Full wwPDB X-ray Structure Validation Report (i)

Jan 2, 2024 – 10:31 pm GMT

PDB ID	:	4ZIT
Title	:	Crystal structure of AcrB in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-28
Resolution	:	3.30 Å(reported)

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

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

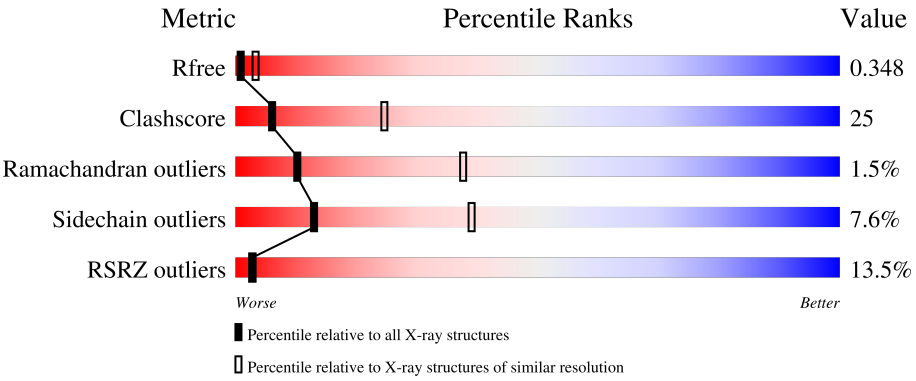
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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

Mol	Chain	Length	Quality of chain
1	A	1049	12% 50% 45%
1	B	1049	11% 54% 41%
1	C	1049	10% 51% 44%
1	D	1049	14% 48% 47%
1	E	1049	17% 49% 46% 5%

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Mol	Chain	Length	Quality of chain
1	F	1049	

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	1101	-	-	-	X
2	LMT	C	1101	X	-	-	-
2	LMT	E	1101	-	-	-	X

2 Entry composition (i)

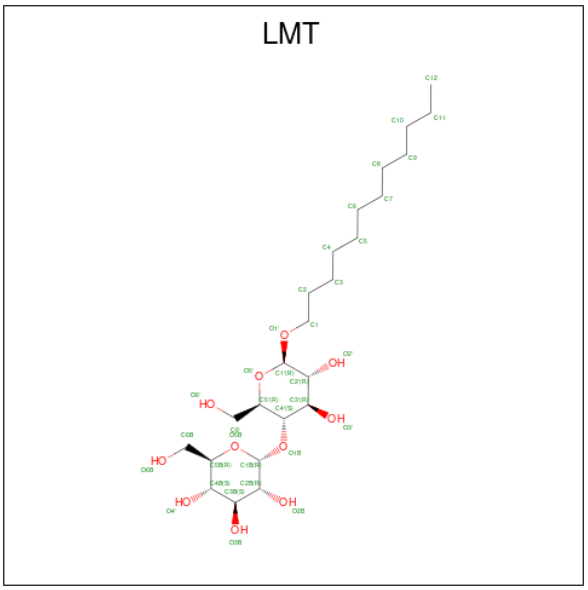
There are 3 unique types of molecules in this entry. The entry contains 47773 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	B	1043	Total	C	N	O	S	0	0	0
			7935	5101	1314	1477	43			
1	C	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	D	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	E	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			
1	F	1042	Total	C	N	O	S	0	0	0
			7925	5095	1311	1476	43			

- 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
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).

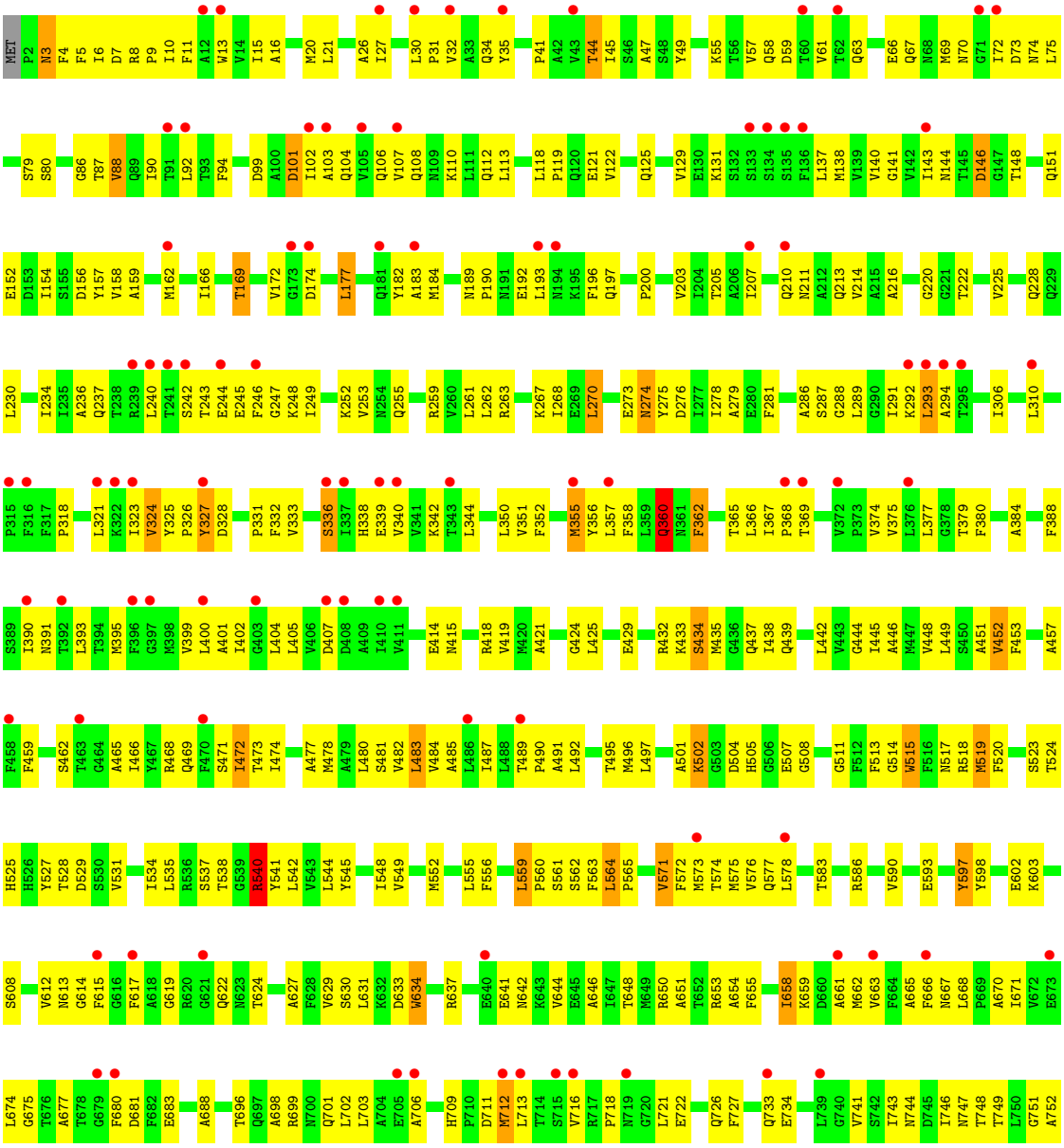
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ni 1 1	0	0
3	C	1	Total Ni 1 1	0	0
3	E	1	Total Ni 1 1	0	0

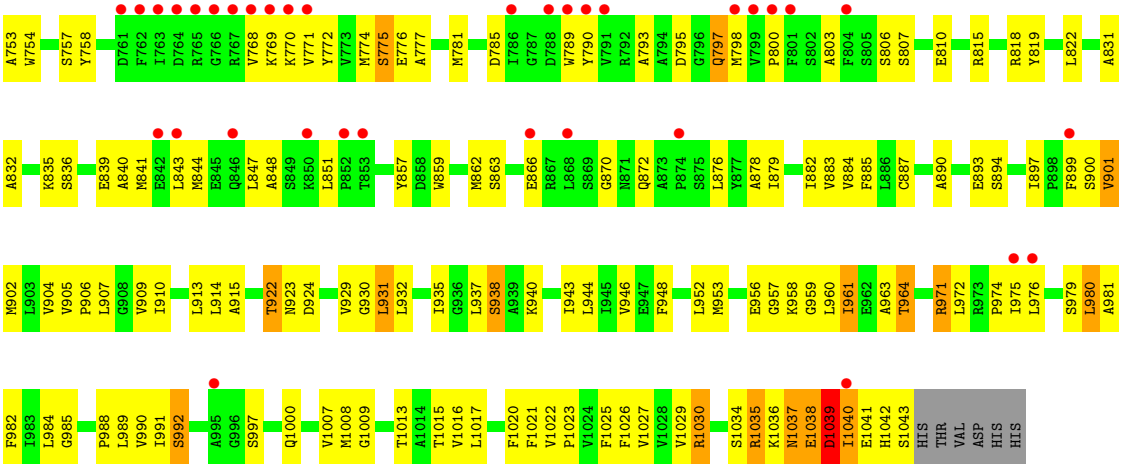
3 Residue-property plots (i)

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

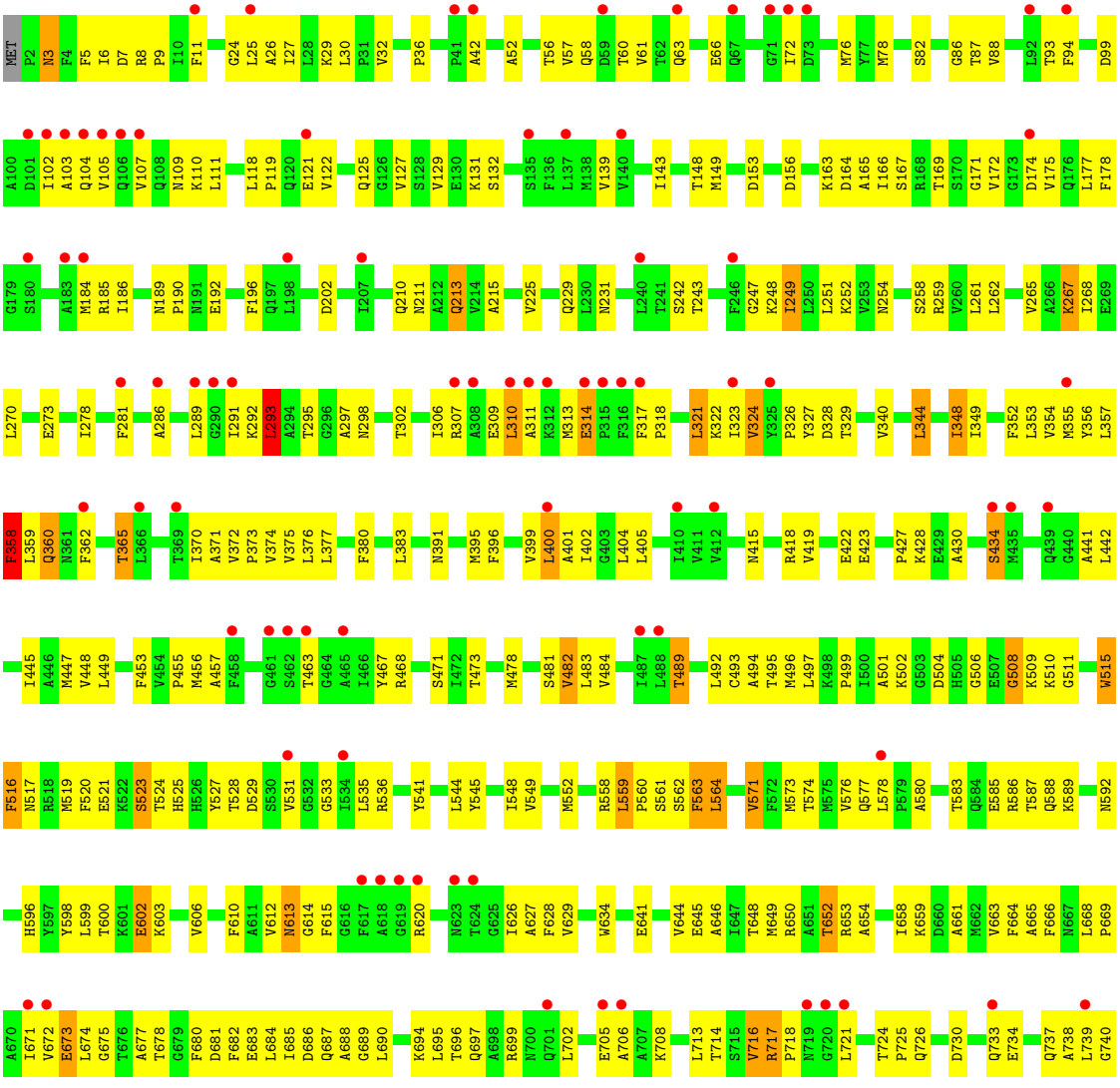
Chain A:

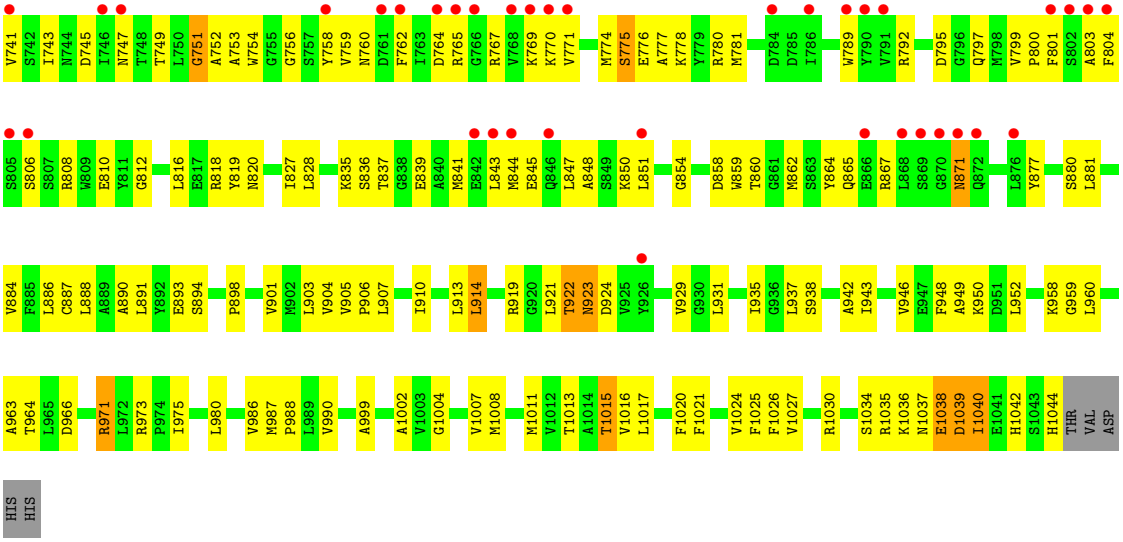




• Molecule 1: Multidrug efflux pump subunit AcrB

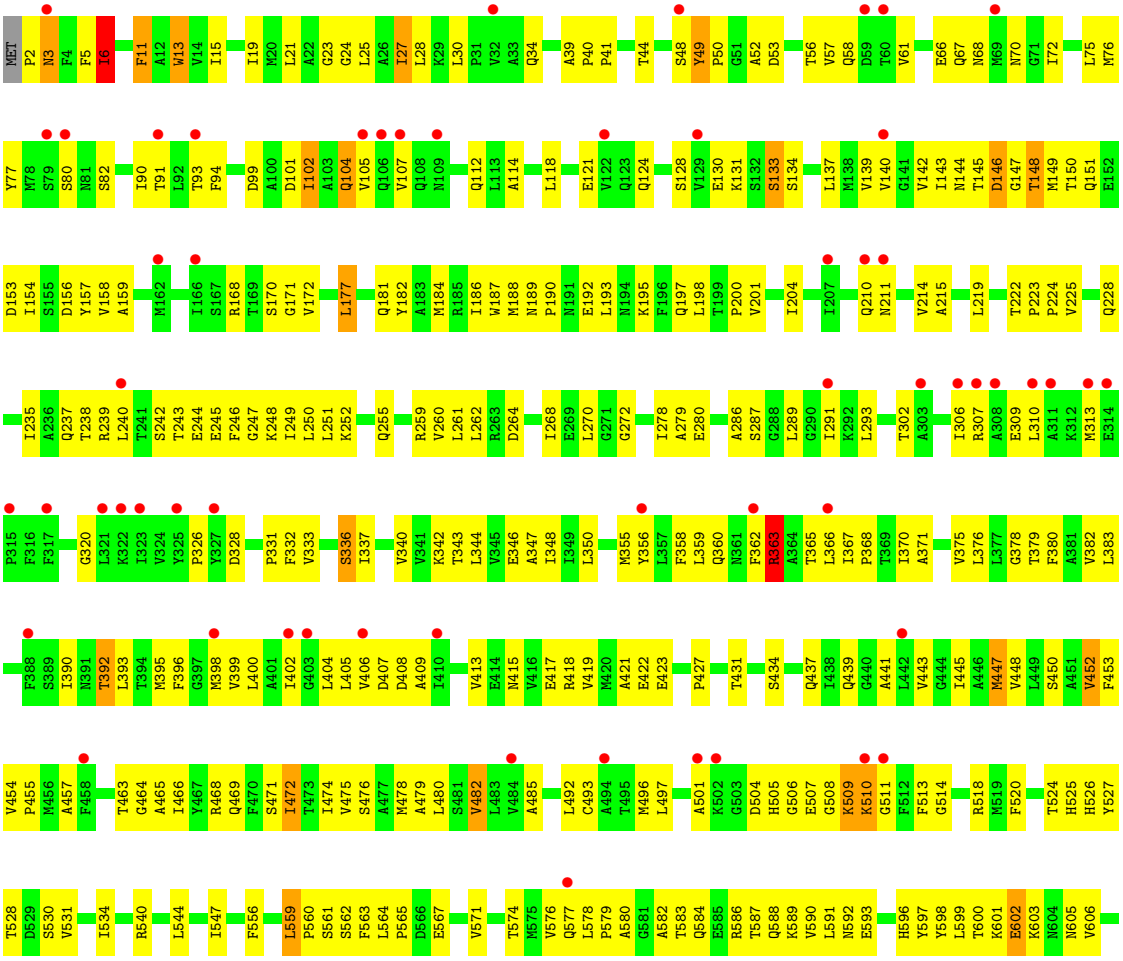
Chain B:

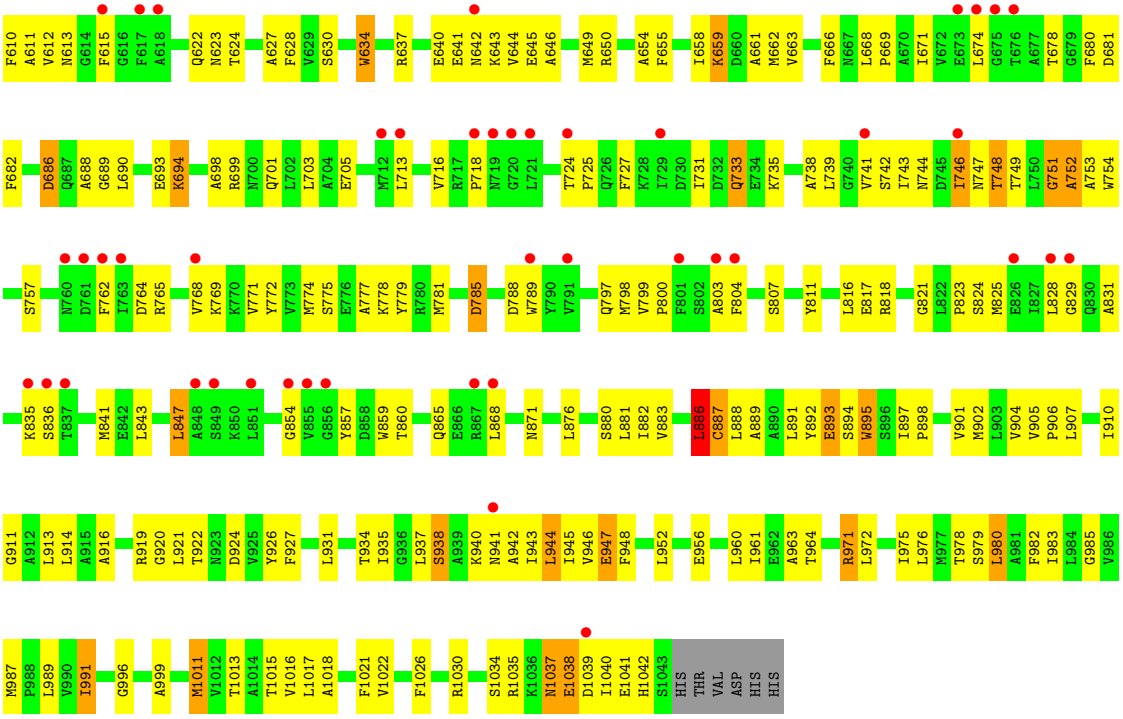




• Molecule 1: Multidrug efflux pump subunit AcrB

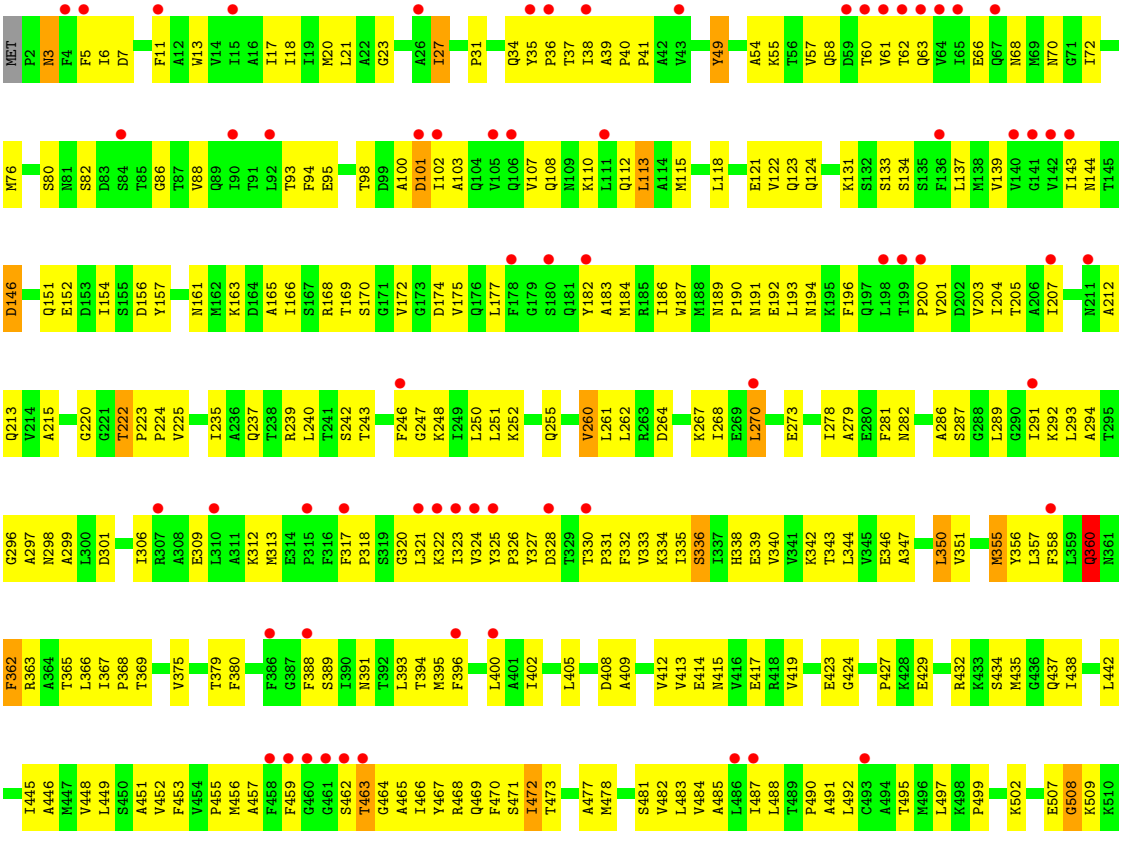
Chain C:

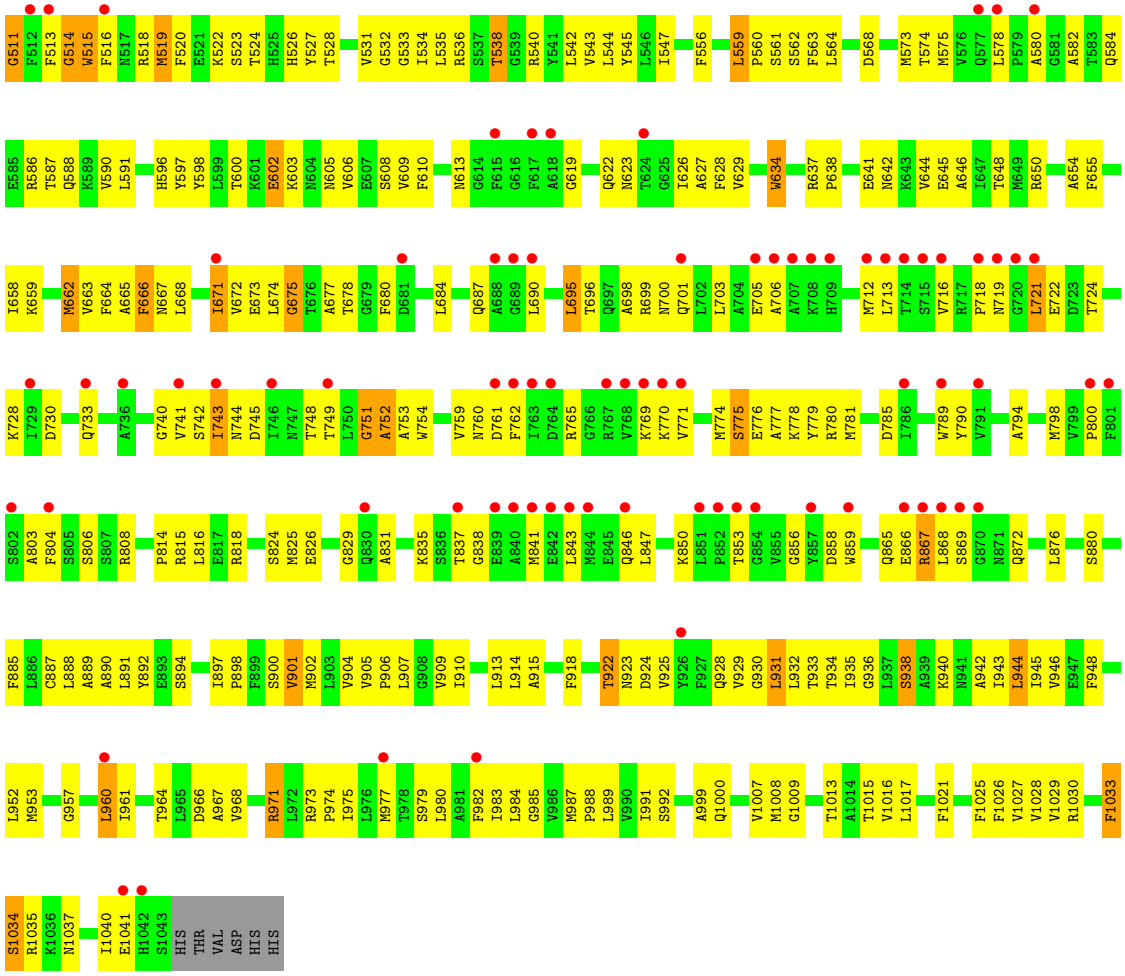




• Molecule 1: Multidrug efflux pump subunit AcrB

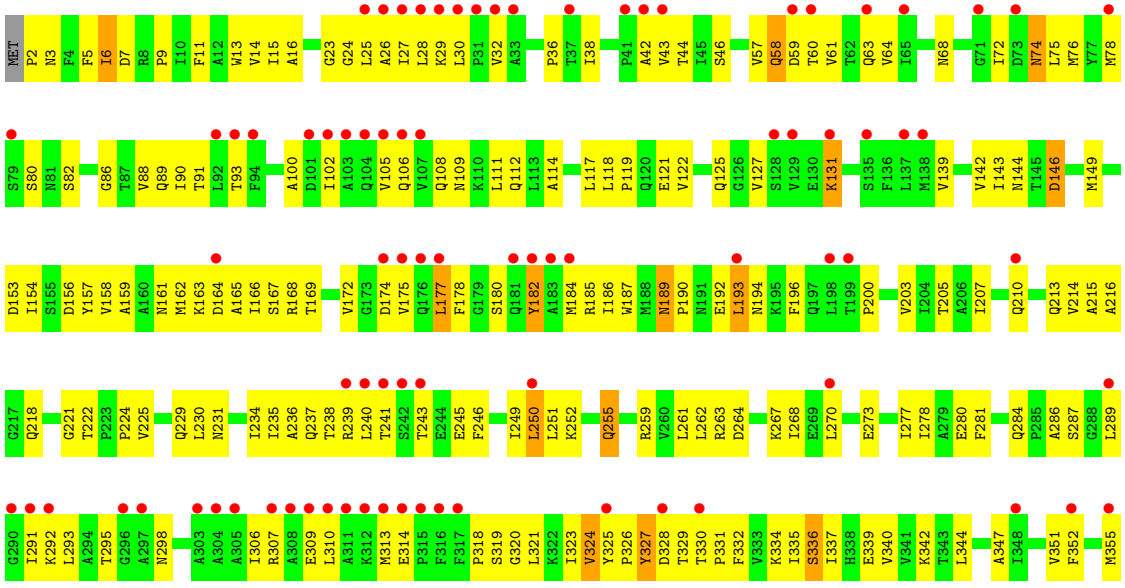
Chain D:

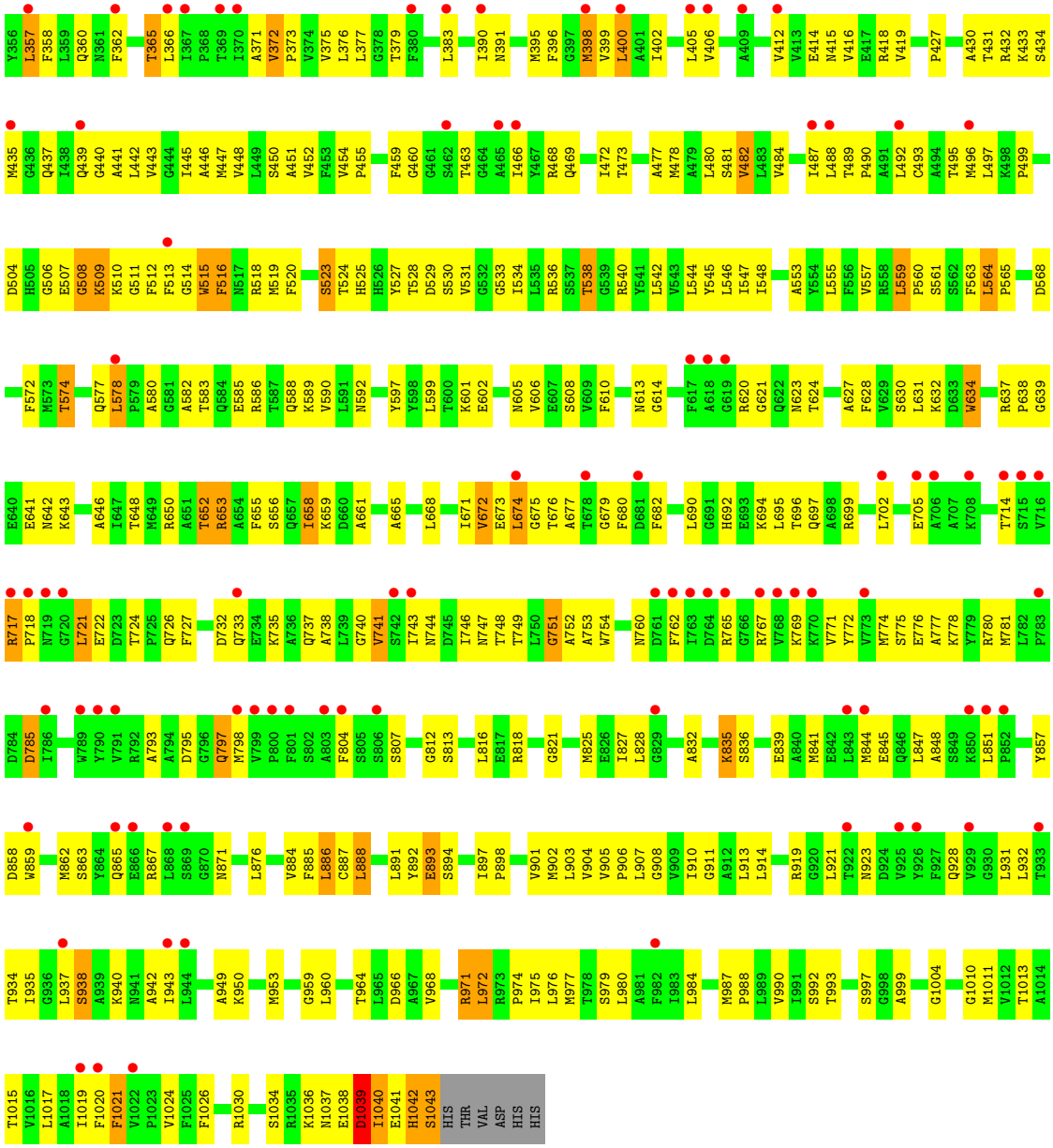




• Molecule 1: Multidrug efflux pump subunit AcrB

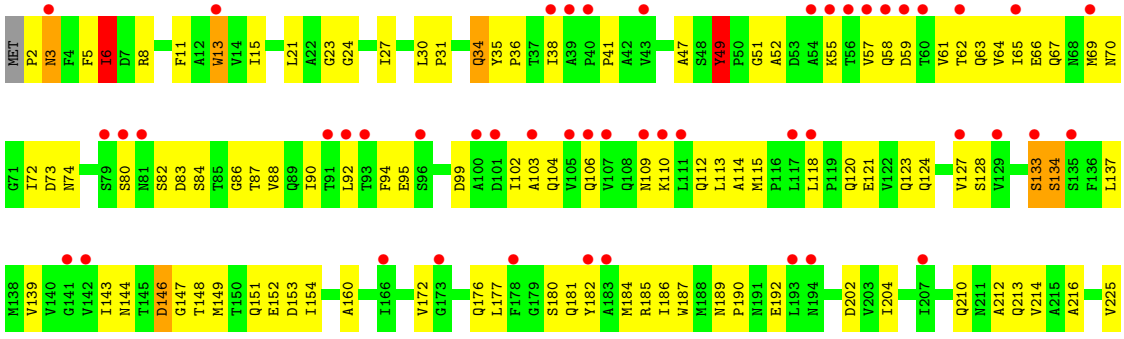
Chain E:

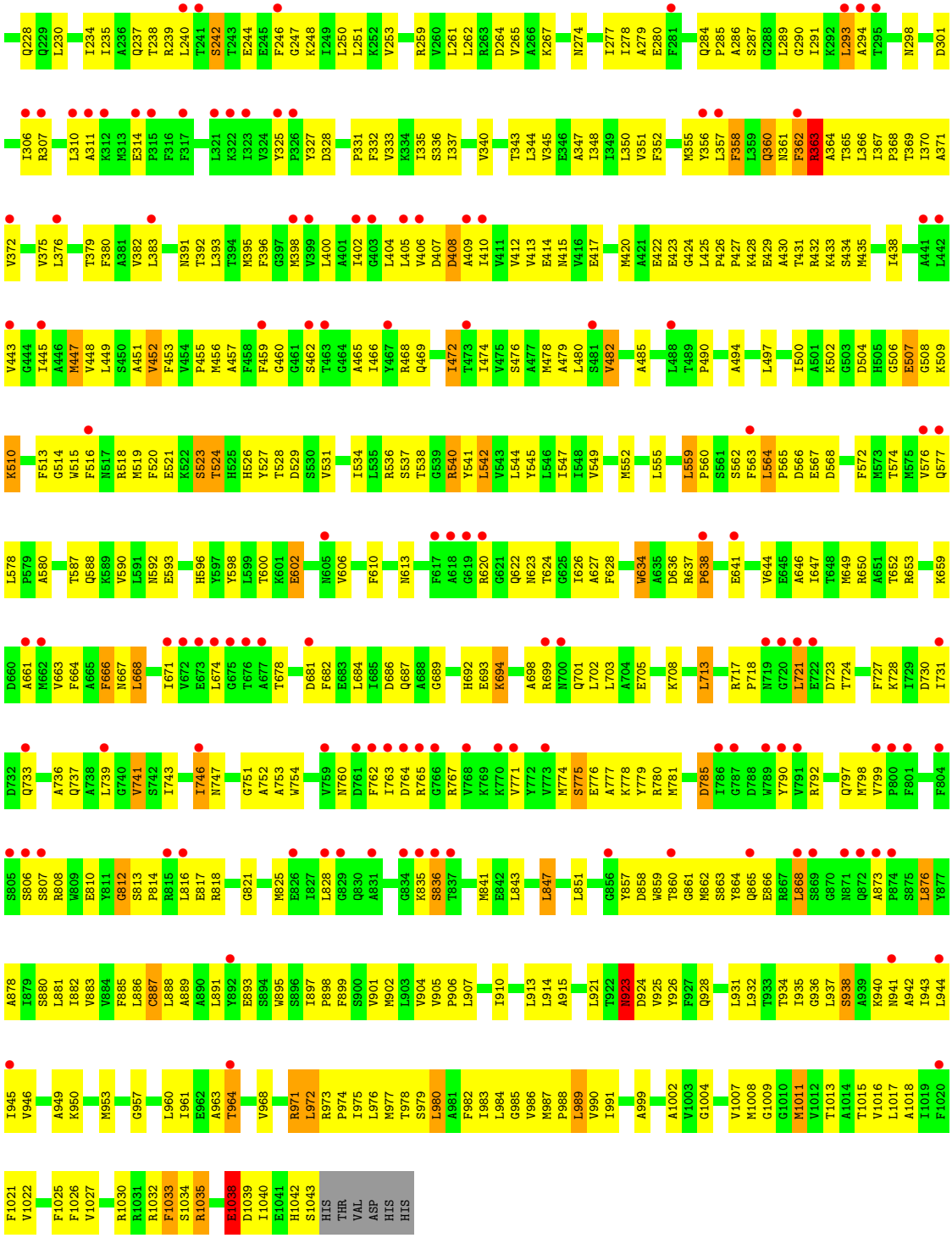




• Molecule 1: Multidrug efflux pump subunit AcrB

Chain F:




