Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 09:54 am GMT

PDB ID	:	4ZIW
Title	:	Crystal structure of AcrB deletion mutant in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-28
Resolution	:	3.40 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

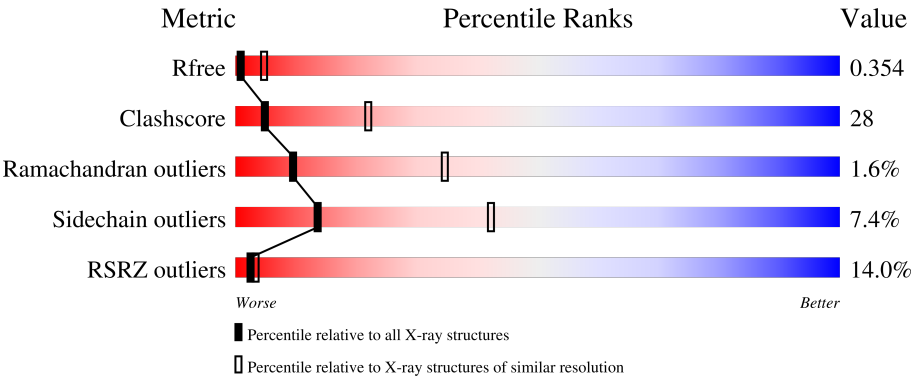
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1044	12% 47% 47% 5% •
1	B	1044	10% 50% 45% •
1	C	1044	12% 47% 47% 5% •
1	D	1044	16% 44% 50% 5% ••
1	E	1044	17% 47% 47% 5% •

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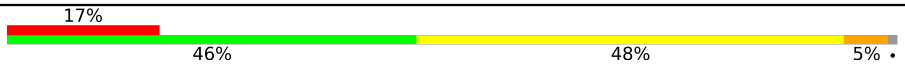
Mol	Chain	Length	Quality of chain
1	F	1044	

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	B	2000	-	-	-	X
2	LMT	D	2000	X	-	-	-
2	LMT	E	1101	X	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47532 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	B	1039	Total	C	N	O	S	0	0	0
			7900	5076	1307	1474	43			
1	C	1035	Total	C	N	O	S	0	0	0
			7867	5057	1299	1468	43			
1	D	1038	Total	C	N	O	S	0	0	0
			7893	5072	1306	1472	43			
1	E	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			
1	F	1037	Total	C	N	O	S	0	0	0
			7883	5066	1303	1471	43			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	615	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	615	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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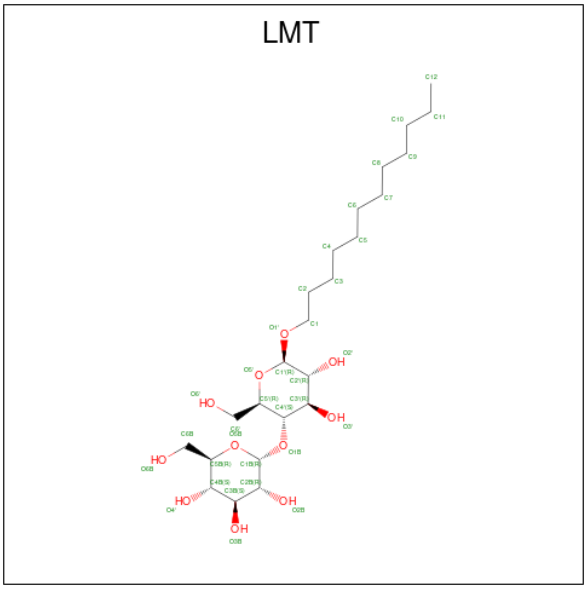
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	615	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	615	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	615	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- 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 35 24 11	0	0

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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

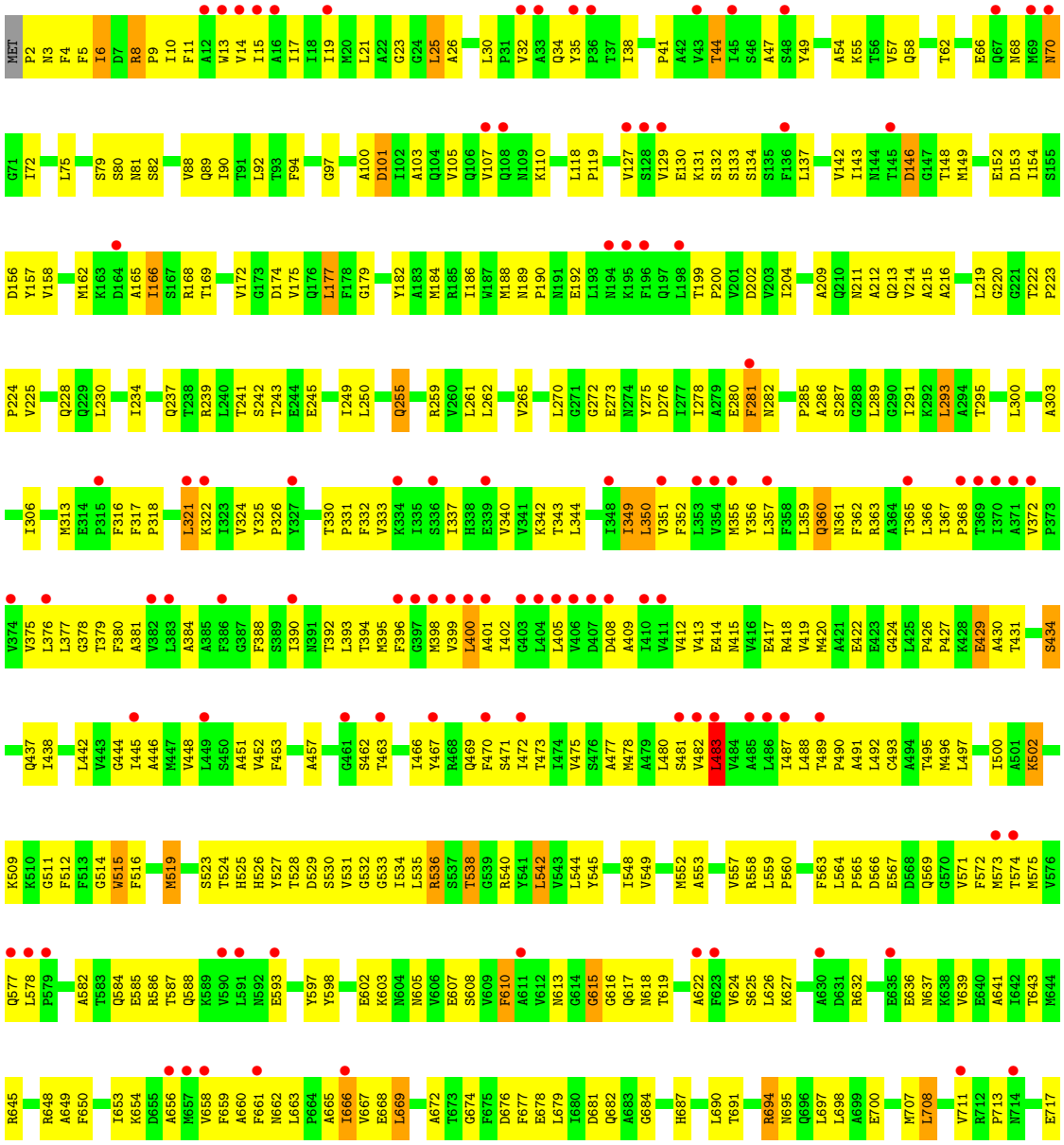
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	E	1	Total Ni 1 1	0	0

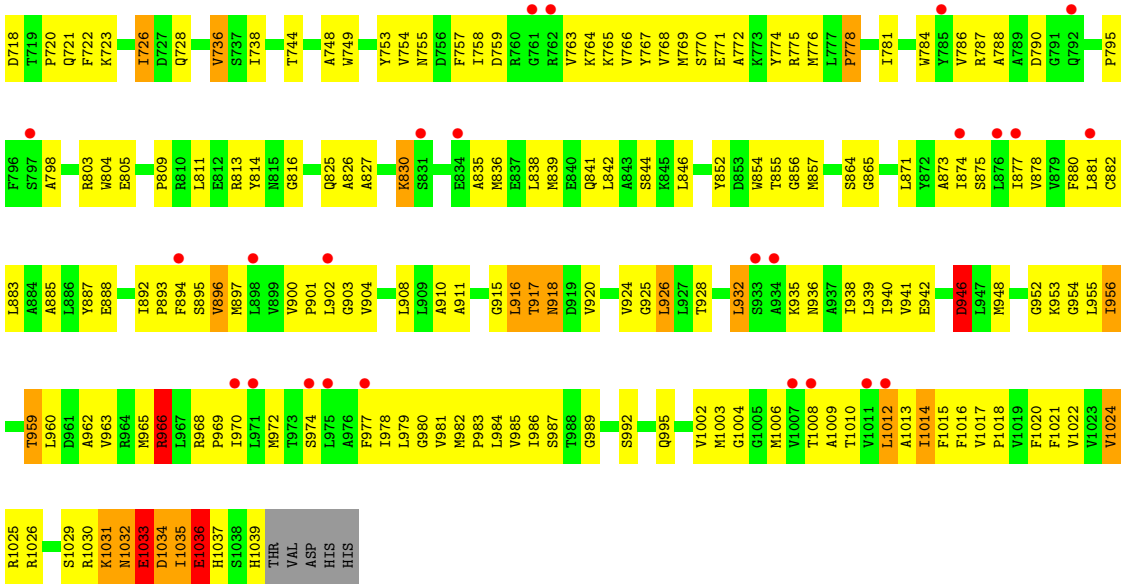
3 Residue-property plots (i)

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

- Molecule 1: Multidrug efflux pump subunit AcrB

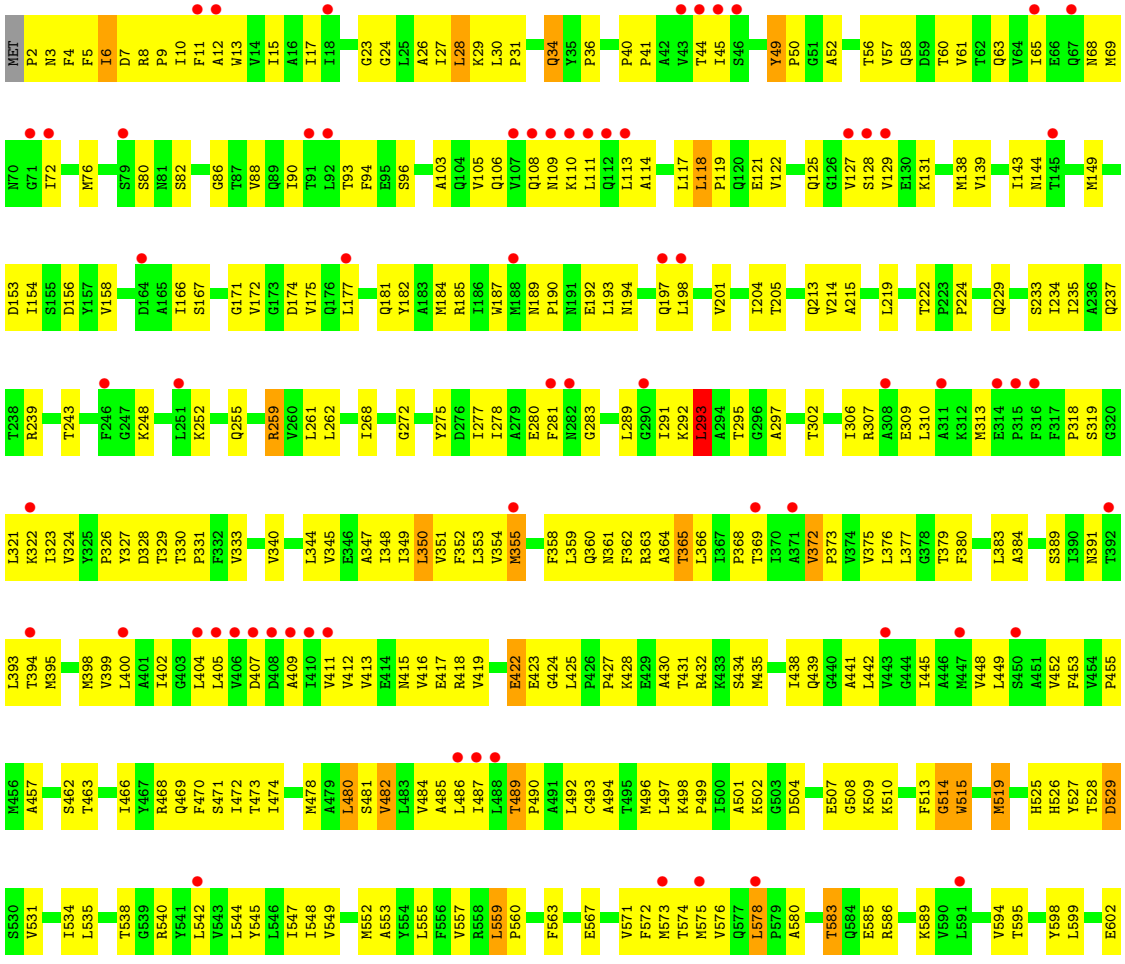
Chain A:

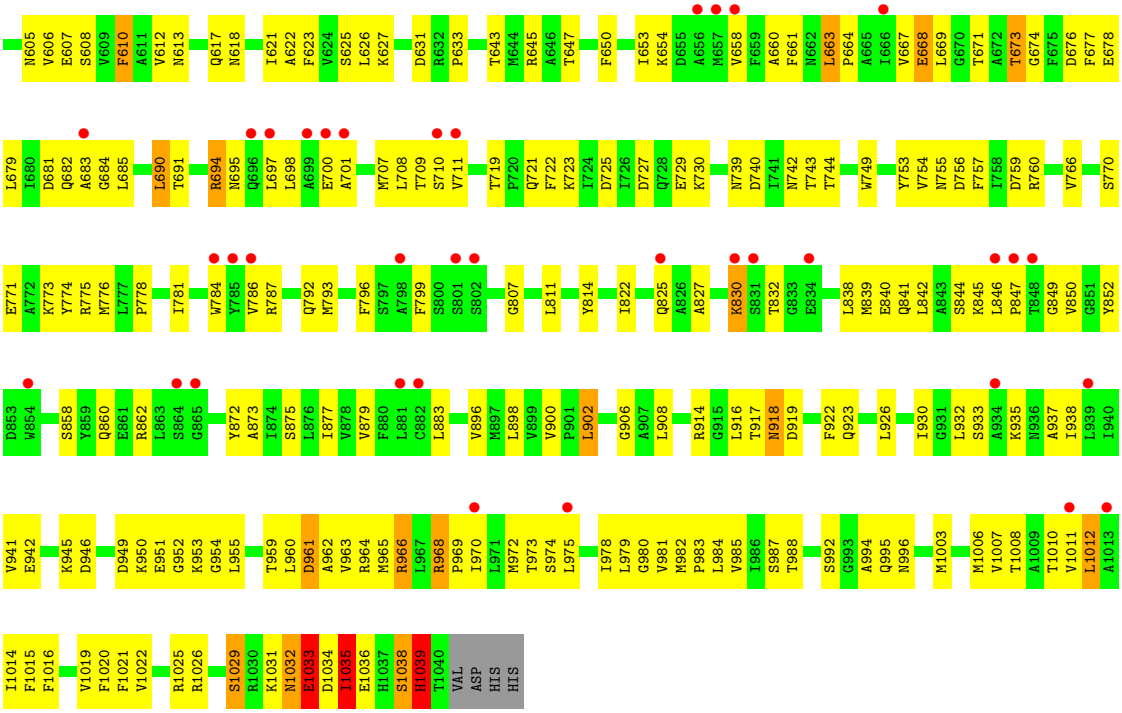




• Molecule 1: Multidrug efflux pump subunit AcrB

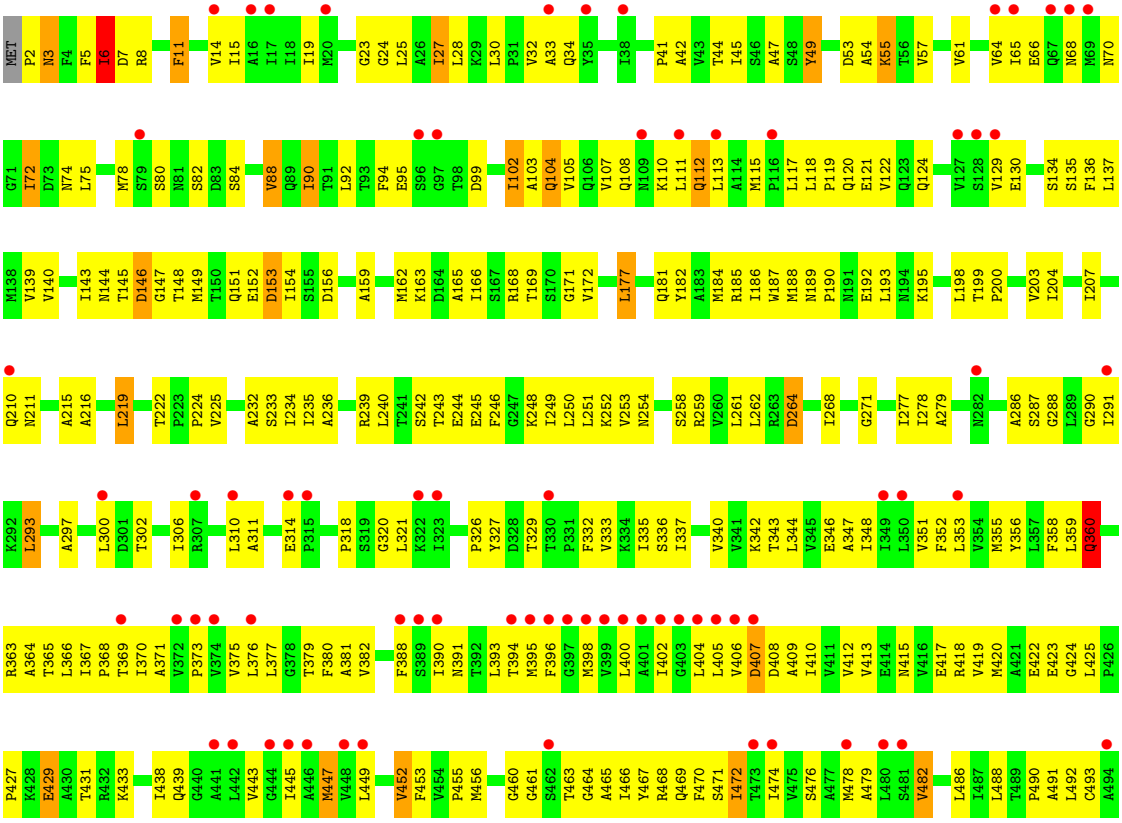
Chain B:

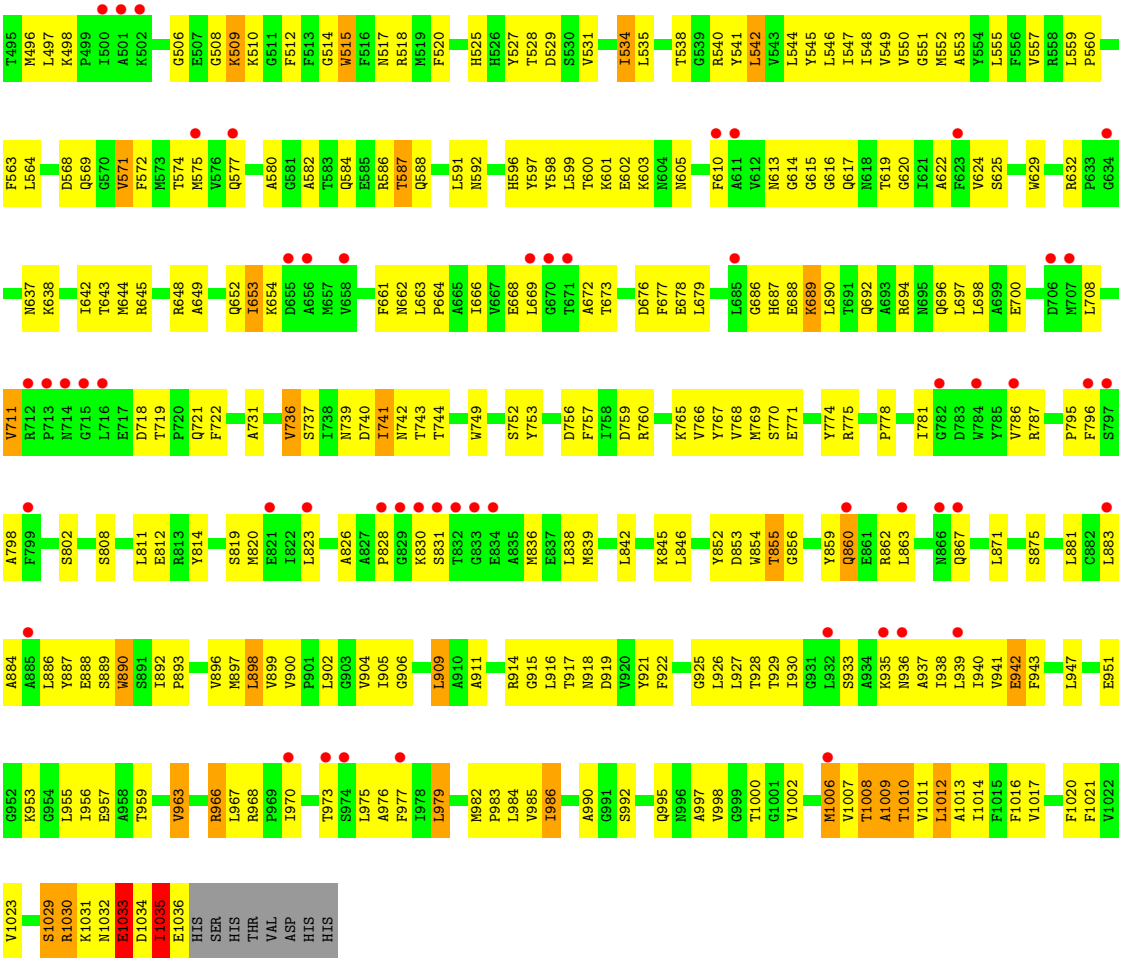




• Molecule 1: Multidrug efflux pump subunit AcrB

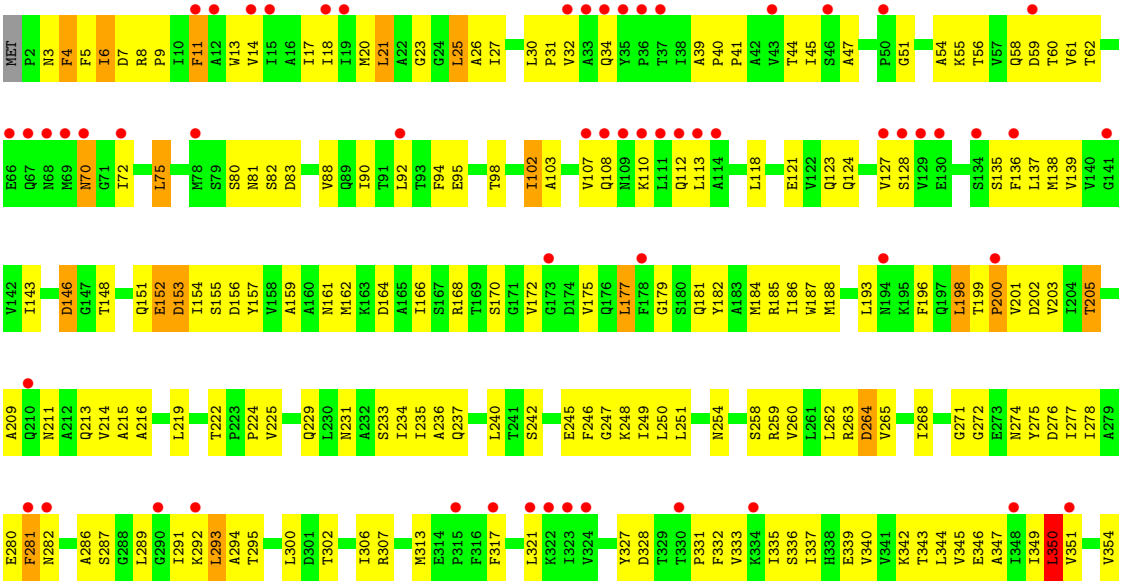
Chain C:

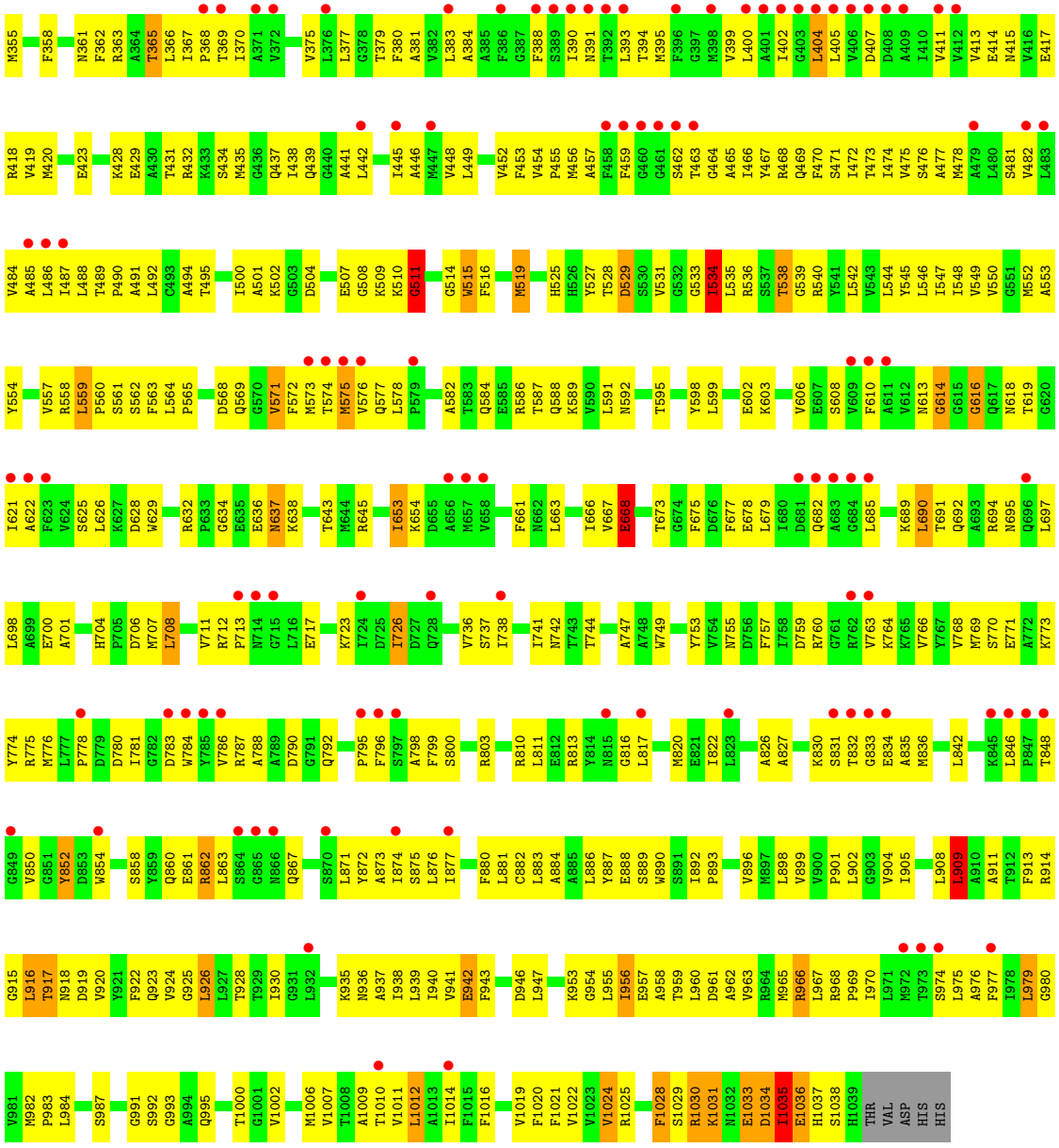




• Molecule 1: Multidrug efflux pump subunit AcrB

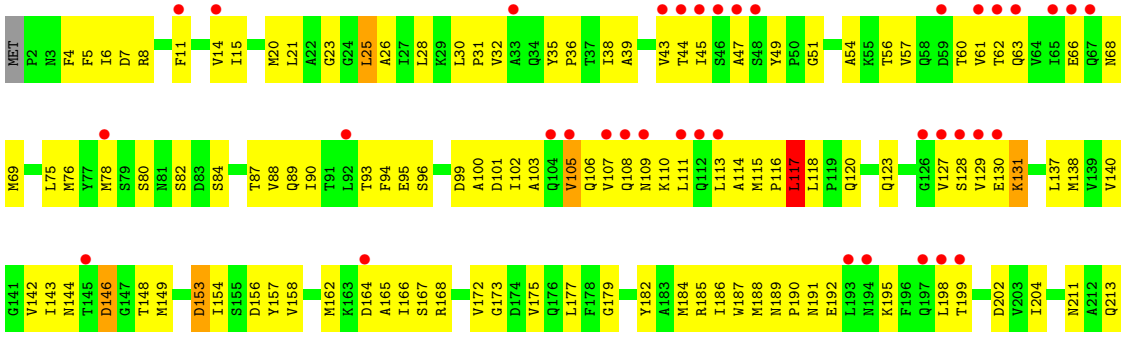
Chain D:

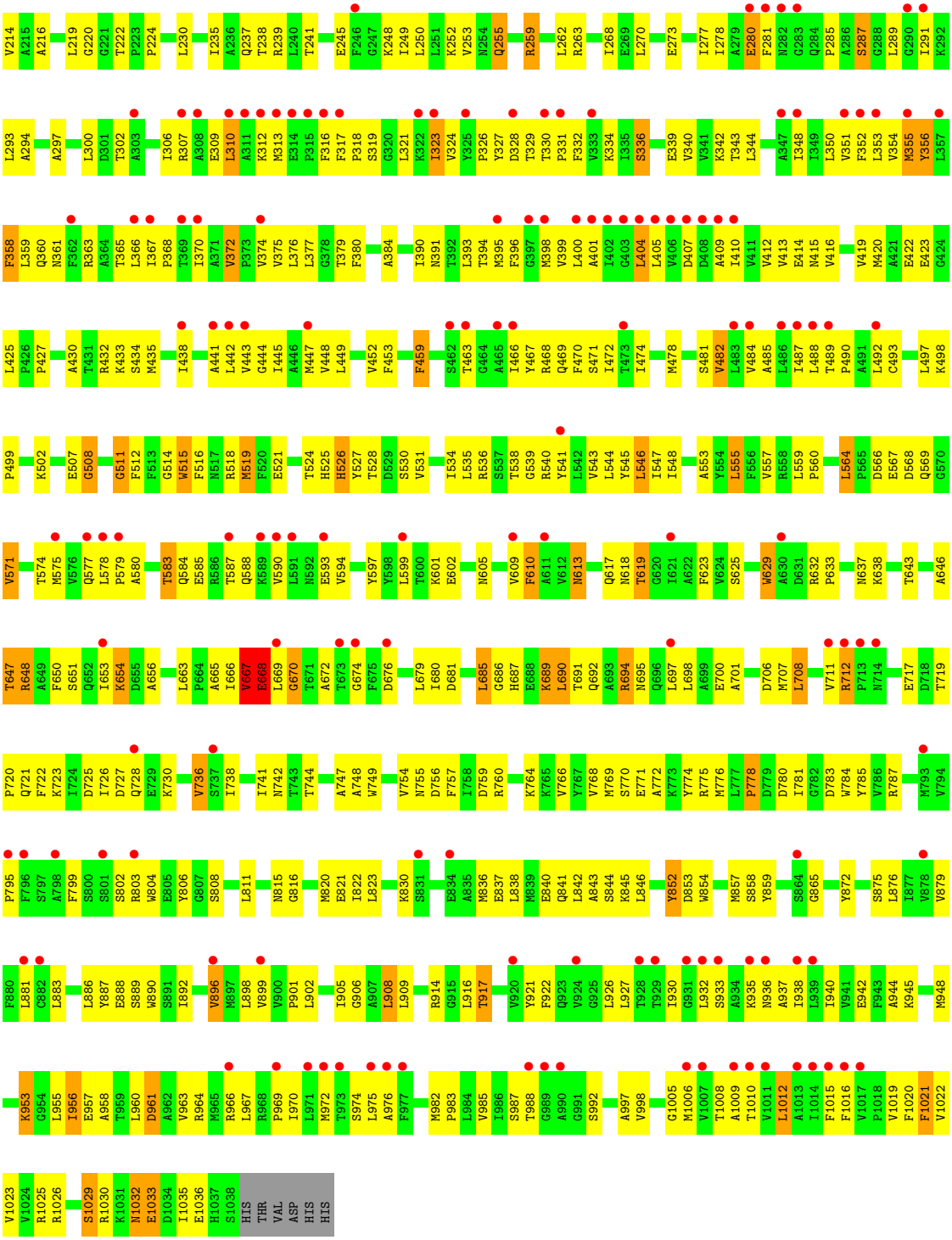




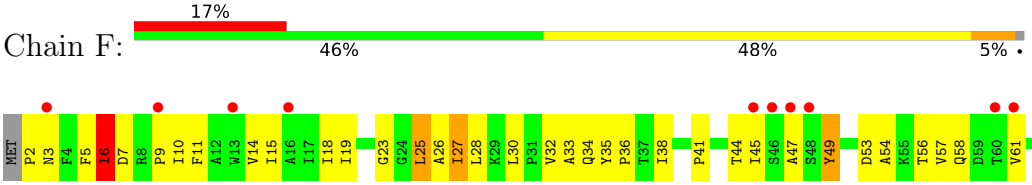
• Molecule 1: Multidrug efflux pump subunit AcrB

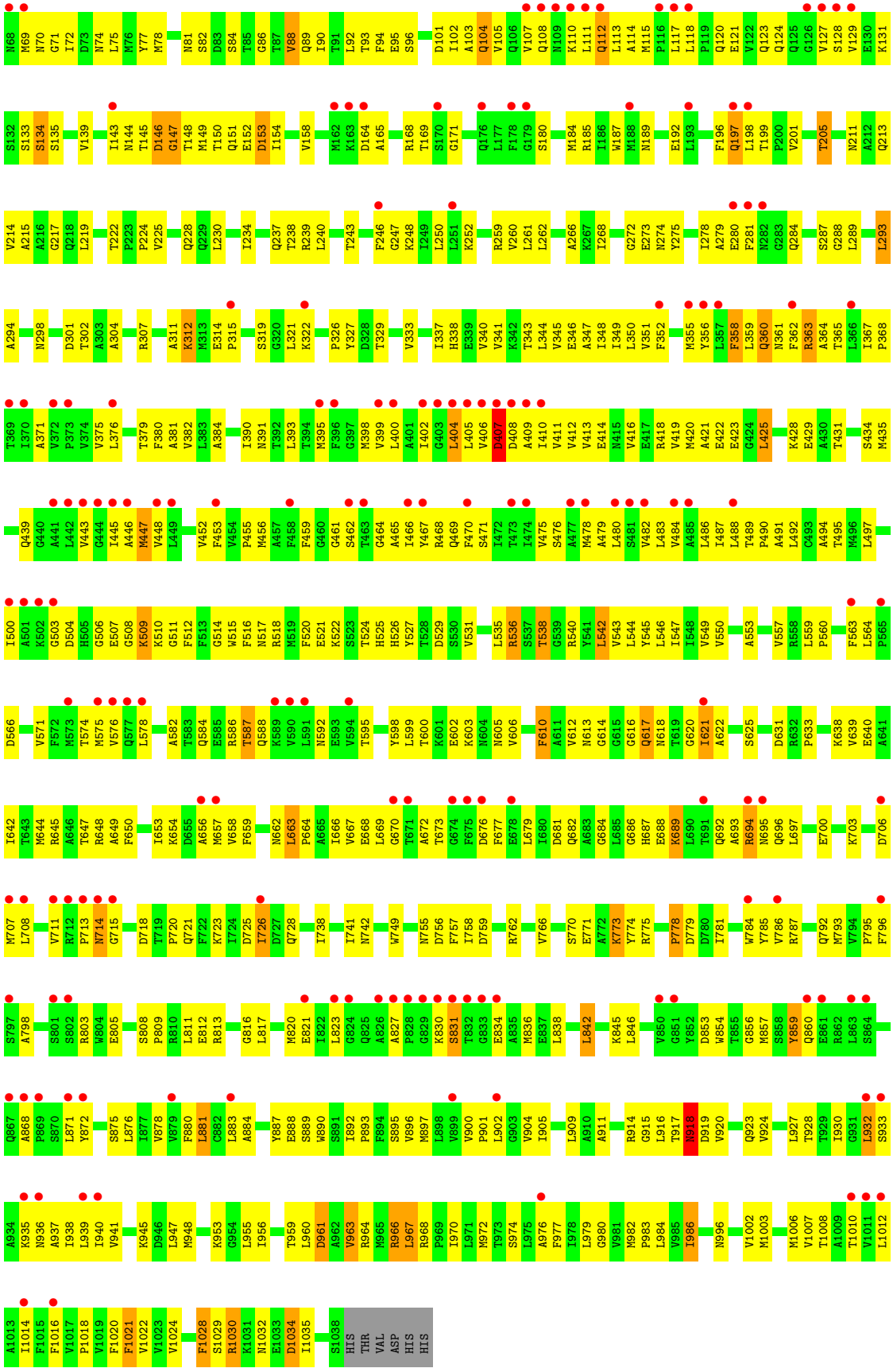
Chain E:





• Molecule 1: Multidrug efflux pump subunit AcrB




N68 M69 N70 G71 I72 D73 N74 L75 M76 Y77 M78 N81 S82 D83 S84 T85 G86 T87 V88 Q89 I90 T91 L92 T93 F94 E95 S96 D101 I102 A103 Q104 V105 Q106 V107 Q108 N109 K110 L111 Q112 L113 A114 M115 P116 L117 L118 P119 Q120 E121 V122 Q123 Q124 Q125 G126 V127 S128 V129 E130 K131
S132 S133 S134 S135 V139 I143 N144 T145 D146 G147 T148 M149 T150 Q151 E152 D153 I154 V158 M162 K163 D164 A165 R168 T169 S170 G171 Q176 L177 F178 G179 S180 M184 R185 I186 W187 M188 N189 E192 L193 F196 Q197 L198 T199 P200 V201 T205 N211 A212 Q213
V214 A215 A216 G217 Q218 L219 T222 P223 P224 V225 Q228 Q229 L230 I234 Q237 T238 R239 L240 T243 F246 G247 K248 I249 L250 L251 K252 R259 V260 L261 L262 A266 K267 I268 G272 E273 N274 Y275 I278 A279 E280 F281 N282 G283 Q284 S287 G288 L289 L293
A294 N298 D301 T302 A303 A304 R307 A311 K312 M313 E314 P315 S319 G320 L321 K322 P326 Y327 D328 T329 V333 I337 H338 E339 V340 V341 K342 T343 L344 V345 E346 A347 I348 I349 L350 V351 F352 M355 Y356 L357 F358 L359 Q360 N361 F362 R363 A364 T365 L366 I367 P368
T369 I370 A371 V372 P373 V374 V375 L376 T379 F380 A381 V382 L383 A384 I390 N391 T392 L393 T394 M395 F396 G397 M398 V399 L400 A401 I402 G403 L404 L405 V406 D407 D408 A409 I410 V411 V412 V413 E414 N415 V416 E417 R418 V419 M420 A421 E422 E423 G424 L425 K428 E429 A430 T431 S434 M435
Q439 G440 A441 L442 V443 G444 I445 A446 M447 V448 L449 V452 F453 V454 P455 M456 A457 F458 F459 G460 G461 S462 T463 G464 A465 I466 Y467 R468 Q469 F470 S471 I472 T473 I474 V475 S476 A477 M478 A479 L480 S481 V482 L483 V484 A485 L486 I487 L488 T489 P490 A491 L492 C493 A494 T495 M496 L497
I500 A501 K502 G503 D504 H505 G506 E507 G508 K509 K510 G511 F512 F513 G514 W515 F516 N517 R518 M519 F520 E521 K522 S523 T524 H525 H526 Y527 T528 D529 S530 V531 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547 I548 V549 V550 A553 V557 R558 L559 P560 F563 L564 P565
D566 V571 F572 M573 T574 M575 V576 Q577 L578 A582 T583 Q584 E585 R586 T587 Q588 K589 V590 L591 N592 E593 V594 T595 Y598 L599 T600 K601 E602 K603 N604 N605 V606 F610 A611 V612 N613 G614 G615 G616 Q617 N618 T619 G620 I621 A622 S625 D631 R632 P633 K638 V639 E640 A641
I642 T643 M644 R645 A646 T647 R648 A649 F650 I653 K654 D655 A656 M657 V658 F659 N662 L663 P664 A665 I666 V667 E668 L669 G670 T671 A672 T673 G674 F675 D676 F677 E678 L679 I680 D681 Q682 A683 G684 L685 G686 H687 E688 K689 L690 T691 Q692 A693 R694 N695 Q696 L697 E700 K703 D706
M707 L708 V711 R712 P713 N714 G715 D718 T719 P720 Q721 F722 K723 I724 D725 I726 D727 Q728 I738 I741 N742 W749 N755 D756 F757 I758 D759 R762 V766 S770 E771 A772 K773 Y774 R775 P778 D779 D780 I781 W784 Y785 V786 R787 Q792 M793 V794 P795 F796
S797 A798 S801 S802 R803 W804 E805 S808 P809 R810 L811 E812 R813 G816 L817 M820 E821 I822 L823 G824 Q825 A826 A827 P828 G829 K830 S831 T832 G833 E834 A835 M836 E837 L838 L842 K845 L846 V850 G851 Y852 D853 W854 T855 G856 M857 S858 Y859 Q860 E861 R862 L863 S864
Q867 A868 P869 S870 L871 Y872 S875 L876 I877 V878 V879 F880 L881 C882 L883 A884 Y887 E888 S889 W890 S891 I892 P893 P894 S895 V896 M897 L898 V899 V900 P901 L902 G903 V904 I905 L909 A910 A911 R914 G915 L916 T917 N918 D919 V920 Q923 V924 L927 T928 T929 I930 G931 L932 S933
A934 K935 N936 A937 I938 L939 I940 V941 K945 D946 L947 M948 K953 G954 L955 I956 T959 L960 D961 A962 V963 R964 M965 R966 L967 R968 P969 I970 L971 M972 T973 S974 L975 A976 F977 I978 L979 G980 V981 M982 P983 L984 V985 I986 N996 V1002 M1003 M1006 V1007 T1008 A1009 T1010 V1011 L1012
A1013 I1014 F1015 F1016 V1017 P1018 V1019 F1020 F1021 V1022 V1023 V1024 F1028 S1029 R1030 K1031 N1032 E1033 D1034 I1035 S1038 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	152.07Å 157.78Å 219.39Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 109.53 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.40) 97.9 (109.53-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.275 , 0.349 0.285 , 0.354	Depositor DCC
R_{free} test set	7110 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	98.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 74.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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 47.48 % 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 9.8623e-05.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, 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	0.65	1/8043 (0.0%)	0.89	11/10922 (0.1%)
1	B	0.65	1/8050 (0.0%)	0.89	9/10932 (0.1%)
1	C	0.67	1/8015 (0.0%)	0.91	9/10884 (0.1%)
1	D	0.60	1/8043 (0.0%)	0.89	15/10922 (0.1%)
1	E	0.60	1/8032 (0.0%)	0.87	12/10907 (0.1%)
1	F	0.60	0/8032	0.89	7/10907 (0.1%)
All	All	0.63	5/48215 (0.0%)	0.89	63/65474 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	7.50	1.63	1.50
1	A	515	TRP	CB-CG	6.68	1.62	1.50
1	E	515	TRP	CB-CG	5.77	1.60	1.50
1	B	515	TRP	CB-CG	5.72	1.60	1.50
1	C	515	TRP	CB-CG	5.07	1.59	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	939	LEU	CA-CB-CG	-8.38	96.02	115.30
1	C	529	ASP	CB-CG-OD1	8.07	125.56	118.30
1	F	529	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	529	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	350	LEU	CA-CB-CG	-7.26	98.61	115.30
1	B	480	LEU	CA-CB-CG	-7.17	98.80	115.30
1	D	979	LEU	CA-CB-CG	-6.85	99.55	115.30
1	E	670	GLY	N-CA-C	6.56	129.51	113.10
1	E	908	LEU	CA-CB-CG	6.55	130.37	115.30
1	B	529	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	250	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	939	LEU	CA-CB-CG	-6.47	100.42	115.30
1	C	967	LEU	CA-CB-CG	6.47	130.18	115.30
1	C	72	ILE	CG1-CB-CG2	-6.41	97.31	111.40
1	D	511	GLY	N-CA-C	6.28	128.79	113.10
1	B	690	LEU	CA-CB-CG	6.24	129.65	115.30
1	D	529	ASP	CB-CG-OD1	6.24	123.91	118.30
1	F	425	LEU	CA-CB-CG	6.20	129.56	115.30
1	D	198	LEU	CA-CB-CG	6.20	129.55	115.30
1	E	519	MET	CB-CG-SD	6.13	130.78	112.40
1	F	967	LEU	CA-CB-CG	6.11	129.36	115.30
1	A	946	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	75	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	293	LEU	CA-CB-CG	6.00	129.09	115.30
1	B	519	MET	CB-CG-SD	5.96	130.28	112.40
1	D	534	ILE	CG1-CB-CG2	-5.96	98.30	111.40
1	A	932	LEU	CA-CB-CG	-5.93	101.67	115.30
1	A	483	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	690	LEU	CA-CB-CG	5.92	128.92	115.30
1	E	117	LEU	CA-CB-CG	5.82	128.69	115.30
1	F	842	LEU	CA-CB-CG	5.80	128.64	115.30
1	D	21	LEU	CA-CB-CG	-5.71	102.17	115.30
1	E	1032	ASN	C-N-CA	5.64	135.79	121.70
1	C	979	LEU	CA-CB-CG	-5.61	102.39	115.30
1	D	967	LEU	CA-CB-CG	5.61	128.19	115.30
1	E	546	LEU	CA-CB-CG	5.59	128.17	115.30
1	D	293	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	118	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	534	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	E	674	GLY	N-CA-C	5.42	126.65	113.10
1	B	555	LEU	CA-CB-CG	-5.40	102.88	115.30
1	C	542	LEU	CA-CB-CG	-5.38	102.92	115.30
1	C	30	LEU	CA-CB-CG	5.38	127.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	287	SER	C-N-CA	-5.33	111.11	122.30
1	A	321	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	449	LEU	CA-CB-CG	-5.32	103.07	115.30
1	F	536	ARG	CG-CD-NE	5.29	122.91	111.80
1	C	1006	MET	CB-CG-SD	5.28	128.24	112.40
1	E	407	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	668	GLU	N-CA-C	5.25	125.17	111.00
1	F	932	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	674	GLY	N-CA-C	5.21	126.13	113.10
1	C	898	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	E	293	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	8	ARG	CB-CG-CD	-5.13	98.27	111.60
1	D	1033	GLU	C-N-CA	5.11	134.47	121.70
1	F	404	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	902	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	28	LEU	CB-CG-CD2	5.03	119.56	111.00
1	D	488	LEU	CA-CB-CG	-5.03	103.74	115.30
1	E	865	GLY	N-CA-C	-5.02	100.54	113.10
1	A	966	ARG	CB-CA-C	5.01	120.42	110.40
1	A	357	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	GLU	Peptide
1	A	1034	ASP	Peptide
1	A	1036	GLU	Peptide
1	B	1033	GLU	Peptide
1	B	1035	ILE	Peptide
1	C	6	ILE	Peptide
1	D	1035	ILE	Peptide
1	F	6	ILE	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	7893	0	8034	457	0
1	B	7900	0	8041	384	0
1	C	7867	0	8015	444	0
1	D	7893	0	8034	515	0
1	E	7883	0	8027	461	0
1	F	7883	0	8027	477	0
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	1	0
2	D	35	0	46	3	0
2	E	35	0	46	8	0
2	F	35	0	46	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47532	0	48454	2651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2651) 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:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.46	0.94
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.50	0.92
1:E:214:VAL:HG11	1:F:742:ASN:HB3	1.51	0.91
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.53	0.91
1:E:239:ARG:NH1	1:E:756:ASP:O	2.04	0.90
1:E:354:VAL:HG22	1:E:975:LEU:HD23	1.51	0.90
1:C:151:GLN:NE2	1:C:286:ALA:O	2.05	0.89
1:C:151:GLN:NE2	1:C:279:ALA:O	2.04	0.89
1:D:571:VAL:HG22	1:D:625:SER:HA	1.54	0.89
1:D:776:MET:HE1	1:F:225:VAL:H	1.37	0.89
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.54	0.89
1:E:355:MET:HG2	1:E:365:THR:HA	1.54	0.88
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.55	0.88
1:A:571:VAL:HG22	1:A:625:SER:HA	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.54	0.88
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.56	0.87
1:E:211:ASN:O	1:E:755:ASN:ND2	2.07	0.87
1:E:680:ILE:HD11	1:E:853:ASP:HB2	1.56	0.87
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.56	0.87
1:C:156:ASP:OD1	1:C:760:ARG:NH2	2.08	0.87
1:B:350:LEU:HD22	1:B:979:LEU:HB3	1.57	0.86
1:C:939:LEU:HB3	1:C:966:ARG:HD2	1.58	0.86
1:D:70:ASN:O	1:D:110:LYS:NZ	2.09	0.86
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.57	0.85
1:C:653:ILE:HG13	1:C:654:LYS:HE2	1.58	0.85
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.59	0.85
1:A:723:LYS:NZ	1:C:236:ALA:O	2.09	0.84
1:F:686:GLY:HA3	1:F:689:LYS:HD3	1.58	0.84
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.57	0.84
1:F:961:ASP:OD1	1:F:964:ARG:NH2	2.11	0.83
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.43	0.83
1:C:264:ASP:OD1	1:C:264:ASP:N	2.12	0.83
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.42	0.83
1:D:457:ALA:O	1:D:468:ARG:NE	2.10	0.83
1:D:156:ASP:OD1	1:D:760:ARG:NH2	2.12	0.83
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.59	0.82
1:D:187:TRP:HB3	1:D:771:GLU:HA	1.59	0.82
1:B:664:PRO:HB3	1:B:669:LEU:HD12	1.61	0.82
1:D:706:ASP:O	1:D:830:LYS:NZ	2.11	0.82
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.12	0.82
1:D:400:LEU:HD23	1:D:924:VAL:HG12	1.61	0.81
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.62	0.81
1:D:953:LYS:NZ	1:D:957:GLU:OE1	2.13	0.80
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.63	0.80
1:A:237:GLN:OE1	1:B:742:ASN:ND2	2.14	0.80
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.63	0.80
1:D:453:PHE:O	1:D:471:SER:OG	1.99	0.80
1:A:691:THR:HG23	1:A:694:ARG:HH12	1.47	0.79
1:D:455:PRO:HG2	1:D:875:SER:HB2	1.62	0.79
1:E:1032:ASN:HB3	1:E:1033:GLU:HB3	1.64	0.79
1:A:966:ARG:HE	1:A:970:ILE:HD11	1.46	0.79
1:E:584:GLN:HB2	1:E:617:GLN:HG2	1.64	0.79
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.64	0.79
1:F:930:ILE:O	1:F:933:SER:OG	2.00	0.79
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:THR:HA	1:D:224:PRO:HD3	1.63	0.79
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.00	0.78
1:C:914:ARG:O	1:C:916:LEU:N	2.16	0.78
1:E:516:PHE:HA	1:E:519:MET:HG3	1.65	0.78
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.65	0.78
1:F:356:TYR:HA	1:F:365:THR:HG21	1.65	0.78
1:A:375:VAL:O	1:A:379:THR:OG1	2.01	0.78
1:A:955:LEU:O	1:A:959:THR:OG1	2.01	0.78
1:A:1034:ASP:HB3	1:A:1035:ILE:HA	1.66	0.78
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.65	0.78
1:F:45:ILE:HG12	1:F:129:VAL:HG13	1.66	0.78
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.15	0.78
1:D:414:GLU:OE1	1:D:968:ARG:NH1	2.17	0.78
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.66	0.78
1:D:211:ASN:O	1:D:755:ASN:ND2	2.18	0.77
1:E:966:ARG:O	1:E:970:ILE:HG12	1.84	0.77
1:C:3:ASN:N	1:C:3:ASN:OD1	2.16	0.77
1:B:327:TYR:HB2	1:B:623:PHE:HE2	1.47	0.77
1:F:82:SER:HB2	1:F:811:LEU:HB2	1.65	0.77
1:D:457:ALA:HA	1:D:468:ARG:HG3	1.67	0.77
1:E:156:ASP:OD1	1:E:760:ARG:NH2	2.18	0.77
1:E:708:LEU:HD21	1:E:838:LEU:HD12	1.67	0.77
1:B:602:GLU:HG3	1:B:605:ASN:HB2	1.66	0.77
1:D:632:ARG:HH12	1:D:638:LYS:HA	1.50	0.77
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.66	0.76
1:F:662:ASN:O	1:F:673:THR:OG1	2.03	0.76
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.66	0.76
1:C:427:PRO:O	1:C:431:THR:OG1	2.03	0.76
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.67	0.76
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.17	0.76
1:C:940:ILE:HG12	1:C:966:ARG:CZ	2.15	0.76
1:D:1036:GLU:HB3	1:D:1037:HIS:HB2	1.68	0.76
1:E:144:ASN:ND2	1:E:319:SER:O	2.15	0.76
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.51	0.76
1:A:214:VAL:HG11	1:B:742:ASN:HB3	1.68	0.76
1:A:34:GLN:HE21	1:A:332:PHE:HE2	1.34	0.76
1:A:491:ALA:O	1:A:495:THR:OG1	2.04	0.76
1:A:605:ASN:HD21	1:A:637:ASN:HA	1.51	0.75
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.68	0.75
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.65	0.75
1:E:241:THR:N	1:E:245:GLU:OE1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:LEU:H	1:A:1033:GLU:HA	1.52	0.75
1:C:460:GLY:O	1:C:867:GLN:NE2	2.20	0.75
1:C:632:ARG:NH1	1:C:637:ASN:O	2.19	0.75
1:E:115:MET:O	1:E:123:GLN:NE2	2.18	0.75
1:A:687:HIS:NE2	1:A:718:ASP:OD1	2.19	0.75
1:A:776:MET:HE1	1:C:225:VAL:H	1.50	0.75
1:A:639:VAL:HG11	1:A:662:ASN:HB2	1.67	0.75
1:D:11:PHE:N	1:E:888:GLU:OE1	2.17	0.75
1:C:418:ARG:O	1:C:422:GLU:HB2	1.87	0.75
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.67	0.75
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.68	0.74
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.67	0.74
1:C:708:LEU:HD23	1:C:711:VAL:HG21	1.69	0.74
1:D:770:SER:HB3	1:D:775:ARG:HD3	1.68	0.74
1:D:588:GLN:NE2	1:D:592:ASN:OD1	2.18	0.74
1:B:930:ILE:O	1:B:933:SER:OG	2.05	0.74
1:D:966:ARG:HE	1:D:970:ILE:HD11	1.50	0.74
1:F:715:GLY:HA3	1:F:812:GLU:OE1	1.88	0.74
1:A:955:LEU:HD21	1:A:1022:VAL:HG13	1.68	0.74
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.68	0.74
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.70	0.74
1:E:39:ALA:HB2	1:E:668:GLU:HG3	1.70	0.74
1:F:936:ASN:HD21	1:F:1010:THR:HG22	1.52	0.74
1:A:175:VAL:HG11	1:A:289:LEU:HD13	1.68	0.74
1:A:531:VAL:O	1:A:534:ILE:HG13	1.87	0.74
1:F:165:ALA:O	1:F:169:THR:OG1	2.03	0.74
1:A:707:MET:HG3	1:A:708:LEU:HD13	1.70	0.73
1:D:448:VAL:HG22	1:D:882:CYS:HB3	1.69	0.73
1:C:418:ARG:NH1	1:C:422:GLU:OE1	2.20	0.73
1:C:420:MET:O	1:C:424:GLY:N	2.20	0.73
1:F:887:TYR:O	1:F:889:SER:N	2.17	0.73
1:A:101:ASP:OD1	1:A:101:ASP:N	2.20	0.73
1:A:414:GLU:HG3	1:A:972:MET:HE1	1.70	0.73
1:A:989:GLY:O	1:A:992:SER:OG	2.06	0.73
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.71	0.73
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.53	0.73
1:A:186:ILE:HB	1:A:768:VAL:HG22	1.68	0.73
1:D:587:THR:HB	1:D:613:ASN:ND2	2.02	0.73
1:E:945:LYS:HA	1:E:948:MET:HE3	1.70	0.73
1:D:587:THR:HB	1:D:613:ASN:HD21	1.53	0.73
1:E:759:ASP:OD2	1:E:764:LYS:NZ	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ARG:HB3	1:A:966:ARG:HH11	1.53	0.73
1:A:584:GLN:HB2	1:A:617:GLN:HG2	1.71	0.73
1:B:166:ILE:HD11	1:B:310:LEU:HD11	1.69	0.73
1:D:56:THR:OG1	1:F:213:GLN:NE2	2.22	0.72
1:E:445:ILE:HG22	1:E:938:ILE:HD13	1.69	0.72
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.53	0.72
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.70	0.72
1:E:184:MET:HB3	1:E:766:VAL:HG13	1.71	0.72
1:F:65:ILE:HG21	1:F:90:ILE:HD13	1.70	0.72
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.25	0.72
1:C:453:PHE:HD2	1:C:456:MET:HE1	1.55	0.72
1:D:351:VAL:HG22	1:D:976:ALA:HB1	1.71	0.72
1:E:448:VAL:HG13	1:E:879:VAL:HG13	1.72	0.72
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.72	0.72
1:C:853:ASP:OD2	1:C:862:ARG:NH2	2.23	0.72
1:B:896:VAL:HG21	1:B:938:ILE:HG13	1.68	0.72
1:D:225:VAL:HG22	1:E:776:MET:HE2	1.72	0.72
1:E:375:VAL:O	1:E:379:THR:OG1	2.07	0.72
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.71	0.72
1:C:580:ALA:HB1	1:C:719:THR:HG22	1.69	0.71
1:A:5:PHE:O	1:A:8:ARG:N	2.15	0.71
1:D:137:LEU:HD23	1:D:291:ILE:HG22	1.69	0.71
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.71	0.71
1:D:602:GLU:OE2	1:D:645:ARG:NH1	2.23	0.71
1:B:540:ARG:HH22	2:B:2000:LMT:H6'1	1.54	0.71
1:E:351:VAL:HG22	1:E:976:ALA:HB1	1.72	0.71
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.72	0.71
1:A:225:VAL:H	1:B:776:MET:HE1	1.54	0.71
1:D:575:MET:HG2	1:D:661:PHE:HE1	1.54	0.71
1:B:350:LEU:HD13	1:B:980:GLY:HA2	1.70	0.71
1:B:985:VAL:O	1:B:996:ASN:ND2	2.23	0.71
1:F:955:LEU:HD21	1:F:1022:VAL:HA	1.73	0.71
1:C:896:VAL:HG23	1:C:937:ALA:HB3	1.71	0.71
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.72	0.71
1:B:375:VAL:O	1:B:379:THR:OG1	2.03	0.71
1:D:574:THR:HG23	1:D:622:ALA:HB3	1.71	0.71
1:B:309:GLU:HG3	1:B:313:MET:HE3	1.72	0.71
1:C:2:PRO:O	1:C:6:ILE:HG12	1.90	0.71
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.72	0.70
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.71	0.70
1:A:723:LYS:HG2	1:A:803:ARG:NH1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HG13	1:B:879:VAL:HG13	1.72	0.70
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.73	0.70
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.72	0.70
1:D:880:PHE:CE1	1:D:893:PRO:HB2	2.26	0.70
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.73	0.70
1:F:45:ILE:HD11	1:F:107:VAL:HG12	1.72	0.70
1:C:940:ILE:HG12	1:C:966:ARG:NH2	2.06	0.70
1:F:544:LEU:HA	1:F:547:ILE:HD12	1.74	0.70
1:F:892:ILE:HG23	1:F:941:VAL:HG11	1.72	0.70
1:A:962:ALA:O	1:A:966:ARG:NH1	2.25	0.70
1:B:974:SER:OG	1:B:1010:THR:HG21	1.92	0.70
1:F:574:THR:HG23	1:F:622:ALA:HB3	1.73	0.70
1:D:941:VAL:HG13	1:D:1021:PHE:CE1	2.26	0.69
1:E:82:SER:HB2	1:E:811:LEU:HB2	1.73	0.69
1:A:424:GLY:O	1:A:502:LYS:NZ	2.25	0.69
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.25	0.69
1:A:653:ILE:HG13	1:A:654:LYS:HE2	1.75	0.69
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.73	0.69
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.73	0.69
1:D:6:ILE:HG22	1:D:490:PRO:HB2	1.75	0.69
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.74	0.69
1:F:714:ASN:HB3	1:F:821:GLU:HB3	1.73	0.69
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.75	0.69
1:A:1034:ASP:CB	1:A:1035:ILE:HA	2.22	0.69
1:B:239:ARG:NH1	1:B:756:ASP:HB2	2.08	0.69
1:F:531:VAL:O	1:F:535:LEU:HG	1.92	0.69
1:B:144:ASN:ND2	1:B:319:SER:O	2.23	0.69
1:B:184:MET:HB2	1:B:757:PHE:CE2	2.28	0.69
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.75	0.69
1:B:422:GLU:OE2	1:B:964:ARG:NH1	2.26	0.68
1:C:326:PRO:O	1:C:625:SER:OG	2.11	0.68
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.26	0.68
1:D:209:ALA:O	1:D:237:GLN:NE2	2.23	0.68
1:D:899:VAL:O	1:D:902:LEU:HB2	1.93	0.68
1:E:185:ARG:NH2	1:E:273:GLU:O	2.24	0.68
1:C:456:MET:HE3	1:C:467:TYR:O	1.92	0.68
1:D:254:ASN:ND2	1:D:258:SER:OG	2.20	0.68
1:B:259:ARG:H	1:B:259:ARG:HD3	1.57	0.68
1:C:45:ILE:HB	1:C:90:ILE:HD12	1.75	0.68
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.26	0.68
1:E:192:GLU:HA	1:E:195:LYS:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:O	1:E:502:LYS:NZ	2.22	0.68
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.75	0.68
1:B:383:LEU:HD11	1:B:473:THR:HA	1.74	0.68
1:D:914:ARG:O	1:D:916:LEU:N	2.27	0.68
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.75	0.68
1:F:741:ILE:HG22	1:F:786:VAL:HG21	1.75	0.68
1:B:602:GLU:OE2	1:B:645:ARG:NH1	2.26	0.68
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.75	0.68
1:A:636:GLU:HB2	1:A:645:ARG:HH22	1.59	0.68
1:D:700:GLU:HB3	1:D:842:LEU:HD22	1.74	0.68
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.57	0.68
1:B:559:LEU:HD12	1:B:918:ASN:HB2	1.76	0.68
1:E:908:LEU:HD23	1:E:922:PHE:HZ	1.59	0.68
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.76	0.67
1:A:892:ILE:HG12	1:A:1025:ARG:HD3	1.75	0.67
1:C:3:ASN:ND2	1:C:486:LEU:O	2.28	0.67
1:D:250:LEU:HD13	1:D:259:ARG:HB3	1.75	0.67
1:D:707:MET:HG3	1:D:708:LEU:HD13	1.77	0.67
1:E:184:MET:HB2	1:E:757:PHE:CE2	2.29	0.67
1:C:5:PHE:O	1:C:7:ASP:N	2.27	0.67
1:B:219:LEU:HG	1:B:234:ILE:HD11	1.74	0.67
1:C:453:PHE:HD2	1:C:456:MET:CE	2.07	0.67
1:C:112:GLN:HG3	1:C:115:MET:HG3	1.77	0.67
1:C:696:GLN:HE21	1:C:845:LYS:HE3	1.59	0.67
1:D:884:ALA:HA	1:D:889:SER:O	1.94	0.67
1:F:239:ARG:HB2	1:F:758:ILE:HD12	1.75	0.67
1:A:697:LEU:HD12	1:A:846:LEU:HD21	1.75	0.67
1:C:942:GLU:HG3	1:C:943:PHE:N	2.09	0.67
1:D:47:ALA:HB2	1:D:127:VAL:HG13	1.76	0.67
1:E:536:ARG:HE	2:E:1101:LMT:H3O1	1.39	0.67
1:E:906:GLY:HA3	1:E:1008:THR:HG21	1.76	0.67
1:A:129:VAL:HG23	1:B:113:LEU:HD11	1.77	0.67
1:A:1026:ARG:NH1	1:A:1033:GLU:OE1	2.27	0.67
1:D:375:VAL:O	1:D:379:THR:OG1	2.11	0.67
1:F:211:ASN:O	1:F:755:ASN:ND2	2.28	0.67
1:B:156:ASP:OD1	1:B:760:ARG:NH2	2.27	0.67
1:D:954:GLY:HA2	1:D:1034:ASP:N	2.05	0.67
1:E:1021:PHE:HE2	1:E:1025:ARG:HD3	1.58	0.67
1:B:770:SER:HB3	1:B:775:ARG:HD3	1.77	0.67
1:D:400:LEU:HD21	1:D:925:GLY:HA2	1.77	0.67
1:F:418:ARG:O	1:F:422:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:VAL:O	1:F:447:MET:HB3	1.95	0.67
1:B:982:MET:HB3	1:B:983:PRO:HD3	1.77	0.66
1:C:855:THR:HA	1:C:859:TYR:HB2	1.77	0.66
1:D:452:VAL:HA	1:D:875:SER:OG	1.95	0.66
1:D:545:TYR:HD1	1:D:546:LEU:HD23	1.60	0.66
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.77	0.66
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.31	0.66
1:A:645:ARG:O	1:A:648:ARG:HB3	1.95	0.66
1:B:24:GLY:O	1:B:27:ILE:HG22	1.95	0.66
1:B:966:ARG:O	1:B:970:ILE:HG12	1.96	0.66
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.76	0.66
1:D:343:THR:O	1:D:346:GLU:N	2.28	0.66
1:D:367:ILE:HG12	1:D:492:LEU:HB3	1.78	0.66
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.30	0.66
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.76	0.66
1:C:688:GLU:HB3	1:C:689:LYS:HD2	1.77	0.66
1:D:442:LEU:O	1:D:445:ILE:HG13	1.95	0.66
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.76	0.66
1:E:120:GLN:NE2	1:E:123:GLN:OE1	2.29	0.66
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.77	0.66
1:F:707:MET:O	1:F:827:ALA:N	2.26	0.66
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.76	0.66
1:D:400:LEU:HD11	1:D:1002:VAL:HG21	1.77	0.66
1:D:697:LEU:HD12	1:D:846:LEU:HD11	1.77	0.66
1:E:204:ILE:HG12	1:E:754:VAL:HG21	1.77	0.66
1:B:683:ALA:O	1:B:685:LEU:N	2.28	0.66
1:E:441:ALA:O	1:E:445:ILE:HG23	1.96	0.66
1:E:444:GLY:HA3	1:E:886:LEU:HD22	1.78	0.66
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.78	0.66
1:F:755:ASN:O	1:F:766:VAL:HB	1.94	0.66
1:B:453:PHE:O	1:B:471:SER:OG	2.11	0.66
1:A:960:LEU:O	1:A:963:VAL:HG12	1.95	0.66
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.78	0.66
1:E:774:TYR:O	1:E:784:TRP:NE1	2.25	0.65
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.78	0.65
1:F:902:LEU:HG	1:F:1012:LEU:HB3	1.78	0.65
1:F:939:LEU:HB3	1:F:966:ARG:HD2	1.78	0.65
1:A:626:LEU:HD11	1:A:639:VAL:HG23	1.76	0.65
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.78	0.65
1:F:880:PHE:HD2	1:F:881:LEU:HD22	1.62	0.65
1:F:1016:PHE:HB3	1:F:1020:PHE:CE1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.77	0.65
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.78	0.65
1:D:509:LYS:HG2	1:D:510:LYS:HG3	1.77	0.65
1:E:101:ASP:OD1	1:E:131:LYS:NZ	2.20	0.65
1:F:213:GLN:HA	1:F:237:GLN:O	1.97	0.65
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.79	0.65
1:C:584:GLN:HB2	1:C:617:GLN:HG2	1.79	0.65
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.77	0.65
1:B:567:GLU:OE2	1:B:994:ALA:N	2.29	0.65
1:C:146:ASP:O	1:C:148:THR:N	2.29	0.65
1:F:198:LEU:HD21	1:F:252:LYS:HB2	1.77	0.65
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.28	0.65
1:A:940:ILE:HG12	1:A:966:ARG:CZ	2.26	0.65
1:C:82:SER:HB2	1:C:811:LEU:HB2	1.79	0.65
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.79	0.65
1:F:527:TYR:CE1	1:F:1014:ILE:HD12	2.32	0.65
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.78	0.65
1:D:1028:PHE:O	1:D:1030:ARG:N	2.29	0.65
1:E:156:ASP:OD2	1:E:764:LYS:NZ	2.26	0.65
1:F:197:GLN:HA	1:F:793:MET:SD	2.36	0.65
1:F:612:VAL:HB	1:F:621:ILE:HG22	1.78	0.65
1:B:573:MET:HG3	1:B:661:PHE:CE2	2.32	0.65
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.31	0.65
1:E:5:PHE:HA	1:E:8:ARG:HB2	1.78	0.65
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.79	0.65
1:F:966:ARG:HH21	1:F:970:ILE:HD11	1.60	0.65
1:A:527:TYR:OH	1:A:1014:ILE:O	2.06	0.65
1:D:694:ARG:NH2	1:D:717:GLU:OE1	2.29	0.65
1:A:143:ILE:O	1:A:321:LEU:HD22	1.96	0.64
1:A:883:LEU:HD22	1:A:887:TYR:CE2	2.32	0.64
1:B:350:LEU:CD2	1:B:979:LEU:HB3	2.27	0.64
1:E:326:PRO:O	1:E:625:SER:OG	2.15	0.64
1:A:538:THR:HG22	1:A:542:LEU:HD22	1.79	0.64
1:A:1037:HIS:HB3	1:A:1039:HIS:H	1.62	0.64
1:B:61:VAL:HG13	1:B:118:LEU:HD22	1.79	0.64
1:A:182:TYR:O	1:A:764:LYS:HD3	1.98	0.64
1:F:664:PRO:HG3	1:F:670:GLY:HA3	1.78	0.64
1:A:184:MET:HB2	1:A:757:PHE:CE2	2.32	0.64
1:B:197:GLN:HA	1:B:793:MET:SD	2.37	0.64
1:F:420:MET:HB3	1:F:500:ILE:HB	1.80	0.64
1:A:368:PRO:HB3	1:A:409:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ALA:O	1:E:723:LYS:NZ	2.30	0.64
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.80	0.64
1:B:139:VAL:O	1:B:326:PRO:HD2	1.98	0.64
1:C:32:VAL:HG22	1:C:390:ILE:HB	1.80	0.64
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.80	0.64
1:E:213:GLN:HA	1:E:237:GLN:O	1.97	0.64
1:E:687:HIS:NE2	1:E:808:SER:HB2	2.13	0.64
1:F:582:ALA:HB2	1:F:586:ARG:HH21	1.63	0.64
1:C:388:PHE:CZ	1:C:472:ILE:HG21	2.33	0.64
1:D:200:PRO:HA	1:D:203:VAL:HG23	1.79	0.64
1:E:610:PHE:N	1:E:623:PHE:O	2.26	0.64
1:A:643:THR:HB	1:A:660:ALA:O	1.98	0.64
1:A:827:ALA:HB3	1:A:830:LYS:HB2	1.78	0.64
1:E:605:ASN:OD1	1:E:637:ASN:ND2	2.31	0.64
1:F:164:ASP:HB3	1:F:168:ARG:NH2	2.13	0.64
1:B:572:PHE:HA	1:B:663:LEU:HD21	1.80	0.64
1:F:527:TYR:CE2	1:F:963:VAL:HG13	2.33	0.64
1:F:895:SER:HB3	1:F:1024:VAL:HG11	1.80	0.64
1:A:564:LEU:HB2	1:A:666:ILE:HD11	1.78	0.63
1:A:966:ARG:O	1:A:970:ILE:HG12	1.98	0.63
