0.40
1:F:213:GLN:NE2	1:F:238:THR:HG23	2.36	0.40
1:F:582:ALA:HB1	1:F:586:ARG:HE	1.86	0.40
1:A:103:ALA:HA	1:A:106:GLN:OE1	2.21	0.40
1:A:262:LEU:O	1:A:265:VAL:HG22	2.22	0.40
1:B:108:GLN:NE2	1:C:112:GLN:CD	2.75	0.40
1:C:182:TYR:HD1	1:C:182:TYR:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:785:ASP:N	1:C:785:ASP:OD2	2.52	0.40
1:C:801:PHE:HD1	1:C:804:PHE:HE2	1.68	0.40
1:D:3:ASN:HA	1:D:6:ILE:HG23	2.01	0.40
1:D:66:GLU:OE1	1:D:821:GLY:HA2	2.22	0.40
1:D:190:PRO:HG3	1:D:779:TYR:HB3	2.03	0.40
1:D:249:ILE:HD13	1:D:249:ILE:HA	1.95	0.40
1:D:393:LEU:HD11	1:D:466:ILE:HG12	2.03	0.40
1:D:811:TYR:HD2	1:D:811:TYR:HA	1.77	0.40
1:E:4:PHE:HZ	1:E:8:ARG:NH1	2.20	0.40
1:E:200:PRO:HB2	1:E:749:THR:HA	2.03	0.40
1:E:459:PHE:HD2	1:E:459:PHE:HA	1.75	0.40
1:E:510:LYS:HD2	1:E:510:LYS:HA	1.92	0.40
1:E:531:VAL:HA	1:E:534:ILE:HG13	2.03	0.40
1:E:618:ALA:HB1	1:E:720:GLY:HA2	2.04	0.40
1:E:746:ILE:HG22	1:E:791:VAL:HG21	2.03	0.40
1:E:974:PRO:O	1:E:977:MET:HB2	2.21	0.40
1:F:160:ALA:HA	1:F:767:ARG:HH12	1.87	0.40
1:F:163:LYS:HB2	1:F:289:LEU:HD21	2.03	0.40
1:F:300:LEU:HD12	1:F:300:LEU:N	2.36	0.40
1:F:348:ILE:CD1	1:F:372:VAL:HG11	2.50	0.40
1:F:597:TYR:CE1	1:F:601:LYS:HB2	2.56	0.40
1:F:603:LYS:HE2	1:F:603:LYS:HB3	1.86	0.40
1:A:281:PHE:HD1	1:A:610:PHE:CD1	2.32	0.40
1:A:451:ALA:CB	1:A:883:VAL:HG13	2.45	0.40
1:A:634:TRP:CD1	1:A:634:TRP:N	2.83	0.40
1:A:754:TRP:HZ3	1:C:219:LEU:HA	1.87	0.40
1:A:909:VAL:HG13	1:A:931:LEU:HD21	2.03	0.40
1:B:368:PRO:HB3	1:B:410:ILE:HD12	2.02	0.40
1:B:792:ARG:HG2	1:B:792:ARG:NH1	2.36	0.40
1:B:885:PHE:CE1	1:B:899:PHE:HE1	2.39	0.40
1:C:446:ALA:O	1:C:450:SER:OG	2.40	0.40
1:C:545:TYR:HB2	1:C:1021:PHE:CE2	2.45	0.40
1:C:982:PHE:O	1:C:983:ILE:C	2.60	0.40
1:D:177:LEU:CD1	1:D:180:SER:HA	2.51	0.40
1:D:431:THR:HG21	1:D:490:PRO:O	2.21	0.40
1:D:616:GLY:HA2	1:D:626:ILE:HB	2.02	0.40
1:D:669:PRO:HB2	1:D:671:ILE:HD12	2.02	0.40
1:D:751:GLY:O	1:D:753:ALA:N	2.54	0.40
1:D:864:TYR:HD1	1:D:864:TYR:HA	1.67	0.40
1:E:644:VAL:O	1:E:648:THR:HG23	2.20	0.40
1:E:790:TYR:HB3	1:E:798:MET:HG2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:540:ARG:O	1:F:543:VAL:HB	2.22	0.40
1:F:572:PHE:HD2	1:F:631:LEU:HD11	1.86	0.40
1:F:960:LEU:HD23	1:F:1031:ARG:HH21	1.87	0.40
1:F:1016:VAL:O	1:F:1016:VAL:HG12	2.20	0.40
1:A:122:VAL:O	1:A:123:GLN:C	2.60	0.40
1:A:382:VAL:O	1:A:386:PHE:HB2	2.22	0.40
1:A:504:ASP:C	1:A:506:GLY:H	2.25	0.40
1:A:792:ARG:HH11	1:A:792:ARG:HG2	1.86	0.40
1:A:848:ALA:HA	1:A:851:LEU:CD1	2.51	0.40
1:A:1017:LEU:HA	1:A:1017:LEU:HD13	1.80	0.40
1:B:78:MET:HG3	1:B:90:ILE:CG2	2.50	0.40
1:B:214:VAL:HG22	1:B:237:GLN:HB3	2.03	0.40
1:B:376:LEU:O	1:B:377:LEU:C	2.59	0.40
1:C:41:PRO:HG2	1:C:94:PHE:HB2	2.03	0.40
1:C:62:THR:C	1:C:64:VAL:H	2.25	0.40
1:C:62:THR:CG2	1:C:80:SER:HB2	2.50	0.40
1:C:185:ARG:HD3	1:C:772:TYR:HB3	2.04	0.40
1:C:401:ALA:O	1:C:405:LEU:HB3	2.20	0.40
1:C:986:VAL:O	1:C:987:MET:C	2.59	0.40
1:D:32:VAL:O	1:D:300:LEU:HD13	2.21	0.40
1:D:137:LEU:HB2	1:D:293:LEU:HB2	2.03	0.40
1:D:583:THR:H	1:D:586:ARG:HG3	1.87	0.40
1:E:199:THR:HG21	1:E:791:VAL:HA	2.04	0.40
1:E:350:LEU:HD23	1:E:350:LEU:HA	1.86	0.40
1:E:751:GLY:C	1:E:753:ALA:N	2.75	0.40
1:F:307:ARG:HA	1:F:307:ARG:HD2	1.81	0.40
1:F:382:VAL:HG11	1:F:476:SER:HB2	2.03	0.40
1:F:483:LEU:O	1:F:487:ILE:HB	2.21	0.40
1:F:574:THR:HG23	1:F:627:ALA:HB3	2.03	0.40
1:F:885:PHE:CE1	1:F:898:PRO:HB2	2.57	0.40
1:F:1034:SER:HG	1:F:1037:ASN:HB2	1.86	0.40
1:A:47:ALA:HB3	1:A:88:VAL:HG13	2.03	0.40
1:A:102:ILE:CD1	1:C:101:ASP:HB3	2.51	0.40
1:A:117:LEU:HD11	1:C:125:GLN:NE2	2.36	0.40
1:A:372:VAL:HA	1:A:375:VAL:CG1	2.52	0.40
1:A:448:VAL:HB	1:A:884:VAL:HG23	2.03	0.40
1:A:637:ARG:HA	1:A:642:ASN:HD22	1.86	0.40
1:A:732:ASP:OD2	1:A:735:LYS:HE2	2.22	0.40
1:A:866:GLU:H	1:A:866:GLU:HG2	1.61	0.40
1:A:888:LEU:HD11	1:A:943:ILE:HD11	2.03	0.40
1:B:30:LEU:HD12	1:B:31:PRO:CD	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:MET:HA	1:B:118:LEU:CD1	2.42	0.40
1:B:184:MET:HB2	1:B:762:PHE:CD2	2.57	0.40
1:B:277:ILE:H	1:B:277:ILE:HG13	1.72	0.40
1:B:314:GLU:HA	1:B:317:PHE:CD2	2.56	0.40
1:B:356:TYR:O	1:B:360:GLN:N	2.49	0.40
1:B:578:LEU:HD23	1:B:578:LEU:HA	1.84	0.40
1:B:837:THR:O	1:B:840:ALA:HB3	2.22	0.40
1:B:957:GLY:O	1:B:1040:ILE:HG22	2.22	0.40
1:C:2:PRO:HB2	1:C:3:ASN:H	1.76	0.40
1:C:411:VAL:HG22	1:C:944:LEU:HD11	2.04	0.40
1:C:444:GLY:O	1:C:448:VAL:HG22	2.22	0.40
1:D:63:GLN:NE2	1:F:767:ARG:HA	2.31	0.40
1:D:186:ILE:CB	1:D:773:VAL:HG12	2.50	0.40
1:D:199:THR:HB	1:D:749:THR:CG2	2.52	0.40
1:D:281:PHE:CE1	1:D:608:SER:HB2	2.57	0.40
1:D:525:HIS:O	1:D:526:HIS:C	2.59	0.40
1:D:895:TRP:CE2	1:F:10:ILE:HD12	2.57	0.40
1:D:1037:ASN:HA	1:D:1038:GLU:O	2.21	0.40
1:E:778:LYS:HA	1:E:781:MET:CE	2.52	0.40
1:E:1020:PHE:HZ	2:E:2000:LMT:H52	1.86	0.40
1:F:172:VAL:HG21	1:F:306:ILE:HD11	2.03	0.40
1:F:405:LEU:HD21	1:F:477:ALA:HB1	2.04	0.40
1:F:578:LEU:HD21	1:F:586:ARG:HB2	2.04	0.40
1:F:833:PRO:O	1:F:835:LYS:N	2.50	0.40
1:F:835:LYS:NZ	1:F:836:SER:H	2.18	0.40
1:F:870:GLY:C	1:F:872:GLN:N	2.73	0.40
1:F:952:LEU:HD22	1:F:956:GLU:HG3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:ASP:OD2	1:B:525:HIS:NE2[2_555]	1.98	0.22