Q228 Q229 L230 I234 I235 A236 Q237 T238 R239 L240 T241 S242 T243 E244 E245 F246 G247 K248 I249 L250 L251 K252 V253 R259 V260 L261 L262 R263 D264 V265 A266 K267 N274 I277 I278 A279 E280 F281 Q284 P285 A286 S287 G288 L289 G290 I291 K292 L293 A294 T295 N298 D301
I306 R307 L310 A311 K312 M313 E314 P315 F316 F317 L321 K322 I323 V324 Y325 P326 Y327 D328 P331 F332 V333 K334 I335 S336 I337 V340 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 V375 L376 T379 F380 A381 V382 L383 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 M420 A421 E422 E423 G424 L425 P426 P427 K428 E429 A430 T431 R432 K433 S434 M435 I438 A441 L442
V443 G444 I445 A446 M447 V448 L449 S450 A451 V452 F453 V454 P455 M456 A457 F458 F459 G460 G461 S462 T463 G464 A465 I466 Y467 R468 Q469 I472 T473 I474 V475 S476 A477 M478 A479 L480 S481 V482 A485 L488 T489 P490 A494 L497 I500 A501 K502 G503 D504 H505 G506 E507 G508 K509
K510 F513 G514 W515 F516 N517 R518 M519 F520 E521 K522 S523 T524 H525 H526 Y527 T528 D529 S530 V531 I534 L535 R536 S537 T538 G539 R540 Y541 L542 V543 L544 Y545 L546 I547 I548 V549 M552 L555 L559 P560 S561 S562 F563 L564 P565 D566 E567 D568 F572 M573 T574 M575 V576 Q577
L578 P579 A580 T587 Q588 K589 V590 L591 N592 E593 H596 Y597 Y598 L599 T600 K601 E602 N605 V606 F610 N613 F617 A618 G619 R620 G621 Q622 N623 T624 G625 I626 A627 F628 W634 A635 D636 R637 P638 E641 V644 E645 A646 I647 T648 M649 R650 A651 T652 R653 K659
D660 A661 M662 V663 F664 A665 F666 N667 L668 I671 V672 E673 L674 G675 T676 A677 T678 D681 F682 E683 L684 I685 D686 Q687 A688 G689 H692 E693 K694 A698 R699 N700 Q701 L702 L703 A704 E705 K708 L713 R717 P718 N719 G720 L721 E722 D723 T724 F727 K728 I729 D730 I731
D732 Q733 A736 Q737 A738 L739 G740 V741 S742 I743 I746 N747 G751 A752 A753 W754 V759 N760 D761 F762 I763 D764 R765 G766 R767 V768 K769 K770 V771 Y772 V773 M774 S775 E776 A777 K778 Y779 R780 M781 D785 I786 G787 D788 W789 Y790 V791 R792 Q797 M798 V799 P800 F801 F804
S805 S806 S807 R808 W809 E810 Y811 G812 S813 P814 R815 L816 E817 R818 G821 M825 E826 I827 L828 G829 Q830 A831 G834 K835 S836 T837 M841 E842 L843 L847 L851 C856 Y857 D858 W859 T860 G861 M862 S863 Y864 Q865 E866 R867 L868 S869 G870 N871 Q872 A873 P874 S875 L876 Y877
A878 I879 S880 L881 I882 V883 V884 F885 L886 C887 L888 A889 A890 L891 Y892 E893 S894 W895 S896 I897 P898 F899 S900 V901 M902 L903 V904 V905 P906 L907 I910 L913 L914 A915 L921 T922 N923 D924 V925 Y926 F927 Q928 L931 L932 T933 T934 I935 G936 L937 S938 A939 K940 N941 A942 I943 L944
I945 V946 A949 K950 M953 G957 L960 I961 E962 A963 T964 V968 R971 L972 R973 P974 I975 L976 M977 T978 S979 L980 A981 F982 I983 L984 G985 V986 M987 P988 L989 V990 I991 A999 A1002 V1003 G1004 V1007 M1008 G1009 G1010 M1011 V1012 T1013 A1014 T1015 V1016 L1017 A1018 I1019 F1020
F1021 V1022 F1025 F1026 V1027 R1030 R1031 R1032 F1033 S1034 R1035 E1038 D1039 I1040 E1041 H1042 S1043 HIS THR VAL ASP HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	151.84Å 156.86Å 218.58Å 90.00° 92.70° 90.00°	Depositor
Resolution (Å)	19.95 – 3.30 127.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.95-3.30) 97.3 (127.41-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.268 , 0.339 0.275 , 0.348	Depositor DCC
R_{free} test set	7703 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	92.0	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.095 for -k,-h,-l 0.105 for k,h,-l 0.105 for h,-k,-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	47773	wwPDB-VP
Average B, all atoms (Å^2)	82.0	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 47.49 % 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 9.8479e-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	0.61	1/8076 (0.0%)	0.85	6/10965 (0.1%)
1	B	0.62	1/8087 (0.0%)	0.86	5/10980 (0.0%)
1	C	0.62	0/8076	0.86	6/10965 (0.1%)
1	D	0.56	1/8076 (0.0%)	0.82	8/10965 (0.1%)
1	E	0.58	2/8076 (0.0%)	0.83	6/10965 (0.1%)
1	F	0.58	1/8076 (0.0%)	0.85	10/10965 (0.1%)
All	All	0.60	6/48467 (0.0%)	0.84	41/65805 (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	2
1	B	0	1
1	C	0	2
1	E	0	1
1	F	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	515	TRP	CB-CG	7.59	1.64	1.50
1	B	515	TRP	CB-CG	6.22	1.61	1.50
1	D	515	TRP	CB-CG	6.04	1.61	1.50
1	E	515	TRP	CB-CG	5.75	1.60	1.50
1	E	493	CYS	CB-SG	-5.49	1.72	1.81
1	F	887	CYS	CB-SG	5.43	1.91	1.82

