Full wwPDB X-ray Structure Validation Report

Dec 15, 2016 – 12:02 PM EST

PDB ID	:	2J8S
Title	:	Drug Export Pathway of Multidrug Exporter AcrB Revealed by DARPin Inhibitors
Authors	:	Sennhauser, G.; Amstutz, P.; Briand, C.; Storchenegger, O.; Gruetter, M.G.
Deposited on	:	2006-10-27
Resolution	:	2.54 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

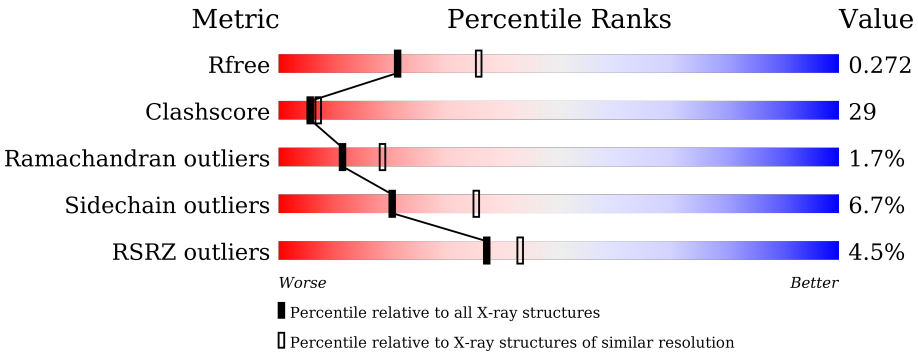
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.54 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	1055	7% 55% 40% 5%
1	B	1055	3% 53% 40%
1	C	1055	3% 59% 36%
2	D	169	60% 29% 8%
2	E	169	7% 49% 36% 5% 9%

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
3	LMT	A	3047	-	-	X	X
3	LMT	A	3048	-	-	X	-
3	LMT	B	3035	-	-	-	X
3	LMT	B	3036	-	-	-	X
3	LMT	B	3037	-	-	X	X
3	LMT	C	3042	-	-	-	X
3	LMT	C	3043	-	-	-	X
3	LMT	C	3044	-	-	-	X
3	LMT	C	3046	-	-	-	X
4	LMU	A	3049	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

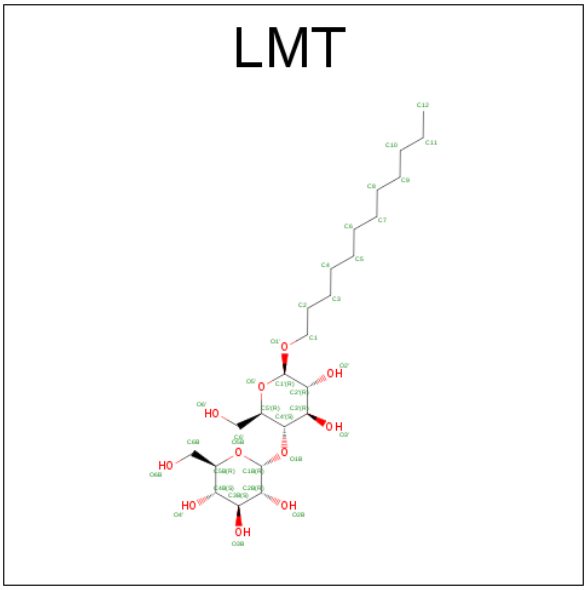
- Molecule 1 is a protein called ACRIFLAVINE RESISTANCE PROTEIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7943	5106	1315	1478	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7849	5052	1295	1458	44			
1	C	1040	Total	C	N	O	S	0	0	0
			7908	5086	1307	1471	44			

- Molecule 2 is a protein called DARPIN.

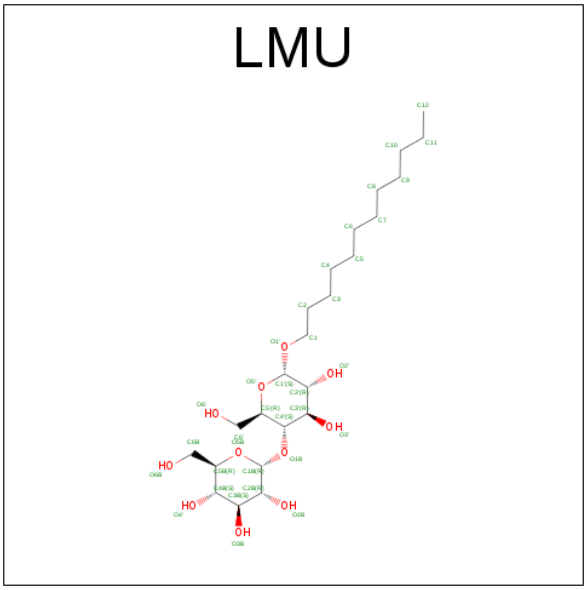
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	153	Total	C	N	O	S	0	0	0
			1159	732	203	223	1			

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 35 24 11	0	0
3	A	1	Total C O 35 24 11	0	0
3	A	1	Total C O 35 24 11	0	0
3	B	1	Total C O 35 24 11	0	0
3	B	1	Total C O 35 24 11	0	0
3	B	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0
3	C	1	Total C O 35 24 11	0	0

- Molecule 4 is DODECYL-ALPHA-D-MALTOSIDE (three-letter code: LMU) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 35 24 11	0	0

- Molecule 5 is water.

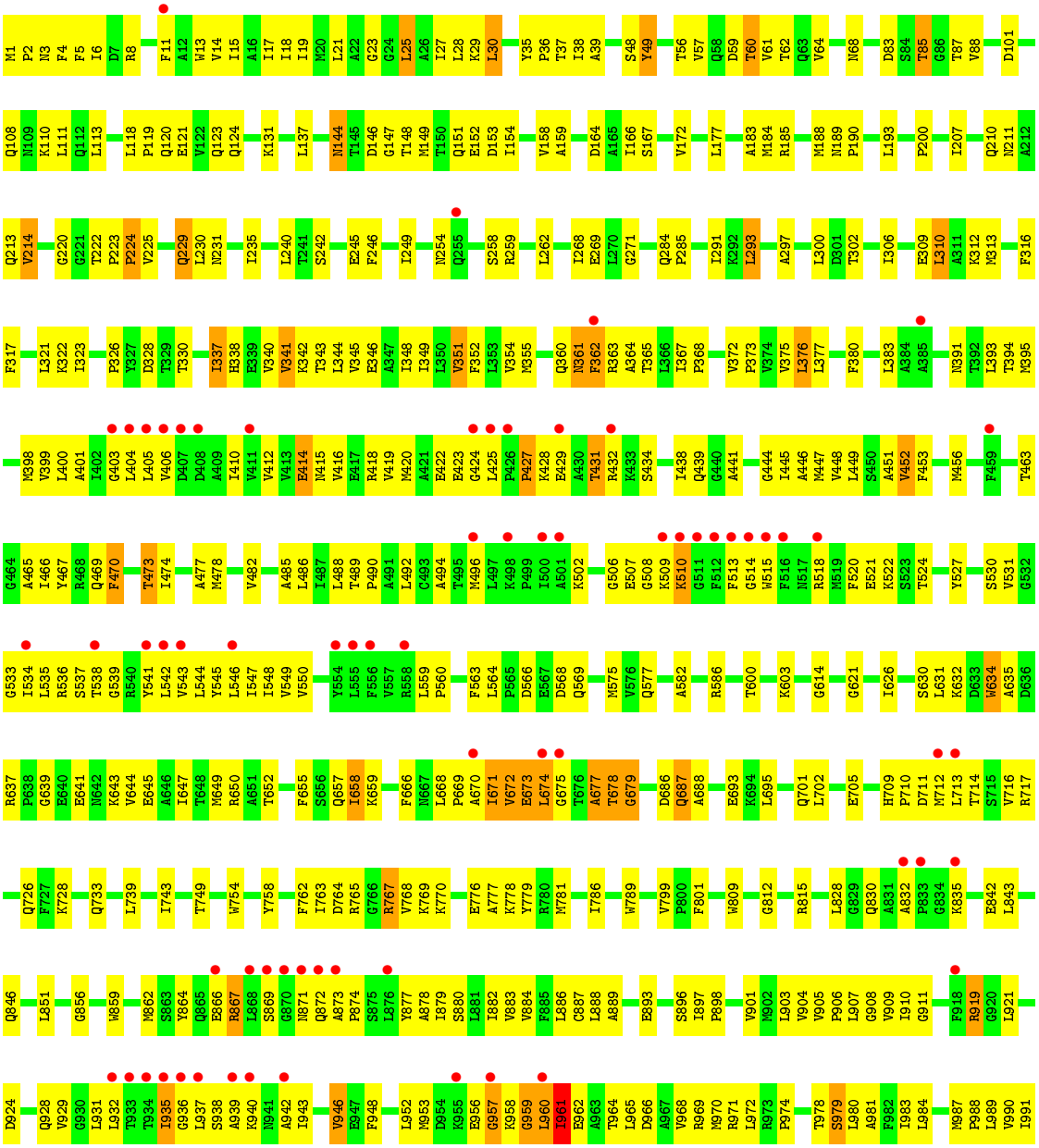
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	118	Total O 118 118	0	0
5	B	99	Total O 99 99	0	0
5	C	117	Total O 117 117	0	0
5	D	10	Total O 10 10	0	0
5	E	6	Total O 6 6	0	0

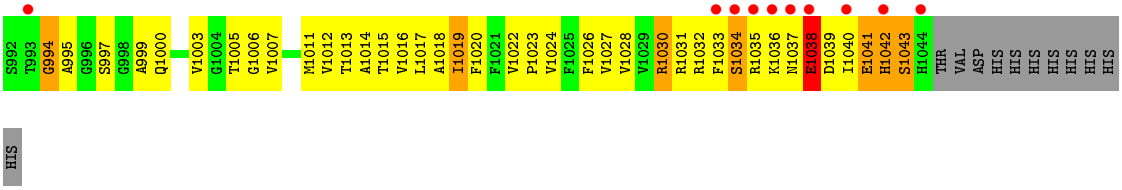
3 Residue-property plots (i)

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

- Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B

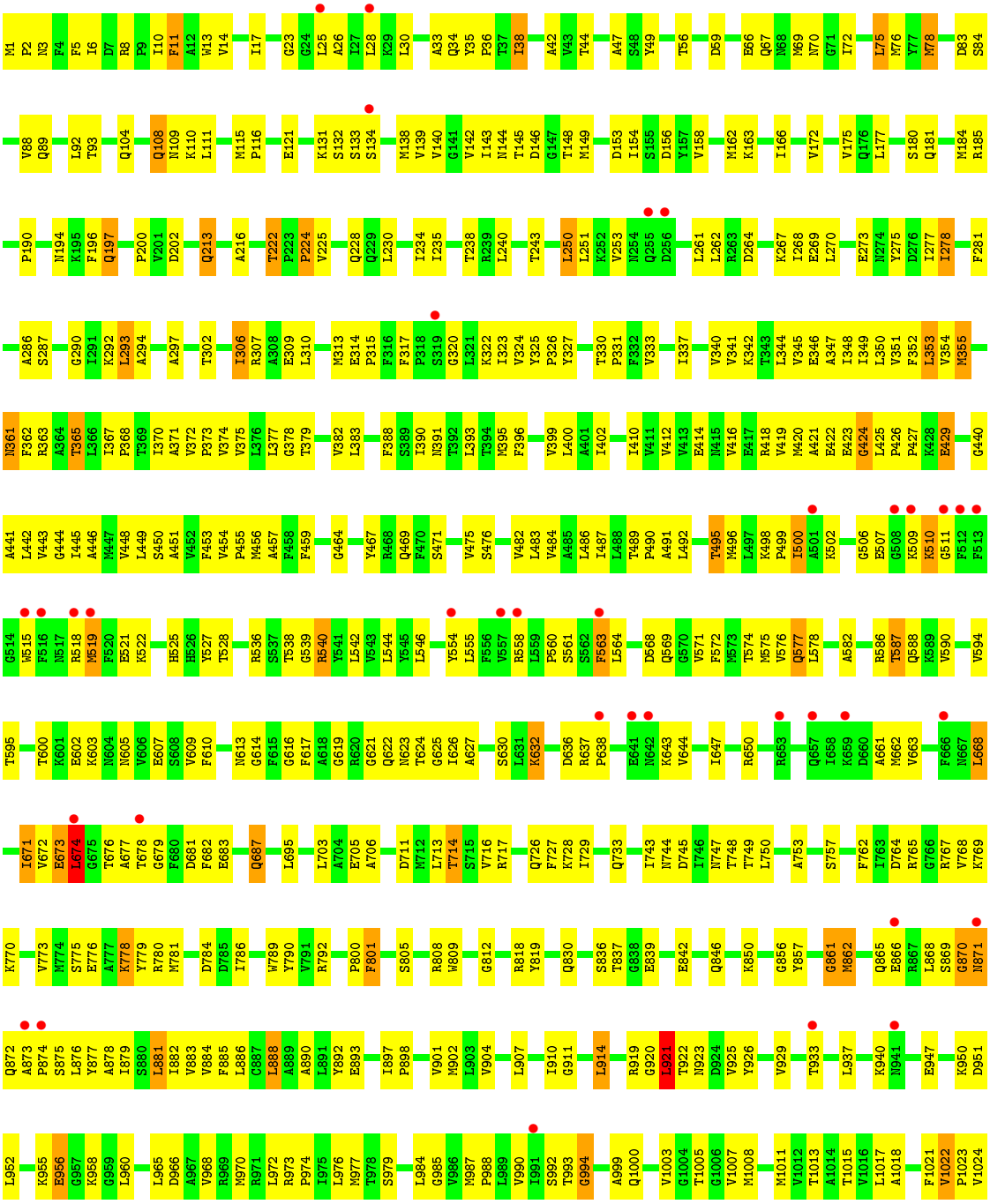
Chain A: 





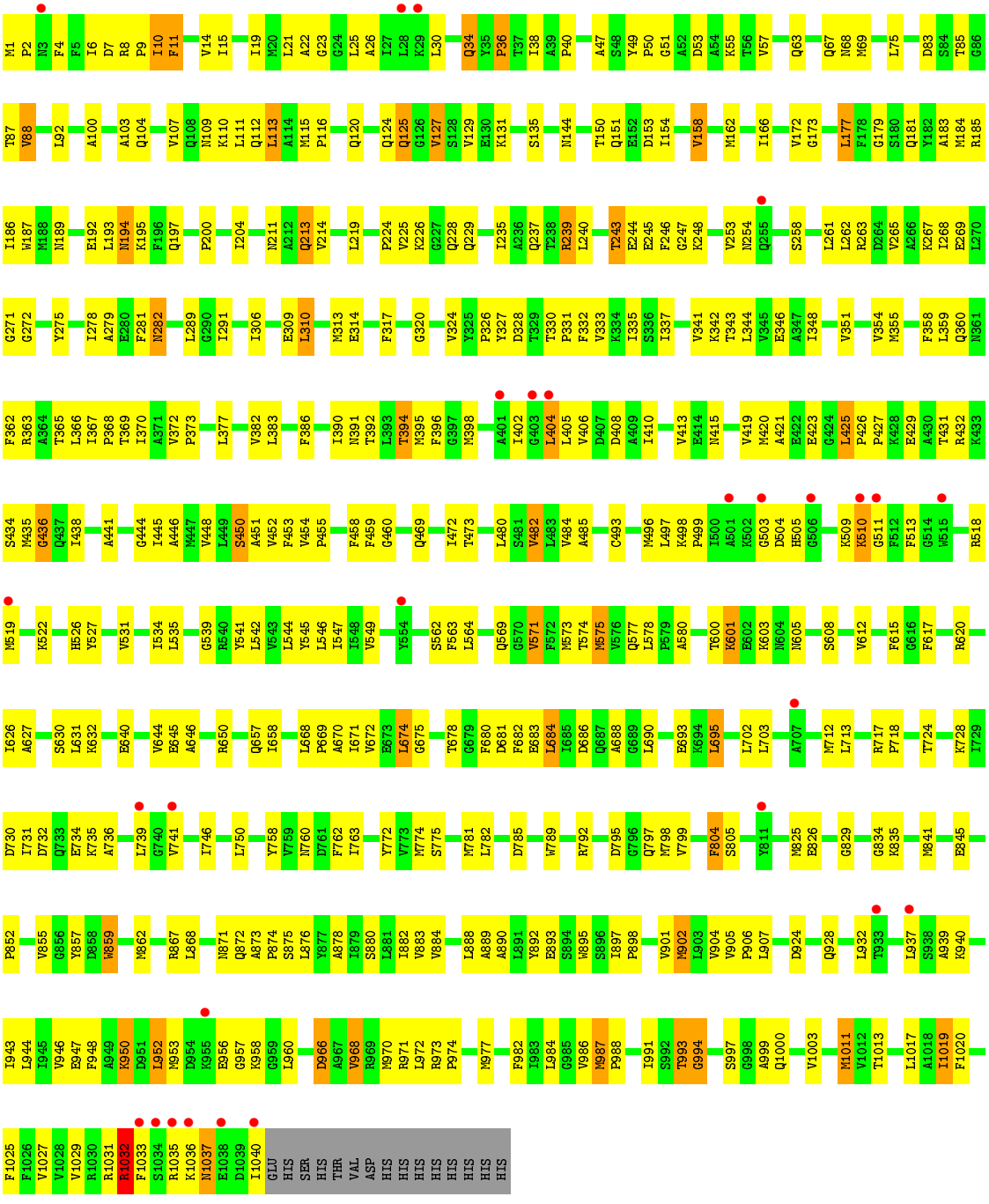
• Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B

Chain B:



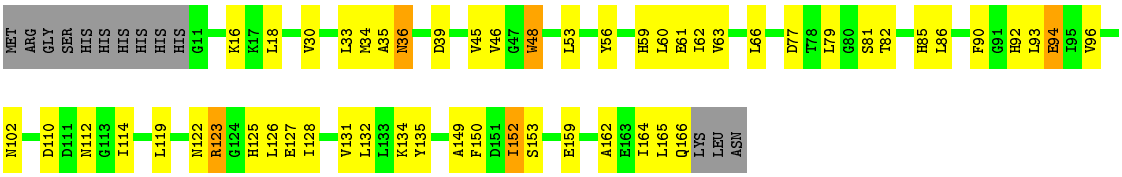
• Molecule 1: ACRIFLAVINE RESISTANCE PROTEIN B

Chain C:

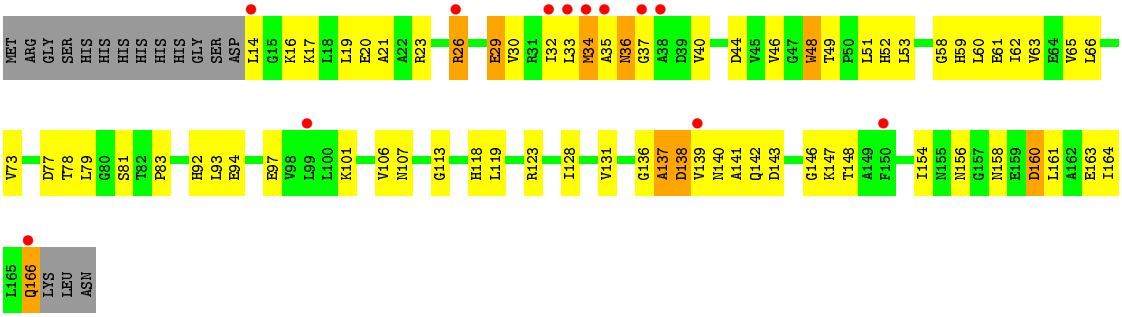


• Molecule 2: DARPIN

Chain D:



- Molecule 2: DARPIN



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	146.18Å 157.41Å 246.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.36 – 2.54 34.36 – 2.55	Depositor EDS
% Data completeness (in resolution range)	95.1 (34.36-2.54) 95.9 (34.36-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.11 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.271 0.229 , 0.272	Depositor DCC
R_{free} test set	3552 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	26771	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, LMU

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	0.38	0/8095	0.63	0/10991
1	B	0.38	0/7999	0.62	0/10863
1	C	0.39	0/8058	0.63	0/10941
2	D	0.34	0/1196	0.59	0/1626
2	E	0.33	0/1178	0.55	0/1602
All	All	0.38	0/26526	0.62	0/36023