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%)	891 (86%)	117 (11%)	34 (3%)	4	30
1	B	1040/1069 (97%)	893 (86%)	126 (12%)	21 (2%)	7	41
1	C	1040/1069 (97%)	874 (84%)	132 (13%)	34 (3%)	4	30
1	D	1042/1069 (98%)	904 (87%)	113 (11%)	25 (2%)	6	36
1	E	1040/1069 (97%)	899 (86%)	124 (12%)	17 (2%)	9	45
1	F	1040/1069 (97%)	898 (86%)	110 (11%)	32 (3%)	4	32
All	All	6244/6414 (97%)	5359 (86%)	722 (12%)	163 (3%)	5	34

All (163) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	SER
1	A	507	GLU
1	A	512	PHE
1	A	992	SER
1	A	995	ALA
1	A	1035	ARG
1	B	147	GLY
1	B	516	PHE
1	B	622	GLN
1	B	638	PRO
1	B	892	TYR
1	B	1040	ILE
1	C	99	ASP
1	C	638	PRO
1	C	893	GLU
1	C	996	GLY
1	C	1037	ASN
1	C	1042	HIS
1	D	147	GLY
1	D	509	LYS
1	D	638	PRO
1	D	991	ILE
1	D	992	SER
1	E	147	GLY
1	E	377	LEU
1	E	638	PRO

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Mol	Chain	Res	Type
1	E	896	SER
1	E	1034	SER
1	E	1038	GLU
1	E	1042	HIS
1	F	507	GLU
1	F	509	LYS
1	F	510	LYS
1	F	672	VAL
1	F	673	GLU
1	F	995	ALA
1	F	996	GLY
1	F	1034	SER
1	F	1035	ARG
1	F	1039	ASP
1	F	1041	GLU
1	A	509	LYS
1	A	511	GLY
1	A	638	PRO
1	A	672	VAL
1	A	673	GLU
1	A	674	LEU
1	A	991	ILE
1	A	1036	LYS
1	A	1038	GLU
1	A	1043	SER
1	B	505	HIS
1	B	508	GLY
1	B	617	ALA
1	B	672	VAL
1	B	673	GLU
1	B	689	GLY
1	B	893	GLU
1	B	1038	GLU
1	B	1042	HIS
1	C	6	ILE
1	C	66	GLU
1	C	98	THR
1	C	105	VAL
1	C	126	GLY
1	C	894	SER
1	D	507	GLU
1	D	617	ALA

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Mol	Chain	Res	Type
1	D	673	GLU
1	D	765	ARG
1	D	919	ARG
1	E	515	TRP
1	E	1040	ILE
1	F	3	ASN
1	F	6	ILE
1	F	134	SER
1	F	505	HIS
1	F	618	ALA
1	F	638	PRO
1	F	834	GLY
1	A	326	PRO
1	A	1031	ARG
1	B	514	GLY
1	B	788	ASP
1	C	507	GLU
1	C	722	GLU
1	C	814	PRO
1	C	890	ALA
1	D	123	GLN
1	D	920	GLY
1	D	1035	ARG
1	D	1037	ASN
1	D	1038	GLU
1	E	511	GLY
1	E	617	ALA
1	E	677	ALA
1	F	215	ALA
1	F	788	ASP
1	F	814	PRO
1	F	1042	HIS
1	A	66	GLU
1	A	148	THR
1	A	360	GLN
1	A	691	GLY
1	A	1037	ASN
1	B	295	THR
1	B	923	ASN
1	C	37	THR
1	C	63	GLN
1	C	123	GLN

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Mol	Chain	Res	Type
1	C	299	ALA
1	C	919	ARG
1	C	920	GLY
1	D	691	GLY
1	D	1040	ILE
1	E	123	GLN
1	E	788	ASP
1	F	147	GLY
1	F	357	LEU
1	F	688	ALA
1	F	835	LYS
1	A	4	PHE
1	A	215	ALA
1	A	920	GLY
1	B	995	ALA
1	C	62	THR
1	C	295	THR
1	C	357	LEU
1	C	377	LEU
1	C	558	ARG
1	C	848	ALA
1	C	1033	PHE
1	C	1038	GLU
1	D	215	ALA
1	D	505	HIS
1	D	558	ARG
1	D	766	GLY
1	D	923	ASN
1	E	357	LEU
1	F	126	GLY
1	F	360	GLN
1	A	204	ILE
1	A	960	LEU
1	B	621	GLY
1	C	83	ASP
1	C	1041	GLU
1	D	871	ASN
1	E	378	GLY
1	F	833	PRO
1	A	126	GLY
1	C	834	GLY
1	A	296	GLY

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Mol	Chain	Res	Type
1	A	330	THR
1	D	910	ILE
1	F	204	ILE
1	A	171	GLY
1	A	508	GLY
1	A	616	GLY
1	E	870	GLY
1	F	330	THR
1	C	330	THR
1	D	639	GLY
1	F	751	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	848/870 (98%)	725 (86%)	123 (14%)	3	19
1	B	846/870 (97%)	721 (85%)	125 (15%)	3	18
1	C	846/870 (97%)	723 (86%)	123 (14%)	3	19
1	D	848/870 (98%)	753 (89%)	95 (11%)	6	29
1	E	846/870 (97%)	748 (88%)	98 (12%)	5	27
1	F	846/870 (97%)	741 (88%)	105 (12%)	4	24
All	All	5080/5220 (97%)	4411 (87%)	669 (13%)	4	22

All (669) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	27	ILE
1	A	34	GLN
1	A	45	ILE
1	A	49	TYR
1	A	53	ASP
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	88	VAL
1	A	91	THR
1	A	102	ILE
1	A	104	GLN
1	A	115	MET
1	A	127	VAL
1	A	131	LYS
1	A	138	MET
1	A	146	ASP
1	A	149	MET
1	A	152	GLU
1	A	157	TYR
1	A	161	ASN
1	A	164	ASP
1	A	169	THR
1	A	185	ARG
1	A	195	LYS
1	A	196	PHE
1	A	201	VAL
1	A	205	THR
1	A	214	VAL
1	A	222	THR
1	A	231	ASN
1	A	243	THR
1	A	253	VAL
1	A	263	ARG
1	A	287	SER
1	A	293	LEU
1	A	324	VAL
1	A	327	TYR
1	A	337	ILE
1	A	348	ILE
1	A	353	LEU
1	A	355	MET
1	A	360	GLN
1	A	362	PHE
1	A	365	THR
1	A	366	LEU
1	A	372	VAL
1	A	386	PHE
1	A	393	LEU
1	A	394	THR

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Mol	Chain	Res	Type
1	A	395	MET
1	A	399	VAL
1	A	404	LEU
1	A	405	LEU
1	A	429	GLU
1	A	445	ILE
1	A	452	VAL
1	A	463	THR
1	A	483	LEU
1	A	502	LYS
1	A	522	LYS
1	A	523	SER
1	A	524	THR
1	A	526	HIS
1	A	534	ILE
1	A	538	THR
1	A	561	SER
1	A	564	LEU
1	A	602	GLU
1	A	604	ASN
1	A	605	ASN
1	A	623	ASN
1	A	624	THR
1	A	630	SER
1	A	644	VAL
1	A	647	ILE
1	A	649	MET
1	A	659	LYS
1	A	666	PHE
1	A	671	ILE
1	A	680	PHE
1	A	695	LEU
1	A	722	GLU
1	A	744	ASN
1	A	760	ASN
1	A	768	VAL
1	A	791	VAL
1	A	797	GLN
1	A	802	SER
1	A	804	PHE
1	A	810	GLU
1	A	813	SER

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Mol	Chain	Res	Type
1	A	816	LEU
1	A	827	ILE
1	A	828	LEU
1	A	836	SER
1	A	843	LEU
1	A	853	THR
1	A	866	GLU
1	A	867	ARG
1	A	886	LEU
1	A	888	LEU
1	A	893	GLU
1	A	894	SER
1	A	897	ILE
1	A	903	LEU
1	A	931	LEU
1	A	933	THR
1	A	946	VAL
1	A	950	LYS
1	A	951	ASP
1	A	965	LEU
1	A	968	VAL
1	A	971	ARG
1	A	980	LEU
1	A	983	ILE
1	A	984	LEU
1	A	986	VAL
1	A	993	THR
1	A	1007	VAL
1	A	1021	PHE
1	A	1040	ILE
1	A	1042	HIS
1	A	1045	THR
1	B	6	ILE
1	B	10	ILE
1	B	35	TYR
1	B	57	VAL
1	B	60	THR
1	B	64	VAL
1	B	65	ILE
1	B	70	ASN
1	B	72	ILE
1	B	88	VAL