1:B:222:THR:HA	1:B:224:PRO:HD3	1.81	0.63
1:D:45:ILE:HA	1:D:128:SER:O	1.97	0.63
1:E:579:PRO:HD3	1:E:656:ALA:HB2	1.78	0.63
1:F:75:LEU:HD21	1:F:78:MET:HB2	1.81	0.63
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.33	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:E:94:PHE:CE1	1:E:103:ALA:HB1	2.34	0.63
1:F:914:ARG:O	1:F:916:LEU:N	2.28	0.63
1:F:932:LEU:HD22	1:F:1006:MET:HE1	1.80	0.63
1:B:201:VAL:O	1:B:205:THR:OG1	2.11	0.63
1:F:144:ASN:O	1:F:148:THR:OG1	2.11	0.63
1:F:151:GLN:NE2	1:F:279:ALA:O	2.31	0.63
1:F:653:ILE:HD12	1:F:654:LYS:HE2	1.79	0.63
1:B:190:PRO:HG3	1:B:774:TYR:HB3	1.78	0.63
1:B:455:PRO:HG2	1:B:875:SER:OG	1.97	0.63
1:B:527:TYR:OH	1:B:1014:ILE:O	2.11	0.63
1:E:445:ILE:HG21	1:E:935:LYS:HD2	1.80	0.63
1:F:344:LEU:O	1:F:348:ILE:HG13	1.98	0.63
1:F:689:LYS:H	1:F:689:LYS:HD2	1.62	0.63
1:E:778:PRO:O	1:E:781:ILE:HG12	1.98	0.63
1:F:45:ILE:HB	1:F:90:ILE:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:SER:HB3	1:F:668:GLU:HB3	1.80	0.63
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.80	0.63
1:D:632:ARG:NH1	1:D:637:ASN:O	2.32	0.63
1:D:677:PHE:HD2	1:D:822:ILE:HD12	1.61	0.63
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.80	0.63
1:E:840:GLU:HG2	1:E:852:TYR:CE1	2.33	0.63
1:F:890:TRP:CE3	1:F:890:TRP:HA	2.33	0.63
1:C:464:GLY:O	1:C:468:ARG:HB2	1.98	0.63
1:D:198:LEU:HD11	1:D:251:LEU:O	1.98	0.63
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.79	0.63
1:D:536:ARG:NH1	2:D:2000:LMT:O3B	2.32	0.63
1:F:54:ALA:HB2	1:F:809:PRO:O	1.99	0.63
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.80	0.63
1:A:241:THR:N	1:A:245:GLU:OE2	2.29	0.63
1:A:883:LEU:HD22	1:A:887:TYR:HE2	1.63	0.63
1:E:14:VAL:HG22	1:F:881:LEU:HD12	1.79	0.63
1:F:44:THR:HA	1:F:90:ILE:O	1.99	0.63
1:F:66:GLU:OE1	1:F:816:GLY:HA2	1.99	0.63
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.80	0.62
1:E:953:LYS:HB3	1:E:958:ALA:HB2	1.81	0.62
1:F:663:LEU:HD23	1:F:663:LEU:H	1.64	0.62
1:B:978:ILE:HG23	1:B:1003:MET:HG3	1.81	0.62
1:D:361:ASN:O	1:D:365:THR:HG22	1.99	0.62
1:E:100:ALA:HB1	1:E:131:LYS:HE3	1.81	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:201:VAL:O	1:F:205:THR:OG1	2.14	0.62
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.79	0.62
1:D:216:ALA:N	1:E:51:GLY:O	2.30	0.62
1:D:871:LEU:HD23	1:D:874:ILE:HD12	1.80	0.62
1:C:577:GLN:HG3	1:C:619:THR:HG22	1.82	0.62
1:E:525:HIS:HA	1:E:528:THR:HG22	1.81	0.62
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.81	0.62
1:C:757:PHE:CE1	1:C:759:ASP:HB2	2.35	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.30	0.62
1:F:211:ASN:ND2	1:F:246:PHE:HZ	1.97	0.62
1:A:462:SER:O	1:A:466:ILE:HG12	1.99	0.62
1:B:24:GLY:O	1:B:28:LEU:HD23	1.99	0.62
1:C:396:PHE:O	1:C:400:LEU:HB2	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	2.00	0.62
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.82	0.62
1:A:966:ARG:HB3	1:A:966:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:LEU:O	1:B:845:LYS:HB2	2.00	0.62
1:C:453:PHE:HB3	1:C:471:SER:HA	1.82	0.62
1:C:947:LEU:HD23	1:C:951:GLU:HG3	1.81	0.62
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.81	0.62
1:B:355:MET:HG3	1:B:359:LEU:HD12	1.81	0.62
1:C:545:TYR:CE2	1:C:1020:PHE:HZ	2.17	0.62
1:C:553:ALA:O	1:C:557:VAL:HG23	2.00	0.62
1:D:219:LEU:HG	1:D:234:ILE:HD11	1.81	0.62
1:E:679:LEU:HD22	1:E:822:ILE:HD11	1.81	0.62
1:F:645:ARG:O	1:F:648:ARG:HB3	2.00	0.62
1:A:326:PRO:O	1:A:625:SER:OG	2.17	0.61
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.82	0.61
1:B:435:MET:SD	1:B:490:PRO:HB3	2.40	0.61
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.35	0.61
1:E:908:LEU:HD23	1:E:922:PHE:CZ	2.34	0.61
1:E:691:THR:HG23	1:E:694:ARG:HH12	1.65	0.61
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.82	0.61
1:A:901:PRO:O	1:A:904:VAL:N	2.33	0.61
1:F:522:LYS:O	1:F:525:HIS:N	2.32	0.61
1:B:941:VAL:HG13	1:B:1021:PHE:HE1	1.64	0.61
1:A:974:SER:OG	1:A:1010:THR:HG21	2.01	0.61
1:B:204:ILE:HG12	1:B:754:VAL:HG21	1.83	0.61
1:D:219:LEU:HD23	1:E:749:TRP:CZ3	2.36	0.61
1:F:902:LEU:HD21	1:F:1016:PHE:HB2	1.82	0.61
1:A:75:LEU:HD13	1:A:92:LEU:HD23	1.81	0.61
1:D:445:ILE:HG21	1:D:935:LYS:HD2	1.81	0.61
1:B:80:SER:HB3	1:B:90:ILE:HG23	1.82	0.61
1:B:1006:MET:O	1:B:1010:THR:HG23	2.00	0.61
1:C:453:PHE:CD2	1:C:456:MET:HE1	2.34	0.61
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.30	0.61
1:E:280:GLU:HG3	1:E:285:PRO:HA	1.81	0.61
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.83	0.61
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.83	0.61
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.83	0.61
1:C:200:PRO:HB2	1:C:744:THR:HG22	1.83	0.61
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.83	0.61
1:E:531:VAL:O	1:E:534:ILE:HG13	2.01	0.61
1:C:254:ASN:ND2	1:C:258:SER:OG	2.22	0.61
1:C:1032:ASN:H	1:C:1033:GLU:HB2	1.65	0.61
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.36	0.61
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:HD2	1:B:50:PRO:HD2	1.66	0.61
1:E:694:ARG:HB3	1:E:694:ARG:HH11	1.65	0.61
1:F:34:GLN:O	1:F:391:ASN:HB2	2.01	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.28	0.61
1:F:121:GLU:O	1:F:124:GLN:HG2	2.00	0.60
1:A:525:HIS:HA	1:A:528:THR:HG22	1.82	0.60
1:B:395:MET:O	1:B:398:MET:HB2	2.00	0.60
1:B:697:LEU:HD22	1:B:846:LEU:HD11	1.83	0.60
1:C:697:LEU:HD12	1:C:846:LEU:HD11	1.82	0.60
1:D:695:ASN:HA	1:D:698:LEU:HD12	1.83	0.60
1:E:76:MET:HE3	1:E:95:GLU:HA	1.83	0.60
1:B:1038:SER:OG	1:B:1039:HIS:N	2.31	0.60
1:C:752:SER:O	1:C:767:TYR:HA	2.00	0.60
1:D:26:ALA:HB1	1:D:384:ALA:HB2	1.84	0.60
1:E:332:PHE:O	1:E:336:SER:OG	2.15	0.60
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.60
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.82	0.60
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.83	0.60
1:A:448:VAL:HG22	1:A:882:CYS:HB3	1.84	0.60
1:A:723:LYS:HD2	1:C:235:ILE:O	2.01	0.60
1:C:925:GLY:HA2	1:C:1002:VAL:HG22	1.84	0.60
1:E:1006:MET:O	1:E:1010:THR:HG23	2.00	0.60
1:F:896:VAL:HG23	1:F:937:ALA:CB	2.32	0.60
1:A:281:PHE:CE1	1:A:324:VAL:HG21	2.36	0.60
1:A:605:ASN:OD1	1:A:637:ASN:ND2	2.34	0.60
1:C:515:TRP:HD1	1:C:518:ARG:HH12	1.49	0.60
1:C:689:LYS:HA	1:C:692:GLN:OE1	2.01	0.60
1:C:892:ILE:O	1:C:896:VAL:HG12	2.02	0.60
1:E:670:GLY:HA2	1:E:857:MET:SD	2.42	0.60
1:F:576:VAL:HG13	1:F:658:VAL:HG22	1.84	0.60
1:F:638:LYS:HE2	1:F:640:GLU:HG3	1.84	0.60
1:F:935:LYS:HE2	1:F:936:ASN:OD1	2.01	0.60
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.34	0.60
1:B:213:GLN:HA	1:B:237:GLN:O	2.02	0.60
1:C:676:ASP:HB3	1:C:823:LEU:HD23	1.82	0.60
1:E:57:VAL:HB	1:E:88:VAL:HG23	1.84	0.60
1:A:188:MET:O	1:A:771:GLU:HB2	2.02	0.60
1:B:778:PRO:O	1:B:781:ILE:HG12	2.02	0.60
1:D:3:ASN:O	1:D:6:ILE:N	2.35	0.60
1:E:1008:THR:O	1:E:1012:LEU:HB2	2.01	0.60
1:F:359:LEU:HB2	1:F:365:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:PHE:HD1	1:A:897:MET:CE	2.15	0.60
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.01	0.60
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.67	0.60
1:C:694:ARG:HD3	1:C:820:MET:SD	2.42	0.60
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.84	0.60
1:F:379:THR:HG23	1:F:476:SER:OG	2.02	0.60
1:B:757:PHE:HE1	1:B:759:ASP:HB2	1.65	0.59
1:C:884:ALA:HB1	1:C:890:TRP:CZ3	2.37	0.59
1:C:1030:ARG:HH21	1:C:1030:ARG:HB2	1.66	0.59
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.36	0.59
1:E:396:PHE:O	1:E:400:LEU:HB2	2.02	0.59
1:F:239:ARG:NH1	1:F:756:ASP:HB2	2.17	0.59
1:A:549:VAL:O	1:A:552:MET:HB3	2.02	0.59
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.59
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.02	0.59
1:F:61:VAL:HG13	1:F:118:LEU:HD13	1.83	0.59
1:F:470:PHE:CD2	1:F:924:VAL:HG11	2.37	0.59
1:F:892:ILE:HD12	1:F:1021:PHE:HE1	1.67	0.59
1:A:216:ALA:HB1	1:A:234:ILE:O	2.02	0.59
1:A:602:GLU:HG3	1:A:605:ASN:HB2	1.84	0.59
1:A:771:GLU:HB3	1:A:774:TYR:HD1	1.68	0.59
1:B:187:TRP:HB3	1:B:771:GLU:HA	1.85	0.59
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.84	0.59
1:D:414:GLU:CD	1:D:969:PRO:HG3	2.22	0.59
1:D:467:TYR:HE1	1:D:920:VAL:HG22	1.66	0.59
1:D:941:VAL:HG13	1:D:1021:PHE:HE1	1.68	0.59
1:D:1036:GLU:HB3	1:D:1037:HIS:CB	2.32	0.59
1:E:361:ASN:O	1:E:365:THR:HG22	2.01	0.59
1:F:54:ALA:HB2	1:F:809:PRO:C	2.22	0.59
1:A:523:SER:O	1:A:526:HIS:HB2	2.03	0.59
1:A:700:GLU:HB3	1:A:842:LEU:HD22	1.84	0.59
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.37	0.59
1:B:327:TYR:HB2	1:B:623:PHE:CE2	2.34	0.59
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.82	0.59
1:F:15:ILE:O	1:F:19:ILE:HG13	2.01	0.59
1:A:721:GLN:HB3	1:C:233:SER:O	2.02	0.59
1:C:249:ILE:O	1:C:262:LEU:N	2.35	0.59
1:C:545:TYR:OH	1:C:898:LEU:O	2.13	0.59
1:E:1032:ASN:CB	1:E:1033:GLU:HB3	2.32	0.59
1:A:610:PHE:O	1:A:622:ALA:HA	2.03	0.59
1:B:143:ILE:HG12	1:B:322:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LYS:HZ1	1:B:1025:ARG:HH21	1.50	0.59
1:E:545:TYR:OH	1:E:898:LEU:O	2.19	0.59
1:B:677:PHE:HE2	1:B:679:LEU:HB2	1.67	0.59
1:E:853:ASP:OD1	1:E:854:TRP:N	2.35	0.59
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.33	0.59
1:D:213:GLN:HA	1:D:237:GLN:O	2.02	0.59
1:E:140:VAL:HG13	1:E:324:VAL:O	2.02	0.59
1:B:492:LEU:O	1:B:496:MET:HG2	2.03	0.59
1:B:858:SER:O	1:B:862:ARG:HB2	2.02	0.59
1:D:737:SER:O	1:D:741:ILE:HG13	2.03	0.59
1:D:795:PRO:HG2	1:D:798:ALA:HB2	1.84	0.59
1:A:920:VAL:O	1:A:924:VAL:HG23	2.03	0.58
1:C:455:PRO:HG2	1:C:875:SER:HA	1.85	0.58
1:D:694:ARG:NH1	1:D:820:MET:SD	2.76	0.58
1:F:595:THR:O	1:F:599:LEU:HG	2.03	0.58
1:A:593:GLU:OE2	1:A:654:LYS:NZ	2.34	0.58
1:E:599:LEU:HD21	1:E:609:VAL:HG23	1.84	0.58
1:E:955:LEU:HD21	1:E:1022:VAL:HA	1.85	0.58
1:F:133:SER:O	1:F:134:SER:HB2	2.02	0.58
1:F:689:LYS:H	1:F:689:LYS:CD	2.16	0.58
1:A:582:ALA:HB2	1:A:586:ARG:HH21	1.68	0.58
1:A:736:VAL:HG22	1:A:788:ALA:HB2	1.85	0.58
1:D:465:ALA:O	1:D:469:GLN:HG2	2.02	0.58
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.07	0.58
1:C:700:GLU:OE1	1:C:845:LYS:HE2	2.03	0.58
1:D:549:VAL:O	1:D:552:MET:HB3	2.03	0.58
1:D:887:TYR:CD2	1:D:892:ILE:HG22	2.38	0.58
1:E:540:ARG:HH22	2:E:1101:LMT:H6'2	1.68	0.58
1:F:184:MET:HB2	1:F:757:PHE:CE2	2.38	0.58
1:F:452:VAL:O	1:F:455:PRO:HD2	2.03	0.58
1:F:693:ALA:O	1:F:696:GLN:HB3	2.03	0.58
1:A:400:LEU:HD12	1:A:928:THR:HG21	1.85	0.58
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.32	0.58
1:B:908:LEU:HD23	1:B:922:PHE:HZ	1.68	0.58
1:D:181:GLN:HG2	1:D:182:TYR:N	2.18	0.58
1:D:773:LYS:HB3	1:F:225:VAL:HG11	1.85	0.58
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.85	0.58
1:E:367:ILE:HD11	1:E:497:LEU:HD13	1.84	0.58
1:E:415:ASN:O	1:E:419:VAL:HG23	2.03	0.58
1:E:463:THR:O	1:E:467:TYR:HD1	1.86	0.58
1:F:571:VAL:HG22	1:F:625:SER:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:616:GLY:O	1:F:618:ASN:N	2.37	0.58
1:F:884:ALA:HB2	1:F:893:PRO:HG2	1.85	0.58
1:A:530:SER:HG	2:A:1101:LMT:H2O2	1.49	0.58
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.68	0.58
1:E:166:ILE:HA	1:E:309:GLU:HG2	1.84	0.58
1:E:526:HIS:O	1:E:530:SER:HB2	2.03	0.58
1:A:770:SER:HB3	1:A:775:ARG:HD3	1.83	0.58
1:A:881:LEU:HB3	1:C:14:VAL:HG13	1.85	0.58
1:B:906:GLY:HA3	1:B:1008:THR:OG1	2.04	0.58
1:D:388:PHE:HE1	1:D:472:ILE:HG21	1.69	0.58
1:A:130:GLU:OE1	1:A:174:ASP:HB2	2.04	0.58
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.86	0.58
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.86	0.58
1:C:336:SER:O	1:C:340:VAL:HG23	2.04	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HD13	1.84	0.58
1:E:687:HIS:CE1	1:E:808:SER:HB2	2.38	0.58
1:F:563:PHE:CZ	1:F:564:LEU:HD13	2.39	0.58
1:A:728:GLN:HE22	1:A:738:ILE:HG21	1.69	0.58
1:A:1032:ASN:N	1:A:1035:ILE:HD11	2.18	0.58
1:B:545:TYR:CE2	1:B:1020:PHE:HZ	2.21	0.58
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.04	0.58
1:B:602:GLU:OE1	1:B:645:ARG:HD2	2.04	0.58
1:C:222:THR:HA	1:C:224:PRO:HD3	1.85	0.58
1:D:438:ILE:O	1:D:441:ALA:HB3	2.03	0.58
1:F:185:ARG:NH2	1:F:273:GLU:O	2.28	0.58
1:F:536:ARG:HD2	2:F:2000:LMT:O4'	2.04	0.58
1:A:105:VAL:HG13	1:B:109:ASN:HD21	1.68	0.57
1:A:749:TRP:HZ3	1:C:219:LEU:HD23	1.67	0.57
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.85	0.57
1:E:239:ARG:NH1	1:E:755:ASN:OD1	2.37	0.57
1:E:653:ILE:HG13	1:E:654:LYS:HD2	1.86	0.57
1:E:686:GLY:H	1:E:689:LYS:HB2	1.68	0.57
1:C:216:ALA:HB1	1:C:234:ILE:O	2.05	0.57
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.39	0.57
1:F:164:ASP:CG	1:F:762:ARG:HH22	2.07	0.57
1:F:187:TRP:HB3	1:F:771:GLU:HA	1.85	0.57
1:A:531:VAL:O	1:A:535:LEU:HG	2.05	0.57
1:E:78:MET:N	1:E:815:ASN:OD1	2.33	0.57
1:E:354:VAL:HG21	1:E:976:ALA:HB2	1.86	0.57
1:F:982:MET:HB3	1:F:983:PRO:HD3	1.86	0.57
1:A:1022:VAL:O	1:A:1026:ARG:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:264:ASP:N	1:D:264:ASP:OD1	2.37	0.57
1:D:1035:ILE:O	1:D:1036:GLU:HG3	2.04	0.57
1:E:902:LEU:HG	1:E:1012:LEU:HB3	1.85	0.57
1:E:1029:SER:OG	1:E:1030:ARG:N	2.31	0.57
1:A:280:GLU:HG3	1:A:285:PRO:HA	1.85	0.57
1:B:677:PHE:CE2	1:B:822:ILE:HD12	2.39	0.57
1:D:525:HIS:HA	1:D:528:THR:HG22	1.86	0.57
1:A:350:LEU:HD13	1:A:980:GLY:HA2	1.86	0.57
1:B:415:ASN:O	1:B:419:VAL:HG23	2.05	0.57
1:C:756:ASP:OD1	1:C:765:LYS:HA	2.04	0.57
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.35	0.57
1:E:854:TRP:CE3	1:E:858:SER:HB3	2.40	0.57
1:B:676:ASP:N	1:B:858:SER:OG	2.33	0.57
1:C:75:LEU:HD11	1:C:92:LEU:HD12	1.86	0.57
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.39	0.57
1:C:739:ASN:O	1:C:743:THR:OG1	2.18	0.57
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.57
1:E:889:SER:HB3	1:E:892:ILE:HG13	1.87	0.57
1:A:259:ARG:NH1	1:B:729:GLU:OE2	2.38	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.87	0.57
1:C:563:PHE:O	1:C:919:ASP:HB2	2.05	0.57
1:C:884:ALA:HB2	1:C:893:PRO:HG2	1.85	0.57
1:C:939:LEU:C	1:C:966:ARG:HD2	2.24	0.57
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.87	0.57
1:D:405:LEU:HD21	1:D:477:ALA:HB1	1.87	0.57
1:E:577:GLN:NE2	1:E:618:ASN:OD1	2.38	0.57
1:E:643:THR:O	1:E:647:THR:OG1	2.23	0.57
1:B:484:VAL:O	1:B:489:THR:HG23	2.05	0.57
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.40	0.57
1:D:677:PHE:CD2	1:D:822:ILE:HD12	2.39	0.57
1:D:1030:ARG:HE	1:D:1031:LYS:HB2	1.69	0.57
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.86	0.57
1:E:540:ARG:HH22	2:E:1101:LMT:C6B	2.18	0.57
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.86	0.57
1:F:435:MET:HE1	1:F:490:PRO:HB3	1.85	0.57
1:F:771:GLU:HB2	1:F:774:TYR:CD1	2.39	0.57
1:A:916:LEU:HD13	1:A:917:THR:HG22	1.87	0.57
1:A:963:VAL:HA	1:A:966:ARG:HH22	1.69	0.57
1:E:697:LEU:HD11	1:E:842:LEU:HB3	1.86	0.57
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.86	0.57
1:A:133:SER:OG	1:A:134:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ALA:HB2	1:A:471:SER:OG	2.04	0.56
1:D:225:VAL:H	1:E:776:MET:HE1	1.70	0.56
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.87	0.56
1:A:363:ARG:O	1:A:366:LEU:HB2	2.05	0.56
1:A:448:VAL:O	1:A:451:ALA:HB3	2.05	0.56
1:B:560:PRO:O	1:B:918:ASN:HB3	2.04	0.56
1:C:890:TRP:CE3	1:C:890:TRP:HA	2.41	0.56
1:D:247:GLY:O	1:D:263:ARG:N	2.33	0.56
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.69	0.56
1:D:516:PHE:HA	1:D:519:MET:HG3	1.86	0.56
1:D:564:LEU:HB2	1:D:666:ILE:HD11	1.87	0.56
1:D:966:ARG:HB3	1:D:966:ARG:HH11	1.70	0.56
1:E:597:TYR:OH	1:E:646:ALA:HA	2.05	0.56
1:A:418:ARG:O	1:A:422:GLU:HB2	2.05	0.56
1:C:185:ARG:HH12	1:C:769:MET:HB2	1.70	0.56
1:C:188:MET:SD	1:C:200:PRO:HG3	2.45	0.56
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.70	0.56
1:C:449:LEU:O	1:C:452:VAL:HG23	2.06	0.56
1:D:124:GLN:HA	1:E:117:LEU:HD12	1.87	0.56
1:E:470:PHE:O	1:E:474:ILE:HG13	2.04	0.56
1:E:697:LEU:HD13	1:E:846:LEU:HD21	1.87	0.56
1:E:842:LEU:O	1:E:845:LYS:HB2	2.05	0.56
1:F:375:VAL:O	1:F:379:THR:OG1	2.09	0.56
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.88	0.56
1:A:399:VAL:HG11	1:A:984:LEU:HD11	1.86	0.56
1:A:534:ILE:HD12	1:A:535:LEU:HD23	1.87	0.56
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.87	0.56
1:C:355:MET:CG	1:C:410:ILE:HD11	2.36	0.56
1:A:978:ILE:HG23	1:A:1003:MET:HG3	1.88	0.56
1:B:525:HIS:NE2	1:B:529:ASP:OD1	2.38	0.56
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.86	0.56
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.71	0.56
1:E:1022:VAL:O	1:E:1026:ARG:HG3	2.06	0.56
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.06	0.56
1:F:945:LYS:HA	1:F:948:MET:HE3	1.88	0.56
1:A:10:ILE:O	1:A:14:VAL:HG23	2.04	0.56
1:A:776:MET:O	1:C:219:LEU:HB3	2.05	0.56
1:D:272:GLY:N	1:D:275:TYR:OH	2.35	0.56
1:E:280:GLU:O	1:E:610:PHE:HA	2.06	0.56
1:F:892:ILE:HD12	1:F:1021:PHE:CE1	2.40	0.56
1:A:795:PRO:HG2	1:A:798:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:GLU:O	1:D:502:LYS:HB3	2.06	0.56
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.56
1:F:414:GLU:HG3	1:F:972:MET:HE1	1.87	0.56
1:C:602:GLU:OE2	1:C:645:ARG:NH1	2.39	0.56
1:E:840:GLU:HG2	1:E:852:TYR:HE1	1.71	0.56
1:B:412:VAL:O	1:B:416:VAL:HG23	2.05	0.56
1:D:455:PRO:HG2	1:D:875:SER:CB	2.35	0.56
1:E:380:PHE:O	1:E:384:ALA:N	2.39	0.56
1:E:442:LEU:O	1:E:445:ILE:HG13	2.06	0.56
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.88	0.56
1:C:921:TYR:HD1	1:C:997:ALA:HB3	1.69	0.56
1:D:423:GLU:C	1:D:502:LYS:HB3	2.26	0.56
1:F:723:LYS:HG2	1:F:803:ARG:NH2	2.20	0.56
1:A:276:ASP:HA	1:C:222:THR:HG21	1.88	0.55
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.88	0.55
1:A:632:ARG:HB3	1:A:637:ASN:HB3	1.88	0.55
1:F:351:VAL:HG22	1:F:976:ALA:HB1	1.87	0.55
1:A:273:GLU:HG2	1:A:765:LYS:HD2	1.89	0.55
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.55
1:B:463:THR:HA	1:B:466:ILE:HD12	1.88	0.55
1:B:908:LEU:HD23	1:B:922:PHE:CZ	2.41	0.55
1:C:391:ASN:O	1:C:394:THR:OG1	2.21	0.55
1:D:185:ARG:HH12	1:D:769:MET:HB2	1.70	0.55
1:D:347:ALA:O	1:D:351:VAL:HG23	2.06	0.55
1:D:701:ALA:HB1	1:D:711:VAL:HG11	1.88	0.55
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.41	0.55
1:F:578:LEU:HD12	1:F:587:THR:HG22	1.88	0.55
1:A:544:LEU:O	1:A:548:ILE:HG13	2.07	0.55
1:D:170:SER:HB2	1:E:75:LEU:H	1.71	0.55
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.71	0.55
1:E:412:VAL:O	1:E:416:VAL:HG23	2.07	0.55
1:F:58:GLN:OE1	1:F:811:LEU:HB3	2.07	0.55
1:F:896:VAL:HG23	1:F:937:ALA:HB1	1.89	0.55
1:A:222:THR:HA	1:A:224:PRO:HD3	1.88	0.55
1:A:572:PHE:HB2	1:A:661:PHE:O	2.05	0.55
1:B:898:LEU:HB3	1:B:1020:PHE:CE2	2.42	0.55
1:C:184:MET:HB3	1:C:766:VAL:HG13	1.88	0.55
1:C:896:VAL:HG23	1:C:937:ALA:CB	2.36	0.55
1:D:59:ASP:OD2	1:F:758:ILE:HD13	2.07	0.55
1:D:888:GLU:OE1	1:F:11:PHE:HB2	2.07	0.55
1:B:1031:LYS:H	1:B:1033:GLU:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:O	1:C:169:THR:OG1	2.09	0.55
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.07	0.55
1:D:470:PHE:CD2	1:D:924:VAL:HG21	2.42	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.88	0.55
1:E:281:PHE:HB2	1:E:610:PHE:CE1	2.41	0.55
1:F:135:SER:HB2	1:F:667:VAL:HG12	1.89	0.55
1:F:1028:PHE:O	1:F:1030:ARG:N	2.40	0.55
1:A:146:ASP:OD2	1:A:146:ASP:N	2.36	0.55
1:C:68:ASN:HB3	1:C:110:LYS:O	2.07	0.55
1:D:448:VAL:HG22	1:D:882:CYS:CB	2.37	0.55
1:D:778:PRO:O	1:D:781:ILE:HG12	2.06	0.55
1:E:613:ASN:HD22	1:E:613:ASN:C	2.10	0.55
1:A:3:ASN:HA	1:A:6:ILE:HG23	1.89	0.55
1:A:514:GLY:C	1:A:516:PHE:H	2.10	0.55
1:B:184:MET:HB2	1:B:757:PHE:CD2	2.42	0.55
1:C:508:GLY:O	1:C:509:LYS:HB2	2.06	0.55
1:C:722:PHE:CE2	1:C:802:SER:HB2	2.42	0.55
1:C:942:GLU:HG3	1:C:943:PHE:HD1	1.71	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.46	0.55
1:D:836:MET:HG2	1:D:854:TRP:CZ2	2.42	0.55
1:E:105:VAL:HG21	1:F:105:VAL:HG13	1.89	0.55
1:F:143:ILE:O	1:F:321:LEU:HD22	2.06	0.55
1:F:298:ASN:HB3	1:F:301:ASP:OD2	2.07	0.55
1:F:412:VAL:O	1:F:416:VAL:HG23	2.06	0.55
1:F:728:GLN:OE1	1:F:738:ILE:HG12	2.07	0.55
1:F:974:SER:HA	1:F:1006:MET:HE3	1.89	0.55
1:D:501:ALA:O	1:D:504:ASP:HB2	2.06	0.55
1:D:723:LYS:HG2	1:D:803:ARG:CZ	2.37	0.55
1:E:569:GLN:NE2	1:E:665:ALA:HA	2.21	0.55
1:A:105:VAL:HG13	1:B:109:ASN:ND2	2.22	0.55
1:A:281:PHE:CD1	1:A:324:VAL:HG11	2.42	0.55
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.72	0.55
1:D:143:ILE:O	1:D:321:LEU:HD22	2.07	0.55
1:E:149:MET:HG3	1:E:154:ILE:HG13	1.89	0.55
1:E:220:GLY:HA3	1:E:230:LEU:O	2.07	0.55
1:A:778:PRO:O	1:A:781:ILE:HG12	2.07	0.55
1:A:1002:VAL:O	1:A:1006:MET:HG2	2.07	0.55
1:B:757:PHE:CE1	1:B:759:ASP:HB2	2.41	0.55
1:C:200:PRO:HA	1:C:203:VAL:CG2	2.37	0.55
1:D:175:VAL:HG11	1:D:289:LEU:HD13	1.88	0.55
1:D:366:LEU:HD23	1:D:369:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:188:MET:O	1:E:771:GLU:HB2	2.06	0.55
1:E:712:ARG:HH21	1:E:823:LEU:HB3	1.71	0.55
1:F:352:PHE:HA	1:F:355:MET:HE2	1.88	0.55
1:F:688:GLU:HB3	1:F:689:LYS:HD2	1.89	0.55
1:A:396:PHE:HZ	1:A:995:GLN:HG2	1.70	0.54
1:B:425:LEU:HD12	1:B:430:ALA:HA	1.89	0.54
1:C:108:GLN:O	1:C:112:GLN:HB2	2.07	0.54
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.89	0.54
1:C:531:VAL:HA	1:C:534:ILE:HG12	1.89	0.54
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.88	0.54
1:D:595:THR:O	1:D:599:LEU:HG	2.05	0.54
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.72	0.54
1:E:435:MET:SD	1:E:490:PRO:HB3	2.46	0.54
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.89	0.54
1:B:404:LEU:HD12	1:B:932:LEU:HD21	1.89	0.54
1:B:631:ASP:C	1:B:633:PRO:HD3	2.28	0.54
1:C:568:ASP:O	1:C:629:TRP:CH2	2.61	0.54
1:C:795:PRO:HG2	1:C:798:ALA:HB2	1.90	0.54
1:D:449:LEU:O	1:D:452:VAL:HG22	2.07	0.54
1:E:355:MET:HB3	1:E:365:THR:OG1	2.06	0.54
1:E:613:ASN:ND2	1:E:619:THR:O	2.40	0.54
1:E:940:ILE:HD11	1:E:970:ILE:HD11	1.90	0.54
1:F:455:PRO:HG3	1:F:878:VAL:HG21	1.89	0.54
1:F:974:SER:OG	1:F:1010:THR:HG21	2.07	0.54
1:A:377:LEU:O	1:A:380:PHE:HB2	2.07	0.54
1:B:586:ARG:O	1:B:589:LYS:HB3	2.07	0.54
1:C:355:MET:HG2	1:C:410:ILE:HD11	1.88	0.54
1:D:188:MET:HB3	1:D:193:LEU:HD11	1.88	0.54
1:E:887:TYR:O	1:E:889:SER:N	2.40	0.54
1:A:158:VAL:HG22	1:A:162:MET:HE3	1.89	0.54
1:A:202:ASP:OD1	1:A:787:ARG:NH2	2.38	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.87	0.54
1:B:739:ASN:O	1:B:743:THR:OG1	2.09	0.54
1:C:408:ASP:O	1:C:412:VAL:HG23	2.07	0.54
1:D:108:GLN:O	1:D:112:GLN:HG2	2.08	0.54
1:D:135:SER:O	1:D:292:LYS:HG2	2.07	0.54
1:D:242:SER:O	1:D:246:PHE:HD1	1.91	0.54
1:D:955:LEU:N	1:D:1033:GLU:O	2.37	0.54
1:A:420:MET:HB3	1:A:500:ILE:HB	1.90	0.54
1:B:423:GLU:O	1:B:502:LYS:HD2	2.06	0.54
1:D:54:ALA:HB1	1:D:811:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:631:ASP:C	1:F:633:PRO:HD3	2.27	0.54
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.07	0.54
1:C:883:LEU:HD21	1:C:938:ILE:HD11	1.89	0.54
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.28	0.54
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.38	0.54
1:C:136:PHE:HB2	1:C:327:TYR:HE2	1.72	0.54
1:D:947:LEU:HB2	1:D:958:ALA:HB1	1.90	0.54
1:F:681:ASP:O	1:F:817:LEU:HD13	2.07	0.54
1:F:936:ASN:ND2	1:F:1010:THR:HG22	2.22	0.54
1:A:565:PRO:HG2	1:A:567:GLU:OE2	2.08	0.54
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.89	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:642:ILE:O	1:C:645:ARG:HG2	2.08	0.54
1:C:1006:MET:O	1:C:1010:THR:OG1	2.25	0.54
1:D:538:THR:HG23	1:D:542:LEU:HD13	1.90	0.54
1:D:904:VAL:HG22	1:D:926:LEU:HD21	1.89	0.54
1:D:962:ALA:O	1:D:965:MET:HG2	2.07	0.54
1:E:44:THR:HA	1:E:90:ILE:O	2.07	0.54
1:E:444:GLY:O	1:E:448:VAL:HG23	2.08	0.54
1:E:545:TYR:CE2	1:E:1020:PHE:HZ	2.25	0.54
1:E:663:LEU:HD23	1:E:663:LEU:H	1.72	0.54
1:F:677:PHE:HB2	1:F:854:TRP:CZ3	2.43	0.54
1:A:936:ASN:O	1:A:940:ILE:HG13	2.08	0.54
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.89	0.54
1:B:771:GLU:HB3	1:B:774:TYR:CD1	2.43	0.54
1:B:941:VAL:HG13	1:B:1021:PHE:CE1	2.42	0.54
1:C:395:MET:O	1:C:398:MET:HB2	2.07	0.54
1:D:692:GLN:HA	1:D:695:ASN:HB2	1.89	0.54
1:D:1033:GLU:HB3	1:D:1034:ASP:HB2	1.90	0.54
1:E:536:ARG:CZ	2:E:1101:LMT:O3B	2.55	0.54
1:E:770:SER:HB3	1:E:775:ARG:HD3	1.89	0.54
1:F:164:ASP:OD1	1:F:762:ARG:NH2	2.40	0.54
1:A:34:GLN:HE22	1:A:569:GLN:NE2	2.06	0.54
1:B:198:LEU:HD21	1:B:252:LYS:HB2	1.90	0.54
1:B:272:GLY:N	1:B:275:TYR:OH	2.21	0.54
1:C:520:PHE:CE2	1:C:968:ARG:HD2	2.43	0.54
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.90	0.54
1:E:138:MET:HG3	1:E:327:TYR:O	2.08	0.54
1:E:593:GLU:OE1	1:E:654:LYS:NZ	2.34	0.54
1:F:114:ALA:O	1:F:118:LEU:HG	2.08	0.54
1:F:435:MET:O	1:F:439:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:LEU:O	1:F:491:ALA:HB3	2.07	0.54
1:A:166:ILE:HD11	1:A:306:ILE:HG23	1.90	0.53
1:A:220:GLY:HA3	1:A:230:LEU:O	2.08	0.53
1:A:545:TYR:O	1:A:549:VAL:HG23	2.08	0.53
1:A:577:GLN:OE1	1:A:619:THR:HG23	2.08	0.53
1:A:769:MET:HG2	1:A:770:SER:H	1.72	0.53
1:B:468:ARG:HG2	1:B:472:ILE:HD13	1.89	0.53
1:D:694:ARG:HD2	1:D:713:PRO:HB3	1.90	0.53
1:E:1019:VAL:O	1:E:1023:VAL:HG23	2.08	0.53
1:F:38:ILE:HD13	1:F:466:ILE:HD13	1.90	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.90	0.53
1:A:896:VAL:HG21	1:A:938:ILE:HG13	1.90	0.53
1:B:945:LYS:NZ	1:B:1025:ARG:HH21	2.07	0.53
1:B:1034:ASP:N	1:B:1035:ILE:HG22	2.24	0.53
1:D:21:LEU:O	1:D:25:LEU:HB2	2.08	0.53
1:D:185:ARG:HB2	1:D:271:GLY:HA3	1.89	0.53
1:D:186:ILE:HB	1:D:768:VAL:HG22	1.91	0.53
1:D:908:LEU:HD23	1:D:922:PHE:CZ	2.43	0.53
1:A:451:ALA:HB1	1:A:878:VAL:HG12	1.91	0.53
1:A:492:LEU:O	1:A:496:MET:HG2	2.08	0.53
1:A:728:GLN:NE2	1:A:738:ILE:HG21	2.23	0.53
1:A:940:ILE:HG12	1:A:966:ARG:NE	2.23	0.53
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.89	0.53
1:C:935:LYS:NZ	1:C:973:THR:HG21	2.24	0.53
1:D:17:ILE:HA	1:D:20:MET:HE2	1.89	0.53
1:D:491:ALA:O	1:D:495:THR:OG1	2.24	0.53
1:D:776:MET:HE1	1:F:225:VAL:HG22	1.89	0.53
1:A:143:ILE:HG22	1:A:286:ALA:HB1	1.91	0.53
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.44	0.53
1:A:281:PHE:HB2	1:A:610:PHE:CE1	2.43	0.53
1:B:902:LEU:HD11	1:B:1016:PHE:HD2	1.73	0.53
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.91	0.53
1:C:366:LEU:O	1:C:370:ILE:HG13	2.08	0.53
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.53
1:C:935:LYS:HE2	1:C:936:ASN:OD1	2.09	0.53
1:D:873:ALA:O	1:D:877:ILE:HG12	2.08	0.53
1:E:553:ALA:O	1:E:557:VAL:HG23	2.08	0.53
1:F:184:MET:HB2	1:F:757:PHE:CD2	2.42	0.53
1:F:446:ALA:HB3	1:F:482:VAL:HG22	1.89	0.53
1:B:108:GLN:HA	1:B:129:VAL:HG21	1.90	0.53
1:C:574:THR:HG21	1:C:598:TYR:CE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LYS:O	1:D:431:THR:N	2.42	0.53
1:D:559:LEU:HD12	1:D:908:LEU:HD22	1.90	0.53
1:D:578:LEU:HB2	1:D:618:ASN:O	2.09	0.53
1:E:482:VAL:O	1:E:485:ALA:HB3	2.09	0.53
1:E:926:LEU:O	1:E:930:ILE:HG13	2.09	0.53