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	529	ASP	CB-CG-OD1	10.05	127.35	118.30
1	B	483	LEU	CA-CB-CG	8.63	135.14	115.30
1	A	972	LEU	CA-CB-CG	7.07	131.55	115.30
1	B	529	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	357	LEU	CA-CB-CG	6.93	131.25	115.30
1	E	888	LEU	CA-CB-CG	-6.90	99.44	115.30
1	A	529	ASP	CB-CG-OD1	6.89	124.50	118.30
1	E	250	LEU	CA-CB-CG	6.75	130.82	115.30
1	F	529	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	C	75	LEU	CA-CB-CG	6.49	130.22	115.30
1	D	944	LEU	CA-CB-CG	-6.45	100.47	115.30
1	A	483	LEU	CA-CB-CG	6.22	129.60	115.30
1	F	989	LEU	CA-CB-CG	6.18	129.52	115.30
1	D	113	LEU	CA-CB-CG	6.01	129.12	115.30
1	D	350	LEU	CA-CB-CG	-6.00	101.49	115.30
1	D	483	LEU	CA-CB-CG	6.00	129.11	115.30
1	C	363	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	293	LEU	CA-CB-CG	5.88	128.83	115.30
1	A	519	MET	CB-CG-SD	5.87	130.01	112.40
1	C	980	LEU	CA-CB-CG	-5.75	102.06	115.30
1	F	49	TYR	CA-CB-CG	5.75	124.32	113.40
1	D	519	MET	CB-CG-SD	5.74	129.63	112.40
1	A	1030	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	F	721	LEU	CA-CB-CG	5.59	128.15	115.30
1	D	673	GLU	N-CA-C	5.48	125.79	111.00
1	C	886	LEU	CA-CB-CG	5.47	127.88	115.30
1	E	357	LEU	CA-CB-CG	5.38	127.69	115.30
1	E	193	LEU	CA-CB-CG	5.36	127.62	115.30
1	F	812	GLY	N-CA-C	-5.35	99.72	113.10
1	E	599	LEU	CA-CB-CG	5.29	127.47	115.30
1	F	847	LEU	CA-CB-CG	5.26	127.39	115.30
1	D	721	LEU	CA-CB-CG	5.25	127.37	115.30
1	E	529	ASP	CB-CG-OD1	5.22	123.00	118.30
1	F	921	LEU	CA-CB-CG	-5.21	103.33	115.30
1	C	944	LEU	CA-CB-CG	5.19	127.25	115.30
1	A	932	LEU	CA-CB-CG	5.19	127.24	115.30
1	B	344	LEU	CA-CB-CG	5.19	127.24	115.30
1	F	363	ARG	CG-CD-NE	5.17	122.65	111.80
1	F	972	LEU	CA-CB-CG	5.09	127.02	115.30
1	D	488	LEU	CA-CB-CG	-5.09	103.59	115.30
1	C	270	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1038	GLU	Peptide
1	A	540	ARG	Sidechain
1	B	1039	ASP	Peptide
1	C	540	ARG	Sidechain
1	C	6	ILE	Peptide
1	E	1039	ASP	Peptide
1	F	6	ILE	Peptide
1	F	812	GLY	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	7925	0	8066	432	0
1	B	7935	0	8073	340	0
1	C	7925	0	8066	397	1
1	D	7925	0	8066	418	1
1	E	7925	0	8066	425	0
1	F	7925	0	8066	439	0
2	A	35	0	46	3	0
2	B	35	0	46	7	0
2	C	35	0	46	0	0
2	D	35	0	46	7	0
2	E	35	0	46	9	0
2	F	35	0	46	3	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47773	0	48679	2382	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (2382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:MET:HE1	1:C:225:VAL:H	1.22	1.04
1:D:781:MET:HE1	1:F:225:VAL:H	1.19	1.03
1:A:971:ARG:HG2	1:A:974:PRO:HG2	1.44	0.96
1:B:1035:ARG:HG3	1:B:1036:LYS:HG3	1.49	0.95
1:B:959:GLY:HA2	1:B:1040:ILE:HB	1.46	0.95
1:B:541:TYR:HH	2:B:1101:LMT:H6'	1.00	0.93
1:C:944:LEU:HB3	1:C:971:ARG:HD2	1.50	0.93
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.48	0.92
1:A:1034:SER:HB3	1:A:1035:ARG:HA	1.50	0.92
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.52	0.90
1:D:344:LEU:HD22	1:D:402:ILE:HD11	1.53	0.90
1:B:225:VAL:HG12	1:C:777:ALA:HB1	1.52	0.89
2:E:1101:LMT:H5B	2:E:1101:LMT:H6D	1.54	0.89
1:F:559:LEU:HD22	1:F:560:PRO:HD2	1.53	0.89
1:A:619:GLY:HA3	1:A:815:ARG:HH22	1.36	0.88
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.37	0.88
1:F:731:ILE:HD13	1:F:746:ILE:HD11	1.54	0.87
1:E:733:GLN:HE22	1:E:743:ILE:HG21	1.39	0.87
1:E:699:ARG:NH2	1:E:722:GLU:OE2	2.08	0.86
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.57	0.86
1:C:919:ARG:O	1:C:921:LEU:N	2.09	0.86
1:D:57:VAL:HG21	1:D:86:GLY:HA2	1.55	0.86
1:E:146:ASP:OD2	1:E:146:ASP:N	2.07	0.86
1:D:696:THR:HG23	1:D:699:ARG:HH12	1.41	0.86
1:E:196:PHE:O	1:E:252:LYS:NZ	2.09	0.85
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.58	0.85
1:A:445:ILE:HD13	1:A:940:LYS:HE3	1.58	0.85
1:B:1037:ASN:HA	1:B:1038:GLU:HG2	1.59	0.84
1:F:897:ILE:HG23	1:F:946:VAL:HG11	1.59	0.84
1:A:957:GLY:HA2	1:A:1042:HIS:HB3	1.59	0.84
1:C:892:TYR:O	1:C:894:SER:N	2.11	0.84
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.59	0.84
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.60	0.84
1:E:950:LYS:HA	1:E:953:MET:HE3	1.58	0.83
1:A:537:SER:OG	1:A:540:ARG:HD2	1.78	0.83
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.61	0.82
1:D:360:GLN:NE2	1:D:513:PHE:O	2.12	0.82
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.60	0.82
1:C:240:LEU:HB2	1:C:246:PHE:CE1	2.15	0.81
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.62	0.81
1:A:578:LEU:HD21	1:A:590:VAL:HG21	1.62	0.81
1:C:578:LEU:HD21	1:C:590:VAL:HG21	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HD22	1:C:293:LEU:HD23	1.61	0.81
1:B:652:THR:HG23	1:B:665:ALA:H	1.46	0.80
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.63	0.80
1:C:151:GLN:NE2	1:C:279:ALA:O	2.13	0.80
1:D:400:LEU:HD23	1:D:929:VAL:HG12	1.64	0.80
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.61	0.80
1:B:422:GLU:O	1:B:502:LYS:NZ	2.15	0.80
1:E:441:ALA:HA	1:E:891:LEU:HD21	1.64	0.79
1:E:156:ASP:OD2	1:E:769:LYS:NZ	2.14	0.79
1:F:82:SER:HB2	1:F:816:LEU:HB2	1.65	0.79
1:D:596:HIS:O	1:D:600:THR:OG1	2.01	0.79
1:A:243:THR:HG23	1:A:268:ILE:HG22	1.64	0.78
1:D:564:LEU:HB2	1:D:671:ILE:HD11	1.65	0.78
1:A:196:PHE:O	1:A:252:LYS:NZ	2.17	0.78
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.17	0.78
1:C:641:GLU:HB2	1:C:650:ARG:HH22	1.49	0.78
1:A:703:LEU:HD21	1:A:718:PRO:HD3	1.66	0.77
1:B:668:LEU:HD23	1:B:668:LEU:H	1.48	0.77
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.63	0.77
1:A:129:VAL:O	1:B:110:LYS:NZ	2.17	0.77
1:C:53:ASP:OD1	1:C:56:THR:OG1	2.01	0.77
1:F:358:PHE:HD1	1:F:977:MET:HG3	1.47	0.77
1:D:55:LYS:NZ	1:F:238:THR:OG1	2.16	0.77
1:E:530:SER:CB	2:E:1101:LMT:H2O2	1.97	0.77
1:E:699:ARG:HE	1:E:718:PRO:HG3	1.49	0.77
1:F:307:ARG:NH2	1:F:314:GLU:OE2	2.18	0.77
1:C:578:LEU:HG	1:C:587:THR:HG22	1.66	0.76
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.67	0.76
1:D:536:ARG:NH2	2:D:1101:LMT:O3B	2.18	0.76
1:E:641:GLU:HA	1:E:646:ALA:HB3	1.66	0.76
1:E:976:LEU:HD21	2:E:1101:LMT:H111	1.68	0.76
1:A:1041:GLU:HB3	1:A:1042:HIS:HA	1.67	0.76
1:B:9:PRO:HB3	1:B:495:THR:HG21	1.68	0.76
1:F:910:ILE:O	1:F:914:LEU:HB2	1.85	0.76
1:A:451:ALA:HB1	1:A:883:VAL:HG12	1.67	0.76
1:D:82:SER:HB2	1:D:816:LEU:HB2	1.67	0.76
1:F:596:HIS:O	1:F:600:THR:OG1	2.04	0.75
1:A:225:VAL:H	1:B:781:MET:HE1	1.49	0.75
1:F:733:GLN:HE22	1:F:743:ILE:HG21	1.50	0.75
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.69	0.75
1:A:70:ASN:O	1:A:110:LYS:NZ	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:LEU:HB2	1:C:246:PHE:HE1	1.49	0.75
1:E:326:PRO:O	1:E:630:SER:OG	2.04	0.75
1:A:146:ASP:HB2	1:A:148:THR:HG23	1.69	0.75
1:C:159:ALA:HB2	1:C:177:LEU:HD11	1.67	0.75
1:E:508:GLY:HA3	1:E:518:ARG:HE	1.52	0.75
1:A:400:LEU:HD21	1:A:930:GLY:HA2	1.69	0.74
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.67	0.74
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.69	0.74
1:C:587:THR:HG21	1:C:622:GLN:O	1.86	0.74
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.69	0.74
1:C:356:TYR:HA	1:C:365:THR:HG21	1.68	0.74
1:D:133:SER:OG	1:D:134:SER:N	2.20	0.74
1:D:156:ASP:OD2	1:D:769:LYS:NZ	2.20	0.74
1:D:225:VAL:H	1:E:781:MET:HE1	1.51	0.74
1:E:174:ASP:HB3	1:E:292:LYS:HB2	1.69	0.74
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.67	0.74
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.70	0.74
1:F:343:THR:HG21	1:F:989:LEU:HD23	1.67	0.74
1:A:144:ASN:HD22	1:A:321:LEU:HD23	1.50	0.74
1:A:1040:ILE:HG13	1:A:1041:GLU:H	1.51	0.74
1:B:508:GLY:O	1:B:510:LYS:N	2.21	0.74
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.70	0.74
1:F:664:PHE:HD2	1:F:717:ARG:HD3	1.50	0.74
1:F:298:ASN:ND2	1:F:301:ASP:OD2	2.21	0.74
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.21	0.73
1:C:3:ASN:N	1:C:3:ASN:OD1	2.21	0.73
1:C:251:LEU:HD11	1:C:262:LEU:HA	1.70	0.73
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.71	0.73
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.69	0.73
1:B:362:PHE:O	1:B:365:THR:HG22	1.89	0.73
1:D:137:LEU:HD13	1:D:293:LEU:HD12	1.71	0.73
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.71	0.72
1:C:143:ILE:HG22	1:C:286:ALA:HB2	1.71	0.72
1:B:213:GLN:HE22	1:C:52:ALA:HA	1.54	0.72
1:B:658:ILE:O	1:B:659:LYS:HD2	1.89	0.72
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.69	0.72
1:B:423:GLU:HA	1:B:502:LYS:HZ3	1.53	0.72
1:B:536:ARG:NH2	2:B:1101:LMT:O2B	2.20	0.72
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.71	0.72
1:D:777:ALA:HB1	1:F:225:VAL:HG12	1.70	0.72
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.71	0.72
1:A:655:PHE:HB3	1:A:663:VAL:HB	1.71	0.72
1:C:201:VAL:HA	1:C:204:ILE:HD12	1.71	0.72
1:D:712:MET:HB3	1:D:713:LEU:HD22	1.70	0.72
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.72	0.72
1:D:427:PRO:HD3	1:D:499:PRO:HB3	1.72	0.72
1:F:58:GLN:OE1	1:F:818:ARG:NH1	2.23	0.72
1:F:537:SER:OG	1:F:540:ARG:NH2	2.23	0.72
1:F:668:LEU:HD23	1:F:668:LEU:H	1.54	0.72
1:E:156:ASP:OD1	1:E:765:ARG:NH2	2.22	0.71
1:E:508:GLY:O	1:E:510:LYS:N	2.23	0.71
1:B:24:GLY:O	1:B:27:ILE:HG22	1.89	0.71
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.23	0.71
1:C:450:SER:HB2	1:C:475:VAL:HG22	1.72	0.71
1:C:746:ILE:HG13	1:C:747:ASN:N	2.06	0.71
1:F:133:SER:OG	1:F:293:LEU:O	2.07	0.71
1:C:596:HIS:O	1:C:600:THR:OG1	2.08	0.71
1:C:588:GLN:O	1:C:592:ASN:ND2	2.23	0.71
1:D:982:PHE:O	1:D:985:GLY:N	2.24	0.71
1:E:971:ARG:O	1:E:975:ILE:HG12	1.91	0.71
1:F:360:GLN:NE2	1:F:513:PHE:O	2.16	0.71
1:E:743:ILE:HA	1:E:746:ILE:HD12	1.72	0.71
1:D:225:VAL:HG22	1:E:781:MET:HE2	1.71	0.71
1:D:335:ILE:O	1:D:339:GLU:HG2	1.91	0.71
1:E:540:ARG:NH1	2:E:1101:LMT:O6B	2.19	0.71
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.54	0.71
1:C:668:LEU:HD23	1:C:668:LEU:H	1.56	0.70
1:F:187:TRP:HB3	1:F:776:GLU:HG2	1.73	0.70
1:A:259:ARG:HH21	1:A:261:LEU:HD11	1.55	0.70
1:D:170:SER:HB2	1:E:75:LEU:H	1.56	0.70
1:E:1013:THR:O	1:E:1017:LEU:HB2	1.92	0.70
1:A:1016:VAL:HG13	2:A:1101:LMT:H112	1.74	0.70
1:C:564:LEU:HG	1:C:565:PRO:HD2	1.73	0.70
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.72	0.70
1:D:540:ARG:NH2	2:D:1101:LMT:O6B	2.24	0.70
1:C:960:LEU:HB3	1:C:1040:ILE:HG23	1.74	0.70
1:D:6:ILE:HG13	1:D:7:ASP:N	2.06	0.70
1:D:66:GLU:OE2	1:D:80:SER:OG	2.07	0.69
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.75	0.69
1:F:456:MET:HB3	1:F:876:LEU:HD21	1.73	0.69
1:A:61:VAL:HG22	1:A:118:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.74	0.69
1:E:637:ARG:HB3	1:E:642:ASN:HB3	1.74	0.69
1:F:352:PHE:HA	1:F:355:MET:HE2	1.73	0.69
1:A:400:LEU:HD11	1:A:1007:VAL:HG21	1.74	0.69
1:B:423:GLU:HA	1:B:502:LYS:NZ	2.07	0.69
1:C:897:ILE:HG23	1:C:946:VAL:HG11	1.74	0.69
1:E:589:LYS:HA	1:E:592:ASN:HD22	1.57	0.69
1:E:901:VAL:HG21	1:E:943:ILE:HG13	1.73	0.69
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.75	0.69
1:C:727:PHE:CZ	1:C:807:SER:HB2	2.28	0.69
1:D:298:ASN:HB3	1:D:301:ASP:HB2	1.75	0.69
1:B:907:LEU:HG	1:B:1017:LEU:HD23	1.75	0.69
1:D:1040:ILE:HG12	1:D:1041:GLU:H	1.58	0.69
1:E:139:VAL:HG13	1:E:178:PHE:HE1	1.57	0.69
1:E:149:MET:HB2	1:E:153:ASP:HB3	1.74	0.69
1:C:982:PHE:O	1:C:985:GLY:N	2.25	0.69
1:D:491:ALA:O	1:D:495:THR:OG1	2.09	0.69
1:E:157:TYR:O	1:E:161:ASN:ND2	2.21	0.69
1:E:959:GLY:HA2	1:E:1040:ILE:HB	1.75	0.69
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.75	0.69
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.74	0.69
1:A:712:MET:HB3	1:A:713:LEU:HD22	1.73	0.69
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.73	0.69
1:D:196:PHE:HB3	1:D:252:LYS:NZ	2.07	0.69
1:E:57:VAL:HG11	1:E:86:GLY:HA2	1.74	0.69
1:E:588:GLN:O	1:E:592:ASN:ND2	2.26	0.69
1:A:654:ALA:O	1:A:658:ILE:HG12	1.92	0.69
1:E:169:THR:HG21	1:E:306:ILE:HG13	1.74	0.69
1:E:1037:ASN:H	1:E:1038:GLU:HA	1.58	0.69
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.73	0.69
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.74	0.69
1:A:747:ASN:ND2	1:C:237:GLN:OE1	2.25	0.69
1:B:196:PHE:O	1:B:252:LYS:NZ	2.24	0.69
1:D:70:ASN:O	1:D:110:LYS:NZ	2.25	0.69
1:D:598:TYR:HB3	1:D:606:VAL:HG21	1.74	0.69
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.74	0.68
1:E:362:PHE:O	1:E:365:THR:HG22	1.92	0.68
1:F:509:LYS:O	1:F:518:ARG:NH1	2.26	0.68
1:F:739:LEU:HD13	1:F:799:VAL:HG11	1.75	0.68
1:D:49:TYR:HB3	1:D:57:VAL:HG22	1.74	0.68
1:D:115:MET:O	1:D:123:GLN:NE2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:702:LEU:HD12	1:F:851:LEU:HD11	1.76	0.68
1:F:3:ASN:OD1	1:F:3:ASN:N	2.26	0.68
1:A:158:VAL:HG22	1:A:162:MET:HE2	1.75	0.68
1:F:73:ASP:OD2	1:F:106:GLN:NE2	2.24	0.68
1:F:667:ASN:O	1:F:678:THR:OG1	2.11	0.68
1:A:564:LEU:HD23	1:A:565:PRO:HD2	1.75	0.68
1:E:146:ASP:OD2	1:E:320:GLY:HA3	1.94	0.68
1:F:577:GLN:HG3	1:F:624:THR:HG22	1.76	0.68
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.76	0.68
1:E:949:ALA:HB3	1:E:1026:PHE:HE1	1.59	0.68
1:A:768:VAL:HG12	1:B:63:GLN:HE21	1.58	0.68
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.74	0.68
1:C:363:ARG:HB3	1:C:363:ARG:HH11	1.59	0.68
1:D:170:SER:OG	1:E:74:ASN:N	2.22	0.68
1:F:452:VAL:HG12	1:F:880:SER:HB3	1.76	0.68
1:A:491:ALA:O	1:A:495:THR:OG1	2.06	0.67
1:E:675:GLY:HA2	1:E:862:MET:SD	2.34	0.67
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.76	0.67
1:B:26:ALA:O	1:B:30:LEU:HB2	1.94	0.67
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.76	0.67
1:E:9:PRO:HB3	1:E:495:THR:HG21	1.76	0.67
1:F:24:GLY:O	1:F:27:ILE:HG12	1.94	0.67
1:A:156:ASP:OD2	1:A:769:LYS:NZ	2.28	0.67
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.77	0.67
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.29	0.67
1:F:527:TYR:HB2	2:F:1101:LMT:H101	1.77	0.67
1:A:350:LEU:HD22	1:A:984:LEU:HB3	1.76	0.67
1:D:562:SER:HB2	1:D:924:ASP:HB3	1.77	0.67
1:B:775:SER:OG	1:B:776:GLU:O	2.13	0.67
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.77	0.67
1:E:376:LEU:O	1:E:379:THR:N	2.27	0.67
1:E:531:VAL:O	1:E:534:ILE:HG13	1.93	0.67
1:E:858:ASP:OD1	1:E:859:TRP:N	2.27	0.67
1:B:267:LYS:HD3	1:B:776:GLU:OE2	1.95	0.67
1:F:251:LEU:HD11	1:F:262:LEU:HA	1.74	0.67
1:A:531:VAL:O	1:A:534:ILE:HG13	1.94	0.67
1:E:213:GLN:HE22	1:F:52:ALA:HA	1.60	0.67
1:F:180:SER:OG	1:F:274:ASN:O	2.07	0.67
1:F:578:LEU:HG	1:F:587:THR:HG22	1.75	0.67
1:C:889:ALA:HB1	1:C:895:TRP:HZ3	1.59	0.67
1:E:237:GLN:OE1	1:F:747:ASN:ND2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:739:LEU:HD13	1:B:799:VAL:HG11	1.77	0.66
1:F:358:PHE:CD1	1:F:977:MET:HG3	2.30	0.66
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.77	0.66
1:B:167:SER:CB	1:B:175:VAL:HG21	2.25	0.66
1:F:808:ARG:NH1	1:F:810:GLU:OE2	2.28	0.66
1:A:957:GLY:CA	1:A:1042:HIS:HB3	2.25	0.66
1:D:330:THR:HG23	1:D:334:LYS:HD2	1.75	0.66
1:D:448:VAL:HG22	1:D:887:CYS:HB3	1.76	0.66
1:D:904:VAL:HG21	1:D:942:ALA:HB2	1.77	0.66
1:F:885:PHE:HD2	1:F:886:LEU:HD22	1.60	0.66
1:D:641:GLU:HB2	1:D:650:ARG:HH22	1.60	0.66
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.77	0.66
1:A:421:ALA:HB1	1:A:505:HIS:CE1	2.30	0.66
1:E:901:VAL:HG23	1:E:942:ALA:HB3	1.78	0.66
1:E:931:LEU:O	1:E:935:ILE:HG13	1.96	0.66
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.29	0.66
1:A:573:MET:HG3	1:A:666:PHE:CE2	2.31	0.66
1:B:58:GLN:O	1:B:63:GLN:HG3	1.95	0.66
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.78	0.66
1:A:971:ARG:C	1:A:974:PRO:HD2	2.16	0.65
1:A:571:VAL:HG22	1:A:630:SER:HA	1.77	0.65
1:D:897:ILE:HA	1:D:1029:VAL:HG11	1.78	0.65
1:F:365:THR:O	1:F:368:PRO:HD2	1.95	0.65
1:C:686:ASP:OD1	1:C:690:LEU:HB2	1.96	0.65
1:A:137:LEU:HB2	1:A:293:LEU:HB2	1.79	0.65
1:A:362:PHE:O	1:A:365:THR:HG22	1.96	0.65
1:A:540:ARG:HG3	1:A:541:TYR:HD1	1.62	0.65
1:A:540:ARG:HG3	1:A:541:TYR:CD1	2.31	0.65
1:D:184:MET:HB3	1:D:771:VAL:HG13	1.79	0.65
1:D:967:ALA:O	1:D:971:ARG:NH1	2.28	0.65
1:E:658:ILE:O	1:E:659:LYS:HD2	1.96	0.65
1:B:610:PHE:HB3	1:B:628:PHE:HB3	1.77	0.65
1:C:947:GLU:HG3	1:C:948:PHE:HD1	1.61	0.65
1:A:923:ASN:ND2	1:A:923:ASN:O	2.30	0.65
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.79	0.65
1:E:702:LEU:HD13	1:E:851:LEU:HD21	1.79	0.65
1:C:744:ASN:O	1:C:748:THR:HG23	1.97	0.65
1:B:139:VAL:O	1:B:326:PRO:HD2	1.96	0.64
1:D:174:ASP:HB3	1:D:292:LYS:HB2	1.79	0.64
1:A:781:MET:HE1	1:C:225:VAL:N	2.05	0.64
1:B:511:GLY:HA2	1:B:515:TRP:CD1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:971:ARG:O	1:B:975:ILE:HG12	1.98	0.64
1:D:453:PHE:O	1:D:471:SER:OG	2.12	0.64
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.80	0.64
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.32	0.64
1:F:452:VAL:O	1:F:455:PRO:HD2	1.97	0.64
1:A:960:LEU:HD21	1:A:1027:VAL:HG13	1.78	0.64
1:B:1013:THR:O	1:B:1017:LEU:HB2	1.96	0.64
1:A:143:ILE:HG22	1:A:286:ALA:HB2	1.80	0.64
1:B:536:ARG:NE	2:B:1101:LMT:O3B	2.30	0.64
1:D:243:THR:HG23	1:D:268:ILE:HG22	1.80	0.64
1:D:568:ASP:O	1:D:634:TRP:HZ3	1.81	0.64
1:E:261:LEU:HD12	1:E:263:ARG:HH12	1.63	0.64
1:B:156:ASP:OD1	1:B:765:ARG:NH2	2.30	0.64
1:D:318:PRO:HD2	1:D:321:LEU:HD12	1.78	0.64
1:F:424:GLY:HA3	1:F:502:LYS:HB2	1.79	0.64
1:A:73:ASP:OD2	1:A:106:GLN:NE2	2.30	0.64
1:E:907:LEU:HG	1:E:1017:LEU:HD23	1.80	0.64
1:C:944:LEU:HB3	1:C:971:ARG:CD	2.27	0.64
1:C:682:PHE:CE1	1:C:857:TYR:HB2	2.33	0.64
1:E:14:VAL:HG22	1:F:886:LEU:HD12	1.78	0.64
1:D:894:SER:HB3	1:D:897:ILE:HB	1.79	0.64
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.80	0.64
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.80	0.64
1:D:931:LEU:O	1:D:935:ILE:HG13	1.98	0.64
1:D:869:SER:OG	1:D:872:GLN:NE2	2.31	0.63
1:D:971:ARG:HB3	1:D:971:ARG:HH11	1.63	0.63
1:F:213:GLN:HG2	1:F:239:ARG:HG3	1.80	0.63
1:F:671:ILE:HD13	1:F:674:LEU:HD12	1.81	0.63
1:D:388:PHE:CE1	1:D:472:ILE:HG21	2.34	0.63
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.79	0.63
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.80	0.63
1:C:671:ILE:HD13	1:C:674:LEU:HD12	1.80	0.63
1:E:108:GLN:HE22	1:F:109:ASN:HA	1.64	0.63
1:F:379:THR:HG23	1:F:476:SER:OG	1.97	0.63
1:F:479:ALA:O	1:F:482:VAL:HG23	1.99	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.80	0.63
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.80	0.63
1:D:507:GLU:O	1:D:509:LYS:N	2.29	0.63
1:E:318:PRO:HD2	1:E:321:LEU:HD22	1.80	0.63
1:E:445:ILE:HG21	1:E:940:LYS:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:ARG:HB3	1:B:921:LEU:HD23	1.80	0.63
1:C:184:MET:HB3	1:C:771:VAL:HG13	1.80	0.63
1:C:559:LEU:HD23	1:C:560:PRO:HD2	1.79	0.63
1:D:358:PHE:CD1	1:D:977:MET:HG2	2.33	0.63
1:A:668:LEU:HD23	1:A:668:LEU:H	1.62	0.63
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.64	0.63
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.80	0.63
1:E:776:GLU:HG2	1:E:777:ALA:H	1.63	0.63
1:A:457:ALA:HB1	1:A:468:ARG:HG3	1.81	0.63
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.13	0.63
1:E:415:ASN:ND2	1:E:437:GLN:OE1	2.28	0.63
1:A:520:PHE:O	1:A:524:THR:HG23	1.98	0.63
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.81	0.63
1:F:971:ARG:NE	1:F:971:ARG:O	2.31	0.63
1:A:832:ALA:HB3	1:A:835:LYS:HD3	1.82	0.62
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.79	0.62
1:D:644:VAL:HG11	1:D:667:ASN:HB2	1.80	0.62
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.80	0.62
1:F:358:PHE:HE2	1:F:516:PHE:HZ	1.45	0.62
1:A:357:LEU:HD23	1:A:358:PHE:CD1	2.34	0.62
1:B:1011:MET:O	1:B:1015:THR:HG23	1.99	0.62
1:D:412:VAL:HG22	1:D:438:ILE:HD12	1.81	0.62
1:D:728:LYS:HG2	1:D:808:ARG:NH1	2.14	0.62
1:B:682:PHE:HE2	1:B:684:LEU:HB2	1.63	0.62
1:E:64:VAL:HG11	1:E:117:LEU:HB2	1.80	0.62
1:E:149:MET:HB2	1:E:153:ASP:CB	2.29	0.62
1:A:174:ASP:HB3	1:A:292:LYS:HB2	1.80	0.62
1:C:493:CYS:O	1:C:497:LEU:HB2	1.99	0.62
1:C:694:LYS:HE3	1:C:694:LYS:H	1.65	0.62
1:D:580:ALA:HB1	1:D:724:THR:HG22	1.80	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.33	0.62
1:F:713:LEU:HD21	1:F:843:LEU:HD12	1.80	0.62
1:B:441:ALA:HA	1:B:891:LEU:HD21	1.79	0.62
1:C:261:LEU:N	1:C:264:ASP:OD2	2.32	0.62
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.63	0.62
1:C:960:LEU:O	1:C:964:THR:HG23	1.99	0.62
1:D:282:ASN:HD21	1:D:608:SER:HA	1.63	0.62
1:F:506:GLY:C	1:F:508:GLY:H	2.01	0.62
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.80	0.62
1:C:937:LEU:HD13	1:C:1011:MET:HE1	1.80	0.62
1:F:578:LEU:HB2	1:F:623:ASN:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:958:LYS:O	1:A:1040:ILE:HG12	2.00	0.62
1:C:171:GLY:HA3	1:C:302:THR:OG1	1.99	0.62
1:B:950:LYS:HZ1	1:B:1030:ARG:HH21	1.48	0.62
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.30	0.62
1:A:276:ASP:HA	1:C:222:THR:HG21	1.82	0.62
1:C:637:ARG:HB3	1:C:642:ASN:HB3	1.82	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.81	0.62
1:A:733:GLN:NE2	1:A:743:ILE:HG21	2.15	0.62
1:D:674:LEU:HD23	1:D:675:GLY:N	2.14	0.62
1:F:372:VAL:HG22	1:F:405:LEU:HD11	1.81	0.62
1:C:101:ASP:OD1	1:C:131:LYS:NZ	2.33	0.61
1:C:520:PHE:O	1:C:524:THR:HG23	2.00	0.61
1:D:144:ASN:HA	1:D:320:GLY:O	2.00	0.61
1:D:700:ASN:HA	1:D:703:LEU:HD12	1.81	0.61
1:F:363:ARG:HG2	1:F:363:ARG:HH11	1.65	0.61
1:A:184:MET:HG2	1:A:246:PHE:CE2	2.36	0.61
1:B:759:VAL:HG12	1:B:760:ASN:HB2	1.81	0.61
1:F:674:LEU:HD22	1:F:861:GLY:HA2	1.83	0.61
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.65	0.61
1:E:680:PHE:HB2	1:E:863:SER:OG	2.00	0.61
1:F:120:GLN:HA	1:F:123:GLN:HB2	1.81	0.61
1:A:225:VAL:HG12	1:B:777:ALA:HB1	1.82	0.61
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.66	0.61
1:B:484:VAL:O	1:B:489:THR:HG23	2.00	0.61
1:C:187:TRP:HA	1:C:774:MET:O	2.00	0.61
1:C:944:LEU:HD13	1:C:975:ILE:HG12	1.82	0.61
1:D:578:LEU:HD21	1:D:590:VAL:HG21	1.81	0.61
1:D:641:GLU:HA	1:D:646:ALA:HB3	1.82	0.61
1:F:139:VAL:HG22	1:F:290:GLY:HA2	1.81	0.61
1:F:429:GLU:O	1:F:433:LYS:HB2	2.01	0.61
1:F:610:PHE:HB3	1:F:628:PHE:HB2	1.82	0.61
1:D:225:VAL:HG12	1:E:777:ALA:HB1	1.82	0.61
1:F:408:ASP:OD2	1:F:408:ASP:N	2.32	0.61
1:F:897:ILE:HG23	1:F:946:VAL:CG1	2.30	0.61
1:F:1021:PHE:HB3	1:F:1025:PHE:CE1	2.35	0.61
1:A:559:LEU:HD13	1:A:923:ASN:HB2	1.82	0.61
1:B:648:THR:O	1:B:652:THR:OG1	2.19	0.61
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.83	0.61
1:B:1037:ASN:HA	1:B:1038:GLU:CG	2.29	0.61
1:C:326:PRO:O	1:C:630:SER:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:795:ASP:OD2	1:E:797:GLN:HG3	2.00	0.61
1:F:455:PRO:HG3	1:F:883:VAL:HG21	1.83	0.61
1:A:244:GLU:O	1:A:247:GLY:N	2.34	0.60
1:A:768:VAL:HG12	1:B:63:GLN:NE2	2.16	0.60
1:A:795:ASP:OD2	1:A:797:GLN:HG3	2.00	0.60
1:B:82:SER:HB2	1:B:816:LEU:HB2	1.82	0.60
1:A:944:LEU:HB3	1:A:971:ARG:CZ	2.31	0.60
1:B:52:ALA:HB1	1:B:56:THR:HB	1.83	0.60
1:B:596:HIS:O	1:B:600:THR:OG1	2.09	0.60
1:C:479:ALA:O	1:C:482:VAL:HG23	2.02	0.60
1:D:368:PRO:HG3	1:D:413:VAL:HG21	1.82	0.60
1:E:583:THR:HG22	1:E:585:GLU:H	1.66	0.60
1:D:18:ILE:HG13	1:E:886:LEU:HD23	1.83	0.60
1:D:247:GLY:O	1:D:261:LEU:HB3	2.01	0.60
1:D:900:SER:HA	1:D:1025:PHE:HB3	1.83	0.60
1:E:165:ALA:HB3	1:E:313:MET:HE3	1.82	0.60
1:A:514:GLY:HA2	1:A:517:ASN:HD22	1.66	0.60
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.82	0.60
1:C:576:VAL:HG21	1:C:591:LEU:HD23	1.83	0.60
1:C:889:ALA:HB1	1:C:895:TRP:CZ3	2.35	0.60
1:D:251:LEU:HD11	1:D:262:LEU:HA	1.83	0.60
1:A:326:PRO:HA	1:A:630:SER:OG	2.00	0.60
1:A:515:TRP:O	1:A:519:MET:HG3	2.01	0.60
1:A:959:GLY:HA2	1:A:1040:ILE:HB	1.84	0.60
1:D:514:GLY:HA2	1:D:516:PHE:HB3	1.83	0.60
1:F:979:SER:CB	1:F:1015:THR:HG21	2.32	0.60
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.60
1:D:531:VAL:O	1:D:534:ILE:HG13	2.01	0.60
1:E:26:ALA:O	1:E:30:LEU:HB2	2.01	0.60
1:E:525:HIS:HA	1:E:528:THR:HG22	1.84	0.60
1:F:351:VAL:HG11	1:F:406:VAL:HG11	1.84	0.60
1:F:519:MET:O	1:F:523:SER:OG	2.18	0.60
1:A:6:ILE:HG13	1:A:7:ASP:N	2.16	0.60
1:A:549:VAL:O	1:A:552:MET:HB3	2.00	0.60
1:C:359:LEU:HB2	1:C:365:THR:HG22	1.84	0.60
1:C:556:PHE:HD1	1:C:913:LEU:HD21	1.66	0.60
1:D:429:GLU:OE1	1:D:432:ARG:NH1	2.34	0.60
1:E:1037:ASN:N	1:E:1038:GLU:HA	2.16	0.60
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.37	0.60
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.82	0.60
1:E:166:ILE:O	1:E:169:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:559:LEU:HD12	1:F:923:ASN:HB2	1.83	0.60
1:A:445:ILE:CD1	1:A:940:LYS:HE3	2.30	0.60
1:B:493:CYS:O	1:B:497:LEU:HB2	2.00	0.60
1:D:910:ILE:O	1:D:914:LEU:HB2	2.01	0.60
1:E:733:GLN:NE2	1:E:743:ILE:HG21	2.13	0.60
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.82	0.60
1:A:193:LEU:HD13	1:A:200:PRO:HD3	1.83	0.60
1:A:360:GLN:NE2	1:A:513:PHE:HB3	2.16	0.60
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.84	0.60
1:B:652:THR:HG22	1:B:664:PHE:HD1	1.66	0.59
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.83	0.59
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.83	0.59
1:A:248:LYS:HA	1:A:261:LEU:HD13	1.83	0.59
1:A:355:MET:HA	1:A:355:MET:HE3	1.84	0.59
1:B:990:VAL:HG22	1:B:1004:GLY:HA3	1.85	0.59
1:D:400:LEU:HD11	1:D:1007:VAL:HG21	1.84	0.59
1:D:578:LEU:HB2	1:D:623:ASN:HB2	1.85	0.59
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.59
1:F:762:PHE:CE1	1:F:764:ASP:HB2	2.37	0.59
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.85	0.59
1:D:157:TYR:O	1:D:161:ASN:ND2	2.26	0.59
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.85	0.59
1:A:859:TRP:HE3	1:A:863:SER:HG	1.48	0.59
1:B:60:THR:HG22	1:B:119:PRO:HD3	1.83	0.59
1:C:393:LEU:HD12	1:C:469:GLN:HG3	1.82	0.59
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.38	0.59
1:E:653:ARG:O	1:E:656:SER:OG	2.19	0.59
1:F:1035:ARG:HD3	1:F:1038:GLU:OE1	2.03	0.59
1:B:166:ILE:O	1:B:169:THR:HB	2.02	0.59
1:D:201:VAL:HA	1:D:204:ILE:HD12	1.84	0.59
1:E:520:PHE:O	1:E:523:SER:OG	2.20	0.59
1:A:699:ARG:NH2	1:A:722:GLU:OE2	2.35	0.59
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.84	0.59
1:D:442:LEU:O	1:D:445:ILE:HG13	2.02	0.59
1:D:733:GLN:OE1	1:D:743:ILE:HG21	2.02	0.59
2:B:1101:LMT:H5B	2:B:1101:LMT:H6D	1.84	0.59
1:D:457:ALA:O	1:D:468:ARG:NE	2.30	0.59
1:F:671:ILE:HD12	1:F:862:MET:SD	2.43	0.59
1:C:945:ILE:HA	1:C:971:ARG:NH1	2.18	0.59
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.02	0.59
1:D:1013:THR:O	1:D:1017:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:76:MET:HB2	1:E:93:THR:O	2.03	0.59
1:E:142:VAL:HG21	1:E:158:VAL:HG21	1.84	0.59
1:C:733:GLN:OE1	1:C:743:ILE:HG21	2.03	0.59
1:D:699:ARG:NH2	1:D:722:GLU:OE2	2.36	0.59
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.85	0.59
1:E:200:PRO:HB2	1:E:749:THR:HG22	1.85	0.59
1:E:213:GLN:HA	1:E:237:GLN:O	2.02	0.59
1:E:702:LEU:HD11	1:E:847:LEU:HB3	1.84	0.59
1:F:859:TRP:HE3	1:F:863:SER:HG	1.50	0.59
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.85	0.59
1:B:519:MET:O	1:B:523:SER:OG	2.21	0.59
1:B:910:ILE:O	1:B:914:LEU:HB2	2.03	0.59
1:D:366:LEU:HA	1:D:369:THR:HB	1.85	0.59
1:E:932:LEU:HA	1:E:935:ILE:HD12	1.84	0.59
1:F:172:VAL:HG13	1:F:291:ILE:HG23	1.85	0.59
1:F:455:PRO:HG2	1:F:880:SER:HA	1.84	0.59
1:B:167:SER:HB2	1:B:175:VAL:HG21	1.84	0.58
1:B:184:MET:HB3	1:B:771:VAL:HG13	1.85	0.58
1:C:139:VAL:HG21	1:C:628:PHE:CE2	2.38	0.58
1:F:267:LYS:HB2	1:F:776:GLU:OE1	2.02	0.58
1:B:696:THR:HG23	1:B:699:ARG:HH12	1.67	0.58
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.84	0.58
1:C:743:ILE:H	1:C:743:ILE:HD12	1.69	0.58
1:D:154:ILE:O	1:D:157:TYR:N	2.37	0.58
1:E:960:LEU:O	1:E:964:THR:HG23	2.03	0.58
1:A:332:PHE:O	1:A:336:SER:HB3	2.03	0.58
1:A:66:GLU:OE2	1:A:80:SER:OG	2.21	0.58
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.85	0.58
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.39	0.58
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.85	0.58
1:C:881:LEU:HB3	1:C:902:MET:HE1	1.85	0.58
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.18	0.58
1:D:932:LEU:HA	1:D:935:ILE:HD12	1.85	0.58
1:F:987:MET:HG3	1:F:1008:MET:HE1	1.85	0.58
1:B:167:SER:HB2	1:C:70:ASN:ND2	2.18	0.58
1:B:359:LEU:C	1:B:360:GLN:HG2	2.21	0.58
1:B:545:TYR:HB2	1:B:1021:PHE:HE2	1.69	0.58
1:D:223:PRO:O	1:E:780:ARG:NH2	2.36	0.58
1:A:1040:ILE:HG13	1:A:1041:GLU:N	2.18	0.58
1:C:347:ALA:HB3	1:C:402:ILE:HD12	1.84	0.58
1:F:527:TYR:CE2	1:F:968:VAL:HG13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ALA:HB2	1:E:488:LEU:HD13	1.85	0.58
1:E:435:MET:SD	1:E:490:PRO:HB3	2.44	0.58
1:F:520:PHE:O	1:F:524:THR:HG22	2.03	0.58
1:F:664:PHE:CD2	1:F:717:ARG:HD3	2.35	0.58
1:A:253:VAL:HG12	1:A:259:ARG:HG2	1.86	0.58
1:A:644:VAL:HG11	1:A:667:ASN:HB2	1.84	0.58
1:B:415:ASN:ND2	1:B:418:ARG:HH12	2.02	0.58
1:F:817:GLU:OE2	1:F:825:MET:HA	2.03	0.58
1:B:905:VAL:HG13	1:B:935:ILE:HG23	1.85	0.58
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.85	0.58
1:D:721:LEU:HB2	1:D:814:PRO:HG2	1.86	0.58
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.18	0.58
1:A:375:VAL:HG21	1:A:481:SER:HA	1.86	0.58
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.85	0.58
1:B:511:GLY:HA2	1:B:515:TRP:NE1	2.19	0.58
1:B:535:LEU:HD13	1:B:1027:VAL:HG21	1.86	0.58
1:C:197:GLN:HA	1:C:798:MET:SD	2.43	0.58
1:D:17:ILE:HA	1:D:20:MET:HE2	1.85	0.58
1:D:776:GLU:HB3	1:D:779:TYR:CE1	2.39	0.58
1:E:210:GLN:HE22	1:E:250:LEU:HB3	1.69	0.58
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.84	0.58
1:F:462:SER:O	1:F:466:ILE:HG12	2.03	0.58
1:A:680:PHE:HB2	1:A:859:TRP:HZ3	1.68	0.57
1:C:363:ARG:NH1	1:C:363:ARG:H	2.01	0.57
1:E:1019:ILE:HG13	1:E:1020:PHE:CD1	2.39	0.57
1:F:11:PHE:O	1:F:15:ILE:HG13	2.03	0.57
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.86	0.57
1:B:688:ALA:O	1:B:690:LEU:HG	2.04	0.57
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.34	0.57
1:E:310:LEU:HD23	1:E:325:TYR:OH	2.04	0.57
1:E:919:ARG:HB3	1:E:921:LEU:HD23	1.85	0.57
1:F:937:LEU:HD13	1:F:1011:MET:SD	2.44	0.57
1:C:971:ARG:NE	1:C:971:ARG:O	2.37	0.57
1:B:72:ILE:HD13	1:B:107:VAL:HA	1.86	0.57
1:E:44:THR:OG1	1:E:91:THR:OG1	2.22	0.57
1:F:858:ASP:OD2	1:F:859:TRP:N	2.37	0.57
1:A:424:GLY:HA3	1:A:502:LYS:CG	2.35	0.57
1:C:452:VAL:HG12	1:C:880:SER:HB3	1.85	0.57
1:D:137:LEU:HB2	1:D:293:LEU:HB2	1.87	0.57
1:E:144:ASN:ND2	1:E:319:SER:O	2.37	0.57
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:LEU:HD21	1:E:477:ALA:HB1	1.87	0.57
1:F:239:ARG:HB2	1:F:763:ILE:HD12	1.85	0.57
1:C:66:GLU:OE2	1:C:80:SER:OG	2.09	0.57
1:F:949:ALA:HB3	1:F:1026:PHE:HE2	1.70	0.57
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.87	0.57
1:C:492:LEU:O	1:C:496:MET:HG2	2.05	0.57
1:D:201:VAL:HG23	1:D:749:THR:HG23	1.86	0.57
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.87	0.57
1:F:915:ALA:HB2	1:F:1009:GLY:HA3	1.85	0.57
1:B:907:LEU:HD21	1:B:1021:PHE:HB2	1.87	0.57
1:E:932:LEU:HD23	1:E:935:ILE:HD12	1.86	0.57
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.87	0.57
1:F:940:LYS:NZ	1:F:978:THR:HG21	2.18	0.57
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.87	0.57
1:D:240:LEU:HB2	1:D:246:PHE:CE1	2.40	0.57
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.87	0.57
1:C:450:SER:O	1:C:454:VAL:HG23	2.04	0.57
1:F:507:GLU:HG2	1:F:518:ARG:HA	1.86	0.57
1:A:709:HIS:HB2	1:A:713:LEU:HD23	1.87	0.56
1:B:57:VAL:HG11	1:B:86:GLY:O	2.05	0.56
1:B:66:GLU:OE2	1:B:818:ARG:HD3	2.04	0.56
1:D:242:SER:O	1:D:246:PHE:HD1	1.87	0.56
1:F:409:ALA:O	1:F:413:VAL:HG23	2.05	0.56
1:F:976:LEU:O	1:F:980:LEU:HB2	2.05	0.56
1:A:140:VAL:N	1:A:289:LEU:O	2.36	0.56
1:C:393:LEU:HD13	1:C:466:ILE:HA	1.86	0.56
1:F:907:LEU:HD23	1:F:1017:LEU:HB3	1.87	0.56
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.04	0.56
1:A:743:ILE:HA	1:A:746:ILE:HD12	1.87	0.56
1:B:186:ILE:HG12	1:B:268:ILE:HG12	1.86	0.56
1:B:189:ASN:OD1	1:B:190:PRO:HD2	2.06	0.56
1:B:696:THR:HG23	1:B:699:ARG:NH1	2.21	0.56
1:C:713:LEU:HD21	1:C:843:LEU:HD12	1.88	0.56
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.88	0.56
1:D:412:VAL:HG22	1:D:438:ILE:CD1	2.35	0.56
1:F:69:MET:HG3	1:F:92:LEU:HD11	1.86	0.56
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.86	0.56
1:A:4:PHE:HB3	1:A:8:ARG:NH1	2.20	0.56
1:A:492:LEU:O	1:A:496:MET:HG2	2.06	0.56
1:A:519:MET:O	1:A:523:SER:OG	2.15	0.56
1:A:577:GLN:OE1	1:A:624:THR:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:TYR:HB3	1:A:655:PHE:HZ	1.71	0.56
1:B:535:LEU:HD21	1:B:1024:VAL:HA	1.87	0.56
1:C:3:ASN:O	1:C:6:ILE:N	2.38	0.56
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.87	0.56
1:D:934:THR:O	1:D:938:SER:OG	2.20	0.56
1:E:327:TYR:HB2	1:E:628:PHE:CZ	2.40	0.56
1:E:375:VAL:HG22	1:E:484:VAL:HG21	1.86	0.56
1:A:57:VAL:HG21	1:A:86:GLY:CA	2.35	0.56
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.41	0.56
1:B:251:LEU:HD11	1:B:262:LEU:HA	1.86	0.56
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.88	0.56
1:C:681:ASP:HB2	1:C:828:LEU:HD23	1.86	0.56
1:D:100:ALA:HB1	1:D:131:LYS:HD2	1.87	0.56
1:E:186:ILE:HG12	1:E:268:ILE:HG12	1.86	0.56
1:F:968:VAL:O	1:F:972:LEU:HB2	2.05	0.56
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.05	0.56
1:B:950:LYS:NZ	1:B:1030:ARG:HH21	2.03	0.56
1:D:248:LYS:HA	1:D:261:LEU:HD13	1.86	0.56
1:D:556:PHE:HD1	1:D:913:LEU:HD21	1.71	0.56
1:E:752:ALA:O	1:E:774:MET:HA	2.05	0.56
1:F:160:ALA:HA	1:F:767:ARG:HE	1.71	0.56
1:F:404:LEU:HB3	1:F:478:MET:SD	2.45	0.56
1:A:259:ARG:NH1	1:B:734:GLU:OE1	2.36	0.56
1:A:344:LEU:HD21	1:A:399:VAL:HA	1.87	0.56
1:A:393:LEU:HD11	1:A:466:ILE:HD13	1.88	0.56
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.86	0.56
1:E:175:VAL:HG23	1:F:70:ASN:ND2	2.20	0.56
1:E:911:GLY:HA3	1:E:1013:THR:OG1	2.05	0.56
1:B:455:PRO:HG2	1:B:880:SER:OG	2.04	0.56
1:D:605:ASN:HD21	1:D:642:ASN:CG	2.09	0.56
1:D:751:GLY:O	1:D:753:ALA:N	2.39	0.56
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.41	0.56
1:C:688:ALA:O	1:C:690:LEU:N	2.39	0.56
1:D:239:ARG:NH1	1:D:761:ASP:O	2.38	0.56
1:E:415:ASN:O	1:E:419:VAL:HG23	2.06	0.56
1:F:298:ASN:HB3	1:F:301:ASP:HB2	1.87	0.56
1:C:11:PHE:O	1:C:11:PHE:HD2	1.88	0.55
1:E:979:SER:HB3	1:E:1015:THR:HG21	1.88	0.55
1:B:211:ASN:O	1:B:760:ASN:ND2	2.39	0.55
1:B:717:ARG:NE	1:B:828:LEU:HB2	2.22	0.55
1:B:745:ASP:O	1:B:749:THR:OG1	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:ALA:HA	1:F:314:GLU:CD	2.27	0.55
1:F:780:ARG:O	1:F:781:MET:HE2	2.06	0.55
1:A:99:ASP:HB3	1:A:102:ILE:HB	1.88	0.55
1:B:888:LEU:HD21	1:B:943:ILE:HD11	1.89	0.55
1:C:407:ASP:OD2	1:C:940:LYS:HD2	2.06	0.55
1:C:1026:PHE:O	1:C:1030:ARG:HG2	2.06	0.55
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.89	0.55
1:D:989:LEU:HB3	1:D:1000:GLN:O	2.06	0.55
1:E:58:GLN:O	1:E:63:GLN:HG3	2.06	0.55
1:F:186:ILE:HD13	1:F:262:LEU:HD21	1.87	0.55
1:F:414:GLU:OE1	1:F:973:ARG:HD3	2.07	0.55
1:F:443:VAL:O	1:F:447:MET:HB3	2.06	0.55
1:F:945:ILE:HA	1:F:971:ARG:NH1	2.20	0.55
1:A:753:ALA:O	1:A:775:SER:HB3	2.06	0.55
1:D:196:PHE:HB3	1:D:252:LYS:HZ3	1.71	0.55
1:D:261:LEU:N	1:D:264:ASP:OD2	2.40	0.55
1:F:187:TRP:HA	1:F:774:MET:O	2.06	0.55
1:D:733:GLN:NE2	1:F:210:GLN:HG2	2.21	0.55
1:E:241:THR:N	1:E:245:GLU:OE1	2.36	0.55
1:E:261:LEU:HD12	1:E:263:ARG:NH1	2.21	0.55
1:E:261:LEU:N	1:E:264:ASP:OD2	2.38	0.55
1:F:506:GLY:O	1:F:508:GLY:N	2.32	0.55
1:A:1037:ASN:N	1:A:1038:GLU:HB2	2.22	0.55
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.87	0.55
1:C:501:ALA:O	1:C:504:ASP:HB2	2.06	0.55
1:C:762:PHE:CE1	1:C:764:ASP:HB2	2.42	0.55
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.88	0.55
1:E:934:THR:O	1:E:938:SER:OG	2.23	0.55
1:C:421:ALA:HB1	1:C:505:HIS:H	1.71	0.55
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.88	0.55
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.89	0.55
2:E:1101:LMT:H6D	2:E:1101:LMT:C5B	2.34	0.55
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.89	0.55
1:A:58:GLN:NE2	1:A:59:ASP:OD1	2.36	0.55
1:D:58:GLN:OE1	1:D:818:ARG:NH1	2.38	0.55
1:E:524:THR:O	1:E:527:TYR:HB3	2.07	0.55
1:E:577:GLN:NE2	1:E:721:LEU:HD11	2.21	0.55
1:A:622:GLN:HE21	1:C:222:THR:HG22	1.72	0.55
1:B:699:ARG:HD2	1:B:718:PRO:HB3	1.89	0.55
1:D:1016:VAL:HG12	2:D:1101:LMT:H91	1.89	0.55
1:F:65:ILE:HB	1:F:90:ILE:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:O	1:A:157:TYR:N	2.40	0.55
1:A:424:GLY:HA3	1:A:502:LYS:CB	2.37	0.55
1:B:76:MET:SD	1:B:864:TYR:HE2	2.30	0.55
1:B:327:TYR:HB2	1:B:628:PHE:CE2	2.41	0.55
1:B:583:THR:HG22	1:B:585:GLU:H	1.71	0.55
1:B:752:ALA:O	1:B:774:MET:HA	2.07	0.55
1:C:343:THR:HA	1:C:346:GLU:OE1	2.07	0.55
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.88	0.55
1:E:430:ALA:O	1:E:433:LYS:HB3	2.07	0.55
1:F:112:GLN:HA	1:F:115:MET:HB2	1.87	0.55
1:F:214:VAL:HG23	1:F:237:GLN:HB2	1.89	0.55
1:A:982:PHE:O	1:A:985:GLY:N	2.40	0.54
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.90	0.54
1:B:356:TYR:C	1:B:358:PHE:H	2.11	0.54
1:B:573:MET:HA	1:B:629:VAL:HG23	1.89	0.54
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.88	0.54
1:C:599:LEU:O	1:C:603:LYS:HG2	2.07	0.54
1:E:559:LEU:HD13	1:E:923:ASN:HB2	1.89	0.54
1:F:414:GLU:HG2	1:F:973:ARG:NH1	2.21	0.54
1:A:101:ASP:OD1	1:A:101:ASP:N	2.41	0.54
1:A:121:GLU:O	1:A:125:GLN:HB2	2.07	0.54
1:A:573:MET:HA	1:A:629:VAL:HG23	1.88	0.54
1:A:976:LEU:O	1:A:980:LEU:HB2	2.07	0.54
1:B:442:LEU:O	1:B:445:ILE:HG13	2.06	0.54
1:B:492:LEU:O	1:B:496:MET:HG2	2.07	0.54
1:D:408:ASP:OD2	1:D:940:LYS:NZ	2.28	0.54
1:D:745:ASP:O	1:D:749:THR:OG1	2.22	0.54
1:E:355:MET:SD	1:E:365:THR:HA	2.47	0.54
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.89	0.54
1:E:910:ILE:O	1:E:914:LEU:HB2	2.07	0.54
1:F:776:GLU:HB2	1:F:779:TYR:CE1	2.43	0.54
1:F:960:LEU:HD21	1:F:1027:VAL:HA	1.89	0.54
1:F:982:PHE:O	1:F:985:GLY:N	2.41	0.54
1:F:1042:HIS:CG	1:F:1043:SER:H	2.24	0.54
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.90	0.54
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.08	0.54
1:E:335:ILE:O	1:E:339:GLU:HG2	2.08	0.54
1:A:702:LEU:HD12	1:A:851:LEU:HD21	1.89	0.54
1:B:588:GLN:O	1:B:592:ASN:ND2	2.40	0.54
1:C:725:PRO:HG3	1:C:811:TYR:CE1	2.43	0.54
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:945:ILE:HG12	1:D:971:ARG:CZ	2.37	0.54
1:E:175:VAL:HG23	1:F:70:ASN:HD22	1.73	0.54
1:E:448:VAL:HG13	1:E:884:VAL:HG22	1.89	0.54
1:F:420:MET:HB3	1:F:500:ILE:HB	1.88	0.54