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Mol	Chain	Res	Type
1	B	96	SER
1	B	110	LYS
1	B	117	LEU
1	B	121	GLU
1	B	124	GLN
1	B	125	GLN
1	B	136	PHE
1	B	145	THR
1	B	164	ASP
1	B	166	ILE
1	B	169	THR
1	B	175	VAL
1	B	189	ASN
1	B	195	LYS
1	B	205	THR
1	B	207	ILE
1	B	213	GLN
1	B	214	VAL
1	B	225	VAL
1	B	229	GLN
1	B	243	THR
1	B	256	ASP
1	B	259	ARG
1	B	270	LEU
1	B	278	ILE
1	B	293	LEU
1	B	295	THR
1	B	324	VAL
1	B	330	THR
1	B	353	LEU
1	B	362	PHE
1	B	365	THR
1	B	367	ILE
1	B	372	VAL
1	B	379	THR
1	B	393	LEU
1	B	395	MET
1	B	396	PHE
1	B	410	ILE
1	B	445	ILE
1	B	447	MET
1	B	448	VAL

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Mol	Chain	Res	Type
1	B	449	LEU
1	B	459	PHE
1	B	463	THR
1	B	468	ARG
1	B	480	LEU
1	B	510	LYS
1	B	519	MET
1	B	524	THR
1	B	534	ILE
1	B	536	ARG
1	B	538	THR
1	B	540	ARG
1	B	542	LEU
1	B	544	LEU
1	B	547	ILE
1	B	559	LEU
1	B	563	PHE
1	B	564	LEU
1	B	586	ARG
1	B	599	LEU
1	B	630	SER
1	B	644	VAL
1	B	657	GLN
1	B	659	LYS
1	B	666	PHE
1	B	668	LEU
1	B	673	GLU
1	B	680	PHE
1	B	699	ARG
1	B	705	GLU
1	B	714	THR
1	B	717	ARG
1	B	721	LEU
1	B	744	ASN
1	B	746	ILE
1	B	795	ASP
1	B	804	PHE
1	B	813	SER
1	B	824	SER
1	B	825	MET
1	B	837	THR
1	B	843	LEU

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Mol	Chain	Res	Type
1	B	844	MET
1	B	847	LEU
1	B	867	ARG
1	B	871	ASN
1	B	872	GLN
1	B	879	ILE
1	B	881	LEU
1	B	886	LEU
1	B	887	CYS
1	B	894	SER
1	B	897	ILE
1	B	903	LEU
1	B	910	ILE
1	B	914	LEU
1	B	919	ARG
1	B	922	THR
1	B	923	ASN
1	B	925	VAL
1	B	931	LEU
1	B	945	ILE
1	B	947	GLU
1	B	971	ARG
1	B	983	ILE
1	B	984	LEU
1	B	986	VAL
1	B	993	THR
1	B	1011	MET
1	B	1024	VAL
1	B	1032	ARG
1	B	1041	GLU
1	B	1042	HIS
1	C	6	ILE
1	C	8	ARG
1	C	11	PHE
1	C	17	ILE
1	C	18	ILE
1	C	27	ILE
1	C	35	TYR
1	C	44	THR
1	C	45	ILE
1	C	49	TYR
1	C	69	MET

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Mol	Chain	Res	Type
1	C	76	MET
1	C	78	MET
1	C	91	THR
1	C	92	LEU
1	C	102	ILE
1	C	111	LEU
1	C	149	MET
1	C	164	ASP
1	C	169	THR
1	C	177	LEU
1	C	195	LYS
1	C	205	THR
1	C	226	LYS
1	C	228	GLN
1	C	240	LEU
1	C	243	THR
1	C	245	GLU
1	C	291	ILE
1	C	293	LEU
1	C	302	THR
1	C	309	GLU
1	C	312	LYS
1	C	322	LYS
1	C	327	TYR
1	C	329	THR
1	C	337	ILE
1	C	343	THR
1	C	350	LEU
1	C	353	LEU
1	C	372	VAL
1	C	392	THR
1	C	398	MET
1	C	399	VAL
1	C	405	LEU
1	C	407	ASP
1	C	420	MET
1	C	422	GLU
1	C	425	LEU
1	C	432	ARG
1	C	435	MET
1	C	437	GLN
1	C	443	VAL

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Mol	Chain	Res	Type
1	C	445	ILE
1	C	447	MET
1	C	452	VAL
1	C	456	MET
1	C	466	ILE
1	C	487	ILE
1	C	489	THR
1	C	498	LYS
1	C	502	LYS
1	C	510	LYS
1	C	512	PHE
1	C	520	PHE
1	C	523	SER
1	C	524	THR
1	C	526	HIS
1	C	534	ILE
1	C	538	THR
1	C	540	ARG
1	C	559	LEU
1	C	602	GLU
1	C	613	ASN
1	C	624	THR
1	C	634	TRP
1	C	647	ILE
1	C	659	LYS
1	C	673	GLU
1	C	684	LEU
1	C	692	HIS
1	C	694	LYS
1	C	695	LEU
1	C	724	THR
1	C	728	LYS
1	C	743	ILE
1	C	746	ILE
1	C	772	TYR
1	C	774	MET
1	C	775	SER
1	C	785	ASP
1	C	804	PHE
1	C	813	SER
1	C	818	ARG
1	C	835	LYS

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Mol	Chain	Res	Type
1	C	842	GLU
1	C	847	LEU
1	C	850	LYS
1	C	860	THR
1	C	881	LEU
1	C	891	LEU
1	C	904	VAL
1	C	923	ASN
1	C	925	VAL
1	C	931	LEU
1	C	935	ILE
1	C	940	LYS
1	C	943	ILE
1	C	950	LYS
1	C	953	MET
1	C	961	ILE
1	C	970	MET
1	C	971	ARG
1	C	976	LEU
1	C	978	THR
1	C	980	LEU
1	C	983	ILE
1	C	984	LEU
1	C	986	VAL
1	C	1007	VAL
1	C	1030	ARG
1	C	1032	ARG
1	C	1035	ARG
1	D	6	ILE
1	D	17	ILE
1	D	45	ILE
1	D	48	SER
1	D	49	TYR
1	D	69	MET
1	D	138	MET
1	D	150	THR
1	D	151	GLN
1	D	157	TYR
1	D	166	ILE
1	D	195	LYS
1	D	205	THR
1	D	238	THR

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Mol	Chain	Res	Type
1	D	243	THR
1	D	267	LYS
1	D	270	LEU
1	D	278	ILE
1	D	293	LEU
1	D	324	VAL
1	D	337	ILE
1	D	341	VAL
1	D	353	LEU
1	D	362	PHE
1	D	363	ARG
1	D	372	VAL
1	D	399	VAL
1	D	400	LEU
1	D	413	VAL
1	D	428	LYS
1	D	437	GLN
1	D	449	LEU
1	D	452	VAL
1	D	463	THR
1	D	483	LEU
1	D	489	THR
1	D	507	GLU
1	D	509	LYS
1	D	524	THR
1	D	538	THR
1	D	557	VAL
1	D	561	SER
1	D	563	PHE
1	D	564	LEU
1	D	574	THR
1	D	575	MET
1	D	602	GLU
1	D	623	ASN
1	D	629	VAL
1	D	633	ASP
1	D	634	TRP
1	D	649	MET
1	D	659	LYS
1	D	666	PHE
1	D	668	LEU
1	D	671	ILE

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Mol	Chain	Res	Type
1	D	673	GLU
1	D	676	THR
1	D	678	THR
1	D	687	GLN
1	D	695	LEU
1	D	703	LEU
1	D	716	VAL
1	D	726	GLN
1	D	786	ILE
1	D	791	VAL
1	D	801	PHE
1	D	802	SER
1	D	804	PHE
1	D	811	TYR
1	D	813	SER
1	D	825	MET
1	D	835	LYS
1	D	842	GLU
1	D	843	LEU
1	D	850	LYS
1	D	864	TYR
1	D	867	ARG
1	D	872	GLN
1	D	875	SER
1	D	893	GLU
1	D	894	SER
1	D	900	SER
1	D	921	LEU
1	D	931	LEU
1	D	965	LEU
1	D	971	ARG
1	D	972	LEU
1	D	984	LEU
1	D	986	VAL
1	D	1015	THR
1	D	1035	ARG
1	D	1040	ILE
1	D	1041	GLU
1	D	1042	HIS
1	E	4	PHE
1	E	13	TRP
1	E	32	VAL

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Mol	Chain	Res	Type
1	E	35	TYR
1	E	44	THR
1	E	45	ILE
1	E	70	ASN
1	E	73	ASP
1	E	96	SER
1	E	138	MET
1	E	145	THR
1	E	164	ASP
1	E	166	ILE
1	E	169	THR
1	E	182	TYR
1	E	192	GLU
1	E	195	LYS
1	E	196	PHE
1	E	200	PRO
1	E	205	THR
1	E	229	GLN
1	E	244	GLU
1	E	253	VAL
1	E	256	ASP
1	E	259	ARG
1	E	261	LEU
1	E	267	LYS
1	E	270	LEU
1	E	278	ILE
1	E	293	LEU
1	E	295	THR
1	E	319	SER
1	E	323	ILE
1	E	334	LYS
1	E	342	LYS
1	E	343	THR
1	E	348	ILE
1	E	353	LEU
1	E	355	MET
1	E	372	VAL
1	E	376	LEU
1	E	393	LEU
1	E	400	LEU
1	E	420	MET
1	E	459	PHE