1:E:942:GLU:O	1:E:945:LYS:N	2.42	0.53
1:F:197:GLN:HG3	1:F:793:MET:SD	2.49	0.53
1:A:954:GLY:HA2	1:A:1034:ASP:H	1.74	0.53
1:B:952:GLY:O	1:B:1036:GLU:HA	2.08	0.53
1:C:184:MET:HB3	1:C:766:VAL:HG22	1.91	0.53
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.90	0.53
1:D:219:LEU:HD23	1:E:749:TRP:HZ3	1.73	0.53
1:D:723:LYS:HG2	1:D:803:ARG:NH1	2.23	0.53
1:E:26:ALA:O	1:E:30:LEU:HB2	2.09	0.53
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.90	0.53
1:E:974:SER:OG	1:E:1010:THR:HG21	2.09	0.53
1:A:953:LYS:O	1:A:1035:ILE:HB	2.09	0.53
1:C:479:ALA:O	1:C:482:VAL:HG23	2.09	0.53
1:D:233:SER:HB2	1:E:721:GLN:HB3	1.91	0.53
1:D:428:LYS:HG2	1:D:494:ALA:HB1	1.91	0.53
1:E:20:MET:HG3	1:E:374:VAL:HG22	1.91	0.53
1:E:140:VAL:HA	1:E:326:PRO:HD2	1.91	0.53
1:E:468:ARG:HG2	1:E:472:ILE:CD1	2.39	0.53
1:E:670:GLY:C	1:E:672:ALA:H	2.12	0.53
1:A:888:GLU:OE1	1:C:11:PHE:HB2	2.09	0.53
1:B:902:LEU:HD21	1:B:1016:PHE:HB2	1.90	0.53
1:C:544:LEU:O	1:C:547:ILE:HB	2.08	0.53
1:C:770:SER:HB3	1:C:775:ARG:HD3	1.91	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:E:1005:GLY:O	1:E:1009:ALA:HB2	2.08	0.53
1:F:700:GLU:HA	1:F:703:LYS:NZ	2.24	0.53
1:A:13:TRP:HE1	1:A:492:LEU:HD21	1.73	0.53
1:A:21:LEU:O	1:A:25:LEU:HB2	2.09	0.53
1:A:44:THR:HA	1:A:90:ILE:O	2.09	0.53
1:A:626:LEU:HD11	1:A:639:VAL:CG2	2.39	0.53
1:B:82:SER:HA	1:B:88:VAL:HG22	1.89	0.53
1:B:154:ILE:O	1:B:158:VAL:HG23	2.09	0.53
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.90	0.53
1:C:571:VAL:HG22	1:C:625:SER:HA	1.91	0.53
1:C:899:VAL:O	1:C:902:LEU:HB2	2.09	0.53
1:A:234:ILE:HD11	1:B:749:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:O	1:A:478:MET:HB3	2.08	0.52
1:A:763:VAL:HG12	1:B:63:GLN:HE21	1.73	0.52
1:C:415:ASN:O	1:C:419:VAL:HG23	2.10	0.52
1:E:701:ALA:HB1	1:E:711:VAL:HG11	1.90	0.52
1:F:3:ASN:ND2	1:F:435:MET:SD	2.77	0.52
1:F:45:ILE:HD13	1:F:111:LEU:HG	1.89	0.52
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.91	0.52
1:F:676:ASP:HB3	1:F:823:LEU:HD23	1.91	0.52
1:F:966:ARG:O	1:F:966:ARG:NE	2.40	0.52
1:A:527:TYR:CE1	1:A:1014:ILE:HD12	2.44	0.52
1:A:536:ARG:NH1	2:A:1101:LMT:O4'	2.41	0.52
1:A:910:ALA:HB2	1:A:1004:GLY:HA3	1.90	0.52
1:B:377:LEU:O	1:B:380:PHE:HB2	2.09	0.52
1:B:841:GLN:O	1:B:844:SER:OG	2.26	0.52
1:C:151:GLN:HE22	1:C:286:ALA:H	1.56	0.52
1:C:663:LEU:HA	1:C:672:ALA:HA	1.91	0.52
1:C:917:THR:O	1:C:919:ASP:N	2.43	0.52
1:C:977:PHE:HE2	1:C:1002:VAL:HG12	1.75	0.52
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.91	0.52
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.09	0.52
1:D:991:GLY:O	1:D:993:GLY:N	2.42	0.52
1:E:15:ILE:HD12	1:E:487:ILE:HG21	1.91	0.52
1:E:355:MET:SD	1:E:368:PRO:HG2	2.48	0.52
1:E:854:TRP:HE3	1:E:858:SER:HB3	1.72	0.52
1:F:452:VAL:C	1:F:455:PRO:HD2	2.30	0.52
1:A:8:ARG:O	1:A:11:PHE:N	2.42	0.52
1:A:940:ILE:HD12	1:A:1017:VAL:HG11	1.90	0.52
1:B:677:PHE:CD2	1:B:822:ILE:HD12	2.45	0.52
1:C:371:ALA:O	1:C:375:VAL:HG23	2.10	0.52
1:D:366:LEU:HA	1:D:369:THR:HB	1.90	0.52
1:D:896:VAL:HG21	1:D:938:ILE:HG13	1.90	0.52
1:E:445:ILE:HG22	1:E:938:ILE:CD1	2.38	0.52
1:E:961:ASP:O	1:E:964:ARG:HB3	2.09	0.52
1:F:47:ALA:HB2	1:F:127:VAL:HG13	1.92	0.52
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.90	0.52
1:F:446:ALA:CB	1:F:482:VAL:HG22	2.40	0.52
1:A:272:GLY:N	1:A:275:TYR:OH	2.34	0.52
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.90	0.52
1:C:600:THR:O	1:C:603:LYS:HG3	2.09	0.52
1:D:278:ILE:CG1	1:D:613:ASN:HB3	2.40	0.52
1:D:434:SER:O	1:D:438:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HA	1:A:875:SER:OG	2.09	0.52
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.30	0.52
1:C:190:PRO:HG3	1:C:774:TYR:CG	2.44	0.52
1:C:940:ILE:HA	1:C:966:ARG:NH1	2.25	0.52
1:D:121:GLU:O	1:D:124:GLN:HG2	2.10	0.52
1:D:546:LEU:O	1:D:550:VAL:HG23	2.10	0.52
1:D:673:THR:HA	1:D:832:THR:OG1	2.10	0.52
1:E:982:MET:HB3	1:E:983:PRO:HD3	1.91	0.52
1:F:329:THR:O	1:F:333:VAL:HG23	2.09	0.52
1:F:456:MET:HA	1:F:459:PHE:CD1	2.45	0.52
1:B:796:PHE:HA	1:B:799:PHE:CZ	2.45	0.52
1:B:953:LYS:O	1:B:1035:ILE:HG12	2.09	0.52
1:C:11:PHE:O	1:C:15:ILE:HG13	2.10	0.52
1:C:355:MET:SD	1:C:368:PRO:HB2	2.50	0.52
1:D:153:ASP:OD2	1:D:153:ASP:N	2.42	0.52
1:F:184:MET:HB3	1:F:766:VAL:HG22	1.91	0.52
1:A:4:PHE:HB3	1:A:8:ARG:CZ	2.39	0.52
1:A:966:ARG:C	1:A:969:PRO:HD2	2.30	0.52
1:B:510:LYS:HB3	1:B:513:PHE:HB3	1.92	0.52
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.91	0.52
1:C:662:ASN:O	1:C:673:THR:N	2.37	0.52
1:D:278:ILE:HD13	1:D:584:GLN:OE1	2.09	0.52
1:E:199:THR:HG21	1:E:787:ARG:H	1.73	0.52
1:E:524:THR:O	1:E:527:TYR:HB3	2.09	0.52
1:F:408:ASP:O	1:F:412:VAL:HG23	2.09	0.52
1:A:708:LEU:HD21	1:A:838:LEU:HD12	1.90	0.52
1:C:251:LEU:HD11	1:C:262:LEU:HD13	1.92	0.52
1:C:549:VAL:O	1:C:552:MET:HB3	2.10	0.52
1:D:478:MET:O	1:D:482:VAL:HG23	2.09	0.52
1:D:653:ILE:HG13	1:D:654:LYS:HE2	1.92	0.52
1:D:771:GLU:HB3	1:D:774:TYR:HD1	1.75	0.52
1:D:940:ILE:HG12	1:D:966:ARG:CZ	2.39	0.52
1:E:47:ALA:O	1:E:87:THR:HA	2.10	0.52
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.45	0.52
1:F:314:GLU:HB2	1:F:315:PRO:HD3	1.92	0.52
1:F:559:LEU:HD11	1:F:911:ALA:HB1	1.92	0.52
1:A:968:ARG:HG2	1:A:972:MET:CE	2.40	0.52
1:C:545:TYR:CE2	1:C:1020:PHE:CZ	2.98	0.52
1:C:884:ALA:HB1	1:C:890:TRP:HZ3	1.74	0.52
1:D:17:ILE:HA	1:D:20:MET:CE	2.40	0.52
1:D:542:LEU:O	1:D:546:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:858:SER:HA	1:D:861:GLU:CD	2.31	0.52
1:F:757:PHE:HE1	1:F:759:ASP:HB2	1.74	0.52
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.74	0.52
1:A:902:LEU:HD21	1:A:1016:PHE:CD1	2.44	0.52
1:B:58:GLN:O	1:B:63:GLN:HG3	2.09	0.52
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.52
1:D:23:GLY:HA2	1:D:381:ALA:HB2	1.90	0.52
1:D:27:ILE:HG23	1:D:390:ILE:HD11	1.91	0.52
1:D:137:LEU:HB3	1:D:291:ILE:O	2.10	0.52
1:D:276:ASP:O	1:D:614:GLY:HA2	2.10	0.52
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.74	0.52
1:D:936:ASN:ND2	1:D:970:ILE:HG23	2.25	0.52
1:E:695:ASN:O	1:E:698:LEU:HB2	2.10	0.52
1:F:453:PHE:HB2	1:F:475:VAL:HG23	1.90	0.52
1:F:778:PRO:O	1:F:781:ILE:HG12	2.10	0.52
1:F:986:ILE:HG23	1:F:986:ILE:O	2.10	0.52
1:A:442:LEU:O	1:A:445:ILE:HG13	2.10	0.51
1:A:553:ALA:O	1:A:557:VAL:HG23	2.10	0.51
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.92	0.51
1:B:413:VAL:O	1:B:417:GLU:HG2	2.11	0.51
1:C:493:CYS:O	1:C:497:LEU:HB2	2.11	0.51
1:D:225:VAL:H	1:E:776:MET:CE	2.22	0.51
1:E:757:PHE:HD2	1:E:766:VAL:HG22	1.75	0.51
1:F:872:TYR:O	1:F:876:LEU:HD12	2.09	0.51
1:F:905:ILE:O	1:F:909:LEU:HB2	2.10	0.51
1:A:694:ARG:NH2	1:A:717:GLU:OE1	2.43	0.51
1:B:549:VAL:O	1:B:552:MET:HB3	2.10	0.51
1:B:578:LEU:HB2	1:B:618:ASN:O	2.10	0.51
1:D:201:VAL:O	1:D:205:THR:OG1	2.26	0.51
1:D:974:SER:OG	1:D:1010:THR:HG21	2.10	0.51
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.90	0.51
1:E:76:MET:HB2	1:E:93:THR:O	2.09	0.51
1:E:514:GLY:C	1:E:516:PHE:N	2.63	0.51
1:A:13:TRP:O	1:A:17:ILE:HG13	2.09	0.51
1:C:219:LEU:HD12	1:C:232:ALA:HB3	1.92	0.51
1:C:906:GLY:HA3	1:C:1008:THR:OG1	2.10	0.51
1:D:636:GLU:HB2	1:D:645:ARG:NH2	2.25	0.51
1:D:881:LEU:HD13	1:F:18:ILE:HG13	1.92	0.51
1:D:966:ARG:C	1:D:969:PRO:HD2	2.30	0.51
1:E:534:ILE:HG21	2:E:1101:LMT:H12	1.92	0.51
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:GLN:HA	1:A:62:THR:HB	1.92	0.51
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.45	0.51
1:B:52:ALA:HB1	1:B:56:THR:HB	1.93	0.51
1:B:700:GLU:HB3	1:B:842:LEU:HD22	1.92	0.51
1:B:950:LYS:O	1:B:951:GLU:HG2	2.10	0.51
1:C:110:LYS:O	1:C:113:LEU:HB2	2.10	0.51
1:C:781:ILE:O	1:C:796:PHE:HB2	2.11	0.51
1:C:985:VAL:HG13	1:C:1000:THR:OG1	2.10	0.51
1:D:56:THR:O	1:D:60:THR:HG22	2.10	0.51
1:D:575:MET:HG2	1:D:661:PHE:CE1	2.42	0.51
1:D:757:PHE:CE1	1:D:759:ASP:HB2	2.45	0.51
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.92	0.51
1:A:417:GLU:HG2	1:A:497:LEU:HD21	1.92	0.51
1:A:632:ARG:NH1	1:A:637:ASN:O	2.44	0.51
1:A:841:GLN:O	1:A:844:SER:OG	2.25	0.51
1:B:515:TRP:O	1:B:519:MET:HG3	2.11	0.51
1:B:560:PRO:HG2	1:B:917:THR:HA	1.93	0.51
1:B:673:THR:HA	1:B:832:THR:OG1	2.11	0.51
1:C:445:ILE:HG12	1:C:935:LYS:HG3	1.91	0.51
1:C:568:ASP:CG	1:C:632:ARG:HH22	2.13	0.51
1:D:113:LEU:HD11	1:F:128:SER:CB	2.30	0.51
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.92	0.51
1:D:363:ARG:O	1:D:366:LEU:HB2	2.10	0.51
1:F:110:LYS:O	1:F:113:LEU:HB2	2.10	0.51
1:F:395:MET:O	1:F:398:MET:HB2	2.11	0.51
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.93	0.51
1:F:666:ILE:HD12	1:F:857:MET:SD	2.51	0.51
1:F:667:VAL:HB	1:F:668:GLU:OE2	2.10	0.51
1:B:44:THR:HA	1:B:90:ILE:O	2.10	0.51
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.92	0.51
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.92	0.51
1:C:538:THR:CG2	1:C:542:LEU:HD13	2.41	0.51
1:C:568:ASP:O	1:C:629:TRP:HH2	1.94	0.51
1:C:982:MET:O	1:C:985:VAL:N	2.44	0.51
1:D:225:VAL:HG12	1:E:772:ALA:HB1	1.93	0.51
1:D:457:ALA:CA	1:D:468:ARG:HG3	2.37	0.51
1:D:899:VAL:HA	1:D:902:LEU:HD22	1.92	0.51
1:E:162:MET:HA	1:E:313:MET:HE1	1.91	0.51
1:E:1016:PHE:O	1:E:1019:VAL:HB	2.10	0.51
1:F:639:VAL:HA	1:F:642:ILE:HD12	1.92	0.51
1:F:892:ILE:CG2	1:F:941:VAL:HG11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:925:GLY:HA2	1.92	0.51
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.76	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.92	0.51
1:C:778:PRO:O	1:C:781:ILE:HG12	2.10	0.51
1:E:438:ILE:O	1:E:441:ALA:HB3	2.11	0.51
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.76	0.51
1:F:144:ASN:O	1:F:284:GLN:NE2	2.42	0.51
1:F:375:VAL:HA	1:F:480:LEU:HD13	1.91	0.51
1:F:455:PRO:HG2	1:F:875:SER:HA	1.91	0.51
1:F:770:SER:HB2	1:F:784:TRP:CZ2	2.46	0.51
1:A:166:ILE:HG22	1:A:175:VAL:HG21	1.93	0.51
1:D:573:MET:HG3	1:D:661:PHE:CE2	2.45	0.51
1:E:68:ASN:HB3	1:E:114:ALA:HB2	1.92	0.51
1:A:209:ALA:O	1:A:237:GLN:NE2	2.43	0.51
1:A:219:LEU:HD13	1:A:230:LEU:HD21	1.93	0.51
1:B:143:ILE:O	1:B:321:LEU:HG	2.11	0.51
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.44	0.51
1:B:678:GLU:HG2	1:B:814:TYR:CG	2.46	0.51
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.93	0.51
1:C:329:THR:O	1:C:332:PHE:HB3	2.11	0.51
1:C:616:GLY:N	1:C:619:THR:OG1	2.43	0.51
1:C:966:ARG:O	1:C:970:ILE:HG13	2.11	0.51
1:C:982:MET:HB3	1:C:983:PRO:HD3	1.93	0.51
1:D:562:SER:N	1:D:917:THR:OG1	2.39	0.51
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.44	0.51
1:E:109:ASN:OD1	1:E:110:LYS:N	2.44	0.51
1:E:237:GLN:OE1	1:F:742:ASN:ND2	2.44	0.51
1:F:409:ALA:O	1:F:413:VAL:HG23	2.11	0.51
1:F:542:LEU:O	1:F:546:LEU:HG	2.11	0.51
1:F:687:HIS:NE2	1:F:718:ASP:OD1	2.43	0.51
1:A:571:VAL:CG2	1:A:625:SER:HA	2.35	0.51
1:B:372:VAL:O	1:B:376:LEU:HG	2.10	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:287:SER:OG	1:C:288:GLY:N	2.42	0.51
1:D:168:ARG:NH2	1:E:816:GLY:HA3	2.26	0.51
1:D:216:ALA:HB1	1:D:234:ILE:O	2.10	0.51
1:D:577:GLN:OE1	1:D:619:THR:HG22	2.11	0.51
1:D:678:GLU:OE1	1:D:678:GLU:HA	2.11	0.51
1:F:406:VAL:O	1:F:407:ASP:C	2.49	0.51
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.25	0.51
1:A:228:GLN:NE2	1:A:230:LEU:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLU:OE1	1:A:627:LYS:HA	2.12	0.50
1:B:181:GLN:HG2	1:B:182:TYR:N	2.25	0.50
1:B:574:THR:HA	1:B:660:ALA:HA	1.92	0.50
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.46	0.50
1:E:423:GLU:O	1:E:502:LYS:HB2	2.11	0.50
1:E:953:LYS:HG3	1:E:957:GLU:CD	2.31	0.50
1:F:445:ILE:HG12	1:F:935:LYS:HG3	1.93	0.50
1:F:830:LYS:HG3	1:F:831:SER:N	2.26	0.50
1:A:605:ASN:ND2	1:A:637:ASN:HA	2.24	0.50
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.44	0.50
1:B:375:VAL:HG11	1:B:481:SER:HB3	1.92	0.50
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.50
1:D:368:PRO:HD3	1:D:413:VAL:HG21	1.94	0.50
1:F:836:MET:HG2	1:F:854:TRP:CH2	2.46	0.50
1:A:511:GLY:CA	1:A:515:TRP:CD1	2.94	0.50
1:A:908:LEU:O	1:A:911:ALA:HB3	2.10	0.50
1:B:493:CYS:O	1:B:497:LEU:HB2	2.11	0.50
1:C:129:VAL:O	1:C:130:GLU:HG3	2.10	0.50
1:C:377:LEU:O	1:C:380:PHE:HB2	2.12	0.50
1:C:666:ILE:HD13	1:C:669:LEU:HD12	1.94	0.50
1:C:939:LEU:HB3	1:C:966:ARG:CD	2.37	0.50
1:D:200:PRO:HA	1:D:203:VAL:CG2	2.41	0.50
1:D:899:VAL:HG21	1:D:937:ALA:HB2	1.93	0.50
1:E:583:THR:HG23	1:E:585:GLU:H	1.77	0.50
1:F:49:TYR:N	1:F:86:GLY:O	2.40	0.50
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.93	0.50
1:F:508:GLY:O	1:F:509:LYS:HB2	2.09	0.50
1:F:947:LEU:HD22	1:F:953:LYS:CE	2.42	0.50
1:A:372:VAL:HG13	1:A:405:LEU:HD12	1.94	0.50
1:A:567:GLU:HG2	1:A:665:ALA:HB2	1.92	0.50
1:B:917:THR:O	1:B:919:ASP:N	2.45	0.50
1:C:737:SER:O	1:C:741:ILE:HG22	2.10	0.50
1:C:927:LEU:O	1:C:930:ILE:HB	2.11	0.50
1:D:83:ASP:OD2	1:D:810:ARG:NH1	2.44	0.50
1:D:691:THR:HG23	1:D:694:ARG:NH2	2.26	0.50
1:E:115:MET:SD	1:E:123:GLN:HG2	2.52	0.50
1:F:3:ASN:OD1	1:F:486:LEU:HB3	2.11	0.50
1:F:338:HIS:O	1:F:341:VAL:HB	2.12	0.50
1:F:918:ASN:O	1:F:918:ASN:ND2	2.39	0.50
1:A:894:PHE:HA	1:A:897:MET:HE3	1.93	0.50
1:C:11:PHE:O	1:C:11:PHE:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:MET:HB3	1:C:871:LEU:HD21	1.94	0.50
1:C:860:GLN:O	1:C:863:LEU:HB3	2.11	0.50
1:C:887:TYR:O	1:C:889:SER:N	2.42	0.50
1:C:927:LEU:O	1:C:928:THR:C	2.50	0.50
1:C:953:LYS:HG2	1:C:957:GLU:OE2	2.11	0.50
1:D:616:GLY:N	1:D:619:THR:OG1	2.44	0.50
1:E:45:ILE:O	1:E:89:GLN:HA	2.12	0.50
1:E:355:MET:HB3	1:E:365:THR:CB	2.41	0.50
1:E:700:GLU:HB3	1:E:842:LEU:HD22	1.93	0.50
1:A:375:VAL:HG13	1:A:480:LEU:CB	2.42	0.50
1:A:649:ALA:O	1:A:653:ILE:HG12	2.12	0.50
1:A:989:GLY:N	1:A:992:SER:OG	2.44	0.50
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.94	0.50
1:B:573:MET:HG3	1:B:661:PHE:HE2	1.77	0.50
1:C:68:ASN:O	1:C:110:LYS:HB3	2.11	0.50
1:C:963:VAL:HA	1:C:966:ARG:HH22	1.77	0.50
1:D:172:VAL:HG22	1:D:302:THR:HG23	1.93	0.50
1:D:917:THR:O	1:D:919:ASP:N	2.45	0.50
1:F:406:VAL:O	1:F:408:ASP:N	2.45	0.50
1:F:773:LYS:HG3	1:F:774:TYR:CZ	2.47	0.50
1:A:394:THR:HG22	1:A:473:THR:OG1	2.12	0.50
1:B:27:ILE:HD13	1:B:380:PHE:CG	2.47	0.50
1:C:311:ALA:O	1:C:314:GLU:HB2	2.12	0.50
1:D:242:SER:OG	1:D:245:GLU:HG2	2.11	0.50
1:D:545:TYR:HB2	1:D:1016:PHE:HE2	1.76	0.50
1:D:747:ALA:O	1:D:769:MET:HA	2.12	0.50
1:E:697:LEU:HD12	1:E:700:GLU:HB2	1.94	0.50
1:F:355:MET:SD	1:F:368:PRO:HB2	2.52	0.50
1:F:893:PRO:O	1:F:897:MET:HG2	2.11	0.50
1:B:595:THR:O	1:B:599:LEU:HG	2.12	0.50
2:B:2000:LMT:H6E	2:B:2000:LMT:O5B	2.11	0.50
1:C:162:MET:O	1:C:166:ILE:N	2.41	0.50
1:D:188:MET:HB3	1:D:193:LEU:CD1	2.42	0.50
1:D:222:THR:HA	1:D:224:PRO:CD	2.38	0.50
1:D:249:ILE:O	1:D:262:LEU:N	2.45	0.50
1:D:525:HIS:NE2	1:D:529:ASP:OD1	2.45	0.50
1:D:854:TRP:CE3	1:D:858:SER:HB2	2.46	0.50
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.94	0.50
1:E:632:ARG:NH1	1:E:637:ASN:O	2.45	0.50
1:F:1016:PHE:HB3	1:F:1020:PHE:CZ	2.46	0.50
1:B:771:GLU:HB3	1:B:774:TYR:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.93	0.50
1:D:248:LYS:HG2	1:D:263:ARG:HH21	1.76	0.50
1:E:76:MET:SD	1:E:859:TYR:HE2	2.35	0.50
1:F:112:GLN:HG3	1:F:115:MET:HG3	1.93	0.50
1:F:219:LEU:H	1:F:219:LEU:HD12	1.76	0.50
1:F:966:ARG:NH2	1:F:970:ILE:HD11	2.25	0.50
1:A:408:ASP:O	1:A:412:VAL:HG23	2.12	0.49
1:A:431:THR:HG21	1:A:490:PRO:O	2.12	0.49
1:B:709:THR:HB	1:B:827:ALA:HA	1.94	0.49
1:B:962:ALA:O	1:B:965:MET:HG2	2.12	0.49
1:C:602:GLU:OE1	1:C:645:ARG:HD2	2.12	0.49
1:C:740:ASP:O	1:C:744:THR:OG1	2.22	0.49
1:D:51:GLY:O	1:F:217:GLY:N	2.44	0.49
1:D:337:ILE:HA	1:D:340:VAL:HG23	1.94	0.49
1:D:632:ARG:NH1	1:D:638:LYS:HA	2.23	0.49
1:D:889:SER:HB3	1:D:892:ILE:HB	1.92	0.49
1:D:920:VAL:HA	1:D:923:GLN:OE1	2.11	0.49
1:E:452:VAL:HA	1:E:875:SER:OG	2.12	0.49
1:F:5:PHE:O	1:F:7:ASP:N	2.42	0.49
1:F:484:VAL:O	1:F:487:ILE:N	2.38	0.49
1:C:687:HIS:NE2	1:C:718:ASP:OD2	2.35	0.49
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.94	0.49
1:E:281:PHE:HB2	1:E:610:PHE:HE1	1.77	0.49
1:A:753:TYR:HB2	1:A:767:TYR:CE1	2.47	0.49
1:B:412:VAL:HG22	1:B:438:ILE:CD1	2.41	0.49
1:C:465:ALA:O	1:C:469:GLN:HG2	2.12	0.49
1:D:1006:MET:O	1:D:1009:ALA:HB3	2.11	0.49
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.95	0.49
1:E:356:TYR:HD1	1:E:365:THR:HG21	1.76	0.49
1:E:478:MET:O	1:E:482:VAL:HG12	2.12	0.49
1:E:748:ALA:O	1:E:770:SER:HB3	2.12	0.49
1:E:769:MET:HG2	1:E:770:SER:H	1.77	0.49
1:F:479:ALA:O	1:F:483:LEU:HG	2.12	0.49
1:F:893:PRO:HA	1:F:896:VAL:HG12	1.93	0.49
1:A:212:ALA:HA	1:A:239:ARG:HE	1.78	0.49
1:A:475:VAL:HA	1:A:478:MET:HE1	1.95	0.49
1:B:57:VAL:HG11	1:B:86:GLY:O	2.11	0.49
1:C:425:LEU:HB3	1:C:429:GLU:CG	2.42	0.49
1:C:569:GLN:OE1	1:C:663:LEU:HD11	2.12	0.49
1:D:18:ILE:HG13	1:E:881:LEU:HD23	1.93	0.49
1:D:695:ASN:O	1:D:698:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ASP:OD2	1:E:146:ASP:N	2.45	0.49
1:E:987:SER:O	1:E:992:SER:HB2	2.12	0.49
1:A:177:LEU:HD13	1:A:179:GLY:O	2.11	0.49
1:A:475:VAL:HA	1:A:478:MET:CE	2.43	0.49
1:B:770:SER:HG	1:B:775:ARG:HG2	1.76	0.49
1:D:249:ILE:HB	1:D:262:LEU:HB2	1.94	0.49
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.94	0.49
1:D:415:ASN:O	1:D:419:VAL:HG23	2.13	0.49
1:D:691:THR:HG23	1:D:694:ARG:HH22	1.77	0.49
1:D:826:ALA:HB2	1:D:835:ALA:HB2	1.93	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.95	0.49
1:F:272:GLY:N	1:F:275:TYR:OH	2.22	0.49
1:A:695:ASN:HA	1:A:698:LEU:HD12	1.94	0.49
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.95	0.49
1:B:574:THR:HG23	1:B:622:ALA:HB3	1.92	0.49
1:B:906:GLY:HA3	1:B:1008:THR:HG21	1.95	0.49
1:B:961:ASP:O	1:B:964:ARG:HB3	2.11	0.49
1:E:434:SER:O	1:E:438:ILE:HG12	2.13	0.49
1:E:514:GLY:C	1:E:516:PHE:H	2.15	0.49
1:E:747:ALA:O	1:E:769:MET:HA	2.13	0.49
1:A:952:GLY:HA2	1:A:1035:ILE:HG22	1.93	0.49
1:B:56:THR:O	1:B:60:THR:OG1	2.19	0.49
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.94	0.49
1:B:280:GLU:HG2	1:B:283:GLY:C	2.32	0.49
1:B:362:PHE:HA	1:B:365:THR:CG2	2.42	0.49
1:E:527:TYR:O	1:E:531:VAL:HG23	2.13	0.49
1:F:365:THR:O	1:F:368:PRO:HD2	2.13	0.49
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.12	0.49
1:B:896:VAL:HG23	1:B:937:ALA:HB3	1.93	0.49
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.93	0.49
1:D:475:VAL:HA	1:D:478:MET:HE1	1.94	0.49
1:E:43:VAL:HG13	1:E:130:GLU:C	2.33	0.49
1:E:356:TYR:C	1:E:358:PHE:H	2.16	0.49
1:E:375:VAL:HG11	1:E:481:SER:HB3	1.95	0.49
1:F:81:ASN:HB2	1:F:89:GLN:HB2	1.95	0.49
1:F:213:GLN:OE1	1:F:238:THR:HA	2.13	0.49
1:F:406:VAL:O	1:F:409:ALA:N	2.45	0.49
1:A:199:THR:HG21	1:A:786:VAL:HA	1.95	0.49
1:A:636:GLU:HA	1:A:641:ALA:CB	2.42	0.49
1:B:988:THR:HA	1:B:992:SER:OG	2.13	0.49
1:C:599:LEU:O	1:C:603:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLN:HG3	1:D:152:GLU:N	2.28	0.49
1:F:75:LEU:CD1	1:F:92:LEU:HD12	2.43	0.49
1:F:144:ASN:ND2	1:F:319:SER:O	2.40	0.49
1:A:330:THR:HB	1:A:331:PRO:HD3	1.95	0.49
1:A:453:PHE:O	1:A:471:SER:OG	2.23	0.49
1:A:574:THR:HG23	1:A:622:ALA:HB3	1.94	0.49
1:A:1016:PHE:HB3	1:A:1020:PHE:CE1	2.48	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.12	0.49
1:C:678:GLU:HG2	1:C:814:TYR:CG	2.48	0.49
1:C:708:LEU:HD21	1:C:839:MET:HG2	1.95	0.49
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.47	0.49
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.95	0.49
1:F:133:SER:OG	1:F:293:LEU:O	2.14	0.49
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.95	0.49
1:A:225:VAL:HG11	1:B:773:LYS:HA	1.95	0.48
1:A:645:ARG:HA	1:A:648:ARG:HB3	1.95	0.48
1:D:462:SER:O	1:D:466:ILE:HG12	2.13	0.48
1:D:527:TYR:CE1	1:D:1014:ILE:HD12	2.47	0.48
1:D:860:GLN:O	1:D:863:LEU:HB2	2.13	0.48
1:F:311:ALA:HA	1:F:314:GLU:HG3	1.95	0.48
1:F:900:VAL:O	1:F:904:VAL:HG23	2.12	0.48
1:A:697:LEU:HD21	1:A:839:MET:HE1	1.95	0.48
1:B:508:GLY:O	1:B:510:LYS:N	2.42	0.48
1:C:686:GLY:O	1:C:690:LEU:N	2.37	0.48
1:D:155:SER:OG	1:D:179:GLY:HA3	2.13	0.48
1:D:413:VAL:O	1:D:417:GLU:HG2	2.13	0.48
1:D:749:TRP:HZ3	1:F:219:LEU:HG	1.78	0.48
1:E:101:ASP:HA	1:E:131:LYS:HZ2	1.78	0.48
1:A:378:GLY:O	1:A:381:ALA:HB3	2.14	0.48
1:A:401:ALA:O	1:A:405:LEU:HG	2.13	0.48
1:A:948:MET:O	1:A:1035:ILE:HG21	2.13	0.48
1:B:441:ALA:HB2	1:B:942:GLU:OE1	2.13	0.48
1:C:520:PHE:HE2	1:C:968:ARG:HD2	1.76	0.48
1:C:538:THR:HG23	1:C:542:LEU:HD13	1.94	0.48
1:D:184:MET:HB3	1:D:766:VAL:HG22	1.95	0.48
1:D:966:ARG:HB3	1:D:966:ARG:NH1	2.28	0.48
1:E:187:TRP:CZ3	1:E:769:MET:HB3	2.48	0.48
1:E:359:LEU:C	1:E:360:GLN:HG2	2.32	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.13	0.48
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.94	0.48
1:A:573:MET:HG3	1:A:661:PHE:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:PRO:O	1:A:798:ALA:HB3	2.13	0.48
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.78	0.48
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.95	0.48
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.77	0.48
1:C:645:ARG:O	1:C:648:ARG:HB3	2.13	0.48
1:D:7:ASP:OD2	1:D:432:ARG:NH2	2.41	0.48
1:D:354:VAL:HG22	1:D:975:LEU:HD23	1.96	0.48
1:D:375:VAL:HG11	1:D:481:SER:HB3	1.96	0.48
1:D:391:ASN:O	1:D:395:MET:HG2	2.13	0.48
1:D:568:ASP:OD1	1:D:632:ARG:NH2	2.43	0.48
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.94	0.48
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.29	0.48
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.95	0.48
1:A:225:VAL:HG22	1:B:776:MET:HE2	1.95	0.48
1:A:577:GLN:O	1:A:656:ALA:HB1	2.14	0.48
1:B:277:ILE:H	1:B:277:ILE:HG13	1.44	0.48
1:C:185:ARG:HB2	1:C:271:GLY:HA3	1.95	0.48
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.94	0.48
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.94	0.48
1:E:372:VAL:O	1:E:376:LEU:HG	2.12	0.48
1:E:757:PHE:CD2	1:E:766:VAL:HG22	2.49	0.48
1:F:9:PRO:HB3	1:F:495:THR:HG21	1.96	0.48
1:F:361:ASN:ND2	1:F:364:ALA:HB2	2.28	0.48
1:B:344:LEU:HD23	1:B:402:ILE:HG12	1.96	0.48
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.45	0.48
1:C:6:ILE:HG12	1:C:6:ILE:H	1.43	0.48
1:C:54:ALA:HB3	1:C:808:SER:O	2.14	0.48
1:C:925:GLY:O	1:C:929:THR:OG1	2.24	0.48
1:D:830:LYS:HG2	1:D:834:GLU:OE2	2.13	0.48
1:D:836:MET:HE1	1:D:862:ARG:HD2	1.94	0.48
1:D:896:VAL:HG23	1:D:937:ALA:HB3	1.95	0.48
1:D:936:ASN:O	1:D:940:ILE:HG13	2.14	0.48
1:E:239:ARG:HH12	1:E:756:ASP:H	1.60	0.48
1:F:400:LEU:O	1:F:404:LEU:HD22	2.14	0.48
1:F:587:THR:HG21	1:F:617:GLN:O	2.13	0.48
1:F:940:ILE:HA	1:F:966:ARG:NH1	2.28	0.48
1:A:607:GLU:HB2	1:A:627:LYS:N	2.28	0.48
1:B:349:ILE:O	1:B:352:PHE:HB3	2.13	0.48
1:B:872:TYR:HA	1:B:875:SER:HB2	1.95	0.48
1:B:954:GLY:HA2	1:B:1035:ILE:HG23	1.96	0.48
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:HD23	1:F:168:ARG:HB3	1.96	0.48
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.49	0.48
1:D:514:GLY:C	1:D:516:PHE:H	2.16	0.48
1:D:571:VAL:CG2	1:D:625:SER:HA	2.35	0.48
1:E:317:PHE:CZ	1:E:323:ILE:HG12	2.49	0.48
1:E:422:GLU:O	1:E:502:LYS:HG3	2.13	0.48
1:F:362:PHE:H	1:F:363:ARG:NH2	2.12	0.48
1:F:414:GLU:OE1	1:F:968:ARG:NH1	2.43	0.48
1:F:900:VAL:HG22	1:F:930:ILE:HG23	1.95	0.48
1:B:535:LEU:HD21	1:B:1019:VAL:HA	1.96	0.48
1:C:902:LEU:HG	1:C:1012:LEU:HB3	1.95	0.48
1:C:1031:LYS:HD2	1:C:1033:GLU:HB2	1.95	0.48
1:F:58:GLN:OE1	1:F:813:ARG:HD2	2.14	0.48
1:F:152:GLU:HG2	1:F:275:TYR:HE2	1.79	0.48
1:F:853:ASP:OD2	1:F:854:TRP:N	2.46	0.48
1:A:70:ASN:OD1	1:A:110:LYS:HD2	2.14	0.48
1:A:361:ASN:O	1:A:365:THR:HG22	2.14	0.48
1:A:532:GLY:O	1:A:536:ARG:HG2	2.14	0.48
1:A:723:LYS:HB2	1:A:805:GLU:OE2	2.14	0.48
1:B:952:GLY:HA2	1:B:1035:ILE:HD11	1.95	0.48
1:C:278:ILE:HD13	1:C:584:GLN:OE1	2.14	0.48
1:C:654:LYS:HA	1:C:654:LYS:HD3	1.51	0.48
1:C:893:PRO:O	1:C:897:MET:HG2	2.14	0.48
1:D:956:ILE:HD12	1:D:957:GLU:H	1.79	0.48
1:E:78:MET:O	1:E:815:ASN:N	2.35	0.48
1:E:143:ILE:O	1:E:321:LEU:HG	2.13	0.48
1:E:887:TYR:HB3	1:E:892:ILE:HD12	1.95	0.48
1:E:906:GLY:HA3	1:E:1008:THR:CG2	2.41	0.48
1:F:459:PHE:CE1	1:F:871:LEU:HG	2.48	0.48
1:A:893:PRO:HB2	1:A:897:MET:HE2	1.94	0.48
1:B:535:LEU:HD13	1:B:1022:VAL:HG21	1.96	0.48
1:C:110:LYS:HA	1:C:110:LYS:HD3	1.68	0.48
1:D:61:VAL:HG13	1:D:118:LEU:HD13	1.95	0.48
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.96	0.48
1:E:414:GLU:HG3	1:E:969:PRO:HB3	1.96	0.48
1:F:901:PRO:O	1:F:904:VAL:N	2.47	0.48
1:F:956:ILE:H	1:F:956:ILE:HD12	1.79	0.48
1:A:157:TYR:OH	1:A:316:PHE:O	2.32	0.47
1:B:277:ILE:HD12	1:B:277:ILE:O	2.14	0.47
1:B:708:LEU:HG	1:B:838:LEU:HD12	1.95	0.47
1:B:753:TYR:OH	1:B:756:ASP:OD1	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:ASN:CG	1:C:240:LEU:HG	2.35	0.47
1:C:1032:ASN:OD1	1:C:1033:GLU:HA	2.14	0.47
1:D:164:ASP:HB3	1:D:168:ARG:NH2	2.28	0.47
1:D:890:TRP:NE1	1:F:10:ILE:HG12	2.29	0.47
1:D:908:LEU:HD23	1:D:922:PHE:HZ	1.79	0.47
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.95	0.47
1:E:906:GLY:CA	1:E:1008:THR:HG21	2.44	0.47
1:F:54:ALA:HB3	1:F:808:SER:O	2.13	0.47
1:F:103:ALA:O	1:F:107:VAL:HG23	2.14	0.47
1:F:120:GLN:HG3	1:F:123:GLN:OE1	2.14	0.47
1:F:398:MET:HE3	1:F:398:MET:HB3	1.77	0.47
1:F:692:GLN:HA	1:F:695:ASN:HB2	1.96	0.47
1:F:770:SER:HB3	1:F:775:ARG:HD3	1.95	0.47
1:F:983:PRO:HA	1:F:986:ILE:HG22	1.94	0.47
1:A:278:ILE:CG1	1:A:613:ASN:HB3	2.44	0.47
1:B:352:PHE:HZ	1:B:362:PHE:CE1	2.32	0.47
1:B:422:GLU:O	1:B:502:LYS:NZ	2.47	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.13	0.47
1:C:551:GLY:O	1:C:555:LEU:HB2	2.14	0.47
1:D:233:SER:O	1:E:721:GLN:HB2	2.14	0.47
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.96	0.47
1:E:99:ASP:HB3	1:E:102:ILE:HB	1.96	0.47
1:E:887:TYR:C	1:E:889:SER:H	2.17	0.47
1:F:917:THR:O	1:F:919:ASP:N	2.47	0.47
1:A:165:ALA:HB3	1:A:313:MET:CE	2.44	0.47
1:A:241:THR:HG23	1:A:758:ILE:O	2.14	0.47
1:A:669:LEU:HD23	1:A:669:LEU:HA	1.61	0.47
1:B:45:ILE:HA	1:B:128:SER:O	2.14	0.47
1:D:137:LEU:HD22	1:D:293:LEU:HB2	1.96	0.47
1:E:20:MET:CG	1:E:374:VAL:HG22	2.44	0.47
1:E:638:LYS:NZ	1:E:988:THR:HG23	2.29	0.47
1:F:914:ARG:C	1:F:916:LEU:H	2.16	0.47
1:F:959:THR:O	1:F:963:VAL:HB	2.14	0.47
1:A:2:PRO:HB2	1:A:3:ASN:H	1.45	0.47
1:A:127:VAL:O	1:B:113:LEU:HD13	2.15	0.47
1:A:143:ILE:HG12	1:A:322:LYS:O	2.15	0.47
1:A:317:PHE:CD2	1:A:321:LEU:HD12	2.49	0.47
1:B:625:SER:O	1:B:626:LEU:HD23	2.14	0.47
1:B:773:LYS:HG3	1:B:774:TYR:CZ	2.49	0.47
1:C:242:SER:HB2	1:C:245:GLU:H	1.78	0.47
1:C:826:ALA:HB3	1:C:830:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:THR:HG21	1:D:598:TYR:CE2	2.49	0.47
1:D:872:TYR:O	1:D:876:LEU:HB2	2.14	0.47
1:A:169:THR:HB	1:A:172:VAL:CG2	2.45	0.47
1:C:544:LEU:HD12	1:C:547:ILE:HD12	1.97	0.47
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.52	0.47
1:E:35:TYR:CE2	1:E:393:LEU:HD21	2.49	0.47
1:E:148:THR:HG21	1:E:319:SER:HB2	1.96	0.47
1:E:165:ALA:HB3	1:E:313:MET:HE2	1.97	0.47
1:E:356:TYR:O	1:E:358:PHE:N	2.47	0.47