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7943	0	8084	601	0
1	B	7849	0	8001	448	0
1	C	7908	0	8059	405	0
2	D	1177	0	1159	50	0
2	E	1159	0	1147	56	0
3	A	105	0	136	84	0
3	B	105	0	138	50	0
3	C	140	0	184	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	35	0	46	50	0
5	A	118	0	0	6	0
5	B	99	0	0	11	0
5	C	117	0	0	6	0
5	D	10	0	0	2	0
5	E	6	0	0	1	0
All	All	26771	0	26954	1565	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (1565) 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)
3:C:3043:LMT:C1	3:C:3043:LMT:C2	1.78	1.61
3:C:3046:LMT:H11	3:C:3046:LMT:O3'	1.28	1.27
1:A:348:ILE:CB	4:A:3049:LMU:H123	1.71	1.18
1:A:932:LEU:HD12	3:A:3048:LMT:H81	1.21	1.16
1:A:932:LEU:HA	3:A:3048:LMT:H82	1.21	1.15
1:A:348:ILE:HB	4:A:3049:LMU:C12	1.76	1.15
1:C:544:LEU:HD11	3:C:3043:LMT:H72	1.27	1.14
1:A:932:LEU:HG	3:A:3048:LMT:H101	1.30	1.13
1:C:875:SER:HB2	3:C:3044:LMT:O2B	1.47	1.12
1:B:919:ARG:HD2	1:B:1005:THR:HG21	1.31	1.12
1:B:883:VAL:HG22	3:B:3037:LMT:H91	1.11	1.07
3:C:3044:LMT:O5B	3:C:3044:LMT:H6E	1.53	1.07
1:A:447:MET:HB2	3:A:3047:LMT:H41	1.37	1.07
1:A:344:LEU:HB3	4:A:3049:LMU:H101	1.34	1.06
3:A:3046:LMT:H112	4:A:3049:LMU:H91	1.33	1.05
1:A:18:ILE:HG12	3:B:3037:LMT:H112	1.36	1.05
3:C:3046:LMT:O2'	3:C:3046:LMT:H5'	1.50	1.03
1:A:451:ALA:HB2	3:A:3047:LMT:H81	1.38	1.02
1:C:458:PHE:CZ	3:C:3046:LMT:H31	1.95	1.02
1:A:341:VAL:HG12	4:A:3049:LMU:H62	1.36	1.01
1:B:278:ILE:HG23	1:B:613:ASN:HB3	1.42	1.01
1:A:671:ILE:HG23	1:A:672:VAL:H	1.20	1.01
3:C:3046:LMT:O3'	3:C:3046:LMT:C1	2.10	0.99
1:A:8:ARG:HH22	3:B:3036:LMT:H6'2	1.23	0.98
1:A:887:CYS:SG	3:A:3047:LMT:H71	2.03	0.98
1:B:883:VAL:HG13	3:B:3037:LMT:C10	1.93	0.98
1:A:372:VAL:HA	1:A:405:LEU:HD21	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:883:VAL:CG1	3:B:3037:LMT:H102	1.93	0.98
1:A:883:VAL:CG1	3:A:3047:LMT:H111	1.93	0.97
1:A:883:VAL:HG11	3:A:3047:LMT:H111	1.46	0.97
1:A:348:ILE:HB	4:A:3049:LMU:H123	0.97	0.97
1:B:222:THR:HG23	1:C:275:TYR:HB2	1.48	0.96
3:A:3046:LMT:H112	4:A:3049:LMU:C9	1.94	0.95
1:A:414:GLU:HG2	1:A:974:PRO:HB3	1.43	0.95
1:A:932:LEU:HA	3:A:3048:LMT:C8	1.97	0.94
1:B:883:VAL:HG13	3:B:3037:LMT:H102	0.97	0.94
1:A:887:CYS:HB3	3:A:3047:LMT:H51	1.49	0.94
1:A:448:VAL:HA	3:A:3047:LMT:H61	1.49	0.94
1:A:447:MET:HB2	3:A:3047:LMT:C4	1.98	0.94
1:A:932:LEU:O	3:A:3048:LMT:H102	1.68	0.93
1:A:451:ALA:HA	3:A:3047:LMT:H102	1.47	0.93
1:A:8:ARG:NH2	3:B:3036:LMT:H6'2	1.81	0.93
1:A:448:VAL:CA	3:A:3047:LMT:H61	1.99	0.92
1:B:560:PRO:HG2	1:B:922:THR:HG22	1.51	0.92
1:B:901:VAL:O	1:B:904:VAL:HG22	1.70	0.92
1:A:448:VAL:N	3:A:3047:LMT:H61	1.85	0.92
4:A:3049:LMU:O2'	4:A:3049:LMU:H12	1.67	0.91
2:D:122:ASN:HA	2:D:152:ILE:HD11	1.49	0.91
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.51	0.90
1:C:342:LYS:O	1:C:346:GLU:HG3	1.70	0.90
1:C:953:MET:HE2	1:C:960:LEU:HA	1.52	0.90
1:A:25:LEU:HD21	3:B:3037:LMT:H41	1.51	0.89
1:B:361:ASN:H	1:B:361:ASN:HD22	0.97	0.89
1:C:575:MET:HE3	1:C:617:PHE:HB2	1.54	0.89
3:C:3042:LMT:O2B	3:C:3042:LMT:H5B	1.71	0.89
1:A:451:ALA:HB1	1:A:884:VAL:HG22	1.52	0.88
1:B:139:VAL:HG13	1:B:327:TYR:HB3	1.54	0.88
1:B:873:ALA:HB3	1:B:874:PRO:HD3	1.54	0.88
1:A:428:LYS:HE3	1:A:432:ARG:HH21	1.38	0.87
1:A:444:GLY:HA2	3:A:3047:LMT:H11	1.57	0.87
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.57	0.87
1:B:361:ASN:N	1:B:361:ASN:HD22	1.71	0.87
1:A:510:LYS:HD3	1:A:513:PHE:HB2	1.57	0.86
3:A:3046:LMT:O4'	3:B:3037:LMT:O6B	1.93	0.86
3:A:3047:LMT:H12	3:A:3047:LMT:O2'	1.74	0.86
1:A:932:LEU:CG	3:A:3048:LMT:H101	2.04	0.86
1:A:451:ALA:CB	3:A:3047:LMT:H81	2.05	0.86
1:B:729:ILE:HD11	1:B:805:SER:HB2	1.55	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:741:VAL:HG11	1:C:799:VAL:HG11	1.56	0.85
1:B:361:ASN:H	1:B:361:ASN:ND2	1.73	0.85
1:B:363:ARG:HD2	1:B:498:LYS:HE3	1.56	0.85
1:A:932:LEU:HD12	3:A:3048:LMT:C8	2.06	0.85
1:A:254:ASN:HD22	1:A:258:SER:HB2	1.40	0.84
1:C:544:LEU:HD21	3:C:3043:LMT:H81	1.59	0.84
1:A:344:LEU:HB2	4:A:3049:LMU:H82	1.59	0.84
1:A:355:MET:HE2	1:A:368:PRO:HG3	1.59	0.84
1:B:367:ILE:HG12	1:B:496:MET:HE3	1.58	0.84
1:A:887:CYS:HB3	3:A:3047:LMT:C5	2.07	0.84
1:A:18:ILE:CG1	3:B:3037:LMT:H112	2.07	0.84
1:C:522:LYS:HG2	1:C:526:HIS:HE1	1.41	0.84
1:A:669:PRO:HB3	1:A:675:GLY:HA3	1.59	0.84
1:B:883:VAL:HG22	3:B:3037:LMT:C9	2.04	0.84
1:A:60:THR:HG22	1:A:61:VAL:HG23	1.59	0.83
1:A:428:LYS:CE	1:A:432:ARG:HH21	1.91	0.83
1:A:452:VAL:HB	3:A:3048:LMT:H112	1.59	0.83
1:B:875:SER:O	1:B:879:ILE:HD13	1.78	0.83
1:A:341:VAL:HG12	4:A:3049:LMU:C6	2.07	0.83
1:A:344:LEU:CB	4:A:3049:LMU:H82	2.09	0.83
1:B:555:LEU:HD21	1:B:914:LEU:HD13	1.61	0.83
3:A:3047:LMT:H3B	1:C:8:ARG:HH21	1.42	0.82
1:A:344:LEU:O	4:A:3049:LMU:H112	1.79	0.82
1:A:341:VAL:CG1	4:A:3049:LMU:H62	2.09	0.82
1:A:687:GLN:HE22	1:A:856:GLY:HA3	1.45	0.82
1:B:673:GLU:HB3	1:B:674:LEU:HD12	1.60	0.82
1:C:937:LEU:HD13	1:C:1011:MET:HG2	1.60	0.82
1:A:451:ALA:HA	3:A:3047:LMT:C10	2.09	0.82
1:A:867:ARG:HA	1:A:867:ARG:HE	1.42	0.81
1:A:21:LEU:O	1:A:25:LEU:HD22	1.81	0.81
1:A:635:ALA:HB2	4:A:3049:LMU:O4'	1.81	0.81
1:C:875:SER:HB2	3:C:3044:LMT:H2O1	1.45	0.81
1:B:879:ILE:O	1:B:883:VAL:HG23	1.81	0.81
1:A:444:GLY:CA	3:A:3047:LMT:H11	2.09	0.81
1:A:542:LEU:HD21	1:A:1028:VAL:HG21	1.62	0.81
1:B:515:TRP:HE3	1:B:518:ARG:HH21	1.29	0.81
1:B:866:GLU:O	1:B:870:GLY:HA2	1.82	0.80
1:A:38:ILE:HG13	1:A:39:ALA:N	1.96	0.80
1:B:72:ILE:HD11	1:B:110:LYS:HG3	1.63	0.80
3:C:3044:LMT:O5B	3:C:3044:LMT:C6'	2.30	0.80
1:B:420:MET:HE1	1:B:427:PRO:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:3042:LMT:C6'	3:C:3042:LMT:O1'	2.30	0.80
1:A:345:VAL:HG23	4:A:3049:LMU:C7	2.11	0.80
1:A:887:CYS:SG	3:A:3047:LMT:C7	2.69	0.80
1:A:449:LEU:C	1:A:451:ALA:H	1.85	0.80
1:C:458:PHE:CE1	3:C:3046:LMT:H31	2.17	0.80
1:C:688:ALA:HB3	1:C:690:LEU:HD13	1.64	0.80
1:C:960:LEU:HD11	1:C:1027:VAL:HG13	1.63	0.80
1:A:444:GLY:HA2	3:A:3047:LMT:C1	2.12	0.79
1:B:809:TRP:HB2	2:D:48:TRP:CH2	2.17	0.79
1:C:531:VAL:HG21	1:C:968:VAL:HG11	1.64	0.79
1:C:640:GLU:H	1:C:640:GLU:CD	1.83	0.79
1:B:879:ILE:HG21	3:B:3037:LMT:H31	1.63	0.79
1:B:425:LEU:HD12	1:B:429:GLU:HB2	1.65	0.79
1:B:441:ALA:O	1:B:445:ILE:HD12	1.82	0.79
1:B:310:LEU:HD13	1:B:323:ILE:HD12	1.63	0.78
4:A:3049:LMU:C1	4:A:3049:LMU:O2'	2.30	0.78
1:A:8:ARG:HH12	3:B:3036:LMT:H5B	1.46	0.78
1:A:424:GLY:HA3	1:A:502:LYS:HB2	1.64	0.78
1:B:379:THR:O	1:B:382:VAL:HG22	1.84	0.78
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.63	0.78
1:A:14:VAL:HG13	1:B:886:LEU:HB3	1.65	0.78
1:A:345:VAL:N	4:A:3049:LMU:H81	1.98	0.78
1:A:345:VAL:O	1:A:348:ILE:HG22	1.83	0.78
1:B:423:GLU:HA	1:B:502:LYS:HE2	1.64	0.78
1:A:671:ILE:HG12	1:A:672:VAL:HG22	1.66	0.78
3:C:3042:LMT:C5B	3:C:3042:LMT:O2B	2.30	0.78
1:A:348:ILE:O	1:A:351:VAL:HG12	1.83	0.78
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.65	0.78
1:A:669:PRO:O	1:A:671:ILE:HG22	1.83	0.77
1:A:932:LEU:CA	3:A:3048:LMT:H82	2.08	0.77
1:C:509:LYS:O	1:C:510:LYS:HB2	1.82	0.77
1:C:952:LEU:HD12	1:C:958:LYS:HD2	1.64	0.77
1:A:527:TYR:HE2	1:A:1019:ILE:HG23	1.50	0.77
1:C:359:LEU:HD12	1:C:365:THR:HA	1.66	0.77
1:C:63:GLN:HE22	1:C:67:GLN:HE21	1.29	0.77
1:A:428:LYS:O	1:A:432:ARG:HG3	1.84	0.77
1:B:574:THR:CG2	1:B:627:ALA:HB3	2.14	0.77
1:A:1038:GLU:HG2	1:A:1040:ILE:H	1.49	0.77
1:A:452:VAL:CG2	3:A:3048:LMT:H112	2.15	0.77
1:C:15:ILE:O	1:C:19:ILE:HG12	1.85	0.77
1:C:987:MET:HB3	1:C:988:PRO:HD3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:O	1:A:60:THR:HB	1.86	0.76
1:A:383:LEU:HD21	1:A:473:THR:HG22	1.68	0.75
1:A:509:LYS:O	1:A:514:GLY:HA3	1.85	0.75
1:B:637:ARG:N	1:B:638:PRO:HD3	2.01	0.75
1:A:188:MET:HE1	1:A:200:PRO:HG3	1.69	0.75
1:A:671:ILE:HG23	1:A:672:VAL:N	2.00	0.75
1:A:18:ILE:HG12	3:B:3037:LMT:C11	2.14	0.75
1:C:404:LEU:HD11	1:C:937:LEU:HD21	1.67	0.75
2:E:62:ILE:O	2:E:66:LEU:HG	1.86	0.75
1:A:188:MET:HE3	1:A:200:PRO:HA	1.68	0.75
3:C:3046:LMT:H11	3:C:3046:LMT:H3O2	1.47	0.75
1:A:144:ASN:OD1	1:A:149:MET:HG2	1.85	0.74
1:C:888:LEU:HD13	1:C:901:VAL:HG21	1.66	0.74
1:A:964:THR:O	1:A:968:VAL:HG23	1.88	0.74
1:C:363:ARG:HD3	1:C:496:MET:O	1.86	0.74
1:A:25:LEU:HD21	3:B:3037:LMT:H61	1.68	0.74
1:A:375:VAL:HB	1:A:405:LEU:HD11	1.66	0.74
1:A:3:ASN:HA	1:A:6:ILE:HD12	1.69	0.74
1:C:85:THR:OG1	1:C:87:THR:HG22	1.87	0.74
1:A:428:LYS:HE3	1:A:432:ARG:NH2	2.03	0.73
2:E:34:MET:HA	2:E:34:MET:HE3	1.68	0.73
1:C:154:ILE:O	1:C:158:VAL:HG12	1.88	0.73
1:C:458:PHE:HZ	3:C:3046:LMT:H51	1.53	0.73
1:B:250:LEU:HD12	1:C:734:GLU:HG2	1.70	0.73
1:A:465:ALA:O	1:A:469:GLN:HG2	1.88	0.73
1:B:131:LYS:HE3	1:B:133:SER:HB2	1.69	0.73
1:B:703:LEU:HD23	1:B:716:VAL:HG22	1.69	0.73
1:C:852:PRO:O	1:C:855:VAL:HG12	1.89	0.73
1:A:452:VAL:CB	3:A:3048:LMT:H112	2.18	0.73
1:C:309:GLU:O	1:C:313:MET:HG3	1.89	0.73
1:A:11:PHE:CZ	3:B:3036:LMT:O6'	2.41	0.73
1:A:25:LEU:CD2	3:B:3037:LMT:H41	2.19	0.73
1:A:1037:ASN:ND2	1:A:1038:GLU:H	1.86	0.73
1:B:42:ALA:HB3	1:B:132:SER:HB2	1.70	0.73
1:A:448:VAL:HG12	3:A:3047:LMT:H52	1.71	0.72
1:B:1022:VAL:HG22	1:B:1023:PRO:HD3	1.70	0.72
1:B:956:GLU:HB2	1:B:958:LYS:HG3	1.70	0.72
1:A:887:CYS:CB	3:A:3047:LMT:H72	2.19	0.72
1:A:887:CYS:HB2	3:A:3047:LMT:H72	1.69	0.72
1:C:120:GLN:O	1:C:124:GLN:HG2	1.89	0.72
1:C:953:MET:O	1:C:957:GLY:HA2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:GLY:HA3	1:A:1013:THR:OG1	1.89	0.72
1:A:445:ILE:HA	1:A:448:VAL:HG22	1.71	0.72
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.72	0.72
2:D:36:ASN:HD22	2:D:36:ASN:N	1.86	0.72
1:A:932:LEU:C	3:A:3048:LMT:H102	2.10	0.72
1:A:316:PHE:CD1	1:B:687:GLN:HG2	2.25	0.72
1:B:527:TYR:CE2	1:B:968:VAL:HG13	2.25	0.72
1:C:69:MET:HE1	1:C:107:VAL:HG13	1.72	0.72
3:C:3043:LMT:O1'	3:C:3043:LMT:C2	2.37	0.72
1:B:26:ALA:O	1:B:30:LEU:HB2	1.90	0.71
1:A:453:PHE:CE2	3:A:3048:LMT:H122	2.25	0.71
1:B:1018:ALA:O	1:B:1022:VAL:HG13	1.91	0.71
1:B:352:PHE:HD2	1:B:353:LEU:HD12	1.56	0.71
1:B:577:GLN:O	1:B:661:ALA:HB1	1.91	0.71
1:A:449:LEU:C	1:A:451:ALA:N	2.42	0.71
1:A:712:MET:HA	1:A:832:ALA:CB	2.21	0.71
1:B:34:GLN:HG2	1:B:35:TYR:CD1	2.25	0.71
1:A:425:LEU:HD23	1:A:429:GLU:HG3	1.72	0.71
1:A:214:VAL:HG11	1:B:747:ASN:HB3	1.71	0.71
1:B:66:GLU:OE1	1:B:818:ARG:HD3	1.90	0.71
1:C:539:GLY:HA2	1:C:542:LEU:HD23	1.72	0.71
1:B:582:ALA:HB3	1:B:623:ASN:HB3	1.71	0.71
2:E:26:ARG:HD3	2:E:29:GLU:HG3	1.72	0.70
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.73	0.70
1:B:726:GLN:HG2	5:B:2063:HOH:O	1.92	0.70
1:C:845:GLU:HG3	1:C:859:TRP:CH2	2.26	0.70
1:B:868:LEU:C	1:B:870:GLY:H	1.92	0.70
1:A:712:MET:HA	1:A:832:ALA:HB3	1.74	0.70
1:A:687:GLN:NE2	1:A:856:GLY:HA3	2.05	0.70
1:C:460:GLY:HA2	5:C:2062:HOH:O	1.91	0.70
1:A:946:VAL:HG23	1:A:1026:PHE:CE1	2.27	0.70
1:B:302:THR:O	1:B:306:ILE:HG23	1.92	0.70
1:B:744:ASN:O	1:B:748:THR:HG23	1.92	0.70
1:A:8:ARG:HH12	3:B:3036:LMT:C5B	2.05	0.69
1:B:293:LEU:CD2	1:B:297:ALA:HB3	2.22	0.69
1:B:947:GLU:O	1:B:951:ASP:HB2	1.92	0.69
1:C:446:ALA:HB2	1:C:482:VAL:HG13	1.72	0.69
1:A:880:SER:O	1:A:884:VAL:HG23	1.91	0.69
1:B:444:GLY:N	3:B:3036:LMT:O2'	2.25	0.69
1:C:875:SER:OG	3:C:3044:LMT:H3B	1.92	0.69
1:B:445:ILE:HG12	1:B:940:LYS:HG3	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:ILE:HG13	1:A:39:ALA:H	1.57	0.69
1:B:2:PRO:O	1:B:6:ILE:HG13	1.91	0.69
1:B:883:VAL:CG2	3:B:3037:LMT:H91	2.07	0.69
1:B:184:MET:HE1	1:B:268:ILE:HG22	1.74	0.69
1:A:534:ILE:O	1:A:537:SER:HB3	1.92	0.69
1:B:554:TYR:O	1:B:558:ARG:HG2	1.93	0.69