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Mol	Chain	Res	Type
1	E	480	LEU
1	E	489	THR
1	E	500	ILE
1	E	521	GLU
1	E	523	SER
1	E	524	THR
1	E	535	LEU
1	E	559	LEU
1	E	586	ARG
1	E	592	ASN
1	E	629	VAL
1	E	636	ASP
1	E	640	GLU
1	E	659	LYS
1	E	668	LEU
1	E	672	VAL
1	E	673	GLU
1	E	682	PHE
1	E	717	ARG
1	E	721	LEU
1	E	744	ASN
1	E	760	ASN
1	E	772	TYR
1	E	785	ASP
1	E	797	GLN
1	E	798	MET
1	E	804	PHE
1	E	805	SER
1	E	813	SER
1	E	836	SER
1	E	844	MET
1	E	865	GLN
1	E	867	ARG
1	E	871	ASN
1	E	894	SER
1	E	910	ILE
1	E	928	GLN
1	E	931	LEU
1	E	938	SER
1	E	944	LEU
1	E	965	LEU
1	E	966	ASP

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Mol	Chain	Res	Type
1	E	971	ARG
1	E	978	THR
1	E	983	ILE
1	E	984	LEU
1	E	993	THR
1	E	1007	VAL
1	E	1016	VAL
1	E	1017	LEU
1	E	1032	ARG
1	E	1035	ARG
1	E	1041	GLU
1	F	5	PHE
1	F	13	TRP
1	F	15	ILE
1	F	27	ILE
1	F	45	ILE
1	F	49	TYR
1	F	62	THR
1	F	77	TYR
1	F	93	THR
1	F	102	ILE
1	F	115	MET
1	F	121	GLU
1	F	124	GLN
1	F	131	LYS
1	F	138	MET
1	F	152	GLU
1	F	174	ASP
1	F	177	LEU
1	F	193	LEU
1	F	195	LYS
1	F	196	PHE
1	F	205	THR
1	F	219	LEU
1	F	222	THR
1	F	225	VAL
1	F	253	VAL
1	F	278	ILE
1	F	293	LEU
1	F	329	THR
1	F	330	THR
1	F	337	ILE

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Mol	Chain	Res	Type
1	F	353	LEU
1	F	358	PHE
1	F	363	ARG
1	F	376	LEU
1	F	382	VAL
1	F	404	LEU
1	F	429	GLU
1	F	447	MET
1	F	448	VAL
1	F	454	VAL
1	F	463	THR
1	F	472	ILE
1	F	474	ILE
1	F	478	MET
1	F	489	THR
1	F	500	ILE
1	F	510	LYS
1	F	523	SER
1	F	526	HIS
1	F	534	ILE
1	F	535	LEU
1	F	547	ILE
1	F	561	SER
1	F	589	LYS
1	F	599	LEU
1	F	602	GLU
1	F	623	ASN
1	F	624	THR
1	F	626	ILE
1	F	630	SER
1	F	649	MET
1	F	659	LYS
1	F	666	PHE
1	F	668	LEU
1	F	671	ILE
1	F	673	GLU
1	F	686	ASP
1	F	694	LYS
1	F	695	LEU
1	F	708	LYS
1	F	721	LEU
1	F	734	GLU

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Mol	Chain	Res	Type
1	F	746	ILE
1	F	748	THR
1	F	759	VAL
1	F	767	ARG
1	F	785	ASP
1	F	788	ASP
1	F	797	GLN
1	F	804	PHE
1	F	808	ARG
1	F	813	SER
1	F	835	LYS
1	F	836	SER
1	F	843	LEU
1	F	847	LEU
1	F	860	THR
1	F	865	GLN
1	F	868	LEU
1	F	914	LEU
1	F	919	ARG
1	F	922	THR
1	F	929	VAL
1	F	931	LEU
1	F	940	LYS
1	F	945	ILE
1	F	954	ASP
1	F	971	ARG
1	F	977	MET
1	F	980	LEU
1	F	983	ILE
1	F	984	LEU
1	F	986	VAL
1	F	991	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	70	ASN
1	A	109	ASN
1	A	151	GLN
1	A	161	ASN
1	A	391	ASN

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Mol	Chain	Res	Type
1	A	733	GLN
1	B	108	GLN
1	B	123	GLN
1	B	124	GLN
1	B	181	GLN
1	B	228	GLN
1	B	622	GLN
1	B	692	HIS
1	B	726	GLN
1	B	865	GLN
1	B	923	ASN
1	C	58	GLN
1	C	104	GLN
1	C	109	ASN
1	C	112	GLN
1	C	120	GLN
1	C	505	HIS
1	C	719	ASN
1	C	760	ASN
1	D	151	GLN
1	D	210	GLN
1	D	211	ASN
1	D	517	ASN
1	D	726	GLN
1	D	865	GLN
1	D	1042	HIS
1	E	68	ASN
1	E	108	GLN
1	E	709	HIS
1	F	109	ASN
1	F	584	GLN
1	F	733	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	2000	-	36,36,36	1.82	8 (22%)	47,47,47	1.37	8 (17%)
2	LMT	E	2000	-	36,36,36	1.82	10 (27%)	47,47,47	2.51	15 (31%)
2	LMT	F	2000	-	36,36,36	1.89	11 (30%)	47,47,47	2.15	15 (31%)
2	LMT	D	2000	-	36,36,36	1.92	9 (25%)	47,47,47	1.49	9 (19%)
2	LMT	B	2000	-	36,36,36	1.85	9 (25%)	47,47,47	1.58	7 (14%)
2	LMT	A	2000	-	36,36,36	1.98	9 (25%)	47,47,47	1.67	9 (19%)

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	C	2000	-	3/3/10/10	12/21/61/61	0/2/2/2
2	LMT	E	2000	-	2/2/10/10	12/21/61/61	0/2/2/2
2	LMT	F	2000	-	3/3/10/10	15/21/61/61	0/2/2/2
2	LMT	D	2000	-	2/2/10/10	14/21/61/61	0/2/2/2
2	LMT	B	2000	-	2/2/10/10	10/21/61/61	0/2/2/2
2	LMT	A	2000	-	2/2/10/10	10/21/61/61	0/2/2/2