1:E:543:VAL:HA	1:E:546:LEU:HG	1.95	0.47
1:A:864:SER:OG	1:A:865:GLY:N	2.47	0.47
1:A:880:PHE:HD1	1:A:897:MET:HE2	1.79	0.47
1:B:167:SER:HB3	1:B:175:VAL:HG21	1.97	0.47
1:B:364:ALA:O	1:B:368:PRO:HD3	2.14	0.47
1:C:119:PRO:O	1:C:122:VAL:HB	2.15	0.47
1:C:203:VAL:O	1:C:207:ILE:HG13	2.14	0.47
1:C:395:MET:HA	1:C:398:MET:HG3	1.97	0.47
1:C:966:ARG:HE	1:C:970:ILE:HD11	1.79	0.47
1:D:235:ILE:O	1:E:723:LYS:HD2	2.14	0.47
1:D:282:ASN:HD21	1:D:608:SER:HA	1.78	0.47
1:D:531:VAL:HG13	1:D:534:ILE:HD11	1.96	0.47
1:D:675:PHE:HB2	1:D:854:TRP:CZ3	2.49	0.47
1:E:518:ARG:O	1:E:521:GLU:N	2.47	0.47
1:E:749:TRP:CZ2	1:E:781:ILE:HD13	2.50	0.47
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.95	0.47
1:F:248:LYS:O	1:F:261:LEU:HD22	2.14	0.47
1:A:157:TYR:HE2	1:A:317:PHE:CD1	2.33	0.47
1:A:587:THR:HB	1:A:613:ASN:ND2	2.30	0.47
1:A:602:GLU:OE1	1:A:645:ARG:HD2	2.14	0.47
1:A:770:SER:HG	1:A:775:ARG:HG2	1.80	0.47
1:B:49:TYR:HB3	1:B:57:VAL:HG12	1.97	0.47
1:B:418:ARG:O	1:B:422:GLU:HB2	2.15	0.47
1:B:513:PHE:O	1:B:515:TRP:N	2.48	0.47
1:B:653:ILE:O	1:B:654:LYS:HD2	2.15	0.47
1:B:770:SER:HB2	1:B:784:TRP:CZ2	2.50	0.47
1:B:1035:ILE:H	1:B:1036:GLU:HG3	1.79	0.47
1:C:203:VAL:HG12	1:C:207:ILE:HD11	1.97	0.47
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.97	0.47
1:D:188:MET:SD	1:D:200:PRO:HG3	2.55	0.47
1:D:456:MET:HE2	1:D:471:SER:HA	1.97	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:736:VAL:HG21	1:D:799:PHE:CE1	2.50	0.47
1:D:776:MET:CE	1:F:225:VAL:HG22	2.45	0.47
1:D:905:ILE:O	1:D:909:LEU:HB2	2.15	0.47
1:D:1030:ARG:HE	1:D:1031:LYS:N	2.13	0.47
1:E:182:TYR:O	1:E:764:LYS:HD3	2.15	0.47
1:E:351:VAL:O	1:E:354:VAL:HB	2.13	0.47
1:E:355:MET:CE	1:E:410:ILE:HG12	2.44	0.47
1:E:508:GLY:HA2	1:E:514:GLY:O	2.14	0.47
1:E:571:VAL:HG13	1:E:623:PHE:HE1	1.80	0.47
1:E:578:LEU:O	1:E:618:ASN:ND2	2.38	0.47
1:E:780:ASP:O	1:E:783:ASP:HB2	2.14	0.47
1:E:836:MET:O	1:E:840:GLU:HG3	2.13	0.47
1:F:228:GLN:NE2	1:F:230:LEU:O	2.45	0.47
1:F:480:LEU:O	1:F:484:VAL:HG23	2.15	0.47
1:F:689:LYS:HD2	1:F:689:LYS:N	2.29	0.47
1:F:1008:THR:O	1:F:1012:LEU:HB2	2.15	0.47
1:B:960:LEU:O	1:B:963:VAL:HG12	2.15	0.47
1:B:1007:VAL:O	1:B:1011:VAL:HG23	2.14	0.47
1:C:204:ILE:O	1:C:207:ILE:HB	2.15	0.47
1:C:402:ILE:O	1:C:406:VAL:HG22	2.15	0.47
1:D:103:ALA:O	1:D:107:VAL:HG23	2.15	0.47
1:D:199:THR:O	1:D:202:ASP:N	2.47	0.47
1:D:770:SER:HB2	1:D:784:TRP:CZ2	2.49	0.47
1:E:944:ALA:HB3	1:E:1021:PHE:HE1	1.78	0.47
1:F:356:TYR:C	1:F:358:PHE:H	2.16	0.47
1:F:407:ASP:O	1:F:411:VAL:HG23	2.15	0.47
1:F:516:PHE:O	1:F:520:PHE:N	2.43	0.47
1:F:1006:MET:O	1:F:1010:THR:HG23	2.15	0.47
1:A:23:GLY:HA3	1:A:377:LEU:O	2.14	0.47
1:A:41:PRO:HD3	1:A:97:GLY:H	1.79	0.47
1:A:300:LEU:O	1:A:303:ALA:HB3	2.15	0.47
1:A:826:ALA:HB2	1:A:835:ALA:HB2	1.97	0.47
1:B:740:ASP:O	1:B:744:THR:OG1	2.23	0.47
1:E:410:ILE:HD13	1:E:972:MET:HB3	1.97	0.47
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.97	0.47
1:F:154:ILE:O	1:F:158:VAL:HG23	2.15	0.47
1:F:222:THR:HA	1:F:224:PRO:HD3	1.97	0.47
1:A:68:ASN:O	1:A:110:LYS:HB3	2.16	0.47
1:A:190:PRO:HG3	1:A:784:TRP:CH2	2.50	0.47
1:A:559:LEU:HD13	1:A:918:ASN:HB2	1.96	0.47
1:A:1032:ASN:O	1:A:1033:GLU:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:THR:O	1:B:1012:LEU:HB2	2.15	0.47
1:C:413:VAL:O	1:C:417:GLU:HG2	2.15	0.47
1:C:422:GLU:HB3	1:C:423:GLU:HG3	1.96	0.47
1:C:669:LEU:HD23	1:C:669:LEU:HA	1.61	0.47
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.96	0.47
1:E:61:VAL:HG22	1:E:118:LEU:HD22	1.97	0.47
1:E:594:VAL:HG22	1:E:650:PHE:CE2	2.50	0.47
1:E:932:LEU:HA	1:E:932:LEU:HD23	1.72	0.47
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.28	0.47
1:F:69:MET:SD	1:F:72:ILE:HD11	2.55	0.47
1:F:371:ALA:O	1:F:375:VAL:HG23	2.15	0.47
1:F:471:SER:O	1:F:475:VAL:HB	2.14	0.47
1:F:506:GLY:C	1:F:508:GLY:H	2.18	0.47
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.49	0.47
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.68	0.46
1:B:583:THR:HG23	1:B:585:GLU:H	1.80	0.46
1:B:959:THR:HG21	1:B:1022:VAL:HG23	1.97	0.46
1:C:104:GLN:HG3	1:C:105:VAL:N	2.29	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.43	0.46
1:D:742:ASN:ND2	1:F:214:VAL:HG21	2.30	0.46
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.97	0.46
1:E:356:TYR:CD1	1:E:365:THR:HG21	2.50	0.46
1:E:728:GLN:NE2	1:E:738:ILE:HG21	2.30	0.46
1:E:785:TYR:CZ	1:E:795:PRO:HB3	2.50	0.46
1:F:510:LYS:O	1:F:512:PHE:N	2.40	0.46
1:F:697:LEU:HD12	1:F:846:LEU:HD11	1.97	0.46
1:F:723:LYS:HG2	1:F:803:ARG:CZ	2.45	0.46
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.59	0.46
1:A:340:VAL:O	1:A:343:THR:HB	2.15	0.46
1:B:344:LEU:HD11	1:B:398:MET:HE2	1.98	0.46
1:B:393:LEU:HD22	1:B:470:PHE:CE1	2.50	0.46
1:B:709:THR:O	1:B:710:SER:OG	2.31	0.46
1:C:527:TYR:HE2	1:C:963:VAL:HG13	1.80	0.46
1:D:880:PHE:HA	1:D:883:LEU:HD12	1.97	0.46
1:F:486:LEU:O	1:F:490:PRO:HG2	2.15	0.46
1:F:563:PHE:CE2	1:F:564:LEU:HD13	2.50	0.46
1:A:190:PRO:HG2	1:A:774:TYR:CG	2.51	0.46
1:A:200:PRO:HB2	1:A:744:THR:HG22	1.98	0.46
1:A:281:PHE:HB2	1:A:610:PHE:HE1	1.80	0.46
1:A:772:ALA:HB1	1:C:225:VAL:HG12	1.97	0.46
1:A:932:LEU:HD23	1:A:932:LEU:HA	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:O	1:B:369:THR:HB	2.15	0.46
1:C:572:PHE:CE1	1:C:643:THR:HG22	2.51	0.46
1:C:587:THR:HG21	1:C:617:GLN:O	2.15	0.46
1:C:899:VAL:CG2	1:C:1017:VAL:HG22	2.45	0.46
1:D:23:GLY:O	1:D:27:ILE:HG13	2.15	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.16	0.46
1:E:101:ASP:HA	1:E:131:LYS:NZ	2.30	0.46
1:F:351:VAL:O	1:F:355:MET:HE2	2.15	0.46
1:F:419:VAL:HG21	1:F:434:SER:HB3	1.96	0.46
1:F:859:TYR:HD2	1:F:859:TYR:O	1.98	0.46
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.96	0.46
1:A:412:VAL:HG22	1:A:438:ILE:HD11	1.96	0.46
1:A:574:THR:HG22	1:A:624:VAL:CG2	2.45	0.46
1:A:836:MET:HG2	1:A:854:TRP:CH2	2.49	0.46
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.97	0.46
1:B:507:GLU:O	1:B:509:LYS:HG3	2.16	0.46
1:C:45:ILE:HG21	1:C:111:LEU:HG	1.96	0.46
1:C:293:LEU:HD22	1:C:297:ALA:HB3	1.96	0.46
1:C:1007:VAL:O	1:C:1011:VAL:HG23	2.16	0.46
1:D:55:LYS:HB3	1:D:55:LYS:HE2	1.71	0.46
1:D:749:TRP:CZ3	1:F:219:LEU:HG	2.51	0.46
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.98	0.46
1:E:653:ILE:C	1:E:654:LYS:HD2	2.36	0.46
1:E:841:GLN:O	1:E:844:SER:OG	2.33	0.46
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.35	0.46
1:F:288:GLY:O	1:F:289:LEU:HD23	2.16	0.46
1:F:795:PRO:HG2	1:F:798:ALA:HB2	1.97	0.46
1:A:379:THR:HG21	1:A:477:ALA:HB2	1.96	0.46
1:B:462:SER:O	1:B:466:ILE:HG13	2.15	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.97	0.46
1:B:527:TYR:CE1	1:B:1014:ILE:HD12	2.51	0.46
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.78	0.46
1:C:153:ASP:OD2	1:C:153:ASP:N	2.47	0.46
1:D:621:ILE:HD12	1:D:622:ALA:H	1.79	0.46
1:D:698:LEU:HD21	1:D:713:PRO:HD3	1.96	0.46
1:D:796:PHE:O	1:D:800:SER:OG	2.30	0.46
1:E:453:PHE:O	1:E:471:SER:OG	2.32	0.46
1:E:484:VAL:O	1:E:489:THR:HG23	2.15	0.46
1:E:720:PRO:HA	1:E:806:TYR:HA	1.96	0.46
1:F:6:ILE:H	1:F:6:ILE:HG12	1.40	0.46
1:F:96:SER:HB3	1:F:461:GLY:HA2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:VAL:O	1:F:326:PRO:HD2	2.15	0.46
1:F:293:LEU:HD13	1:F:294:ALA:O	2.15	0.46
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.74	0.46
1:A:211:ASN:O	1:A:755:ASN:ND2	2.46	0.46
1:A:359:LEU:C	1:A:360:GLN:HG2	2.34	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB2	1.97	0.46
1:A:749:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.46
1:B:76:MET:HB2	1:B:93:THR:O	2.16	0.46
1:B:394:THR:HG23	1:B:469:GLN:OE1	2.15	0.46
1:B:840:GLU:HG2	1:B:852:TYR:CE1	2.51	0.46
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.98	0.46
1:C:242:SER:O	1:C:246:PHE:HD1	1.99	0.46
1:C:855:THR:HG23	1:C:856:GLY:N	2.31	0.46
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.57	0.46
1:D:30:LEU:CD1	1:D:384:ALA:HA	2.46	0.46
1:D:420:MET:HB3	1:D:500:ILE:HB	1.98	0.46
1:D:749:TRP:CE3	1:F:234:ILE:HD11	2.51	0.46
1:E:222:THR:HA	1:E:224:PRO:HD3	1.98	0.46
1:E:896:VAL:HG23	1:E:937:ALA:HB3	1.98	0.46
1:F:664:PRO:HD3	1:F:672:ALA:C	2.36	0.46
1:F:967:LEU:HA	1:F:970:ILE:HD12	1.98	0.46
1:A:1006:MET:O	1:A:1010:THR:HG23	2.16	0.46
1:B:352:PHE:C	1:B:352:PHE:CD2	2.88	0.46
1:C:135:SER:HB3	1:C:668:GLU:HA	1.98	0.46
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.15	0.46
1:C:900:VAL:O	1:C:904:VAL:HG23	2.16	0.46
1:D:136:PHE:CE2	1:D:292:LYS:HE3	2.50	0.46
1:D:277:ILE:HG12	1:D:614:GLY:HA3	1.98	0.46
1:D:787:ARG:HA	1:D:792:GLN:O	2.15	0.46
1:A:100:ALA:HB1	1:A:131:LYS:HD2	1.98	0.46
1:A:212:ALA:HA	1:A:239:ARG:NE	2.30	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.97	0.46
1:A:255:GLN:H	1:A:255:GLN:HG3	1.57	0.46
1:A:375:VAL:HG21	1:A:481:SER:HA	1.97	0.46
1:A:636:GLU:HA	1:A:641:ALA:HB3	1.98	0.46
1:B:727:ASP:OD1	1:B:730:LYS:HG3	2.16	0.46
1:B:906:GLY:HA3	1:B:1008:THR:CG2	2.46	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:250:LEU:CD1	1:C:259:ARG:HB3	2.45	0.46
1:C:277:ILE:HA	1:C:614:GLY:HA2	1.98	0.46
1:C:534:ILE:HG21	1:C:534:ILE:HD13	1.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:757:PHE:HE1	1:D:759:ASP:HB2	1.81	0.46
1:E:648:ARG:O	1:E:651:SER:OG	2.34	0.46
1:F:10:ILE:O	1:F:14:VAL:HG23	2.16	0.46
1:F:105:VAL:HA	1:F:108:GLN:HE21	1.80	0.46
1:F:421:ALA:O	1:F:503:GLY:N	2.30	0.46
1:F:757:PHE:CE1	1:F:759:ASP:HB2	2.50	0.46
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.86	0.46
1:A:438:ILE:O	1:A:442:LEU:HG	2.16	0.46
1:B:667:VAL:HB	1:B:668:GLU:CD	2.36	0.46
1:B:677:PHE:HB3	1:B:822:ILE:O	2.16	0.46
1:B:900:VAL:HG22	1:B:930:ILE:HG23	1.98	0.46
1:C:731:ALA:HA	1:C:736:VAL:HG23	1.97	0.46
1:C:902:LEU:HD23	1:C:1013:ALA:HA	1.97	0.46
1:D:30:LEU:HD13	1:D:384:ALA:HA	1.98	0.46
1:F:425:LEU:HB3	1:F:429:GLU:HG2	1.98	0.46
1:F:738:ILE:O	1:F:741:ILE:HG13	2.16	0.46
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.98	0.46
1:B:68:ASN:CB	1:B:114:ALA:HB2	2.46	0.46
1:B:457:ALA:HB2	1:B:471:SER:OG	2.16	0.46
1:B:544:LEU:O	1:B:547:ILE:HB	2.16	0.46
1:B:787:ARG:HA	1:B:792:GLN:O	2.15	0.46
1:C:2:PRO:HB2	1:C:3:ASN:OD1	2.15	0.46
1:C:836:MET:HA	1:C:854:TRP:CH2	2.51	0.46
1:E:4:PHE:O	1:E:8:ARG:HD2	2.15	0.46
1:E:190:PRO:HB3	1:E:784:TRP:CE2	2.51	0.46
1:E:691:THR:HA	1:E:694:ARG:NH1	2.31	0.46
1:E:748:ALA:O	1:E:769:MET:HG2	2.16	0.46
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.45	0.46
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.98	0.46
1:F:352:PHE:HA	1:F:355:MET:CE	2.46	0.46
1:F:566:ASP:CG	1:F:673:THR:HG23	2.36	0.46
1:F:945:LYS:O	1:F:948:MET:N	2.49	0.46
1:A:488:LEU:O	1:A:491:ALA:HB3	2.15	0.45
1:A:514:GLY:C	1:A:516:PHE:N	2.69	0.45
1:A:516:PHE:HA	1:A:519:MET:HG3	1.98	0.45
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.51	0.45
1:B:427:PRO:O	1:B:430:ALA:HB3	2.17	0.45
1:B:455:PRO:HG2	1:B:875:SER:HG	1.81	0.45
1:C:423:GLU:HB2	1:C:425:LEU:HG	1.98	0.45
1:C:986:ILE:O	1:C:986:ILE:HD13	2.16	0.45
1:D:136:PHE:HD2	1:D:292:LYS:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:CD1	1:D:259:ARG:HB3	2.44	0.45
1:D:332:PHE:CD1	1:D:569:GLN:HG2	2.50	0.45
1:D:559:LEU:HD13	1:D:918:ASN:HB2	1.96	0.45
1:E:748:ALA:HB3	1:E:749:TRP:HD1	1.81	0.45
1:F:110:LYS:HD3	1:F:110:LYS:HA	1.61	0.45
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.98	0.45
1:F:654:LYS:HB3	1:F:656:ALA:H	1.81	0.45
1:A:681:ASP:OD1	1:A:684:GLY:N	2.47	0.45
1:B:470:PHE:O	1:B:474:ILE:HG13	2.15	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.16	0.45
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.98	0.45
1:C:343:THR:HG23	1:C:983:PRO:HB2	1.98	0.45
1:C:542:LEU:O	1:C:546:LEU:HG	2.16	0.45
1:C:890:TRP:HA	1:C:890:TRP:HE3	1.81	0.45
1:D:3:ASN:O	1:D:5:PHE:N	2.49	0.45
1:D:184:MET:HB3	1:D:766:VAL:HG13	1.97	0.45
1:E:106:GLN:HA	1:E:109:ASN:ND2	2.31	0.45
1:E:172:VAL:CG2	1:E:306:ILE:HD11	2.46	0.45
1:E:445:ILE:HG21	1:E:935:LYS:CD	2.46	0.45
1:E:955:LEU:HD13	1:E:1025:ARG:HG2	1.98	0.45
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.46	0.45
1:F:171:GLY:HA3	1:F:302:THR:OG1	2.15	0.45
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.97	0.45
1:A:363:ARG:O	1:A:366:LEU:N	2.49	0.45
1:B:23:GLY:HA3	1:B:377:LEU:HB3	1.99	0.45
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.46	0.45
1:B:363:ARG:HD2	1:B:498:LYS:HD2	1.97	0.45
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.45
1:B:510:LYS:HB2	1:B:514:GLY:H	1.82	0.45
1:C:514:GLY:O	1:C:518:ARG:HD3	2.16	0.45
1:C:1006:MET:HA	1:C:1009:ALA:HB3	1.97	0.45
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.99	0.45
1:D:470:PHE:CE2	1:D:924:VAL:HG21	2.51	0.45
1:D:974:SER:CB	1:D:1010:THR:HG21	2.47	0.45
1:E:186:ILE:O	1:E:768:VAL:HA	2.16	0.45
1:F:65:ILE:HD13	1:F:90:ILE:HD11	1.97	0.45
1:F:77:TYR:CE1	1:F:93:THR:HG21	2.52	0.45
1:F:676:ASP:HB3	1:F:823:LEU:CD2	2.46	0.45
1:F:941:VAL:HG13	1:F:1021:PHE:CZ	2.52	0.45
1:F:1003:MET:O	1:F:1007:VAL:HG23	2.16	0.45
1:A:349:ILE:O	1:A:352:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LYS:HD3	1:A:654:LYS:HA	1.62	0.45
1:B:347:ALA:O	1:B:351:VAL:HG23	2.16	0.45
1:B:418:ARG:HD2	1:B:965:MET:HB2	1.98	0.45
1:C:407:ASP:N	1:C:407:ASP:OD1	2.48	0.45
1:C:662:ASN:OD1	1:C:663:LEU:HD23	2.16	0.45
1:E:54:ALA:N	1:E:84:SER:HA	2.31	0.45
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.99	0.45
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.82	0.45
1:E:982:MET:O	1:E:985:VAL:HG23	2.16	0.45
1:F:459:PHE:CZ	1:F:871:LEU:HG	2.52	0.45
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.78	0.45
1:A:981:VAL:O	1:A:984:LEU:N	2.46	0.45
1:C:527:TYR:OH	1:C:1014:ILE:O	2.24	0.45
1:C:527:TYR:CE2	1:C:963:VAL:HG13	2.52	0.45
1:C:812:GLU:HB2	1:C:819:SER:O	2.16	0.45
1:C:892:ILE:HD12	1:C:1021:PHE:HE1	1.81	0.45
1:D:3:ASN:O	1:D:4:PHE:C	2.55	0.45
1:D:293:LEU:HD13	1:D:294:ALA:O	2.16	0.45
1:D:414:GLU:OE2	1:D:969:PRO:HG3	2.16	0.45
1:D:572:PHE:CE1	1:D:643:THR:HG22	2.50	0.45
1:E:331:PRO:HA	1:E:334:LYS:HD2	1.98	0.45
1:E:697:LEU:HD12	1:E:697:LEU:HA	1.75	0.45
1:F:694:ARG:HD3	1:F:820:MET:SD	2.57	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.98	0.45
1:A:708:LEU:HA	1:A:825:GLN:O	2.16	0.45
1:A:900:VAL:O	1:A:904:VAL:HG23	2.17	0.45
1:A:948:MET:HG3	1:A:954:GLY:O	2.17	0.45
1:B:373:PRO:O	1:B:376:LEU:HB2	2.17	0.45
1:B:442:LEU:O	1:B:445:ILE:HG13	2.16	0.45
1:B:961:ASP:OD2	1:B:964:ARG:NH2	2.50	0.45
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.45
1:C:786:VAL:HG23	1:C:796:PHE:CE2	2.51	0.45
1:D:251:LEU:HD12	1:D:265:VAL:HG21	1.99	0.45
1:E:377:LEU:O	1:E:380:PHE:HB2	2.17	0.45
1:E:415:ASN:HD22	1:E:434:SER:CB	2.27	0.45
1:F:250:LEU:HD13	1:F:259:ARG:HB3	1.98	0.45
1:F:642:ILE:O	1:F:645:ARG:HG2	2.17	0.45
1:F:980:GLY:O	1:F:983:PRO:HD2	2.17	0.45
1:A:941:VAL:HG22	1:A:1021:PHE:CD1	2.52	0.45
1:B:580:ALA:HB1	1:B:719:THR:HG22	1.99	0.45
1:B:647:THR:CG2	1:B:660:ALA:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:THR:O	1:C:398:MET:HG2	2.17	0.45
1:D:383:LEU:HD22	1:D:388:PHE:CD1	2.52	0.45
1:D:383:LEU:HD22	1:D:388:PHE:HD1	1.81	0.45
1:D:618:ASN:N	1:D:618:ASN:OD1	2.50	0.45
1:D:977:PHE:HD2	1:D:1006:MET:HG3	1.82	0.45
1:D:1016:PHE:O	1:D:1019:VAL:HB	2.17	0.45
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.98	0.45
1:E:354:VAL:CG1	1:E:972:MET:HG2	2.46	0.45
1:E:708:LEU:H	1:E:708:LEU:HG	1.42	0.45
1:F:5:PHE:HD2	1:F:6:ILE:HG12	1.82	0.45
1:F:361:ASN:HD22	1:F:364:ALA:HB2	1.80	0.45
1:F:932:LEU:O	1:F:935:LYS:HB3	2.17	0.45
1:A:184:MET:HB3	1:A:766:VAL:HG13	1.98	0.45
1:A:597:TYR:CD2	1:A:650:PHE:CZ	3.05	0.45
1:A:873:ALA:O	1:A:877:ILE:HG12	2.16	0.45
1:A:956:ILE:H	1:A:956:ILE:HG13	1.38	0.45
1:B:139:VAL:HA	1:B:289:LEU:O	2.16	0.45
1:B:293:LEU:HD11	1:B:297:ALA:O	2.17	0.45
1:B:428:LYS:O	1:B:431:THR:N	2.49	0.45
1:C:376:LEU:HD22	1:C:398:MET:CE	2.47	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.17	0.45
1:D:7:ASP:O	1:D:8:ARG:HG3	2.16	0.45
1:D:240:LEU:HD22	1:D:245:GLU:OE1	2.16	0.45
1:D:763:VAL:HG12	1:E:63:GLN:OE1	2.17	0.45
1:D:880:PHE:O	1:D:883:LEU:HB2	2.17	0.45
1:D:979:LEU:HA	1:D:979:LEU:HD23	1.34	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.99	0.45
1:E:564:LEU:CD1	1:E:666:ILE:HD12	2.47	0.45
1:E:564:LEU:HD13	1:E:666:ILE:HD12	1.98	0.45
1:F:521:GLU:O	1:F:524:THR:HB	2.16	0.45
1:F:700:GLU:HA	1:F:703:LYS:HZ2	1.82	0.45
1:F:787:ARG:HA	1:F:792:GLN:O	2.17	0.45
1:A:158:VAL:HA	1:A:162:MET:HE2	1.99	0.45
1:A:882:CYS:O	1:A:885:ALA:HB3	2.16	0.45
1:B:445:ILE:HG21	1:B:935:LYS:HD2	1.98	0.45
1:C:181:GLN:HG2	1:C:182:TYR:N	2.31	0.45
1:D:441:ALA:HB2	1:D:942:GLU:OE2	2.17	0.45
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.47	0.45
1:A:444:GLY:O	1:A:448:VAL:HG23	2.17	0.45
1:A:720:PRO:HA	1:A:805:GLU:O	2.16	0.45
1:B:354:VAL:HG22	1:B:975:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:LEU:HD22	1:B:472:ILE:HG22	1.99	0.45
1:B:650:PHE:HB3	1:B:658:VAL:HB	1.99	0.45
1:C:461:GLY:HA3	1:C:863:LEU:HD21	1.99	0.45
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.45
1:D:685:LEU:O	1:D:689:LYS:HD2	2.16	0.45
1:E:108:GLN:CD	1:F:112:GLN:HG2	2.37	0.45
1:E:367:ILE:CD1	1:E:497:LEU:HD13	2.47	0.45
1:E:427:PRO:O	1:E:430:ALA:HB3	2.16	0.45
1:F:363:ARG:CZ	1:F:363:ARG:H	2.29	0.45
1:F:887:TYR:C	1:F:889:SER:N	2.70	0.45
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.52	0.44
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.52	0.44
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.83	0.44
1:B:525:HIS:O	1:B:528:THR:HG22	2.17	0.44
1:B:674:GLY:HA2	1:B:825:GLN:HA	1.98	0.44
1:B:723:LYS:HE3	1:B:725:ASP:OD2	2.17	0.44
1:B:873:ALA:O	1:B:877:ILE:HG13	2.17	0.44
1:C:163:LYS:HE3	1:C:177:LEU:HB2	1.99	0.44
1:C:694:ARG:HG2	1:C:698:LEU:HD12	1.98	0.44
1:C:845:LYS:HD2	1:C:845:LYS:O	2.17	0.44
1:D:214:VAL:HG21	1:E:742:ASN:ND2	2.32	0.44
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.99	0.44
1:D:685:LEU:HD21	1:D:848:THR:O	2.18	0.44
1:D:831:SER:OG	1:D:832:THR:N	2.49	0.44
1:E:108:GLN:HA	1:E:129:VAL:HG21	1.98	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.44
1:E:571:VAL:HG22	1:E:625:SER:HA	1.98	0.44
1:F:187:TRP:O	1:F:266:ALA:HB1	2.17	0.44
1:F:614:GLY:O	1:F:616:GLY:HA3	2.16	0.44
1:A:388:PHE:CE2	1:A:472:ILE:HD13	2.53	0.44
1:A:470:PHE:CD2	1:A:924:VAL:HG11	2.52	0.44
1:A:722:PHE:CD1	1:A:804:TRP:CE2	3.05	0.44
1:A:904:VAL:HA	1:A:926:LEU:HD21	1.99	0.44
1:B:329:THR:O	1:B:333:VAL:HG23	2.16	0.44
1:B:576:VAL:HG22	1:B:658:VAL:HG22	1.99	0.44
1:D:214:VAL:HG11	1:E:742:ASN:CG	2.38	0.44
1:D:307:ARG:HD3	1:D:307:ARG:HA	1.88	0.44
1:D:336:SER:O	1:D:340:VAL:HG23	2.17	0.44
1:D:723:LYS:HB3	1:D:803:ARG:HG2	2.00	0.44
1:E:102:ILE:O	1:E:106:GLN:HG3	2.17	0.44
1:E:255:GLN:H	1:E:255:GLN:HG3	1.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:THR:O	1:E:332:PHE:HB3	2.18	0.44
1:E:409:ALA:O	1:E:413:VAL:HG23	2.17	0.44
1:E:568:ASP:O	1:E:629:TRP:CZ3	2.70	0.44
1:E:770:SER:OG	1:E:775:ARG:HG2	2.18	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.17	0.44
1:F:940:ILE:HG12	1:F:966:ARG:NH2	2.32	0.44
1:A:213:GLN:HA	1:A:237:GLN:O	2.17	0.44
1:A:663:LEU:HD12	1:A:667:VAL:HG13	1.98	0.44
1:A:871:LEU:O	1:A:874:ILE:HB	2.17	0.44
1:B:65:ILE:O	1:B:69:MET:HG2	2.17	0.44
1:B:235:ILE:HD11	1:C:721:GLN:OE1	2.17	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.98	0.44
1:B:984:LEU:HB3	1:B:995:GLN:O	2.17	0.44
1:C:615:GLY:HA2	1:C:616:GLY:HA3	1.69	0.44
1:D:123:GLN:HB3	1:E:116:PRO:HB3	1.99	0.44
1:D:463:THR:HG22	1:D:467:TYR:CE2	2.51	0.44
1:D:827:ALA:O	1:D:830:LYS:N	2.39	0.44
1:A:34:GLN:O	1:A:392:THR:OG1	2.16	0.44
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.45	0.44
1:A:376:LEU:HD22	1:A:398:MET:SD	2.57	0.44
1:A:650:PHE:HD1	1:A:653:ILE:HD11	1.83	0.44
1:D:531:VAL:O	1:D:535:LEU:HG	2.17	0.44
1:D:833:GLY:O	1:D:836:MET:HB2	2.17	0.44
1:D:871:LEU:HD23	1:D:871:LEU:HA	1.66	0.44
1:D:911:ALA:HB2	1:D:922:PHE:CE1	2.53	0.44
1:E:344:LEU:O	1:E:348:ILE:HG13	2.18	0.44
1:E:632:ARG:HB3	1:E:637:ASN:HB3	1.99	0.44
1:E:837:GLU:O	1:E:840:GLU:HB2	2.18	0.44
1:F:247:GLY:O	1:F:261:LEU:HB3	2.18	0.44
1:F:312:LYS:O	1:F:312:LYS:HD3	2.17	0.44
1:A:892:ILE:HG12	1:A:1025:ARG:CD	2.46	0.44
1:C:53:ASP:HA	1:C:84:SER:HB2	1.99	0.44
1:C:103:ALA:O	1:C:107:VAL:HG23	2.18	0.44
1:C:343:THR:HA	1:C:346:GLU:OE1	2.17	0.44
1:D:328:ASP:O	1:D:331:PRO:HD2	2.18	0.44
1:D:366:LEU:HD22	1:D:370:ILE:HG13	2.00	0.44
1:D:982:MET:HB3	1:D:983:PRO:HD3	2.00	0.44
1:E:568:ASP:O	1:E:629:TRP:HZ3	2.00	0.44
1:E:685:LEU:HD11	1:E:690:LEU:HG	1.99	0.44
1:F:400:LEU:HD11	1:F:1002:VAL:HG21	1.99	0.44
1:F:728:GLN:HE22	1:F:738:ILE:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HA	1:A:493:CYS:SG	2.57	0.44
1:A:691:THR:HG23	1:A:694:ARG:NH1	2.25	0.44
1:A:769:MET:HG2	1:A:770:SER:N	2.33	0.44
1:A:959:THR:HG21	1:A:1022:VAL:HG23	1.99	0.44
1:B:61:VAL:HG22	1:B:119:PRO:HD2	1.99	0.44
1:B:399:VAL:HA	1:B:402:ILE:HG13	2.00	0.44
1:B:707:MET:SD	1:B:830:LYS:HG2	2.58	0.44
1:C:6:ILE:HG22	1:C:8:ARG:O	2.17	0.44
1:C:538:THR:HG21	1:C:1023:VAL:CG2	2.48	0.44
1:D:345:VAL:O	1:D:349:ILE:HD12	2.18	0.44
1:D:400:LEU:HG	1:D:928:THR:OG1	2.18	0.44
1:D:682:GLN:HG3	1:D:817:LEU:HD13	2.00	0.44
1:E:198:LEU:HD21	1:E:252:LYS:HB2	1.99	0.44
1:E:309:GLU:OE2	1:E:313:MET:HE3	2.17	0.44
1:E:420:MET:SD	1:E:499:PRO:HA	2.58	0.44
1:E:610:PHE:HB2	1:E:623:PHE:HB3	2.00	0.44
1:E:728:GLN:HE22	1:E:738:ILE:HG21	1.82	0.44
1:F:484:VAL:C	1:F:486:LEU:N	2.71	0.44
1:F:647:THR:HG23	1:F:659:PHE:CE1	2.53	0.44
1:F:927:LEU:O	1:F:928:THR:C	2.55	0.44
1:F:1018:PRO:O	1:F:1022:VAL:HG23	2.18	0.44
1:A:415:ASN:O	1:A:419:VAL:HG23	2.17	0.44
1:A:424:GLY:C	1:A:502:LYS:HZ2	2.20	0.44
1:B:478:MET:O	1:B:482:VAL:HG12	2.17	0.44
1:C:65:ILE:HD11	1:C:118:LEU:HD11	1.99	0.44
1:C:574:THR:HG23	1:C:622:ALA:HB3	1.98	0.44
1:C:955:LEU:O	1:C:959:THR:HG23	2.17	0.44
1:C:975:LEU:O	1:C:976:ALA:C	2.55	0.44
1:D:346:GLU:O	1:D:350:LEU:HD12	2.17	0.44
1:D:395:MET:O	1:D:399:VAL:HG23	2.17	0.44
1:D:514:GLY:C	1:D:516:PHE:N	2.71	0.44
1:D:975:LEU:HD12	1:D:975:LEU:HA	1.82	0.44
1:E:21:LEU:O	1:E:25:LEU:HB2	2.18	0.44
1:E:694:ARG:NH2	1:E:717:GLU:OE1	2.50	0.44
1:F:101:ASP:O	1:F:105:VAL:HG23	2.17	0.44
1:F:345:VAL:O	1:F:349:ILE:HD12	2.18	0.44
1:F:468:ARG:HA	1:F:471:SER:OG	2.18	0.44
1:B:13:TRP:O	1:B:17:ILE:HG13	2.17	0.44
1:B:72:ILE:HG12	1:B:106:GLN:HB3	1.99	0.44
1:D:164:ASP:HB3	1:D:168:ARG:HH21	1.82	0.44
1:D:956:ILE:H	1:D:956:ILE:HG13	1.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.99	0.44
1:F:916:LEU:HD23	1:F:916:LEU:HA	1.76	0.44
1:A:130:GLU:HB3	1:A:132:SER:HB2	2.00	0.44
1:A:324:VAL:HG22	1:A:325:TYR:H	1.82	0.44
1:A:483:LEU:HD13	1:A:487:ILE:HD12	1.99	0.44
1:A:636:GLU:HB2	1:A:645:ARG:NH2	2.30	0.44
1:A:895:SER:HB2	1:A:1021:PHE:HA	1.99	0.44
1:B:399:VAL:O	1:B:402:ILE:HG13	2.18	0.44
1:B:445:ILE:HD12	1:B:449:LEU:HD12	2.00	0.44
1:B:721:GLN:CD	1:B:807:GLY:HA3	2.38	0.44
1:B:975:LEU:O	1:B:979:LEU:HB2	2.18	0.44
1:C:429:GLU:O	1:C:433:LYS:HB2	2.18	0.44
1:C:663:LEU:HD23	1:C:663:LEU:H	1.83	0.44
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.44
2:D:2000:LMT:H6E	2:D:2000:LMT:O5B	2.18	0.44
1:E:172:VAL:HG22	1:E:302:THR:HG23	2.00	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.18	0.44
1:E:905:ILE:HG23	1:E:906:GLY:N	2.33	0.44
1:F:669:LEU:HD22	1:F:856:GLY:HA2	1.98	0.44
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.85	0.43
1:A:451:ALA:CB	1:A:878:VAL:HG12	2.48	0.43
1:B:194:ASN:HA	1:B:793:MET:HE2	2.00	0.43
1:B:214:VAL:HG21	1:C:742:ASN:ND2	2.32	0.43
1:B:902:LEU:HD11	1:B:1016:PHE:CD2	2.53	0.43
1:B:959:THR:HG21	1:B:1022:VAL:CG2	2.48	0.43
1:C:370:ILE:C	1:C:373:PRO:HD2	2.39	0.43
1:C:722:PHE:CZ	1:C:802:SER:HB2	2.53	0.43
1:D:196:PHE:CG	1:D:260:VAL:HG11	2.53	0.43
1:D:377:LEU:O	1:D:380:PHE:HB2	2.17	0.43
1:D:712:ARG:O	1:D:822:ILE:HG23	2.17	0.43
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.60	0.43
1:E:149:MET:HB2	1:E:153:ASP:CB	2.43	0.43
1:F:35:TYR:HB3	1:F:38:ILE:HD12	2.00	0.43
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.52	0.43
1:F:146:ASP:OD2	1:F:147:GLY:N	2.49	0.43
1:F:281:PHE:HB2	1:F:610:PHE:CE1	2.53	0.43
1:F:343:THR:O	1:F:346:GLU:N	2.51	0.43
1:F:425:LEU:HB3	1:F:429:GLU:HB3	2.00	0.43
1:F:770:SER:OG	1:F:775:ARG:HG2	2.18	0.43
1:A:788:ALA:HB3	1:A:790:ASP:OD2	2.18	0.43
1:A:1035:ILE:O	1:A:1036:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.00	0.43
1:B:526:HIS:O	1:B:529:ASP:HB2	2.18	0.43
1:B:691:THR:HG23	1:B:694:ARG:NH1	2.33	0.43
1:B:755:ASN:O	1:B:766:VAL:HB	2.18	0.43
1:D:34:GLN:HB2	1:D:333:VAL:HG22	2.00	0.43
1:D:960:LEU:HD23	1:D:960:LEU:HA	1.75	0.43
1:D:1020:PHE:O	1:D:1024:VAL:HB	2.18	0.43
1:E:187:TRP:HZ3	1:E:769:MET:HB3	1.82	0.43
1:E:370:ILE:HD12	1:E:492:LEU:HD13	2.00	0.43
1:E:676:ASP:HA	1:E:823:LEU:HD23	1.99	0.43
1:E:821:GLU:HG2	1:E:822:ILE:N	2.33	0.43
1:F:343:THR:HA	1:F:346:GLU:OE1	2.18	0.43
1:F:610:PHE:O	1:F:622:ALA:HA	2.18	0.43
1:A:158:VAL:HA	1:A:162:MET:CE	2.48	0.43
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.78	0.43
1:A:527:TYR:O	1:A:530:SER:HB3	2.18	0.43
1:A:667:VAL:HG12	1:A:668:GLU:OE1	2.19	0.43
1:A:770:SER:OG	1:A:775:ARG:HG2	2.18	0.43
1:A:962:ALA:O	1:A:965:MET:HG2	2.18	0.43
1:B:544:LEU:O	1:B:548:ILE:HG13	2.18	0.43
1:C:405:LEU:HD12	1:C:406:VAL:N	2.34	0.43
1:C:679:LEU:O	1:C:819:SER:HB2	2.18	0.43
1:C:905:ILE:HG13	1:C:909:LEU:HD23	2.00	0.43
1:C:911:ALA:HB2	1:C:922:PHE:CE1	2.52	0.43
1:D:246:PHE:O	1:D:262:LEU:HD23	2.18	0.43
1:D:343:THR:HG21	1:D:984:LEU:HD21	2.00	0.43
1:D:415:ASN:ND2	1:D:943:PHE:HZ	2.15	0.43
1:D:559:LEU:HA	1:D:560:PRO:HD2	1.68	0.43
1:D:588:GLN:NE2	1:D:588:GLN:O	2.51	0.43
1:D:691:THR:HA	1:D:694:ARG:NH1	2.33	0.43
1:E:238:THR:HG22	1:E:239:ARG:O	2.17	0.43
1:E:559:LEU:CD2	1:E:560:PRO:HD2	2.46	0.43
1:F:143:ILE:HG12	1:F:322:LYS:O	2.19	0.43
1:F:348:ILE:HG12	1:F:402:ILE:HD13	2.00	0.43
1:F:650:PHE:HB2	1:F:658:VAL:O	2.18	0.43
1:F:707:MET:HB2	1:F:708:LEU:HD12	2.00	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.01	0.43
1:A:615:GLY:HA2	1:A:617:GLN:H	1.82	0.43
1:A:695:ASN:O	1:A:698:LEU:HB2	2.18	0.43
1:A:722:PHE:HD1	1:A:804:TRP:CE2	2.37	0.43
1:A:932:LEU:O	1:A:935:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.53	0.43
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.83	0.43
1:B:594:VAL:HG22	1:B:650:PHE:CZ	2.53	0.43
1:B:1031:LYS:HA	1:B:1032:ASN:HA	1.68	0.43
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.48	0.43
1:C:146:ASP:O	1:C:148:THR:OG1	2.36	0.43
1:C:363:ARG:NH2	1:C:498:LYS:HD2	2.33	0.43
1:C:1031:LYS:HD2	1:C:1033:GLU:CB	2.49	0.43
1:D:81:ASN:O	1:D:88:VAL:HG23	2.19	0.43
1:D:124:GLN:NE2	1:D:753:TYR:HD2	2.16	0.43
1:D:454:VAL:O	1:D:457:ALA:HB3	2.19	0.43