1:B:919:ARG:CD	1:B:1005:THR:HG21	2.15	0.69
1:C:445:ILE:HG23	1:C:940:LYS:HG3	1.74	0.69
1:C:541:TYR:OH	3:C:3043:LMT:H21	1.92	0.69
1:C:966:ASP:O	1:C:970:MET:HG3	1.92	0.69
2:E:34:MET:HE1	2:E:40:VAL:HG12	1.75	0.69
1:A:447:MET:C	3:A:3047:LMT:H61	2.12	0.69
1:C:991:ILE:HG23	3:C:3042:LMT:H42	1.74	0.69
1:A:932:LEU:CD1	3:A:3048:LMT:H81	2.13	0.68
1:C:527:TYR:CE2	1:C:968:VAL:HG13	2.28	0.68
1:C:544:LEU:HD11	3:C:3043:LMT:C7	2.16	0.68
1:B:196:PHE:C	1:B:197:GLN:HE21	1.97	0.68
1:C:7:ASP:C	1:C:9:PRO:HD3	2.14	0.68
1:A:897:ILE:N	1:A:898:PRO:HD2	2.08	0.68
1:C:162:MET:HA	1:C:313:MET:HE1	1.74	0.68
1:C:544:LEU:HD21	3:C:3043:LMT:C8	2.23	0.68
1:C:876:LEU:HD11	1:C:932:LEU:HD11	1.74	0.68
2:D:127:GLU:O	2:D:131:VAL:HG23	1.94	0.68
1:C:104:GLN:HE21	1:C:129:VAL:HG13	1.59	0.68
3:C:3042:LMT:H2B	3:C:3042:LMT:C3'	2.24	0.68
1:C:328:ASP:O	1:C:331:PRO:HD2	1.93	0.68
1:B:879:ILE:CG2	3:B:3037:LMT:H31	2.23	0.68
1:A:259:ARG:HD2	5:D:2008:HOH:O	1.93	0.68
1:B:910:ILE:HG23	1:B:1013:THR:HG21	1.76	0.68
1:C:544:LEU:CD1	3:C:3043:LMT:H72	2.16	0.67
1:A:568:ASP:CG	1:A:637:ARG:HH22	1.96	0.67
1:B:362:PHE:O	1:B:365:THR:HG22	1.93	0.67
2:E:30:VAL:O	2:E:34:MET:HB2	1.95	0.67
1:B:871:ASN:HD22	1:B:872:GLN:N	1.92	0.67
2:E:23:ARG:HB2	2:E:53:LEU:HD13	1.76	0.67
1:A:1007:VAL:O	1:A:1011:MET:HB2	1.94	0.67
1:A:960:LEU:HD12	1:A:961:ILE:N	2.09	0.67
1:C:547:ILE:HG12	3:C:3043:LMT:H121	1.77	0.67
3:A:3046:LMT:C11	4:A:3049:LMU:H91	2.20	0.67
1:A:543:VAL:O	1:A:547:ILE:HG13	1.95	0.67
1:B:1025:PHE:O	1:B:1029:VAL:HG23	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:VAL:HG23	1:C:453:PHE:CD1	2.30	0.67
1:A:344:LEU:HB3	4:A:3049:LMU:C10	2.18	0.67
1:B:420:MET:HB3	1:B:500:ILE:HG23	1.76	0.67
1:C:924:ASP:O	1:C:928:GLN:HG3	1.95	0.67
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.25	0.66
1:A:568:ASP:OD2	1:A:637:ARG:NH2	2.28	0.66
1:A:942:ALA:O	1:A:946:VAL:HG12	1.95	0.66
1:B:184:MET:HE3	1:B:185:ARG:H	1.60	0.66
1:A:931:LEU:O	1:A:935:ILE:HG22	1.95	0.66
3:C:3042:LMT:H2'	3:C:3042:LMT:H6E	1.78	0.66
1:A:932:LEU:CA	3:A:3048:LMT:H102	2.25	0.66
1:B:419:VAL:O	1:B:423:GLU:HG2	1.94	0.66
1:C:953:MET:CE	1:C:960:LEU:HA	2.25	0.66
2:D:110:ASP:OD2	2:D:114:ILE:HB	1.95	0.66
1:B:871:ASN:HD22	1:B:872:GLN:H	1.43	0.66
1:C:332:PHE:HA	1:C:335:ILE:HG22	1.78	0.66
1:A:432:ARG:HH11	1:A:432:ARG:HG2	1.59	0.66
1:B:414:GLU:HG3	1:B:977:MET:CE	2.25	0.66
3:B:3037:LMT:O2B	3:B:3037:LMT:C3'	2.44	0.66
1:B:350:LEU:O	1:B:354:VAL:HG13	1.96	0.66
1:A:18:ILE:CD1	3:B:3037:LMT:H112	2.25	0.66
1:B:910:ILE:HG13	1:B:914:LEU:CD2	2.26	0.66
3:C:3042:LMT:H1B	3:C:3042:LMT:O3'	1.95	0.66
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.76	0.66
1:C:944:LEU:O	1:C:971:ARG:HG3	1.95	0.66
1:A:345:VAL:HG23	4:A:3049:LMU:H72	1.78	0.65
2:D:150:PHE:O	2:D:153:SER:HB3	1.95	0.65
2:E:97:GLU:HG2	2:E:131:VAL:HG11	1.76	0.65
1:B:871:ASN:HD21	1:B:873:ALA:HB3	1.61	0.65
1:C:522:LYS:HG2	1:C:526:HIS:CE1	2.29	0.65
3:B:3035:LMT:H6E	3:B:3035:LMT:H5B	1.78	0.65
1:A:453:PHE:CZ	3:A:3048:LMT:H122	2.32	0.65
1:B:72:ILE:HD11	1:B:110:LYS:CG	2.27	0.65
1:B:440:GLY:O	3:B:3036:LMT:O3'	2.14	0.65
1:B:489:THR:OG1	1:B:490:PRO:HD3	1.97	0.65
2:E:34:MET:CE	2:E:34:MET:HA	2.27	0.65
1:B:185:ARG:HB2	1:B:269:GLU:O	1.97	0.65
1:B:213:GLN:NE2	1:B:238:THR:HG22	2.12	0.65
1:C:144:ASN:HA	1:C:320:GLY:O	1.97	0.65
1:C:406:VAL:O	1:C:410:ILE:HG13	1.97	0.64
3:C:3042:LMT:H6E	3:C:3042:LMT:O1'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:875:SER:CB	3:C:3044:LMT:H3B	2.27	0.64
1:A:544:LEU:HA	1:A:547:ILE:HD12	1.78	0.64
1:C:69:MET:CE	1:C:107:VAL:HG13	2.26	0.64
1:A:702:LEU:HD13	1:A:851:LEU:HD11	1.79	0.64
1:A:337:ILE:O	1:A:341:VAL:HG23	1.97	0.64
1:A:520:PHE:O	1:A:524:THR:HG23	1.98	0.64
1:C:151:GLN:NE2	1:C:279:ALA:O	2.30	0.64
1:A:341:VAL:HB	4:A:3049:LMU:C4	2.28	0.64
1:A:781:MET:HG3	1:C:228:GLN:OE1	1.97	0.64
1:A:726:GLN:OE1	1:A:812:GLY:HA3	1.98	0.64
1:A:908:GLY:HA2	1:A:1014:ALA:HB2	1.79	0.64
1:A:687:GLN:HE22	1:A:856:GLY:CA	2.09	0.64
1:C:21:LEU:O	1:C:25:LEU:HG	1.98	0.64
1:C:795:ASP:OD1	1:C:797:GLN:HG2	1.98	0.64
1:B:536:ARG:HD2	3:B:3035:LMT:O3B	1.98	0.64
2:D:126:LEU:HD22	2:D:164:ILE:HD12	1.78	0.64
1:A:326:PRO:O	1:A:630:SER:HB2	1.98	0.64
1:A:568:ASP:O	1:A:634:TRP:CZ3	2.51	0.64
1:C:162:MET:HA	1:C:313:MET:CE	2.28	0.64
1:B:454:VAL:HG22	1:B:455:PRO:HD3	1.79	0.63
1:A:235:ILE:O	1:B:728:LYS:HD2	1.98	0.63
1:A:1040:ILE:HG23	1:A:1041:GLU:N	2.13	0.63
1:B:25:LEU:HA	1:B:28:LEU:HD12	1.80	0.63
1:B:674:LEU:HD12	1:B:674:LEU:H	1.62	0.63
1:C:736:ALA:O	1:C:741:VAL:HG22	1.99	0.63
1:A:445:ILE:HG21	1:A:940:LYS:HE2	1.79	0.63
1:C:563:PHE:O	1:C:564:LEU:HD12	1.99	0.63
1:C:575:MET:CE	1:C:617:PHE:HB2	2.27	0.63
1:C:834:GLY:O	1:C:835:LYS:HD3	1.97	0.63
1:A:400:LEU:HD12	1:A:470:PHE:CE2	2.33	0.63
1:A:527:TYR:CE2	1:A:1019:ILE:HG23	2.34	0.63
1:A:883:VAL:HB	3:A:3047:LMT:C11	2.29	0.63
1:C:354:VAL:CG2	1:C:984:LEU:HD12	2.29	0.63
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.64	0.63
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.81	0.63
1:A:11:PHE:CE1	3:B:3036:LMT:O6'	2.50	0.63
1:B:342:LYS:O	1:B:346:GLU:HG2	1.99	0.63
1:B:367:ILE:HG12	1:B:496:MET:CE	2.28	0.63
1:C:671:ILE:CD1	1:C:674:LEU:HD11	2.28	0.63
2:D:131:VAL:O	2:D:134:LYS:HB3	1.99	0.63
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:TYR:HE1	1:A:968:VAL:HG12	1.64	0.62
1:B:764:ASP:OD1	1:B:765:ARG:HD3	1.99	0.62
1:C:544:LEU:CD1	3:C:3043:LMT:H92	2.28	0.62
1:C:735:LYS:O	1:C:739:LEU:HD13	1.99	0.62
1:B:363:ARG:HD3	1:B:498:LYS:HG3	1.81	0.62
1:B:681:ASP:HB3	1:B:861:GLY:H	1.64	0.62
1:A:1038:GLU:HG2	1:A:1040:ILE:N	2.13	0.62
1:A:872:GLN:HE21	1:A:874:PRO:HD3	1.65	0.62
1:A:932:LEU:HA	3:A:3048:LMT:H102	1.79	0.62
1:C:901:VAL:O	1:C:904:VAL:HG12	1.99	0.62
1:A:546:LEU:O	1:A:550:VAL:HG23	2.00	0.62
1:A:569:GLN:HA	1:A:634:TRP:HH2	1.63	0.62
1:A:904:VAL:HG23	1:A:907:LEU:HD12	1.82	0.62
1:C:601:LYS:HB3	1:C:601:LYS:NZ	2.14	0.62
2:E:61:GLU:O	2:E:65:VAL:HG23	1.99	0.62
1:A:932:LEU:HA	3:A:3048:LMT:C10	2.29	0.62
1:B:69:MET:HG3	1:B:78:MET:HE3	1.81	0.62
1:C:151:GLN:OE1	1:C:278:ILE:HG23	1.99	0.62
1:B:674:LEU:C	1:B:676:THR:H	2.01	0.62
2:E:34:MET:CE	2:E:40:VAL:HG12	2.29	0.62
1:B:197:GLN:HE21	1:B:197:GLN:N	1.98	0.62
1:C:531:VAL:O	1:C:534:ILE:HG12	1.99	0.62
1:C:939:ALA:O	1:C:943:ILE:HG12	2.00	0.62
1:B:987:MET:HA	1:B:1008:MET:HE3	1.82	0.62
1:B:576:VAL:HG22	1:B:663:VAL:HG13	1.81	0.62
1:C:370:ILE:O	1:C:373:PRO:HD2	2.00	0.62
2:D:62:ILE:O	2:D:66:LEU:HG	2.00	0.62
1:A:709:HIS:N	1:A:710:PRO:HD3	2.14	0.61
1:A:879:ILE:O	1:A:883:VAL:HG23	2.00	0.61
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.65	0.61
2:D:112:ASN:HB2	2:D:114:ILE:HG12	1.81	0.61
1:A:418:ARG:HE	1:A:970:MET:HG3	1.64	0.61
1:B:757:SER:HB3	1:B:773:VAL:HG12	1.80	0.61
1:B:575:MET:HA	1:B:626:ILE:HD13	1.81	0.61
1:C:425:LEU:HB3	1:C:429:GLU:HG2	1.81	0.61
1:C:63:GLN:HE22	1:C:67:GLN:NE2	1.97	0.61
1:A:960:LEU:HD22	1:A:1030:ARG:HB3	1.80	0.61
1:A:28:LEU:C	1:A:29:LYS:HD2	2.20	0.61
1:A:341:VAL:C	4:A:3049:LMU:H62	2.21	0.61
1:A:717:ARG:HH12	1:A:828:LEU:HD23	1.65	0.61
1:B:177:LEU:H	1:B:177:LEU:HD23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:ILE:O	1:B:914:LEU:HD22	2.00	0.61
1:C:247:GLY:O	1:C:263:ARG:HB2	2.01	0.61
1:A:185:ARG:HB2	1:A:269:GLU:O	2.00	0.61
1:A:338:HIS:HB3	4:A:3049:LMU:H2'	1.82	0.61
1:B:314:GLU:HA	1:B:317:PHE:CE2	2.35	0.61
1:B:571:VAL:HG12	1:B:630:SER:HA	1.82	0.61
1:A:8:ARG:HH22	3:B:3036:LMT:C6B	2.07	0.61
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.83	0.61
1:B:519:MET:HA	1:B:522:LYS:HE2	1.83	0.61
1:B:972:LEU:O	1:B:976:LEU:HD13	2.00	0.61
1:A:533:GLY:HA2	1:A:536:ARG:HD3	1.82	0.61
1:A:83:ASP:OD2	1:A:815:ARG:HD3	2.01	0.61
2:E:77:ASP:OD1	2:E:81:SER:HB3	2.00	0.61
1:A:537:SER:C	1:A:539:GLY:H	2.03	0.61
1:A:883:VAL:HG11	3:A:3047:LMT:C11	2.27	0.61
1:A:956:GLU:O	1:A:958:LYS:HG3	2.01	0.61
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.83	0.61
1:B:489:THR:HG21	5:B:2040:HOH:O	2.01	0.61
3:C:3042:LMT:O1'	3:C:3042:LMT:H6D	2.00	0.61
2:E:142:GLN:HB3	2:E:146:GLY:HA2	1.81	0.61
1:B:555:LEU:CD2	1:B:914:LEU:HD13	2.30	0.61
1:C:875:SER:CB	3:C:3044:LMT:O2B	2.37	0.61
2:E:48:TRP:HZ3	2:E:77:ASP:OD1	1.84	0.61
1:C:671:ILE:HG12	1:C:862:MET:SD	2.40	0.60
1:A:341:VAL:O	1:A:344:LEU:HB2	2.01	0.60
1:A:341:VAL:CB	4:A:3049:LMU:H62	2.30	0.60
3:C:3042:LMT:H122	3:C:3042:LMT:H82	1.82	0.60
1:A:582:ALA:HA	1:A:586:ARG:NH2	2.16	0.60
1:B:910:ILE:HG13	1:B:914:LEU:HD22	1.84	0.60
3:C:3046:LMT:O6'	3:C:3046:LMT:C5B	2.50	0.60
1:C:254:ASN:HD22	1:C:258:SER:HB2	1.67	0.60
1:A:671:ILE:HG21	1:A:675:GLY:HA2	1.84	0.60
1:B:69:MET:HG3	1:B:78:MET:CE	2.32	0.60
1:A:657:GLN:HG2	1:A:658:ILE:N	2.16	0.60
1:C:459:PHE:CE1	1:C:876:LEU:HD23	2.37	0.60
1:A:310:LEU:HG	1:A:323:ILE:HD13	1.84	0.60
1:B:910:ILE:CG2	1:B:1013:THR:HG21	2.31	0.60
1:B:492:LEU:HD22	1:B:496:MET:CE	2.32	0.60
1:B:420:MET:HE2	1:B:499:PRO:HA	1.83	0.60
1:C:110:LYS:NZ	1:C:113:LEU:HD23	2.17	0.60
3:C:3042:LMT:H6E	3:C:3042:LMT:C2'	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:PHE:CD1	1:C:569:GLN:HA	2.36	0.60
3:A:3046:LMT:H112	4:A:3049:LMU:H92	1.82	0.59
1:B:38:ILE:HD11	1:B:671:ILE:HG21	1.83	0.59
1:C:129:VAL:HG13	1:C:129:VAL:O	2.02	0.59
1:C:243:THR:HG21	1:C:269:GLU:HA	1.84	0.59
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.84	0.59
2:E:158:ASN:ND2	2:E:161:LEU:HB2	2.17	0.59
1:A:28:LEU:O	1:A:29:LYS:HD2	2.01	0.59
1:A:522:LYS:HB3	1:A:522:LYS:NZ	2.18	0.59
1:C:337:ILE:O	1:C:341:VAL:HG23	2.02	0.59
2:E:163:GLU:O	2:E:166:GLN:HB2	2.02	0.59
1:B:337:ILE:O	1:B:341:VAL:HG23	2.02	0.59
3:C:3042:LMT:O3'	3:C:3042:LMT:C1B	2.50	0.59
1:C:458:PHE:CZ	3:C:3046:LMT:H51	2.37	0.59
1:C:982:PHE:CD2	1:C:1011:MET:HG3	2.38	0.59
1:A:302:THR:O	1:A:306:ILE:HG13	2.01	0.59
1:A:887:CYS:CB	3:A:3047:LMT:C7	2.80	0.59
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.83	0.59
1:C:434:SER:O	1:C:438:ILE:HG12	2.02	0.59
1:B:1011:MET:O	1:B:1015:THR:HG23	2.02	0.59
1:B:492:LEU:HB3	1:B:496:MET:HE2	1.83	0.59
1:B:872:GLN:O	1:B:876:LEU:N	2.35	0.59
1:C:547:ILE:HG12	3:C:3043:LMT:C12	2.33	0.59
1:A:1022:VAL:HB	1:A:1023:PRO:HD3	1.83	0.59
1:A:5:PHE:HE2	1:A:11:PHE:CE1	2.20	0.59
1:A:393:LEU:HD23	1:A:470:PHE:HD1	1.67	0.59
1:A:739:LEU:HD13	1:A:799:VAL:HG11	1.84	0.59
1:A:929:VAL:O	1:A:932:LEU:HB3	2.03	0.59
1:A:344:LEU:HB3	4:A:3049:LMU:H82	1.81	0.59
1:A:809:TRP:CD1	2:E:79:LEU:HD23	2.38	0.59
1:C:1011:MET:HE2	1:C:1011:MET:HA	1.84	0.59
3:C:3042:LMT:H2B	3:C:3042:LMT:H3'	1.83	0.59
1:A:25:LEU:CG	3:B:3037:LMT:H41	2.33	0.59
1:B:482:VAL:O	1:B:486:LEU:HG	2.02	0.59
1:B:491:ALA:O	1:B:495:THR:HB	2.02	0.59
1:A:6:ILE:HG23	1:A:494:ALA:CB	2.32	0.58
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.33	0.58
1:C:104:GLN:NE2	1:C:129:VAL:HG13	2.16	0.58
1:A:1037:ASN:CG	1:A:1038:GLU:H	2.04	0.58
1:A:345:VAL:HG23	4:A:3049:LMU:H81	1.84	0.58
1:A:463:THR:HG23	1:A:563:PHE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:GLY:N	1:A:997:SER:OG	2.36	0.58
1:C:369:THR:O	1:C:372:VAL:HG13	2.04	0.58
1:A:485:ALA:C	1:A:486:LEU:HD12	2.23	0.58
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.03	0.58
1:B:1013:THR:HG22	1:B:1017:LEU:HD12	1.84	0.58
1:B:351:VAL:O	1:B:355:MET:HB2	2.03	0.58
1:C:193:LEU:HD13	1:C:265:VAL:HB	1.84	0.58
1:A:343:THR:HG21	1:A:1000:GLN:HE22	1.68	0.58
1:A:469:GLN:O	1:A:473:THR:HG23	2.04	0.58
1:C:510:LYS:HG2	1:C:511:GLY:H	1.67	0.58