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	LMT	O1'-C1'	4.63	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2000	LMT	O5'-C5'	4.45	1.55	1.44
2	F	2000	LMT	O1'-C1'	4.41	1.47	1.40
2	C	2000	LMT	O5'-C5'	4.30	1.54	1.44
2	F	2000	LMT	O5'-C5'	4.27	1.54	1.44
2	B	2000	LMT	O3B-C3B	4.14	1.52	1.43
2	A	2000	LMT	O3B-C3B	4.10	1.52	1.43
2	E	2000	LMT	O1'-C1'	4.06	1.47	1.40
2	A	2000	LMT	O5B-C1B	4.04	1.52	1.41
2	B	2000	LMT	O1'-C1'	3.94	1.46	1.40
2	E	2000	LMT	O5B-C1B	3.92	1.51	1.41
2	E	2000	LMT	O5'-C5'	3.89	1.53	1.44
2	C	2000	LMT	O5B-C1B	3.86	1.51	1.41
2	A	2000	LMT	O1'-C1'	3.86	1.46	1.40
2	B	2000	LMT	O5'-C5'	3.80	1.53	1.44
2	D	2000	LMT	O5B-C1B	3.78	1.51	1.41
2	C	2000	LMT	O5'-C1'	3.73	1.51	1.41
2	D	2000	LMT	O3B-C3B	3.68	1.51	1.43
2	D	2000	LMT	C6'-C5'	-3.67	1.39	1.51
2	D	2000	LMT	O5'-C5'	3.61	1.53	1.44
2	C	2000	LMT	O1'-C1'	3.54	1.46	1.40
2	F	2000	LMT	C6'-C5'	-3.49	1.40	1.51
2	F	2000	LMT	O3B-C3B	3.49	1.51	1.43
2	B	2000	LMT	O5B-C1B	3.46	1.50	1.41
2	D	2000	LMT	O5'-C1'	3.44	1.50	1.41
2	A	2000	LMT	C6'-C5'	-3.44	1.40	1.51
2	F	2000	LMT	O5B-C1B	3.44	1.50	1.41
2	B	2000	LMT	O5'-C1'	3.39	1.50	1.41
2	A	2000	LMT	O5'-C1'	3.08	1.49	1.41
2	C	2000	LMT	O3B-C3B	3.04	1.50	1.43
2	E	2000	LMT	O5'-C1'	3.03	1.49	1.41
2	E	2000	LMT	C6'-C5'	-2.91	1.42	1.51
2	B	2000	LMT	C6'-C5'	-2.91	1.42	1.51
2	F	2000	LMT	O5'-C1'	2.83	1.49	1.41
2	C	2000	LMT	O2'-C2'	2.77	1.49	1.43
2	C	2000	LMT	C6'-C5'	-2.75	1.42	1.51
2	A	2000	LMT	O2'-C2'	2.62	1.49	1.43
2	D	2000	LMT	C3'-C2'	-2.46	1.46	1.52
2	E	2000	LMT	O3'-C3'	2.39	1.48	1.43
2	C	2000	LMT	C3'-C2'	-2.36	1.46	1.52
2	F	2000	LMT	O2'-C2'	2.32	1.48	1.43
2	D	2000	LMT	O2'-C2'	2.32	1.48	1.43
2	B	2000	LMT	O2'-C2'	2.30	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	LMT	O3'-C3'	2.23	1.48	1.43
2	E	2000	LMT	O2B-C2B	2.20	1.48	1.43
2	E	2000	LMT	O1B-C1B	-2.12	1.35	1.41
2	F	2000	LMT	C3'-C2'	-2.11	1.46	1.52
2	E	2000	LMT	O2'-C2'	2.11	1.48	1.43
2	A	2000	LMT	O3'-C3'	2.10	1.47	1.43
2	B	2000	LMT	C4'-C5'	2.09	1.58	1.52
2	F	2000	LMT	O3'-C3'	2.06	1.47	1.43
2	A	2000	LMT	C5-C4	2.06	1.63	1.51
2	F	2000	LMT	C5-C4	2.06	1.63	1.51
2	D	2000	LMT	C5-C4	2.03	1.63	1.51
2	F	2000	LMT	C2-C1	2.02	1.59	1.51
2	E	2000	LMT	O1B-C4'	-2.00	1.38	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2000	LMT	O3B-C3B-C4B	-7.15	93.83	110.35
2	E	2000	LMT	C4B-C3B-C2B	7.14	123.29	110.82
2	A	2000	LMT	O5B-C5B-C4B	5.58	119.82	109.69
2	F	2000	LMT	O1B-C1B-C2B	5.48	122.29	108.10
2	B	2000	LMT	C1'-C2'-C3'	5.35	121.13	110.00
2	E	2000	LMT	O5B-C1B-C2B	5.30	121.57	110.35
2	E	2000	LMT	O3B-C3B-C2B	-4.65	99.61	110.35
2	F	2000	LMT	O6'-C6'-C5'	-4.53	95.74	111.29
2	F	2000	LMT	O1'-C1'-C2'	4.40	115.17	108.30
2	F	2000	LMT	C1B-O1B-C4'	-4.13	107.75	117.96
2	E	2000	LMT	C1B-O5B-C5B	4.08	121.69	113.69
2	F	2000	LMT	C1'-O5'-C5'	4.05	121.64	113.69
2	A	2000	LMT	O5B-C1B-C2B	4.05	118.92	110.35
2	F	2000	LMT	O5'-C5'-C4'	3.84	117.84	109.75
2	D	2000	LMT	C1'-O5'-C5'	3.74	121.03	113.69
2	A	2000	LMT	C1'-O5'-C5'	3.73	121.00	113.69
2	E	2000	LMT	O5B-C5B-C4B	3.73	116.46	109.69
2	E	2000	LMT	C3B-C4B-C5B	3.58	116.63	110.24
2	E	2000	LMT	C1'-C2'-C3'	3.56	117.41	110.00
2	E	2000	LMT	O1B-C4'-C5'	-3.54	99.75	109.45
2	D	2000	LMT	O5B-C5B-C4B	3.54	116.12	109.69
2	F	2000	LMT	O3B-C3B-C4B	-3.54	102.17	110.35
2	B	2000	LMT	O5'-C1'-C2'	3.50	117.77	110.35
2	C	2000	LMT	O5'-C1'-C2'	3.50	117.76	110.35
2	D	2000	LMT	C2'-C3'-C4'	3.40	117.44	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2000	LMT	O5'-C5'-C6'	3.32	114.70	106.44
2	A	2000	LMT	C1B-C2B-C3B	3.30	116.87	110.00
2	F	2000	LMT	C2'-C3'-C4'	3.22	117.03	109.68
2	D	2000	LMT	C4B-C3B-C2B	3.16	116.34	110.82
2	B	2000	LMT	O5B-C5B-C4B	3.12	115.36	109.69
2	F	2000	LMT	O1B-C4'-C3'	3.08	115.47	107.28
2	B	2000	LMT	C2'-C3'-C4'	3.02	116.58	109.68
2	E	2000	LMT	C1B-O1B-C4'	-3.00	110.55	117.96
2	E	2000	LMT	C2'-C3'-C4'	2.92	116.36	109.68
2	C	2000	LMT	C1B-O1B-C4'	-2.89	110.82	117.96
2	E	2000	LMT	O2B-C2B-C3B	2.87	116.98	110.35
2	F	2000	LMT	O5'-C5'-C6'	-2.85	99.34	106.44
2	B	2000	LMT	C1-O1'-C1'	2.78	118.46	113.84
2	D	2000	LMT	O1B-C4'-C3'	2.71	114.48	107.28
2	C	2000	LMT	C4B-C3B-C2B	2.70	115.53	110.82
2	C	2000	LMT	O5'-C5'-C6'	2.69	113.12	106.44
2	D	2000	LMT	C3B-C4B-C5B	2.64	114.95	110.24
2	B	2000	LMT	C4B-C3B-C2B	-2.62	106.25	110.82
2	B	2000	LMT	O3B-C3B-C2B	2.57	116.30	110.35
2	F	2000	LMT	C1'-C2'-C3'	2.56	115.33	110.00
2	F	2000	LMT	C1B-O5B-C5B	-2.53	108.72	113.69
2	D	2000	LMT	O3'-C3'-C2'	-2.50	104.58	110.35
2	C	2000	LMT	C3B-C4B-C5B	2.49	114.68	110.24
2	F	2000	LMT	O4'-C4B-C5B	-2.49	103.11	109.30
2	E	2000	LMT	O1B-C1B-C2B	-2.48	101.66	108.10
2	A	2000	LMT	C2'-C3'-C4'	2.41	115.18	109.68
2	A	2000	LMT	C3B-C4B-C5B	2.39	114.50	110.24
2	F	2000	LMT	O3B-C3B-C2B	2.36	115.80	110.35
2	F	2000	LMT	C1-O1'-C1'	2.35	117.73	113.84
2	D	2000	LMT	C1-O1'-C1'	2.30	117.66	113.84
2	C	2000	LMT	C1'-O5'-C5'	2.29	118.18	113.69
2	A	2000	LMT	O1'-C1'-C2'	2.27	111.85	108.30
2	A	2000	LMT	O4'-C4B-C5B	2.23	114.83	109.30
2	C	2000	LMT	C1B-C2B-C3B	2.18	114.53	110.00
2	D	2000	LMT	C6'-C5'-C4'	-2.14	107.09	113.33
2	A	2000	LMT	C1-O1'-C1'	2.11	117.33	113.84
2	E	2000	LMT	O5B-C5B-C6B	2.08	111.61	106.44
2	C	2000	LMT	O5B-C5B-C4B	2.07	113.45	109.69

All (14) chirality outliers are listed below:

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

All (73) torsion outliers are listed below:

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

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

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Mol	Chain	Res	Type	Atoms
2	A	2000	LMT	C2B-C1B-O1B-C4'
2	F	2000	LMT	C2-C3-C4-C5
2	E	2000	LMT	C3'-C4'-O1B-C1B
2	E	2000	LMT	C5'-C4'-O1B-C1B
2	D	2000	LMT	O5B-C1B-O1B-C4'
2	F	2000	LMT	C2B-C1B-O1B-C4'
2	C	2000	LMT	C1-C2-C3-C4
2	C	2000	LMT	C2-C1-O1'-C1'

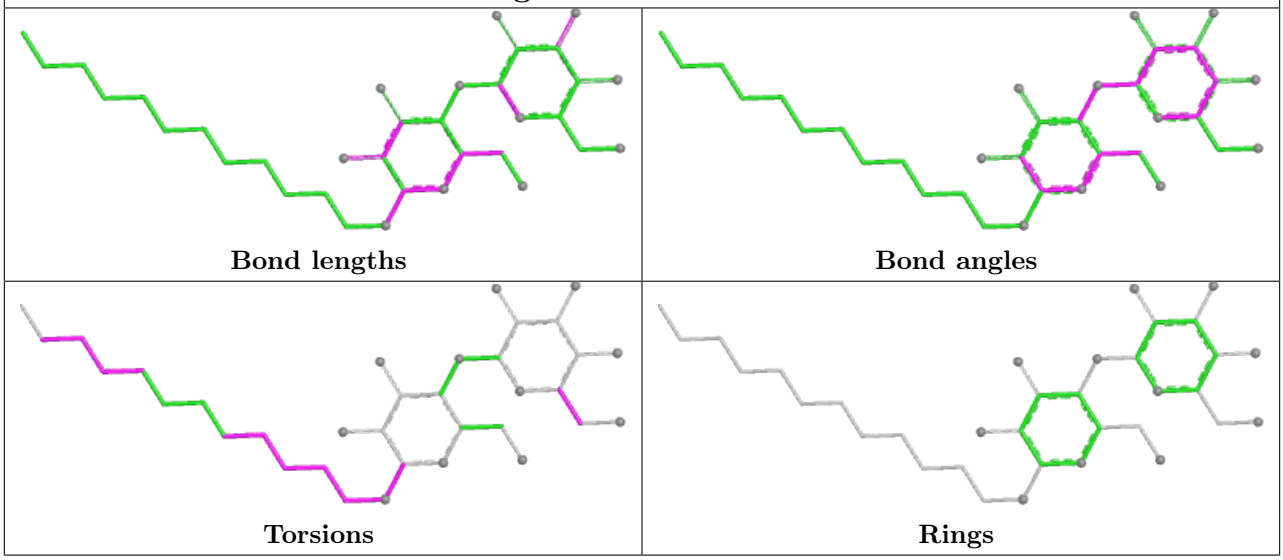
There are no ring outliers.