1:F:568:ASP:OD1	1:F:637:ARG:NH1	2.31	0.54
1:A:901:VAL:HG21	1:A:943:ILE:HG13	1.88	0.54
1:B:318:PRO:HD2	1:B:321:LEU:HD22	1.88	0.54
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.89	0.54
1:D:448:VAL:HG22	1:D:887:CYS:CB	2.37	0.54
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.09	0.54
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.42	0.54
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.90	0.54
1:F:775:SER:OG	1:F:776:GLU:O	2.25	0.54
1:B:986:VAL:HG21	1:B:1007:VAL:HG11	1.89	0.54
1:C:893:GLU:HG3	1:C:893:GLU:O	2.06	0.54
1:E:121:GLU:O	1:E:125:GLN:HB2	2.08	0.54
1:F:13:TRP:CH2	1:F:370:ILE:HD13	2.42	0.54
1:F:284:GLN:HG3	1:F:285:PRO:HD2	1.90	0.54
1:F:926:TYR:HD1	1:F:1002:ALA:HB3	1.73	0.54
1:C:193:LEU:HD13	1:C:200:PRO:HD3	1.89	0.54
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.90	0.54
1:C:895:TRP:HA	1:C:895:TRP:CE3	2.42	0.54
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.72	0.54
1:A:11:PHE:CD2	1:B:890:ALA:HB1	2.43	0.54
1:A:27:ILE:HD11	1:A:380:PHE:CD1	2.43	0.54
1:B:415:ASN:OD1	1:B:434:SER:HB2	2.08	0.54
1:B:730:ASP:OD1	1:B:808:ARG:NH2	2.40	0.54
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.90	0.54
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.38	0.54
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.90	0.54
1:E:785:ASP:N	1:E:785:ASP:OD1	2.41	0.54
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.89	0.54
1:C:44:THR:OG1	1:C:91:THR:OG1	2.25	0.54
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.88	0.54
1:E:751:GLY:O	1:E:753:ALA:N	2.41	0.54
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.55	0.53
1:E:375:VAL:O	1:E:379:THR:OG1	2.24	0.53
1:E:460:GLY:O	1:E:463:THR:OG1	2.25	0.53
1:A:73:ASP:CG	1:A:106:GLN:HE22	2.12	0.53
1:B:668:LEU:H	1:B:668:LEU:CD2	2.21	0.53
1:B:705:GLU:HA	1:B:708:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:TYR:CD1	1:D:60:THR:HG21	2.44	0.53
1:D:584:GLN:N	1:D:622:GLN:HB3	2.24	0.53
1:D:699:ARG:NE	1:D:718:PRO:HB3	2.24	0.53
1:E:218:GLN:HG3	1:E:221:GLY:HA3	1.90	0.53
1:E:1040:ILE:O	1:E:1041:GLU:HG3	2.07	0.53
1:A:279:ALA:HB3	1:A:286:ALA:O	2.09	0.53
1:B:356:TYR:O	1:B:358:PHE:N	2.34	0.53
1:B:602:GLU:OE2	1:B:650:ARG:HD2	2.09	0.53
1:D:156:ASP:OD1	1:D:765:ARG:NH2	2.41	0.53
1:D:563:PHE:O	1:D:564:LEU:HD12	2.09	0.53
1:F:587:THR:HG21	1:F:622:GLN:O	2.07	0.53
1:F:686:ASP:OD1	1:F:687:GLN:N	2.41	0.53
1:A:210:GLN:HE21	1:B:733:GLN:HE21	1.56	0.53
1:C:34:GLN:O	1:C:392:THR:OG1	2.26	0.53
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.90	0.53
1:C:453:PHE:HB3	1:C:471:SER:HA	1.88	0.53
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.90	0.53
1:D:72:ILE:HD13	1:D:107:VAL:HA	1.91	0.53
1:D:419:VAL:HG13	1:D:423:GLU:OE2	2.09	0.53
1:E:262:LEU:HG	1:E:268:ILE:HD11	1.90	0.53
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.89	0.53
1:F:376:LEU:O	1:F:379:THR:N	2.41	0.53
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.43	0.53
1:D:564:LEU:HD22	1:D:671:ILE:HG12	1.90	0.53
1:E:214:VAL:HG21	1:F:747:ASN:ND2	2.23	0.53
1:F:699:ARG:HE	1:F:718:PRO:HB3	1.72	0.53
1:A:108:GLN:NE2	1:B:109:ASN:O	2.41	0.53
1:A:465:ALA:O	1:A:469:GLN:HG2	2.09	0.53
1:C:654:ALA:O	1:C:658:ILE:HG12	2.08	0.53
1:C:731:ILE:HD13	1:C:746:ILE:HD11	1.90	0.53
1:D:68:ASN:O	1:D:110:LYS:HB3	2.08	0.53
1:D:151:GLN:HG3	1:D:152:GLU:N	2.24	0.53
1:E:240:LEU:HB2	1:E:246:PHE:CE1	2.44	0.53
1:E:448:VAL:HG13	1:E:884:VAL:HG13	1.90	0.53
1:E:492:LEU:O	1:E:496:MET:HG2	2.09	0.53
1:E:606:VAL:HA	1:E:631:LEU:HD23	1.89	0.53
1:F:462:SER:HB3	1:F:865:GLN:HG2	1.91	0.53
1:A:434:SER:O	1:A:438:ILE:HG12	2.09	0.53
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.90	0.53
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.90	0.53
1:E:506:GLY:HA2	1:E:509:LYS:HD2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:555:LEU:HD11	1:E:914:LEU:HD12	1.89	0.53
1:E:578:LEU:HD13	1:E:661:ALA:HB2	1.91	0.53
1:A:448:VAL:O	1:A:451:ALA:HB3	2.08	0.53
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.29	0.53
1:B:789:TRP:O	1:B:801:PHE:HD2	1.92	0.53
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.90	0.53
1:C:882:ILE:O	1:C:886:LEU:HD22	2.08	0.53
1:E:632:LYS:O	1:E:637:ARG:NE	2.42	0.53
1:E:753:ALA:O	1:E:775:SER:HB3	2.08	0.53
1:F:396:PHE:O	1:F:400:LEU:HB2	2.09	0.53
1:A:242:SER:OG	1:A:245:GLU:HG2	2.08	0.53
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.73	0.53
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.53
1:B:396:PHE:O	1:B:400:LEU:HB2	2.08	0.53
1:C:363:ARG:HH11	1:C:363:ARG:CB	2.21	0.53
1:C:686:ASP:HB3	1:C:823:PRO:O	2.09	0.53
1:D:58:GLN:O	1:D:62:THR:HB	2.08	0.53
1:D:582:ALA:HB3	1:D:623:ASN:HB3	1.91	0.53
2:D:1101:LMT:H5B	2:D:1101:LMT:H6D	1.91	0.53
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.89	0.53
1:F:212:ALA:HA	1:F:239:ARG:HG2	1.90	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.91	0.53
1:B:169:THR:HG21	1:B:306:ILE:HG13	1.90	0.53
1:D:298:ASN:OD1	1:D:301:ASP:N	2.40	0.53
1:E:189:ASN:ND2	1:E:190:PRO:HD2	2.24	0.53
1:E:445:ILE:HG12	1:E:940:LYS:HE3	1.90	0.53
1:A:744:ASN:O	1:A:748:THR:HG23	2.09	0.52
1:A:952:LEU:O	1:A:956:GLU:HB2	2.08	0.52
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.44	0.52
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.09	0.52
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.91	0.52
1:D:587:THR:HB	1:D:613:ASN:HD21	1.74	0.52
1:E:57:VAL:HG11	1:E:86:GLY:CA	2.39	0.52
1:E:60:THR:HG22	1:E:119:PRO:HD3	1.92	0.52
1:F:137:LEU:HB2	1:F:293:LEU:HB2	1.91	0.52
1:F:143:ILE:HG22	1:F:286:ALA:HB2	1.90	0.52
1:A:26:ALA:O	1:A:30:LEU:HB2	2.09	0.52
1:B:3:ASN:HA	1:B:6:ILE:HD12	1.90	0.52
1:B:800:PRO:HG2	1:B:803:ALA:HB2	1.91	0.52
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.52
1:D:235:ILE:HD11	1:E:726:GLN:NE2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.34	0.52
1:D:775:SER:HB2	1:D:789:TRP:HZ2	1.74	0.52
1:F:753:ALA:O	1:F:775:SER:HB3	2.09	0.52
1:B:354:VAL:O	1:B:358:PHE:HB2	2.10	0.52
1:B:456:MET:O	1:B:467:TYR:HB3	2.09	0.52
1:B:457:ALA:HB2	1:B:471:SER:OG	2.10	0.52
1:B:987:MET:HA	1:B:1008:MET:HE3	1.90	0.52
1:C:937:LEU:HD13	1:C:1011:MET:CE	2.40	0.52
1:D:451:ALA:O	1:D:880:SER:OG	2.22	0.52
1:E:544:LEU:HA	1:E:547:ILE:HD12	1.90	0.52
1:F:247:GLY:O	1:F:261:LEU:HB3	2.09	0.52
1:A:401:ALA:O	1:A:405:LEU:HG	2.10	0.52
1:A:902:MET:O	1:A:905:VAL:HG23	2.09	0.52
1:C:137:LEU:HB2	1:C:293:LEU:HB2	1.91	0.52
1:C:452:VAL:O	1:C:455:PRO:HD2	2.08	0.52
1:C:916:ALA:HB2	1:C:927:PHE:CE1	2.43	0.52
1:E:447:MET:HB3	1:E:887:CYS:SG	2.49	0.52
1:E:1039:ASP:N	1:E:1040:ILE:HG13	2.24	0.52
1:F:580:ALA:HB1	1:F:724:THR:HG22	1.91	0.52
1:F:986:VAL:HG21	1:F:1007:VAL:HG11	1.90	0.52
1:A:776:GLU:HG2	1:A:777:ALA:H	1.75	0.52
1:C:940:LYS:NZ	1:C:978:THR:HG21	2.25	0.52
1:D:456:MET:HG3	1:D:471:SER:HB2	1.92	0.52
1:D:987:MET:HA	1:D:1008:MET:HE3	1.92	0.52
1:F:451:ALA:HB1	1:F:883:VAL:HG12	1.90	0.52
1:F:1015:THR:OG1	1:F:1016:VAL:N	2.43	0.52
1:A:650:ARG:O	1:A:653:ARG:HB3	2.08	0.52
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.40	0.52
1:F:187:TRP:CB	1:F:776:GLU:HG2	2.40	0.52
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.45	0.52
1:F:985:GLY:O	1:F:988:PRO:HD2	2.09	0.52
1:A:958:LYS:C	1:A:1040:ILE:HG12	2.30	0.52
1:A:971:ARG:O	1:A:974:PRO:HD2	2.10	0.52
1:B:87:THR:HG21	1:B:620:ARG:NH2	2.25	0.52
1:B:586:ARG:O	1:B:589:LYS:HB3	2.09	0.52
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.92	0.52
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.92	0.52
1:D:678:THR:HA	1:D:837:THR:OG1	2.10	0.52
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.91	0.52
1:E:80:SER:HB3	1:E:90:ILE:HG12	1.91	0.52
1:E:533:GLY:HA2	1:E:536:ARG:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:778:LYS:HG3	1:F:779:TYR:CZ	2.45	0.52
1:F:971:ARG:HH21	1:F:975:ILE:HD11	1.75	0.52
1:A:407:ASP:HB3	1:A:940:LYS:HZ3	1.74	0.52
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.44	0.52
1:C:901:VAL:HG23	1:C:942:ALA:CB	2.36	0.52
1:D:892:TYR:CD2	1:D:897:ILE:HG22	2.45	0.52
1:E:225:VAL:HG12	1:F:777:ALA:HB1	1.90	0.52
1:F:698:ALA:O	1:F:701:GLN:HB3	2.10	0.52
1:A:485:ALA:O	1:A:490:PRO:HD3	2.10	0.52
1:B:267:LYS:N	1:B:267:LYS:HD2	2.24	0.52
1:B:669:PRO:HB3	1:B:674:LEU:HD12	1.91	0.52
1:C:82:SER:HB2	1:C:816:LEU:HB2	1.92	0.52
1:E:42:ALA:HB2	1:E:93:THR:HG23	1.91	0.52
1:F:250:LEU:HD11	1:F:259:ARG:HB3	1.92	0.52
1:F:682:PHE:CE1	1:F:857:TYR:HB2	2.44	0.52
1:A:11:PHE:HE1	1:A:15:ILE:HD11	1.75	0.52
1:A:836:SER:HB3	1:A:839:GLU:HG3	1.92	0.52
1:A:841:MET:HG2	1:A:859:TRP:CH2	2.45	0.52
1:E:59:ASP:OD1	1:E:63:GLN:NE2	2.43	0.52
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.92	0.52
1:A:216:ALA:HB2	1:A:236:ALA:HB2	1.92	0.51
1:A:711:ASP:O	1:A:835:LYS:NZ	2.36	0.51
1:A:1020:PHE:CZ	2:A:1101:LMT:H32	2.46	0.51
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.92	0.51
1:C:336:SER:O	1:C:340:VAL:HG23	2.09	0.51
1:D:332:PHE:O	1:D:336:SER:HB3	2.10	0.51
1:E:184:MET:HB2	1:E:762:PHE:CE2	2.46	0.51
1:E:339:GLU:OE1	1:E:342:LYS:HD3	2.11	0.51
1:E:1038:GLU:OE1	1:E:1040:ILE:HG12	2.10	0.51
1:F:521:GLU:O	1:F:524:THR:HG23	2.10	0.51
1:F:841:MET:HG2	1:F:859:TRP:CH2	2.45	0.51
2:A:1101:LMT:H6D	2:A:1101:LMT:O5B	2.09	0.51
1:B:82:SER:HA	1:B:88:VAL:HG22	1.92	0.51
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.92	0.51
1:C:247:GLY:O	1:C:261:LEU:HB3	2.11	0.51
1:C:940:LYS:HE2	1:C:941:ASN:OD1	2.10	0.51
1:D:163:LYS:HD2	1:D:289:LEU:HD21	1.91	0.51
1:D:362:PHE:HE2	1:D:363:ARG:HH21	1.59	0.51
1:D:775:SER:OG	1:D:780:ARG:HG2	2.10	0.51
1:D:971:ARG:O	1:D:975:ILE:HG12	2.11	0.51
1:E:527:TYR:CE2	1:E:972:LEU:HG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:897:ILE:N	1:E:898:PRO:HD2	2.25	0.51
1:F:83:ASP:HB2	1:F:87:THR:O	2.10	0.51
1:F:754:TRP:CH2	1:F:780:ARG:HA	2.45	0.51
1:F:760:ASN:O	1:F:771:VAL:HB	2.11	0.51
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.92	0.51
1:C:1038:GLU:HA	1:C:1039:ASP:CB	2.40	0.51
1:D:143:ILE:HG22	1:D:286:ALA:HB2	1.93	0.51
1:D:637:ARG:HB3	1:D:642:ASN:HB3	1.92	0.51
1:D:776:GLU:HB3	1:D:779:TYR:CD1	2.45	0.51
1:F:733:GLN:NE2	1:F:743:ILE:HG21	2.22	0.51
1:A:3:ASN:O	1:A:6:ILE:HG12	2.10	0.51
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.45	0.51
1:A:790:TYR:HB3	1:A:798:MET:HB3	1.92	0.51
1:D:182:TYR:HD2	1:D:765:ARG:HH22	1.59	0.51
1:D:586:ARG:O	1:D:590:VAL:HG23	2.11	0.51
1:F:340:VAL:HG22	1:F:396:PHE:CE2	2.46	0.51
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.93	0.51
1:A:992:SER:OG	1:A:1000:GLN:OE1	2.26	0.51
1:B:61:VAL:HG22	1:B:118:LEU:HD22	1.91	0.51
1:C:739:LEU:HD13	1:C:799:VAL:HG11	1.92	0.51
1:C:751:GLY:O	1:C:753:ALA:N	2.43	0.51
1:D:212:ALA:HA	1:D:239:ARG:HD3	1.92	0.51
1:D:690:LEU:HD21	1:D:853:THR:O	2.09	0.51
1:E:441:ALA:O	1:E:445:ILE:HG23	2.10	0.51
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.93	0.51
1:F:431:THR:HG21	1:F:490:PRO:O	2.11	0.51
1:F:650:ARG:O	1:F:653:ARG:HB3	2.10	0.51
1:A:905:VAL:HG13	1:A:935:ILE:HD13	1.93	0.51
1:B:415:ASN:O	1:B:419:VAL:HG23	2.10	0.51
1:B:654:ALA:O	1:B:658:ILE:HG12	2.11	0.51
1:C:686:ASP:OD2	1:C:823:PRO:HD2	2.11	0.51
1:D:728:LYS:HA	1:F:235:ILE:HB	1.92	0.51
1:E:102:ILE:O	1:E:106:GLN:HG3	2.10	0.51
1:E:139:VAL:O	1:E:326:PRO:HD2	2.10	0.51
1:E:904:VAL:HG21	1:E:942:ALA:CB	2.40	0.51
1:F:261:LEU:N	1:F:264:ASP:OD2	2.43	0.51
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.40	0.51
1:F:524:THR:O	1:F:528:THR:HG22	2.11	0.51
1:F:937:LEU:HD11	1:F:982:PHE:HE2	1.76	0.51
1:F:944:LEU:HD13	1:F:975:ILE:HG12	1.91	0.51
1:A:612:VAL:HG12	1:A:615:PHE:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:PHE:CE1	1:A:899:PHE:CE2	2.98	0.51
1:C:979:SER:HA	1:C:1011:MET:HE3	1.93	0.51
1:D:169:THR:HG21	1:D:306:ILE:HG13	1.92	0.51
1:E:184:MET:HG2	1:E:246:PHE:CD2	2.46	0.51
1:E:597:TYR:CD2	1:E:655:PHE:HZ	2.29	0.51
1:A:113:LEU:HD11	1:C:128:SER:HB3	1.93	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HB3	1.93	0.51
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.91	0.51
1:A:459:PHE:CE2	1:A:876:LEU:HD12	2.45	0.51
1:C:693:GLU:HB3	1:C:694:LYS:HE2	1.93	0.51
1:D:800:PRO:HG2	1:D:803:ALA:HB2	1.93	0.51
1:A:213:GLN:HA	1:A:237:GLN:O	2.11	0.51
1:C:396:PHE:O	1:C:400:LEU:HB2	2.11	0.51
1:C:400:LEU:O	1:C:404:LEU:HD13	2.10	0.51
1:D:328:ASP:O	1:D:331:PRO:HD2	2.11	0.51
1:D:728:LYS:HG2	1:D:808:ARG:CZ	2.41	0.51
1:D:953:MET:SD	1:D:960:LEU:HA	2.51	0.51
1:E:165:ALA:HA	1:E:168:ARG:HB2	1.93	0.51
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.91	0.51
1:E:643:LYS:NZ	1:E:993:THR:HG23	2.26	0.51
1:F:63:GLN:OE1	1:F:818:ARG:NH2	2.44	0.51
1:A:971:ARG:CZ	1:A:971:ARG:HB3	2.41	0.51
1:B:3:ASN:O	1:B:6:ILE:HB	2.11	0.51
1:B:254:ASN:HB2	1:B:258:SER:O	2.11	0.51
1:C:156:ASP:OD2	1:C:769:LYS:NZ	2.41	0.51
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.93	0.51
1:E:58:GLN:HE21	1:E:816:LEU:HD13	1.76	0.51
1:F:23:GLY:O	1:F:27:ILE:HG23	2.11	0.51
1:F:404:LEU:HG	1:F:449:LEU:HD13	1.92	0.51
1:A:151:GLN:HE22	1:A:278:ILE:HG22	1.76	0.50
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.41	0.50
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.76	0.50
1:C:531:VAL:O	1:C:534:ILE:HG13	2.11	0.50
1:D:23:GLY:O	1:D:27:ILE:HB	2.11	0.50
1:D:58:GLN:O	1:D:63:GLN:HG3	2.12	0.50
1:D:336:SER:O	1:D:340:VAL:HG23	2.11	0.50
1:D:544:LEU:O	1:D:547:ILE:HB	2.11	0.50
1:F:380:PHE:HD2	1:F:383:LEU:HD12	1.75	0.50
1:F:901:VAL:HG23	1:F:942:ALA:CB	2.37	0.50
1:B:5:PHE:HE2	1:B:11:PHE:CD2	2.29	0.50
1:C:222:THR:HA	1:C:224:PRO:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:GLU:HG3	1:C:605:ASN:HD22	1.77	0.50
1:D:112:GLN:HG3	1:E:112:GLN:OE1	2.10	0.50
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.46	0.50
1:D:602:GLU:HB3	1:D:606:VAL:HG23	1.93	0.50
1:D:730:ASP:HB2	1:D:808:ARG:NH2	2.26	0.50
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.92	0.50
1:E:696:THR:HG23	1:E:699:ARG:HH12	1.75	0.50
1:A:151:GLN:HG3	1:A:152:GLU:N	2.27	0.50
1:C:343:THR:HG21	1:C:989:LEU:HD21	1.92	0.50
1:E:357:LEU:O	1:E:358:PHE:HD1	1.94	0.50
1:F:694:LYS:H	1:F:694:LYS:HD2	1.77	0.50
1:F:898:PRO:O	1:F:902:MET:HG2	2.10	0.50
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.92	0.50
1:C:578:LEU:HD12	1:C:582:ALA:HB1	1.92	0.50
1:C:934:THR:O	1:C:938:SER:OG	2.28	0.50
1:D:971:ARG:C	1:D:974:PRO:HD2	2.32	0.50
1:E:6:ILE:HD11	1:E:431:THR:HG22	1.92	0.50
1:E:82:SER:HB2	1:E:816:LEU:HB2	1.94	0.50
1:E:442:LEU:O	1:E:445:ILE:HG13	2.11	0.50
1:E:901:VAL:HG23	1:E:942:ALA:CB	2.42	0.50
1:F:310:LEU:O	1:F:314:GLU:HG3	2.12	0.50
1:F:428:LYS:O	1:F:432:ARG:HG3	2.11	0.50
1:F:923:ASN:O	1:F:923:ASN:ND2	2.36	0.50
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.93	0.50
1:A:293:LEU:HD22	1:A:294:ALA:H	1.76	0.50
1:A:360:GLN:HE22	1:A:513:PHE:HB3	1.76	0.50
1:D:379:THR:HG21	1:D:477:ALA:HB2	1.93	0.50
1:E:216:ALA:HB1	1:E:234:ILE:HG22	1.92	0.50
1:A:572:PHE:HB2	1:A:666:PHE:O	2.11	0.50
1:A:971:ARG:O	1:A:975:ILE:HG12	2.11	0.50
1:B:210:GLN:HG2	1:C:733:GLN:NE2	2.27	0.50
1:B:588:GLN:HG3	1:B:592:ASN:HD21	1.76	0.50
1:C:952:LEU:HD23	1:C:956:GLU:HG3	1.93	0.50
1:D:400:LEU:HD21	1:D:930:GLY:HA2	1.93	0.50
1:D:915:ALA:HB2	1:D:1009:GLY:HA3	1.93	0.50
1:E:46:SER:OG	1:E:89:GLN:HG2	2.11	0.50
1:E:222:THR:HA	1:E:224:PRO:HD3	1.93	0.50
1:E:340:VAL:HG22	1:E:396:PHE:CE2	2.47	0.50
1:E:379:THR:HA	1:E:480:LEU:HD12	1.94	0.50
1:A:734:GLU:HG2	1:C:250:LEU:HD22	1.93	0.50
1:A:907:LEU:HD21	1:A:1021:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.92	0.50
1:B:177:LEU:HD23	1:B:178:PHE:N	2.26	0.50
1:B:401:ALA:O	1:B:405:LEU:HG	2.11	0.50
1:B:894:SER:HB3	1:B:898:PRO:HD3	1.92	0.50
1:C:634:TRP:CD1	1:C:634:TRP:N	2.72	0.50
1:E:177:LEU:HG	1:E:289:LEU:HD21	1.93	0.50
1:E:396:PHE:O	1:E:400:LEU:HB2	2.12	0.50
1:E:564:LEU:HD13	1:E:674:LEU:HD21	1.94	0.50
1:E:892:TYR:O	1:E:893:GLU:HB2	2.11	0.50
1:F:66:GLU:OE1	1:F:821:GLY:HA2	2.11	0.50
1:F:431:THR:HG22	1:F:435:MET:CE	2.41	0.50
1:F:445:ILE:HG12	1:F:940:LYS:HG3	1.94	0.50
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.27	0.50
1:A:197:GLN:HA	1:A:798:MET:SD	2.52	0.50
1:C:658:ILE:O	1:C:659:LYS:NZ	2.37	0.50
1:D:609:VAL:HG22	1:D:629:VAL:HG13	1.94	0.50
1:D:909:VAL:HG22	1:D:931:LEU:HD21	1.94	0.50
1:E:184:MET:HG2	1:E:246:PHE:CE2	2.46	0.50
1:F:69:MET:SD	1:F:72:ILE:HD11	2.52	0.50
1:F:189:ASN:OD1	1:F:190:PRO:HD2	2.12	0.50
1:F:527:TYR:O	1:F:531:VAL:HG23	2.11	0.50
1:F:590:VAL:O	1:F:593:GLU:HB2	2.11	0.50
1:F:723:ASP:HA	1:F:813:SER:HA	1.94	0.50
1:F:746:ILE:HG13	1:F:747:ASN:N	2.26	0.50
1:A:140:VAL:HG11	1:A:310:LEU:HD21	1.93	0.50
1:A:350:LEU:HD13	1:A:985:GLY:HA2	1.93	0.50
1:C:27:ILE:HG13	1:C:28:LEU:N	2.27	0.50
1:C:144:ASN:O	1:C:148:THR:HG23	2.11	0.50
1:C:612:VAL:HG12	1:C:615:PHE:HB3	1.94	0.50
1:C:946:VAL:HG13	1:C:1026:PHE:CE1	2.47	0.50
1:D:222:THR:HA	1:D:224:PRO:HD3	1.93	0.50
1:D:668:LEU:H	1:D:668:LEU:HD23	1.77	0.50
1:E:580:ALA:HB1	1:E:724:THR:HG22	1.92	0.50
1:F:121:GLU:O	1:F:124:GLN:HG2	2.11	0.50
1:F:413:VAL:O	1:F:417:GLU:HG2	2.12	0.50
1:F:485:ALA:O	1:F:490:PRO:HD3	2.11	0.50
1:F:764:ASP:OD2	1:F:765:ARG:NH2	2.45	0.50
1:A:352:PHE:HD1	1:A:369:THR:HG21	1.77	0.49
1:B:249:ILE:HG12	1:B:262:LEU:HB2	1.94	0.49
1:B:527:TYR:O	1:B:531:VAL:HG23	2.12	0.49
1:B:871:ASN:OD1	1:B:871:ASN:N	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:987:MET:HB3	1:B:988:PRO:HD3	1.93	0.49
1:C:379:THR:HG23	1:C:476:SER:OG	2.11	0.49
1:D:415:ASN:HB3	1:D:434:SER:HB2	1.94	0.49
1:D:778:LYS:HG3	1:D:779:TYR:CE2	2.47	0.49
1:E:58:GLN:OE1	1:E:818:ARG:NH1	2.45	0.49
1:E:440:GLY:C	1:E:891:LEU:HD11	2.32	0.49
1:E:602:GLU:HG3	1:E:605:ASN:HB2	1.94	0.49
1:F:64:VAL:HG12	1:F:114:ALA:HB1	1.93	0.49
1:F:332:PHE:HD1	1:F:634:TRP:CH2	2.30	0.49
1:F:587:THR:OG1	1:F:588:GLN:N	2.45	0.49
1:A:577:GLN:O	1:A:661:ALA:HB1	2.12	0.49
1:A:887:CYS:O	1:A:890:ALA:HB3	2.12	0.49
1:A:915:ALA:HB2	1:A:1009:GLY:HA3	1.94	0.49
1:C:817:GLU:HB2	1:C:824:SER:O	2.12	0.49
1:D:267:LYS:HD2	1:D:776:GLU:CD	2.33	0.49
1:D:957:GLY:O	1:D:1040:ILE:HG21	2.11	0.49
1:E:358:PHE:CD2	1:E:977:MET:HG3	2.47	0.49
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.94	0.49
1:E:671:ILE:HB	1:E:674:LEU:HG	1.94	0.49
1:F:426:PRO:O	1:F:430:ALA:N	2.42	0.49
1:F:457:ALA:HB1	1:F:468:ARG:HG3	1.94	0.49
1:A:444:GLY:O	1:A:448:VAL:HG23	2.12	0.49
1:B:354:VAL:HG21	1:B:980:LEU:HB3	1.93	0.49
1:B:478:MET:O	1:B:482:VAL:HG12	2.12	0.49
1:B:563:PHE:O	1:B:564:LEU:HD12	2.11	0.49
1:E:339:GLU:O	1:E:342:LYS:HB3	2.13	0.49
1:E:415:ASN:HD22	1:E:434:SER:CB	2.17	0.49
1:E:583:THR:H	1:E:586:ARG:HG3	1.77	0.49
1:F:352:PHE:HA	1:F:355:MET:CE	2.39	0.49
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.47	0.49
1:B:525:HIS:HA	1:B:528:THR:HG22	1.93	0.49
1:B:877:TYR:HA	1:B:880:SER:HB2	1.93	0.49
1:B:1020:PHE:HZ	2:B:1101:LMT:H62	1.76	0.49
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.94	0.49
1:D:445:ILE:HG12	1:D:940:LYS:HE3	1.94	0.49
1:F:184:MET:HB3	1:F:771:VAL:HG13	1.95	0.49
1:F:904:VAL:O	1:F:907:LEU:N	2.45	0.49
1:A:177:LEU:HD23	1:A:288:GLY:O	2.13	0.49
1:A:501:ALA:O	1:A:504:ASP:HB2	2.13	0.49
1:B:671:ILE:O	1:B:673:GLU:N	2.40	0.49
1:C:455:PRO:HG2	1:C:880:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:600:THR:O	1:C:603:LYS:HG3	2.11	0.49
1:D:5:PHE:HE2	1:D:11:PHE:HD1	1.59	0.49
1:D:175:VAL:HG12	1:D:289:LEU:HD22	1.94	0.49
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.92	0.49
1:D:575:MET:HA	1:D:626:ILE:HD12	1.93	0.49
1:D:626:ILE:HG13	1:D:627:ALA:N	2.28	0.49
1:D:678:THR:HB	1:D:831:ALA:HB3	1.95	0.49
1:E:162:MET:HA	1:E:313:MET:CE	2.43	0.49
1:F:937:LEU:HD22	1:F:1011:MET:HE2	1.94	0.49
1:B:559:LEU:HD12	1:B:923:ASN:HB2	1.95	0.49
1:C:201:VAL:O	1:C:204:ILE:HB	2.13	0.49
1:C:668:LEU:HB2	1:C:669:PRO:HD2	1.93	0.49
1:D:449:LEU:HB3	1:D:478:MET:SD	2.53	0.49
1:D:459:PHE:CB	1:D:464:GLY:HA2	2.43	0.49
1:D:1034:SER:OG	1:D:1035:ARG:N	2.46	0.49
1:E:46:SER:HA	1:E:88:VAL:O	2.13	0.49
1:E:154:ILE:CG2	1:E:287:SER:HB3	2.42	0.49
1:F:587:THR:HG21	1:F:623:ASN:HA	1.94	0.49
1:F:923:ASN:HD22	1:F:923:ASN:C	2.14	0.49
1:A:544:LEU:O	1:A:548:ILE:HG13	2.13	0.49
1:B:87:THR:HG21	1:B:620:ARG:HH22	1.78	0.49
1:B:405:LEU:HD22	1:B:481:SER:HB3	1.93	0.49
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.95	0.49
1:A:800:PRO:HG2	1:A:803:ALA:HB2	1.94	0.49
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.94	0.49
1:D:520:PHE:O	1:D:524:THR:HG23	2.13	0.49
1:F:65:ILE:HD11	1:F:118:LEU:HD11	1.95	0.49
1:F:623:ASN:N	1:F:623:ASN:OD1	2.45	0.49
1:A:442:LEU:O	1:A:445:ILE:HG13	2.12	0.49
1:A:831:ALA:HB2	1:A:840:ALA:HB2	1.93	0.49
1:A:900:SER:HB3	1:A:1029:VAL:HG21	1.93	0.49
1:B:577:GLN:O	1:B:661:ALA:HB1	2.13	0.49
1:C:150:THR:HG23	1:C:153:ASP:OD1	2.12	0.49
1:C:405:LEU:HD12	1:C:406:VAL:N	2.27	0.49
1:C:544:LEU:O	1:C:547:ILE:HB	2.13	0.49
1:C:578:LEU:CG	1:C:587:THR:HG22	2.39	0.49
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.95	0.49
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.95	0.49
1:E:177:LEU:HA	1:E:289:LEU:HD23	1.95	0.49
1:E:362:PHE:HA	1:E:365:THR:HG22	1.94	0.49
1:F:415:ASN:OD1	1:F:434:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:GLU:OE1	1:C:996:GLY:HA2	2.12	0.49
1:C:623:ASN:N	1:C:623:ASN:OD1	2.46	0.49
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.95	0.49
1:D:108:GLN:NE2	1:E:109:ASN:O	2.46	0.49
1:E:530:SER:OG	2:E:1101:LMT:H1'	2.12	0.49
1:E:717:ARG:HD2	1:E:828:LEU:HB2	1.94	0.49
1:F:507:GLU:HG2	1:F:518:ARG:HG3	1.94	0.49
1:F:983:ILE:HG23	1:F:1008:MET:HE2	1.95	0.49
1:B:463:THR:HG22	1:B:563:PHE:HE2	1.78	0.48
1:B:516:PHE:O	1:B:520:PHE:N	2.37	0.48
1:C:343:THR:HG21	1:C:989:LEU:CD2	2.43	0.48
1:C:742:SER:O	1:C:746:ILE:HG23	2.13	0.48
1:D:455:PRO:HG2	1:D:880:SER:OG	2.13	0.48
1:D:527:TYR:O	1:D:531:VAL:HG23	2.13	0.48
1:F:427:PRO:O	1:F:431:THR:OG1	2.26	0.48
1:F:451:ALA:O	1:F:883:VAL:HG11	2.13	0.48
1:A:583:THR:H	1:A:586:ARG:HG3	1.78	0.48
1:B:251:LEU:HD21	1:B:262:LEU:HB2	1.95	0.48
1:C:332:PHE:O	1:C:336:SER:HB3	2.13	0.48
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.94	0.48
1:D:452:VAL:HA	1:D:880:SER:OG	2.12	0.48
1:D:532:GLY:O	1:D:536:ARG:HG3	2.13	0.48
1:D:744:ASN:O	1:D:748:THR:HG23	2.12	0.48
1:F:80:SER:OG	1:F:818:ARG:HB2	2.13	0.48
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.28	0.48
1:B:166:ILE:HD12	1:B:309:GLU:HG3	1.95	0.48
1:C:13:TRP:HH2	1:C:370:ILE:HD13	1.78	0.48
1:E:327:TYR:C	1:E:327:TYR:CD2	2.87	0.48
1:E:602:GLU:OE2	1:E:650:ARG:NH1	2.46	0.48
1:F:562:SER:HB2	1:F:924:ASP:HB3	1.95	0.48
1:A:391:ASN:O	1:A:395:MET:HG2	2.12	0.48
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.94	0.48
1:A:1037:ASN:CA	1:A:1038:GLU:HB2	2.43	0.48
1:B:427:PRO:CD	1:B:499:PRO:HB3	2.41	0.48
1:C:590:VAL:HA	1:C:593:GLU:OE1	2.14	0.48
1:D:889:ALA:HA	1:D:894:SER:O	2.14	0.48
1:E:324:VAL:O	1:E:326:PRO:HD3	2.14	0.48
1:E:399:VAL:O	1:E:402:ILE:HG13	2.13	0.48
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.48	0.48
1:A:79:SER:HA	1:A:818:ARG:O	2.14	0.48
1:A:138:MET:O	1:A:291:ILE:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:HA	1:A:931:LEU:HD21	1.95	0.48
1:B:121:GLU:O	1:B:125:GLN:HB2	2.14	0.48
1:B:371:ALA:O	1:B:375:VAL:HG23	2.13	0.48
1:E:36:PRO:HG3	1:E:469:GLN:HG3	1.95	0.48
1:F:363:ARG:HH11	1:F:363:ARG:CG	2.26	0.48
1:B:383:LEU:HD11	1:B:473:THR:HG23	1.96	0.48
1:B:682:PHE:HB3	1:B:827:ILE:O	2.14	0.48
1:B:1020:PHE:CZ	2:B:1101:LMT:H62	2.48	0.48
1:D:838:GLY:O	1:D:841:MET:HB2	2.14	0.48
1:E:520:PHE:O	1:E:524:THR:HG23	2.13	0.48
1:E:832:ALA:HB3	1:E:835:LYS:HD2	1.95	0.48
1:F:343:THR:HG21	1:F:989:LEU:CD2	2.39	0.48
1:F:375:VAL:O	1:F:379:THR:OG1	2.15	0.48
1:F:776:GLU:HB2	1:F:779:TYR:HE1	1.78	0.48
1:A:593:GLU:OE2	1:A:659:LYS:NZ	2.36	0.48
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.34	0.48
1:B:327:TYR:CD1	1:B:571:VAL:HG11	2.48	0.48
1:F:11:PHE:CE2	1:F:15:ILE:HD11	2.49	0.48
1:F:120:GLN:HG3	1:F:123:GLN:CD	2.34	0.48
1:F:133:SER:O	1:F:134:SER:HB2	2.14	0.48
1:F:340:VAL:HG11	1:F:395:MET:CB	2.43	0.48
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.96	0.48
1:A:58:GLN:O	1:A:63:GLN:HG3	2.13	0.48
1:A:108:GLN:O	1:A:112:GLN:HG2	2.14	0.48
1:A:326:PRO:HA	1:A:630:SER:HG	1.78	0.48
1:B:327:TYR:HD1	1:B:571:VAL:HG11	1.79	0.48
1:C:443:VAL:HG11	1:C:891:LEU:HD11	1.95	0.48
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.49	0.48
1:D:901:VAL:HG21	1:D:943:ILE:HG13	1.95	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.14	0.48
1:F:242:SER:HB2	1:F:244:GLU:HB3	1.95	0.48
1:F:412:VAL:HA	1:F:438:ILE:CD1	2.43	0.48
1:A:421:ALA:HB1	1:A:505:HIS:HE1	1.78	0.48
1:A:979:SER:CB	1:A:1015:THR:HG21	2.44	0.48
1:B:717:ARG:CD	1:B:828:LEU:HB2	2.44	0.48
1:B:960:LEU:HD13	1:B:1030:ARG:HG2	1.96	0.48
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.96	0.48
1:D:193:LEU:HD13	1:D:200:PRO:HD3	1.96	0.48
1:D:293:LEU:HD11	1:D:299:ALA:HA	1.94	0.48
1:D:960:LEU:O	1:D:964:THR:HG23	2.13	0.48
1:E:351:VAL:HG21	1:E:406:VAL:HG22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:676:THR:O	1:E:679:GLY:N	2.47	0.48
1:E:699:ARG:HE	1:E:718:PRO:CG	2.24	0.48
1:E:903:LEU:O	1:E:906:PRO:HD2	2.13	0.48
1:F:949:ALA:HB3	1:F:1026:PHE:CE2	2.49	0.48
1:A:16:ALA:O	1:A:20:MET:HG3	2.14	0.48
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.95	0.48
1:A:435:MET:HE3	1:A:439:GLN:HB2	1.95	0.48
1:B:904:VAL:HG21	1:B:942:ALA:CB	2.43	0.48
1:D:27:ILE:HD11	1:D:380:PHE:CE1	2.48	0.48
1:D:705:GLU:HB3	1:D:847:LEU:HD22	1.96	0.48
1:D:719:ASN:HB3	1:D:826:GLU:HG2	1.95	0.48
1:E:327:TYR:C	1:E:327:TYR:HD2	2.16	0.48
1:E:680:PHE:HB2	1:E:863:SER:HG	1.77	0.48
1:F:383:LEU:HD23	1:F:472:ILE:HD13	1.96	0.48
1:C:66:GLU:OE1	1:C:821:GLY:HA2	2.14	0.47
1:C:527:TYR:O	1:C:531:VAL:HG23	2.14	0.47
1:D:740:GLY:O	1:D:794:ALA:N	2.40	0.47
1:D:985:GLY:O	1:D:988:PRO:HD2	2.14	0.47
1:A:63:GLN:O	1:A:67:GLN:HG3	2.15	0.47
1:A:152:GLU:HB2	1:A:182:TYR:HE1	1.79	0.47
1:A:425:LEU:HB3	1:A:429:GLU:HB2	1.96	0.47
1:A:757:SER:O	1:A:772:TYR:HA	2.14	0.47
1:A:979:SER:HB2	1:A:1015:THR:HG21	1.96	0.47
1:A:1021:PHE:HB3	1:A:1025:PHE:CE1	2.48	0.47
1:B:743:ILE:HD12	1:B:743:ILE:H	1.78	0.47
1:C:690:LEU:HD11	1:C:854:GLY:O	2.14	0.47
1:D:391:ASN:O	1:D:395:MET:HG2	2.14	0.47
1:E:440:GLY:O	1:E:891:LEU:HD11	2.15	0.47
1:E:776:GLU:HG2	1:E:777:ALA:N	2.29	0.47
1:F:350:LEU:HD23	1:F:984:LEU:HB3	1.96	0.47
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.49	0.47
1:A:681:ASP:HB2	1:A:862:MET:HE3	1.96	0.47
1:B:717:ARG:HE	1:B:828:LEU:HB2	1.78	0.47
1:C:39:ALA:HA	1:C:40:PRO:HD2	1.67	0.47
1:D:34:GLN:HB2	1:D:333:VAL:HG22	1.94	0.47
1:E:281:PHE:CE1	1:E:608:SER:HB2	2.49	0.47
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.97	0.47
1:F:746:ILE:HG13	1:F:747:ASN:H	1.78	0.47
1:A:960:LEU:O	1:A:964:THR:HG23	2.15	0.47
1:B:225:VAL:HG13	1:C:781:MET:SD	2.54	0.47
1:B:678:THR:HA	1:B:837:THR:OG1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:TYR:O	1:B:881:LEU:HG	2.13	0.47
1:D:455:PRO:HG2	1:D:880:SER:CB	2.44	0.47
1:E:572:PHE:CD1	1:E:648:THR:HG22	2.49	0.47
1:E:992:SER:O	1:E:997:SER:HB2	2.14	0.47
1:E:1037:ASN:HB2	1:E:1038:GLU:O	2.15	0.47
1:F:202:ASP:OD1	1:F:792:ARG:NH2	2.47	0.47
1:F:368:PRO:O	1:F:371:ALA:HB3	2.13	0.47
1:F:885:PHE:HE1	1:F:899:PHE:CE2	2.32	0.47
1:A:67:GLN:NE2	1:C:768:VAL:HG13	2.29	0.47
1:B:32:VAL:HG22	1:B:298:ASN:ND2	2.29	0.47
1:C:146:ASP:O	1:C:148:THR:N	2.47	0.47
1:D:343:THR:O	1:D:346:GLU:N	2.47	0.47
1:D:634:TRP:CD1	1:D:634:TRP:N	2.82	0.47
1:E:61:VAL:HG21	1:E:122:VAL:HG21	1.96	0.47
1:E:246:PHE:HA	1:E:249:ILE:HG23	1.97	0.47
1:F:361:ASN:HB3	1:F:364:ALA:HB3	1.95	0.47
1:F:405:LEU:HD12	1:F:406:VAL:N	2.29	0.47
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.95	0.47
1:A:535:LEU:HD23	1:A:535:LEU:HA	1.65	0.47
1:A:637:ARG:HB3	1:A:642:ASN:HB3	1.96	0.47
1:A:937:LEU:O	1:A:940:LYS:HB3	2.15	0.47
1:B:574:THR:HA	1:B:665:ALA:HA	1.96	0.47
1:B:685:ILE:HD11	1:B:819:TYR:CD2	2.49	0.47
1:D:610:PHE:HB3	1:D:628:PHE:HB2	1.97	0.47
1:E:61:VAL:HA	1:E:118:LEU:HD22	1.97	0.47
1:E:158:VAL:HB	1:E:177:LEU:HD11	1.96	0.47
1:F:345:VAL:O	1:F:348:ILE:HB	2.14	0.47
1:A:220:GLY:HA3	1:A:230:LEU:O	2.14	0.47
1:A:641:GLU:HA	1:A:646:ALA:HB3	1.96	0.47
1:A:671:ILE:HG21	1:A:674:LEU:HB3	1.95	0.47
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.80	0.47
1:B:164:ASP:OD2	1:C:67:GLN:HG2	2.15	0.47
1:B:501:ALA:O	1:B:504:ASP:HB2	2.15	0.47
1:B:645:GLU:O	1:B:649:MET:HB2	2.15	0.47
1:C:133:SER:OG	1:C:293:LEU:O	2.31	0.47
1:C:139:VAL:HA	1:C:289:LEU:O	2.14	0.47
1:C:375:VAL:HA	1:C:480:LEU:HD13	1.96	0.47
1:C:383:LEU:HD23	1:C:472:ILE:HD12	1.97	0.47
1:C:778:LYS:HG3	1:C:779:TYR:CZ	2.50	0.47
1:D:191:ASN:O	1:D:194:ASN:N	2.48	0.47
1:D:559:LEU:CD2	1:D:922:THR:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.96	0.47
1:E:238:THR:HG22	1:E:239:ARG:O	2.13	0.47
1:E:525:HIS:HA	1:E:528:THR:CG2	2.44	0.47
1:E:538:THR:HG22	1:E:1024:VAL:HG13	1.97	0.47
1:E:987:MET:HB3	1:E:988:PRO:HD3	1.96	0.47
1:F:253:VAL:HG13	1:F:259:ARG:HG2	1.96	0.47
1:F:588:GLN:O	1:F:592:ASN:ND2	2.48	0.47
1:A:44:THR:HA	1:A:90:ILE:O	2.13	0.47
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.63	0.47
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.35	0.47
1:A:514:GLY:HA2	1:A:517:ASN:ND2	2.29	0.47
1:B:273:GLU:CD	1:B:770:LYS:HD2	2.35	0.47
1:C:30:LEU:HD23	1:C:390:ILE:HD11	1.97	0.47
1:C:831:ALA:HB3	1:C:835:LYS:HG2	1.97	0.47
1:D:21:LEU:HD13	1:D:21:LEU:HA	1.63	0.47
1:D:183:ALA:HB2	1:D:273:GLU:HG3	1.97	0.47
1:D:196:PHE:HB3	1:D:252:LYS:HZ1	1.77	0.47
1:D:573:MET:HG3	1:D:666:PHE:HE2	1.80	0.47
1:D:888:LEU:HD11	1:D:901:VAL:HG22	1.96	0.47
1:E:621:GLY:O	1:E:624:THR:HG22	2.14	0.47
1:F:453:PHE:HE1	1:F:474:ILE:HG21	1.80	0.47
1:A:69:MET:SD	1:A:72:ILE:HD11	2.55	0.47
1:A:75:LEU:HD23	1:C:168:ARG:HD3	1.97	0.47
1:A:578:LEU:CD2	1:A:590:VAL:HG21	2.40	0.47
1:B:231:ASN:HB2	1:C:583:THR:HG22	1.97	0.47
1:B:725:PRO:HA	1:B:810:GLU:O	2.15	0.47
1:B:795:ASP:OD2	1:B:797:GLN:HG2	2.15	0.47
1:B:888:LEU:HA	1:B:888:LEU:HD23	1.65	0.47
1:D:121:GLU:O	1:D:124:GLN:HG2	2.15	0.47
1:D:538:THR:HG21	1:D:1028:VAL:HG22	1.97	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:CB	2.45	0.47
1:D:907:LEU:HD21	1:D:1021:PHE:HB2	1.96	0.47
1:E:371:ALA:O	1:E:375:VAL:HG23	2.15	0.47
1:E:751:GLY:O	1:E:754:TRP:N	2.48	0.47
1:E:888:LEU:HA	1:E:888:LEU:HD23	1.49	0.47
1:A:613:ASN:OD1	1:A:614:GLY:N	2.48	0.47
1:A:793:ALA:HB3	1:A:795:ASP:OD2	2.14	0.47
1:C:457:ALA:HB2	1:C:471:SER:OG	2.15	0.47
1:C:895:TRP:HA	1:C:895:TRP:HE3	1.78	0.47
1:D:888:LEU:HD12	1:D:902:MET:HG3	1.97	0.47
1:D:948:PHE:O	1:D:952:LEU:HG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:732:ASP:OD1	1:E:735:LYS:HG3	2.14	0.47
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.97	0.47
1:F:382:VAL:HG11	1:F:476:SER:CB	2.45	0.47
1:F:736:ALA:O	1:F:741:VAL:HG23	2.15	0.47
1:A:146:ASP:OD2	1:A:146:ASP:N	2.29	0.46
1:A:169:THR:HG22	1:A:172:VAL:HG23	1.97	0.46
1:A:563:PHE:CD2	1:A:671:ILE:HD11	2.50	0.46
1:B:399:VAL:O	1:B:402:ILE:HG13	2.15	0.46
1:B:404:LEU:HD21	1:B:449:LEU:HD22	1.97	0.46
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.96	0.46
1:C:504:ASP:C	1:C:506:GLY:H	2.18	0.46
1:C:641:GLU:HA	1:C:646:ALA:HB3	1.96	0.46
1:E:249:ILE:CG1	1:E:262:LEU:HB2	2.45	0.46
1:E:568:ASP:O	1:E:634:TRP:HZ3	1.98	0.46
1:E:841:MET:O	1:E:845:GLU:HG3	2.14	0.46
1:F:602:GLU:OE2	1:F:650:ARG:HD2	2.16	0.46
1:F:682:PHE:HE1	1:F:857:TYR:HB2	1.80	0.46
1:A:648:THR:HB	1:A:665:ALA:O	2.15	0.46
1:B:42:ALA:HB3	1:B:132:SER:HB3	1.96	0.46
1:B:213:GLN:NE2	1:C:52:ALA:HA	2.28	0.46
1:B:447:MET:HB3	1:B:887:CYS:SG	2.56	0.46
1:C:371:ALA:O	1:C:375:VAL:HG23	2.15	0.46
1:C:524:THR:O	1:C:528:THR:HG22	2.14	0.46
1:C:888:LEU:CD1	1:C:901:VAL:HG11	2.45	0.46
1:D:163:LYS:HE3	1:D:177:LEU:HB2	1.97	0.46
1:D:776:GLU:HG2	1:D:777:ALA:H	1.81	0.46
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.97	0.46
1:E:332:PHE:O	1:E:336:SER:HB2	2.15	0.46
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.30	0.46
1:F:578:LEU:HD21	1:F:590:VAL:HG21	1.97	0.46
1:F:743:ILE:H	1:F:743:ILE:HD12	1.80	0.46
1:F:835:LYS:HG2	1:F:836:SER:H	1.80	0.46
1:B:706:ALA:HB1	1:B:713:LEU:HD13	1.97	0.46
1:C:375:VAL:HB	1:C:405:LEU:HD22	1.97	0.46
1:C:725:PRO:HG3	1:C:811:TYR:HE1	1.81	0.46
1:C:944:LEU:CD1	1:C:975:ILE:HG12	2.45	0.46
1:D:347:ALA:O	1:D:351:VAL:HG23	2.16	0.46
1:D:540:ARG:O	1:D:543:VAL:HB	2.16	0.46
1:E:527:TYR:O	1:E:530:SER:HB3	2.14	0.46
1:F:566:ASP:OD1	1:F:678:THR:HG23	2.16	0.46
1:A:556:PHE:HD1	1:A:913:LEU:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:THR:HA	1:A:622:GLN:OE1	2.15	0.46
1:B:143:ILE:HG12	1:B:322:LYS:O	2.16	0.46
1:B:578:LEU:HD21	1:B:587:THR:HA	1.97	0.46
1:B:753:ALA:O	1:B:775:SER:HB3	2.16	0.46
1:C:562:SER:HB2	1:C:924:ASP:HB3	1.96	0.46
1:C:735:LYS:O	1:C:738:ALA:HB3	2.15	0.46
1:D:184:MET:HB3	1:D:771:VAL:HG22	1.98	0.46
1:D:485:ALA:O	1:D:490:PRO:HD3	2.15	0.46
1:D:545:TYR:HB2	1:D:1021:PHE:HE2	1.81	0.46
1:E:450:SER:HB2	1:E:454:VAL:HG23	1.97	0.46
1:E:508:GLY:HA3	1:E:518:ARG:NE	2.25	0.46
1:E:652:THR:OG1	1:E:665:ALA:HB3	2.15	0.46
1:F:151:GLN:NE2	1:F:279:ALA:H	2.14	0.46
1:A:69:MET:HE1	1:A:107:VAL:O	2.14	0.46
1:B:310:LEU:HG	1:B:323:ILE:HG13	1.98	0.46
1:B:713:LEU:HD11	1:B:843:LEU:HD12	1.97	0.46
1:C:76:MET:N	1:C:93:THR:O	2.46	0.46
1:C:170:SER:O	1:C:302:THR:HA	2.14	0.46
1:C:841:MET:HG2	1:C:859:TRP:CH2	2.51	0.46
1:D:55:LYS:HZ1	1:F:238:THR:HG1	1.56	0.46
1:D:250:LEU:HD23	1:E:737:GLN:NE2	2.30	0.46
1:D:417:GLU:OE1	1:D:497:LEU:HD11	2.16	0.46
1:E:13:TRP:HA	1:E:13:TRP:CE3	2.49	0.46
1:F:152:GLU:HB3	1:F:182:TYR:HE1	1.80	0.46
1:F:278:ILE:CG1	1:F:613:ASN:HB3	2.45	0.46
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.97	0.46
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.96	0.46
1:F:549:VAL:O	1:F:552:MET:HB3	2.15	0.46
1:F:873:ALA:HB2	1:F:928:GLN:NE2	2.29	0.46
1:A:659:LYS:HA	1:A:659:LYS:HD3	1.67	0.46
1:B:104:GLN:HG3	1:B:129:VAL:HG12	1.98	0.46
1:B:758:TYR:CE1	1:B:770:LYS:HD3	2.50	0.46
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:366:LEU:O	1:C:370:ILE:HG13	2.16	0.46
1:D:449:LEU:HD13	1:D:478:MET:SD	2.55	0.46
1:D:712:MET:HE3	1:D:835:LYS:HG2	1.96	0.46
1:E:162:MET:O	1:E:164:ASP:N	2.48	0.46
1:E:255:GLN:H	1:E:255:GLN:HG3	1.21	0.46
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.45	0.46
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:895:TRP:HA	1:F:895:TRP:CE3	2.50	0.46
1:A:449:LEU:HB3	1:A:478:MET:SD	2.56	0.46
1:A:457:ALA:HB2	1:A:471:SER:CB	2.46	0.46
1:A:597:TYR:CG	1:A:655:PHE:CZ	3.04	0.46
1:A:1039:ASP:H	1:A:1040:ILE:HB	1.80	0.46
1:B:600:THR:O	1:B:603:LYS:HB2	2.15	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.50	0.46
1:C:427:PRO:O	1:C:431:THR:OG1	2.30	0.46
1:C:611:ALA:HA	1:C:627:ALA:HA	1.97	0.46
1:C:947:GLU:HG3	1:C:948:PHE:CD1	2.47	0.46
1:D:189:ASN:HB3	1:D:192:GLU:HB2	1.97	0.46
1:D:423:GLU:O	1:D:502:LYS:HB3	2.16	0.46
1:D:562:SER:OG	1:D:922:THR:HG21	2.16	0.46
1:D:957:GLY:O	1:D:1040:ILE:HD13	2.16	0.46
1:E:727:PHE:CE1	1:E:807:SER:HB2	2.51	0.46
1:F:574:THR:HG23	1:F:627:ALA:HB3	1.97	0.46
1:F:971:ARG:C	1:F:974:PRO:HD2	2.36	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB3	1.98	0.46
1:B:166:ILE:HG12	1:B:310:LEU:HD13	1.97	0.46
1:B:517:ASN:O	1:B:521:GLU:N	2.45	0.46
1:B:702:LEU:HD22	1:B:851:LEU:HD11	1.97	0.46
1:C:2:PRO:O	1:C:5:PHE:HB3	2.16	0.46
1:D:57:VAL:HG21	1:D:86:GLY:CA	2.36	0.46
1:D:463:THR:HG23	1:D:467:TYR:CD1	2.51	0.46
1:D:897:ILE:HA	1:D:1029:VAL:CG1	2.43	0.46
1:D:987:MET:HB3	1:D:988:PRO:HD3	1.98	0.46
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.97	0.46
1:E:478:MET:O	1:E:482:VAL:HG12	2.15	0.46
1:E:741:VAL:HB	1:E:746:ILE:HD11	1.97	0.46
1:F:366:LEU:HA	1:F:369:THR:HB	1.97	0.46
1:F:449:LEU:HD23	1:F:936:GLY:HA3	1.96	0.46
1:F:534:ILE:HB	1:F:541:TYR:CZ	2.51	0.46
1:F:652:THR:HG23	1:F:664:PHE:HD1	1.80	0.46
1:F:885:PHE:CD2	1:F:886:LEU:HD22	2.47	0.46
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.61	0.46
1:B:641:GLU:HA	1:B:646:ALA:HB3	1.98	0.46
1:C:238:THR:HG22	1:C:239:ARG:O	2.16	0.46
1:C:445:ILE:HG12	1:C:940:LYS:HG3	1.98	0.46
1:C:641:GLU:OE2	1:C:641:GLU:N	2.37	0.46
1:C:972:LEU:O	1:C:975:ILE:HB	2.16	0.46
1:D:139:VAL:HA	1:D:289:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:ILE:HG12	1:E:262:LEU:HB2	1.98	0.46
1:E:344:LEU:HD23	1:E:402:ILE:HD11	1.98	0.46
1:F:447:MET:SD	1:F:891:LEU:HD22	2.56	0.46
1:A:375:VAL:HG22	1:A:484:VAL:HG21	1.98	0.46
1:B:903:LEU:HB3	1:B:1025:PHE:CE2	2.51	0.46
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.16	0.46
1:C:698:ALA:O	1:C:701:GLN:HB3	2.16	0.46
1:C:785:ASP:O	1:C:789:TRP:HD1	1.98	0.46
1:D:165:ALA:HB3	1:D:313:MET:HE1	1.97	0.46
1:D:252:LYS:HE2	1:D:260:VAL:HG21	1.98	0.46
1:D:346:GLU:O	1:D:350:LEU:HD12	2.16	0.46
1:D:424:GLY:HA3	1:D:502:LYS:HB3	1.97	0.46
1:D:459:PHE:CE2	1:D:876:LEU:HD12	2.51	0.46
1:D:515:TRP:O	1:D:519:MET:HG3	2.16	0.46
1:D:752:ALA:O	1:D:774:MET:HA	2.15	0.46
1:E:184:MET:HB3	1:E:771:VAL:HG13	1.98	0.46
1:E:185:ARG:HH12	1:E:774:MET:HE3	1.81	0.46
1:F:73:ASP:CG	1:F:106:GLN:HE22	2.19	0.46
1:F:564:LEU:HD12	1:F:564:LEU:HA	1.85	0.46
1:B:149:MET:HB2	1:B:153:ASP:CB	2.45	0.45
1:B:247:GLY:O	1:B:261:LEU:HB3	2.16	0.45
1:B:310:LEU:CD2	1:B:323:ILE:HG21	2.46	0.45
1:B:702:LEU:HD13	1:B:848:ALA:HA	1.97	0.45
1:C:562:SER:OG	1:C:922:THR:HG21	2.16	0.45
1:C:584:GLN:N	1:C:622:GLN:HB3	2.31	0.45
1:D:445:ILE:O	1:D:449:LEU:HB2	2.16	0.45
1:E:193:LEU:HD13	1:E:200:PRO:HD3	1.97	0.45
1:E:597:TYR:CD1	1:E:601:LYS:HD2	2.51	0.45
1:E:680:PHE:CE1	1:E:682:PHE:HB2	2.50	0.45
1:E:682:PHE:CE1	1:E:857:TYR:HB2	2.52	0.45
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.33	0.45
1:A:110:LYS:O	1:A:113:LEU:N	2.45	0.45
1:A:377:LEU:O	1:A:380:PHE:HB2	2.16	0.45
1:A:404:LEU:HD23	1:A:449:LEU:HD13	1.98	0.45
1:A:758:TYR:CD1	1:A:770:LYS:HD3	2.51	0.45
1:B:558:ARG:HD3	1:B:558:ARG:HA	1.77	0.45
1:B:847:LEU:O	1:B:850:LYS:HB2	2.15	0.45
1:C:48:SER:O	1:C:50:PRO:HD3	2.17	0.45
1:D:172:VAL:HG13	1:D:291:ILE:HG23	1.98	0.45
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.53	0.45
1:D:435:MET:HE3	1:D:435:MET:HB3	1.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:535:LEU:HD22	1:D:1027:VAL:HG21	1.98	0.45