2:E:59:HIS:O	2:E:63:VAL:HG23	2.03	0.58
1:A:14:VAL:O	1:A:18:ILE:HG13	2.04	0.58
1:A:859:TRP:CD1	1:A:867:ARG:HD2	2.39	0.58
1:B:347:ALA:O	1:B:351:VAL:HG23	2.03	0.58
1:B:671:ILE:HG22	1:B:672:VAL:N	2.19	0.58
1:C:103:ALA:O	1:C:107:VAL:HG23	2.04	0.58
1:C:183:ALA:N	1:C:271:GLY:O	2.37	0.58
1:A:164:ASP:HB2	5:A:2032:HOH:O	2.04	0.58
1:C:172:VAL:HG12	1:C:173:GLY:O	2.03	0.58
1:C:868:LEU:O	1:C:872:GLN:HG2	2.03	0.58
1:A:1038:GLU:C	1:A:1040:ILE:H	2.06	0.58
1:A:412:VAL:O	1:A:416:VAL:HG23	2.03	0.58
1:B:222:THR:HG23	1:C:275:TYR:CB	2.30	0.58
2:D:152:ILE:HD13	2:D:152:ILE:C	2.24	0.58
1:A:146:ASP:O	1:A:148:THR:HG23	2.04	0.57
1:A:345:VAL:HG23	4:A:3049:LMU:C8	2.34	0.57
1:A:444:GLY:HA3	3:A:3047:LMT:H11	1.86	0.57
1:A:862:MET:O	1:A:866:GLU:HG2	2.04	0.57
1:B:776:GLU:CD	1:B:778:LYS:HZ2	2.07	0.57
1:A:354:VAL:CG2	1:A:984:LEU:HD12	2.34	0.57
1:B:349:ILE:O	1:B:352:PHE:HB3	2.05	0.57
1:B:703:LEU:CD2	1:B:716:VAL:HG22	2.33	0.57
1:C:1011:MET:CE	1:C:1011:MET:HA	2.35	0.57
1:A:414:GLU:HG3	1:A:415:ASN:N	2.19	0.57
1:A:453:PHE:CD2	3:A:3048:LMT:H122	2.39	0.57
1:A:531:VAL:O	1:A:534:ILE:HG12	2.04	0.57
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.39	0.57
3:B:3037:LMT:H2O1	3:B:3037:LMT:C3'	2.17	0.57
1:C:544:LEU:HD11	3:C:3043:LMT:H92	1.85	0.57
1:B:444:GLY:CA	3:B:3036:LMT:O2'	2.52	0.57
1:B:893:GLU:HG3	1:B:893:GLU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:LEU:HD21	1:A:1028:VAL:CG2	2.34	0.57
1:B:104:GLN:NE2	1:C:109:ASN:HB3	2.20	0.57
1:B:382:VAL:HG21	1:B:476:SER:HB3	1.86	0.57
1:C:878:ALA:O	1:C:882:ILE:HG12	2.05	0.57
2:E:29:GLU:OE2	2:E:33:LEU:HD23	2.05	0.57
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.86	0.57
1:B:330:THR:HB	1:B:331:PRO:HD3	1.87	0.57
1:B:590:VAL:O	1:B:594:VAL:HG23	2.03	0.57
1:B:582:ALA:HB3	1:B:623:ASN:CB	2.35	0.57
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.85	0.57
2:E:51:LEU:HD23	2:E:83:PRO:HG2	1.86	0.57
1:A:1:MET:N	1:A:2:PRO:CD	2.68	0.57
1:A:418:ARG:HE	1:A:970:MET:CG	2.18	0.57
1:A:445:ILE:HG21	1:A:940:LYS:HG3	1.87	0.57
1:A:568:ASP:O	1:A:634:TRP:HZ3	1.87	0.57
1:A:312:LYS:NZ	1:A:312:LYS:HB3	2.20	0.57
1:B:302:THR:O	1:B:306:ILE:CG2	2.53	0.57
1:B:30:LEU:HD23	1:B:390:ILE:HG13	1.87	0.57
1:B:515:TRP:HE3	1:B:518:ARG:NH2	2.01	0.57
2:E:160:ASP:O	2:E:164:ILE:HG22	2.05	0.57
1:B:133:SER:HB3	1:B:292:LYS:HE2	1.87	0.57
1:C:185:ARG:HB2	1:C:269:GLU:O	2.05	0.57
2:E:113:GLY:O	2:E:143:ASP:HA	2.05	0.57
1:A:351:VAL:O	1:A:355:MET:HG2	2.05	0.56
1:A:809:TRP:HB2	2:E:48:TRP:CH2	2.40	0.56
1:B:340:VAL:HG21	1:B:395:MET:HB3	1.87	0.56
1:C:192:GLU:HA	1:C:195:LYS:HG2	1.86	0.56
1:C:875:SER:HB2	3:C:3044:LMT:H3B	1.87	0.56
1:C:901:VAL:HG23	1:C:902:MET:N	2.21	0.56
1:A:563:PHE:O	1:A:924:ASP:HB2	2.04	0.56
1:B:378:GLY:O	1:B:382:VAL:HG13	2.05	0.56
1:B:767:ARG:HA	5:B:2072:HOH:O	2.04	0.56
1:B:907:LEU:O	1:B:1013:THR:HG22	2.06	0.56
1:C:263:ARG:HD3	5:C:2047:HOH:O	2.04	0.56
1:C:509:LYS:O	1:C:510:LYS:CB	2.51	0.56
1:C:695:LEU:HD13	1:C:825:MET:HG3	1.86	0.56
1:A:447:MET:C	3:A:3047:LMT:C6	2.74	0.56
1:A:842:GLU:O	1:A:846:GLN:HG3	2.05	0.56
1:B:729:ILE:HD11	1:B:805:SER:CB	2.32	0.56
1:C:480:LEU:O	1:C:484:VAL:HG23	2.05	0.56
1:A:345:VAL:HG23	4:A:3049:LMU:C6	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:VAL:HA	1:A:405:LEU:CD2	2.30	0.56
1:A:639:GLY:O	1:A:643:LYS:HD3	2.06	0.56
1:A:678:THR:O	1:A:679:GLY:O	2.24	0.56
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.88	0.56
2:D:77:ASP:OD2	2:D:81:SER:HB3	2.06	0.56
1:A:979:SER:OG	1:A:1015:THR:HG21	2.06	0.56
1:C:454:VAL:HB	1:C:455:PRO:HD3	1.88	0.56
1:B:865:GLN:O	1:B:869:SER:HB2	2.06	0.56
1:B:919:ARG:HG2	1:B:919:ARG:HH11	1.69	0.56
1:A:539:GLY:CA	1:A:542:LEU:HD13	2.36	0.56
1:B:363:ARG:NE	1:B:496:MET:O	2.39	0.56
1:A:309:GLU:HG3	1:A:313:MET:CE	2.35	0.55
1:B:444:GLY:HA2	3:B:3036:LMT:O2'	2.07	0.55
1:B:527:TYR:HE2	1:B:968:VAL:HG13	1.70	0.55
1:C:497:LEU:O	1:C:497:LEU:HD12	2.06	0.55
3:B:3037:LMT:H3'	3:B:3037:LMT:O2B	2.06	0.55
1:C:845:GLU:HG3	1:C:859:TRP:CZ3	2.41	0.55
1:C:888:LEU:HD13	1:C:901:VAL:CG2	2.35	0.55
2:D:48:TRP:CZ3	2:D:77:ASP:OD2	2.59	0.55
1:B:293:LEU:HD21	1:B:297:ALA:HB3	1.88	0.55
1:A:400:LEU:HD12	1:A:470:PHE:HE2	1.70	0.55
1:A:958:LYS:O	1:A:959:GLY:C	2.44	0.55
1:B:355:MET:HG2	1:B:365:THR:HA	1.87	0.55
1:B:424:GLY:H	1:B:502:LYS:HB2	1.71	0.55
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.88	0.55
1:C:150:THR:O	1:C:154:ILE:HG13	2.06	0.55
1:C:573:MET:HE3	1:C:626:ILE:HD11	1.88	0.55
1:A:427:PRO:O	1:A:431:THR:HG22	2.07	0.55
1:B:412:VAL:O	1:B:416:VAL:HG23	2.07	0.55
1:B:569:GLN:O	1:B:571:VAL:HG22	2.06	0.55
1:B:84:SER:HB3	5:B:2017:HOH:O	2.06	0.55
1:C:580:ALA:CB	1:C:724:THR:HG22	2.31	0.55
2:D:128:ILE:O	2:D:132:LEU:HG	2.07	0.55
1:A:18:ILE:HD13	3:B:3036:LMT:H61	1.89	0.55
1:A:712:MET:CB	1:A:835:LYS:HG3	2.36	0.55
1:B:333:VAL:O	1:B:337:ILE:HG13	2.06	0.55
1:B:745:ASP:O	1:B:749:THR:HG23	2.05	0.55
1:B:775:SER:O	1:B:780:ARG:NH1	2.40	0.55
1:C:686:ASP:OD1	1:C:690:LEU:HB2	2.06	0.55
3:A:3047:LMT:C3B	1:C:8:ARG:HH21	2.14	0.55
1:C:7:ASP:O	1:C:9:PRO:HD3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ARG:NH1	1:A:432:ARG:HG2	2.22	0.55
1:B:563:PHE:CE2	1:B:564:LEU:HD13	2.41	0.55
1:A:341:VAL:O	4:A:3049:LMU:H61	2.06	0.55
1:A:527:TYR:CE1	1:A:968:VAL:HG12	2.42	0.55
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.88	0.55
1:B:674:LEU:C	1:B:676:THR:N	2.58	0.55
1:B:919:ARG:HD2	1:B:1005:THR:CG2	2.20	0.55
1:A:919:ARG:HE	1:A:1005:THR:HG21	1.72	0.55
1:B:143:ILE:HG21	1:B:281:PHE:HB3	1.88	0.55
1:B:393:LEU:HD12	1:B:469:GLN:HG3	1.89	0.55
1:B:561:SER:HA	1:B:923:ASN:HB3	1.88	0.55
1:C:690:LEU:H	1:C:690:LEU:HD12	1.71	0.55
1:C:83:ASP:HB2	1:C:87:THR:CG2	2.37	0.55
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.89	0.54
1:A:530:SER:O	1:A:534:ILE:HG23	2.08	0.54
1:B:842:GLU:O	1:B:846:GLN:HG3	2.07	0.54
1:C:68:ASN:O	1:C:110:LYS:HE2	2.07	0.54
1:B:396:PHE:HA	1:B:399:VAL:HG22	1.89	0.54
1:B:445:ILE:HG22	1:B:449:LEU:HD12	1.90	0.54
1:B:563:PHE:CD2	1:B:564:LEU:HD13	2.42	0.54
1:B:878:ALA:O	1:B:882:ILE:HG13	2.06	0.54
2:E:48:TRP:CZ3	2:E:77:ASP:OD1	2.60	0.54
1:A:675:GLY:C	1:A:677:ALA:H	2.11	0.54
1:A:873:ALA:N	1:A:874:PRO:CD	2.70	0.54
1:B:423:GLU:HA	1:B:502:LYS:CE	2.34	0.54
1:B:492:LEU:HD22	1:B:496:MET:HE1	1.88	0.54
1:C:83:ASP:HB2	1:C:87:THR:HG23	1.88	0.54
1:A:1035:ARG:O	1:A:1037:ASN:N	2.41	0.54
1:B:144:ASN:OD1	1:B:148:THR:HG22	2.07	0.54
1:B:426:PRO:HD2	1:B:429:GLU:HG3	1.90	0.54
1:B:885:PHE:HD1	1:B:902:MET:CE	2.20	0.54
2:D:35:ALA:C	2:D:36:ASN:HD22	2.10	0.54
1:A:420:MET:O	1:A:424:GLY:HA2	2.07	0.54
1:A:488:LEU:O	1:A:492:LEU:HD13	2.08	0.54
1:B:446:ALA:HB2	1:B:482:VAL:HG21	1.89	0.54
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.89	0.54
1:C:446:ALA:O	1:C:450:SER:HB2	2.07	0.54
1:C:575:MET:HG3	5:C:2076:HOH:O	2.06	0.54
1:C:892:TYR:O	1:C:893:GLU:C	2.45	0.54
1:A:348:ILE:CG2	4:A:3049:LMU:H123	2.35	0.54
1:A:300:LEU:HD23	1:A:330:THR:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:TRP:O	1:B:17:ILE:HG13	2.07	0.54
1:B:341:VAL:O	1:B:345:VAL:HG23	2.07	0.54
1:B:5:PHE:CG	1:B:487:ILE:HG23	2.42	0.54
1:A:1038:GLU:OE1	1:A:1039:ASP:N	2.31	0.54
3:A:3048:LMT:H5B	3:A:3048:LMT:H6D	1.89	0.54
1:A:524:THR:O	1:A:527:TYR:HB3	2.08	0.54
1:C:541:TYR:CE1	3:C:3043:LMT:H41	2.42	0.54
1:C:741:VAL:HG11	1:C:799:VAL:CG1	2.35	0.54
1:C:875:SER:HB2	3:C:3044:LMT:C2B	2.35	0.54
2:D:61:GLU:OE1	2:D:61:GLU:N	2.41	0.54
1:A:901:VAL:HG11	1:A:943:ILE:HG13	1.90	0.54
1:B:868:LEU:C	1:B:870:GLY:N	2.61	0.54
1:C:423:GLU:CB	1:C:425:LEU:HD13	2.38	0.54
1:A:953:MET:HE1	1:A:1026:PHE:HE2	1.72	0.54
1:A:344:LEU:HB3	4:A:3049:LMU:C8	2.38	0.54
1:A:354:VAL:HG21	1:A:981:ALA:HA	1.88	0.54
1:A:445:ILE:O	1:A:448:VAL:HG22	2.07	0.54
1:B:146:ASP:HB2	1:B:320:GLY:HA3	1.90	0.54
1:C:534:ILE:HG22	1:C:541:TYR:OH	2.07	0.54
1:C:991:ILE:O	1:C:991:ILE:HG22	2.08	0.54
2:E:106:VAL:HG21	2:E:136:GLY:O	2.08	0.54
1:A:1:MET:H3	1:A:2:PRO:HD3	1.73	0.54
1:A:563:PHE:CD1	1:A:564:LEU:HG	2.42	0.54
1:A:867:ARG:HA	1:A:867:ARG:NE	2.16	0.54
1:B:344:LEU:HD23	1:B:402:ILE:HD11	1.90	0.54
2:D:123:ARG:HB3	2:D:125:HIS:CD2	2.42	0.54
1:A:230:LEU:HD12	1:A:231:ASN:N	2.22	0.53
1:A:393:LEU:CD2	1:A:466:ILE:HG23	2.38	0.53
1:A:671:ILE:CG2	1:A:672:VAL:H	2.05	0.53
2:E:139:VAL:HG23	2:E:140:ASN:OD1	2.07	0.53
1:B:133:SER:O	1:B:134:SER:HB3	2.08	0.53
1:B:678:THR:HG22	1:B:830:GLN:HB2	1.90	0.53
1:C:372:VAL:HG22	1:C:373:PRO:HD3	1.90	0.53
1:C:50:PRO:HG2	1:C:125:GLN:HE21	1.73	0.53
2:E:26:ARG:NH1	2:E:26:ARG:HB3	2.23	0.53
1:A:415:ASN:O	1:A:419:VAL:HG23	2.08	0.53
1:A:448:VAL:HA	3:A:3047:LMT:C6	2.32	0.53
1:B:616:GLY:O	1:B:619:GLY:N	2.42	0.53
1:C:10:ILE:O	1:C:14:VAL:HG13	2.07	0.53
1:C:23:GLY:HA3	1:C:377:LEU:O	2.09	0.53
1:A:254:ASN:HD22	1:A:258:SER:CB	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1031:ARG:C	1:C:1033:PHE:H	2.11	0.53
1:C:1037:ASN:O	1:C:1040:ILE:HG23	2.08	0.53
1:C:50:PRO:CG	1:C:125:GLN:HE21	2.22	0.53
1:A:953:MET:CE	1:A:1026:PHE:HE2	2.22	0.53
1:A:338:HIS:HA	1:A:341:VAL:HG23	1.91	0.53
1:A:675:GLY:C	1:A:677:ALA:N	2.61	0.53
1:A:929:VAL:HA	1:A:932:LEU:HB2	1.91	0.53
1:B:968:VAL:HG21	1:B:1023:PRO:HG3	1.89	0.53
1:A:412:VAL:HG11	1:A:489:THR:HG22	1.90	0.53
1:A:889:ALA:HB1	1:C:10:ILE:HD11	1.91	0.53
1:B:144:ASN:HD21	1:B:148:THR:CG2	2.22	0.53
2:D:48:TRP:HD1	2:D:53:LEU:HD13	1.73	0.53
1:A:341:VAL:C	4:A:3049:LMU:C6	2.77	0.53
1:A:35:TYR:CZ	1:A:564:LEU:HD13	2.43	0.53
3:C:3042:LMT:O3'	3:C:3042:LMT:H2B	2.08	0.53
2:D:122:ASN:HA	2:D:152:ILE:CD1	2.30	0.53
1:A:489:THR:HB	1:A:490:PRO:HD3	1.90	0.53
1:A:872:GLN:NE2	1:A:874:PRO:HD3	2.23	0.53
1:B:213:GLN:HE21	1:B:238:THR:HG22	1.74	0.53
1:A:893:GLU:CD	1:C:10:ILE:HG23	2.29	0.53
1:C:194:ASN:ND2	1:C:798:MET:HG3	2.24	0.53
1:B:448:VAL:HG13	1:B:884:VAL:HG13	1.91	0.53
1:B:776:GLU:HG2	1:B:778:LYS:HD2	1.91	0.53
1:B:979:SER:OG	1:B:1015:THR:HG21	2.09	0.53
1:C:111:LEU:HD21	1:C:127:VAL:HG23	1.90	0.53
1:C:563:PHE:O	1:C:924:ASP:HB2	2.09	0.53
1:A:883:VAL:CB	3:A:3047:LMT:H111	2.38	0.53
1:A:537:SER:O	1:A:539:GLY:N	2.39	0.53
1:A:85:THR:HG22	1:A:87:THR:H	1.73	0.53
1:A:948:PHE:O	1:A:952:LEU:HG	2.09	0.53
2:E:60:LEU:HD22	2:E:94:GLU:OE2	2.08	0.53
1:A:1037:ASN:O	1:A:1038:GLU:HB3	2.08	0.52
1:A:108:GLN:NE2	1:B:109:ASN:HB3	2.24	0.52
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.90	0.52
1:B:871:ASN:ND2	1:B:872:GLN:N	2.57	0.52
1:C:541:TYR:HA	1:C:544:LEU:HB2	1.90	0.52
2:E:35:ALA:C	2:E:37:GLY:H	2.12	0.52
1:A:677:ALA:O	1:A:678:THR:C	2.47	0.52
1:A:883:VAL:CG1	3:A:3047:LMT:C11	2.79	0.52
1:B:650:ARG:HB2	1:B:650:ARG:HH11	1.73	0.52
1:C:36:PRO:HG3	1:C:469:GLN:CD	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:390:ILE:HA	1:C:394:THR:HG21	1.90	0.52
1:C:415:ASN:HD22	1:C:434:SER:CB	2.22	0.52
1:C:575:MET:HE1	1:C:617:PHE:CD2	2.44	0.52
3:A:3047:LMT:C1	3:A:3047:LMT:O2'	2.54	0.52
1:A:447:MET:HB2	3:A:3047:LMT:H42	1.89	0.52
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.91	0.52
1:A:214:VAL:HG21	5:B:2066:HOH:O	2.09	0.52
1:A:883:VAL:CB	3:A:3047:LMT:C11	2.87	0.52
1:B:184:MET:CE	1:B:268:ILE:HG22	2.40	0.52
1:B:587:THR:HG21	1:B:622:GLN:O	2.10	0.52
1:B:668:LEU:HD23	1:B:668:LEU:N	2.24	0.52
1:A:889:ALA:O	1:C:10:ILE:HD11	2.09	0.52
1:B:148:THR:HG23	1:B:149:MET:HG2	1.91	0.52
1:B:363:ARG:HH11	1:B:498:LYS:HE3	1.74	0.52
5:A:2018:HOH:O	1:C:104:GLN:HG3	2.09	0.52
1:C:937:LEU:HB3	1:C:1011:MET:CE	2.39	0.52
1:A:712:MET:HB3	1:A:835:LYS:HG3	1.92	0.52