1:D:771:GLU:HB3	1:D:774:TYR:CD1	2.53	0.43
1:D:786:VAL:HG23	1:D:796:PHE:CE2	2.53	0.43
1:D:1007:VAL:O	1:D:1011:VAL:HG23	2.18	0.43
1:E:173:GLY:O	1:F:71:GLY:HA3	2.18	0.43
1:F:54:ALA:HB1	1:F:811:LEU:HG	2.00	0.43
1:F:84:SER:HB3	1:F:809:PRO:O	2.17	0.43
1:F:144:ASN:OD1	1:F:148:THR:HA	2.18	0.43
1:A:137:LEU:HD13	1:A:293:LEU:HG	1.99	0.43
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.74	0.43
1:B:681:ASP:HA	1:B:849:GLY:O	2.18	0.43
1:C:546:LEU:O	1:C:550:VAL:HG23	2.18	0.43
1:D:199:THR:HG21	1:D:787:ARG:H	1.82	0.43
1:D:959:THR:HG21	1:D:1022:VAL:CG2	2.49	0.43
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.78	0.43
1:E:597:TYR:O	1:E:601:LYS:HB2	2.18	0.43
1:F:196:PHE:CD2	1:F:260:VAL:HG21	2.54	0.43
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.43
1:F:771:GLU:HB2	1:F:774:TYR:HD1	1.82	0.43
1:A:3:ASN:O	1:A:4:PHE:C	2.57	0.43
1:A:79:SER:HA	1:A:813:ARG:O	2.19	0.43
1:A:530:SER:O	1:A:533:GLY:N	2.51	0.43
1:A:639:VAL:CG1	1:A:662:ASN:HB2	2.42	0.43
1:A:814:TYR:OH	1:A:854:TRP:O	2.29	0.43
1:B:281:PHE:HB2	1:B:610:PHE:CE1	2.53	0.43
1:B:407:ASP:OD1	1:B:973:THR:HG21	2.19	0.43
1:B:949:ASP:O	1:B:951:GLU:N	2.52	0.43
1:B:981:VAL:O	1:B:982:MET:C	2.57	0.43
1:B:1033:GLU:OE2	1:B:1034:ASP:HB2	2.18	0.43
1:C:531:VAL:O	1:C:535:LEU:HG	2.19	0.43
1:C:836:MET:HG2	1:C:854:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:927:LEU:O	1:C:930:ILE:N	2.51	0.43
1:C:963:VAL:HA	1:C:966:ARG:HH12	1.82	0.43
1:D:852:TYR:CD2	1:D:852:TYR:N	2.86	0.43
1:D:966:ARG:O	1:D:970:ILE:HG12	2.18	0.43
1:E:250:LEU:HD21	1:E:253:VAL:HG22	2.00	0.43
1:F:38:ILE:HD13	1:F:466:ILE:CD1	2.49	0.43
1:F:462:SER:O	1:F:466:ILE:HG12	2.19	0.43
1:F:602:GLU:HG3	1:F:605:ASN:HB2	2.01	0.43
1:A:142:VAL:O	1:A:286:ALA:HB1	2.18	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.79	0.43
1:A:540:ARG:HH22	2:A:1101:LMT:H6'2	1.84	0.43
1:A:728:GLN:OE1	1:A:738:ILE:HG12	2.19	0.43
1:A:946:ASP:C	1:A:946:ASP:OD1	2.56	0.43
1:A:1013:ALA:C	1:A:1015:PHE:H	2.21	0.43
1:B:26:ALA:HB1	1:B:384:ALA:CB	2.49	0.43
1:B:535:LEU:CD2	1:B:1019:VAL:HA	2.49	0.43
1:C:188:MET:HB3	1:C:193:LEU:CD1	2.46	0.43
1:C:677:PHE:CE1	1:C:852:TYR:HB2	2.53	0.43
1:C:966:ARG:O	1:C:966:ARG:HG2	2.19	0.43
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.01	0.43
1:E:324:VAL:O	1:E:326:PRO:HD3	2.19	0.43
1:E:602:GLU:HG3	1:E:602:GLU:O	2.19	0.43
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.53	0.43
1:F:49:TYR:CG	1:F:57:VAL:HG12	2.54	0.43
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.48	0.43
1:F:376:LEU:HD22	1:F:398:MET:CE	2.49	0.43
1:F:706:ASP:OD1	1:F:706:ASP:N	2.49	0.43
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.43
1:A:722:PHE:HB2	1:A:804:TRP:CZ3	2.52	0.43
1:A:893:PRO:O	1:A:896:VAL:HG13	2.18	0.43
1:C:66:GLU:HG2	1:C:78:MET:SD	2.59	0.43
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.99	0.43
1:C:166:ILE:HG23	1:C:172:VAL:HG11	2.01	0.43
1:C:211:ASN:OD1	1:C:239:ARG:HA	2.18	0.43
1:C:979:LEU:HD23	1:C:979:LEU:HA	1.51	0.43
1:D:14:VAL:HG13	1:E:881:LEU:HB3	2.01	0.43
1:D:339:GLU:HA	1:D:342:LYS:HB2	2.00	0.43
1:D:464:GLY:O	1:D:468:ARG:HB2	2.18	0.43
1:D:470:PHE:HD2	1:D:924:VAL:HG11	1.84	0.43
1:D:507:GLU:O	1:D:509:LYS:N	2.52	0.43
1:D:531:VAL:HA	1:D:534:ILE:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:553:ALA:O	1:D:557:VAL:HG23	2.18	0.43
1:D:663:LEU:HD23	1:D:663:LEU:H	1.83	0.43
1:E:45:ILE:HA	1:E:128:SER:O	2.19	0.43
1:E:248:LYS:HG2	1:E:263:ARG:NH2	2.33	0.43
1:E:350:LEU:O	1:E:353:LEU:HB2	2.19	0.43
1:F:180:SER:CB	1:F:274:ASN:H	2.31	0.43
1:F:681:ASP:CG	1:F:682:GLN:N	2.71	0.43
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.43
1:A:748:ALA:HB3	1:A:749:TRP:HD1	1.83	0.43
1:A:966:ARG:NE	1:A:970:ILE:HD11	2.25	0.43
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.84	0.43
1:C:393:LEU:HD13	1:C:466:ILE:HA	2.00	0.43
1:C:548:ILE:CD1	1:C:1016:PHE:HE1	2.32	0.43
1:C:992:SER:HA	1:C:995:GLN:HG3	2.00	0.43
1:D:83:ASP:OD1	1:D:810:ARG:HD3	2.18	0.43
1:D:293:LEU:HD22	1:D:294:ALA:H	1.83	0.43
1:D:485:ALA:O	1:D:490:PRO:HD3	2.18	0.43
1:D:867:GLN:HB3	1:D:871:LEU:HD12	2.00	0.43
1:D:1035:ILE:HG22	1:D:1036:GLU:O	2.19	0.43
1:E:32:VAL:HA	1:E:390:ILE:O	2.19	0.43
1:E:899:VAL:CG1	1:E:933:SER:HB2	2.48	0.43
1:F:344:LEU:CD1	1:F:402:ILE:HD11	2.48	0.43
1:F:871:LEU:HD22	1:F:927:LEU:HD21	2.01	0.43
1:A:763:VAL:HG12	1:B:63:GLN:NE2	2.33	0.43
1:A:969:PRO:HA	1:A:972:MET:CE	2.49	0.43
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.01	0.43
1:C:544:LEU:O	1:C:548:ILE:HG13	2.19	0.43
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.77	0.43
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.53	0.43
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.81	0.43
1:D:992:SER:HA	1:D:995:GLN:HG3	2.00	0.43
1:E:219:LEU:HD23	1:F:749:TRP:CZ3	2.53	0.43
1:E:580:ALA:HB1	1:E:719:THR:HG21	2.00	0.43
1:E:685:LEU:HD12	1:E:686:GLY:O	2.18	0.43
1:E:723:LYS:HE3	1:E:725:ASP:HB2	2.01	0.43
1:F:53:ASP:O	1:F:57:VAL:HG13	2.19	0.43
1:F:355:MET:CG	1:F:410:ILE:HD11	2.49	0.43
1:A:26:ALA:O	1:A:30:LEU:HB2	2.19	0.42
1:A:726:ILE:H	1:A:726:ILE:HG12	1.13	0.42
1:B:612:VAL:HB	1:B:621:ILE:HG23	2.01	0.42
1:B:695:ASN:O	1:B:698:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:969:PRO:HA	1:B:972:MET:HE3	2.00	0.42
1:B:982:MET:HB3	1:B:983:PRO:CD	2.48	0.42
1:C:356:TYR:HA	1:C:365:THR:HG21	2.01	0.42
1:C:415:ASN:ND2	1:C:438:ILE:HG21	2.34	0.42
1:C:447:MET:SD	1:C:886:LEU:HD22	2.59	0.42
1:C:1034:ASP:O	1:C:1035:ILE:HG12	2.19	0.42
1:D:25:LEU:HA	1:D:25:LEU:HD12	1.64	0.42
1:D:82:SER:HB2	1:D:811:LEU:HB2	2.00	0.42
1:D:157:TYR:O	1:D:161:ASN:ND2	2.46	0.42
1:E:164:ASP:O	1:E:168:ARG:HG3	2.19	0.42
1:E:190:PRO:HG3	1:E:774:TYR:CG	2.54	0.42
1:E:191:ASN:O	1:E:195:LYS:HB2	2.19	0.42
1:E:597:TYR:HH	1:E:646:ALA:HA	1.84	0.42
1:F:114:ALA:HA	1:F:117:LEU:HD12	2.00	0.42
1:F:344:LEU:HD11	1:F:376:LEU:HD11	2.01	0.42
1:F:356:TYR:C	1:F:358:PHE:N	2.73	0.42
1:A:1008:THR:O	1:A:1012:LEU:HB2	2.20	0.42
1:B:9:PRO:O	1:B:12:ALA:HB3	2.18	0.42
1:C:184:MET:HE3	1:C:185:ARG:N	2.34	0.42
1:C:649:ALA:O	1:C:653:ILE:HG12	2.19	0.42
1:D:564:LEU:HA	1:D:565:PRO:HD2	1.84	0.42
1:D:959:THR:HG21	1:D:1022:VAL:HG22	2.01	0.42
1:E:459:PHE:HE1	1:E:872:TYR:HH	1.65	0.42
1:F:686:GLY:CA	1:F:689:LYS:HD3	2.40	0.42
1:F:920:VAL:HA	1:F:923:GLN:OE1	2.19	0.42
1:A:776:MET:HE2	1:C:225:VAL:HG22	2.02	0.42
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.53	0.42
1:B:219:LEU:HD23	1:C:749:TRP:HZ3	1.84	0.42
1:B:984:LEU:HD23	1:B:984:LEU:HA	1.77	0.42
1:C:352:PHE:C	1:C:352:PHE:CD2	2.93	0.42
1:D:13:TRP:HB3	1:E:890:TRP:HZ2	1.84	0.42
1:D:576:VAL:HG21	1:D:591:LEU:HD21	2.00	0.42
1:D:1012:LEU:O	1:D:1016:PHE:HB2	2.19	0.42
1:E:430:ALA:O	1:E:433:LYS:HB3	2.19	0.42
1:F:464:GLY:HA2	1:F:467:TYR:CD1	2.53	0.42
1:F:483:LEU:O	1:F:486:LEU:HB2	2.19	0.42
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.00	0.42
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.42
1:B:2:PRO:HB2	1:B:439:GLN:OE1	2.19	0.42
1:B:667:VAL:HB	1:B:668:GLU:OE2	2.20	0.42
1:B:847:PRO:O	1:B:850:VAL:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:HA	1:C:92:LEU:O	2.19	0.42
1:C:192:GLU:O	1:C:195:LYS:HB3	2.19	0.42
1:C:347:ALA:HB3	1:C:402:ILE:HD12	2.01	0.42
1:C:836:MET:HG2	1:C:854:TRP:CH2	2.54	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.76	0.42
1:D:626:LEU:HB3	1:D:632:ARG:HD3	2.01	0.42
1:D:883:LEU:CB	1:D:893:PRO:HB3	2.49	0.42
1:D:976:ALA:O	1:D:980:GLY:N	2.52	0.42
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.49	0.42
1:E:356:TYR:C	1:E:358:PHE:N	2.71	0.42
1:E:404:LEU:HA	1:E:404:LEU:HD12	1.84	0.42
1:E:588:GLN:NE2	1:E:588:GLN:O	2.52	0.42
1:E:898:LEU:O	1:E:901:PRO:HD2	2.19	0.42
1:F:32:VAL:HG22	1:F:390:ILE:HB	2.01	0.42
1:F:603:LYS:HB3	1:F:603:LYS:HE2	1.65	0.42
1:A:219:LEU:HD11	1:B:722:PHE:HB2	2.01	0.42
1:A:368:PRO:HB3	1:A:409:ALA:CB	2.47	0.42
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.54	0.42
1:A:916:LEU:HB3	1:A:917:THR:H	1.66	0.42
1:A:1030:ARG:O	1:A:1031:LYS:HG2	2.20	0.42
1:B:525:HIS:O	1:B:526:HIS:C	2.58	0.42
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.55	0.42
1:C:249:ILE:HB	1:C:262:LEU:CB	2.49	0.42
1:C:423:GLU:OE1	1:C:425:LEU:HD11	2.19	0.42
1:C:1008:THR:C	1:C:1010:THR:H	2.23	0.42
1:D:30:LEU:HD12	1:D:31:PRO:CD	2.48	0.42
1:D:182:TYR:O	1:D:764:LYS:HD3	2.20	0.42
1:D:586:ARG:O	1:D:589:LYS:HB3	2.19	0.42
1:D:813:ARG:NH2	1:D:816:GLY:O	2.53	0.42
1:D:1021:PHE:O	1:D:1025:ARG:HG2	2.19	0.42
1:E:69:MET:HE1	1:E:107:VAL:HG13	2.01	0.42
1:E:692:GLN:O	1:E:695:ASN:HB2	2.20	0.42
1:E:695:ASN:HA	1:E:698:LEU:HD12	2.01	0.42
1:F:307:ARG:NH2	1:F:311:ALA:HB2	2.35	0.42
1:F:638:LYS:HE2	1:F:640:GLU:CG	2.48	0.42
1:F:723:LYS:HG3	1:F:725:ASP:OD1	2.20	0.42
1:A:142:VAL:O	1:A:287:SER:N	2.51	0.42
1:A:679:LEU:HA	1:A:679:LEU:HD12	1.76	0.42
1:A:895:SER:HB3	1:A:1024:VAL:HB	2.02	0.42
1:B:5:PHE:C	1:B:8:ARG:H	2.22	0.42
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD11	1:C:333:VAL:HG11	2.02	0.42
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.79	0.42
1:C:360:GLN:HE21	1:C:360:GLN:HB3	1.66	0.42
1:C:425:LEU:HB3	1:C:429:GLU:HG3	1.99	0.42
1:C:506:GLY:O	1:C:508:GLY:N	2.48	0.42
1:C:541:TYR:OH	2:C:1101:LMT:O6'	2.34	0.42
1:D:251:LEU:CD1	1:D:265:VAL:HG21	2.50	0.42
1:D:538:THR:HG22	1:D:539:GLY:N	2.34	0.42
1:D:562:SER:H	1:D:917:THR:HG1	1.61	0.42
1:E:443:VAL:O	1:E:447:MET:HG2	2.20	0.42
1:E:534:ILE:CG2	2:E:1101:LMT:H12	2.49	0.42
1:E:633:PRO:HD2	1:E:637:ASN:OD1	2.19	0.42
1:E:690:LEU:HB3	1:E:820:MET:SD	2.59	0.42
1:E:883:LEU:HD23	1:E:883:LEU:HA	1.85	0.42
1:E:944:ALA:HB3	1:E:1021:PHE:CE1	2.54	0.42
1:F:152:GLU:HG2	1:F:275:TYR:CE2	2.55	0.42
1:F:831:SER:HB3	1:F:834:GLU:HG3	2.01	0.42
1:F:1010:THR:O	1:F:1014:ILE:HG23	2.20	0.42
1:A:81:ASN:O	1:A:88:VAL:HA	2.20	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.20	0.42
1:A:855:THR:OG1	1:A:856:GLY:N	2.52	0.42
1:A:982:MET:HB3	1:A:983:PRO:HD3	2.01	0.42
1:B:345:VAL:O	1:B:348:ILE:HB	2.20	0.42
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.01	0.42
1:B:553:ALA:O	1:B:557:VAL:HG23	2.20	0.42
1:B:1022:VAL:O	1:B:1026:ARG:HG3	2.19	0.42
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.78	0.42
1:C:186:ILE:O	1:C:768:VAL:HG23	2.19	0.42
1:C:488:LEU:O	1:C:491:ALA:HB3	2.20	0.42
1:C:571:VAL:HG22	1:C:624:VAL:O	2.19	0.42
1:D:146:ASP:OD2	1:D:146:ASP:N	2.52	0.42
1:D:200:PRO:HB2	1:D:744:THR:HG22	2.02	0.42
1:D:435:MET:O	1:D:439:GLN:HB2	2.20	0.42
1:D:578:LEU:HD11	1:D:587:THR:N	2.35	0.42
1:D:914:ARG:HD2	1:D:1000:THR:HG21	2.02	0.42
1:E:463:THR:O	1:E:467:TYR:CD1	2.69	0.42
1:F:211:ASN:OD1	1:F:240:LEU:HG	2.19	0.42
1:F:304:ALA:O	1:F:307:ARG:HB3	2.19	0.42
1:F:932:LEU:HD11	1:F:977:PHE:CE2	2.55	0.42
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.35	0.42
1:A:166:ILE:HG23	1:A:166:ILE:HD12	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:MET:SD	1:A:955:LEU:HA	2.58	0.42
1:B:26:ALA:O	1:B:30:LEU:HB2	2.20	0.42
1:B:409:ALA:O	1:B:413:VAL:HG23	2.20	0.42
1:B:607:GLU:OE1	1:B:627:LYS:HG2	2.20	0.42
1:B:701:ALA:HB3	1:B:711:VAL:HG11	2.01	0.42
1:D:475:VAL:O	1:D:478:MET:HB3	2.20	0.42
1:D:886:LEU:HD12	1:D:886:LEU:HA	1.76	0.42
1:F:399:VAL:HG11	1:F:984:LEU:HD21	2.02	0.42
1:F:509:LYS:HA	1:F:509:LYS:HD2	1.83	0.42
1:A:199:THR:HG21	1:A:787:ARG:H	1.85	0.42
1:B:3:ASN:O	1:B:6:ILE:HB	2.20	0.42
1:B:671:THR:O	1:B:671:THR:OG1	2.35	0.42
1:B:898:LEU:HB3	1:B:1020:PHE:CZ	2.54	0.42
1:C:55:LYS:HB3	1:C:55:LYS:HE2	1.72	0.42
1:C:343:THR:HG21	1:C:984:LEU:HD23	2.02	0.42
1:C:926:LEU:HA	1:C:926:LEU:HD23	1.82	0.42
1:D:852:TYR:N	1:D:852:TYR:HD2	2.18	0.42
1:E:30:LEU:HA	1:E:31:PRO:HD3	1.82	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.80	0.42
1:E:235:ILE:HD11	1:F:721:GLN:OE1	2.20	0.42
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.01	0.42
1:E:544:LEU:O	1:E:547:ILE:HB	2.19	0.42
1:E:843:ALA:O	1:E:846:LEU:HG	2.20	0.42
1:E:921:TYR:HB3	1:E:998:VAL:HG23	2.02	0.42
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.62	0.42
1:F:41:PRO:O	1:F:94:PHE:HB2	2.20	0.42
1:F:883:LEU:HD11	1:F:938:ILE:HD11	2.00	0.42
1:F:974:SER:HA	1:F:1006:MET:CE	2.49	0.42
1:A:282:ASN:HD21	1:A:608:SER:CB	2.33	0.42
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.84	0.42
1:A:563:PHE:O	1:A:564:LEU:HD12	2.20	0.42
1:A:694:ARG:HB3	1:A:694:ARG:HH11	1.85	0.42
1:B:955:LEU:O	1:B:959:THR:HG23	2.20	0.42
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.42
1:C:335:ILE:HG12	1:C:990:ALA:HB2	2.02	0.42
1:C:753:TYR:HD1	1:C:767:TYR:HE2	1.66	0.42
1:D:193:LEU:CD2	1:D:265:VAL:HB	2.50	0.42
1:D:836:MET:CE	1:D:862:ARG:HD2	2.49	0.42
1:D:941:VAL:HG22	1:D:1021:PHE:CD1	2.55	0.42
1:E:43:VAL:HG13	1:E:130:GLU:O	2.20	0.42
1:E:722:PHE:CZ	1:E:802:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:PHE:CD1	1:E:804:TRP:CE2	3.08	0.42
1:E:960:LEU:O	1:E:963:VAL:HG12	2.20	0.42
1:E:1029:SER:HG	1:E:1030:ARG:H	1.61	0.42
1:F:364:ALA:O	1:F:368:PRO:HD3	2.19	0.42
1:F:786:VAL:HG23	1:F:796:PHE:CE2	2.55	0.42
1:F:960:LEU:HD23	1:F:960:LEU:HA	1.89	0.42
1:A:585:GLU:O	1:A:588:GLN:HB3	2.20	0.41
1:B:15:ILE:HD13	1:B:15:ILE:HG21	1.86	0.41
1:C:24:GLY:CA	1:C:27:ILE:HG23	2.50	0.41
1:C:148:THR:HG22	1:C:149:MET:O	2.20	0.41
1:C:278:ILE:CG1	1:C:613:ASN:HB3	2.48	0.41
1:C:453:PHE:CD2	1:C:456:MET:CE	2.95	0.41
1:C:855:THR:CA	1:C:859:TYR:HB2	2.47	0.41
1:C:899:VAL:HG12	1:C:933:SER:HB2	2.02	0.41
1:C:977:PHE:HE2	1:C:1002:VAL:CG1	2.32	0.41
1:D:152:GLU:CD	1:D:152:GLU:H	2.24	0.41
1:D:235:ILE:HG23	1:D:235:ILE:HD12	1.74	0.41
1:D:393:LEU:HD13	1:D:466:ILE:HA	2.02	0.41
1:D:470:PHE:CD2	1:D:924:VAL:HG11	2.54	0.41
1:E:579:PRO:HD3	1:E:656:ALA:CB	2.48	0.41
1:E:727:ASP:OD1	1:E:730:LYS:HG3	2.20	0.41
1:E:741:ILE:O	1:E:744:THR:OG1	2.34	0.41
1:F:3:ASN:HD21	1:F:486:LEU:HA	1.85	0.41
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.01	0.41
1:F:587:THR:HG21	1:F:618:ASN:HA	2.02	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.76	0.41
1:A:149:MET:HG3	1:A:154:ILE:HG13	2.02	0.41
1:A:427:PRO:O	1:A:430:ALA:HB3	2.19	0.41
1:A:901:PRO:HA	1:A:904:VAL:HB	2.02	0.41
1:B:4:PHE:CZ	1:B:8:ARG:HD3	2.55	0.41
1:B:248:LYS:O	1:B:261:LEU:HD22	2.20	0.41
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.02	0.41
1:B:486:LEU:HA	1:B:486:LEU:HD23	1.77	0.41
1:B:914:ARG:NH1	1:B:985:VAL:HG12	2.35	0.41
1:B:1015:PHE:CZ	2:B:2000:LMT:H52	2.55	0.41
1:C:187:TRP:HB3	1:C:771:GLU:HA	2.02	0.41
1:C:443:VAL:O	1:C:447:MET:HB3	2.20	0.41
1:C:584:GLN:N	1:C:617:GLN:HB3	2.34	0.41
1:E:363:ARG:CZ	1:E:498:LYS:HE3	2.49	0.41
1:E:493:CYS:O	1:E:497:LEU:HB2	2.19	0.41
1:F:344:LEU:HD22	1:F:402:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:ASP:C	1:F:506:GLY:N	2.72	0.41
1:A:169:THR:HB	1:A:172:VAL:HG23	2.02	0.41
1:B:363:ARG:NH1	1:B:498:LYS:HG3	2.35	0.41
1:B:463:THR:O	1:B:466:ILE:HB	2.20	0.41
1:B:480:LEU:O	1:B:484:VAL:HG23	2.20	0.41
1:B:482:VAL:O	1:B:485:ALA:HB3	2.20	0.41
1:B:527:TYR:O	1:B:531:VAL:HG23	2.20	0.41
1:B:701:ALA:CB	1:B:711:VAL:HG11	2.50	0.41
1:C:443:VAL:HG12	1:C:886:LEU:HD21	2.01	0.41
1:C:753:TYR:HD1	1:C:767:TYR:CE2	2.38	0.41
1:C:966:ARG:HH21	1:C:970:ILE:HD11	1.85	0.41
1:D:459:PHE:O	1:D:468:ARG:NH2	2.54	0.41
1:D:482:VAL:O	1:D:486:LEU:HG	2.20	0.41
1:E:62:THR:O	1:E:66:GLU:HG3	2.21	0.41
1:E:158:VAL:HG11	1:E:289:LEU:HG	2.01	0.41
1:E:202:ASP:OD2	1:E:787:ARG:NH2	2.46	0.41
1:E:306:ILE:O	1:E:309:GLU:HB3	2.20	0.41
1:E:927:LEU:HA	1:E:930:ILE:HD12	2.02	0.41
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.84	0.41
1:F:578:LEU:HA	1:F:656:ALA:HB1	2.02	0.41
1:A:54:ALA:HB2	1:A:809:PRO:O	2.20	0.41
1:A:273:GLU:CG	1:A:765:LYS:HD2	2.50	0.41
1:A:1017:VAL:HB	1:A:1018:PRO:HD3	2.02	0.41
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.86	0.41
1:B:576:VAL:HG13	1:B:658:VAL:HG22	2.01	0.41
1:B:676:ASP:H	1:B:858:SER:HG	1.62	0.41
1:B:968:ARG:O	1:B:972:MET:HE2	2.20	0.41
1:C:614:GLY:O	1:C:616:GLY:HA3	2.20	0.41
1:C:664:PRO:HG2	1:C:666:ILE:O	2.20	0.41
1:D:5:PHE:CE1	1:D:487:ILE:HG12	2.55	0.41
1:D:234:ILE:HA	1:E:722:PHE:O	2.20	0.41
1:D:432:ARG:HH11	1:D:432:ARG:HD2	1.68	0.41
1:D:531:VAL:O	1:D:534:ILE:HG13	2.20	0.41
1:D:544:LEU:O	1:D:547:ILE:HB	2.20	0.41
1:D:679:LEU:HD11	1:D:850:VAL:HG12	2.02	0.41
1:D:726:ILE:H	1:D:726:ILE:HG12	1.24	0.41
1:D:898:LEU:O	1:D:901:PRO:HD2	2.20	0.41
1:D:941:VAL:HG13	1:D:1021:PHE:CD1	2.56	0.41
1:E:7:ASP:O	1:E:8:ARG:HG3	2.20	0.41
1:E:448:VAL:HG13	1:E:879:VAL:CG1	2.47	0.41
1:E:1015:PHE:O	1:E:1019:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:LEU:CD1	1:F:587:THR:HG22	2.50	0.41
1:A:165:ALA:HA	1:A:168:ARG:NH1	2.35	0.41
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.51	0.41
1:B:572:PHE:CE1	1:B:643:THR:HG22	2.56	0.41
1:D:9:PRO:O	1:D:13:TRP:CD1	2.74	0.41
1:D:473:THR:O	1:D:476:SER:OG	2.38	0.41
1:D:531:VAL:HA	1:D:534:ILE:HD11	2.01	0.41
1:D:634:GLY:O	1:D:638:LYS:HG3	2.20	0.41
1:E:697:LEU:HA	1:E:700:GLU:HB2	2.02	0.41
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.41
1:F:199:THR:HG22	1:F:785:TYR:O	2.20	0.41
1:F:620:GLY:O	1:F:621:ILE:HD12	2.20	0.41
1:F:666:ILE:HD13	1:F:669:LEU:HD12	2.03	0.41
1:F:694:ARG:HE	1:F:713:PRO:HB3	1.85	0.41
1:F:720:PRO:HA	1:F:805:GLU:O	2.20	0.41
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.77	0.41
1:A:204:ILE:HG12	1:A:754:VAL:HG21	2.02	0.41
1:A:578:LEU:HB2	1:A:618:ASN:HA	2.02	0.41
1:A:650:PHE:HB3	1:A:658:VAL:HB	2.02	0.41
1:B:121:GLU:O	1:B:125:GLN:HB2	2.21	0.41
1:B:149:MET:H	1:B:149:MET:HG2	1.75	0.41
1:B:167:SER:HB2	1:C:70:ASN:HB3	2.02	0.41
1:C:376:LEU:HD22	1:C:398:MET:HE3	2.02	0.41
1:C:836:MET:O	1:C:854:TRP:HZ2	2.03	0.41
1:D:44:THR:HA	1:D:90:ILE:O	2.20	0.41
1:D:58:GLN:HA	1:D:62:THR:HB	2.03	0.41
1:D:138:MET:CG	1:D:291:ILE:HB	2.51	0.41
1:D:355:MET:HE2	1:D:368:PRO:HG2	2.03	0.41
1:D:418:ARG:HH21	1:D:943:PHE:HE2	1.69	0.41
1:E:175:VAL:HG11	1:E:289:LEU:HD13	2.02	0.41
1:E:189:ASN:O	1:E:192:GLU:HB2	2.21	0.41
1:E:262:LEU:HG	1:E:268:ILE:HD11	2.02	0.41
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.55	0.41
1:E:585:GLU:O	1:E:588:GLN:HB3	2.20	0.41
1:E:914:ARG:NH1	1:E:985:VAL:HG12	2.36	0.41
1:E:927:LEU:O	1:E:930:ILE:HB	2.21	0.41
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.41
1:F:679:LEU:HD23	1:F:820:MET:HB2	2.03	0.41
1:F:970:ILE:H	1:F:970:ILE:HG13	1.64	0.41
1:A:66:GLU:OE1	1:A:816:GLY:HA2	2.20	0.41
1:A:367:ILE:HG21	1:A:367:ILE:HD13	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HA	1:B:321:LEU:HA	2.02	0.41
1:C:370:ILE:O	1:C:373:PRO:HD2	2.20	0.41
1:C:591:LEU:HD11	1:C:620:GLY:HA3	2.01	0.41
1:C:689:LYS:H	1:C:689:LYS:CD	2.33	0.41
1:C:1012:LEU:HD12	1:C:1012:LEU:HA	1.85	0.41
1:D:366:LEU:HD23	1:D:366:LEU:HA	1.74	0.41
1:D:572:PHE:CD1	1:D:643:THR:HG22	2.56	0.41
1:D:667:VAL:HG12	1:D:668:GLU:OE1	2.20	0.41
1:D:788:ALA:HB3	1:D:790:ASP:OD2	2.20	0.41
1:E:250:LEU:HD13	1:E:259:ARG:HB2	2.02	0.41
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.86	0.41
1:F:914:ARG:NH1	1:F:996:ASN:HB3	2.36	0.41
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.56	0.41
1:A:57:VAL:CG1	1:A:88:VAL:HB	2.50	0.41
1:A:82:SER:HB2	1:A:811:LEU:HB2	2.02	0.41
1:A:343:THR:HG21	1:A:984:LEU:HD21	2.02	0.41
1:A:355:MET:HE1	1:A:368:PRO:HG2	2.02	0.41
1:A:574:THR:OG1	1:A:659:PHE:O	2.22	0.41
1:A:694:ARG:HD2	1:A:713:PRO:HB3	2.03	0.41
1:A:979:LEU:HD23	1:A:979:LEU:HA	1.80	0.41
2:A:1101:LMT:H81	2:A:1101:LMT:H51	1.51	0.41
1:B:82:SER:HB2	1:B:811:LEU:HB2	2.03	0.41
1:B:883:LEU:HD23	1:B:883:LEU:HA	1.88	0.41
1:B:923:GLN:O	1:B:926:LEU:HB2	2.21	0.41
1:C:153:ASP:HA	1:C:182:TYR:OH	2.20	0.41
1:E:186:ILE:HG12	1:E:268:ILE:HG12	2.02	0.41
1:E:219:LEU:HD23	1:F:749:TRP:HZ3	1.85	0.41
1:E:224:PRO:HD2	1:F:584:GLN:NE2	2.35	0.41
1:E:555:LEU:HB3	1:E:908:LEU:HD13	2.03	0.41
1:E:916:LEU:HD11	1:E:997:ALA:HA	2.03	0.41
1:F:61:VAL:O	1:F:65:ILE:HG13	2.19	0.41
1:F:120:GLN:O	1:F:123:GLN:HB2	2.21	0.41
1:F:345:VAL:HA	1:F:348:ILE:HD12	2.03	0.41
1:F:356:TYR:O	1:F:358:PHE:N	2.53	0.41
1:F:407:ASP:HB3	1:F:445:ILE:HD13	2.03	0.41
1:F:600:THR:C	1:F:602:GLU:H	2.22	0.41
1:F:649:ALA:O	1:F:653:ILE:HG12	2.20	0.41
1:F:741:ILE:HG22	1:F:786:VAL:HG11	2.03	0.41
1:F:803:ARG:NH1	1:F:805:GLU:OE2	2.54	0.41
1:A:75:LEU:HD23	1:C:168:ARG:HB3	2.03	0.41
1:A:189:ASN:O	1:A:192:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HD2	1:B:775:ARG:NH2	2.36	0.41
1:A:261:LEU:O	1:A:265:VAL:HG22	2.21	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.61	0.41
1:A:645:ARG:C	1:A:648:ARG:HB3	2.41	0.41
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.82	0.41
1:B:80:SER:CB	1:B:90:ILE:HG12	2.51	0.41
1:B:105:VAL:HG21	1:C:105:VAL:HG13	2.03	0.41
1:B:361:ASN:O	1:B:365:THR:HG22	2.21	0.41
1:C:64:VAL:HG11	1:C:117:LEU:HB2	2.01	0.41
1:C:605:ASN:HD21	1:C:637:ASN:HA	1.85	0.41
1:C:930:ILE:HG21	1:C:930:ILE:HD13	1.87	0.41
1:C:1029:SER:OG	1:C:1030:ARG:N	2.48	0.41
1:D:11:PHE:HB2	1:E:888:GLU:OE2	2.21	0.41
1:D:166:ILE:HD13	1:D:166:ILE:HA	1.91	0.41
1:D:293:LEU:HD22	1:D:294:ALA:N	2.36	0.41
1:D:770:SER:OG	1:D:775:ARG:HG2	2.20	0.41
1:D:963:VAL:HA	1:D:966:ARG:HH12	1.85	0.41
1:E:103:ALA:O	1:E:107:VAL:HG23	2.21	0.41
1:E:313:MET:HA	1:E:316:PHE:HD2	1.86	0.41
1:E:527:TYR:CE2	1:E:967:LEU:HG	2.56	0.41
1:E:535:LEU:HD13	1:E:1022:VAL:HG21	2.02	0.41
1:E:559:LEU:HD22	1:E:917:THR:HA	2.03	0.41
1:E:685:LEU:HD13	1:E:689:LYS:HB3	2.02	0.41
1:F:33:ALA:HB2	1:F:298:ASN:OD1	2.21	0.41
1:F:379:THR:N	1:F:480:LEU:HD11	2.35	0.41
1:F:510:LYS:HA	1:F:518:ARG:NH1	2.35	0.41
1:F:545:TYR:O	1:F:549:VAL:HG23	2.21	0.41
1:F:553:ALA:O	1:F:557:VAL:HG23	2.20	0.41
1:F:932:LEU:HD11	1:F:977:PHE:HE2	1.85	0.41
1:A:757:PHE:CE1	1:A:759:ASP:HB2	2.55	0.41
1:A:903:GLY:HA2	1:A:1009:ALA:HB2	2.03	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.21	0.41
1:B:914:ARG:HH12	1:B:985:VAL:HG12	1.86	0.41
1:B:914:ARG:NH2	1:B:996:ASN:HB3	2.36	0.41
1:B:926:LEU:HA	1:B:926:LEU:HD23	1.69	0.41
1:C:65:ILE:HG21	1:C:90:ILE:HD13	2.03	0.41
1:C:199:THR:HG21	1:C:787:ARG:H	1.86	0.41
1:C:404:LEU:HB3	1:C:478:MET:SD	2.61	0.41
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.83	0.41
1:D:317:PHE:CD1	1:D:321:LEU:HD12	2.56	0.41
1:D:339:GLU:OE1	1:D:342:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ASP:O	1:D:783:ASP:HB2	2.20	0.41
1:E:142:VAL:O	1:E:154:ILE:HD13	2.21	0.41
1:E:235:ILE:HB	1:F:723:LYS:HA	2.01	0.41
1:E:567:GLU:O	1:E:569:GLN:HG3	2.21	0.41
1:E:838:LEU:HD22	1:E:841:GLN:HB2	2.02	0.41
1:F:726:ILE:H	1:F:726:ILE:HG13	1.65	0.41
1:F:979:LEU:HD23	1:F:979:LEU:HA	1.75	0.41
1:A:678:GLU:HG2	1:A:814:TYR:CG	2.56	0.40
1:B:138:MET:HE2	1:B:138:MET:HB2	1.94	0.40
1:B:773:LYS:HG3	1:B:774:TYR:CE2	2.56	0.40
1:C:497:LEU:HD12	1:C:497:LEU:HA	1.82	0.40
1:C:632:ARG:HH12	1:C:638:LYS:HA	1.86	0.40
1:C:1010:THR:O	1:C:1014:ILE:HG23	2.21	0.40
1:D:143:ILE:HG22	1:D:286:ALA:HB2	2.02	0.40
1:D:442:LEU:HD23	1:D:442:LEU:HA	1.70	0.40
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.71	0.40
1:D:654:LYS:HA	1:D:654:LYS:HD3	1.77	0.40
1:D:940:ILE:HG12	1:D:966:ARG:NH2	2.36	0.40
1:E:56:THR:O	1:E:60:THR:OG1	2.25	0.40
1:E:343:THR:HG21	1:E:399:VAL:CG1	2.43	0.40
1:E:723:LYS:HG2	1:E:803:ARG:NH1	2.36	0.40
1:E:736:VAL:HB	1:E:741:ILE:HD11	2.03	0.40
1:F:104:GLN:OE1	1:F:108:GLN:NE2	2.54	0.40
1:F:217:GLY:O	1:F:234:ILE:HB	2.22	0.40
1:C:527:TYR:O	1:C:531:VAL:HG23	2.21	0.40
1:C:963:VAL:HA	1:C:966:ARG:NH2	2.37	0.40
1:C:984:LEU:HB3	1:C:995:GLN:O	2.21	0.40
1:D:162:MET:HA	1:D:313:MET:SD	2.62	0.40
1:D:404:LEU:HD21	1:D:449:LEU:HD22	2.02	0.40
1:D:540:ARG:NH2	2:D:2000:LMT:H6'2	2.36	0.40
1:D:564:LEU:HD22	1:D:666:ILE:HG12	2.04	0.40
1:D:564:LEU:CD2	1:D:666:ILE:HG12	2.51	0.40
1:E:330:THR:HB	1:E:331:PRO:HD3	2.03	0.40
1:E:516:PHE:HA	1:E:519:MET:CG	2.45	0.40
1:E:541:TYR:HH	2:E:1101:LMT:H6'	1.54	0.40
1:E:956:ILE:H	1:E:956:ILE:HG13	1.27	0.40
1:F:489:THR:HA	1:F:492:LEU:HB2	2.03	0.40
1:F:868:ALA:HB2	1:F:923:GLN:NE2	2.36	0.40
1:F:941:VAL:HG13	1:F:1021:PHE:CE1	2.56	0.40
1:A:676:ASP:HB2	1:A:857:MET:HE3	2.04	0.40
1:A:697:LEU:HA	1:A:700:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PHE:HB2	1:A:804:TRP:CH2	2.56	0.40
1:A:969:PRO:HA	1:A:972:MET:HE2	2.03	0.40
1:B:233:SER:HB2	1:C:721:GLN:HG2	2.03	0.40
1:B:786:VAL:HG23	1:B:796:PHE:CE2	2.55	0.40
1:B:983:PRO:O	1:B:987:SER:HB2	2.22	0.40
1:C:152:GLU:H	1:C:152:GLU:CD	2.24	0.40
1:C:364:ALA:O	1:C:368:PRO:HD3	2.21	0.40
1:C:584:GLN:N	1:C:617:GLN:OE1	2.31	0.40
1:D:231:ASN:ND2	1:E:617:GLN:HE22	2.20	0.40
1:D:511:GLY:CA	1:D:515:TRP:CD1	3.01	0.40
1:E:667:VAL:H	1:E:667:VAL:HG23	1.58	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.83	0.40
1:A:340:VAL:HB	1:A:395:MET:HE2	2.02	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.22	0.40
1:A:467:TYR:CE2	1:A:920:VAL:HG22	2.55	0.40
1:C:55:LYS:HA	1:C:811:LEU:HD11	2.03	0.40
1:C:137:LEU:HB2	1:C:293:LEU:HB2	2.03	0.40
1:C:188:MET:O	1:C:771:GLU:HG3	2.20	0.40
1:C:252:LYS:HE2	1:C:253:VAL:O	2.21	0.40
1:C:431:THR:HG21	1:C:490:PRO:O	2.22	0.40
1:D:188:MET:HB2	1:D:188:MET:HE3	1.78	0.40
1:D:281:PHE:CD2	1:D:281:PHE:C	2.95	0.40
1:E:587:THR:HB	1:E:613:ASN:OD1	2.21	0.40
1:E:681:ASP:HB2	1:E:690:LEU:HG	2.04	0.40
1:E:722:PHE:HD1	1:E:804:TRP:CE2	2.40	0.40
1:F:180:SER:HB3	1:F:273:GLU:CB	2.51	0.40
1:F:525:HIS:O	1:F:526:HIS:C	2.60	0.40
1:F:546:LEU:O	1:F:550:VAL:HG23	2.21	0.40
1:A:142:VAL:N	1:A:287:SER:O	2.44	0.40
1:A:615:GLY:HA2	1:A:616:GLY:HA2	1.75	0.40
1:A:778:PRO:HG3	1:A:804:TRP:HZ2	1.87	0.40
1:B:58:GLN:OE1	1:B:811:LEU:HB3	2.21	0.40
1:B:534:ILE:HD13	1:B:534:ILE:HG21	1.91	0.40
1:C:44:THR:HA	1:C:90:ILE:O	2.21	0.40
1:C:359:LEU:HB2	1:C:365:THR:HG22	2.03	0.40
1:C:1031:LYS:HA	1:C:1031:LYS:HD3	1.86	0.40
1:D:407:ASP:O	1:D:411:VAL:HG23	2.22	0.40
1:D:554:TYR:CE2	1:D:558:ARG:HG3	2.56	0.40
1:D:704:HIS:CE1	1:D:842:LEU:HD21	2.56	0.40
1:D:916:LEU:HB3	1:D:917:THR:H	1.68	0.40
1:D:984:LEU:HB3	1:D:995:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:936:ASN:ND2	1:E:970:ILE:HG23	2.36	0.40
1:F:337:ILE:HD11	1:F:391:ASN:HA	2.04	0.40
1:F:343:THR:HG21	1:F:984:LEU:HD23	2.03	0.40
1:F:348:ILE:HG13	1:F:348:ILE:H	1.68	0.40
1:F:478:MET:O	1:F:482:VAL:HG23	2.21	0.40
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.75	0.40
1:F:527:TYR:O	1:F:531:VAL:HG23	2.21	0.40
1:F:887:TYR:C	1:F:889:SER:H	2.13	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1044 (99%)	942 (91%)	79 (8%)	15 (1%)	11	37
1	B	1037/1044 (99%)	942 (91%)	85 (8%)	10 (1%)	15	46
1	C	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	9	34
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	8	32
1	E	1035/1044 (99%)	937 (90%)	87 (8%)	11 (1%)	14	44
1	F	1035/1044 (99%)	926 (90%)	84 (8%)	25 (2%)	6	28
All	All	6212/6264 (99%)	5612 (90%)	502 (8%)	98 (2%)	9	34