1:D:713:LEU:CD2	1:D:843:LEU:HD12	2.46	0.45
1:E:414:GLU:HG3	1:E:974:PRO:HB3	1.98	0.45
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.98	0.45
1:A:293:LEU:HD22	1:A:294:ALA:N	2.32	0.45
1:A:819:TYR:N	1:A:822:LEU:O	2.48	0.45
1:C:346:GLU:O	1:C:350:LEU:HD13	2.17	0.45
1:C:817:GLU:OE2	1:C:825:MET:HA	2.16	0.45
1:C:818:ARG:NH2	1:C:821:GLY:O	2.49	0.45
1:C:947:GLU:HG3	1:C:948:PHE:N	2.30	0.45
1:E:158:VAL:HG13	1:E:162:MET:HE2	1.97	0.45
1:E:445:ILE:CG2	1:E:940:LYS:HD2	2.46	0.45
1:E:972:LEU:HD22	1:E:972:LEU:HA	1.67	0.45
1:F:398:MET:HE3	1:F:398:MET:HB3	1.81	0.45
1:F:460:GLY:O	1:F:868:LEU:HD21	2.16	0.45
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.97	0.45
1:A:597:TYR:CB	1:A:655:PHE:HZ	2.30	0.45
1:A:964:THR:HG21	1:A:1027:VAL:HG23	1.99	0.45
1:B:310:LEU:HD23	1:B:323:ILE:HG21	1.98	0.45
1:C:434:SER:O	1:C:437:GLN:N	2.45	0.45
1:D:237:GLN:OE1	1:E:747:ASN:ND2	2.40	0.45
1:D:293:LEU:HD23	1:D:294:ALA:N	2.30	0.45
1:D:933:THR:O	1:D:936:GLY:N	2.49	0.45
1:E:545:TYR:O	1:E:548:ILE:N	2.50	0.45
1:E:597:TYR:HD1	1:E:601:LYS:HD2	1.81	0.45
1:F:69:MET:HA	1:F:72:ILE:HD11	1.98	0.45
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.85	0.45
1:A:910:ILE:O	1:A:914:LEU:HB2	2.17	0.45
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.99	0.45
1:C:408:ASP:HB3	1:C:485:ALA:HB2	1.99	0.45
1:C:644:VAL:HG12	1:C:645:GLU:N	2.31	0.45
1:D:609:VAL:HG13	1:D:629:VAL:HG22	1.99	0.45
1:D:654:ALA:O	1:D:658:ILE:HG12	2.16	0.45
1:D:781:MET:SD	1:F:225:VAL:HG13	2.56	0.45
1:E:443:VAL:O	1:E:446:ALA:HB3	2.16	0.45
1:F:291:ILE:HD13	1:F:306:ILE:HD13	1.99	0.45
1:F:527:TYR:CZ	1:F:968:VAL:HG13	2.51	0.45
1:A:69:MET:HE1	1:A:107:VAL:HG13	1.99	0.45
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.16	0.45
1:B:419:VAL:HG13	1:B:423:GLU:OE1	2.16	0.45
1:B:544:LEU:O	1:B:548:ILE:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:HG21	1:C:158:VAL:HG22	1.99	0.45
1:C:443:VAL:O	1:C:447:MET:HB3	2.16	0.45
1:D:644:VAL:CG1	1:D:667:ASN:HB2	2.45	0.45
1:E:512:PHE:HB3	1:E:513:PHE:CD1	2.51	0.45
1:E:572:PHE:CE1	1:E:648:THR:HG22	2.51	0.45
1:F:228:GLN:NE2	1:F:230:LEU:O	2.41	0.45
1:A:848:ALA:HA	1:A:851:LEU:HG	1.99	0.45
1:B:545:TYR:CE2	1:B:1025:PHE:HZ	2.34	0.45
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.98	0.45
1:C:637:ARG:HD2	1:C:642:ASN:O	2.16	0.45
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.45
1:D:362:PHE:O	1:D:365:THR:HG22	2.16	0.45
1:D:434:SER:O	1:D:438:ILE:HG12	2.17	0.45
1:E:516:PHE:HA	1:E:519:MET:HG3	1.98	0.45
1:E:564:LEU:CD1	1:E:671:ILE:HD12	2.47	0.45
1:E:680:PHE:HE1	1:E:682:PHE:HB2	1.81	0.45
1:E:836:SER:OG	1:E:839:GLU:HG3	2.16	0.45
1:E:894:SER:HB3	1:E:897:ILE:H	1.82	0.45
1:F:466:ILE:HG21	1:F:925:VAL:HG11	1.98	0.45
1:F:705:GLU:HA	1:F:708:LYS:HE3	1.99	0.45
1:F:960:LEU:O	1:F:963:ALA:N	2.49	0.45
1:A:727:PHE:CZ	1:A:807:SER:HB2	2.52	0.45
1:A:953:MET:HE2	1:A:963:ALA:HB3	1.99	0.45
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.47	0.45
1:D:182:TYR:O	1:D:769:LYS:HD3	2.17	0.45
1:D:325:TYR:HA	1:D:326:PRO:HD2	1.93	0.45
1:D:591:LEU:HD12	1:D:613:ASN:HB2	1.99	0.45
1:E:216:ALA:HB1	1:E:234:ILE:CG2	2.47	0.45
1:E:949:ALA:HB3	1:E:1026:PHE:CE1	2.45	0.45
1:E:1011:MET:O	1:E:1015:THR:HG23	2.17	0.45
1:F:336:SER:O	1:F:340:VAL:HG23	2.17	0.45
1:A:45:ILE:HD12	1:A:90:ILE:HB	1.98	0.45
1:A:575:MET:O	1:A:575:MET:HG3	2.17	0.45
1:A:1043:SER:O	1:A:1043:SER:OG	2.34	0.45
1:B:999:ALA:O	1:B:1002:ALA:N	2.50	0.45
1:C:800:PRO:HG2	1:C:803:ALA:HB2	1.99	0.45
1:D:101:ASP:OD1	1:D:101:ASP:N	2.49	0.45
1:D:775:SER:HB2	1:D:789:TRP:CZ2	2.51	0.45
1:D:979:SER:CB	1:D:1015:THR:HG21	2.46	0.45
1:D:1030:ARG:HA	1:D:1030:ARG:HD2	1.63	0.45
1:E:240:LEU:HB2	1:E:246:PHE:HE1	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:GLU:HG2	1:E:284:GLN:O	2.17	0.45
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.99	0.45
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.52	0.45
1:F:307:ARG:NH1	1:F:325:TYR:OH	2.48	0.45
1:F:659:LYS:HG3	1:F:661:ALA:H	1.81	0.45
1:A:544:LEU:O	1:A:544:LEU:HG	2.17	0.45
1:C:378:GLY:O	1:C:382:VAL:HG23	2.16	0.45
1:D:309:GLU:O	1:D:312:LYS:HB2	2.17	0.45
1:D:508:GLY:H	1:D:518:ARG:HG3	1.82	0.45
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.99	0.45
1:E:186:ILE:HD13	1:E:262:LEU:HD21	1.99	0.45
1:F:61:VAL:HG11	1:F:88:VAL:HG11	1.99	0.45
1:F:251:LEU:HD21	1:F:262:LEU:HB2	1.98	0.45
1:F:497:LEU:HA	1:F:497:LEU:HD12	1.56	0.45
1:F:641:GLU:HA	1:F:646:ALA:HB3	1.99	0.45
1:A:259:ARG:NH2	1:A:261:LEU:HD11	2.27	0.44
1:A:350:LEU:HD13	1:A:984:LEU:O	2.17	0.44
1:B:377:LEU:O	1:B:380:PHE:HB2	2.17	0.44
1:C:150:THR:N	1:C:153:ASP:HB2	2.32	0.44
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.81	0.44
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.52	0.44
1:D:751:GLY:O	1:D:754:TRP:N	2.49	0.44
1:D:759:VAL:HG12	1:D:760:ASN:HB2	1.99	0.44
2:D:1101:LMT:H72	2:D:1101:LMT:H102	1.66	0.44
1:E:291:ILE:HD13	1:E:306:ILE:HD13	1.99	0.44
1:F:987:MET:HE2	1:F:987:MET:HB3	1.93	0.44
1:A:203:VAL:HG12	1:A:207:ILE:HD11	1.97	0.44
1:B:102:ILE:O	1:B:105:VAL:HG12	2.18	0.44
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.17	0.44
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.53	0.44
1:D:3:ASN:O	1:D:6:ILE:HG12	2.16	0.44
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.44
1:D:891:LEU:HD12	1:D:891:LEU:HA	1.82	0.44
1:E:6:ILE:HD13	1:E:432:ARG:HG2	1.98	0.44
1:E:68:ASN:HB2	1:E:114:ALA:HB2	1.99	0.44
1:E:159:ALA:O	1:E:767:ARG:NH2	2.50	0.44
1:E:399:VAL:HA	1:E:402:ILE:HG13	1.98	0.44
1:E:455:PRO:O	1:E:876:LEU:HD13	2.16	0.44
1:F:563:PHE:HB2	1:F:866:GLU:HB2	1.99	0.44
1:A:32:VAL:HG13	1:A:390:ILE:O	2.17	0.44
1:A:261:LEU:HD12	1:A:263:ARG:NH1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:PHE:CZ	1:A:844:MET:HG3	2.53	0.44
1:A:753:ALA:HB3	1:A:754:TRP:HD1	1.82	0.44
1:A:879:ILE:HD13	1:C:25:LEU:HD21	1.99	0.44
1:B:27:ILE:HD13	1:B:380:PHE:CD1	2.53	0.44
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.52	0.44
1:F:5:PHE:CE2	1:F:8:ARG:HD2	2.52	0.44
1:F:144:ASN:O	1:F:148:THR:HG23	2.17	0.44
1:F:730:ASP:OD1	1:F:808:ARG:NH2	2.51	0.44
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.76	0.44
1:A:58:GLN:OE1	1:A:818:ARG:NH1	2.49	0.44
1:A:211:ASN:OD1	1:A:240:LEU:HG	2.16	0.44
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.86	0.44
1:A:774:MET:HG2	1:A:775:SER:N	2.33	0.44
1:A:885:PHE:HD1	1:A:902:MET:HE1	1.83	0.44
1:B:99:ASP:HB3	1:B:102:ILE:HB	1.99	0.44
1:B:682:PHE:CD2	1:B:827:ILE:HD12	2.52	0.44
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.52	0.44
1:C:242:SER:HB2	1:C:245:GLU:H	1.81	0.44
1:C:699:ARG:HD3	1:C:825:MET:SD	2.56	0.44
1:D:220:GLY:O	1:D:224:PRO:HB3	2.18	0.44
1:E:80:SER:CB	1:E:90:ILE:HG12	2.48	0.44
1:A:183:ALA:HB2	1:A:273:GLU:HG3	1.99	0.44
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.77	0.44
1:B:524:THR:O	1:B:527:TYR:HB3	2.18	0.44
1:B:901:VAL:HG23	1:B:942:ALA:HB3	1.99	0.44
1:D:703:LEU:HD21	1:D:718:PRO:HD3	1.98	0.44
1:E:68:ASN:CB	1:E:114:ALA:HB2	2.48	0.44
1:E:448:VAL:O	1:E:452:VAL:HG13	2.17	0.44
1:E:744:ASN:O	1:E:748:THR:HG23	2.17	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.18	0.44
1:F:185:ARG:HB3	1:F:187:TRP:NE1	2.33	0.44
1:F:587:THR:CG2	1:F:623:ASN:HA	2.46	0.44
1:F:990:VAL:HG22	1:F:1004:GLY:HA3	2.00	0.44
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.98	0.44
1:A:190:PRO:HG3	1:A:789:TRP:CZ2	2.52	0.44
1:A:452:VAL:HG12	1:A:884:VAL:CG2	2.48	0.44
1:A:743:ILE:H	1:A:743:ILE:HD12	1.82	0.44
1:A:781:MET:SD	1:C:225:VAL:HG13	2.58	0.44
1:A:961:ILE:H	1:A:961:ILE:HG13	1.33	0.44
1:B:78:MET:N	1:B:820:ASN:OD1	2.49	0.44
1:B:767:ARG:HH22	1:C:67:GLN:NE2	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HA	1:C:195:LYS:HE3	1.99	0.44
1:C:508:GLY:O	1:C:509:LYS:HB2	2.17	0.44
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.98	0.44
1:C:952:LEU:HB2	1:C:963:ALA:HB1	1.99	0.44
1:C:987:MET:O	1:C:991:ILE:HG22	2.18	0.44
1:D:34:GLN:HG3	1:D:332:PHE:HE2	1.82	0.44
1:D:270:LEU:HD12	1:D:270:LEU:HA	1.89	0.44
1:D:465:ALA:O	1:D:469:GLN:HG2	2.17	0.44
1:E:105:VAL:HG23	1:F:109:ASN:OD1	2.18	0.44
1:E:658:ILE:C	1:E:659:LYS:HD2	2.37	0.44
1:F:149:MET:HB2	1:F:153:ASP:CB	2.47	0.44
1:F:859:TRP:O	1:F:864:TYR:HD1	2.01	0.44
1:A:20:MET:SD	1:A:374:VAL:HG22	2.58	0.44
1:A:74:ASN:O	1:A:94:PHE:HD2	2.00	0.44
1:A:275:TYR:CD1	1:C:223:PRO:HD3	2.53	0.44
1:A:400:LEU:CD2	1:A:929:VAL:HG12	2.48	0.44
1:A:562:SER:OG	1:A:922:THR:HG21	2.17	0.44
1:A:726:GLN:O	1:A:810:GLU:HG2	2.18	0.44
1:B:937:LEU:HD23	1:B:937:LEU:HA	1.80	0.44
1:C:587:THR:HG21	1:C:623:ASN:HA	2.00	0.44
1:E:990:VAL:HG22	1:E:1004:GLY:HA3	2.00	0.44
1:F:151:GLN:HB3	1:F:152:GLU:OE2	2.17	0.44
1:F:506:GLY:C	1:F:508:GLY:N	2.71	0.44
1:F:727:PHE:CZ	1:F:807:SER:HB2	2.52	0.44
1:F:889:ALA:HB1	1:F:895:TRP:CZ3	2.51	0.44
1:A:508:GLY:N	1:A:518:ARG:HG3	2.32	0.44
1:C:587:THR:HA	1:C:590:VAL:HG23	2.00	0.44
1:C:889:ALA:HB2	1:C:898:PRO:HG2	2.00	0.44
1:D:680:PHE:CZ	1:D:829:GLY:HA3	2.53	0.44
1:E:72:ILE:HG23	1:E:106:GLN:OE1	2.18	0.44
1:E:544:LEU:O	1:E:547:ILE:HB	2.17	0.44
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.44
1:F:564:LEU:HD12	1:F:565:PRO:HD2	2.00	0.44
1:A:644:VAL:HG11	1:A:667:ASN:CB	2.48	0.44
1:B:289:LEU:HD23	1:B:289:LEU:HA	1.79	0.44
1:B:549:VAL:O	1:B:552:MET:HB3	2.18	0.44
1:C:904:VAL:O	1:C:907:LEU:HB2	2.17	0.44
1:D:184:MET:HB2	1:D:762:PHE:CE2	2.53	0.44
1:D:239:ARG:HD2	1:D:761:ASP:O	2.18	0.44
1:E:695:LEU:HB3	1:E:825:MET:SD	2.58	0.44
1:E:984:LEU:HD23	1:E:984:LEU:HA	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:GLN:O	1:F:67:GLN:HG3	2.18	0.44
1:F:84:SER:HB3	1:F:814:PRO:O	2.18	0.44
1:F:507:GLU:HG2	1:F:518:ARG:CG	2.47	0.44
1:A:30:LEU:HD11	1:A:384:ALA:HA	2.00	0.43
1:A:339:GLU:HB2	1:A:1000:GLN:HE22	1.83	0.43
1:A:726:GLN:OE1	1:C:235:ILE:HD11	2.18	0.43
1:A:992:SER:O	1:A:997:SER:HB2	2.18	0.43
1:B:61:VAL:HG21	1:B:122:VAL:HG21	2.00	0.43
1:C:368:PRO:HA	1:C:409:ALA:HB1	2.00	0.43
1:C:727:PHE:HZ	1:C:807:SER:HB2	1.76	0.43
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.77	0.43
1:E:32:VAL:HG22	1:E:298:ASN:ND2	2.33	0.43
1:E:100:ALA:HB1	1:E:131:LYS:HE3	2.00	0.43
1:F:937:LEU:HD11	1:F:982:PHE:CE2	2.53	0.43
1:A:646:ALA:O	1:A:650:ARG:HG2	2.18	0.43
1:B:427:PRO:O	1:B:430:ALA:HB3	2.18	0.43
1:B:613:ASN:HD22	1:B:614:GLY:N	2.15	0.43
1:C:1038:GLU:HA	1:C:1039:ASP:HB2	2.00	0.43
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.99	0.43
2:D:1101:LMT:H31	2:D:1101:LMT:H62	1.59	0.43
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.38	0.43
1:E:166:ILE:HD12	1:E:309:GLU:HG3	2.00	0.43
1:E:200:PRO:HA	1:E:203:VAL:HG23	1.99	0.43
1:E:459:PHE:CE1	1:E:876:LEU:HD12	2.53	0.43
1:E:754:TRP:CH2	1:E:780:ARG:HA	2.53	0.43
1:F:692:HIS:NE2	1:F:723:ASP:OD1	2.49	0.43
1:B:610:PHE:O	1:B:628:PHE:N	2.45	0.43
1:B:901:VAL:HG23	1:B:942:ALA:CB	2.49	0.43
1:C:465:ALA:O	1:C:469:GLN:HG2	2.18	0.43
1:C:504:ASP:C	1:C:506:GLY:N	2.72	0.43
1:C:509:LYS:HD2	1:C:509:LYS:HA	1.77	0.43
1:C:883:VAL:O	1:C:887:CYS:HB2	2.19	0.43
1:D:31:PRO:O	1:D:389:SER:HB2	2.18	0.43
1:D:470:PHE:CD2	1:D:929:VAL:HG21	2.52	0.43
1:D:761:ASP:OD1	1:D:770:LYS:HA	2.17	0.43
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.83	0.43
1:E:415:ASN:CG	1:E:418:ARG:HH12	2.15	0.43
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.48	0.43
1:E:542:LEU:O	1:E:546:LEU:HG	2.17	0.43
1:E:652:THR:HG23	1:E:665:ALA:H	1.82	0.43
1:E:931:LEU:HD23	1:E:931:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1020:PHE:CZ	2:E:1101:LMT:H41	2.54	0.43
1:F:647:ILE:O	1:F:650:ARG:HG2	2.18	0.43
1:A:47:ALA:O	1:A:87:THR:HA	2.19	0.43
1:A:225:VAL:HG11	1:B:778:LYS:HA	2.00	0.43
1:A:281:PHE:CE1	1:A:608:SER:HB2	2.53	0.43
1:A:379:THR:HG21	1:A:477:ALA:HB2	2.00	0.43
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.50	0.43
1:B:36:PRO:HD3	1:B:391:ASN:OD1	2.18	0.43
1:B:847:LEU:HA	1:B:847:LEU:HD23	1.83	0.43
1:B:913:LEU:HD23	1:B:913:LEU:HA	1.85	0.43
1:C:751:GLY:O	1:C:754:TRP:N	2.51	0.43
1:D:396:PHE:HE1	1:D:999:ALA:HB1	1.81	0.43
1:D:790:TYR:HB3	1:D:798:MET:HB3	1.99	0.43
1:D:967:ALA:C	1:D:971:ARG:HH12	2.21	0.43
1:E:588:GLN:HG3	1:E:592:ASN:HD21	1.83	0.43
1:E:908:GLY:O	1:E:1010:GLY:HA2	2.18	0.43
1:F:340:VAL:HG22	1:F:396:PHE:HE2	1.82	0.43
1:F:560:PRO:HB2	1:F:836:SER:OG	2.18	0.43
1:F:1015:THR:O	1:F:1017:LEU:N	2.51	0.43
1:A:344:LEU:HD22	1:A:402:ILE:HD11	1.98	0.43
1:A:893:GLU:OE1	1:C:11:PHE:HB2	2.18	0.43
1:A:1038:GLU:HB3	1:A:1039:ASP:C	2.39	0.43
1:B:149:MET:HB2	1:B:153:ASP:HB3	2.01	0.43
1:B:192:GLU:HB3	1:B:265:VAL:HA	2.01	0.43
1:B:504:ASP:C	1:B:506:GLY:H	2.21	0.43
1:B:950:LYS:HZ1	1:B:1030:ARG:NH2	2.14	0.43
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.80	0.43
1:C:139:VAL:O	1:C:326:PRO:HD2	2.18	0.43
1:C:144:ASN:ND2	1:C:149:MET:SD	2.92	0.43
1:C:187:TRP:HZ3	1:C:774:MET:CE	2.32	0.43
1:C:509:LYS:HG2	1:C:513:PHE:HB2	1.99	0.43
1:D:165:ALA:HA	1:D:168:ARG:NH1	2.34	0.43
1:D:619:GLY:HA3	1:D:815:ARG:HH22	1.82	0.43
1:D:659:LYS:HD3	1:D:659:LYS:HA	1.71	0.43
1:E:182:TYR:HD1	1:E:182:TYR:HA	1.74	0.43
1:E:214:VAL:HG11	1:F:747:ASN:HB3	2.00	0.43
1:E:238:THR:OG1	1:F:728:LYS:NZ	2.51	0.43
1:F:412:VAL:HA	1:F:438:ILE:HD12	2.00	0.43
1:A:61:VAL:HG21	1:A:122:VAL:HG21	2.01	0.43
1:A:104:GLN:OE1	1:A:131:LYS:HD3	2.19	0.43
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.78	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LEU:O	1:A:452:VAL:HG22	2.19	0.43
1:A:944:LEU:CB	1:A:971:ARG:NH2	2.81	0.43
1:B:682:PHE:HB3	1:B:827:ILE:HB	2.00	0.43
1:C:189:ASN:OD1	1:C:190:PRO:HD2	2.18	0.43
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.53	0.43
1:D:394:THR:HG22	1:D:473:THR:OG1	2.18	0.43
1:D:457:ALA:HB1	1:D:468:ARG:HG3	1.99	0.43
1:D:887:CYS:O	1:D:890:ALA:HB3	2.19	0.43
1:E:180:SER:HB3	1:E:273:GLU:H	1.83	0.43
1:E:778:LYS:H	1:E:778:LYS:HG2	1.64	0.43
1:F:893:GLU:O	1:F:893:GLU:HG3	2.18	0.43
1:F:984:LEU:HA	1:F:984:LEU:HD23	1.69	0.43
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.01	0.43
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.73	0.43
1:A:379:THR:OG1	1:A:477:ALA:HA	2.19	0.43
1:A:400:LEU:HD23	1:A:929:VAL:HG12	2.01	0.43
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.78	0.43
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.53	0.43
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.54	0.43
1:B:754:TRP:CH2	1:B:780:ARG:HA	2.54	0.43
1:B:952:LEU:HA	1:B:952:LEU:HD23	1.78	0.43
1:C:182:TYR:O	1:C:769:LYS:HD3	2.19	0.43
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.84	0.43
1:D:58:GLN:HA	1:D:62:THR:HB	2.00	0.43
1:D:393:LEU:CD1	1:D:466:ILE:HA	2.49	0.43
1:D:559:LEU:HD23	1:D:560:PRO:CD	2.49	0.43
1:E:668:LEU:HD23	1:E:668:LEU:H	1.83	0.43
1:E:905:VAL:HG13	1:E:935:ILE:HG23	2.00	0.43
1:F:940:LYS:HZ2	1:F:978:THR:HG21	1.83	0.43
1:A:246:PHE:HB3	1:A:268:ILE:HD13	2.00	0.43
1:B:6:ILE:O	1:B:428:LYS:NZ	2.49	0.43
1:B:9:PRO:CB	1:B:495:THR:HG21	2.45	0.43
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.79	0.43
1:B:858:ASP:OD1	1:B:859:TRP:N	2.44	0.43
1:C:328:ASP:O	1:C:331:PRO:HD2	2.19	0.43
1:C:415:ASN:O	1:C:419:VAL:HG23	2.18	0.43
1:D:194:ASN:OD1	1:D:798:MET:HG3	2.18	0.43
1:D:414:GLU:HG3	1:D:974:PRO:HG3	2.01	0.43
1:D:706:ALA:HB3	1:D:716:VAL:HG21	2.00	0.43
1:E:185:ARG:HH12	1:E:774:MET:CE	2.32	0.43
1:E:230:LEU:HG	1:E:231:ASN:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:564:LEU:HD23	1:E:565:PRO:HD2	2.00	0.43
1:F:11:PHE:HE2	1:F:15:ILE:HD11	1.84	0.43
1:F:380:PHE:O	1:F:383:LEU:HB2	2.19	0.43
1:F:1038:GLU:HA	1:F:1039:ASP:HA	1.81	0.43
1:A:267:LYS:HD2	1:A:776:GLU:CD	2.39	0.43
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.01	0.43
2:B:1101:LMT:H6D	2:B:1101:LMT:C5B	2.48	0.43
1:C:982:PHE:O	1:C:983:ILE:C	2.57	0.43
1:D:278:ILE:HG13	1:D:613:ASN:HB3	2.00	0.43
1:D:858:ASP:OD2	1:D:859:TRP:N	2.49	0.43
1:E:589:LYS:O	1:E:592:ASN:HB2	2.19	0.43
1:E:682:PHE:CD2	1:E:827:ILE:HD12	2.53	0.43
1:F:192:GLU:HB3	1:F:265:VAL:HA	2.00	0.43
1:A:75:LEU:HD11	1:A:92:LEU:HB3	2.01	0.43
1:A:228:GLN:NE2	1:A:230:LEU:O	2.43	0.43
1:A:344:LEU:CD2	1:A:399:VAL:HG22	2.49	0.43
1:B:510:LYS:O	1:B:515:TRP:HD1	2.02	0.43
1:C:757:SER:O	1:C:772:TYR:HA	2.18	0.43
1:C:898:PRO:HA	1:C:901:VAL:HG12	2.01	0.43
1:C:945:ILE:HG12	1:C:971:ARG:NH2	2.34	0.43
1:D:35:TYR:HB3	1:D:36:PRO:HD2	2.01	0.43
1:D:37:THR:OG1	1:D:296:GLY:HA2	2.18	0.43
1:D:54:ALA:HB1	1:D:816:LEU:HG	2.00	0.43
1:D:415:ASN:O	1:D:419:VAL:HG23	2.19	0.43
1:D:644:VAL:HG12	1:D:645:GLU:N	2.33	0.43
1:D:742:SER:HG	1:D:744:ASN:HD22	1.64	0.43
1:D:973:ARG:HB3	1:D:974:PRO:HD3	2.01	0.43
1:E:504:ASP:C	1:E:506:GLY:H	2.23	0.43
1:E:555:LEU:HB3	1:E:913:LEU:HB3	2.00	0.43
1:E:1021:PHE:O	1:E:1024:VAL:HB	2.19	0.43
1:F:216:ALA:HB1	1:F:234:ILE:CG2	2.49	0.43
1:F:733:GLN:O	1:F:737:GLN:HG3	2.18	0.43
1:A:216:ALA:HB1	1:A:234:ILE:HG22	2.01	0.42
1:A:400:LEU:HD11	1:A:1007:VAL:CG2	2.46	0.42
1:A:572:PHE:HD1	1:A:666:PHE:O	2.02	0.42
1:A:847:LEU:HD23	1:A:847:LEU:HA	1.83	0.42
1:B:348:ILE:HG22	1:B:349:ILE:N	2.34	0.42
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.53	0.42
1:C:44:THR:HA	1:C:90:ILE:O	2.17	0.42
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.46	0.42
1:C:398:MET:HE3	1:C:398:MET:HB3	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ARG:HH11	1:C:422:GLU:CD	2.23	0.42
1:C:510:LYS:HG2	1:C:511:GLY:N	2.34	0.42
1:C:610:PHE:HB3	1:C:628:PHE:HB2	2.00	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.64	0.42
1:D:187:TRP:HA	1:D:774:MET:O	2.19	0.42
1:E:578:LEU:HB2	1:E:623:ASN:OD1	2.19	0.42
1:F:84:SER:C	1:F:86:GLY:H	2.22	0.42
1:F:139:VAL:HA	1:F:289:LEU:O	2.19	0.42
1:F:293:LEU:HD22	1:F:294:ALA:H	1.84	0.42
1:F:828:LEU:HD23	1:F:828:LEU:HA	1.84	0.42
1:A:542:LEU:HD12	1:A:542:LEU:HA	1.78	0.42
1:A:703:LEU:CD2	1:A:718:PRO:HD3	2.44	0.42
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	2.01	0.42
1:B:165:ALA:HB3	1:B:313:MET:HE1	2.01	0.42
1:B:317:PHE:HE2	1:B:323:ILE:HG12	1.84	0.42
1:B:453:PHE:O	1:B:456:MET:HG2	2.19	0.42
1:B:497:LEU:HD12	1:B:497:LEU:HA	1.77	0.42
1:B:612:VAL:HG12	1:B:615:PHE:HB3	2.01	0.42
1:D:252:LYS:HE2	1:D:252:LYS:HB3	1.72	0.42
1:D:357:LEU:HD23	1:D:357:LEU:O	2.18	0.42
1:D:984:LEU:HD23	1:D:984:LEU:HA	1.81	0.42
1:E:553:ALA:O	1:E:557:VAL:HG23	2.19	0.42
1:E:793:ALA:HB3	1:E:795:ASP:OD2	2.19	0.42
1:F:277:ILE:HD11	1:F:620:ARG:NH1	2.34	0.42
1:F:425:LEU:HD22	1:F:429:GLU:HG2	2.01	0.42
1:F:897:ILE:HD11	1:F:950:LYS:HE2	2.01	0.42
1:F:953:MET:SD	1:F:960:LEU:HA	2.59	0.42
1:A:80:SER:HB3	1:A:90:ILE:HA	2.01	0.42
1:A:166:ILE:HA	1:A:166:ILE:HD13	1.76	0.42
1:A:545:TYR:O	1:A:548:ILE:N	2.53	0.42
1:B:602:GLU:OE2	1:B:650:ARG:NH1	2.52	0.42
1:B:958:LYS:HB3	1:B:963:ALA:HB2	2.01	0.42
1:C:187:TRP:HZ3	1:C:774:MET:HE3	1.84	0.42
1:C:376:LEU:HD22	1:C:398:MET:CE	2.49	0.42
1:C:393:LEU:CD1	1:C:466:ILE:HD13	2.49	0.42
1:C:404:LEU:HB3	1:C:478:MET:SD	2.59	0.42
1:C:931:LEU:O	1:C:935:ILE:HG13	2.19	0.42
1:D:414:GLU:CG	1:D:974:PRO:HG3	2.48	0.42
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.84	0.42
1:E:194:ASN:OD1	1:E:798:MET:HG3	2.18	0.42
1:E:330:THR:O	1:E:334:LYS:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:VAL:O	1:E:416:VAL:HG23	2.19	0.42
1:E:564:LEU:CD1	1:E:674:LEU:HD21	2.49	0.42
1:F:34:GLN:HB2	1:F:333:VAL:HG22	2.00	0.42
1:F:58:GLN:O	1:F:62:THR:HB	2.19	0.42
1:F:181:GLN:HG2	1:F:182:TYR:N	2.34	0.42
1:F:534:ILE:HG22	2:F:1101:LMT:H5'	2.00	0.42
1:F:536:ARG:HD2	2:F:1101:LMT:O4'	2.19	0.42
1:F:898:PRO:HA	1:F:901:VAL:HG12	2.01	0.42
1:A:327:TYR:C	1:A:327:TYR:CD2	2.93	0.42
1:A:375:VAL:CG2	1:A:481:SER:HA	2.49	0.42
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.54	0.42
1:A:781:MET:HE2	1:C:225:VAL:HG22	2.00	0.42
1:A:948:PHE:CE2	1:A:971:ARG:HD3	2.55	0.42
1:B:511:GLY:HA2	1:B:515:TRP:HE1	1.82	0.42
1:B:733:GLN:O	1:B:737:GLN:HG3	2.18	0.42
1:C:640:GLU:O	1:C:643:LYS:HB3	2.20	0.42
1:C:655:PHE:HB3	1:C:663:VAL:HB	2.02	0.42
1:C:847:LEU:HD12	1:C:847:LEU:HA	1.90	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.90	0.42
1:D:684:LEU:O	1:D:824:SER:HB2	2.20	0.42
1:E:57:VAL:HG11	1:E:86:GLY:O	2.19	0.42
1:E:578:LEU:HA	1:E:661:ALA:HB1	2.00	0.42
1:E:682:PHE:CZ	1:E:857:TYR:HB2	2.54	0.42
1:E:902:MET:O	1:E:905:VAL:HG23	2.19	0.42
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.84	0.42
1:A:6:ILE:HD11	1:A:432:ARG:HE	1.85	0.42
1:A:462:SER:O	1:A:466:ILE:HG12	2.19	0.42
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.83	0.42
1:A:835:LYS:HG3	1:A:839:GLU:OE2	2.20	0.42
1:B:76:MET:HB2	1:B:93:THR:O	2.20	0.42
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.02	0.42
1:B:167:SER:HB3	1:B:175:VAL:HG21	2.00	0.42
1:B:887:CYS:O	1:B:890:ALA:HB3	2.18	0.42
1:C:356:TYR:HA	1:C:365:THR:CG2	2.43	0.42
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.84	0.42
1:D:137:LEU:HD22	1:D:293:LEU:HG	2.01	0.42
1:D:365:THR:O	1:D:368:PRO:HD2	2.18	0.42
1:D:578:LEU:HG	1:D:623:ASN:O	2.19	0.42
1:E:58:GLN:NE2	1:E:816:LEU:HD13	2.34	0.42
1:E:281:PHE:CD1	1:E:610:PHE:HD1	2.36	0.42
1:F:504:ASP:C	1:F:506:GLY:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:563:PHE:CD2	1:F:564:LEU:HB2	2.54	0.42
1:F:576:VAL:HG13	1:F:663:VAL:HG22	2.01	0.42
1:F:941:ASN:CG	1:F:975:ILE:HG23	2.40	0.42
1:F:957:GLY:HA3	1:F:1043:SER:HB2	2.01	0.42
1:A:55:LYS:HE2	1:A:55:LYS:HB3	1.92	0.42
1:A:57:VAL:HG21	1:A:86:GLY:O	2.19	0.42
1:A:207:ILE:O	1:A:211:ASN:HB3	2.19	0.42
1:A:583:THR:HG21	1:C:228:GLN:HG3	2.02	0.42
1:A:878:ALA:O	1:A:882:ILE:HG12	2.19	0.42
1:B:344:LEU:HD23	1:B:402:ILE:HD11	2.02	0.42
1:B:1037:ASN:HA	1:B:1038:GLU:CB	2.49	0.42
1:D:445:ILE:HG21	1:D:940:LYS:HD2	2.01	0.42
1:D:753:ALA:O	1:D:775:SER:HB3	2.18	0.42
1:D:946:VAL:HG13	1:D:1026:PHE:CD1	2.55	0.42
1:E:43:VAL:HG22	1:E:131:LYS:HD2	2.02	0.42
1:E:602:GLU:OE1	1:E:650:ARG:HD2	2.20	0.42
1:E:726:GLN:NE2	1:E:812:GLY:HA3	2.35	0.42
1:E:923:ASN:OD1	1:E:928:GLN:NE2	2.49	0.42
1:F:30:LEU:HD12	1:F:30:LEU:HA	1.93	0.42
1:F:931:LEU:HD23	1:F:931:LEU:HA	1.79	0.42
1:A:419:VAL:HG11	1:A:433:LYS:HG2	2.02	0.42
1:A:576:VAL:HG22	1:A:663:VAL:HG22	2.02	0.42
1:A:633:ASP:OD2	1:A:634:TRP:HD1	2.02	0.42
1:A:1030:ARG:HD2	1:A:1030:ARG:HA	1.64	0.42
1:B:599:LEU:HD23	1:B:599:LEU:HA	1.86	0.42
1:C:752:ALA:O	1:C:774:MET:HA	2.20	0.42
1:D:213:GLN:HA	1:D:237:GLN:O	2.19	0.42
1:D:338:HIS:NE2	1:D:342:LYS:HE3	2.35	0.42
1:E:891:LEU:HD12	1:E:891:LEU:HA	1.80	0.42
1:E:972:LEU:HD13	1:E:976:LEU:HD13	2.01	0.42
1:E:1030:ARG:HA	1:E:1030:ARG:HD2	1.77	0.42
1:F:881:LEU:HD23	1:F:935:ILE:HG21	2.01	0.42
1:A:214:VAL:HG21	1:B:747:ASN:CG	2.39	0.42
1:A:525:HIS:HA	1:A:528:THR:HG22	2.01	0.42
1:B:370:ILE:O	1:B:374:VAL:HG23	2.19	0.42
1:B:510:LYS:O	1:B:515:TRP:CD1	2.72	0.42
1:B:1038:GLU:C	1:B:1040:ILE:HG13	2.40	0.42
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.87	0.42
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.74	0.42
1:C:441:ALA:HB2	1:C:948:PHE:HE1	1.85	0.42
1:C:464:GLY:O	1:C:468:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:VAL:HA	1:C:829:GLY:HA2	2.02	0.42
1:D:317:PHE:HA	1:D:318:PRO:HD3	1.83	0.42
1:D:533:GLY:O	1:D:536:ARG:HB2	2.19	0.42
1:D:865:GLN:HA	1:D:868:LEU:HD12	2.01	0.42
1:E:760:ASN:O	1:E:771:VAL:HB	2.20	0.42
1:E:919:ARG:HB3	1:E:921:LEU:CD2	2.50	0.42
1:F:110:LYS:O	1:F:113:LEU:HB2	2.19	0.42
1:F:328:ASP:O	1:F:331:PRO:HD2	2.19	0.42
1:F:376:LEU:HD22	1:F:398:MET:HE3	2.02	0.42
1:F:895:TRP:HA	1:F:895:TRP:HE3	1.85	0.42
1:A:247:GLY:O	1:A:261:LEU:HB3	2.20	0.42
1:A:375:VAL:HG11	1:A:481:SER:HB3	2.01	0.42
1:B:175:VAL:HG23	1:C:70:ASN:HD21	1.85	0.42
1:B:415:ASN:HD21	1:B:948:PHE:HZ	1.67	0.42
1:C:61:VAL:HG13	1:C:118:LEU:HD13	2.02	0.42
1:C:507:GLU:HG2	1:C:518:ARG:HG3	2.01	0.42
1:C:591:LEU:HD12	1:C:613:ASN:HB2	2.02	0.42
1:C:979:SER:CB	1:C:1015:THR:HG21	2.50	0.42
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.54	0.42
1:D:49:TYR:CB	1:D:57:VAL:HG22	2.47	0.42
1:D:459:PHE:HB3	1:D:464:GLY:HA2	2.01	0.42
1:D:885:PHE:CE1	1:D:898:PRO:HB2	2.55	0.42
1:E:143:ILE:HG22	1:E:286:ALA:HB2	2.01	0.42
1:E:215:ALA:HA	1:F:51:GLY:HA3	2.02	0.42
1:E:235:ILE:HB	1:F:728:LYS:HA	2.02	0.42
1:E:347:ALA:CB	1:E:402:ILE:HG21	2.49	0.42
1:E:613:ASN:OD1	1:E:614:GLY:N	2.53	0.42
1:F:382:VAL:HG11	1:F:476:SER:HB3	2.02	0.42
1:F:775:SER:OG	1:F:780:ARG:HG2	2.20	0.42
1:F:907:LEU:CD2	1:F:1017:LEU:HB3	2.50	0.42
1:A:989:LEU:HD22	1:A:1000:GLN:HB3	2.01	0.42
1:B:706:ALA:HB1	1:B:716:VAL:HG11	2.01	0.42
1:C:68:ASN:OD1	1:C:114:ALA:HB2	2.19	0.42
1:C:252:LYS:HB3	1:C:260:VAL:CG2	2.50	0.42
1:C:355:MET:SD	1:C:368:PRO:HB2	2.60	0.42
1:D:61:VAL:CG2	1:D:122:VAL:HG21	2.49	0.42
1:D:76:MET:HB2	1:D:93:THR:O	2.19	0.42
1:D:322:LYS:HG2	1:D:323:ILE:O	2.20	0.42
1:D:867:ARG:HA	1:D:867:ARG:HD3	1.87	0.42
1:E:530:SER:OG	2:E:1101:LMT:C1'	2.68	0.42
1:E:582:ALA:HA	1:E:586:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:ILE:HD11	1:F:497:LEU:HD13	2.01	0.42
1:F:555:LEU:HB3	1:F:913:LEU:HB3	2.02	0.42
1:A:41:PRO:HG2	1:A:94:PHE:CB	2.40	0.41
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.85	0.41
1:A:562:SER:CB	1:A:924:ASP:HB3	2.50	0.41
1:A:698:ALA:O	1:A:701:GLN:HB3	2.20	0.41
1:A:712:MET:HG3	1:A:835:LYS:HE2	2.02	0.41
1:B:652:THR:HG22	1:B:664:PHE:CD1	2.52	0.41
1:B:686:ASP:HA	1:B:854:GLY:O	2.20	0.41
1:C:144:ASN:HB3	1:C:148:THR:HG23	2.02	0.41
1:D:94:PHE:CE2	1:D:103:ALA:HB1	2.56	0.41
1:D:523:SER:O	1:D:526:HIS:HB2	2.20	0.41
1:D:909:VAL:HG22	1:D:931:LEU:CD2	2.50	0.41
1:D:925:VAL:HA	1:D:928:GLN:OE1	2.20	0.41
1:E:15:ILE:HD12	1:E:487:ILE:HG21	2.01	0.41
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.55	0.41
1:F:99:ASP:HB3	1:F:102:ILE:HB	2.02	0.41
1:F:400:LEU:HD11	1:F:1007:VAL:HG21	2.02	0.41
1:F:407:ASP:OD1	1:F:978:THR:HG23	2.20	0.41
1:F:693:GLU:HB3	1:F:694:LYS:HD2	2.02	0.41
1:F:1038:GLU:O	1:F:1038:GLU:HG2	2.19	0.41
1:A:971:ARG:CZ	1:A:971:ARG:CB	2.98	0.41
1:B:165:ALA:HB3	1:B:313:MET:CE	2.50	0.41
1:B:751:GLY:O	1:B:753:ALA:N	2.53	0.41
1:C:244:GLU:O	1:C:247:GLY:N	2.53	0.41
1:C:252:LYS:HB3	1:C:260:VAL:HG21	2.02	0.41
1:C:563:PHE:CD2	1:C:564:LEU:HB2	2.56	0.41
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.20	0.41
1:D:415:ASN:OD1	1:D:434:SER:HB2	2.21	0.41
1:E:214:VAL:HG21	1:F:747:ASN:CG	2.39	0.41
1:E:352:PHE:HE1	1:E:366:LEU:CD2	2.33	0.41
1:F:213:GLN:HA	1:F:237:GLN:O	2.19	0.41
1:F:375:VAL:HG13	1:F:480:LEU:HB2	2.02	0.41
1:F:841:MET:SD	1:F:863:SER:HB2	2.60	0.41
1:F:934:THR:O	1:F:938:SER:OG	2.38	0.41
1:A:34:GLN:NE2	1:A:35:TYR:HE1	2.19	0.41
1:A:200:PRO:HB2	1:A:749:THR:HG22	2.01	0.41
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.73	0.41
1:A:597:TYR:CZ	1:A:651:ALA:HA	2.54	0.41
1:B:7:ASP:C	1:B:8:ARG:HG3	2.41	0.41
1:B:311:ALA:O	1:B:314:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:ARG:CZ	1:B:468:ARG:HB2	2.51	0.41
1:B:681:ASP:O	1:B:860:THR:HG22	2.20	0.41
1:B:738:ALA:O	1:B:740:GLY:N	2.54	0.41
1:C:250:LEU:HD11	1:C:259:ARG:HB3	2.01	0.41
1:C:578:LEU:HB3	1:C:579:PRO:HD2	2.02	0.41
1:C:910:ILE:O	1:C:914:LEU:HB2	2.20	0.41
1:D:58:GLN:HA	1:D:62:THR:OG1	2.20	0.41
1:D:293:LEU:CD2	1:D:297:ALA:HB3	2.50	0.41
1:D:544:LEU:HA	1:D:547:ILE:HD12	2.02	0.41
1:E:277:ILE:HG23	1:E:620:ARG:HH21	1.84	0.41
1:E:602:GLU:HB3	1:E:606:VAL:HG23	2.02	0.41
1:F:358:PHE:HD1	1:F:977:MET:CG	2.26	0.41
1:F:531:VAL:HG11	1:F:968:VAL:HG11	2.03	0.41
1:A:565:PRO:O	1:A:670:ALA:HB2	2.20	0.41
1:B:562:SER:HB2	1:B:922:THR:CG2	2.51	0.41
1:B:717:ARG:HD2	1:B:828:LEU:HB2	2.01	0.41
1:C:184:MET:HG2	1:C:246:PHE:CD2	2.55	0.41
1:C:340:VAL:HG11	1:C:395:MET:HB3	2.02	0.41
1:C:413:VAL:O	1:C:417:GLU:HG2	2.21	0.41
1:C:586:ARG:O	1:C:590:VAL:HG23	2.20	0.41
1:C:693:GLU:HB3	1:C:694:LYS:CE	2.50	0.41
1:C:1016:VAL:HG12	1:C:1016:VAL:O	2.20	0.41
1:D:27:ILE:HD11	1:D:380:PHE:CD1	2.55	0.41
1:D:695:LEU:HD13	1:D:825:MET:SD	2.61	0.41
1:D:974:PRO:O	1:D:975:ILE:C	2.59	0.41
1:E:166:ILE:HD12	1:E:309:GLU:CG	2.49	0.41
1:E:252:LYS:HB3	1:E:252:LYS:HE2	1.61	0.41
1:E:508:GLY:CA	1:E:518:ARG:HE	2.26	0.41
1:F:49:TYR:N	1:F:86:GLY:O	2.42	0.41
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.81	0.41
1:A:75:LEU:CD2	1:C:168:ARG:HD3	2.50	0.41
1:A:140:VAL:O	1:A:289:LEU:N	2.44	0.41
1:A:328:ASP:O	1:A:331:PRO:HD2	2.20	0.41
1:A:524:THR:O	1:A:527:TYR:HB3	2.20	0.41
1:B:680:PHE:HB2	1:B:859:TRP:CZ3	2.55	0.41
1:B:904:VAL:HA	1:B:1025:PHE:HE1	1.86	0.41
1:C:23:GLY:O	1:C:27:ILE:HG23	2.20	0.41
1:C:309:GLU:HG3	1:C:313:MET:CE	2.51	0.41
1:C:713:LEU:CD2	1:C:843:LEU:HD12	2.50	0.41
1:D:34:GLN:NE2	1:D:35:TYR:HE1	2.18	0.41
1:D:355:MET:HA	1:D:355:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:ALA:O	1:D:413:VAL:HG23	2.19	0.41
1:E:24:GLY:O	1:E:27:ILE:HG22	2.21	0.41
1:E:347:ALA:HB1	1:E:402:ILE:HG21	2.02	0.41
1:E:937:LEU:HD23	1:E:937:LEU:HA	1.88	0.41
1:F:566:ASP:CG	1:F:678:THR:HG23	2.40	0.41
1:F:878:ALA:O	1:F:882:ILE:HG13	2.21	0.41
1:A:141:GLY:O	1:A:323:ILE:HA	2.21	0.41
1:A:377:LEU:HD23	1:A:377:LEU:HA	1.84	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.60	0.41
1:A:904:VAL:HG12	1:A:938:SER:HB3	2.03	0.41
1:C:154:ILE:O	1:C:157:TYR:N	2.54	0.41
1:C:181:GLN:O	1:C:272:GLY:HA2	2.20	0.41
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.50	0.41
1:C:422:GLU:HB3	1:C:423:GLU:HG3	2.01	0.41
1:C:703:LEU:CD1	1:C:718:PRO:HD3	2.51	0.41
1:C:1040:ILE:HG22	1:C:1040:ILE:O	2.20	0.41
1:D:38:ILE:HD11	1:D:466:ILE:HD11	2.02	0.41
1:D:113:LEU:HD21	1:F:128:SER:HB3	2.02	0.41
1:D:137:LEU:HD23	1:D:291:ILE:HG22	2.02	0.41
1:F:459:PHE:CE1	1:F:876:LEU:HG	2.56	0.41
1:A:27:ILE:HD11	1:A:380:PHE:CE1	2.56	0.41
1:A:252:LYS:HB3	1:A:252:LYS:HE2	1.75	0.41
1:A:274:ASN:OD1	1:A:276:ASP:HB2	2.20	0.41
1:A:472:ILE:HG22	1:A:473:THR:N	2.35	0.41
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.87	0.41
1:A:507:GLU:HG3	1:A:518:ARG:HA	2.03	0.41
1:A:1035:ARG:HG2	1:A:1036:LYS:H	1.85	0.41
1:A:1040:ILE:HG13	1:A:1042:HIS:HB2	2.02	0.41
1:B:278:ILE:CG1	1:B:613:ASN:HB3	2.49	0.41
1:B:1015:THR:O	1:B:1017:LEU:N	2.54	0.41
1:C:365:THR:O	1:C:368:PRO:HD2	2.20	0.41
1:C:586:ARG:O	1:C:589:LYS:HB2	2.21	0.41
1:D:203:VAL:O	1:D:207:ILE:HG13	2.20	0.41
1:D:524:THR:O	1:D:528:THR:HG22	2.19	0.41
1:D:888:LEU:HD13	1:D:901:VAL:HG13	2.02	0.41
1:D:944:LEU:HD23	1:D:944:LEU:HA	1.78	0.41
1:E:5:PHE:HE2	1:E:11:PHE:CD2	2.39	0.41
1:E:78:MET:HE3	1:E:821:GLY:N	2.35	0.41
1:E:185:ARG:CD	1:E:772:TYR:HB2	2.51	0.41
1:F:392:THR:O	1:F:395:MET:HB2	2.20	0.41
1:F:684:LEU:HB3	1:F:825:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:971:ARG:NH2	1:F:975:ILE:HD11	2.36	0.41
1:A:351:VAL:HG22	1:A:981:ALA:HB1	2.03	0.41
1:A:699:ARG:HE	1:A:718:PRO:HG3	1.85	0.41
1:B:675:GLY:HA2	1:B:862:MET:SD	2.61	0.41
1:B:716:VAL:HG23	1:B:827:ILE:CG2	2.51	0.41
1:B:836:SER:OG	1:B:839:GLU:HG3	2.21	0.41
1:C:48:SER:C	1:C:50:PRO:HD3	2.41	0.41
1:C:80:SER:OG	1:C:818:ARG:HD3	2.20	0.41
1:D:72:ILE:HG21	1:D:107:VAL:HG23	2.03	0.41
1:D:544:LEU:O	1:D:544:LEU:HG	2.21	0.41
1:D:597:TYR:CD2	1:D:655:PHE:CZ	3.09	0.41
1:D:648:THR:HB	1:D:665:ALA:O	2.20	0.41
1:E:310:LEU:HD21	1:E:323:ILE:HG21	2.03	0.41
1:E:565:PRO:HG2	1:E:999:ALA:HA	2.02	0.41
1:E:639:GLY:O	1:E:643:LYS:HG3	2.20	0.41
1:F:356:TYR:CE1	1:F:362:PHE:HD1	2.38	0.41
1:F:1018:ALA:O	1:F:1022:VAL:HG23	2.21	0.41
1:A:11:PHE:CE2	1:B:890:ALA:HB1	2.56	0.41
1:A:30:LEU:HA	1:A:31:PRO:HD3	1.92	0.41
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.02	0.41
1:A:172:VAL:HG22	1:A:306:ILE:HD11	2.03	0.41
1:A:216:ALA:HB3	1:A:234:ILE:O	2.21	0.41
1:A:278:ILE:HG13	1:A:613:ASN:HB3	2.02	0.41
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.62	0.41
1:A:985:GLY:O	1:A:988:PRO:HD2	2.20	0.41
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.56	0.41
1:B:576:VAL:HG22	1:B:663:VAL:HG13	2.03	0.41
1:B:706:ALA:HB2	1:B:844:MET:HE1	2.03	0.41
1:B:949:ALA:HB3	1:B:1026:PHE:CE1	2.55	0.41
1:C:77:TYR:CZ	1:C:93:THR:HG21	2.56	0.41
1:C:150:THR:H	1:C:153:ASP:HB2	1.85	0.41
1:C:151:GLN:NE2	1:C:286:ALA:O	2.54	0.41
1:C:926:TYR:HE1	1:C:999:ALA:HB1	1.86	0.41
1:C:1034:SER:OG	1:C:1037:ASN:HB3	2.21	0.41
1:D:143:ILE:O	1:D:321:LEU:HA	2.21	0.41
1:D:172:VAL:CG2	1:D:306:ILE:HD11	2.51	0.41
1:D:278:ILE:HD13	1:D:584:GLN:HE21	1.85	0.41
1:D:478:MET:HB3	1:D:478:MET:HE2	1.95	0.41
1:D:588:GLN:N	1:D:613:ASN:ND2	2.69	0.41
1:D:671:ILE:H	1:D:671:ILE:HG13	1.70	0.41
1:D:687:GLN:OE1	1:D:856:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:ALA:O	1:D:701:GLN:HB3	2.21	0.41
1:E:187:TRP:HA	1:E:774:MET:O	2.21	0.41
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.82	0.41
1:E:538:THR:CG2	1:E:1024:VAL:HG13	2.51	0.41
1:E:545:TYR:OH	1:E:906:PRO:HG2	2.20	0.41
1:E:738:ALA:C	1:E:740:GLY:H	2.23	0.41
1:E:844:MET:HA	1:E:844:MET:CE	2.50	0.41
1:E:885:PHE:HD2	1:E:886:LEU:HD13	1.85	0.41
1:F:447:MET:HE1	1:F:887:CYS:O	2.21	0.41
1:F:465:ALA:HA	1:F:468:ARG:CZ	2.51	0.41
1:F:542:LEU:O	1:F:545:TYR:HB3	2.21	0.41
1:F:578:LEU:HB2	1:F:623:ASN:CB	2.51	0.41
1:F:1032:ARG:O	1:F:1033:PHE:HB2	2.21	0.41
1:A:478:MET:HB3	1:A:478:MET:HE2	1.91	0.41
1:B:177:LEU:HA	1:B:289:LEU:HD23	2.03	0.41
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.54	0.41
1:B:533:GLY:HA2	1:B:536:ARG:HB2	2.03	0.41
1:B:888:LEU:HD13	1:B:901:VAL:HG11	2.03	0.41
1:B:946:VAL:HG22	1:B:1026:PHE:HD1	1.86	0.41
1:B:960:LEU:O	1:B:964:THR:HG23	2.21	0.41
1:B:1026:PHE:O	1:B:1030:ARG:HB2	2.21	0.41
1:C:104:GLN:HG3	1:C:105:VAL:N	2.35	0.41
1:D:542:LEU:HD12	1:D:542:LEU:HA	1.71	0.41
1:D:662:MET:HG2	1:D:664:PHE:CZ	2.56	0.41
1:E:692:HIS:NE2	1:E:813:SER:HB2	2.35	0.41
1:F:907:LEU:HG	1:F:1017:LEU:HD23	2.03	0.41
1:F:926:TYR:HE1	1:F:999:ALA:HB1	1.86	0.41
1:A:453:PHE:CE2	1:A:474:ILE:HG21	2.56	0.40
1:A:870:GLY:O	1:A:872:GLN:HG3	2.21	0.40
1:A:897:ILE:HG12	1:A:1030:ARG:HD3	2.03	0.40
1:A:990:VAL:HG21	1:A:1008:MET:HE3	2.02	0.40
1:A:1040:ILE:CG1	1:A:1041:GLU:H	2.26	0.40
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.86	0.40
1:B:841:MET:O	1:B:845:GLU:HG3	2.22	0.40
1:C:987:MET:HE2	1:C:987:MET:HB3	1.94	0.40
1:D:393:LEU:HD12	1:D:469:GLN:HG3	2.03	0.40
1:D:514:GLY:C	1:D:516:PHE:N	2.72	0.40
1:E:448:VAL:HA	1:E:451:ALA:HB3	2.03	0.40
1:E:586:ARG:O	1:E:589:LYS:HB3	2.21	0.40
1:F:6:ILE:H	1:F:6:ILE:HG12	1.41	0.40
1:F:47:ALA:HB2	1:F:127:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:55:LYS:HA	1:F:816:LEU:CD1	2.51	0.40
1:F:160:ALA:HA	1:F:767:ARG:NE	2.34	0.40
1:F:563:PHE:CE2	1:F:564:LEU:HD22	2.56	0.40
1:F:565:PRO:HG2	1:F:567:GLU:OE2	2.21	0.40
1:F:572:PHE:HB2	1:F:666:PHE:O	2.22	0.40
1:A:210:GLN:OE1	1:A:249:ILE:HG23	2.22	0.40
1:A:338:HIS:NE2	1:A:342:LYS:HD2	2.37	0.40
1:A:344:LEU:HD21	1:A:399:VAL:HG22	2.04	0.40
1:A:356:TYR:HE2	1:A:513:PHE:HE2	1.68	0.40
1:B:442:LEU:HA	1:B:442:LEU:HD23	1.79	0.40
1:B:760:ASN:O	1:B:771:VAL:HB	2.21	0.40
1:C:182:TYR:HD2	1:C:765:ARG:HH22	1.68	0.40
1:C:1018:ALA:O	1:C:1022:VAL:HG23	2.21	0.40
1:D:146:ASP:OD2	1:D:146:ASP:N	2.44	0.40
1:D:151:GLN:CG	1:D:152:GLU:N	2.84	0.40
1:D:189:ASN:HA	1:D:190:PRO:HD3	1.91	0.40
1:D:251:LEU:HD21	1:D:262:LEU:HD13	2.02	0.40
1:D:279:ALA:HB3	1:D:286:ALA:O	2.20	0.40
1:E:203:VAL:O	1:E:207:ILE:HG13	2.21	0.40
1:E:383:LEU:HD23	1:E:383:LEU:HA	1.92	0.40
1:E:1042:HIS:HB3	1:E:1043:SER:H	1.59	0.40
1:F:752:ALA:O	1:F:774:MET:HA	2.21	0.40
1:F:790:TYR:HB3	1:F:798:MET:HB3	2.01	0.40
1:A:577:GLN:HE22	1:A:624:THR:HG22	1.86	0.40
1:A:706:ALA:HB2	1:A:844:MET:HE3	2.02	0.40
1:A:752:ALA:O	1:A:774:MET:HA	2.22	0.40
1:A:894:SER:HB3	1:A:897:ILE:HB	2.03	0.40
1:B:185:ARG:HH12	1:B:774:MET:CE	2.35	0.40
1:B:448:VAL:HG13	1:B:884:VAL:HG22	2.03	0.40
1:B:756:GLY:CA	1:B:774:MET:HG3	2.52	0.40
1:B:931:LEU:O	1:B:935:ILE:HG13	2.21	0.40
1:B:1015:THR:OG1	1:B:1016:VAL:N	2.53	0.40
1:C:466:ILE:H	1:C:466:ILE:HG12	1.77	0.40
1:C:668:LEU:H	1:C:668:LEU:CD2	2.30	0.40
1:C:701:GLN:HG2	1:C:705:GLU:OE2	2.20	0.40
1:C:940:LYS:O	1:C:943:ILE:HB	2.21	0.40
1:D:356:TYR:O	1:D:360:GLN:N	2.48	0.40
1:D:846:GLN:O	1:D:850:LYS:HD3	2.21	0.40
1:E:2:PRO:HB2	1:E:439:GLN:OE1	2.21	0.40
1:F:238:THR:HG22	1:F:239:ARG:O	2.21	0.40
1:F:453:PHE:CE1	1:F:474:ILE:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:666:PHE:N	1:F:666:PHE:CD1	2.88	0.40
1:A:152:GLU:HB2	1:A:182:TYR:CE1	2.56	0.40
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.56	0.40
1:B:163:LYS:HD2	1:B:177:LEU:HD12	2.03	0.40
1:B:348:ILE:HD13	1:B:348:ILE:HG21	1.80	0.40
1:B:650:ARG:O	1:B:653:ARG:HB3	2.21	0.40
1:C:344:LEU:HA	1:C:399:VAL:HG22	2.03	0.40
1:C:368:PRO:O	1:C:371:ALA:HB3	2.21	0.40
1:C:699:ARG:HE	1:C:718:PRO:HB3	1.87	0.40
1:C:1037:ASN:HB3	1:C:1038:GLU:H	1.81	0.40
1:D:112:GLN:OE1	1:D:115:MET:HG3	2.22	0.40
1:D:706:ALA:HB1	1:D:716:VAL:HG11	2.03	0.40
1:D:777:ALA:CB	1:F:225:VAL:HG12	2.44	0.40
1:D:982:PHE:O	1:D:983:ILE:C	2.59	0.40
2:D:1101:LMT:H6D	2:D:1101:LMT:C5B	2.52	0.40
1:E:167:SER:CB	1:E:175:VAL:HG21	2.52	0.40
1:E:216:ALA:HB2	1:E:236:ALA:HB2	2.04	0.40
1:E:291:ILE:HG21	1:E:306:ILE:HD11	2.02	0.40
1:E:328:ASP:O	1:E:331:PRO:HD2	2.21	0.40
1:E:398:MET:HG2	1:E:473:THR:CG2	2.52	0.40
1:F:30:LEU:HA	1:F:31:PRO:HD3	1.89	0.40
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.40
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.04	0.40
1:F:636:ASP:O	1:F:638:PRO:HD3	2.22	0.40
1:F:778:LYS:H	1:F:778:LYS:HG2	1.58	0.40
1:F:964:THR:O	1:F:968:VAL:HB	2.21	0.40
1:A:110:LYS:HE2	1:C:130:GLU:OE2	2.21	0.40
1:A:261:LEU:HD12	1:A:263:ARG:CZ	2.51	0.40
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.04	0.40
1:A:944:LEU:HB3	1:A:971:ARG:NH2	2.37	0.40
1:B:156:ASP:OD2	1:B:769:LYS:NZ	2.31	0.40
1:C:520:PHE:HE1	1:C:976:LEU:HD22	1.87	0.40
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.82	0.40
1:C:1015:THR:OG1	1:C:1016:VAL:N	2.55	0.40
1:D:586:ARG:HH11	1:D:586:ARG:HD2	1.78	0.40
1:E:157:TYR:CE1	1:E:318:PRO:HD3	2.57	0.40
1:E:158:VAL:HG11	1:E:289:LEU:HD11	2.03	0.40
1:E:189:ASN:HD22	1:E:190:PRO:HD2	1.85	0.40
1:E:527:TYR:HB2	2:E:1101:LMT:H82	2.04	0.40
1:E:848:ALA:HA	1:E:851:LEU:HG	2.04	0.40
1:F:462:SER:HB3	1:F:865:GLN:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:785:ASP:N	1:F:785:ASP:OD1	2.55	0.40
1:F:932:LEU:O	1:F:935:ILE:N	2.54	0.40
1:F:1035:ARG:HH11	1:F:1038:GLU:CD	2.24	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:GLU:OE2	1:D:522:LYS:NZ[1_556]	2.16	0.04