1:A:448:VAL:HG21	1:A:943:ILE:HD13	1.91	0.52
1:B:733:GLN:HE22	1:B:743:ILE:CG1	2.23	0.52
1:C:40:PRO:HD2	1:C:674:LEU:HD12	1.90	0.52
1:A:293:LEU:HD22	1:A:297:ALA:HB3	1.91	0.52
1:B:453:PHE:HB2	1:B:475:VAL:HG12	1.92	0.52
1:B:560:PRO:O	1:B:922:THR:HB	2.09	0.52
1:C:782:LEU:O	1:C:785:ASP:HB2	2.09	0.52
1:A:679:GLY:HA2	1:A:830:GLN:HA	1.92	0.52
1:B:507:GLU:OE2	1:B:521:GLU:HG2	2.09	0.52
1:C:34:GLN:O	1:C:392:THR:HB	2.09	0.52
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.90	0.52
1:A:120:GLN:O	1:A:124:GLN:HG3	2.10	0.52
1:A:184:MET:HG2	1:A:246:PHE:CD1	2.44	0.52
1:A:864:TYR:O	1:A:867:ARG:HB2	2.10	0.52
1:A:456:MET:HE3	1:A:932:LEU:HD13	1.91	0.52
1:B:890:ALA:HB3	3:B:3036:LMT:H12	1.91	0.52
1:A:641:GLU:O	1:A:650:ARG:NH2	2.39	0.52
1:A:18:ILE:CD1	3:B:3036:LMT:H61	2.40	0.52
1:B:424:GLY:N	1:B:502:LYS:HB2	2.24	0.52
1:A:878:ALA:O	1:A:882:ILE:HG12	2.11	0.51
1:B:454:VAL:CG2	1:B:455:PRO:HD3	2.40	0.51
1:B:278:ILE:CG2	1:B:613:ASN:HB3	2.30	0.51
1:B:75:LEU:HD21	1:B:92:LEU:HB3	1.91	0.51
1:C:314:GLU:HG2	1:C:317:PHE:CE1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:ARG:O	1:A:422:GLU:HG3	2.09	0.51
1:B:578:LEU:HD22	1:B:661:ALA:CB	2.40	0.51
1:C:184:MET:HB2	1:C:762:PHE:CE2	2.46	0.51
3:C:3046:LMT:H5'	3:C:3046:LMT:H2O2	1.70	0.51
1:A:539:GLY:HA2	1:A:542:LEU:HD13	1.93	0.51
1:A:559:LEU:HD12	1:A:560:PRO:HD2	1.93	0.51
1:B:668:LEU:HD23	1:B:668:LEU:H	1.76	0.51
1:B:687:GLN:HG3	5:B:2055:HOH:O	2.11	0.51
1:A:220:GLY:HA2	1:B:781:MET:SD	2.50	0.51
1:A:25:LEU:HD21	3:B:3037:LMT:C4	2.33	0.51
1:A:27:ILE:HD13	3:A:3046:LMT:C7	2.41	0.51
1:A:361:ASN:C	1:A:363:ARG:H	2.14	0.51
1:A:575:MET:HE1	1:A:626:ILE:HG13	1.92	0.51
1:B:5:PHE:CD1	1:B:487:ILE:HG23	2.45	0.51
1:B:509:LYS:O	1:B:510:LYS:O	2.29	0.51
1:B:542:LEU:O	1:B:546:LEU:HD13	2.10	0.51
1:C:876:LEU:HD13	1:C:932:LEU:HD21	1.93	0.51
1:A:341:VAL:O	4:A:3049:LMU:C6	2.58	0.51
1:A:60:THR:HG22	1:A:61:VAL:CG2	2.37	0.51
1:A:614:GLY:HA2	1:A:621:GLY:O	2.10	0.51
1:A:953:MET:O	1:A:957:GLY:HA2	2.10	0.51
1:A:991:ILE:O	1:A:991:ILE:CG2	2.58	0.51
1:B:544:LEU:HD23	1:B:1021:PHE:HZ	1.75	0.51
1:B:243:THR:HG23	5:B:2033:HOH:O	2.10	0.51
1:B:717:ARG:HH11	1:B:717:ARG:HG2	1.74	0.51
1:C:21:LEU:HD12	1:C:22:ALA:N	2.26	0.51
1:C:601:LYS:HZ2	1:C:601:LYS:HB3	1.74	0.51
1:A:300:LEU:CD2	1:A:330:THR:HG23	2.41	0.51
1:A:341:VAL:HB	4:A:3049:LMU:H42	1.91	0.51
1:A:344:LEU:C	4:A:3049:LMU:H112	2.31	0.51
1:A:712:MET:HA	1:A:832:ALA:HB2	1.92	0.51
1:A:893:GLU:OE1	1:C:10:ILE:HG23	2.11	0.51
1:B:418:ARG:O	1:B:422:GLU:HG3	2.11	0.51
1:B:47:ALA:HB3	1:B:88:VAL:CG1	2.40	0.51
1:C:291:ILE:CD1	1:C:306:ILE:HD13	2.41	0.51
1:C:451:ALA:HB1	1:C:883:VAL:HG12	1.92	0.51
1:C:575:MET:HE1	1:C:617:PHE:HD2	1.75	0.51
1:A:210:GLN:OE1	1:A:249:ILE:HG23	2.11	0.51
1:A:229:GLN:HA	1:A:229:GLN:HE21	1.76	0.51
1:B:572:PHE:HA	1:B:668:LEU:CD2	2.40	0.51
1:A:341:VAL:HB	4:A:3049:LMU:H41	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:TRP:NE1	2:E:79:LEU:HD23	2.26	0.51
1:B:396:PHE:HD2	1:B:399:VAL:HG21	1.76	0.51
1:B:443:VAL:C	3:B:3036:LMT:O2'	2.48	0.51
1:C:1032:ARG:O	1:C:1032:ARG:HG3	2.11	0.51
1:C:541:TYR:N	1:C:541:TYR:CD2	2.79	0.51
1:B:577:GLN:NE2	1:B:578:LEU:O	2.43	0.50
1:C:690:LEU:H	1:C:690:LEU:CD1	2.23	0.50
1:A:17:ILE:O	1:A:21:LEU:HG	2.11	0.50
1:A:932:LEU:CA	3:A:3048:LMT:C10	2.88	0.50
1:A:645:GLU:O	1:A:649:MET:HG3	2.11	0.50
1:B:162:MET:O	1:B:166:ILE:HG12	2.11	0.50
1:B:253:VAL:O	1:B:253:VAL:HG23	2.11	0.50
1:B:251:LEU:HD11	1:B:262:LEU:HD12	1.93	0.50
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.92	0.50
1:B:643:LYS:O	1:B:647:ILE:HG13	2.11	0.50
1:B:836:SER:OG	1:B:839:GLU:HG3	2.11	0.50
1:B:885:PHE:HD1	1:B:902:MET:HE1	1.76	0.50
2:E:58:GLY:HA3	2:E:92:HIS:CE1	2.46	0.50
1:A:23:GLY:HA3	1:A:377:LEU:O	2.12	0.50
1:A:635:ALA:HB2	4:A:3049:LMU:H4O1	1.75	0.50
1:A:980:LEU:HD23	1:A:980:LEU:O	2.11	0.50
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.32	0.50
1:C:75:LEU:C	1:C:75:LEU:HD13	2.32	0.50
1:A:446:ALA:HB2	1:A:482:VAL:CG2	2.42	0.50
1:A:351:VAL:HG23	1:A:981:ALA:HB1	1.92	0.50
1:B:637:ARG:N	1:B:638:PRO:CD	2.73	0.50
1:B:871:ASN:HD21	1:B:873:ALA:CB	2.25	0.50
1:A:1042:HIS:O	1:A:1043:SER:O	2.30	0.50
1:A:25:LEU:HG	3:B:3037:LMT:H22	1.93	0.50
1:C:359:LEU:CD1	1:C:365:THR:HA	2.41	0.50
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.94	0.50
1:A:149:MET:HB2	1:A:153:ASP:HB2	1.94	0.50
1:B:1013:THR:CG2	1:B:1017:LEU:HD12	2.41	0.50
1:B:968:VAL:CG2	1:B:1023:PRO:HG3	2.42	0.50
1:B:448:VAL:O	1:B:451:ALA:HB3	2.12	0.50
1:B:454:VAL:N	1:B:455:PRO:CD	2.75	0.50
1:B:621:GLY:O	1:B:624:THR:HG22	2.11	0.50
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.47	0.50
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.47	0.50
1:C:100:ALA:HB1	1:C:131:LYS:HD2	1.93	0.50
3:A:3047:LMT:O5B	3:A:3047:LMT:O6'	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:960:LEU:O	1:A:964:THR:HG23	2.11	0.50
1:B:544:LEU:HD23	1:B:1021:PHE:CZ	2.46	0.50
1:B:363:ARG:CD	1:B:498:LYS:HE3	2.37	0.50
1:C:573:MET:CE	1:C:626:ILE:HD11	2.41	0.50
1:A:451:ALA:CB	3:A:3047:LMT:C8	2.85	0.50
1:C:997:SER:HA	1:C:1000:GLN:HB2	1.94	0.50
2:D:92:HIS:O	2:D:96:VAL:HG23	2.12	0.50
1:B:23:GLY:O	1:B:26:ALA:HB3	2.12	0.49
1:B:776:GLU:CD	1:B:778:LYS:NZ	2.66	0.49
1:B:879:ILE:HG12	3:B:3037:LMT:C3	2.42	0.49
1:A:337:ILE:HG22	1:A:338:HIS:HD2	1.78	0.49
1:A:341:VAL:CG1	3:A:3046:LMT:H62	2.42	0.49
1:A:404:LEU:HA	1:A:937:LEU:HD21	1.94	0.49
1:A:8:ARG:CZ	3:B:3036:LMT:H6'2	2.41	0.49
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.91	0.49
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.92	0.49
1:A:35:TYR:HB3	1:A:36:PRO:HD2	1.95	0.49
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.47	0.49
1:A:575:MET:HG2	1:A:666:PHE:HE1	1.77	0.49
1:B:540:ARG:NH1	3:B:3035:LMT:O6B	2.45	0.49
1:B:993:THR:O	1:B:994:GLY:O	2.30	0.49
1:C:184:MET:HG2	1:C:246:PHE:CE1	2.46	0.49
3:C:3042:LMT:O3'	3:C:3042:LMT:C2B	2.60	0.49
1:A:444:GLY:HA2	3:A:3047:LMT:H21	1.95	0.49
1:A:328:ASP:OD1	1:A:330:THR:HB	2.12	0.49
1:A:451:ALA:HA	3:A:3047:LMT:C8	2.41	0.49
1:A:754:TRP:CZ2	1:A:786:ILE:HD13	2.47	0.49
1:B:442:LEU:HA	1:B:445:ILE:HD13	1.93	0.49
2:D:36:ASN:ND2	2:D:36:ASN:N	2.58	0.49
2:E:49:THR:H	2:E:52:HIS:HB2	1.78	0.49
1:A:268:ILE:N	1:A:268:ILE:HD12	2.27	0.49
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.94	0.49
1:B:676:THR:HB	1:B:679:GLY:HA3	1.94	0.49
1:B:83:ASP:C	1:B:83:ASP:OD2	2.50	0.49
1:C:327:TYR:CE1	1:C:571:VAL:HG13	2.47	0.49
1:A:434:SER:O	1:A:438:ILE:HG12	2.12	0.49
1:A:984:LEU:O	1:A:987:MET:HB2	2.12	0.49
1:B:966:ASP:O	1:B:970:MET:HG3	2.13	0.49
1:A:452:VAL:C	3:A:3048:LMT:H121	2.33	0.49
1:A:309:GLU:HG3	1:A:313:MET:HE2	1.95	0.49
1:B:574:THR:HG22	1:B:627:ALA:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:973:ARG:N	1:B:974:PRO:HD2	2.27	0.49
1:C:243:THR:HG22	1:C:268:ILE:HG22	1.94	0.49
1:C:688:ALA:HB3	1:C:690:LEU:CD1	2.40	0.49
1:C:953:MET:HE1	1:C:960:LEU:CD2	2.42	0.49
1:A:444:GLY:HA2	3:A:3047:LMT:C2	2.42	0.49
1:A:453:PHE:CG	3:A:3048:LMT:C12	2.96	0.49
1:B:587:THR:HG21	1:B:623:ASN:HA	1.95	0.49
1:B:674:LEU:O	1:B:676:THR:N	2.46	0.49
3:C:3046:LMT:O6'	3:C:3046:LMT:O5B	2.30	0.49
1:C:398:MET:O	1:C:402:ILE:HG12	2.13	0.49
1:A:1031:ARG:NH1	1:A:1039:ASP:OD2	2.45	0.49
1:A:673:GLU:OE1	1:A:673:GLU:HA	2.12	0.49
1:B:879:ILE:CG1	3:B:3037:LMT:H31	2.43	0.49
1:C:200:PRO:O	1:C:204:ILE:HG13	2.13	0.49
1:C:690:LEU:HD12	1:C:690:LEU:N	2.27	0.49
1:C:758:TYR:HB2	1:C:772:TYR:CE1	2.48	0.49
1:C:888:LEU:HB2	1:C:898:PRO:HB3	1.95	0.49
1:A:649:MET:O	1:A:652:THR:HG22	2.13	0.49
1:A:896:SER:C	1:A:898:PRO:HD2	2.32	0.49
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.92	0.49
1:C:181:GLN:O	1:C:272:GLY:HA2	2.13	0.49
1:C:50:PRO:HG2	1:C:125:GLN:NE2	2.28	0.49
2:D:60:LEU:HD13	2:D:94:GLU:HG2	1.95	0.49
1:A:1016:VAL:HG23	1:A:1017:LEU:N	2.28	0.48
1:A:146:ASP:O	1:A:147:GLY:C	2.51	0.48
1:C:4:PHE:O	1:C:8:ARG:HG2	2.13	0.48
1:A:1020:PHE:O	1:A:1023:PRO:HD2	2.14	0.48
1:B:184:MET:CE	1:B:185:ARG:H	2.25	0.48
1:B:38:ILE:HD13	1:B:38:ILE:H	1.79	0.48
1:B:727:PHE:HE2	1:B:786:ILE:HD12	1.78	0.48
3:C:3046:LMT:O1B	3:C:3046:LMT:O6'	2.30	0.48
1:C:446:ALA:CB	1:C:482:VAL:HG13	2.41	0.48
2:E:65:VAL:HG12	2:E:65:VAL:O	2.11	0.48
1:A:901:VAL:HG22	1:A:946:VAL:HG11	1.96	0.48
3:B:3037:LMT:O3'	3:B:3037:LMT:O2B	2.30	0.48
1:B:344:LEU:O	1:B:348:ILE:HG13	2.13	0.48
1:A:447:MET:C	1:A:449:LEU:H	2.15	0.48
1:A:5:PHE:CE2	1:A:11:PHE:CE1	3.00	0.48
1:A:961:ILE:HG12	1:A:1031:ARG:HH21	1.79	0.48
1:B:625:GLY:O	1:B:626:ILE:HD13	2.14	0.48
1:B:70:ASN:O	1:B:110:LYS:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:THR:HG21	1:C:275:TYR:C	2.34	0.48
1:A:919:ARG:HH21	1:A:1005:THR:CG2	2.26	0.48
1:A:284:GLN:HG3	1:A:285:PRO:HD2	1.94	0.48
1:A:317:PHE:HE2	1:A:323:ILE:HG13	1.79	0.48
1:B:425:LEU:HD13	1:B:426:PRO:CD	2.42	0.48
1:A:969:ARG:HG2	1:A:969:ARG:HH11	1.78	0.48
1:B:572:PHE:HA	1:B:668:LEU:HD22	1.96	0.48
1:B:733:GLN:HE22	1:B:743:ILE:HG13	1.77	0.48
1:B:770:LYS:N	5:B:2073:HOH:O	2.37	0.48
1:C:370:ILE:C	1:C:373:PRO:HD2	2.34	0.48
1:A:544:LEU:O	1:A:548:ILE:HG13	2.14	0.48
1:C:841:MET:O	1:C:859:TRP:HH2	1.97	0.48
1:A:110:LYS:O	1:A:113:LEU:HB2	2.13	0.48
1:A:4:PHE:O	1:A:8:ARG:HG3	2.13	0.48
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.49	0.48
1:B:727:PHE:HE1	2:D:79:LEU:HD21	1.79	0.48
2:E:44:ASP:OD1	2:E:48:TRP:HB2	2.14	0.48
1:A:674:LEU:CD1	1:A:862:MET:HB2	2.44	0.48
1:A:743:ILE:HD12	1:A:743:ILE:N	2.29	0.48
1:B:121:GLU:CD	1:B:121:GLU:H	2.17	0.48
1:B:355:MET:HE1	1:B:410:ILE:HG23	1.95	0.48
1:A:768:VAL:HG12	1:B:67:GLN:NE2	2.28	0.48
1:A:348:ILE:CG1	4:A:3049:LMU:H123	2.39	0.48
1:A:406:VAL:O	1:A:410:ILE:HG13	2.13	0.48
1:A:541:TYR:C	1:A:543:VAL:H	2.15	0.48
1:B:230:LEU:H	1:B:230:LEU:HD23	1.78	0.48
1:B:425:LEU:CD1	1:B:429:GLU:HB2	2.39	0.48
1:C:408:ASP:HB3	1:C:485:ALA:CB	2.44	0.48
1:C:605:ASN:O	1:C:632:LYS:HG2	2.13	0.48
1:C:947:GLU:HG3	1:C:948:PHE:N	2.29	0.48
1:B:542:LEU:HD11	1:B:1028:VAL:HG11	1.95	0.47
1:B:727:PHE:CE2	1:B:786:ILE:HD12	2.49	0.47
1:B:881:LEU:HD13	1:B:881:LEU:O	2.14	0.47
1:C:432:ARG:HH11	1:C:432:ARG:HG2	1.79	0.47
2:E:14:LEU:N	5:E:2001:HOH:O	2.46	0.47
1:A:345:VAL:CG2	4:A:3049:LMU:H72	2.42	0.47
1:A:441:ALA:O	1:A:445:ILE:HD13	2.13	0.47
1:A:506:GLY:C	1:A:508:GLY:H	2.18	0.47
1:A:713:LEU:HD22	1:A:843:LEU:CD2	2.44	0.47
1:B:154:ILE:O	1:B:158:VAL:HG23	2.14	0.47
1:B:879:ILE:CG1	3:B:3037:LMT:C3	2.92	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1019:ILE:HG22	1:C:1020:PHE:CD1	2.48	0.47
1:C:498:LYS:HG2	1:C:499:PRO:HD2	1.96	0.47
1:C:973:ARG:N	1:C:974:PRO:HD2	2.29	0.47
1:A:919:ARG:HB3	1:A:921:LEU:CD2	2.43	0.47
1:A:453:PHE:HE2	1:A:932:LEU:HD23	1.79	0.47
1:C:680:PHE:CZ	1:C:829:GLY:HA3	2.49	0.47
2:D:45:VAL:HG23	2:D:46:VAL:HG13	1.94	0.47
1:A:1038:GLU:C	1:A:1040:ILE:N	2.68	0.47
1:A:27:ILE:HD13	3:A:3046:LMT:H71	1.95	0.47
1:A:884:VAL:HA	3:A:3047:LMT:H92	1.97	0.47
1:B:687:GLN:NE2	1:B:856:GLY:HA3	2.29	0.47
1:C:110:LYS:HZ1	1:C:113:LEU:HD23	1.78	0.47
1:C:396:PHE:CD1	1:C:1003:VAL:HG21	2.49	0.47
1:B:790:TYR:CE1	1:B:800:PRO:HB3	2.50	0.47
2:E:107:ASN:OD1	2:E:137:ALA:HA	2.14	0.47
1:A:452:VAL:HB	3:A:3048:LMT:C11	2.39	0.47
1:A:456:MET:HG2	1:A:467:TYR:HB3	1.97	0.47
1:A:542:LEU:HD12	1:A:542:LEU:N	2.30	0.47
1:B:309:GLU:O	1:B:313:MET:HG2	2.14	0.47
1:B:897:ILE:N	1:B:898:PRO:CD	2.78	0.47
1:C:282:ASN:OD1	1:C:608:SER:HA	2.14	0.47
1:C:946:VAL:O	1:C:947:GLU:C	2.53	0.47