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	ALA
1	A	986	ILE
1	A	1029	SER
1	A	1033	GLU

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Mol	Chain	Res	Type
1	B	617	GLN
1	B	1029	SER
1	B	1038	SER
1	C	509	LYS
1	C	915	GLY
1	C	1009	ALA
1	C	1029	SER
1	C	1035	ILE
1	D	508	GLY
1	D	511	GLY
1	D	668	GLU
1	D	915	GLY
1	D	1029	SER
1	D	1034	ASP
1	D	1035	ILE
1	D	1036	GLU
1	D	1038	SER
1	E	667	VAL
1	E	1029	SER
1	E	1033	GLU
1	E	1036	GLU
1	F	134	SER
1	F	145	THR
1	F	509	LYS
1	F	617	GLN
1	F	888	GLU
1	F	1029	SER
1	F	1032	ASN
1	F	1035	ILE
1	A	915	GLY
1	A	987	SER
1	A	1032	ASN
1	B	514	GLY
1	B	684	GLY
1	B	1035	ILE
1	C	147	GLY
1	C	831	SER
1	D	4	PHE
1	D	987	SER
1	D	1028	PHE
1	D	1031	LYS
1	E	668	GLU

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Mol	Chain	Res	Type
1	F	6	ILE
1	F	146	ASP
1	F	147	GLY
1	F	511	GLY
1	F	684	GLY
1	F	918	ASN
1	F	1028	PHE
1	A	615	GLY
1	A	1031	LYS
1	B	918	ASN
1	C	134	SER
1	C	146	ASP
1	C	360	GLN
1	C	888	GLU
1	F	407	ASP
1	F	507	GLU
1	F	831	SER
1	F	1034	ASP
1	A	215	ALA
1	B	215	ALA
1	C	6	ILE
1	C	1033	GLU
1	D	614	GLY
1	D	653	ILE
1	D	909	LEU
1	F	360	GLN
1	A	918	ASN
1	A	1036	GLU
1	B	1039	HIS
1	C	215	ALA
1	C	918	ASN
1	D	215	ALA
1	E	216	ALA
1	F	150	THR
1	F	215	ALA
1	A	509	LYS
1	E	778	PRO
1	F	773	LYS
1	F	915	GLY
1	A	666	ILE
1	A	778	PRO
1	C	998	VAL

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Mol	Chain	Res	Type
1	E	511	GLY
1	E	1035	ILE
1	D	616	GLY
1	C	828	PRO
1	E	508	GLY
1	E	539	GLY
1	F	778	PRO
1	B	318	PRO
1	C	653	ILE
1	D	200	PRO

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	846/852 (99%)	781 (92%)	65 (8%)	13	40
1	B	847/852 (99%)	789 (93%)	58 (7%)	16	45
1	C	843/852 (99%)	774 (92%)	69 (8%)	11	37
1	D	846/852 (99%)	789 (93%)	57 (7%)	16	46
1	E	845/852 (99%)	775 (92%)	70 (8%)	11	36
1	F	845/852 (99%)	789 (93%)	56 (7%)	16	46
All	All	5072/5112 (99%)	4697 (93%)	375 (7%)	13	42

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	25	LEU
1	A	44	THR
1	A	49	TYR
1	A	70	ASN
1	A	101	ASP
1	A	146	ASP
1	A	148	THR

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Mol	Chain	Res	Type
1	A	152	GLU
1	A	166	ILE
1	A	177	LEU
1	A	243	THR
1	A	255	GLN
1	A	281	PHE
1	A	293	LEU
1	A	295	THR
1	A	337	ILE
1	A	342	LYS
1	A	349	ILE
1	A	350	LEU
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	502	LYS
1	A	512	PHE
1	A	519	MET
1	A	524	THR
1	A	536	ARG
1	A	538	THR
1	A	542	LEU
1	A	558	ARG
1	A	566	ASP
1	A	575	MET
1	A	603	LYS
1	A	610	PHE
1	A	669	LEU
1	A	682	GLN
1	A	690	LEU
1	A	694	ARG
1	A	708	LEU
1	A	711	VAL
1	A	726	ILE
1	A	736	VAL
1	A	830	LYS

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	916	LEU
1	A	917	THR
1	A	926	LEU
1	A	942	GLU
1	A	946	ASP
1	A	956	ILE
1	A	959	THR
1	A	966	ARG
1	A	977	PHE
1	A	985	VAL
1	A	1012	LEU
1	A	1014	ILE
1	A	1024	VAL
1	A	1035	ILE
1	B	6	ILE
1	B	10	ILE
1	B	11	PHE
1	B	29	LYS
1	B	34	GLN
1	B	49	TYR
1	B	96	SER
1	B	117	LEU
1	B	131	LYS
1	B	177	LEU
1	B	185	ARG
1	B	229	GLN
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	293	LEU
1	B	295	THR
1	B	323	ILE
1	B	350	LEU
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	372	VAL
1	B	389	SER
1	B	400	LEU
1	B	422	GLU

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Mol	Chain	Res	Type
1	B	482	VAL
1	B	489	THR
1	B	538	THR
1	B	542	LEU
1	B	559	LEU
1	B	563	PHE
1	B	571	VAL
1	B	575	MET
1	B	578	LEU
1	B	583	THR
1	B	610	PHE
1	B	663	LEU
1	B	668	GLU
1	B	673	THR
1	B	682	GLN
1	B	690	LEU
1	B	694	ARG
1	B	830	LYS
1	B	839	MET
1	B	860	GLN
1	B	916	LEU
1	B	946	ASP
1	B	961	ASP
1	B	966	ARG
1	B	968	ARG
1	B	1012	LEU
1	B	1029	SER
1	B	1032	ASN
1	B	1033	GLU
1	B	1035	ILE
1	B	1039	HIS
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	25	LEU
1	C	27	ILE
1	C	28	LEU
1	C	49	TYR
1	C	55	LYS
1	C	88	VAL
1	C	90	ILE
1	C	102	ILE

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	112	GLN
1	C	120	GLN
1	C	145	THR
1	C	153	ASP
1	C	177	LEU
1	C	219	LEU
1	C	243	THR
1	C	264	ASP
1	C	293	LEU
1	C	337	ILE
1	C	342	LYS
1	C	358	PHE
1	C	360	GLN
1	C	407	ASP
1	C	429	GLU
1	C	439	GLN
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	470	PHE
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	512	PHE
1	C	540	ARG
1	C	564	LEU
1	C	571	VAL
1	C	575	MET
1	C	587	THR
1	C	596	HIS
1	C	610	PHE
1	C	644	MET
1	C	652	GLN
1	C	661	PHE
1	C	689	LYS
1	C	711	VAL
1	C	736	VAL
1	C	741	ILE
1	C	838	LEU
1	C	842	LEU
1	C	855	THR

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Mol	Chain	Res	Type
1	C	860	GLN
1	C	881	LEU
1	C	890	TRP
1	C	909	LEU
1	C	942	GLU
1	C	956	ILE
1	C	963	VAL
1	C	966	ARG
1	C	986	ILE
1	C	1008	THR
1	C	1010	THR
1	C	1012	LEU
1	C	1030	ARG
1	C	1033	GLU
1	C	1035	ILE
1	C	1036	GLU
1	D	6	ILE
1	D	11	PHE
1	D	25	LEU
1	D	70	ASN
1	D	102	ILE
1	D	146	ASP
1	D	148	THR
1	D	152	GLU
1	D	153	ASP
1	D	177	LEU
1	D	205	THR
1	D	229	GLN
1	D	264	ASP
1	D	280	GLU
1	D	281	PHE
1	D	295	THR
1	D	350	LEU
1	D	358	PHE
1	D	362	PHE
1	D	365	THR
1	D	404	LEU
1	D	429	GLU
1	D	437	GLN
1	D	489	THR
1	D	519	MET
1	D	534	ILE

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Mol	Chain	Res	Type
1	D	538	THR
1	D	559	LEU
1	D	561	SER
1	D	571	VAL
1	D	575	MET
1	D	603	LYS
1	D	610	PHE
1	D	628	ASP
1	D	629	TRP
1	D	637	ASN
1	D	690	LEU
1	D	708	LEU
1	D	726	ILE
1	D	738	ILE
1	D	852	TYR
1	D	862	ARG
1	D	909	LEU
1	D	913	PHE
1	D	916	LEU
1	D	917	THR
1	D	926	LEU
1	D	930	ILE
1	D	942	GLU
1	D	946	ASP
1	D	956	ILE
1	D	961	ASP
1	D	966	ARG
1	D	1012	LEU
1	D	1024	VAL
1	D	1030	ARG
1	D	1035	ILE
1	E	6	ILE
1	E	11	PHE
1	E	25	LEU
1	E	28	LEU
1	E	49	TYR
1	E	96	SER
1	E	105	VAL
1	E	117	LEU
1	E	131	LYS
1	E	146	ASP
1	E	153	ASP

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Mol	Chain	Res	Type
1	E	177	LEU
1	E	249	ILE
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	280	GLU
1	E	310	LEU
1	E	312	LYS
1	E	323	ILE
1	E	336	SER
1	E	355	MET
1	E	356	TYR
1	E	358	PHE
1	E	372	VAL
1	E	398	MET
1	E	404	LEU
1	E	459	PHE
1	E	482	VAL
1	E	512	PHE
1	E	526	HIS
1	E	538	THR
1	E	555	LEU
1	E	564	LEU
1	E	566	ASP
1	E	571	VAL
1	E	574	THR
1	E	575	MET
1	E	583	THR
1	E	610	PHE
1	E	613	ASN
1	E	619	THR
1	E	629	TRP
1	E	647	THR
1	E	648	ARG
1	E	654	LYS
1	E	667	VAL
1	E	668	GLU
1	E	669	LEU
1	E	685	LEU
1	E	689	LYS
1	E	690	LEU
1	E	694	ARG

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Mol	Chain	Res	Type
1	E	706	ASP
1	E	707	MET
1	E	708	LEU
1	E	712	ARG
1	E	726	ILE
1	E	736	VAL
1	E	799	PHE
1	E	830	LYS
1	E	852	TYR
1	E	896	VAL
1	E	909	LEU
1	E	917	THR
1	E	953	LYS
1	E	956	ILE
1	E	961	ASP
1	E	1012	LEU
1	E	1021	PHE
1	F	6	ILE
1	F	25	LEU
1	F	27	ILE
1	F	28	LEU
1	F	49	TYR
1	F	70	ASN
1	F	88	VAL
1	F	102	ILE
1	F	104	GLN
1	F	112	GLN
1	F	153	ASP
1	F	197	GLN
1	F	205	THR
1	F	243	THR
1	F	280	GLU
1	F	293	LEU
1	F	312	LYS
1	F	327	TYR
1	F	350	LEU
1	F	358	PHE
1	F	360	GLN
1	F	363	ARG
1	F	407	ASP
1	F	431	THR
1	F	447	MET

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Mol	Chain	Res	Type
1	F	448	VAL
1	F	515	TRP
1	F	538	THR
1	F	542	LEU
1	F	575	MET
1	F	587	THR
1	F	610	PHE
1	F	621	ILE
1	F	644	MET
1	F	657	MET
1	F	663	LEU
1	F	689	LYS
1	F	694	ARG
1	F	711	VAL
1	F	714	ASN
1	F	726	ILE
1	F	779	ASP
1	F	838	LEU
1	F	842	LEU
1	F	845	LYS
1	F	859	TYR
1	F	860	GLN
1	F	881	LEU
1	F	918	ASN
1	F	961	ASP
1	F	963	VAL
1	F	966	ARG
1	F	986	ILE
1	F	1021	PHE
1	F	1030	ARG
1	F	1034	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	237	GLN
1	A	569	GLN
1	B	63	GLN
1	B	109	ASN
1	B	742	ASN
1	C	151	GLN

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Mol	Chain	Res	Type
1	C	613	ASN
1	C	755	ASN
1	D	109	ASN
1	D	231	ASN
1	D	437	GLN
1	D	742	ASN
1	E	34	GLN
1	E	67	GLN
1	E	231	ASN
1	E	569	GLN
1	E	605	ASN
1	E	613	ASN
1	E	637	ASN
1	E	732	GLN
1	F	108	GLN
1	F	584	GLN
1	F	613	ASN
1	F	682	GLN
1	F	704	HIS
1	F	732	GLN
1	F	755	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

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	F	2000	-	36,36,36	1.85	8 (22%)	47,47,47	1.14	4 (8%)
2	LMT	B	2000	-	36,36,36	1.81	12 (33%)	47,47,47	1.50	8 (17%)
2	LMT	E	1101	-	36,36,36	1.83	10 (27%)	47,47,47	1.92	9 (19%)
2	LMT	D	2000	-	36,36,36	1.87	9 (25%)	47,47,47	1.70	8 (17%)
2	LMT	A	1101	-	36,36,36	1.80	11 (30%)	47,47,47	1.37	6 (12%)
2	LMT	C	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.40	6 (12%)

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	F	2000	-	-	15/21/61/61	0/2/2/2
2	LMT	B	2000	-	-	13/21/61/61	0/2/2/2
2	LMT	E	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	D	2000	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	12/21/61/61	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	4.20	1.47	1.40
2	C	1101	LMT	O5'-C5'	4.10	1.54	1.44
2	F	2000	LMT	O5'-C1'	4.07	1.52	1.41
2	B	2000	LMT	O5'-C5'	3.97	1.54	1.44
2	F	2000	LMT	O5'-C5'	3.97	1.54	1.44
2	F	2000	LMT	O1'-C1'	3.95	1.46	1.40
2	D	2000	LMT	O1'-C1'	3.94	1.46	1.40
2	A	1101	LMT	O5'-C5'	3.91	1.53	1.44
2	D	2000	LMT	O5'-C5'	3.85	1.53	1.44
2	C	1101	LMT	O1'-C1'	3.65	1.46	1.40
2	E	1101	LMT	O5'-C5'	3.60	1.53	1.44
2	D	2000	LMT	O5B-C1B	3.52	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O5'-C1'	3.47	1.50	1.41
2	C	1101	LMT	C6'-C5'	-3.46	1.40	1.51
2	F	2000	LMT	C6'-C5'	-3.42	1.40	1.51
2	F	2000	LMT	O5B-C1B	3.40	1.50	1.41
2	A	1101	LMT	O5B-C1B	3.36	1.50	1.41
2	E	1101	LMT	C6'-C5'	-3.35	1.40	1.51
2	A	1101	LMT	O1'-C1'	3.34	1.45	1.40
2	C	1101	LMT	O5'-C1'	3.33	1.50	1.41
2	B	2000	LMT	C6'-C5'	-3.25	1.40	1.51
2	C	1101	LMT	O5B-C1B	3.21	1.50	1.41
2	A	1101	LMT	C6'-C5'	-3.20	1.41	1.51
2	B	2000	LMT	O5B-C1B	3.19	1.50	1.41
2	D	2000	LMT	C3'-C2'	-3.14	1.44	1.52
2	E	1101	LMT	O5B-C1B	3.12	1.49	1.41
2	B	2000	LMT	O1'-C1'	3.07	1.45	1.40
2	D	2000	LMT	C6'-C5'	-3.05	1.41	1.51
2	C	1101	LMT	O3B-C3B	3.05	1.50	1.43
2	B	2000	LMT	O5'-C1'	2.96	1.49	1.41
2	B	2000	LMT	C3'-C2'	-2.94	1.44	1.52
2	B	2000	LMT	C3B-C2B	-2.87	1.45	1.52
2	D	2000	LMT	O5'-C1'	2.86	1.49	1.41
2	D	2000	LMT	O3B-C3B	2.86	1.49	1.43
2	E	1101	LMT	C3'-C2'	-2.83	1.45	1.52
2	F	2000	LMT	C3'-C2'	-2.80	1.45	1.52
2	E	1101	LMT	O3B-C3B	2.68	1.49	1.43
2	D	2000	LMT	C3B-C2B	-2.66	1.45	1.52
2	E	1101	LMT	O1B-C1B	-2.65	1.34	1.41
2	A	1101	LMT	O5'-C1'	2.65	1.48	1.41
2	A	1101	LMT	C3'-C2'	-2.63	1.45	1.52
2	D	2000	LMT	O2'-C2'	2.51	1.48	1.43
2	F	2000	LMT	O3B-C3B	2.38	1.48	1.43
2	A	1101	LMT	O2'-C2'	2.35	1.48	1.43
2	C	1101	LMT	C3'-C2'	-2.33	1.46	1.52
2	C	1101	LMT	O2'-C2'	2.32	1.48	1.43
2	A	1101	LMT	C1'-C2'	-2.28	1.45	1.52
2	A	1101	LMT	O3B-C3B	2.26	1.48	1.43
2	A	1101	LMT	C3B-C2B	-2.23	1.46	1.52
2	B	2000	LMT	O3B-C3B	2.23	1.48	1.43
2	E	1101	LMT	O1B-C4'	-2.16	1.38	1.43
2	B	2000	LMT	C5-C4	2.09	1.63	1.51
2	E	1101	LMT	O3'-C3'	2.07	1.47	1.43
2	C	1101	LMT	O3'-C3'	2.07	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	LMT	O2'-C2'	2.06	1.47	1.43
2	F	2000	LMT	C5-C4	2.05	1.63	1.51
2	B	2000	LMT	O3'-C3'	2.03	1.47	1.43
2	A	1101	LMT	O1B-C1B	-2.03	1.36	1.41
2	C	1101	LMT	C5-C4	2.01	1.62	1.51
2	B	2000	LMT	C4'-C5'	2.00	1.58	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1101	LMT	O1B-C4'-C5'	-5.21	95.18	109.45
2	D	2000	LMT	O1'-C1'-C2'	5.11	116.28	108.30
2	C	1101	LMT	O1'-C1'-C2'	4.87	115.91	108.30
2	E	1101	LMT	C4B-C3B-C2B	4.82	119.23	110.82
2	E	1101	LMT	C3B-C4B-C5B	4.70	118.63	110.24
2	D	2000	LMT	C1-O1'-C1'	4.70	121.63	113.84
2	A	1101	LMT	C1B-O5B-C5B	4.43	122.37	113.69
2	E	1101	LMT	O1'-C1'-C2'	4.15	114.78	108.30
2	A	1101	LMT	O5B-C5B-C4B	4.02	116.99	109.69
2	B	2000	LMT	C1B-O1B-C4'	-3.87	108.39	117.96
2	B	2000	LMT	O5B-C5B-C4B	3.72	116.44	109.69
2	E	1101	LMT	O4'-C4B-C3B	-3.67	101.86	110.35
2	D	2000	LMT	O2'-C2'-C1'	3.62	118.84	110.05
2	B	2000	LMT	C1'-C2'-C3'	-3.57	102.57	110.00
2	D	2000	LMT	C1B-O1B-C4'	-3.33	109.73	117.96
2	E	1101	LMT	O5'-C5'-C6'	3.06	114.03	106.44
2	B	2000	LMT	O3B-C3B-C2B	-3.03	103.34	110.35
2	D	2000	LMT	C1'-O5'-C5'	2.96	119.49	113.69
2	D	2000	LMT	C1'-C2'-C3'	-2.82	104.11	110.00
2	F	2000	LMT	C1B-O5B-C5B	-2.81	108.17	113.69
2	E	1101	LMT	O5B-C5B-C4B	2.76	114.70	109.69
2	E	1101	LMT	O1B-C1B-C2B	-2.70	101.11	108.10
2	C	1101	LMT	C1'-C2'-C3'	-2.69	104.40	110.00
2	B	2000	LMT	O1'-C1'-C2'	2.61	112.38	108.30
2	C	1101	LMT	C3'-C4'-C5'	-2.55	105.07	110.93
2	C	1101	LMT	O3'-C3'-C4'	2.49	116.54	109.94
2	B	2000	LMT	C1B-O5B-C5B	2.46	118.51	113.69
2	B	2000	LMT	O1B-C1B-C2B	2.46	114.46	108.10
2	C	1101	LMT	C1B-O1B-C4'	-2.43	111.94	117.96
2	D	2000	LMT	O3'-C3'-C4'	2.42	116.37	109.94
2	A	1101	LMT	C1B-C2B-C3B	2.38	114.96	110.00
2	F	2000	LMT	O5B-C5B-C4B	2.37	114.00	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2000	LMT	C1'-O5'-C5'	2.32	118.23	113.69
2	A	1101	LMT	O3B-C3B-C4B	-2.29	105.06	110.35
2	D	2000	LMT	C4B-C3B-C2B	2.29	114.81	110.82
2	B	2000	LMT	C1'-O5'-C5'	-2.28	109.21	113.69
2	E	1101	LMT	O2'-C2'-C1'	2.22	115.44	110.05
2	F	2000	LMT	O5B-C5B-C6B	2.17	111.82	106.44
2	C	1101	LMT	C1B-C2B-C3B	2.14	114.46	110.00
2	A	1101	LMT	O5B-C1B-C2B	2.13	114.86	110.35
2	A	1101	LMT	C6B-C5B-C4B	-2.10	108.09	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	E	1101	LMT	C2B

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	C2'-C1'-O1'-C1
2	E	1101	LMT	C4B-C5B-C6B-O6B
2	F	2000	LMT	O5'-C5'-C6'-O6'
2	A	1101	LMT	O5'-C5'-C6'-O6'
2	E	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	E	1101	LMT	O5'-C5'-C6'-O6'
2	D	2000	LMT	O5'-C5'-C6'-O6'
2	E	1101	LMT	C4'-C5'-C6'-O6'
2	A	1101	LMT	C4'-C5'-C6'-O6'
2	D	2000	LMT	C4'-C5'-C6'-O6'
2	B	2000	LMT	C2-C3-C4-C5
2	C	1101	LMT	C4-C5-C6-C7
2	A	1101	LMT	C3-C4-C5-C6
2	C	1101	LMT	O5'-C5'-C6'-O6'
2	F	2000	LMT	C4'-C5'-C6'-O6'
2	F	2000	LMT	O5B-C5B-C6B-O6B
2	B	2000	LMT	C4'-C5'-C6'-O6'
2	C	1101	LMT	C4'-C5'-C6'-O6'
2	F	2000	LMT	C4B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
2	A	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	A	1101	LMT	O5B-C5B-C6B-O6B
2	C	1101	LMT	C6-C7-C8-C9
2	A	1101	LMT	O1'-C1-C2-C3
2	D	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	O5'-C5'-C6'-O6'
2	B	2000	LMT	O1'-C1-C2-C3
2	E	1101	LMT	C5-C6-C7-C8
2	E	1101	LMT	C11-C10-C9-C8
2	C	1101	LMT	C2-C3-C4-C5
2	F	2000	LMT	C11-C10-C9-C8
2	D	2000	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	C4-C5-C6-C7
2	B	2000	LMT	C5-C6-C7-C8
2	B	2000	LMT	C11-C10-C9-C8
2	F	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	C1-C2-C3-C4
2	E	1101	LMT	C3-C4-C5-C6
2	C	1101	LMT	C5-C6-C7-C8
2	D	2000	LMT	O5B-C5B-C6B-O6B
2	F	2000	LMT	C7-C8-C9-C10
2	F	2000	LMT	C1-C2-C3-C4
2	C	1101	LMT	C1-C2-C3-C4
2	E	1101	LMT	C2-C3-C4-C5
2	F	2000	LMT	C2-C3-C4-C5
2	B	2000	LMT	C9-C10-C11-C12
2	B	2000	LMT	O5'-C1'-O1'-C1
2	B	2000	LMT	C7-C8-C9-C10
2	D	2000	LMT	C1-C2-C3-C4
2	D	2000	LMT	C6-C7-C8-C9
2	F	2000	LMT	C9-C10-C11-C12
2	E	1101	LMT	C5'-C4'-O1B-C1B
2	B	2000	LMT	C2-C1-O1'-C1'
2	B	2000	LMT	O5B-C5B-C6B-O6B
2	F	2000	LMT	C4-C5-C6-C7
2	E	1101	LMT	C3'-C4'-O1B-C1B
2	D	2000	LMT	C5-C6-C7-C8
2	D	2000	LMT	C11-C10-C9-C8
2	B	2000	LMT	C4-C5-C6-C7
2	D	2000	LMT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
2	D	2000	LMT	C4-C5-C6-C7
2	F	2000	LMT	C3-C4-C5-C6
2	F	2000	LMT	O1'-C1-C2-C3
2	D	2000	LMT	C9-C10-C11-C12
2	A	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C9-C10-C11-C12
2	C	1101	LMT	O1'-C1-C2-C3

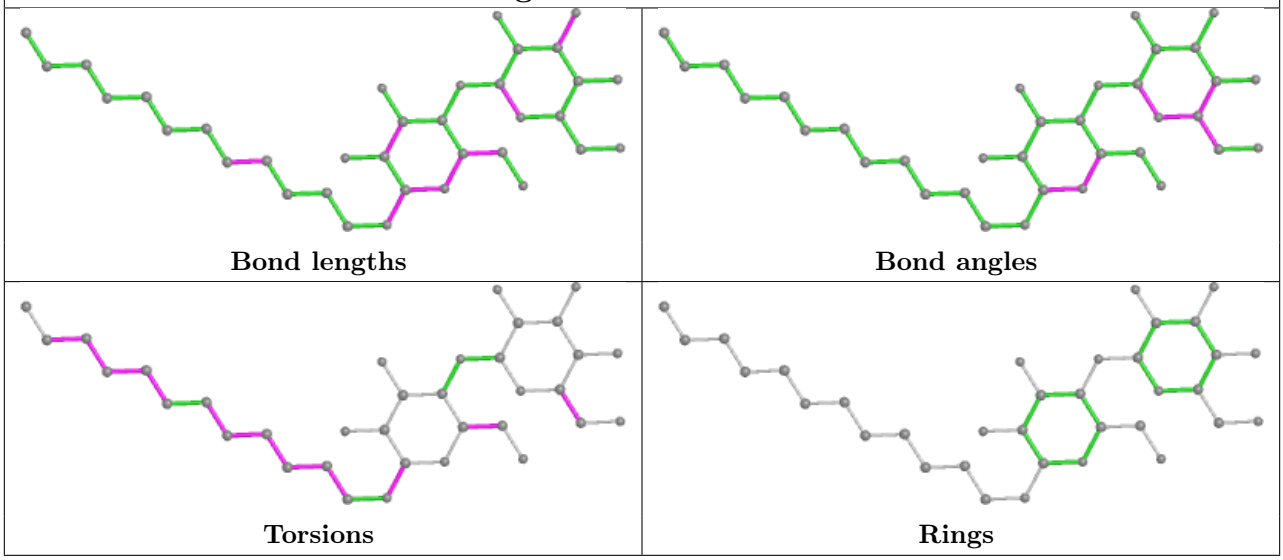
There are no ring outliers.

6 monomers are involved in 20 short contacts:

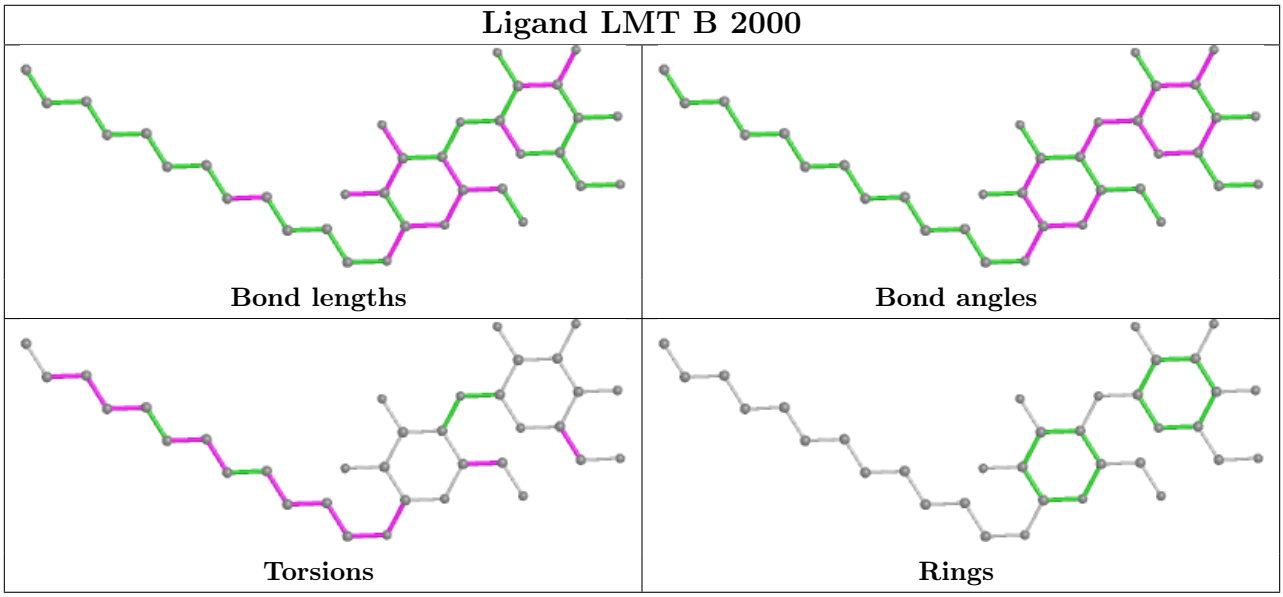
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2000	LMT	1	0
2	B	2000	LMT	3	0
2	E	1101	LMT	8	0
2	D	2000	LMT	3	0
2	A	1101	LMT	4	0
2	C	1101	LMT	1	0

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.

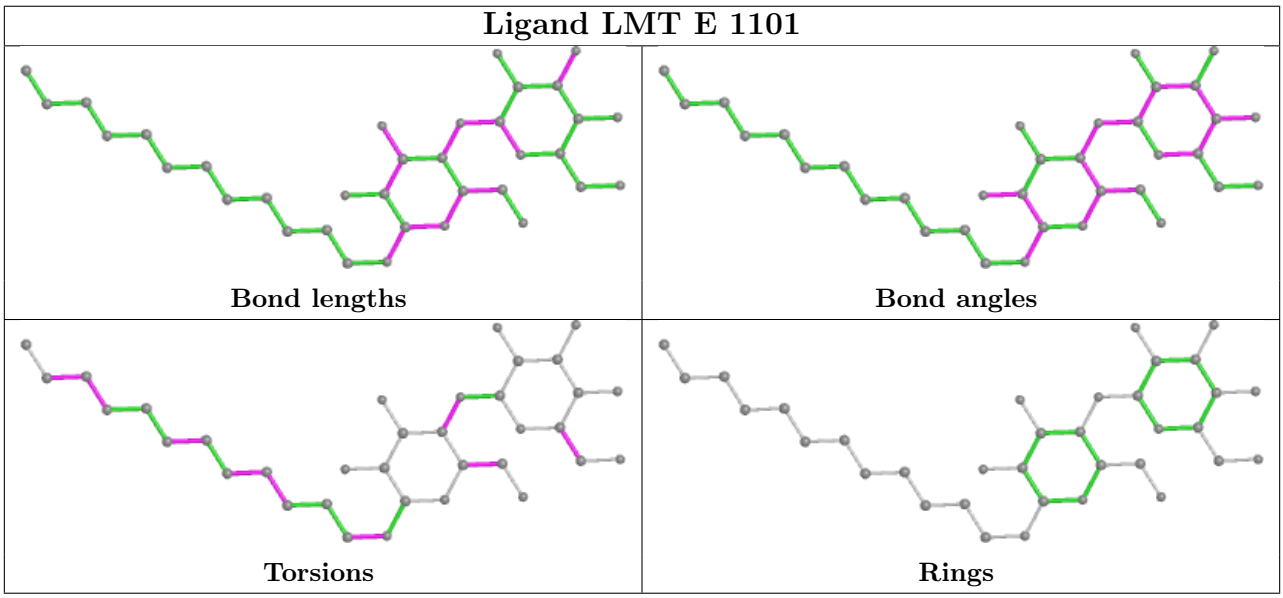
Ligand LMT F 2000



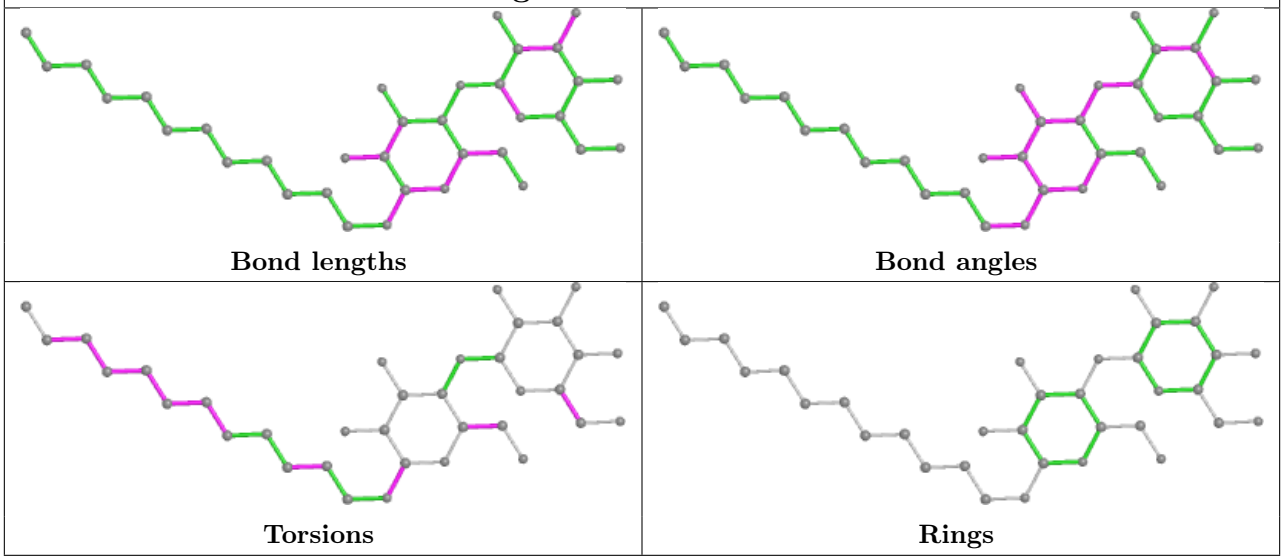
Ligand LMT B 2000



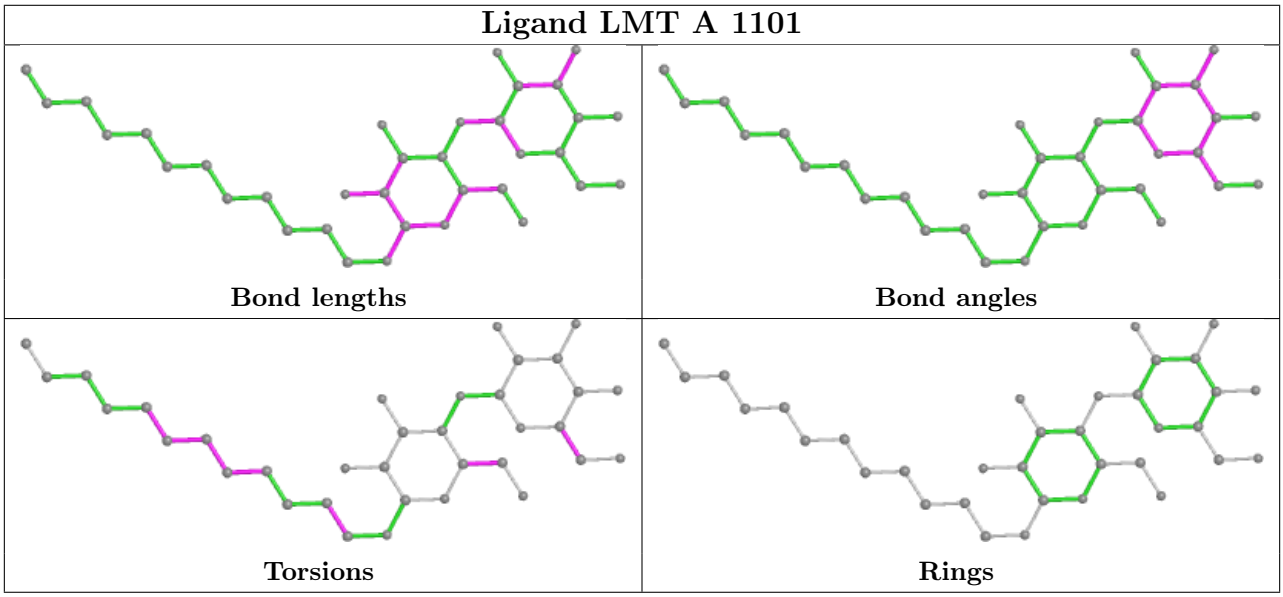
Ligand LMT E 1101



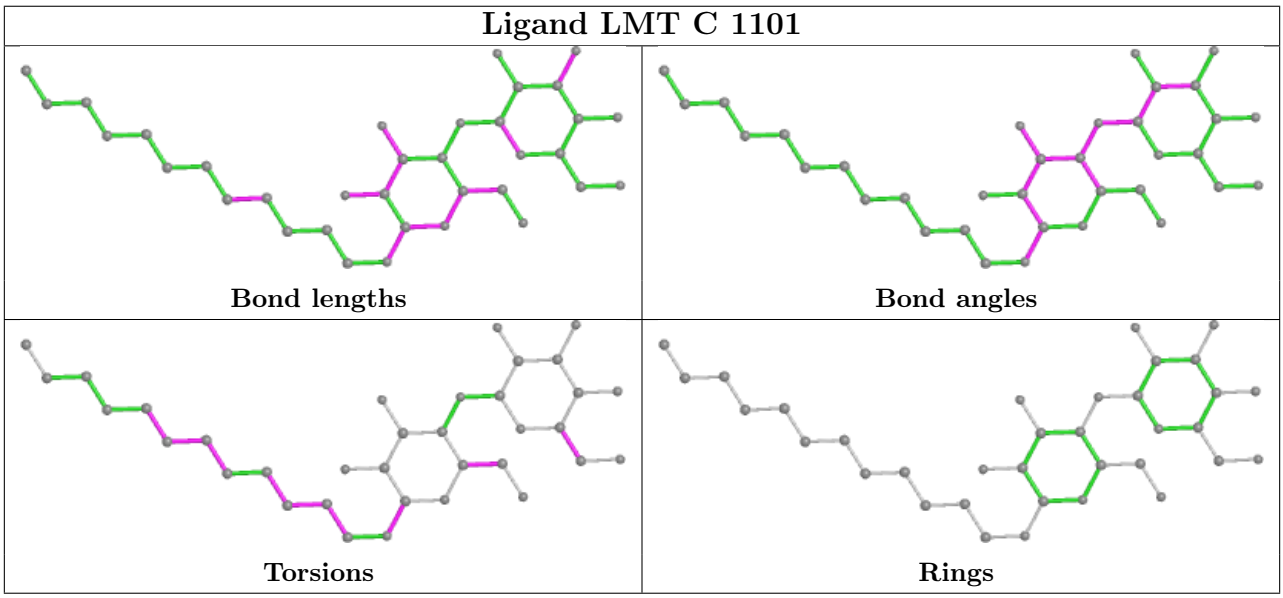
Ligand LMT D 2000



Ligand LMT A 1101



Ligand LMT C 1101



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	1038/1044 (99%)	0.42	127 (12%)	4	5	27, 75, 109, 132	0
1	B	1039/1044 (99%)	0.37	102 (9%)	7	9	18, 68, 104, 130	0
1	C	1035/1044 (99%)	0.49	125 (12%)	4	5	17, 69, 104, 126	0
1	D	1038/1044 (99%)	0.59	162 (15%)	2	2	16, 90, 130, 173	0
1	E	1037/1044 (99%)	0.69	180 (17%)	1	1	40, 91, 115, 134	0
1	F	1037/1044 (99%)	0.73	177 (17%)	1	2	24, 84, 118, 142	0
All	All	6224/6264 (99%)	0.55	873 (14%)	2	3	16, 80, 115, 173	0

All (873) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	128	SER	16.7
1	E	314	GLU	14.0
1	E	315	PRO	12.2
1	F	714	ASN	11.8
1	F	442	LEU	11.2
1	F	128	SER	11.2
1	E	311	ALA	10.4
1	F	832	THR	10.4
1	F	481	SER	10.4
1	F	830	LYS	10.1
1	F	831	SER	10.0
1	C	403	GLY	9.3
1	C	402	ILE	9.2
1	E	406	VAL	9.1
1	C	714	ASN	8.7
1	E	405	LEU	8.5
1	C	715	GLY	8.5
1	B	315	PRO	8.5
1	D	459	PHE	8.4