6 monomers are involved in 38 short contacts:

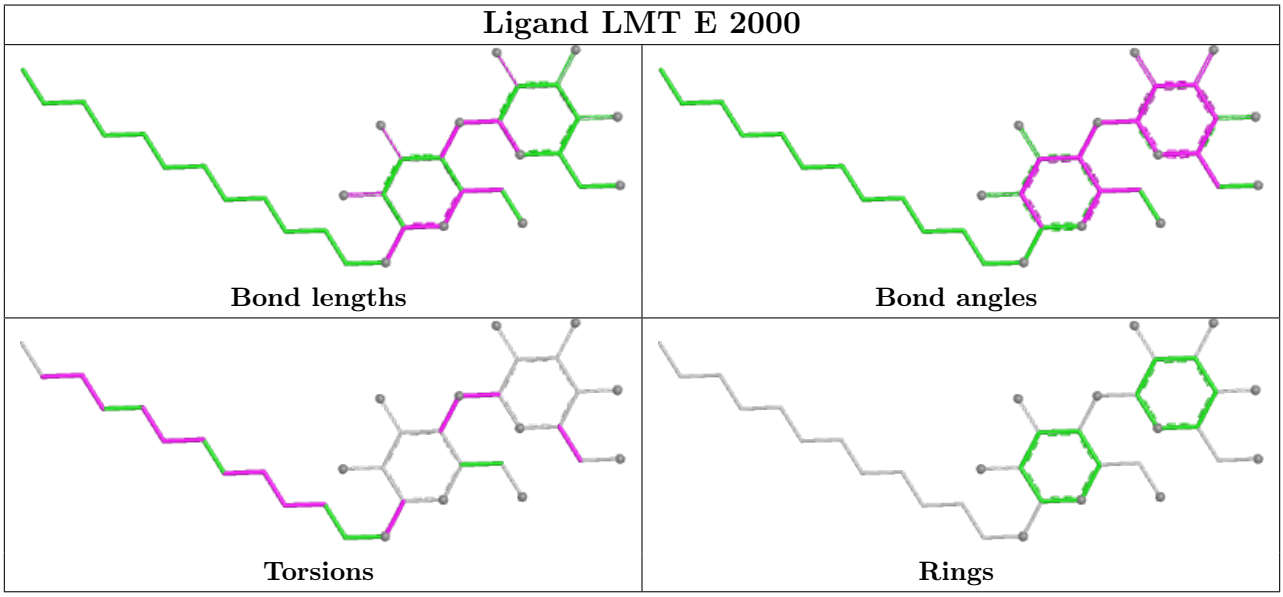
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2000	LMT	5	0
2	E	2000	LMT	17	0
2	F	2000	LMT	2	0
2	D	2000	LMT	4	0
2	B	2000	LMT	3	0
2	A	2000	LMT	7	0

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.