1:A:777:ALA:O	1:A:781:MET:HE3	2.15	0.47
1:A:979:SER:O	1:A:983:ILE:HG13	2.14	0.47
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.48	0.47
1:A:886:LEU:O	1:C:14:VAL:HB	2.15	0.47
3:C:3042:LMT:C1	3:C:3042:LMT:H6D	2.44	0.47
1:C:332:PHE:HA	1:C:335:ILE:CG2	2.44	0.47
1:C:63:GLN:NE2	1:C:67:GLN:HE21	2.05	0.47
1:C:872:GLN:HA	3:C:3044:LMT:H2B	1.96	0.47
2:E:138:ASP:HB3	2:E:141:ALA:HB2	1.96	0.47
1:A:13:TRP:O	1:A:17:ILE:HG13	2.14	0.47
1:A:223:PRO:HD3	1:B:275:TYR:CD1	2.50	0.47
1:A:225:VAL:HG11	1:B:778:LYS:HA	1.96	0.47
1:A:701:GLN:O	1:A:705:GLU:HG2	2.15	0.47
1:B:451:ALA:O	1:B:455:PRO:HG2	2.14	0.47
1:B:278:ILE:HD13	1:B:588:GLN:OE1	2.15	0.47
1:B:733:GLN:NE2	1:B:743:ILE:HD11	2.29	0.47
1:C:186:ILE:HD13	1:C:268:ILE:HG23	1.96	0.47
1:C:408:ASP:OD1	1:C:482:VAL:HG12	2.15	0.47
2:D:61:GLU:HB2	5:D:2002:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD23	1:B:390:ILE:CG1	2.45	0.47
1:B:423:GLU:O	1:B:425:LEU:N	2.48	0.47
1:B:459:PHE:O	1:B:464:GLY:HA3	2.14	0.47
1:A:763:ILE:HD11	1:B:59:ASP:HB3	1.97	0.47
1:C:177:LEU:HD13	1:C:179:GLY:C	2.35	0.47
1:C:253:VAL:O	1:C:253:VAL:HG23	2.14	0.47
1:C:458:PHE:CZ	3:C:3046:LMT:C3	2.83	0.47
1:C:731:ILE:HD13	1:C:746:ILE:CG2	2.45	0.47
1:C:845:GLU:OE1	1:C:859:TRP:HZ3	1.97	0.47
1:A:372:VAL:HG22	1:A:405:LEU:CD2	2.45	0.47
3:C:3046:LMT:H2'	3:C:3046:LMT:H12	1.39	0.47
1:A:338:HIS:HA	1:A:341:VAL:CG2	2.45	0.47
1:A:36:PRO:O	1:A:38:ILE:HG23	2.15	0.47
1:A:671:ILE:CG2	1:A:675:GLY:HA2	2.43	0.47
1:A:871:ASN:CG	1:A:872:GLN:N	2.67	0.47
1:B:144:ASN:HA	1:B:320:GLY:O	2.15	0.47
1:A:428:LYS:HE2	1:A:432:ARG:HH21	1.71	0.46
1:A:62:THR:OG1	1:A:88:VAL:HG13	2.16	0.46
1:B:372:VAL:HB	1:B:373:PRO:HD3	1.96	0.46
1:B:363:ARG:HH11	1:B:498:LYS:CE	2.28	0.46
1:B:420:MET:CB	1:B:500:ILE:HG23	2.45	0.46
1:B:586:ARG:HG2	1:B:586:ARG:HH11	1.80	0.46
1:B:985:GLY:O	1:B:988:PRO:HD2	2.14	0.46
1:C:111:LEU:HD21	1:C:127:VAL:CG2	2.45	0.46
1:C:541:TYR:CZ	3:C:3043:LMT:H41	2.50	0.46
1:C:426:PRO:HG2	1:C:429:GLU:HB3	1.96	0.46
1:A:210:GLN:CD	1:A:249:ILE:HG23	2.36	0.46
1:A:448:VAL:HG21	1:A:943:ILE:CD1	2.45	0.46
1:A:68:ASN:O	1:A:110:LYS:HB3	2.16	0.46
1:A:83:ASP:C	1:A:85:THR:H	2.18	0.46
1:B:156:ASP:HA	1:B:181:GLN:HA	1.96	0.46
1:B:324:VAL:O	1:B:326:PRO:HD3	2.15	0.46
1:B:636:ASP:C	1:B:638:PRO:HD3	2.36	0.46
1:B:869:SER:O	1:B:870:GLY:C	2.53	0.46
1:C:671:ILE:HD11	1:C:674:LEU:HD11	1.95	0.46
1:C:671:ILE:HG12	1:C:862:MET:HE1	1.98	0.46
1:A:344:LEU:CB	4:A:3049:LMU:C8	2.87	0.46
1:A:965:LEU:HD12	1:A:966:ASP:N	2.30	0.46
1:B:650:ARG:NH1	1:B:650:ARG:HB2	2.31	0.46
1:C:775:SER:HB2	1:C:789:TRP:CZ2	2.51	0.46
3:A:3046:LMT:C11	4:A:3049:LMU:C9	2.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:O	1:A:477:ALA:HB3	2.15	0.46
1:B:762:PHE:CE1	1:B:764:ASP:HB2	2.51	0.46
1:C:240:LEU:HD22	1:C:245:GLU:HB3	1.97	0.46
1:C:425:LEU:HB3	1:C:429:GLU:CG	2.45	0.46
1:C:671:ILE:O	1:C:671:ILE:HG13	2.16	0.46
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.46
1:A:544:LEU:O	1:A:547:ILE:HB	2.16	0.46
1:B:383:LEU:HD22	1:B:388:PHE:CD1	2.50	0.46
1:B:571:VAL:O	1:B:668:LEU:HD21	2.16	0.46
1:C:404:LEU:HD13	1:C:982:PHE:CD1	2.51	0.46
1:C:421:ALA:O	1:C:505:HIS:HB3	2.16	0.46
2:E:118:HIS:HE2	2:E:148:THR:HA	1.80	0.46
1:A:1038:GLU:HG2	1:A:1040:ILE:O	2.15	0.46
1:A:423:GLU:HB2	1:A:425:LEU:HD13	1.96	0.46
1:B:595:THR:HG23	1:B:609:VAL:HB	1.97	0.46
1:B:575:MET:HA	1:B:626:ILE:CD1	2.45	0.46
1:C:434:SER:C	1:C:436:GLY:H	2.18	0.46
1:C:631:LEU:HD11	1:C:644:VAL:HG12	1.96	0.46
1:B:261:LEU:O	1:B:264:ASP:HB2	2.16	0.46
1:B:277:ILE:HD13	1:B:614:GLY:HA3	1.98	0.46
1:B:145:THR:HG21	1:B:322:LYS:HE2	1.97	0.46
1:B:578:LEU:HD22	1:B:661:ALA:HB2	1.98	0.46
1:A:56:THR:OG1	1:C:213:GLN:NE2	2.48	0.46
1:C:472:ILE:HG23	1:C:473:THR:N	2.31	0.46
1:C:578:LEU:N	1:C:578:LEU:HD12	2.30	0.46
1:C:888:LEU:CD2	1:C:943:ILE:HD11	2.46	0.46
1:A:240:LEU:HD23	1:A:246:PHE:CG	2.51	0.46
1:A:410:ILE:O	1:A:414:GLU:HB3	2.16	0.46
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.98	0.46
1:C:956:GLU:HG2	1:C:958:LYS:HE3	1.98	0.46
2:D:93:LEU:HD11	2:D:131:VAL:HG21	1.97	0.46
1:A:1033:PHE:O	1:A:1034:SER:HB3	2.16	0.46
1:A:928:GLN:O	1:A:932:LEU:HB2	2.15	0.46
1:A:964:THR:HG21	1:A:1027:VAL:HG12	1.96	0.46
1:B:563:PHE:O	1:B:925:VAL:HG13	2.15	0.46
1:B:764:ASP:HB3	1:B:769:LYS:HD2	1.98	0.46
1:C:355:MET:SD	1:C:368:PRO:HB2	2.56	0.46
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.98	0.46
1:A:360:GLN:OE1	1:A:513:PHE:HB3	2.15	0.46
1:A:887:CYS:HB3	3:A:3047:LMT:H52	1.95	0.46
1:B:1022:VAL:N	1:B:1023:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:MET:HE2	5:B:2045:HOH:O	2.15	0.46
1:B:425:LEU:HD12	1:B:429:GLU:CB	2.43	0.46
1:B:727:PHE:HE2	1:B:786:ILE:CD1	2.29	0.46
1:C:545:TYR:CD2	1:C:1025:PHE:HZ	2.33	0.46
1:C:953:MET:HE1	1:C:960:LEU:HD23	1.97	0.46
2:D:59:HIS:O	2:D:63:VAL:HG23	2.16	0.46
1:A:631:LEU:HD11	1:A:644:VAL:HG12	1.98	0.45
1:B:475:VAL:HG23	1:B:476:SER:N	2.31	0.45
2:D:152:ILE:HD13	2:D:152:ILE:O	2.16	0.45
1:A:167:SER:HB2	1:B:70:ASN:OD1	2.17	0.45
1:C:577:GLN:HG2	5:C:2087:HOH:O	2.16	0.45
1:C:601:LYS:CB	1:C:601:LYS:NZ	2.78	0.45
1:A:404:LEU:HD22	1:A:449:LEU:CD2	2.47	0.45
1:A:537:SER:C	1:A:539:GLY:N	2.69	0.45
1:B:1033:PHE:N	1:B:1033:PHE:CD2	2.82	0.45
1:B:716:VAL:HG13	1:B:716:VAL:O	2.16	0.45
1:B:990:VAL:HG13	1:B:1005:THR:HG22	1.99	0.45
1:C:187:TRP:HA	1:C:774:MET:O	2.16	0.45
1:C:781:MET:O	1:C:782:LEU:HD23	2.15	0.45
1:C:875:SER:HB2	3:C:3044:LMT:C3B	2.46	0.45
1:A:188:MET:CE	1:A:200:PRO:HA	2.42	0.45
1:A:342:LYS:N	4:A:3049:LMU:H41	2.32	0.45
1:A:393:LEU:HD22	1:A:466:ILE:HG23	1.98	0.45
1:A:910:ILE:HG23	1:A:911:GLY:N	2.31	0.45
1:B:190:PRO:HB3	1:B:789:TRP:CD2	2.50	0.45
1:B:175:VAL:HA	1:B:290:GLY:O	2.16	0.45
1:B:36:PRO:HG3	1:B:469:GLN:HG3	1.98	0.45
1:B:632:LYS:HA	1:B:632:LYS:HE2	1.99	0.45
1:C:261:LEU:O	1:C:262:LEU:C	2.54	0.45
1:A:453:PHE:CE1	3:A:3048:LMT:H122	2.52	0.45
1:A:348:ILE:HG23	1:A:349:ILE:N	2.31	0.45
1:A:445:ILE:CA	1:A:448:VAL:HG22	2.45	0.45
1:A:713:LEU:HD12	1:A:713:LEU:HA	1.80	0.45
1:A:778:LYS:HG3	5:A:2097:HOH:O	2.15	0.45
1:A:905:VAL:HG13	1:A:935:ILE:HD12	1.99	0.45
1:A:964:THR:HG21	1:A:1027:VAL:CG1	2.46	0.45
1:B:776:GLU:OE1	1:B:778:LYS:HE3	2.16	0.45
1:C:405:LEU:C	1:C:405:LEU:HD12	2.37	0.45
1:A:11:PHE:CZ	1:A:15:ILE:HD11	2.52	0.45
1:A:1:MET:O	1:A:4:PHE:HB3	2.16	0.45
1:A:655:PHE:C	1:A:657:GLN:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:GLU:HB3	1:B:630:SER:O	2.17	0.45
1:B:76:MET:HE2	1:B:93:THR:HG22	1.99	0.45
1:C:391:ASN:H	1:C:394:THR:CG2	2.29	0.45
1:C:423:GLU:HB2	1:C:425:LEU:HD13	1.99	0.45
1:A:1037:ASN:CG	1:A:1038:GLU:N	2.70	0.45
1:A:345:VAL:HA	4:A:3049:LMU:H111	1.98	0.45
1:A:361:ASN:HB3	1:A:364:ALA:CB	2.47	0.45
1:B:177:LEU:H	1:B:177:LEU:CD2	2.29	0.45
1:B:351:VAL:O	1:B:355:MET:CB	2.65	0.45
1:B:808:ARG:HA	2:D:79:LEU:HD23	1.99	0.45
2:D:165:LEU:O	2:D:166:GLN:OE1	2.35	0.45
1:A:425:LEU:HD12	1:A:425:LEU:N	2.32	0.45
1:A:447:MET:C	1:A:449:LEU:N	2.69	0.45
1:A:972:LEU:C	1:A:972:LEU:HD13	2.36	0.45
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.47	0.45
1:C:184:MET:HG2	1:C:246:PHE:CD1	2.52	0.45
1:C:330:THR:HB	1:C:331:PRO:HD3	1.99	0.45
2:D:82:THR:O	2:D:85:HIS:HB2	2.17	0.45
1:A:367:ILE:HD11	1:A:496:MET:HB2	1.99	0.45
1:A:372:VAL:HG22	1:A:405:LEU:HD22	1.99	0.45
1:A:872:GLN:HE21	1:A:872:GLN:HA	1.82	0.45
1:B:424:GLY:H	1:B:502:LYS:HE3	1.82	0.45
1:B:910:ILE:HG23	1:B:911:GLY:N	2.32	0.45
1:C:999:ALA:O	1:C:1003:VAL:HG23	2.17	0.45
1:C:7:ASP:OD2	1:C:432:ARG:NH2	2.49	0.45
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.52	0.45
1:B:33:ALA:O	1:B:391:ASN:HA	2.17	0.45
3:C:3044:LMT:H6E	3:C:3044:LMT:C5B	2.45	0.45
3:C:3046:LMT:O6B	3:C:3046:LMT:O6'	2.30	0.45
1:C:413:VAL:HG22	1:C:493:CYS:SG	2.57	0.45
1:C:573:MET:HE3	1:C:617:PHE:HE2	1.81	0.45
1:B:10:ILE:HD12	1:C:895:TRP:NE1	2.31	0.45
1:A:1032:ARG:HG3	1:A:1032:ARG:HH11	1.83	0.44
1:A:151:GLN:HG3	5:A:2027:HOH:O	2.17	0.44
1:A:463:THR:CG2	1:A:467:TYR:HE2	2.31	0.44
1:B:968:VAL:HG21	1:B:1023:PRO:CG	2.46	0.44
1:B:1:MET:HB3	1:B:2:PRO:HD3	1.99	0.44
1:B:879:ILE:HG12	3:B:3037:LMT:H31	1.99	0.44
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.98	0.44
1:C:404:LEU:HD11	1:C:937:LEU:CD2	2.41	0.44
1:C:712:MET:C	1:C:713:LEU:HD23	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:TYR:CE1	2:D:90:PHE:CE2	3.05	0.44
1:B:426:PRO:HD2	1:B:429:GLU:CG	2.48	0.44
1:B:762:PHE:CZ	1:B:764:ASP:HB2	2.52	0.44
1:C:904:VAL:HG23	1:C:907:LEU:HD12	1.98	0.44
2:D:48:TRP:HZ3	2:D:77:ASP:CB	2.30	0.44
2:D:94:GLU:CD	2:D:94:GLU:N	2.70	0.44
1:A:184:MET:HG2	1:A:246:PHE:CE1	2.52	0.44
1:A:764:ASP:OD1	1:A:765:ARG:HD3	2.18	0.44
1:A:935:ILE:HA	1:A:938:SER:OG	2.18	0.44
1:B:314:GLU:N	1:B:315:PRO:CD	2.81	0.44
1:B:577:GLN:HE21	1:B:577:GLN:C	2.20	0.44
1:B:681:ASP:HB3	1:B:861:GLY:N	2.31	0.44
1:C:213:GLN:CG	1:C:239:ARG:HD3	2.47	0.44
1:C:244:GLU:H	1:C:244:GLU:CD	2.19	0.44
1:C:328:ASP:OD2	1:C:330:THR:HB	2.17	0.44
1:C:657:GLN:O	1:C:658:ILE:C	2.55	0.44
1:C:730:ASP:O	1:C:805:SER:HA	2.16	0.44
1:A:1016:VAL:HG23	1:A:1017:LEU:CD1	2.48	0.44
1:A:883:VAL:HB	3:A:3047:LMT:H112	1.99	0.44
1:B:143:ILE:HG22	1:B:286:ALA:HB2	2.00	0.44
1:B:139:VAL:O	1:B:326:PRO:HD2	2.17	0.44
1:B:605:ASN:OD1	1:B:637:ARG:HG2	2.16	0.44
1:C:542:LEU:HD22	1:C:542:LEU:N	2.33	0.44
2:E:14:LEU:HA	2:E:17:LYS:HD3	2.00	0.44
1:A:166:ILE:HD12	1:A:306:ILE:HG23	2.00	0.44
1:A:29:LYS:HA	1:A:29:LYS:HE3	2.00	0.44
1:A:36:PRO:HG3	1:A:469:GLN:HG3	1.99	0.44
1:A:632:LYS:O	1:A:637:ARG:HD3	2.18	0.44
1:A:809:TRP:CD1	2:E:46:VAL:HB	2.53	0.44
1:A:897:ILE:N	1:A:898:PRO:CD	2.78	0.44
1:B:952:LEU:CD1	1:B:966:ASP:HB3	2.47	0.44
1:C:950:LYS:HD2	1:C:950:LYS:C	2.38	0.44
1:A:1018:ALA:O	1:A:1022:VAL:HG23	2.18	0.44
1:A:887:CYS:SG	3:A:3047:LMT:H72	2.51	0.44
1:B:222:THR:HA	1:B:224:PRO:HD3	2.00	0.44
1:B:450:SER:O	1:B:454:VAL:HG22	2.17	0.44
1:B:920:GLY:O	1:B:921:LEU:O	2.36	0.44
1:C:2:PRO:O	1:C:6:ILE:HG13	2.17	0.44
2:D:149:ALA:HA	2:D:152:ILE:CG2	2.47	0.44
2:E:16:LYS:O	2:E:19:LEU:HB2	2.16	0.44
1:A:687:GLN:NE2	1:A:856:GLY:CA	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:GLN:HE21	1:A:872:GLN:CA	2.30	0.44
1:B:1007:VAL:O	1:B:1011:MET:HB2	2.18	0.44
1:B:674:LEU:HD12	1:B:674:LEU:N	2.31	0.44
1:C:213:GLN:HG2	1:C:239:ARG:CD	2.47	0.44
1:C:432:ARG:NH1	1:C:432:ARG:HG2	2.33	0.44
1:C:880:SER:O	1:C:884:VAL:HG23	2.18	0.44
1:A:964:THR:HG22	1:A:1026:PHE:HD2	1.83	0.44
1:A:453:PHE:CD2	3:A:3048:LMT:C12	3.01	0.44
1:A:343:THR:HA	1:A:346:GLU:OE2	2.17	0.44
1:B:293:LEU:HD23	1:B:294:ALA:N	2.33	0.44
1:B:420:MET:HE1	1:B:427:PRO:CG	2.40	0.44
1:B:525:HIS:HB3	5:B:2049:HOH:O	2.18	0.44
1:B:778:LYS:HD3	1:B:779:TYR:CE1	2.53	0.44
1:B:400:LEU:O	1:B:933:THR:HG21	2.18	0.44
1:C:372:VAL:HG22	1:C:373:PRO:CD	2.48	0.44
1:C:419:VAL:HG13	1:C:423:GLU:HG3	1.99	0.44
1:C:444:GLY:O	1:C:448:VAL:HB	2.18	0.44
1:C:509:LYS:O	1:C:509:LYS:HG3	2.17	0.44
1:C:574:THR:HB	1:C:627:ALA:HB3	1.98	0.44
1:A:240:LEU:HG	1:A:245:GLU:HB3	2.00	0.44
1:B:355:MET:HA	1:B:355:MET:CE	2.48	0.44
1:C:267:LYS:HE3	1:C:267:LYS:HB2	1.82	0.44
1:C:358:PHE:CD2	1:C:977:MET:HG2	2.52	0.44
1:C:6:ILE:HD11	1:C:431:THR:HG22	2.00	0.44
1:C:452:VAL:HG23	1:C:453:PHE:CE1	2.52	0.44
1:C:867:ARG:HG2	1:C:871:ASN:ND2	2.32	0.44
1:C:902:MET:HA	1:C:902:MET:CE	2.48	0.44
1:A:341:VAL:CA	4:A:3049:LMU:H62	2.48	0.43
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.83	0.43
1:A:733:GLN:OE1	1:A:743:ILE:HG12	2.18	0.43