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	1040/1049 (99%)	940 (90%)	89 (9%)	11 (1%)	14	45
1	B	1041/1049 (99%)	950 (91%)	75 (7%)	16 (2%)	10	38
1	C	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	9	36
1	D	1040/1049 (99%)	954 (92%)	70 (7%)	16 (2%)	10	38
1	E	1040/1049 (99%)	946 (91%)	77 (7%)	17 (2%)	9	36
1	F	1040/1049 (99%)	946 (91%)	76 (7%)	18 (2%)	9	35
All	All	6241/6294 (99%)	5682 (91%)	464 (7%)	95 (2%)	10	38

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	677	ALA
1	A	991	ILE
1	A	1037	ASN
1	A	1040	ILE
1	B	509	LYS

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Mol	Chain	Res	Type
1	B	516	PHE
1	B	673	GLU
1	B	677	ALA
1	B	689	GLY
1	B	1038	GLU
1	C	133	SER
1	C	360	GLN
1	C	509	LYS
1	C	689	GLY
1	C	836	SER
1	C	893	GLU
1	C	920	GLY
1	C	1037	ASN
1	D	508	GLY
1	D	511	GLY
1	D	992	SER
1	E	509	LYS
1	E	893	GLU
1	E	1042	HIS
1	F	133	SER
1	F	134	SER
1	F	146	ASP
1	F	360	GLN
1	F	836	SER
1	F	1035	ARG
1	F	1040	ILE
1	A	360	GLN
1	A	675	GLY
1	A	688	ALA
1	A	992	SER
1	A	1039	ASP
1	B	672	VAL
1	B	751	GLY
1	C	134	SER
1	C	146	ASP
1	C	147	GLY
1	C	751	GLY
1	C	871	ASN
1	D	360	GLN
1	D	675	GLY
1	D	751	GLY
1	D	991	ILE

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Mol	Chain	Res	Type
1	D	1033	PHE
1	E	508	GLY
1	E	672	VAL
1	E	674	LEU
1	E	677	ALA
1	E	1039	ASP
1	F	147	GLY
1	F	507	GLU
1	F	1033	PHE
1	A	751	GLY
1	B	1034	SER
1	B	1040	ILE
1	C	514	GLY
1	C	752	ALA
1	C	1042	HIS
1	D	215	ALA
1	D	752	ALA
1	E	516	PHE
1	E	751	GLY
1	F	514	GLY
1	F	1038	GLU
1	D	514	GLY
1	D	677	ALA
1	D	1034	SER
1	E	163	LYS
1	E	514	GLY
1	E	1034	SER
1	F	689	GLY
1	F	751	GLY
1	F	923	ASN
1	B	358	PHE
1	B	923	ASN
1	C	215	ALA
1	D	923	ASN
1	D	960	LEU
1	E	638	PRO
1	E	1040	ILE
1	B	215	ALA
1	B	893	GLU
1	E	74	ASN
1	F	638	PRO
1	A	658	ILE

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Mol	Chain	Res	Type
1	B	508	GLY
1	B	644	VAL
1	D	638	PRO
1	E	658	ILE
1	F	204	ILE
1	F	644	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	848/855 (99%)	790 (93%)	58 (7%)	16	44
1	B	849/855 (99%)	782 (92%)	67 (8%)	12	37
1	C	848/855 (99%)	775 (91%)	73 (9%)	10	35
1	D	848/855 (99%)	796 (94%)	52 (6%)	18	48
1	E	848/855 (99%)	779 (92%)	69 (8%)	11	36
1	F	848/855 (99%)	780 (92%)	68 (8%)	12	37
All	All	5089/5130 (99%)	4702 (92%)	387 (8%)	13	39

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	44	THR
1	A	49	TYR
1	A	88	VAL
1	A	101	ASP
1	A	146	ASP
1	A	169	THR
1	A	177	LEU
1	A	205	THR
1	A	222	THR
1	A	255	GLN
1	A	270	LEU

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Mol	Chain	Res	Type
1	A	274	ASN
1	A	293	LEU
1	A	324	VAL
1	A	327	TYR
1	A	336	SER
1	A	355	MET
1	A	360	GLN
1	A	362	PHE
1	A	434	SER
1	A	437	GLN
1	A	452	VAL
1	A	472	ILE
1	A	489	THR
1	A	502	LYS
1	A	538	THR
1	A	540	ARG
1	A	559	LEU
1	A	561	SER
1	A	564	LEU
1	A	571	VAL
1	A	597	TYR
1	A	602	GLU
1	A	603	LYS
1	A	617	PHE
1	A	634	TRP
1	A	662	MET
1	A	712	MET
1	A	716	VAL
1	A	721	LEU
1	A	741	VAL
1	A	775	SER
1	A	785	ASP
1	A	797	GLN
1	A	806	SER
1	A	857	TYR
1	A	866	GLU
1	A	901	VAL
1	A	922	THR
1	A	931	LEU
1	A	938	SER
1	A	961	ILE
1	A	964	THR