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Mol	Chain	Res	Type	RSRZ
1	E	129	VAL	8.4
1	F	936	ASN	8.0
1	A	371	ALA	7.9
1	F	127	VAL	7.8
1	D	685	LEU	7.7
1	B	314	GLU	7.7
1	F	823	LEU	7.5
1	C	831	SER	7.5
1	E	973	THR	7.3
1	D	461	GLY	7.2
1	D	322	LYS	7.2
1	D	683	ALA	7.2
1	D	864	SER	7.1
1	F	410	ILE	7.1
1	F	715	GLY	6.9
1	E	409	ALA	6.9
1	C	832	THR	6.8
1	E	407	ASP	6.8
1	A	369	THR	6.7
1	F	406	VAL	6.7
1	E	488	LEU	6.7
1	F	695	ASN	6.7
1	F	448	VAL	6.6
1	D	407	ASP	6.5
1	D	389	SER	6.5
1	F	407	ASP	6.5
1	F	694	ARG	6.5
1	D	462	SER	6.5
1	E	928	THR	6.4
1	B	164	ASP	6.4
1	E	976	ALA	6.4
1	D	35	TYR	6.3
1	C	670	GLY	6.3
1	E	864	SER	6.2
1	F	405	LEU	6.2
1	B	128	SER	6.2
1	F	46	SER	6.1
1	D	282	ASN	6.1
1	E	127	VAL	6.1
1	C	671	THR	6.1
1	F	107	VAL	6.1
1	A	396	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	E	487	ILE	6.0
1	A	372	VAL	6.0
1	D	67	GLN	5.9
1	E	307	ARG	5.9
1	A	404	LEU	5.9
1	E	408	ASP	5.9
1	A	656	ALA	5.9
1	A	400	LEU	5.9
1	F	441	ALA	5.9
1	F	315	PRO	5.9
1	F	111	LEU	5.9
1	D	108	GLN	5.9
1	F	109	ASN	5.8
1	F	500	ILE	5.8
1	A	445	ILE	5.8
1	E	972	MET	5.7
1	F	671	THR	5.7
1	D	70	ASN	5.7
1	A	35	TYR	5.7
1	F	449	LEU	5.7
1	E	310	LEU	5.7
1	C	716	LEU	5.6
1	C	406	VAL	5.6
1	E	932	LEU	5.6
1	F	193	LEU	5.6
1	F	178	PHE	5.6
1	D	486	LEU	5.6
1	F	821	GLU	5.6
1	D	834	GLU	5.5
1	D	460	GLY	5.5
1	C	401	ALA	5.5
1	F	47	ALA	5.5
1	D	111	LEU	5.4
1	B	111	LEU	5.4
1	E	578	LEU	5.4
1	E	410	ILE	5.4
1	E	312	LYS	5.4
1	B	129	VAL	5.4
1	D	658	VAL	5.4
1	A	48	SER	5.4
1	A	894	PHE	5.4
1	F	372	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	487	ILE	5.3
1	C	830	LYS	5.3
1	D	847	PRO	5.3
1	C	821	GLU	5.3
1	E	67	GLN	5.3
1	F	482	VAL	5.3
1	A	16	ALA	5.3
1	C	404	LEU	5.3
1	F	872	TYR	5.3
1	D	404	LEU	5.3
1	C	405	LEU	5.2
1	C	398	MET	5.2
1	E	1014	ILE	5.2
1	F	501	ALA	5.2
1	E	355	MET	5.2
1	E	351	VAL	5.2
1	B	109	ASN	5.2
1	B	831	SER	5.2
1	D	846	LEU	5.2
1	E	352	PHE	5.2
1	E	834	GLU	5.2
1	E	442	LEU	5.2
1	A	482	VAL	5.2
1	F	474	ILE	5.1
1	A	635	GLU	5.1
1	C	445	ILE	5.0
1	F	463	THR	5.0
1	C	707	MET	5.0
1	E	330	THR	5.0
1	E	403	GLY	5.0
1	E	466	ILE	5.0
1	F	833	GLY	4.9
1	F	502	LYS	4.9
1	C	481	SER	4.9
1	F	60	THR	4.9
1	D	32	VAL	4.9
1	B	697	LEU	4.9
1	E	362	PHE	4.9
1	D	141	GLY	4.9
1	E	590	VAL	4.8
1	F	129	VAL	4.8
1	E	366	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	939	LEU	4.8
1	F	443	VAL	4.8
1	D	68	ASN	4.8
1	D	330	THR	4.8
1	D	112	GLN	4.8
1	F	473	THR	4.8
1	B	830	LYS	4.7
1	E	198	LEU	4.7
1	C	833	GLY	4.7
1	F	879	VAL	4.7
1	B	108	GLN	4.7
1	D	411	VAL	4.7
1	E	484	VAL	4.7
1	D	487	ILE	4.6
1	E	483	LEU	4.6
1	A	407	ASP	4.6
1	C	713	PRO	4.6
1	E	291	ILE	4.6
1	A	1008	THR	4.6
1	C	79	SER	4.6
1	C	936	ASN	4.6
1	D	323	ILE	4.6
1	F	467	TYR	4.6
1	B	656	ALA	4.6
1	F	362	PHE	4.6
1	F	408	ASP	4.6
1	C	706	ASP	4.6
1	C	473	THR	4.5
1	F	883	LEU	4.5
1	F	670	GLY	4.5
1	E	107	VAL	4.5
1	E	1010	THR	4.5
1	E	369	THR	4.5
1	D	684	GLY	4.5
1	A	974	SER	4.5
1	A	368	PRO	4.5
1	A	401	ALA	4.4
1	A	578	LEU	4.4
1	B	700	GLU	4.4
1	F	713	PRO	4.4
1	D	714	ASN	4.4
1	C	863	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	128	SER	4.4
1	A	376	LEU	4.4
1	E	443	VAL	4.4
1	F	116	PRO	4.4
1	F	706	ASP	4.4
1	B	864	SER	4.3
1	F	485	ALA	4.3
1	D	849	GLY	4.3
1	B	282	ASN	4.3
1	F	48	SER	4.3
1	E	313	MET	4.3
1	A	486	LEU	4.3
1	B	696	GLN	4.3
1	C	323	ILE	4.3
1	F	824	GLY	4.3
1	C	314	GLU	4.3
1	E	348	ILE	4.3
1	A	127	VAL	4.2
1	E	669	LEU	4.2
1	D	575	MET	4.2
1	D	874	ILE	4.2
1	C	127	VAL	4.2
1	F	282	ASN	4.2
1	C	444	GLY	4.2
1	D	610	PHE	4.2
1	E	1006	MET	4.2
1	A	15	ILE	4.1
1	E	621	ILE	4.1
1	F	402	ILE	4.1
1	B	710	SER	4.1
1	A	397	GLY	4.1
1	D	682	GLN	4.1
1	F	868	ALA	4.1
1	E	402	ILE	4.1
1	C	64	VAL	4.1
1	E	46	SER	4.1
1	F	829	GLY	4.1
1	E	404	LEU	4.1
1	E	924	VAL	4.1
1	C	442	LEU	4.1
1	D	110	LYS	4.1
1	F	357	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	848	THR	4.1
1	C	16	ALA	4.1
1	F	864	SER	4.1
1	D	784	TRP	4.0
1	E	282	ASN	4.0
1	E	463	THR	4.0
1	D	178	PHE	4.0
1	B	447	MET	4.0
1	E	1013	ALA	4.0
1	A	405	LEU	4.0
1	D	681	ASP	4.0
1	C	474	ILE	4.0
1	B	67	GLN	4.0
1	F	589	LYS	4.0
1	E	990	ALA	4.0
1	D	408	ASP	4.0
1	C	68	ASN	4.0
1	D	870	SER	3.9
1	D	371	ALA	3.9
1	D	400	LEU	3.9
1	A	410	ILE	3.9
1	A	339	GLU	3.9
1	E	308	ALA	3.9
1	E	353	LEU	3.9
1	E	400	LEU	3.9
1	F	68	ASN	3.9
1	F	369	THR	3.9
1	F	503	GLY	3.9
1	B	701	ALA	3.9
1	D	656	ALA	3.9
1	B	848	THR	3.8
1	C	784	TRP	3.8
1	C	65	ILE	3.8
1	F	112	GLN	3.8
1	E	975	LEU	3.8
1	E	1009	ALA	3.8
1	D	621	ILE	3.8
1	E	462	SER	3.8
1	F	445	ILE	3.8
1	C	866	ASN	3.8
1	D	136	PHE	3.8
1	F	396	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	18	ILE	3.8
1	B	113	LEU	3.8
1	F	712	ARG	3.7
1	E	370	ILE	3.7
1	C	394	THR	3.7
1	F	707	MET	3.7
1	A	463	THR	3.7
1	D	128	SER	3.7
1	E	65	ILE	3.7
1	C	502	LYS	3.7
1	A	403	GLY	3.7
1	F	446	ALA	3.7
1	B	400	LEU	3.7
1	F	826	ALA	3.7
1	F	65	ILE	3.7
1	B	406	VAL	3.7
1	D	113	LEU	3.6
1	F	356	TYR	3.6
1	E	333	VAL	3.6
1	E	1011	VAL	3.6
1	F	373	PRO	3.6
1	E	111	LEU	3.6
1	F	118	LEU	3.6
1	E	935	LYS	3.6
1	B	107	VAL	3.6
1	C	939	LEU	3.6
1	B	575	MET	3.6
1	F	850	VAL	3.6
1	A	327	TYR	3.6
1	C	400	LEU	3.6
1	C	829	GLY	3.6
1	F	45	ILE	3.6
1	E	989	GLY	3.6
1	C	67	GLN	3.5
1	D	406	VAL	3.5
1	E	936	ASN	3.5
1	E	920	VAL	3.5
1	D	458	PHE	3.5
1	C	390	ILE	3.5
1	E	105	VAL	3.5
1	B	316	PHE	3.5
1	C	823	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	929	THR	3.5
1	E	317	PHE	3.5
1	F	1012	LEU	3.5
1	B	311	ALA	3.5
1	C	935	LYS	3.5
1	C	129	VAL	3.5
1	E	322	LYS	3.5
1	C	69	MET	3.5
1	A	593	GLU	3.5
1	B	410	ILE	3.5
1	F	871	LEU	3.5
1	D	78	MET	3.5
1	B	145	THR	3.5
1	E	882	CYS	3.4
1	E	283	GLY	3.4
1	D	401	ALA	3.4
1	C	867	GLN	3.4
1	E	108	GLN	3.4
1	E	194	ASN	3.4
1	B	683	ALA	3.4
1	F	834	GLU	3.4
1	C	388	PHE	3.4
1	E	712	ARG	3.4
1	A	574	THR	3.4
1	C	860	GLN	3.4
1	E	398	MET	3.4
1	E	357	LEU	3.4
1	C	480	LEU	3.4
1	E	977	PHE	3.4
1	F	198	LEU	3.4
1	C	656	ALA	3.4
1	A	933	SER	3.4
1	D	576	VAL	3.3
1	D	15	ILE	3.3
1	D	92	LEU	3.3
1	C	116	PRO	3.3
1	F	939	LEU	3.3
1	E	673	THR	3.3
1	F	444	GLY	3.3
1	F	197	GLN	3.3
1	F	867	GLN	3.3
1	C	374	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	390	ILE	3.3
1	A	467	TYR	3.3
1	F	179	GLY	3.3
1	D	405	LEU	3.3
1	D	623	PHE	3.3
1	F	575	MET	3.3
1	D	479	ALA	3.3
1	A	406	VAL	3.3
1	B	322	LYS	3.3
1	F	708	LEU	3.3
1	D	210	GLN	3.3
1	C	322	LYS	3.3
1	F	176	GLN	3.3
1	E	48	SER	3.3
1	C	38	ILE	3.3
1	B	881	LEU	3.2
1	A	411	VAL	3.2
1	A	365	THR	3.2
1	D	369	THR	3.2
1	C	448	VAL	3.2
1	A	1012	LEU	3.2
1	D	317	PHE	3.2
1	D	482	VAL	3.2
1	C	395	MET	3.2
1	F	466	ILE	3.2
1	C	407	ASP	3.2
1	F	462	SER	3.2
1	E	931	GLY	3.2
1	F	478	MET	3.2
1	A	13	TRP	3.2
1	A	398	MET	3.2
1	B	44	THR	3.2
1	D	783	ASP	3.2
1	D	609	VAL	3.2
1	A	390	ILE	3.2
1	B	488	LEU	3.2
1	E	33	ALA	3.2
1	A	353	LEU	3.2
1	C	449	LEU	3.2
1	D	972	MET	3.2
1	B	408	ASP	3.2
1	D	483	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	404	LEU	3.1
1	A	69	MET	3.1
1	D	281	PHE	3.1
1	D	66	GLU	3.1
1	E	109	ASN	3.1
1	D	657	MET	3.1
1	F	281	PHE	3.1
1	C	834	GLU	3.1
1	F	484	VAL	3.1
1	C	330	THR	3.1
1	D	36	PRO	3.1
1	E	126	GLY	3.1
1	B	198	LEU	3.1
1	B	443	VAL	3.1
1	D	866	ASN	3.1
1	C	307	ARG	3.1
1	F	869	PRO	3.1
1	F	453	PHE	3.1
1	D	109	ASN	3.1
1	B	65	ILE	3.1
1	D	130	GLU	3.1
1	E	465	ALA	3.1
1	E	969	PRO	3.1
1	A	573	MET	3.1
1	A	902	LEU	3.1
1	E	316	PHE	3.1
1	F	801	SER	3.1
1	E	896	VAL	3.1
1	E	78	MET	3.1
1	A	408	ASP	3.0
1	E	59	ASP	3.0
1	E	112	GLN	3.0
1	E	593	GLU	3.0
1	D	321	LEU	3.0
1	E	674	GLY	3.0
1	B	46	SER	3.0
1	C	109	ASN	3.0
1	B	308	ALA	3.0
1	E	899	VAL	3.0
1	D	114	ALA	3.0
1	E	323	ILE	3.0
1	F	64	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	355	MET	3.0
1	F	355	MET	3.0
1	B	127	VAL	3.0
1	E	104	GLN	3.0
1	B	11	PHE	3.0
1	D	403	GLY	3.0
1	D	865	GLY	3.0
1	A	481	SER	3.0
1	B	45	ILE	3.0
1	F	400	LEU	3.0
1	D	12	ALA	3.0
1	C	885	ALA	3.0
1	B	112	GLN	3.0
1	B	834	GLU	3.0
1	D	715	GLY	2.9
1	D	59	ASP	2.9
1	A	579	PRO	2.9
1	F	656	ALA	2.9
1	D	463	THR	2.9
1	F	110	LYS	2.9
1	C	712	ARG	2.9
1	C	883	LEU	2.9
1	F	117	LEU	2.9
1	B	177	LEU	2.9
1	E	473	THR	2.9
1	F	594	VAL	2.9
1	E	579	PRO	2.9
1	E	44	THR	2.9
1	A	354	VAL	2.9
1	C	494	ALA	2.9
1	A	661	PHE	2.9
1	C	96	SER	2.9
1	C	397	GLY	2.9
1	C	310	LEU	2.9
1	C	399	VAL	2.9
1	F	1011	VAL	2.9
1	F	470	PHE	2.9
1	C	1006	MET	2.9
1	E	938	ILE	2.9
1	D	796	PHE	2.9
1	F	9	PRO	2.9
1	B	251	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	393	LEU	2.9
1	D	797	SER	2.9
1	F	13	TRP	2.9
1	F	784	TRP	2.9
1	F	1016	PHE	2.9
1	B	1013	ALA	2.9
1	D	292	LYS	2.9
1	D	33	ALA	2.8
1	E	798	ALA	2.8
1	C	113	LEU	2.8
1	A	1007	VAL	2.8
1	F	399	VAL	2.8
1	A	145	THR	2.8
1	E	541	TYR	2.8
1	F	932	LEU	2.8
1	D	372	VAL	2.8
1	A	195	LYS	2.8
1	F	935	LYS	2.8
1	B	801	SER	2.8
1	F	67	GLN	2.8
1	E	14	VAL	2.8
1	E	325	TYR	2.8
1	C	111	LEU	2.8
1	D	351	VAL	2.8
1	E	1016	PHE	2.8
1	B	573	MET	2.8
1	D	854	TRP	2.8
1	C	799	PHE	2.8
1	C	373	PRO	2.8
1	E	676	ASP	2.8
1	F	827	ALA	2.8
1	E	803	ARG	2.8
1	F	861	GLU	2.8
1	F	409	ALA	2.8
1	F	591	LEU	2.8
1	A	977	PHE	2.8
1	C	462	SER	2.8
1	C	478	MET	2.8
1	C	786	VAL	2.8
1	C	300	LEU	2.8
1	A	386	PHE	2.8
1	D	324	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	828	PRO	2.8
1	A	383	LEU	2.7
1	C	372	VAL	2.7
1	E	1015	PHE	2.7
1	B	394	THR	2.7
1	D	200	PRO	2.7
1	E	395	MET	2.7
1	D	622	ALA	2.7
1	F	246	PHE	2.7
1	A	577	GLN	2.7
1	A	971	LEU	2.7
1	D	14	VAL	2.7
1	F	108	GLN	2.7
1	D	396	PHE	2.7
1	C	376	LEU	2.7
1	E	591	LEU	2.7
1	A	487	ILE	2.7
1	A	874	ILE	2.7
1	F	726	ILE	2.7
1	D	11	PHE	2.7
1	E	145	THR	2.7
1	F	675	PHE	2.7
1	A	658	VAL	2.7
1	B	369	THR	2.7
1	B	854	TRP	2.7
1	A	970	ILE	2.7
1	F	863	LEU	2.7
1	A	281	PHE	2.7
1	A	1011	VAL	2.7
1	F	576	VAL	2.7
1	A	322	LYS	2.7
1	E	1007	VAL	2.7
1	B	934	ALA	2.7
1	B	110	LYS	2.7
1	E	45	ILE	2.7
1	E	401	ALA	2.7
1	B	407	ASP	2.7
1	B	711	VAL	2.7
1	E	280	GLU	2.7
1	A	630	ALA	2.7
1	B	798	ALA	2.7
1	C	17	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	92	LEU	2.6
1	D	391	ASN	2.6
1	F	188	MET	2.6
1	C	446	ALA	2.6
1	D	973	THR	2.6
1	A	336	SER	2.6
1	D	831	SER	2.6
1	C	210	GLN	2.6
1	F	590	VAL	2.6
1	F	786	VAL	2.6
1	A	785	TYR	2.6
1	B	699	ALA	2.6
1	A	107	VAL	2.6
1	A	70	ASN	2.6
1	E	47	ALA	2.6
1	D	368	PRO	2.6
1	A	590	VAL	2.6
1	E	66	GLU	2.6
1	E	447	MET	2.6
1	F	657	MET	2.6
1	A	666	ILE	2.6
1	A	714	ASN	2.6
1	B	785	TYR	2.6
1	D	579	PRO	2.6
1	A	357	LEU	2.6
1	F	976	ALA	2.6
1	A	374	VAL	2.6
1	D	173	GLY	2.6
1	C	932	LEU	2.6
1	E	290	GLY	2.6
1	A	449	LEU	2.6
1	A	876	LEU	2.6
1	E	577	GLN	2.6
1	A	315	PRO	2.6
1	C	828	PRO	2.6
1	D	69	MET	2.6
1	D	445	ILE	2.6
1	E	697	LEU	2.6
1	E	246	PHE	2.6
1	E	164	ASP	2.6
1	D	786	VAL	2.6
1	F	674	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	851	GLY	2.6
1	E	113	LEU	2.6
1	E	599	LEU	2.6
1	F	1010	THR	2.6
1	D	713	PRO	2.6
1	A	834	GLU	2.5
1	C	97	GLY	2.5
1	F	403	GLY	2.5
1	C	369	THR	2.5
1	F	352	PHE	2.5
1	D	43	VAL	2.5
1	F	370	ILE	2.5
1	B	786	VAL	2.5
1	B	12	ALA	2.5
1	B	91	THR	2.5
1	D	37	THR	2.5
1	E	587	THR	2.5
1	B	882	CYS	2.5
1	A	33	ALA	2.5
1	E	793	MET	2.5
1	A	12	ALA	2.5
1	B	188	MET	2.5
1	E	130	GLU	2.5
1	A	129	VAL	2.5
1	D	290	GLY	2.5
1	F	488	LEU	2.5
1	E	331	PRO	2.5
1	A	877	ILE	2.5
1	B	666	ILE	2.5
1	C	575	MET	2.5
1	D	447	MET	2.5
1	E	711	VAL	2.5
1	E	988	THR	2.5
1	A	485	ALA	2.5
1	F	376	LEU	2.5
1	D	412	VAL	2.4
1	F	899	VAL	2.4
1	D	50	PRO	2.4
1	E	197	GLN	2.4
1	F	164	ASP	2.4
1	D	46	SER	2.4
1	A	198	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	290	GLY	2.4
1	C	441	ALA	2.4
1	D	877	ILE	2.4
1	E	63	GLN	2.4
1	D	376	LEU	2.4
1	B	409	ALA	2.4
1	D	815	ASN	2.4
1	D	778	PRO	2.4
1	F	676	ASP	2.4
1	D	34	GLN	2.4
1	A	196	PHE	2.4
1	A	321	LEU	2.4
1	E	489	THR	2.4
1	A	761	GLY	2.4
1	F	162	MET	2.4
1	D	409	ALA	2.4
1	B	355	MET	2.4
1	F	711	VAL	2.4
1	A	334	LYS	2.4
1	E	367	ILE	2.4
1	E	881	LEU	2.4
1	A	67	GLN	2.4
1	B	450	SER	2.4
1	D	845	LYS	2.4
1	F	860	GLN	2.4
1	D	611	ALA	2.4
1	F	3	ASN	2.4
1	F	16	ALA	2.4
1	B	411	VAL	2.4
1	D	763	VAL	2.4
1	E	43	VAL	2.4
1	F	69	MET	2.4
1	F	395	MET	2.4
1	A	19	ILE	2.4
1	B	591	LEU	2.4
1	D	392	THR	2.4
1	B	43	VAL	2.3
1	C	14	VAL	2.3
1	C	782	GLY	2.3
1	E	966	ARG	2.3
1	E	1017	VAL	2.3
1	E	281	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	348	ILE	2.3
1	B	371	ALA	2.3
1	C	797	SER	2.3
1	C	350	LEU	2.3
1	D	72	ILE	2.3
1	E	796	PHE	2.3
1	A	164	ASP	2.3
1	D	19	ILE	2.3
1	D	383	LEU	2.3
1	B	802	SER	2.3
1	D	977	PHE	2.3
1	E	713	PRO	2.3
1	F	563	PHE	2.3
1	B	542	LEU	2.3
1	B	975	LEU	2.3
1	E	328	ASP	2.3
1	C	973	THR	2.3
1	E	303	ALA	2.3
1	F	61	VAL	2.3
1	F	458	PHE	2.3
1	D	932	LEU	2.3
1	E	92	LEU	2.3
1	E	795	PRO	2.3
1	A	14	VAL	2.3
1	D	833	GLY	2.3
1	F	170	SER	2.3
1	C	970	ILE	2.3
1	A	399	VAL	2.3
1	E	737	SER	2.3
1	E	801	SER	2.3
1	D	107	VAL	2.3
1	D	129	VAL	2.3
1	E	878	VAL	2.3
1	D	832	THR	2.3
1	B	404	LEU	2.3
1	D	573	MET	2.3
1	E	486	LEU	2.3
1	C	128	SER	2.3
1	F	477	ALA	2.3
1	B	486	LEU	2.2
1	E	714	ASN	2.2
1	A	36	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	470	PHE	2.2
1	E	630	ALA	2.2
1	C	685	LEU	2.2
1	D	398	MET	2.2
1	A	370	ILE	2.2
1	D	1014	ILE	2.2
1	E	728	GLN	2.2
1	F	251	LEU	2.2
1	F	480	LEU	2.2
1	A	351	VAL	2.2
1	B	865	GLY	2.2
1	D	696	GLN	2.2
1	F	280	GLU	2.2
1	A	591	LEU	2.2
1	A	975	LEU	2.2
1	B	405	LEU	2.2
1	F	902	LEU	2.2
1	D	334	LYS	2.2
1	F	577	GLN	2.2
1	C	389	SER	2.2
1	F	797	SER	2.2
1	F	802	SER	2.2
1	C	611	ALA	2.2
1	A	657	MET	2.2
1	A	762	ARG	2.2
1	A	797	SER	2.2
1	D	315	PRO	2.2
1	A	898	LEU	2.2
1	D	817	LEU	2.2
1	E	971	LEU	2.2
1	C	610	PHE	2.2
1	B	72	ILE	2.2
1	E	397	GLY	2.2
1	D	823	LEU	2.2
1	B	970	ILE	2.2
1	D	134	SER	2.2
1	A	483	LEU	2.2
1	C	33	ALA	2.2
1	E	611	ALA	2.2
1	F	366	LEU	2.2
1	B	847	PRO	2.2
1	A	382	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	18	ILE	2.2
1	B	392	THR	2.2
1	D	127	VAL	2.2
1	D	574	THR	2.2
1	B	784	TRP	2.2
1	B	846	LEU	2.2
1	B	939	LEU	2.2
1	F	163	LYS	2.2
1	C	349	ILE	2.2
1	E	438	ILE	2.2
1	E	609	VAL	2.2
1	D	485	ALA	2.1
1	E	347	ALA	2.1
1	C	623	PHE	2.1
1	C	977	PHE	2.1
1	F	933	SER	2.1
1	E	589	LYS	2.1
1	A	194	ASN	2.1
1	D	388	PHE	2.1
1	B	658	VAL	2.1
1	E	831	SER	2.1
1	C	669	LEU	2.1
1	D	442	LEU	2.1
1	E	193	LEU	2.1
1	A	934	ALA	2.1
1	C	796	PHE	2.1
1	D	762	ARG	2.1
1	A	43	VAL	2.1
1	D	738	ILE	2.1
1	F	565	PRO	2.1
1	C	501	ALA	2.1
1	D	348	ILE	2.1
1	B	79	SER	2.1
1	C	315	PRO	2.1
1	A	32	VAL	2.1
1	C	658	VAL	2.1
1	C	974	SER	2.1
1	F	322	LYS	2.1
1	A	623	PHE	2.1
1	B	246	PHE	2.1
1	D	785	TYR	2.1
1	E	374	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	678	GLU	2.1
1	A	472	ILE	2.1
1	F	940	ILE	2.1
1	C	634	GLY	2.1
1	E	492	LEU	2.1
1	D	795	PRO	2.1
1	A	611	ALA	2.1
1	A	45	ILE	2.1
1	C	291	ILE	2.1
1	C	35	TYR	2.1
1	F	621	ILE	2.1
1	B	657	MET	2.1
1	C	577	GLN	2.1
1	E	11	PHE	2.1
1	A	622	ALA	2.1
1	A	831	SER	2.1
1	D	724	ILE	2.1
1	E	653	ILE	2.1
1	D	194	ASN	2.1
1	E	933	SER	2.1
1	E	575	MET	2.1
1	F	796	PHE	2.1
1	B	578	LEU	2.1
1	D	402	ILE	2.1
1	A	792	GLN	2.0
1	B	825	GLN	2.0
1	D	728	GLN	2.0
1	A	489	THR	2.0
1	D	1010	THR	2.0
1	C	353	LEU	2.0
1	B	281	PHE	2.0
1	C	20	MET	2.0
1	C	396	PHE	2.0
1	D	386	PHE	2.0
1	C	282	ASN	2.0
1	E	62	THR	2.0
1	F	1014	ILE	2.0
1	A	136	PHE	2.0
1	C	655	ASP	2.0
1	C	500	ILE	2.0
1	F	143	ILE	2.0
1	A	461	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	71	GLY	2.0
1	F	573	MET	2.0
1	A	108	GLN	2.0
1	A	711	VAL	2.0
1	E	61	VAL	2.0
1	A	881	LEU	2.0
1	E	441	ALA	2.0
1	F	691	THR	2.0
1	B	197	GLN	2.0
1	D	974	SER	2.0
1	F	578	LEU	2.0
1	F	126	GLY	2.0
1	E	199	THR	2.0
1	B	1011	VAL	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)

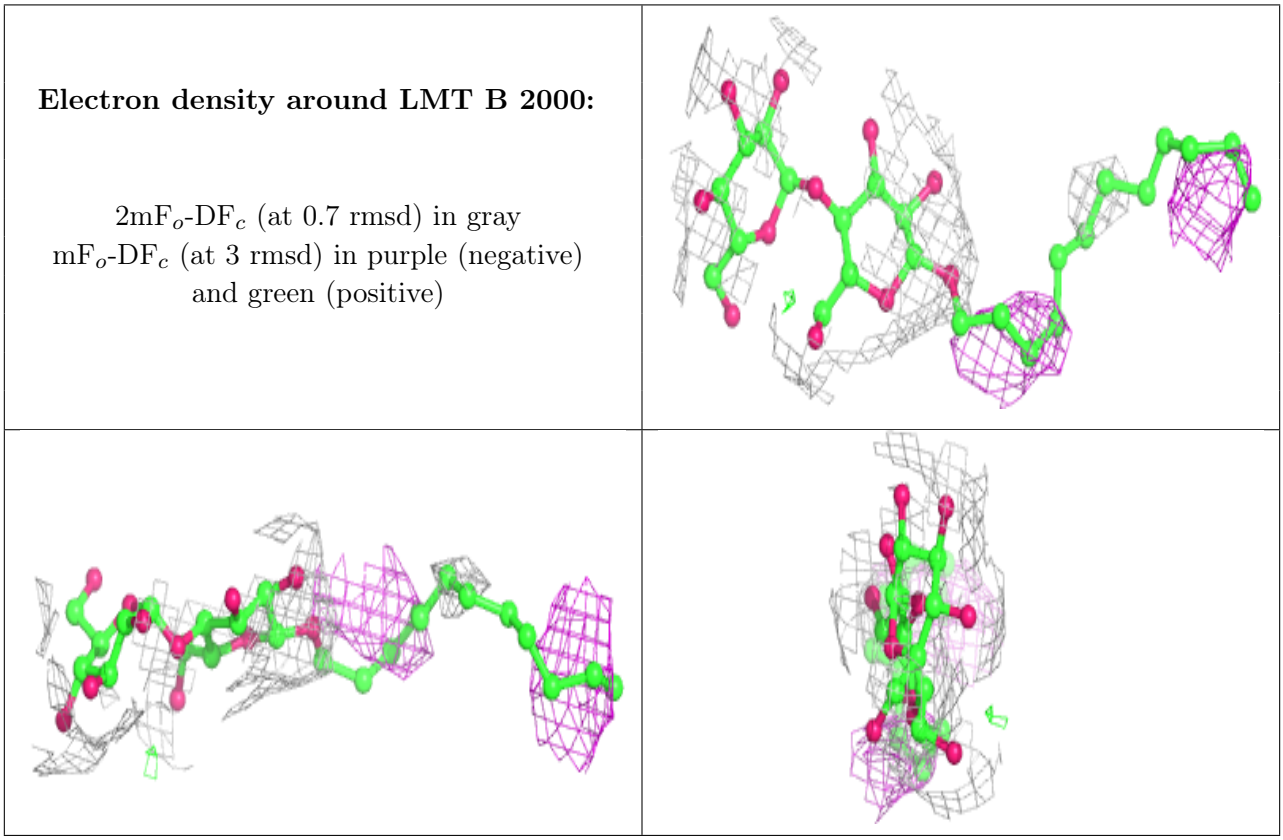
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.73	0.43	31,50,60,69	0
2	LMT	E	1101	35/35	0.78	0.42	41,74,104,107	0
2	LMT	D	2000	35/35	0.82	0.34	21,41,56,63	0
2	LMT	C	1101	35/35	0.82	0.33	12,41,56,72	0
2	LMT	F	2000	35/35	0.82	0.39	40,64,89,94	0
2	LMT	A	1101	35/35	0.86	0.32	31,41,90,99	0
3	NI	E	1102	1/1	0.96	0.15	170,170,170,170	0
3	NI	A	1102	1/1	0.97	0.19	154,154,154,154	0
3	NI	C	1102	1/1	0.98	0.09	41,41,41,41	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.

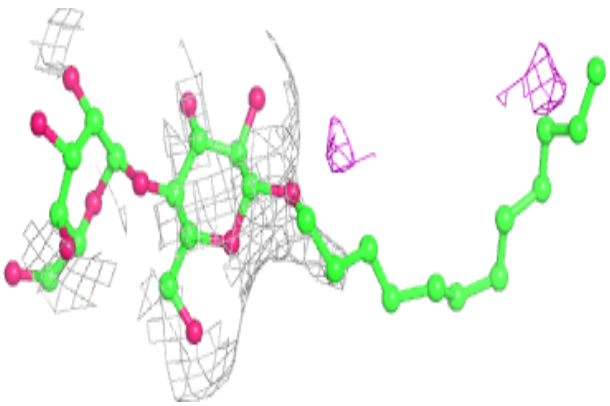
Electron density around LMT B 2000:

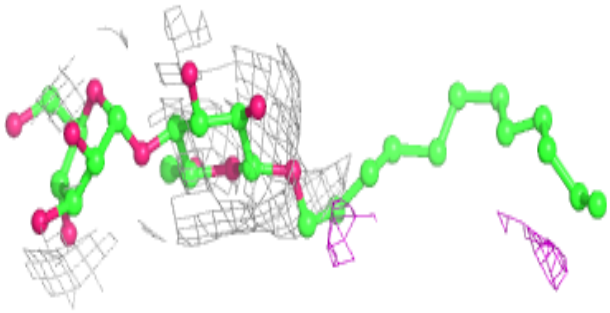
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around LMT E 1101:

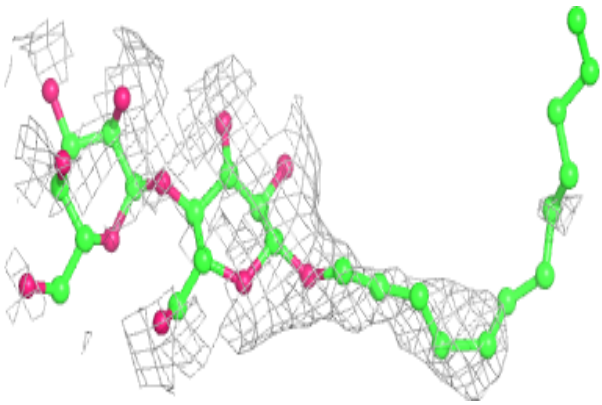
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

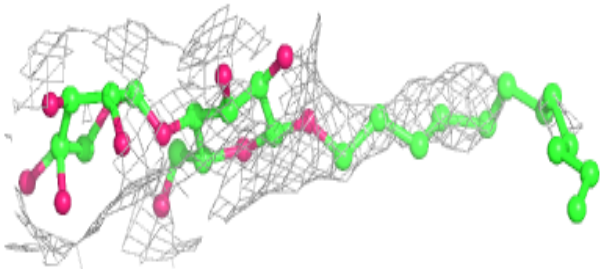


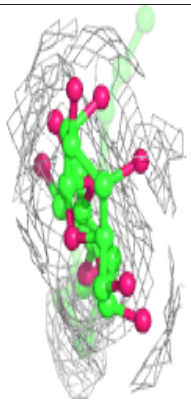


Electron density around LMT D 2000:

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

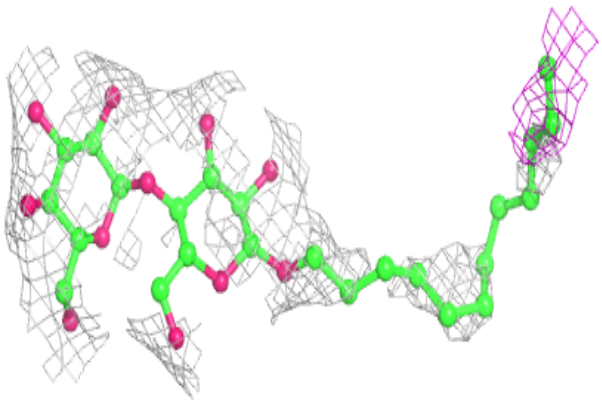


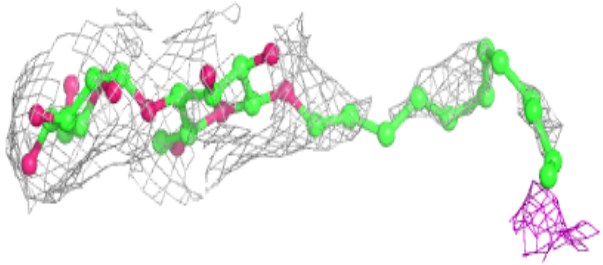


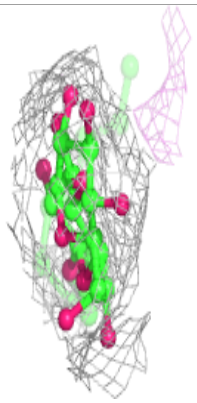


Electron density around LMT C 1101:

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

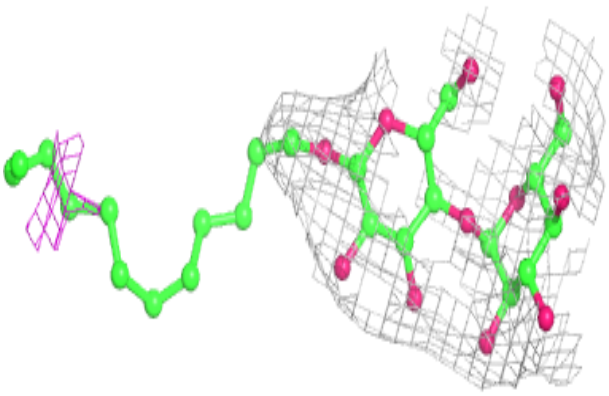


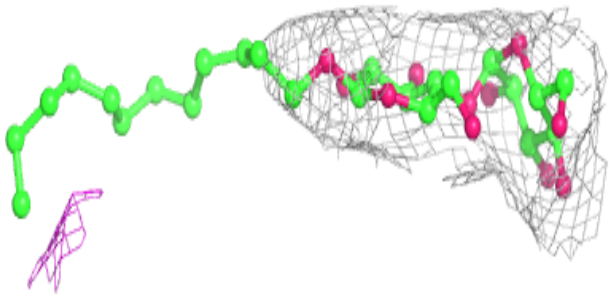


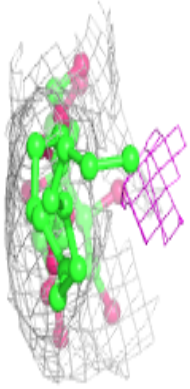


Electron density around LMT F 2000:

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

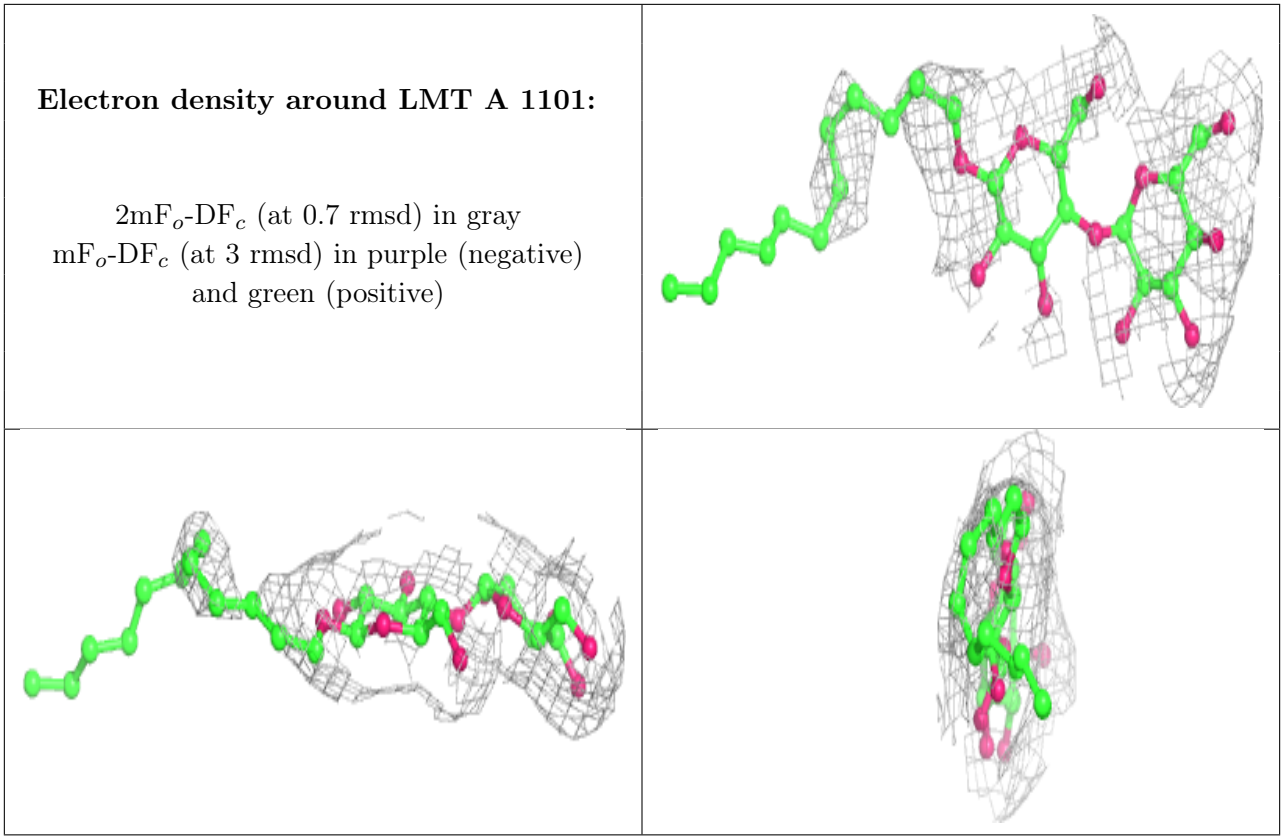






Electron density around LMT A 1101:

$2mF_o$-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.