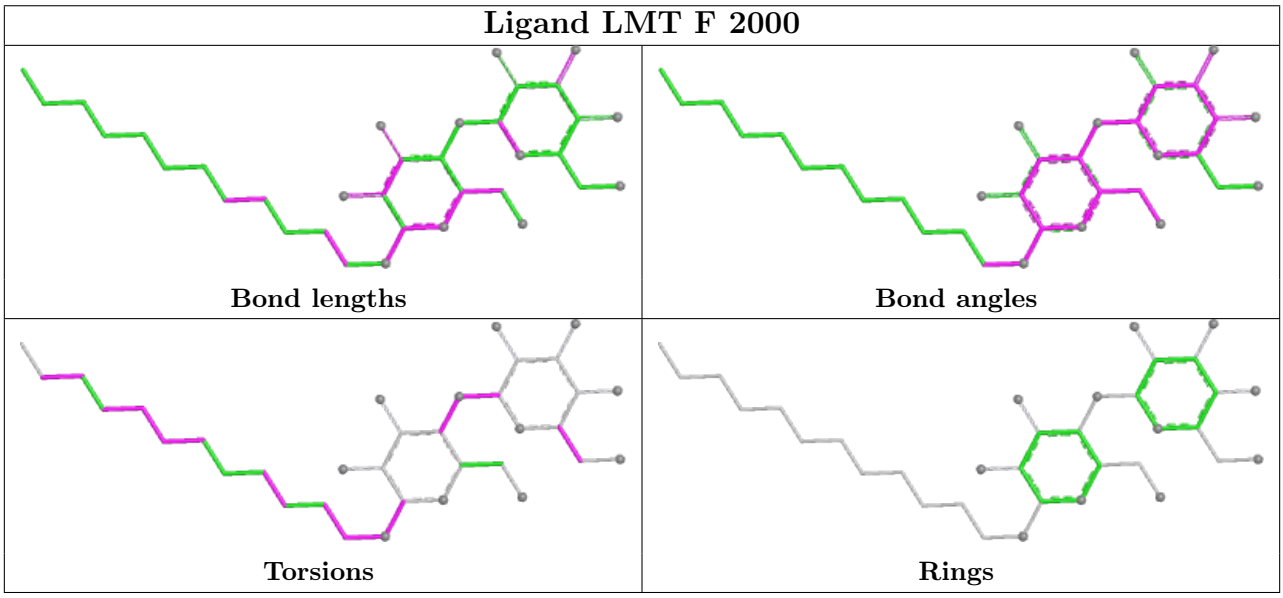
Ligand LMT C 2000



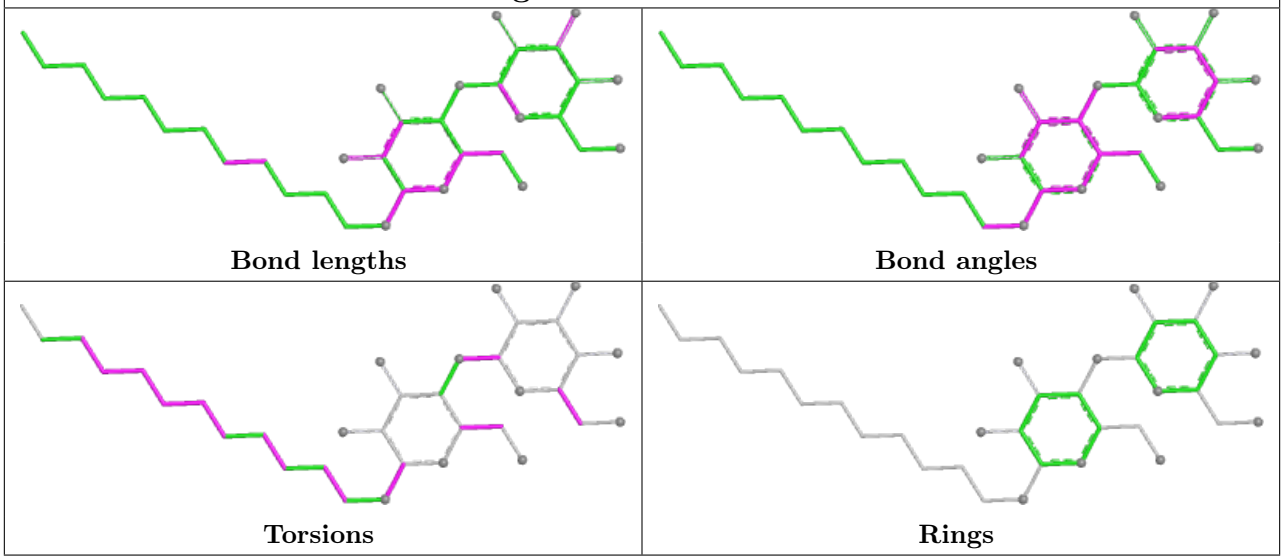
Ligand LMT E 2000



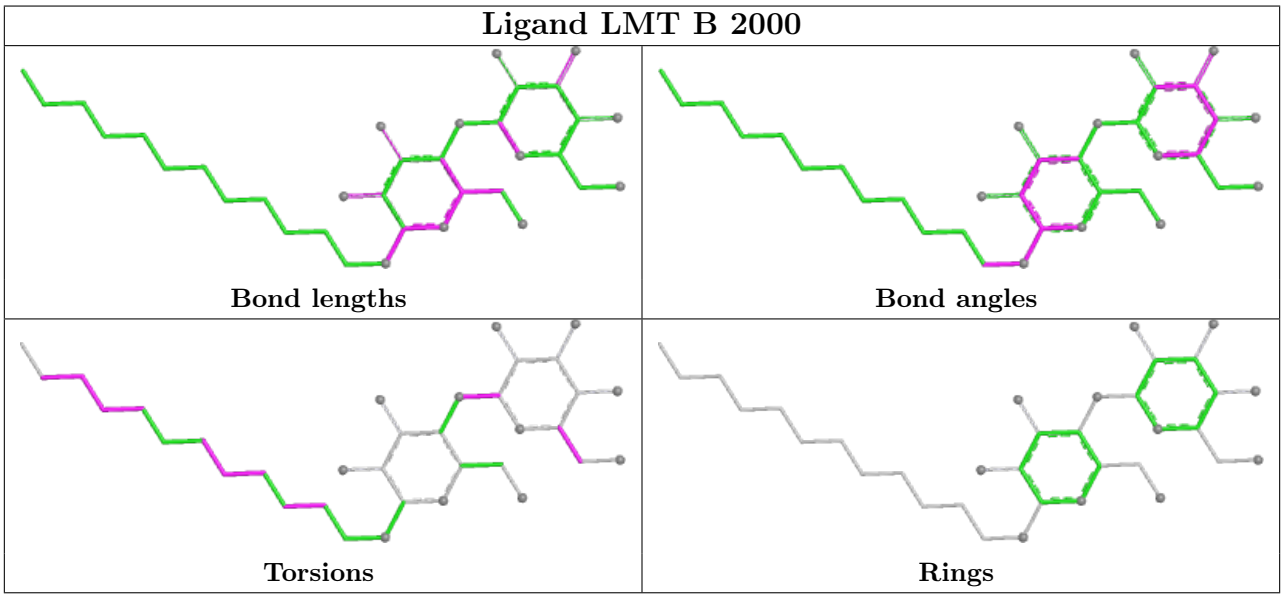
Ligand LMT F 2000



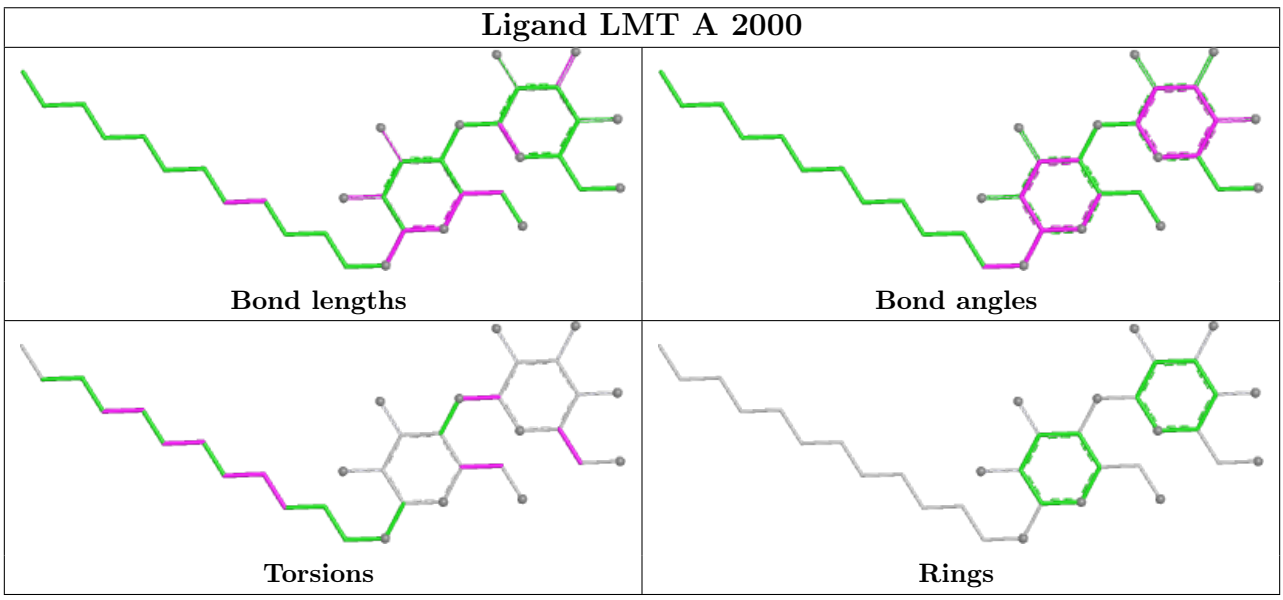
Ligand LMT D 2000



Ligand LMT B 2000



Ligand LMT A 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%)	-0.38	11 (1%)	80	69	13, 49, 91, 117	0
1	B	1042/1069 (97%)	-0.19	31 (2%)	50	37	11, 49, 101, 139	0
1	C	1042/1069 (97%)	-0.17	27 (2%)	56	42	8, 62, 104, 135	0
1	D	1044/1069 (97%)	-0.48	6 (0%)	89	81	9, 36, 74, 116	0
1	E	1042/1069 (97%)	-0.58	3 (0%)	94	89	7, 28, 59, 88	0
1	F	1042/1069 (97%)	-0.57	3 (0%)	94	89	5, 30, 61, 103	0
All	All	6256/6414 (97%)	-0.40	81 (1%)	77	65	5, 40, 91, 139	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	715	SER	15.5
1	B	689	GLY	7.9
1	C	720	GLY	7.0
1	C	856	GLY	5.2
1	B	870	GLY	5.1
1	B	71	GLY	5.0
1	B	170	SER	4.8
1	B	868	LEU	4.6
1	B	79	SER	4.6
1	B	869	SER	4.4
1	C	426	PRO	4.0
1	C	116	PRO	3.9
1	C	301	ASP	3.7
1	B	690	LEU	3.6
1	B	167	SER	3.6
1	B	78	MET	3.4
1	A	1034	SER	3.3
1	C	690	LEU	3.3
1	B	834	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	511	GLY	3.3
1	C	820	ASN	3.3
1	B	295	THR	3.3
1	C	719	ASN	3.2
1	A	870	GLY	3.1
1	B	1034	SER	3.1
1	D	833	PRO	3.0
1	C	496	MET	3.0
1	C	458	PHE	2.9
1	C	712	MET	2.9
1	C	826	GLU	2.9
1	B	714	THR	2.9
1	B	833	PRO	2.9
1	A	1033	PHE	2.8
1	D	320	GLY	2.8
1	C	427	PRO	2.7
1	C	676	THR	2.7
1	C	494	ALA	2.6
1	B	874	PRO	2.6
1	D	869	SER	2.6
1	A	869	SER	2.6
1	C	76	MET	2.5
1	A	678	THR	2.5
1	B	683	GLU	2.5
1	C	54	ALA	2.5
1	D	1034	SER	2.4
1	A	167	SER	2.4
1	B	853	THR	2.4
1	E	833	PRO	2.4
1	B	859	TRP	2.4
1	B	619	GLY	2.4
1	E	678	THR	2.4
1	C	872	GLN	2.3
1	C	858	ASP	2.3
1	A	334	LYS	2.3
1	B	872	GLN	2.3
1	A	871	ASN	2.3
1	B	871	ASN	2.3
1	E	834	GLY	2.3
1	B	292	LYS	2.3
1	B	72	ILE	2.3
1	C	260	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	499	PRO	2.2
1	D	620	ARG	2.2
1	B	677	ALA	2.2
1	F	510	LYS	2.2
1	C	33	ALA	2.2
1	A	148	THR	2.2
1	C	498	LYS	2.2
1	A	290	GLY	2.2
1	B	711	ASP	2.1
1	B	294	ALA	2.1
1	C	827	ILE	2.1
1	F	48	SER	2.1
1	B	858	ASP	2.1
1	B	296	GLY	2.1
1	C	838	GLY	2.1
1	B	174	ASP	2.1
1	C	842	GLU	2.0
1	A	1040	ILE	2.0
1	C	714	THR	2.0
1	D	1043	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	B	2000	35/35	0.83	0.34	11,43,62,64	0
2	LMT	D	2000	35/35	0.86	0.37	20,39,53,62	0
2	LMT	E	2000	35/35	0.86	0.38	14,53,70,88	0

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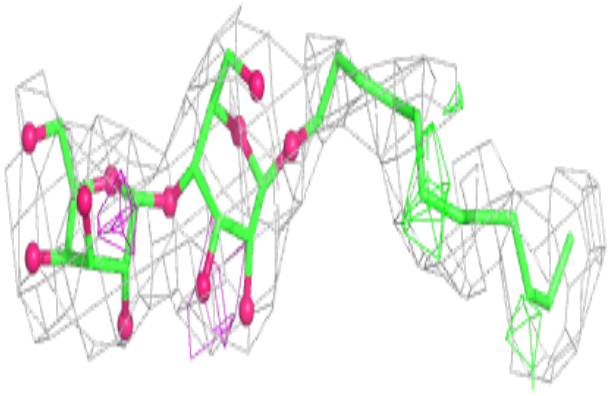
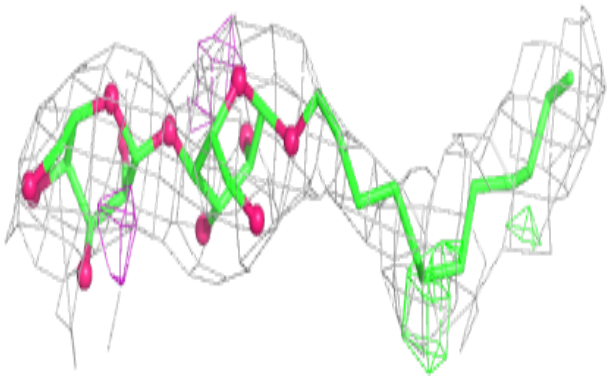
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	C	2000	35/35	0.88	0.38	12,33,43,47	0
2	LMT	F	2000	35/35	0.88	0.30	14,40,70,74	0
2	LMT	A	2000	35/35	0.89	0.30	31,50,62,70	0

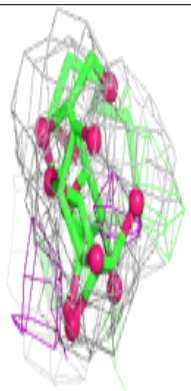
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LMT 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)

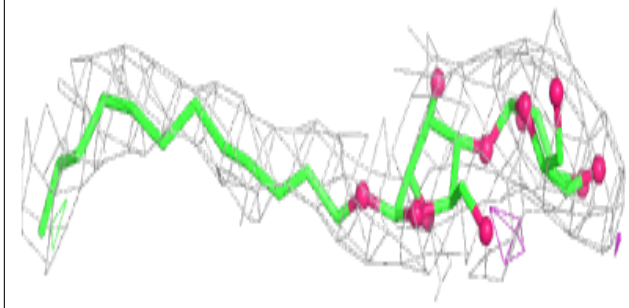


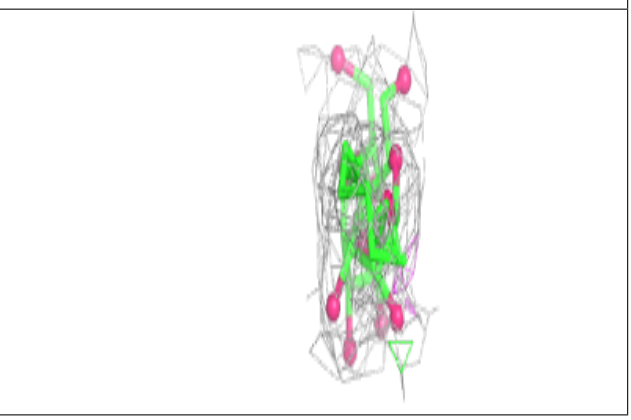




Electron density around LMT D 2000:

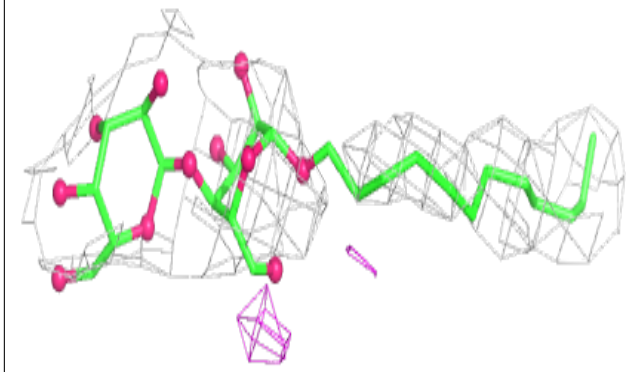
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

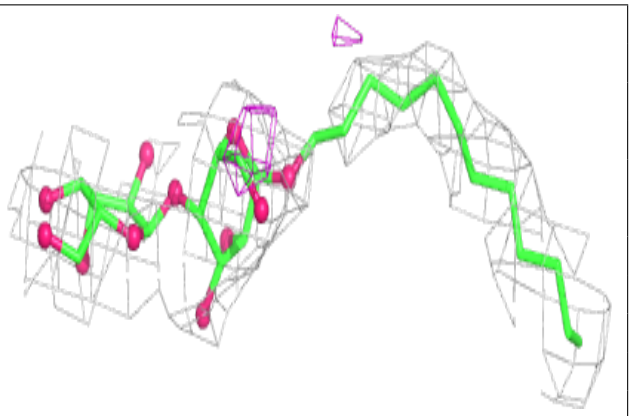




Electron density around LMT E 2000:

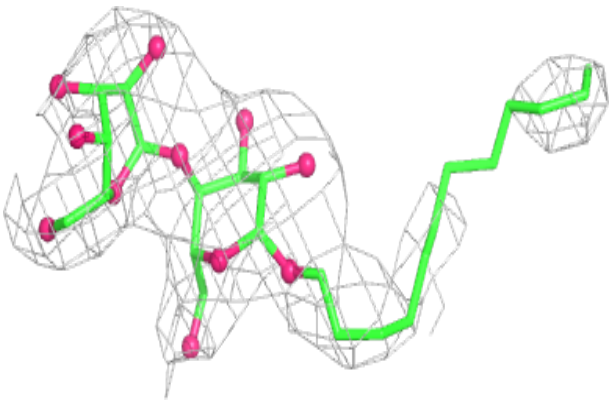
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

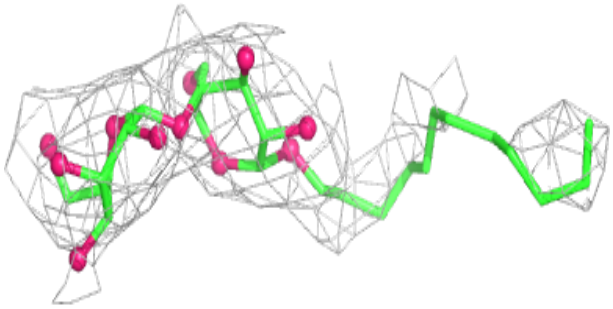


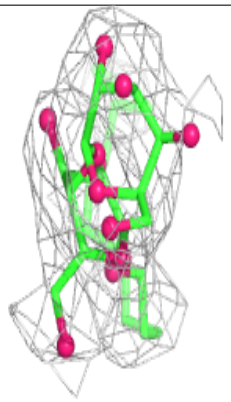


Electron density around LMT C 2000:

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

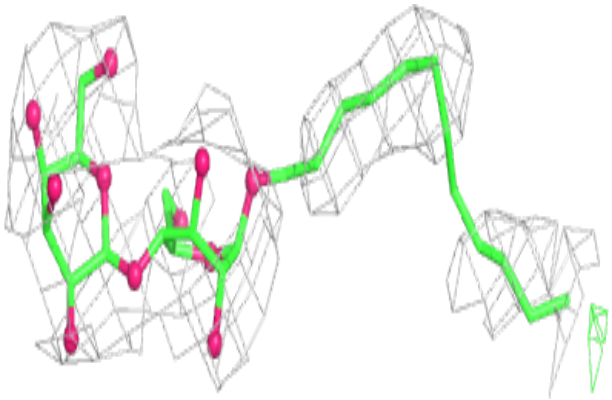


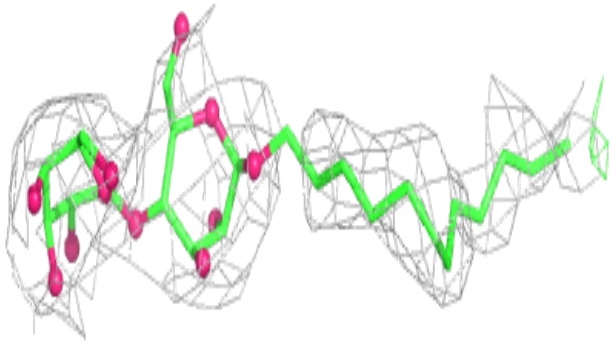


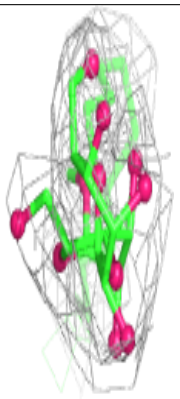


Electron density around LMT F 2000:

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

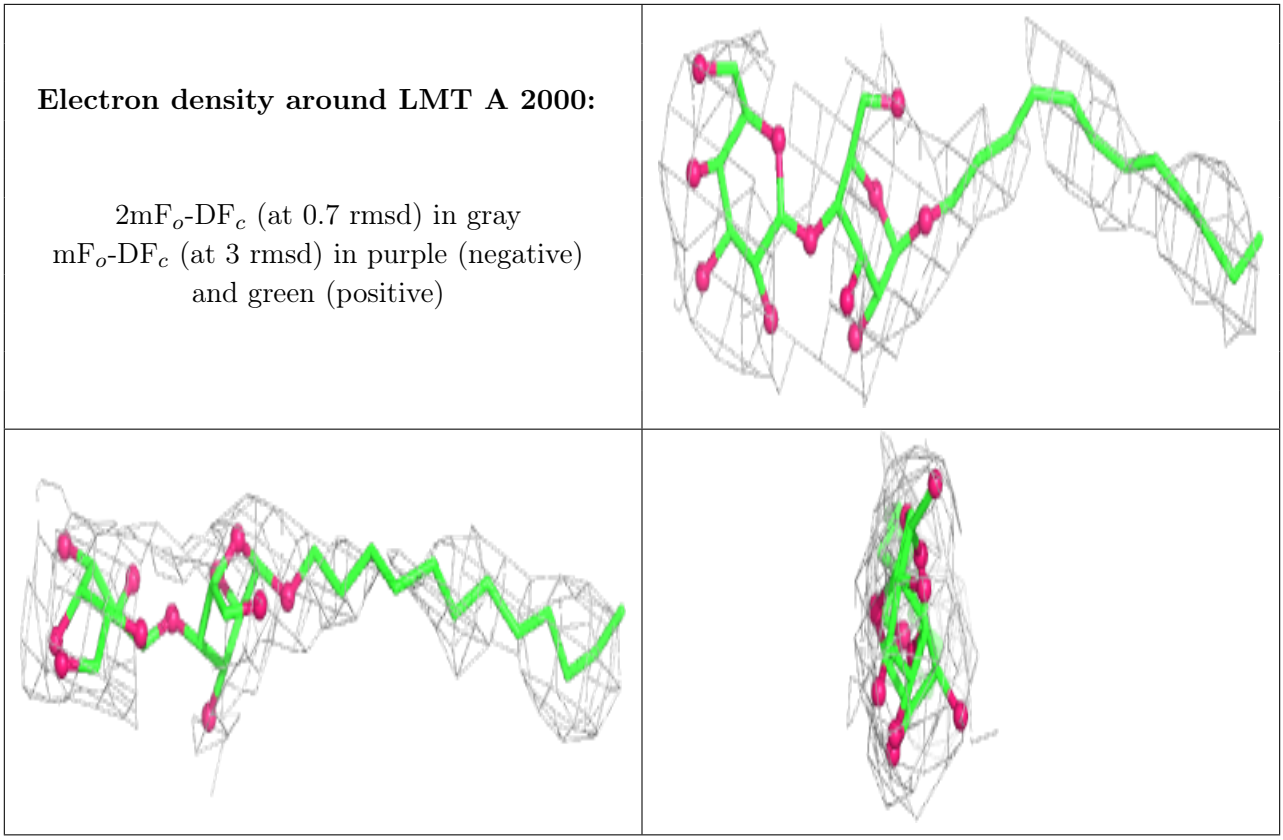






Electron density around LMT A 2000:

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



6.5 Other polymers (i)

There are no such residues in this entry.