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Mol	Chain	Res	Type
1	A	971	ARG
1	A	980	LEU
1	A	1035	ARG
1	A	1039	ASP
1	B	3	ASN
1	B	25	LEU
1	B	29	LYS
1	B	131	LYS
1	B	148	THR
1	B	213	GLN
1	B	229	GLN
1	B	242	SER
1	B	243	THR
1	B	249	ILE
1	B	259	ARG
1	B	267	LYS
1	B	270	LEU
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	314	GLU
1	B	321	LEU
1	B	324	VAL
1	B	329	THR
1	B	348	ILE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	400	LEU
1	B	434	SER
1	B	482	VAL
1	B	489	THR
1	B	523	SER
1	B	559	LEU
1	B	561	SER
1	B	563	PHE
1	B	564	LEU
1	B	571	VAL
1	B	602	GLU
1	B	613	ASN
1	B	626	ILE

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Mol	Chain	Res	Type
1	B	634	TRP
1	B	652	THR
1	B	666	PHE
1	B	687	GLN
1	B	694	LYS
1	B	695	LEU
1	B	697	GLN
1	B	714	THR
1	B	716	VAL
1	B	717	ARG
1	B	721	LEU
1	B	741	VAL
1	B	775	SER
1	B	806	SER
1	B	835	LYS
1	B	865	GLN
1	B	867	ARG
1	B	871	ASN
1	B	886	LEU
1	B	914	LEU
1	B	922	THR
1	B	938	SER
1	B	966	ASP
1	B	971	ARG
1	B	973	ARG
1	B	1015	THR
1	B	1039	ASP
1	B	1042	HIS
1	B	1044	HIS
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	13	TRP
1	C	27	ILE
1	C	49	TYR
1	C	58	GLN
1	C	102	ILE
1	C	104	GLN
1	C	112	GLN
1	C	145	THR
1	C	148	THR
1	C	177	LEU

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Mol	Chain	Res	Type
1	C	243	THR
1	C	255	GLN
1	C	280	GLU
1	C	307	ARG
1	C	336	SER
1	C	337	ILE
1	C	342	LYS
1	C	358	PHE
1	C	362	PHE
1	C	363	ARG
1	C	392	THR
1	C	439	GLN
1	C	447	MET
1	C	448	VAL
1	C	452	VAL
1	C	463	THR
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	526	HIS
1	C	530	SER
1	C	559	LEU
1	C	561	SER
1	C	571	VAL
1	C	602	GLU
1	C	634	TRP
1	C	649	MET
1	C	659	LYS
1	C	662	MET
1	C	666	PHE
1	C	678	THR
1	C	686	ASP
1	C	694	LYS
1	C	733	GLN
1	C	741	VAL
1	C	746	ILE
1	C	748	THR
1	C	749	THR
1	C	785	ASP
1	C	788	ASP
1	C	797	GLN
1	C	804	PHE

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Mol	Chain	Res	Type
1	C	847	LEU
1	C	860	THR
1	C	865	GLN
1	C	868	LEU
1	C	876	LEU
1	C	886	LEU
1	C	887	CYS
1	C	895	TRP
1	C	938	SER
1	C	947	GLU
1	C	961	ILE
1	C	971	ARG
1	C	980	LEU
1	C	991	ILE
1	C	1011	MET
1	C	1035	ARG
1	C	1038	GLU
1	C	1041	GLU
1	D	3	ASN
1	D	27	ILE
1	D	49	TYR
1	D	88	VAL
1	D	101	ASP
1	D	102	ILE
1	D	146	ASP
1	D	205	THR
1	D	222	THR
1	D	255	GLN
1	D	260	VAL
1	D	270	LEU
1	D	324	VAL
1	D	336	SER
1	D	355	MET
1	D	360	GLN
1	D	362	PHE
1	D	437	GLN
1	D	462	SER
1	D	463	THR
1	D	472	ILE
1	D	538	THR
1	D	559	LEU
1	D	561	SER

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Mol	Chain	Res	Type
1	D	602	GLU
1	D	603	LYS
1	D	634	TRP
1	D	662	MET
1	D	666	PHE
1	D	671	ILE
1	D	672	VAL
1	D	695	LEU
1	D	741	VAL
1	D	743	ILE
1	D	775	SER
1	D	785	ASP
1	D	804	PHE
1	D	806	SER
1	D	866	GLU
1	D	867	ARG
1	D	901	VAL
1	D	918	PHE
1	D	922	THR
1	D	931	LEU
1	D	938	SER
1	D	961	ILE
1	D	966	ASP
1	D	968	VAL
1	D	971	ARG
1	D	980	LEU
1	D	1033	PHE
1	D	1037	ASN
1	E	3	ASN
1	E	6	ILE
1	E	25	LEU
1	E	28	LEU
1	E	29	LYS
1	E	58	GLN
1	E	131	LYS
1	E	146	ASP
1	E	177	LEU
1	E	182	TYR
1	E	189	ASN
1	E	205	THR
1	E	229	GLN
1	E	243	THR

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Mol	Chain	Res	Type
1	E	255	GLN
1	E	259	ARG
1	E	267	LYS
1	E	270	LEU
1	E	293	LEU
1	E	295	THR
1	E	314	GLU
1	E	324	VAL
1	E	327	TYR
1	E	329	THR
1	E	336	SER
1	E	337	ILE
1	E	360	GLN
1	E	365	THR
1	E	372	VAL
1	E	398	MET
1	E	400	LEU
1	E	482	VAL
1	E	523	SER
1	E	538	THR
1	E	559	LEU
1	E	561	SER
1	E	563	PHE
1	E	564	LEU
1	E	574	THR
1	E	578	LEU
1	E	634	TRP
1	E	652	THR
1	E	653	ARG
1	E	672	VAL
1	E	673	GLU
1	E	690	LEU
1	E	694	LYS
1	E	697	GLN
1	E	714	THR
1	E	717	ARG
1	E	721	LEU
1	E	741	VAL
1	E	785	ASP
1	E	797	GLN
1	E	804	PHE
1	E	835	LYS

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Mol	Chain	Res	Type
1	E	865	GLN
1	E	867	ARG
1	E	871	ASN
1	E	886	LEU
1	E	938	SER
1	E	966	ASP
1	E	968	VAL
1	E	971	ARG
1	E	972	LEU
1	E	980	LEU
1	E	1021	PHE
1	E	1036	LYS
1	E	1043	SER
1	F	3	ASN
1	F	6	ILE
1	F	13	TRP
1	F	21	LEU
1	F	34	GLN
1	F	49	TYR
1	F	59	ASP
1	F	104	GLN
1	F	176	GLN
1	F	177	LEU
1	F	242	SER
1	F	280	GLU
1	F	293	LEU
1	F	327	TYR
1	F	335	ILE
1	F	337	ILE
1	F	357	LEU
1	F	358	PHE
1	F	362	PHE
1	F	363	ARG
1	F	408	ASP
1	F	447	MET
1	F	448	VAL
1	F	452	VAL
1	F	472	ILE
1	F	482	VAL
1	F	510	LYS
1	F	515	TRP
1	F	523	SER

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Mol	Chain	Res	Type
1	F	524	THR
1	F	526	HIS
1	F	538	THR
1	F	540	ARG
1	F	542	LEU
1	F	559	LEU
1	F	564	LEU
1	F	602	GLU
1	F	626	ILE
1	F	634	TRP
1	F	649	MET
1	F	666	PHE
1	F	668	LEU
1	F	681	ASP
1	F	694	LYS
1	F	703	LEU
1	F	713	LEU
1	F	721	LEU
1	F	741	VAL
1	F	746	ILE
1	F	775	SER
1	F	785	ASP
1	F	797	GLN
1	F	806	SER
1	F	847	LEU
1	F	860	THR
1	F	868	LEU
1	F	876	LEU
1	F	923	ASN
1	F	938	SER
1	F	961	ILE
1	F	964	THR
1	F	971	ARG
1	F	980	LEU
1	F	991	ILE
1	F	1011	MET
1	F	1030	ARG
1	F	1034	SER
1	F	1038	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	151	GLN
1	A	181	GLN
1	A	505	HIS
1	A	517	ASN
1	A	605	ASN
1	A	928	GLN
1	B	63	GLN
1	B	189	ASN
1	B	231	ASN
1	B	588	GLN
1	B	592	ASN
1	B	613	ASN
1	B	642	ASN
1	B	733	GLN
1	B	1037	ASN
1	C	70	ASN
1	D	34	GLN
1	D	605	ASN
1	D	744	ASN
1	E	67	GLN
1	E	108	GLN
1	E	189	ASN
1	E	588	GLN
1	E	592	ASN
1	E	733	GLN
1	E	737	GLN
1	F	89	GLN
1	F	588	GLN
1	F	592	ASN
1	F	733	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	1101	-	36,36,36	1.92	9 (25%)	47,47,47	1.61	10 (21%)
2	LMT	B	1101	-	36,36,36	1.75	10 (27%)	47,47,47	1.42	8 (17%)
2	LMT	F	1101	-	36,36,36	1.76	8 (22%)	47,47,47	1.02	1 (2%)
2	LMT	A	1101	-	36,36,36	1.79	10 (27%)	47,47,47	1.10	3 (6%)
2	LMT	D	1101	-	36,36,36	1.76	7 (19%)	47,47,47	1.26	8 (17%)
2	LMT	E	1101	-	36,36,36	1.83	11 (30%)	47,47,47	1.13	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	C	1101	-	1/1/10/10	13/21/61/61	0/2/2/2
2	LMT	B	1101	-	-	10/21/61/61	0/2/2/2
2	LMT	F	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	A	1101	-	-	11/21/61/61	0/2/2/2
2	LMT	D	1101	-	-	13/21/61/61	0/2/2/2
2	LMT	E	1101	-	-	14/21/61/61	0/2/2/2

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	LMT	O5'-C5'	4.67	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	4.14	1.47	1.40
2	C	1101	LMT	O1'-C1'	4.14	1.47	1.40
2	A	1101	LMT	O5'-C5'	4.00	1.54	1.44
2	B	1101	LMT	O5B-C1B	3.96	1.51	1.41
2	D	1101	LMT	O5'-C5'	3.87	1.53	1.44
2	A	1101	LMT	O5B-C1B	3.83	1.51	1.41
2	E	1101	LMT	O5'-C5'	3.83	1.53	1.44
2	E	1101	LMT	O5B-C1B	3.77	1.51	1.41
2	C	1101	LMT	O5'-C1'	3.74	1.51	1.41
2	D	1101	LMT	O1'-C1'	3.68	1.46	1.40
2	F	1101	LMT	O5'-C5'	3.65	1.53	1.44
2	C	1101	LMT	O5B-C1B	3.64	1.51	1.41
2	F	1101	LMT	O1'-C1'	3.64	1.46	1.40
2	F	1101	LMT	O5B-C1B	3.57	1.50	1.41
2	D	1101	LMT	O5B-C1B	3.51	1.50	1.41
2	F	1101	LMT	C6'-C5'	-3.50	1.40	1.51
2	B	1101	LMT	O1'-C1'	3.39	1.46	1.40
2	B	1101	LMT	O5'-C5'	3.34	1.52	1.44
2	E	1101	LMT	C6'-C5'	-3.32	1.40	1.51
2	F	1101	LMT	O5'-C1'	3.27	1.50	1.41
2	B	1101	LMT	C6'-C5'	-3.24	1.41	1.51
2	A	1101	LMT	O5'-C1'	3.18	1.49	1.41
2	D	1101	LMT	O5'-C1'	3.16	1.49	1.41
2	D	1101	LMT	O3B-C3B	3.14	1.50	1.43
2	E	1101	LMT	O5'-C1'	3.12	1.49	1.41
2	D	1101	LMT	C6'-C5'	-3.11	1.41	1.51
2	A	1101	LMT	C6'-C5'	-3.11	1.41	1.51
2	A	1101	LMT	O1'-C1'	3.08	1.45	1.40
2	C	1101	LMT	C6'-C5'	-2.92	1.42	1.51
2	F	1101	LMT	C3'-C2'	-2.86	1.45	1.52
2	F	1101	LMT	O3B-C3B	2.84	1.49	1.43
2	B	1101	LMT	O3B-C3B	2.77	1.49	1.43
2	C	1101	LMT	C3'-C2'	-2.67	1.45	1.52
2	C	1101	LMT	O3B-C3B	2.64	1.49	1.43
2	A	1101	LMT	O3B-C3B	2.63	1.49	1.43
2	C	1101	LMT	O2'-C2'	2.56	1.49	1.43
2	B	1101	LMT	O5'-C1'	2.55	1.48	1.41
2	A	1101	LMT	C3'-C2'	-2.51	1.45	1.52
2	E	1101	LMT	O2'-C2'	2.44	1.48	1.43
2	D	1101	LMT	O2'-C2'	2.36	1.48	1.43
2	B	1101	LMT	C3B-C2B	-2.35	1.46	1.52
2	B	1101	LMT	O3'-C3'	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O3B-C3B	2.32	1.48	1.43
2	A	1101	LMT	O2'-C2'	2.31	1.48	1.43
2	E	1101	LMT	O3'-C3'	2.24	1.48	1.43
2	B	1101	LMT	C3'-C2'	-2.21	1.46	1.52
2	A	1101	LMT	C3B-C2B	-2.21	1.46	1.52
2	A	1101	LMT	O3'-C3'	2.20	1.48	1.43
2	E	1101	LMT	C3B-C2B	-2.18	1.46	1.52
2	F	1101	LMT	O2'-C2'	2.07	1.47	1.43
2	E	1101	LMT	C3'-C2'	-2.03	1.47	1.52
2	B	1101	LMT	C5-C4	2.03	1.63	1.51
2	E	1101	LMT	C5-C4	2.02	1.62	1.51
2	C	1101	LMT	C5-C4	2.01	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	LMT	C4B-C3B-C2B	4.14	118.05	110.82
2	B	1101	LMT	C1'-O5'-C5'	-4.01	105.82	113.69
2	C	1101	LMT	C3B-C4B-C5B	3.91	117.21	110.24
2	E	1101	LMT	C3B-C4B-C5B	-3.58	103.84	110.24
2	B	1101	LMT	C1B-O5B-C5B	3.52	120.59	113.69
2	B	1101	LMT	O5B-C5B-C4B	3.50	116.06	109.69
2	C	1101	LMT	C1-O1'-C1'	3.42	119.51	113.84
2	A	1101	LMT	C1B-O1B-C4'	-3.29	109.83	117.96
2	C	1101	LMT	C1B-O1B-C4'	-3.21	110.03	117.96
2	C	1101	LMT	C1B-C2B-C3B	3.04	116.34	110.00
2	A	1101	LMT	O5'-C5'-C6'	2.87	113.56	106.44
2	C	1101	LMT	O3B-C3B-C4B	-2.81	103.86	110.35
2	B	1101	LMT	O1'-C1'-C2'	2.79	112.66	108.30
2	D	1101	LMT	C2'-C3'-C4'	2.78	116.03	109.68
2	D	1101	LMT	O1B-C1B-C2B	2.51	114.60	108.10
2	E	1101	LMT	O1'-C1'-C2'	2.46	112.14	108.30
2	B	1101	LMT	C1'-C2'-C3'	2.42	115.04	110.00
2	D	1101	LMT	C1B-C2B-C3B	2.39	114.97	110.00
2	D	1101	LMT	C1B-O1B-C4'	-2.36	112.11	117.96
2	C	1101	LMT	O5'-C5'-C6'	2.36	112.31	106.44
2	E	1101	LMT	C1-O1'-C1'	2.29	117.64	113.84
2	B	1101	LMT	O5'-C5'-C6'	2.28	112.11	106.44
2	F	1101	LMT	O4'-C4B-C3B	-2.26	105.12	110.35
2	E	1101	LMT	C4B-C3B-C2B	-2.19	107.00	110.82
2	D	1101	LMT	C1'-C2'-C3'	2.19	114.55	110.00
2	D	1101	LMT	O5B-C5B-C6B	2.15	111.79	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	LMT	O5'-C5'-C4'	-2.15	105.21	109.75
2	E	1101	LMT	C1B-O1B-C4'	-2.15	112.65	117.96
2	B	1101	LMT	O2'-C2'-C3'	-2.14	105.41	110.35
2	C	1101	LMT	O1B-C1B-C2B	2.11	113.57	108.10
2	C	1101	LMT	O4'-C4B-C3B	-2.08	105.55	110.35
2	A	1101	LMT	C1'-C2'-C3'	-2.04	105.74	110.00
2	D	1101	LMT	O3'-C3'-C2'	-2.04	105.64	110.35
2	C	1101	LMT	O3B-C3B-C2B	-2.03	105.65	110.35
2	D	1101	LMT	C6B-C5B-C4B	-2.02	108.28	113.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1101	LMT	C3B

All (69) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
2	B	1101	LMT	O1'-C1-C2-C3
2	D	1101	LMT	O5'-C5'-C6'-O6'
2	D	1101	LMT	O1'-C1-C2-C3
2	B	1101	LMT	C3-C4-C5-C6
2	D	1101	LMT	C4'-C5'-C6'-O6'
2	D	1101	LMT	C2-C3-C4-C5
2	D	1101	LMT	C4-C5-C6-C7
2	E	1101	LMT	C3-C4-C5-C6
2	B	1101	LMT	C7-C8-C9-C10
2	E	1101	LMT	C5-C6-C7-C8
2	F	1101	LMT	C1-C2-C3-C4
2	C	1101	LMT	O1'-C1-C2-C3
2	E	1101	LMT	C4-C5-C6-C7
2	F	1101	LMT	C3-C4-C5-C6
2	A	1101	LMT	C4B-C5B-C6B-O6B
2	C	1101	LMT	C6-C7-C8-C9
2	C	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C2-C1-O1'-C1'
2	D	1101	LMT	C2-C1-O1'-C1'
2	E	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C7-C8-C9-C10
2	F	1101	LMT	C5-C6-C7-C8
2	C	1101	LMT	C4B-C5B-C6B-O6B
2	B	1101	LMT	C11-C10-C9-C8
2	D	1101	LMT	C11-C10-C9-C8
2	E	1101	LMT	C1-C2-C3-C4
2	A	1101	LMT	C5-C6-C7-C8
2	A	1101	LMT	C7-C8-C9-C10
2	E	1101	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	C2'-C1'-O1'-C1
2	A	1101	LMT	O1'-C1-C2-C3
2	A	1101	LMT	C2'-C1'-O1'-C1
2	C	1101	LMT	C7-C8-C9-C10
2	E	1101	LMT	O5B-C1B-O1B-C4'
2	E	1101	LMT	O1'-C1-C2-C3
2	C	1101	LMT	C1-C2-C3-C4
2	B	1101	LMT	C9-C10-C11-C12
2	C	1101	LMT	O5B-C5B-C6B-O6B
2	D	1101	LMT	O5'-C1'-O1'-C1
2	E	1101	LMT	C2B-C1B-O1B-C4'
2	A	1101	LMT	O5'-C1'-O1'-C1
2	F	1101	LMT	C6-C7-C8-C9

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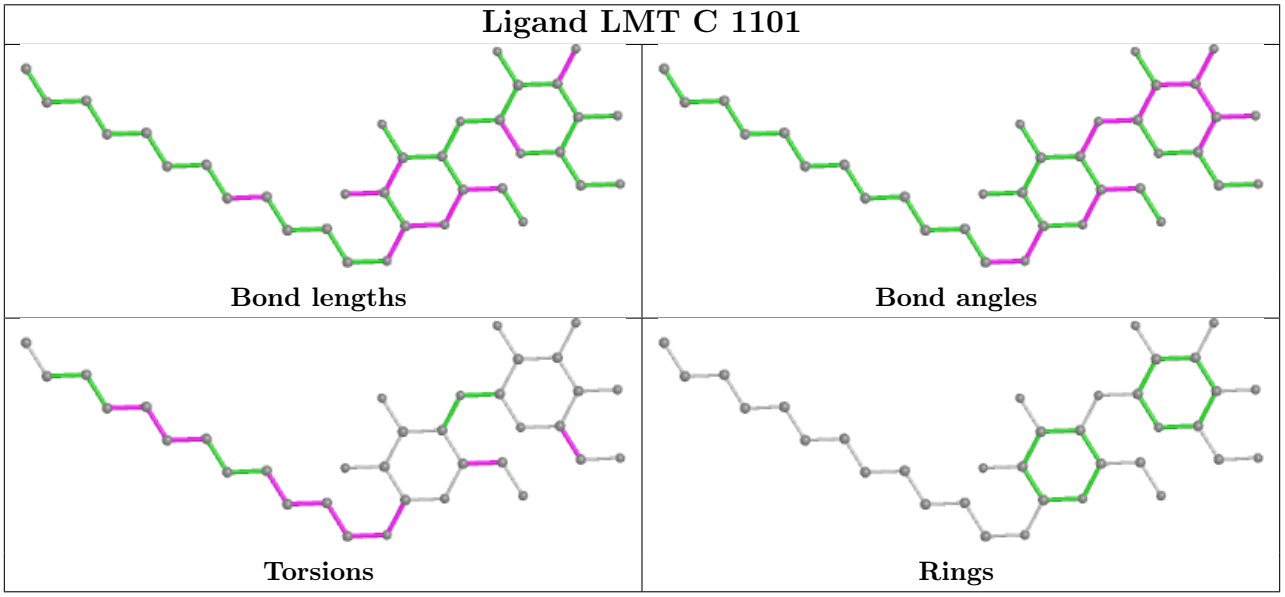
Mol	Chain	Res	Type	Atoms
2	C	1101	LMT	C2-C3-C4-C5
2	A	1101	LMT	C6-C7-C8-C9
2	E	1101	LMT	C11-C10-C9-C8

There are no ring outliers.

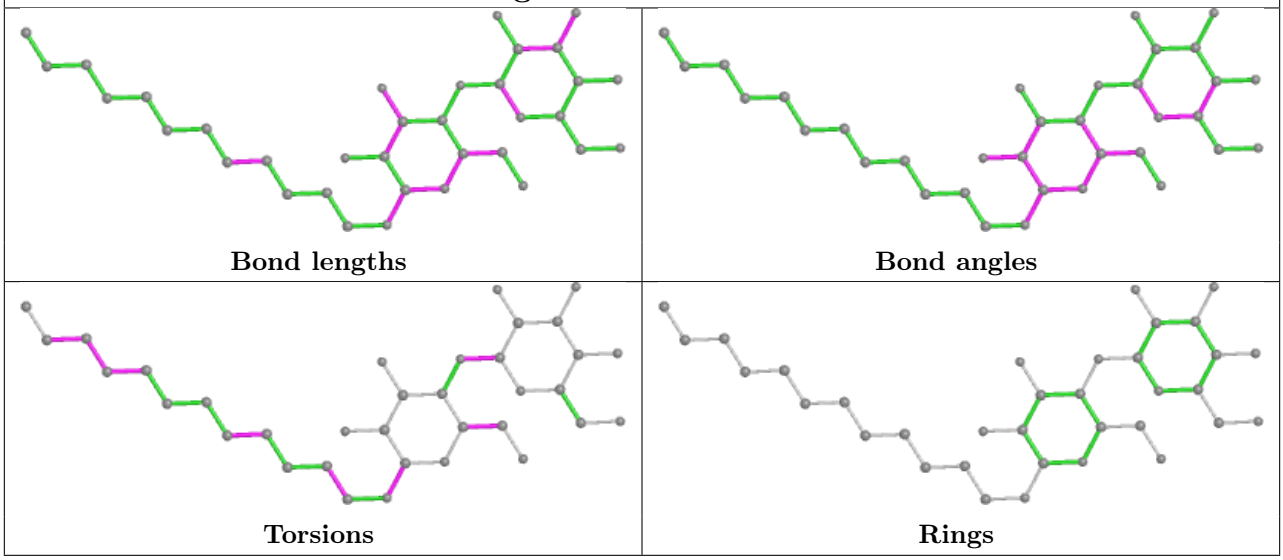
5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	LMT	7	0
2	F	1101	LMT	3	0
2	A	1101	LMT	3	0
2	D	1101	LMT	7	0
2	E	1101	LMT	9	0

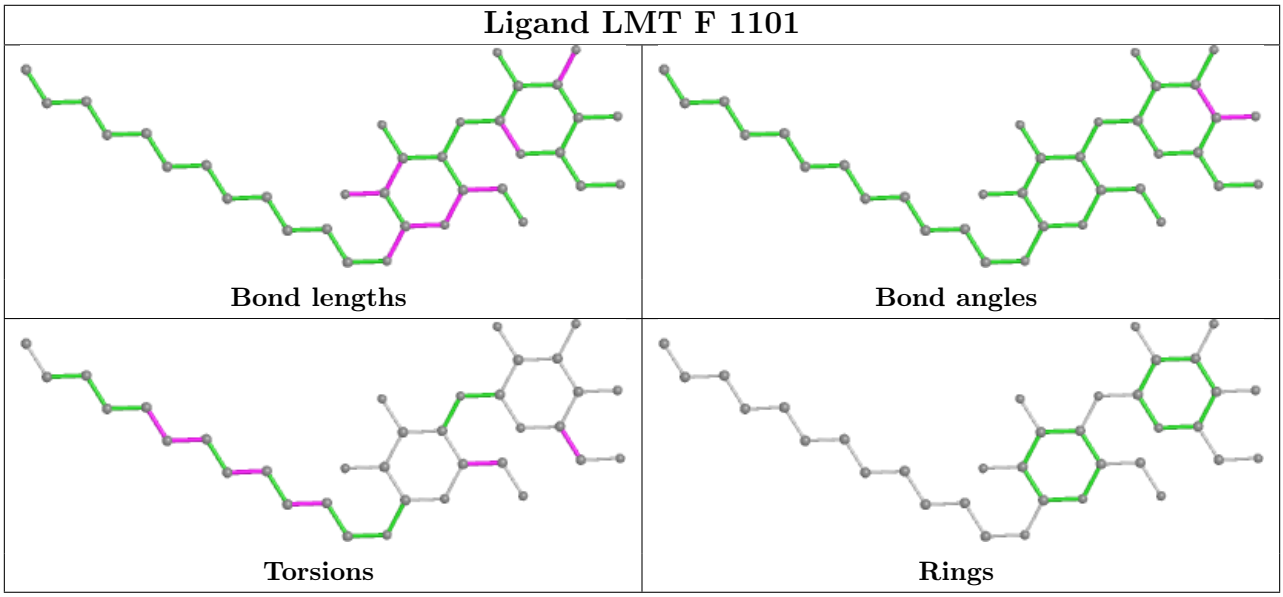
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



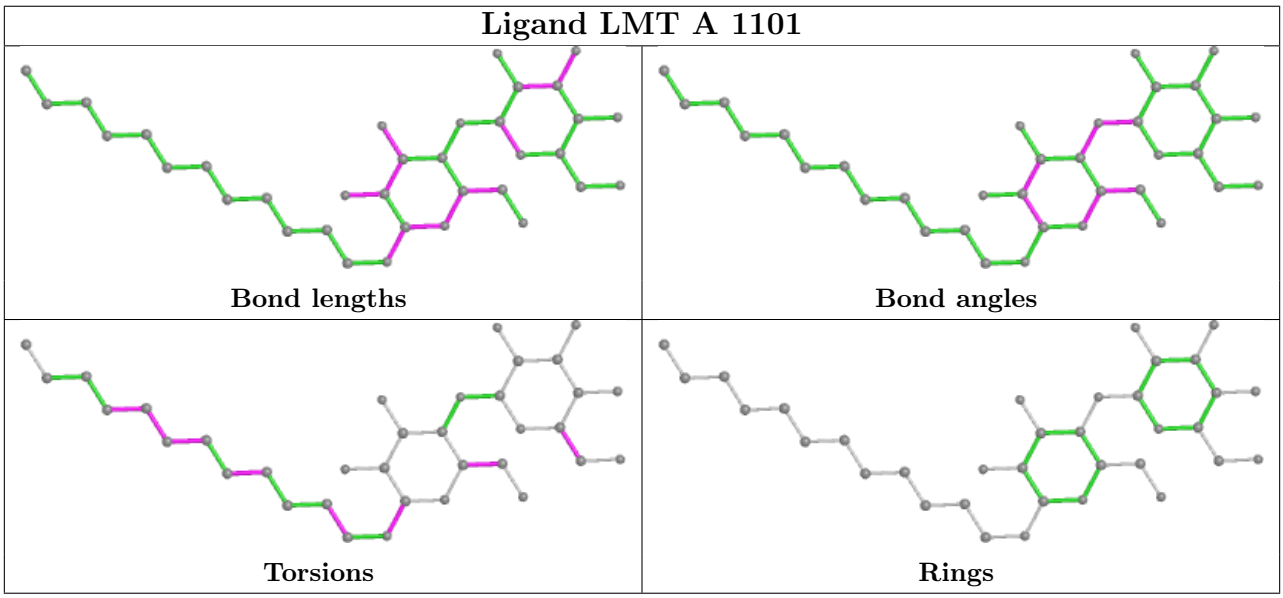
Ligand LMT B 1101



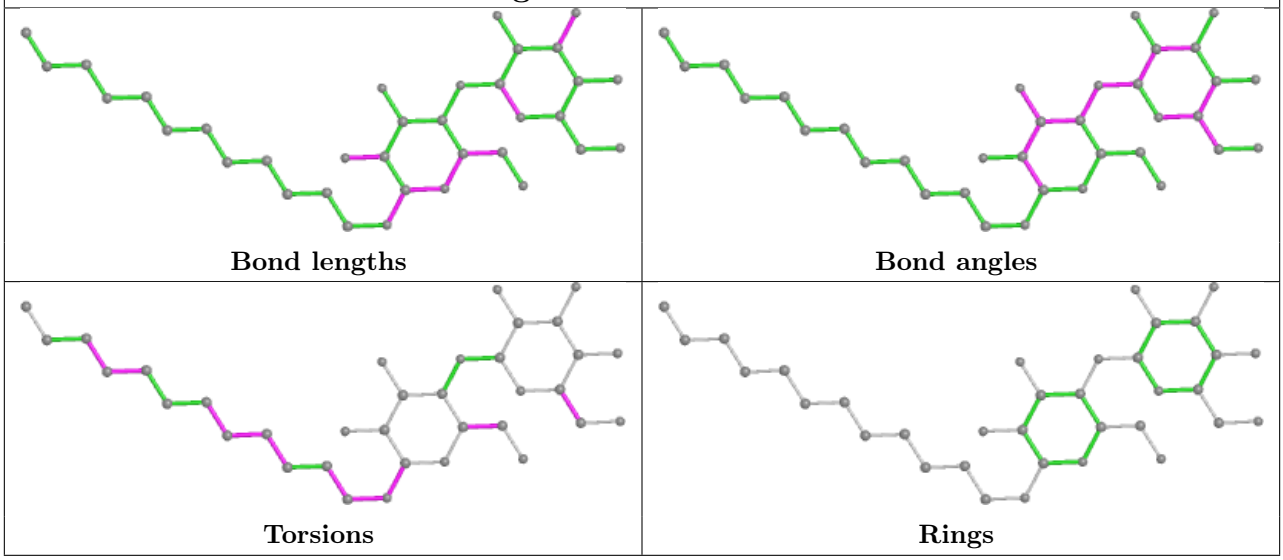
Ligand LMT F 1101



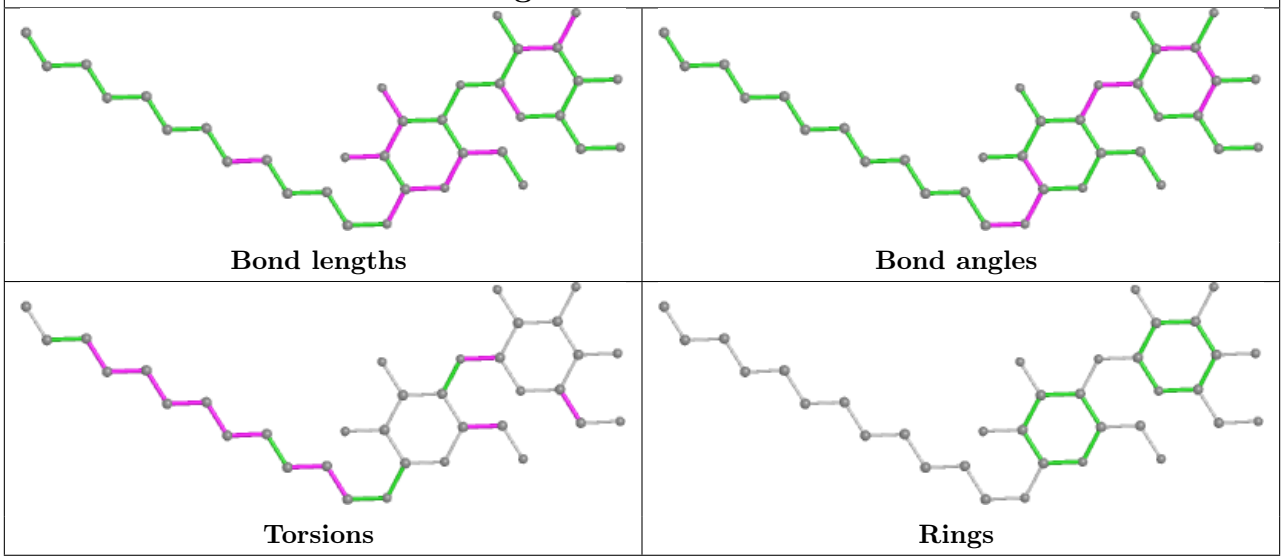
Ligand LMT A 1101



Ligand LMT D 1101



Ligand LMT E 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	1042/1049 (99%)	0.60	130 (12%)	3	3	48, 78, 110, 142	0
1	B	1043/1049 (99%)	0.59	120 (11%)	4	4	36, 72, 102, 149	0
1	C	1042/1049 (99%)	0.54	101 (9%)	7	8	34, 72, 100, 155	0
1	D	1042/1049 (99%)	0.68	145 (13%)	2	2	40, 89, 116, 145	0
1	E	1042/1049 (99%)	0.81	174 (16%)	1	1	57, 90, 113, 158	0
1	F	1042/1049 (99%)	0.80	172 (16%)	1	2	51, 86, 112, 144	0
All	All	6253/6294 (99%)	0.67	842 (13%)	3	3	34, 82, 111, 158	0

All (842) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	869	SER	15.4
1	E	314	GLU	15.3
1	E	315	PRO	14.2
1	E	311	ALA	13.6
1	B	314	GLU	10.8
1	B	315	PRO	10.2
1	F	675	GLY	10.0
1	E	869	SER	9.9
1	D	322	LYS	9.7
1	F	442	LEU	9.7
1	C	314	GLU	9.3
1	E	105	VAL	9.3
1	E	290	GLY	8.6
1	E	291	ILE	8.5
1	D	720	GLY	8.4
1	F	676	THR	8.4
1	E	307	ARG	8.3
1	C	720	GLY	8.2
1	E	310	LEU	8.1

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Mol	Chain	Res	Type	RSRZ
1	D	719	ASN	8.1
1	F	836	SER	7.8
1	C	310	LEU	7.8
1	C	721	LEU	7.7
1	E	769	LYS	7.6
1	C	719	ASN	7.6
1	E	104	GLN	7.5
1	F	117	LEU	7.5
1	C	307	ARG	7.5
1	F	59	ASP	7.2
1	D	141	GLY	7.1
1	D	323	ILE	7.1
1	B	311	ALA	7.1
1	F	109	ASN	7.1
1	E	308	ALA	6.9
1	E	242	SER	6.7
1	F	441	ALA	6.7
1	F	801	PHE	6.5
1	F	791	VAL	6.5
1	A	801	PHE	6.5
1	F	618	ALA	6.4
1	E	765	ARG	6.4
1	E	25	LEU	6.4
1	B	71	GLY	6.4
1	D	791	VAL	6.3
1	D	869	SER	6.3
1	F	719	ASN	6.3
1	F	826	GLU	6.2
1	E	102	ILE	6.2
1	E	764	ASP	6.1
1	D	843	LEU	6.1
1	D	386	PHE	6.0
1	E	303	ALA	5.9
1	C	79	SER	5.9
1	F	403	GLY	5.9
1	F	720	GLY	5.9
1	F	60	THR	5.9
1	F	721	LEU	5.8
1	A	102	ILE	5.8
1	A	761	ASP	5.8
1	E	366	LEU	5.8
1	F	240	LEU	5.8

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Mol	Chain	Res	Type	RSRZ
1	E	33	ALA	5.7
1	A	705	GLU	5.7
1	C	791	VAL	5.7
1	E	106	GLN	5.6
1	F	763	ILE	5.6
1	C	856	GLY	5.6
1	F	815	ARG	5.6
1	B	617	PHE	5.6
1	F	873	ALA	5.6
1	B	73	ASP	5.6
1	F	865	GLN	5.6
1	F	315	PRO	5.6
1	C	804	PHE	5.6
1	B	105	VAL	5.5
1	D	768	VAL	5.5
1	D	459	PHE	5.5
1	B	791	VAL	5.5
1	B	101	ASP	5.5
1	B	102	ILE	5.5
1	B	104	GLN	5.5
1	D	690	LEU	5.5
1	D	325	TYR	5.4
1	A	789	TRP	5.4
1	E	137	LEU	5.4
1	C	311	ALA	5.4
1	E	488	LEU	5.4
1	E	791	VAL	5.4
1	F	402	ILE	5.4
1	D	840	ALA	5.4
1	E	801	PHE	5.3
1	D	853	THR	5.3
1	E	762	PHE	5.3
1	D	868	LEU	5.3
1	A	765	ARG	5.3
1	F	837	THR	5.3
1	A	174	ASP	5.2
1	A	768	VAL	5.2
1	D	321	LEU	5.2
1	B	801	PHE	5.2
1	B	764	ASP	5.2
1	E	768	VAL	5.2
1	D	461	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	308	ALA	5.2
1	F	828	LEU	5.2
1	D	324	VAL	5.2
1	D	842	GLU	5.1
1	F	362	PHE	5.1
1	F	314	GLU	5.1
1	E	129	VAL	5.1
1	D	715	SER	5.1
1	E	789	TRP	5.1
1	F	804	PHE	5.0
1	B	312	LYS	5.0
1	E	770	LYS	5.0
1	F	805	SER	5.0
1	D	801	PHE	5.0
1	A	239	ARG	5.0
1	A	673	GLU	5.0
1	F	80	SER	5.0
1	D	841	MET	5.0
1	A	767	ARG	4.9
1	D	844	MET	4.9
1	C	826	GLU	4.9
1	A	396	PHE	4.9
1	A	369	THR	4.9
1	A	321	LEU	4.9
1	C	801	PHE	4.9
1	E	706	ALA	4.8
1	B	462	SER	4.8
1	A	769	LYS	4.8
1	B	59	ASP	4.8
1	D	59	ASP	4.8
1	B	868	LEU	4.7
1	A	240	LEU	4.7
1	A	846	GLN	4.7
1	E	409	ALA	4.7
1	E	761	ASP	4.7
1	C	855	VAL	4.7
1	E	681	ASP	4.6
1	E	617	PHE	4.6
1	F	107	VAL	4.6
1	D	458	PHE	4.6
1	A	766	GLY	4.6
1	E	513	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	296	GLY	4.6
1	F	410	ILE	4.6
1	E	367	ILE	4.6
1	B	618	ALA	4.5
1	F	293	LEU	4.5
1	E	717	ARG	4.5
1	C	851	LEU	4.5
1	D	851	LEU	4.5
1	F	118	LEU	4.5
1	A	35	TYR	4.5
1	E	674	LEU	4.5
1	C	69	MET	4.5
1	A	716	VAL	4.5
1	C	107	VAL	4.5
1	F	674	LEU	4.5
1	B	720	GLY	4.4
1	E	929	VAL	4.4
1	F	762	PHE	4.4
1	E	71	GLY	4.4
1	F	103	ALA	4.4
1	F	325	TYR	4.4
1	F	746	ILE	4.4
1	D	1042	HIS	4.4
1	D	1041	GLU	4.4
1	B	291	ILE	4.4
1	A	706	ALA	4.4
1	C	315	PRO	4.3
1	E	743	ILE	4.3
1	E	210	GLN	4.3
1	A	790	TYR	4.3
1	E	362	PHE	4.3
1	A	486	LEU	4.3
1	F	356	TYR	4.3
1	D	769	LYS	4.3
1	A	193	LEU	4.3
1	D	764	ASP	4.3
1	E	462	SER	4.2
1	F	786	ILE	4.2
1	F	62	THR	4.2
1	D	837	THR	4.2
1	E	369	THR	4.2
1	F	481	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	789	TRP	4.2
1	D	839	GLU	4.1
1	E	241	THR	4.1
1	D	460	GLY	4.1
1	E	243	THR	4.1
1	E	944	LEU	4.1
1	E	933	THR	4.1
1	F	941	ASN	4.1
1	D	859	TRP	4.1
1	F	79	SER	4.0
1	D	102	ILE	4.0
1	E	78	MET	4.0
1	A	72	ILE	4.0
1	A	791	VAL	4.0
1	F	831	ALA	4.0
1	F	306	ILE	4.0
1	A	762	PHE	4.0
1	C	122	VAL	4.0
1	B	766	GLY	3.9
1	F	619	GLY	3.9
1	B	866	GLU	3.9
1	E	866	GLU	3.9
1	B	246	PHE	3.9
1	C	109	ASN	3.9
1	E	487	ILE	3.9
1	B	619	GLY	3.9
1	C	836	SER	3.9
1	A	679	GLY	3.9
1	F	617	PHE	3.9
1	C	868	LEU	3.9
1	D	713	LEU	3.9
1	F	790	TYR	3.9
1	F	731	ILE	3.9
1	C	129	VAL	3.8
1	E	32	VAL	3.8
1	F	945	ILE	3.8
1	A	400	LEU	3.8
1	D	721	LEU	3.8
1	E	174	ASP	3.8
1	E	92	LEU	3.8
1	D	63	GLN	3.8
1	D	706	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	173	GLY	3.8
1	B	458	PHE	3.8
1	C	402	ILE	3.8
1	D	761	ASP	3.8
1	D	317	PHE	3.8
1	E	309	GLU	3.8
1	D	400	LEU	3.8
1	D	767	ARG	3.8
1	B	719	ASN	3.8
1	C	675	GLY	3.8
1	D	870	GLY	3.8
1	B	307	ARG	3.8
1	E	390	ILE	3.8
1	E	181	GLN	3.8
1	F	770	LYS	3.8
1	A	92	LEU	3.8
1	D	140	VAL	3.8
1	D	310	LEU	3.7
1	C	93	THR	3.7
1	E	790	TYR	3.7
1	A	763	ILE	3.7
1	B	323	ILE	3.7
1	A	315	PRO	3.7
1	C	322	LYS	3.7
1	A	843	LEU	3.7
1	B	72	ILE	3.7
1	F	111	LEU	3.7
1	E	26	ALA	3.7
1	F	93	THR	3.7
1	B	671	ILE	3.7
1	E	312	LYS	3.7
1	D	101	ASP	3.7
1	E	705	GLU	3.7
1	F	856	GLY	3.7
1	C	403	GLY	3.7
1	E	59	ASP	3.7
1	F	69	MET	3.7
1	B	770	LYS	3.7
1	C	166	ILE	3.6
1	F	406	VAL	3.6
1	E	868	LEU	3.6
1	B	876	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	3	ASN	3.6
1	C	325	TYR	3.6
1	E	922	THR	3.6
1	D	60	THR	3.6
1	E	720	GLY	3.6
1	D	180	SER	3.6
1	E	798	MET	3.6
1	B	316	PHE	3.6
1	D	763	ILE	3.6
1	D	714	THR	3.6
1	D	789	TRP	3.6
1	A	372	VAL	3.6
1	F	193	LEU	3.6
1	F	322	LYS	3.5
1	D	688	ALA	3.5
1	B	733	GLN	3.5
1	F	323	ILE	3.5
1	E	733	GLN	3.5
1	A	458	PHE	3.5
1	A	242	SER	3.5
1	C	763	ILE	3.5
1	F	768	VAL	3.5
1	F	868	LEU	3.5
1	B	768	VAL	3.5
1	A	470	PHE	3.5
1	D	762	PHE	3.5
1	B	310	LEU	3.5
1	D	689	GLY	3.5
1	C	674	LEU	3.5
1	F	307	ARG	3.5
1	A	866	GLU	3.5
1	B	721	LEU	3.5
1	C	59	ASP	3.5
1	A	850	LYS	3.5
1	E	103	ALA	3.5
1	F	700	ASN	3.4
1	D	330	THR	3.4
1	D	741	VAL	3.4
1	A	323	ILE	3.4
1	A	713	LEU	3.4
1	D	486	LEU	3.4
1	D	396	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	763	ILE	3.4
1	C	321	LEU	3.4
1	F	57	VAL	3.4
1	C	789	TRP	3.4
1	F	462	SER	3.4
1	C	323	ILE	3.4
1	A	617	PHE	3.4
1	C	768	VAL	3.4
1	B	106	GLN	3.4
1	E	183	ALA	3.4
1	B	624	THR	3.4
1	E	678	THR	3.4
1	A	43	VAL	3.4
1	E	107	VAL	3.4
1	E	177	LEU	3.4
1	C	762	PHE	3.4
1	D	708	LYS	3.4
1	E	708	LYS	3.4
1	E	193	LEU	3.3
1	A	368	PRO	3.3
1	E	804	PHE	3.3
1	F	91	THR	3.3
1	A	976	LEU	3.3
1	A	615	PHE	3.3
1	F	96	SER	3.3
1	E	800	PRO	3.3
1	C	849	SER	3.3
1	D	846	GLN	3.3
1	B	317	PHE	3.3
1	F	681	ASP	3.3
1	F	105	VAL	3.3
1	A	842	GLU	3.3
1	E	843	LEU	3.3
1	A	661	ALA	3.3
1	B	870	GLY	3.3
1	A	376	LEU	3.3
1	E	325	TYR	3.3
1	E	400	LEU	3.3
1	C	803	ALA	3.2
1	F	58	GLN	3.2
1	B	806	SER	3.2
1	E	405	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	712	MET	3.2
1	A	770	LYS	3.2
1	E	128	SER	3.2
1	F	326	PRO	3.2
1	F	733	GLN	3.2
1	E	43	VAL	3.2
1	E	182	TYR	3.2
1	C	712	MET	3.2
1	E	30	LEU	3.2
1	B	805	SER	3.2
1	E	292	LYS	3.2
1	E	317	PHE	3.2
1	F	764	ASP	3.2
1	A	293	LEU	3.2
1	D	733	GLN	3.2
1	E	844	MET	3.2
1	F	563	PHE	3.2
1	C	837	THR	3.2
1	F	673	GLU	3.1
1	D	770	LYS	3.1
1	D	4	PHE	3.1
1	B	92	LEU	3.1
1	C	306	ILE	3.1
1	A	136	PHE	3.1
1	A	680	PHE	3.1
1	C	317	PHE	3.1
1	F	295	THR	3.1
1	F	110	LYS	3.1
1	C	303	ALA	3.1
1	C	106	GLN	3.1
1	F	638	PRO	3.1
1	D	142	VAL	3.1
1	D	462	SER	3.1
1	E	94	PHE	3.1
1	B	844	MET	3.1
1	D	802	SER	3.1
1	E	239	ARG	3.1
1	B	701	GLN	3.1
1	C	501	ALA	3.1
1	A	411	VAL	3.1
1	F	310	LEU	3.1
1	F	463	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	3.1
1	E	783	PRO	3.1
1	D	463	THR	3.1
1	E	138	MET	3.0
1	C	362	PHE	3.0
1	B	846	GLN	3.0
1	D	106	GLN	3.0
1	D	143	ILE	3.0
1	E	398	MET	3.0
1	A	800	PRO	3.0
1	A	292	LYS	3.0
1	F	620	ARG	3.0
1	F	40	PRO	3.0
1	D	617	PHE	3.0
1	F	799	VAL	3.0
1	D	804	PHE	3.0
1	D	182	TYR	3.0
1	D	852	PRO	3.0
1	E	73	ASP	3.0
1	F	399	VAL	3.0
1	A	310	LEU	3.0
1	B	488	LEU	3.0
1	A	407	ASP	3.0
1	C	291	ILE	3.0
1	E	240	LEU	3.0
1	B	94	PHE	3.0
1	F	65	ILE	3.0
1	B	843	LEU	3.0
1	D	681	ASP	3.0
1	A	134	SER	3.0
1	B	369	THR	3.0
1	C	105	VAL	2.9
1	C	724	THR	2.9
1	C	210	GLN	2.9
1	E	786	ILE	2.9
1	A	578	LEU	2.9
1	D	578	LEU	2.9
1	C	761	ASP	2.9
1	D	291	ILE	2.9
1	D	716	VAL	2.9
1	E	799	VAL	2.9
1	D	36	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	493	CYS	2.9
1	B	871	ASN	2.9
1	B	872	GLN	2.9
1	D	671	ILE	2.9
1	D	736	ALA	2.9
1	D	749	THR	2.9
1	D	854	GLY	2.9
1	D	43	VAL	2.9
1	E	937	LEU	2.9
1	F	129	VAL	2.9
1	B	355	MET	2.9
1	F	43	VAL	2.9
1	F	409	ALA	2.9
1	C	828	LEU	2.9
1	A	183	ALA	2.9
1	A	788	ASP	2.9
1	B	25	LEU	2.8
1	F	38	ILE	2.8
1	D	211	ASN	2.8
1	D	64	VAL	2.8
1	D	136	PHE	2.8
1	D	315	PRO	2.8
1	E	943	ILE	2.8
1	E	742	SER	2.8
1	F	39	ALA	2.8
1	C	442	LEU	2.8
1	A	853	THR	2.8
1	E	37	THR	2.8
1	F	383	LEU	2.8
1	C	642	ASN	2.8
1	E	1020	PHE	2.8
1	A	397	GLY	2.8
1	F	398	MET	2.8
1	B	739	LEU	2.8
1	B	412	VAL	2.8
1	E	806	SER	2.8
1	D	709	HIS	2.8
1	F	357	LEU	2.8
1	D	105	VAL	2.8
1	E	865	GLN	2.8
1	A	336	SER	2.8
1	E	79	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	198	LEU	2.8
1	F	246	PHE	2.8
1	A	27	ILE	2.8
1	D	65	ILE	2.8
1	F	834	GLY	2.8
1	A	390	ILE	2.7
1	B	135	SER	2.7
1	C	760	ASN	2.7
1	A	244	GLU	2.7
1	D	487	ILE	2.7
1	F	207	ILE	2.7
1	A	322	LYS	2.7
1	B	762	PHE	2.7
1	F	806	SER	2.7
1	F	81	ASN	2.7
1	B	63	GLN	2.7
1	E	328	ASP	2.7
1	D	35	TYR	2.7
1	F	773	VAL	2.7
1	E	198	LEU	2.7
1	F	835	LYS	2.7
1	E	719	ASN	2.7
1	B	758	TYR	2.7
1	F	166	ILE	2.7
1	F	106	GLN	2.7
1	E	93	THR	2.7
1	B	705	GLU	2.7
1	B	842	GLU	2.7
1	F	311	ALA	2.7
1	F	577	GLN	2.7
1	A	355	MET	2.7
1	B	620	ARG	2.7
1	A	210	GLN	2.7
1	A	246	PHE	2.7
1	A	621	GLY	2.7
1	A	995	ALA	2.7
1	E	357	LEU	2.7
1	E	27	ILE	2.7
1	E	164	ASP	2.7
1	A	181	GLN	2.7
1	B	804	PHE	2.7
1	B	803	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	739	LEU	2.7
1	A	733	GLN	2.7
1	A	30	LEU	2.6
1	F	944	LEU	2.6
1	B	67	GLN	2.6
1	A	1040	ILE	2.6
1	B	790	TYR	2.6
1	D	729	ILE	2.6
1	D	867	ARG	2.6
1	D	577	GLN	2.6
1	D	977	MET	2.6
1	A	327	TYR	2.6
1	E	65	ILE	2.6
1	E	370	ILE	2.6
1	C	1039	ASP	2.6
1	B	410	ILE	2.6
1	E	803	ALA	2.6
1	F	766	GLY	2.6
1	A	12	ALA	2.6
1	D	92	LEU	2.6
1	D	746	ILE	2.6
1	F	142	VAL	2.6
1	F	372	VAL	2.6
1	D	701	GLN	2.6
1	E	718	PRO	2.6
1	E	850	LYS	2.6
1	F	722	GLU	2.6
1	F	829	GLY	2.6
1	B	42	ALA	2.6
1	A	241	THR	2.6
1	F	759	VAL	2.6
1	C	835	LYS	2.6
1	E	348	ILE	2.6
1	D	328	ASP	2.6
1	E	380	PHE	2.6
1	E	313	MET	2.6
1	B	240	LEU	2.6
1	E	28	LEU	2.6
1	F	860	THR	2.6
1	E	289	LEU	2.6
1	F	671	ILE	2.6
1	A	899	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	63	GLN	2.5
1	C	511	GLY	2.5
1	C	366	LEU	2.5
1	B	534	ILE	2.5
1	E	716	VAL	2.5
1	A	764	ASP	2.5
1	F	92	LEU	2.5
1	A	852	PRO	2.5
1	F	56	THR	2.5
1	B	289	LEU	2.5
1	C	848	ALA	2.5
1	C	713	LEU	2.5
1	E	131	LYS	2.5
1	E	702	LEU	2.5
1	C	140	VAL	2.5
1	E	42	ALA	2.5
1	C	510	LYS	2.5
1	E	492	LEU	2.5
1	A	666	PHE	2.5
1	A	804	PHE	2.5
1	B	802	SER	2.5
1	B	107	VAL	2.5
1	F	473	THR	2.5
1	D	712	MET	2.5
1	E	184	MET	2.5
1	E	101	ASP	2.5
1	B	623	ASN	2.5
1	B	531	VAL	2.5
1	E	619	GLY	2.5
1	A	640	GLU	2.5
1	E	412	VAL	2.5
1	F	672	VAL	2.5
1	E	715	SER	2.5
1	F	135	SER	2.5
1	F	871	ASN	2.5
1	A	573	MET	2.5
1	A	32	VAL	2.5
1	E	270	LEU	2.5
1	A	786	ILE	2.5
1	C	207	ILE	2.5
1	A	107	VAL	2.4
1	D	624	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	184	MET	2.4
1	A	103	ALA	2.4
1	A	463	THR	2.4
1	E	316	PHE	2.4
1	A	410	ILE	2.4
1	F	761	ASP	2.4
1	C	617	PHE	2.4
1	D	615	PHE	2.4
1	A	868	LEU	2.4
1	D	5	PHE	2.4
1	F	459	PHE	2.4
1	B	769	LYS	2.4
1	B	461	GLY	2.4
1	C	867	ARG	2.4
1	B	286	ALA	2.4
1	D	11	PHE	2.4
1	C	80	SER	2.4
1	E	297	ALA	2.4
1	D	388	PHE	2.4
1	C	211	ASN	2.4
1	F	127	VAL	2.4
1	F	321	LEU	2.4
1	E	29	LYS	2.4
1	C	162	MET	2.4
1	D	718	PRO	2.4
1	C	618	ALA	2.4
1	D	38	ILE	2.4
1	B	771	VAL	2.4
1	E	925	VAL	2.4
1	E	1022	VAL	2.4
1	C	941	ASN	2.4
1	D	866	GLU	2.4
1	F	294	ALA	2.4
1	E	175	VAL	2.4
1	E	41	PRO	2.4
1	F	54	ALA	2.4
1	E	851	LEU	2.4
1	A	135	SER	2.4
1	A	316	PHE	2.4
1	C	577	GLN	2.4
1	C	91	THR	2.4
1	D	90	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	707	ALA	2.4
1	E	466	ILE	2.4
1	D	246	PHE	2.3
1	D	307	ARG	2.3
1	F	443	VAL	2.3
1	E	465	ALA	2.3
1	E	926	TYR	2.3
1	A	392	THR	2.3
1	C	741	VAL	2.3
1	A	162	MET	2.3
1	A	337	ILE	2.3
1	E	304	ALA	2.3
1	D	830	GLN	2.3
1	E	496	MET	2.3
1	A	357	LEU	2.3
1	B	207	ILE	2.3
1	D	84	SER	2.3
1	B	672	VAL	2.3
1	C	398	MET	2.3
1	B	439	GLN	2.3
1	D	771	VAL	2.3
1	A	798	MET	2.3
1	B	487	ILE	2.3
1	C	729	ILE	2.3
1	F	892	TYR	2.3
1	F	173	GLY	2.3
1	C	356	TYR	2.3
1	C	410	ILE	2.3
1	D	513	PHE	2.3
1	F	662	MET	2.3
1	C	676	THR	2.3
1	C	854	GLY	2.3
1	F	869	SER	2.3
1	C	308	ALA	2.3
1	B	290	GLY	2.3
1	E	31	PRO	2.3
1	C	746	ILE	2.3
1	E	439	GLN	2.3
1	B	183	ALA	2.3
1	D	178	PHE	2.3
1	F	699	ARG	2.3
1	B	706	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	494	ALA	2.3
1	B	121	GLU	2.3
1	A	343	THR	2.3
1	A	489	THR	2.3
1	E	330	THR	2.3
1	D	200	PRO	2.3
1	E	435	MET	2.3
1	B	362	PHE	2.3
1	D	857	TYR	2.3
1	E	859	TRP	2.2
1	F	100	ALA	2.3
1	F	183	ALA	2.3
1	B	465	ALA	2.2
1	F	467	TYR	2.2
1	B	434	SER	2.2
1	C	458	PHE	2.2
1	E	60	THR	2.2
1	F	516	PHE	2.2
1	B	140	VAL	2.2
1	D	580	ALA	2.2
1	E	618	ALA	2.2
1	F	807	SER	2.2
1	B	786	ILE	2.2
1	A	719	ASN	2.2
1	F	771	VAL	2.2
1	B	851	LEU	2.2
1	B	741	VAL	2.2
1	D	15	ILE	2.2
1	E	406	VAL	2.2
1	E	773	VAL	2.2
1	C	673	GLU	2.2
1	F	800	PRO	2.2
1	F	133	SER	2.2
1	A	874	PRO	2.2
1	A	295	THR	2.2
1	F	317	PHE	2.2
1	D	61	VAL	2.2
1	F	576	VAL	2.2
1	A	60	THR	2.2
1	A	294	ALA	2.2
1	E	250	LEU	2.2
1	E	383	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	488	LEU	2.2
1	F	101	ASP	2.2
1	B	463	THR	2.2
1	C	388	PHE	2.2
1	E	352	PHE	2.2
1	E	714	THR	2.2
1	C	240	LEU	2.2
1	D	618	ALA	2.2
1	C	718	PRO	2.2
1	E	852	PRO	2.2
1	F	178	PHE	2.2
1	E	355	MET	2.2
1	D	62	THR	2.2
1	E	305	ALA	2.1
1	D	358	PHE	2.1
1	E	176	GLN	2.1
1	A	339	GLU	2.1
1	C	502	LYS	2.1
1	F	787	GLY	2.1
1	A	194	ASN	2.1
1	F	677	ALA	2.1
1	C	406	VAL	2.1
1	F	445	ILE	2.1
1	A	13	TRP	2.1
1	A	62	THR	2.1
1	B	103	ALA	2.1
1	B	325	TYR	2.1
1	B	789	TRP	2.1
1	C	3	ASN	2.1
1	C	615	PHE	2.1
1	D	512	PHE	2.1
1	A	340	VAL	2.1
1	A	799	VAL	2.1
1	E	1019	ILE	2.1
1	D	960	LEU	2.1
1	C	60	THR	2.1
1	F	55	LYS	2.1
1	F	765	ARG	2.1
1	A	715	SER	2.1
1	E	829	GLY	2.1
1	C	327	TYR	2.1
1	F	13	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	964	THR	2.1
1	B	400	LEU	2.1
1	D	270	LEU	2.1
1	A	408	ASP	2.1
1	B	11	PHE	2.1
1	A	91	THR	2.1
1	A	207	ILE	2.1
1	B	746	ILE	2.1
1	A	71	GLY	2.1
1	D	67	GLN	2.1
1	D	786	ILE	2.1
1	E	578	LEU	2.1
1	A	403	GLY	2.1
1	B	366	LEU	2.1
1	B	281	PHE	2.1
1	E	982	PHE	2.1
1	F	1020	PHE	2.1
1	F	182	TYR	2.1
1	F	312	LYS	2.1
1	D	111	LEU	2.1
1	F	194	ASN	2.1
1	F	241	THR	2.1
1	A	663	VAL	2.1
1	B	180	SER	2.1
1	D	207	ILE	2.1
1	D	743	ILE	2.1
1	B	198	LEU	2.1
1	C	313	MET	2.1
1	D	516	PHE	2.1
1	D	199	THR	2.1
1	D	800	PRO	2.1
1	D	926	TYR	2.1
1	A	771	VAL	2.1
1	E	767	ARG	2.1
1	B	137	LEU	2.1
1	B	761	ASP	2.1
1	C	829	GLY	2.1
1	F	376	LEU	2.1
1	C	32	VAL	2.1
1	F	661	ALA	2.1
1	B	435	MET	2.1
1	F	281	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	705	GLU	2.0
1	B	41	PRO	2.0
1	F	605	ASN	2.0
1	F	872	GLN	2.0
1	F	641	GLU	2.0
1	B	926	TYR	2.0
1	F	816	LEU	2.0
1	D	982	PHE	2.0
1	B	174	ASP	2.0
1	B	784	ASP	2.0
1	E	135	SER	2.0
1	D	26	ALA	2.0
1	F	405	LEU	2.0
1	A	133	SER	2.0
1	C	48	SER	2.0
1	F	874	PRO	2.0
1	C	484	VAL	2.0
1	A	143	ILE	2.0
1	A	739	LEU	2.0
1	A	975	ILE	2.0
1	F	141	GLY	2.0
1	B	747	ASN	2.0
1	E	199	THR	2.0
1	B	578	LEU	2.0
1	B	765	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

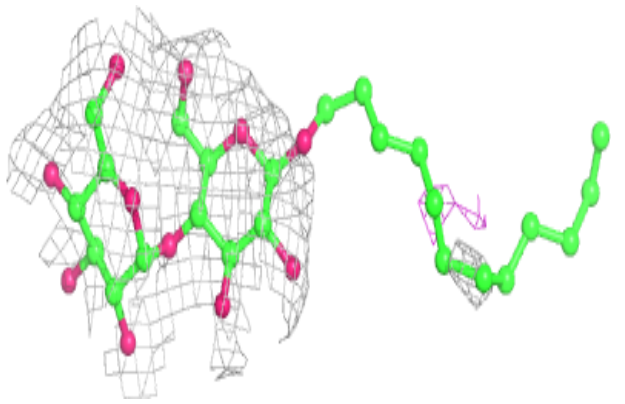
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

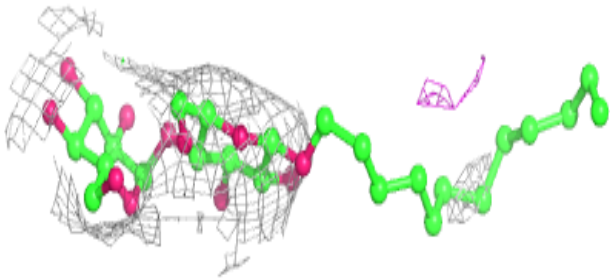
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LMT	E	1101	35/35	0.73	0.48	54,94,105,108	0
2	LMT	B	1101	35/35	0.78	0.49	58,82,95,98	0
2	LMT	D	1101	35/35	0.81	0.38	38,77,87,92	0
2	LMT	C	1101	35/35	0.82	0.32	30,75,84,93	0
2	LMT	A	1101	35/35	0.83	0.36	62,71,84,86	0
2	LMT	F	1101	35/35	0.85	0.39	35,82,93,99	0
3	NI	C	1102	1/1	0.96	0.22	80,80,80,80	0
3	NI	E	1102	1/1	0.96	0.18	96,96,96,96	0
3	NI	A	1102	1/1	0.99	0.16	79,79,79,79	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 E 1101:

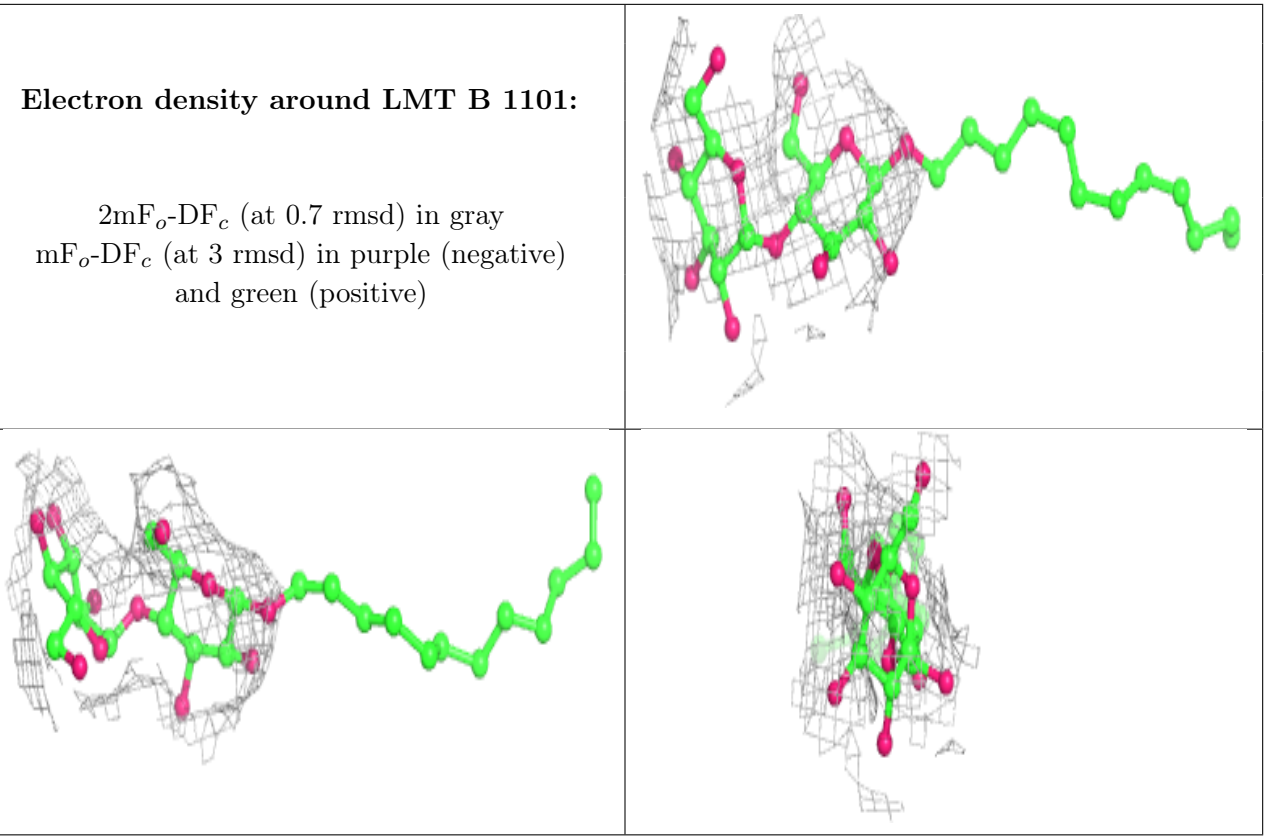
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





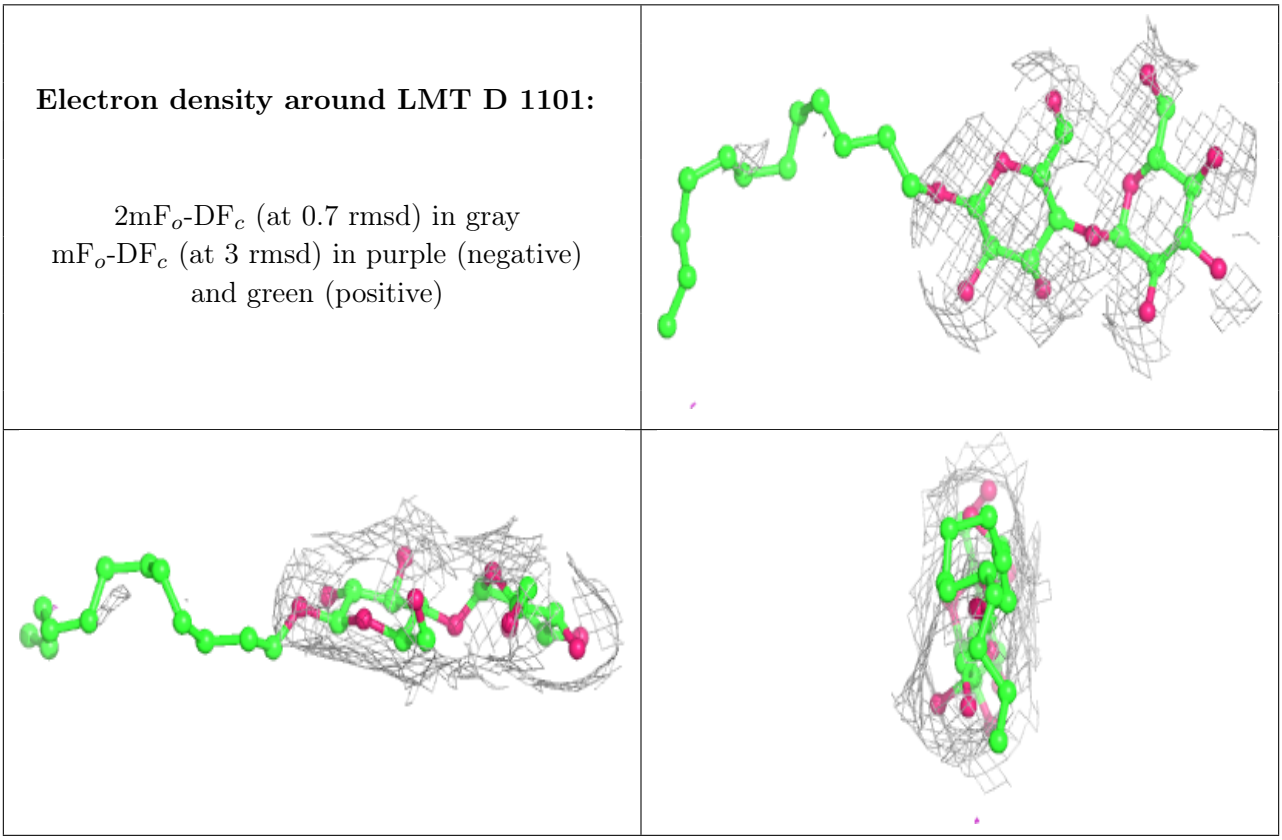
Electron density around LMT B 1101:

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



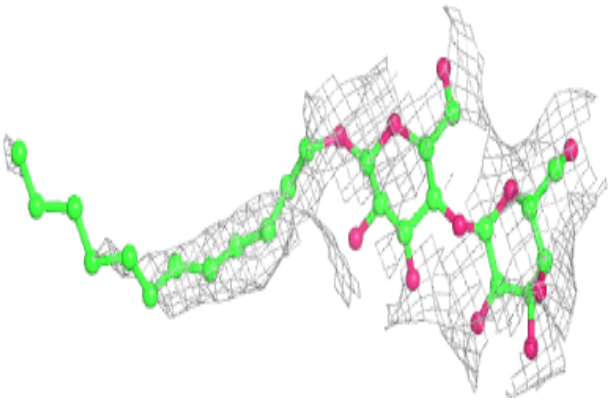
Electron density around LMT D 1101:

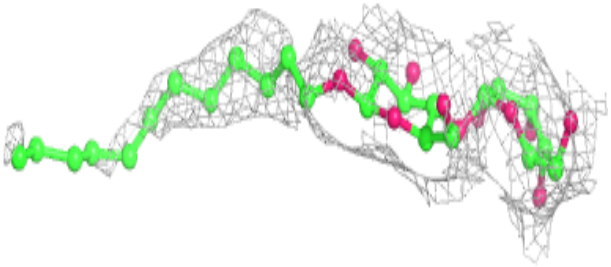
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

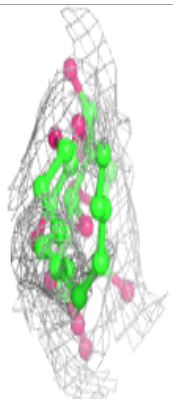


Electron density around LMT C 1101:

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

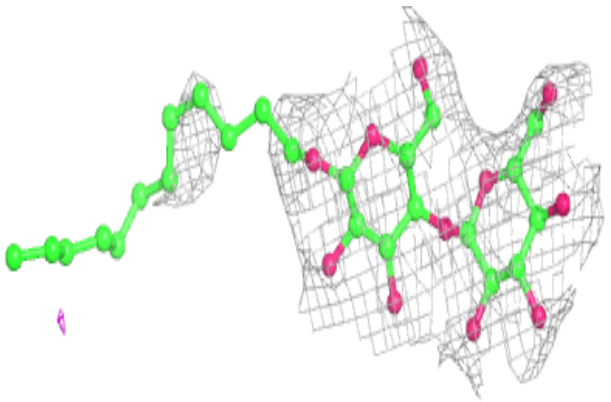


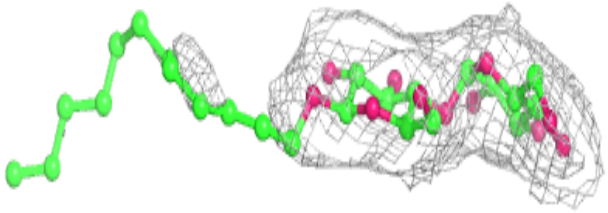


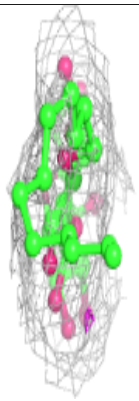


Electron density around LMT A 1101:

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

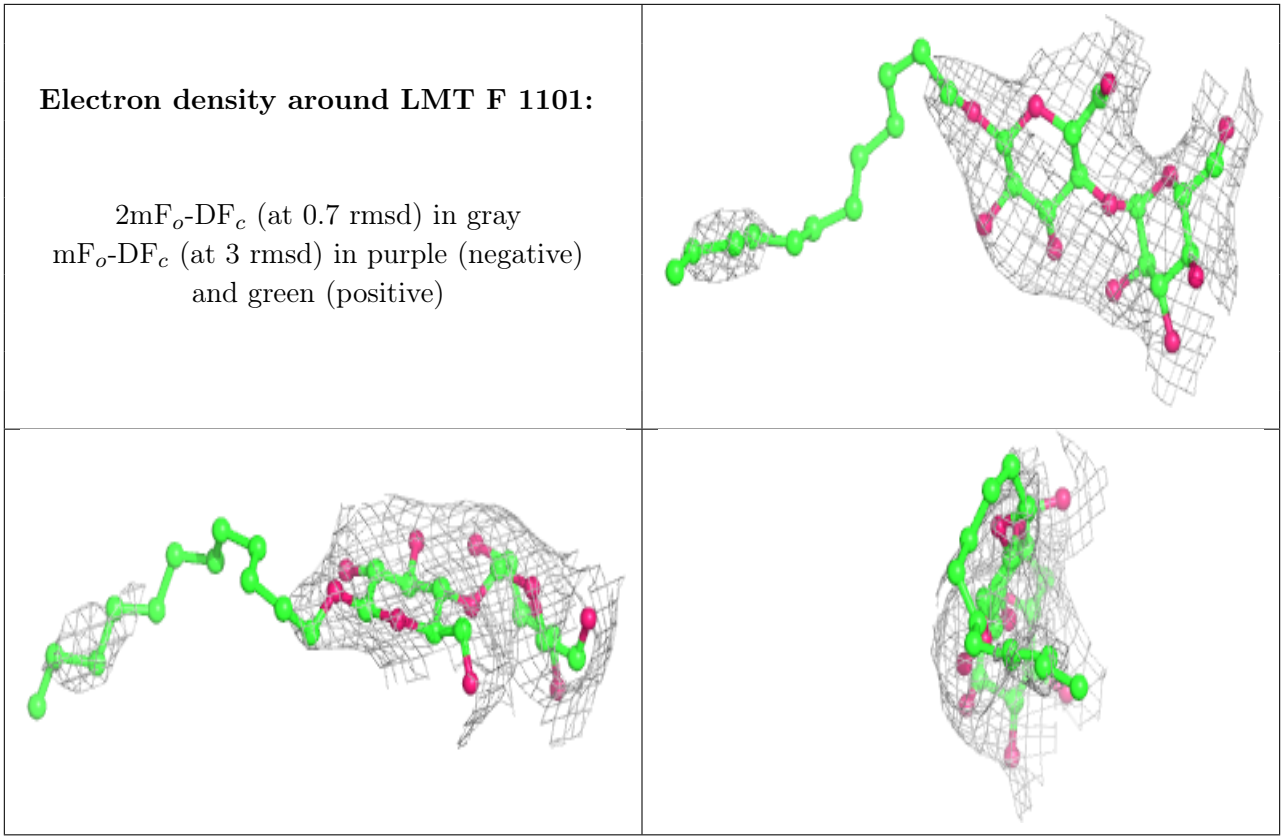






Electron density around LMT F 1101:

$2mF_o$-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.