1:A:758:TYR:CE1	1:A:770:LYS:HG2	2.52	0.43
1:A:888:LEU:HD21	1:A:943:ILE:HD11	1.99	0.43
1:B:180:SER:OG	1:B:273:GLU:HB2	2.18	0.43
1:B:324:VAL:HG22	1:B:325:TYR:N	2.33	0.43
1:B:34:GLN:HG2	1:B:35:TYR:CE1	2.53	0.43
1:C:213:GLN:HG2	1:C:239:ARG:HD2	2.00	0.43
1:C:605:ASN:C	1:C:632:LYS:HG2	2.38	0.43
1:A:3:ASN:HA	1:A:6:ILE:CD1	2.43	0.43
1:A:398:MET:O	1:A:401:ALA:HB3	2.18	0.43
1:A:405:LEU:HD23	1:A:405:LEU:C	2.38	0.43
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:PHE:CG	1:C:977:MET:HG2	2.53	0.43
1:C:703:LEU:HD11	1:C:718:PRO:HG3	2.00	0.43
2:D:159:GLU:HA	2:D:162:ALA:HB3	2.00	0.43
2:E:16:LYS:O	2:E:20:GLU:HG3	2.18	0.43
1:A:317:PHE:CD2	1:A:321:LEU:HD12	2.54	0.43
1:A:403:GLY:O	1:A:406:VAL:HG12	2.19	0.43
1:A:527:TYR:HE2	1:A:1019:ILE:CG2	2.25	0.43
1:B:1032:ARG:HG2	1:B:1032:ARG:HH11	1.83	0.43
1:B:425:LEU:HD13	1:B:426:PRO:HD2	2.00	0.43
1:B:677:ALA:O	1:B:837:THR:HG21	2.19	0.43
1:C:362:PHE:O	1:C:365:THR:HG22	2.18	0.43
1:A:154:ILE:O	1:A:158:VAL:HG13	2.19	0.43
1:A:183:ALA:N	1:A:271:GLY:O	2.51	0.43
1:B:216:ALA:HB3	1:B:234:ILE:O	2.18	0.43
1:B:726:GLN:OE1	1:B:812:GLY:HA3	2.19	0.43
1:B:987:MET:HB3	1:B:988:PRO:HD3	2.01	0.43
1:C:545:TYR:O	1:C:549:VAL:HG23	2.18	0.43
1:C:943:ILE:O	1:C:947:GLU:HB3	2.17	0.43
1:A:506:GLY:O	1:A:508:GLY:N	2.51	0.43
1:A:521:GLU:HA	1:A:521:GLU:OE1	2.19	0.43
1:A:728:LYS:HD2	1:C:235:ILE:O	2.18	0.43
1:A:956:GLU:O	1:A:957:GLY:C	2.56	0.43
1:A:399:VAL:HG11	1:A:989:LEU:HD11	2.00	0.43
1:C:333:VAL:O	1:C:337:ILE:HD13	2.19	0.43
2:D:94:GLU:CD	2:D:94:GLU:H	2.22	0.43
2:E:49:THR:O	2:E:52:HIS:N	2.50	0.43
1:A:887:CYS:CB	3:A:3047:LMT:C5	2.90	0.43
1:A:337:ILE:HG22	1:A:338:HIS:N	2.33	0.43
1:A:600:THR:O	1:A:603:LYS:HG3	2.19	0.43
1:A:781:MET:SD	1:C:228:GLN:CG	3.07	0.43
1:A:969:ARG:CG	1:A:970:MET:N	2.81	0.43
1:B:603:LYS:HG2	1:B:603:LYS:O	2.17	0.43
1:B:911:GLY:HA3	1:B:1013:THR:OG1	2.18	0.43
1:C:993:THR:O	1:C:994:GLY:O	2.36	0.43
1:A:1026:PHE:O	1:A:1030:ARG:HB2	2.19	0.43
1:A:393:LEU:HD21	1:A:466:ILE:HG23	2.00	0.43
1:A:515:TRP:O	1:A:518:ARG:HB3	2.18	0.43
1:B:142:VAL:O	1:B:154:ILE:HG21	2.19	0.43
1:B:293:LEU:HD23	1:B:294:ALA:H	1.84	0.43
1:C:420:MET:HG3	1:C:425:LEU:O	2.18	0.43
1:C:427:PRO:HD3	1:C:499:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLN:NE2	1:C:67:GLN:NE2	2.63	0.43
1:C:732:ASP:CG	1:C:735:LYS:HG3	2.39	0.43
1:C:873:ALA:HB3	1:C:874:PRO:HD3	2.00	0.43
1:C:897:ILE:N	1:C:897:ILE:HD12	2.33	0.43
1:A:60:THR:CG2	1:A:119:PRO:HG2	2.48	0.43
1:A:781:MET:HG3	1:C:228:GLN:CD	2.39	0.43
1:B:992:SER:OG	1:B:1000:GLN:NE2	2.51	0.43
3:B:3036:LMT:H1B	3:B:3036:LMT:O3'	2.18	0.43
1:B:471:SER:O	1:B:475:VAL:HG13	2.19	0.43
1:B:888:LEU:HB3	1:B:898:PRO:HG3	2.01	0.43
1:C:1035:ARG:O	1:C:1035:ARG:HG2	2.18	0.43
1:A:1023:PRO:O	1:A:1027:VAL:HG22	2.19	0.43
1:A:1024:VAL:O	1:A:1028:VAL:HG23	2.19	0.43
1:A:372:VAL:HB	1:A:373:PRO:CD	2.48	0.43
1:A:441:ALA:O	1:A:444:GLY:N	2.52	0.43
1:A:677:ALA:O	1:A:678:THR:O	2.36	0.43
1:A:776:GLU:HG2	5:A:2097:HOH:O	2.18	0.43
1:B:138:MET:HE2	1:B:140:VAL:CG2	2.48	0.43
1:B:373:PRO:O	1:B:377:LEU:HD13	2.19	0.43
1:C:503:GLY:C	1:C:505:HIS:H	2.22	0.43
1:C:669:PRO:HG2	1:C:675:GLY:O	2.18	0.43
1:C:69:MET:HE3	1:C:92:LEU:HD21	2.00	0.43
1:C:888:LEU:O	1:C:889:ALA:C	2.56	0.43
1:A:952:LEU:HD21	1:A:970:MET:HE1	2.01	0.43
1:B:420:MET:CE	1:B:499:PRO:HA	2.48	0.43
1:B:706:ALA:HB3	1:B:716:VAL:HG11	2.01	0.43
1:B:733:GLN:HE22	1:B:743:ILE:HD11	1.83	0.43
1:C:68:ASN:O	1:C:110:LYS:HB3	2.19	0.43
1:C:11:PHE:O	1:C:14:VAL:HG22	2.19	0.43
1:C:127:VAL:O	1:C:127:VAL:CG2	2.66	0.43
1:C:539:GLY:CA	1:C:542:LEU:HD23	2.44	0.43
1:A:101:ASP:OD1	1:A:131:LYS:HE2	2.18	0.42
1:A:531:VAL:O	1:A:535:LEU:HG	2.19	0.42
1:A:687:GLN:HB2	1:A:687:GLN:HE21	1.56	0.42
1:A:762:PHE:CE1	1:A:764:ASP:HB2	2.54	0.42
1:A:449:LEU:HD11	1:A:936:GLY:O	2.19	0.42
1:C:225:VAL:O	1:C:226:LYS:C	2.58	0.42
1:C:448:VAL:HG22	1:C:884:VAL:HG13	2.01	0.42
1:A:510:LYS:HB2	1:A:510:LYS:HE3	1.81	0.42
1:A:712:MET:HB2	1:A:835:LYS:HG3	2.00	0.42
1:B:674:LEU:HD22	1:B:862:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:VAL:O	1:B:907:LEU:HB2	2.19	0.42
3:C:3046:LMT:H6B	3:C:3046:LMT:H6'	1.63	0.42
1:C:527:TYR:O	1:C:531:VAL:HG23	2.19	0.42
1:C:535:LEU:HD11	1:C:1027:VAL:HG21	1.99	0.42
2:E:136:GLY:O	2:E:137:ALA:HB2	2.18	0.42
2:E:137:ALA:O	2:E:139:VAL:N	2.52	0.42
2:E:49:THR:O	2:E:52:HIS:HB2	2.19	0.42
1:A:118:LEU:O	1:A:123:GLN:NE2	2.52	0.42
1:A:887:CYS:CB	3:A:3047:LMT:H51	2.34	0.42
1:B:371:ALA:O	1:B:375:VAL:HG23	2.19	0.42
1:B:717:ARG:NH1	1:B:717:ARG:HG2	2.33	0.42
1:C:426:PRO:HG2	1:C:429:GLU:CB	2.50	0.42
1:B:457:ALA:HB2	1:B:471:SER:OG	2.19	0.42
1:B:973:ARG:HG2	1:B:977:MET:HE2	2.02	0.42
1:C:366:LEU:O	1:C:369:THR:HB	2.19	0.42
1:C:562:SER:O	1:C:924:ASP:HA	2.19	0.42
1:C:948:PHE:HD2	1:C:971:ARG:NH2	2.17	0.42
1:A:341:VAL:HG13	3:A:3046:LMT:H62	2.01	0.42
1:A:959:GLY:O	1:A:960:LEU:C	2.58	0.42
1:A:999:ALA:O	1:A:1003:VAL:HG23	2.20	0.42
1:B:414:GLU:CG	1:B:977:MET:HE1	2.49	0.42
1:B:750:LEU:HB2	1:B:801:PHE:CZ	2.54	0.42
1:B:873:ALA:CB	1:B:874:PRO:HD3	2.37	0.42
1:C:686:ASP:OD2	1:C:690:LEU:O	2.38	0.42
1:C:671:ILE:HG12	1:C:862:MET:CE	2.48	0.42
2:E:44:ASP:OD2	2:E:44:ASP:C	2.58	0.42
1:A:1016:VAL:HG23	1:A:1017:LEU:HD12	2.01	0.42
1:A:159:ALA:HB2	1:A:177:LEU:CD2	2.50	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD12	1.82	0.42
1:A:341:VAL:HG12	4:A:3049:LMU:C7	2.47	0.42
1:A:709:HIS:N	1:A:710:PRO:CD	2.81	0.42
1:A:901:VAL:HG11	1:A:943:ILE:CG1	2.50	0.42
1:A:990:VAL:O	1:A:990:VAL:HG22	2.18	0.42
1:B:306:ILE:HD11	1:B:310:LEU:HD11	2.02	0.42
1:C:197:GLN:HA	1:C:798:MET:SD	2.59	0.42
1:C:670:ALA:HB3	1:C:862:MET:HE1	2.01	0.42
2:D:30:VAL:O	2:D:34:MET:HG2	2.19	0.42
1:A:152:GLU:HG3	5:A:2027:HOH:O	2.18	0.42
1:A:211:ASN:HB2	1:A:240:LEU:HD22	2.01	0.42
1:A:352:PHE:CD1	1:A:352:PHE:C	2.93	0.42
1:A:686:ASP:OD1	1:A:688:ALA:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:LEU:O	1:A:906:PRO:HD2	2.20	0.42
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.01	0.42
1:B:703:LEU:HD23	1:B:716:VAL:CG2	2.46	0.42
1:C:404:LEU:HD13	1:C:982:PHE:HD1	1.85	0.42
2:D:18:LEU:HA	2:D:33:LEU:HD13	2.02	0.42
2:D:48:TRP:CZ3	2:D:77:ASP:CB	3.03	0.42
1:A:207:ILE:O	1:A:211:ASN:HB3	2.19	0.42
1:A:575:MET:HG2	1:A:666:PHE:CE1	2.55	0.42
1:A:83:ASP:HB2	1:A:85:THR:HG22	2.02	0.42
1:B:979:SER:CB	1:B:1015:THR:HG21	2.50	0.42
1:B:441:ALA:C	1:B:445:ILE:HD12	2.40	0.42
1:B:421:ALA:HB2	1:B:500:ILE:CD1	2.49	0.42
1:C:876:LEU:CD1	1:C:932:LEU:HD21	2.50	0.42
2:D:60:LEU:HD22	2:D:94:GLU:HG3	2.01	0.42
1:A:522:LYS:HZ2	1:A:522:LYS:HB3	1.85	0.42
1:B:396:PHE:O	1:B:399:VAL:HG22	2.19	0.42
1:C:683:GLU:O	1:C:857:TYR:HA	2.20	0.42
2:D:114:ILE:HG21	2:D:119:LEU:HD21	2.01	0.42
2:D:30:VAL:HG21	2:D:62:ILE:HD13	2.01	0.42
2:E:128:ILE:HD12	2:E:128:ILE:N	2.34	0.42
1:A:229:GLN:HA	1:A:229:GLN:NE2	2.35	0.42
1:B:768:VAL:N	5:B:2072:HOH:O	2.49	0.42
1:C:668:LEU:O	1:C:678:THR:HG23	2.20	0.42
2:E:32:ILE:HG22	2:E:36:ASN:ND2	2.34	0.42
1:A:391:ASN:H	1:A:394:THR:HB	1.84	0.41
1:B:355:MET:HA	1:B:355:MET:HE2	2.02	0.41
1:B:577:GLN:NE2	1:B:577:GLN:C	2.74	0.41
1:B:600:THR:C	1:B:602:GLU:H	2.24	0.41
1:B:8:ARG:HG3	1:B:8:ARG:HH11	1.85	0.41
1:C:115:MET:N	1:C:116:PRO:HD2	2.34	0.41
1:C:382:VAL:O	1:C:386:PHE:HD1	2.03	0.41
1:C:38:ILE:HD11	1:C:671:ILE:HG22	2.03	0.41
1:C:47:ALA:HB3	1:C:88:VAL:HG13	2.02	0.41
2:D:77:ASP:OD1	2:D:79:LEU:N	2.51	0.41
1:A:658:ILE:H	1:A:658:ILE:HG13	1.72	0.41
1:A:668:LEU:C	1:A:670:ALA:N	2.72	0.41
1:A:671:ILE:CG2	1:A:675:GLY:CA	2.98	0.41
1:B:925:VAL:HG23	1:B:926:TYR:N	2.34	0.41
1:C:365:THR:O	1:C:368:PRO:HD2	2.20	0.41
1:C:612:VAL:CG1	1:C:615:PHE:HB3	2.50	0.41
1:C:852:PRO:O	1:C:855:VAL:CG1	2.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:PHE:N	1:A:666:PHE:CD1	2.89	0.41
1:B:149:MET:HB2	1:B:153:ASP:CB	2.47	0.41
1:B:506:GLY:HA2	1:B:509:LYS:HG2	2.02	0.41
1:B:733:GLN:HE22	1:B:743:ILE:CD1	2.33	0.41
1:C:804:PHE:HD2	1:C:804:PHE:O	2.03	0.41
1:C:681:ASP:OD2	1:C:826:GLU:OE2	2.38	0.41
2:D:92:HIS:HB3	2:D:94:GLU:OE2	2.20	0.41
1:A:1012:VAL:O	1:A:1016:VAL:HG13	2.20	0.41
1:A:337:ILE:O	1:A:341:VAL:CG2	2.67	0.41
1:A:509:LYS:HB3	1:A:509:LYS:HE2	1.79	0.41
1:C:348:ILE:HG12	1:C:402:ILE:HD12	2.01	0.41
1:C:615:PHE:C	1:C:615:PHE:CD1	2.93	0.41
1:C:682:PHE:HE2	1:C:684:LEU:HD23	1.86	0.41
1:C:670:ALA:HB3	1:C:862:MET:CE	2.49	0.41
1:A:189:ASN:ND2	1:A:779:TYR:OH	2.53	0.41
1:A:449:LEU:HB3	1:A:478:MET:SD	2.61	0.41
1:A:404:LEU:HD22	1:A:449:LEU:HD21	2.03	0.41
1:A:768:VAL:HG12	1:B:67:GLN:HE22	1.84	0.41
1:B:952:LEU:HD13	1:B:966:ASP:HB3	2.03	0.41
1:C:395:MET:HE1	1:C:398:MET:SD	2.61	0.41
1:C:535:LEU:HA	1:C:535:LEU:HD12	1.88	0.41
1:C:646:ALA:HB1	1:C:650:ARG:NH1	2.35	0.41
1:C:441:ALA:HB2	1:C:947:GLU:HG2	2.01	0.41
1:C:354:VAL:HG22	1:C:984:LEU:HD12	2.02	0.41
1:A:1005:THR:OG1	1:A:1006:GLY:N	2.54	0.41
1:A:449:LEU:HB2	1:A:478:MET:HE1	2.03	0.41
1:A:643:LYS:O	1:A:647:ILE:HG13	2.21	0.41
1:A:452:VAL:CG1	1:A:880:SER:OG	2.69	0.41
1:B:540:ARG:HB2	1:B:540:ARG:HE	1.70	0.41
1:C:712:MET:HG3	1:C:713:LEU:HD23	2.02	0.41
2:E:21:ALA:HB1	2:E:29:GLU:HB3	2.03	0.41
1:A:25:LEU:N	1:A:25:LEU:HD13	2.35	0.41
1:A:321:LEU:HD13	1:A:322:LYS:N	2.36	0.41
1:B:492:LEU:HB3	1:B:496:MET:CE	2.51	0.41
1:C:11:PHE:HD1	1:C:11:PHE:O	2.03	0.41
1:C:189:ASN:O	1:C:193:LEU:HB2	2.21	0.41
1:C:248:LYS:HE2	2:E:156:ASN:OD1	2.20	0.41
1:C:26:ALA:O	1:C:30:LEU:HG	2.21	0.41
1:C:544:LEU:HD13	3:C:3043:LMT:H92	2.02	0.41
1:C:563:PHE:CD2	1:C:862:MET:HE3	2.56	0.41
1:C:774:MET:HB3	5:C:2032:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:ILE:CG2	1:A:1041:GLU:N	2.80	0.41
1:A:190:PRO:HB3	1:A:789:TRP:CD2	2.56	0.41
1:A:348:ILE:HD12	4:A:3049:LMU:C12	2.50	0.41
1:A:972:LEU:O	1:A:972:LEU:HD13	2.21	0.41
1:C:1029:VAL:O	1:C:1033:PHE:HD1	2.04	0.41
1:C:135:SER:HB2	1:C:672:VAL:HB	2.02	0.41
1:C:739:LEU:HD23	1:C:799:VAL:HG21	2.01	0.41
2:E:141:ALA:O	2:E:148:THR:HG22	2.21	0.41
2:E:118:HIS:NE2	2:E:147:LYS:O	2.54	0.41
1:A:60:THR:HG23	1:A:119:PRO:CG	2.51	0.41
1:A:164:ASP:OD2	1:A:767:ARG:NH2	2.54	0.41
1:A:343:THR:HG21	1:A:1000:GLN:NE2	2.32	0.41
1:A:678:THR:C	1:A:679:GLY:O	2.60	0.41
1:A:87:THR:HG22	1:A:88:VAL:N	2.35	0.41
1:A:958:LYS:O	1:A:959:GLY:O	2.39	0.41
1:A:893:GLU:OE2	1:C:10:ILE:HG23	2.21	0.41
1:C:125:GLN:OE1	1:C:125:GLN:HA	2.20	0.41
1:C:445:ILE:HD11	1:C:944:LEU:HD21	2.01	0.41
1:C:600:THR:O	1:C:603:LYS:NZ	2.42	0.41
1:C:952:LEU:HD13	1:C:956:GLU:HB3	2.03	0.41
1:C:971:ARG:C	1:C:974:PRO:HD2	2.40	0.41
1:A:19:ILE:CG1	3:B:3036:LMT:H101	2.51	0.41
1:A:393:LEU:HD23	1:A:470:PHE:CD1	2.52	0.41
1:A:5:PHE:HE2	1:A:11:PHE:CD1	2.38	0.41
1:B:1024:VAL:O	1:B:1028:VAL:HG22	2.21	0.41
1:B:568:ASP:OD2	1:B:644:VAL:HG12	2.21	0.41
1:C:326:PRO:O	1:C:630:SER:HB2	2.20	0.41
1:C:510:LYS:HG2	1:C:511:GLY:N	2.34	0.41
1:C:972:LEU:HD13	1:C:972:LEU:C	2.41	0.41
2:D:166:GLN:OE1	2:D:166:GLN:HA	2.20	0.41
2:D:48:TRP:HZ3	2:D:77:ASP:OD2	2.02	0.41
2:E:158:ASN:ND2	2:E:161:LEU:CB	2.83	0.41
1:A:137:LEU:HD13	1:A:293:LEU:HG	2.03	0.41
1:A:345:VAL:HG23	4:A:3049:LMU:H61	2.01	0.41
1:A:361:ASN:O	1:A:363:ARG:N	2.53	0.41
1:A:376:LEU:O	1:A:380:PHE:HD1	2.04	0.41
1:A:939:ALA:O	1:A:943:ILE:HG13	2.21	0.41
1:B:228:GLN:HE21	1:B:230:LEU:HD23	1.86	0.41
1:B:876:LEU:HG	3:B:3037:LMT:O2'	2.21	0.41
1:C:211:ASN:ND2	1:C:760:ASN:HD21	2.19	0.41
1:C:53:ASP:O	1:C:57:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:898:PRO:O	1:C:901:VAL:HG22	2.21	0.41
1:C:937:LEU:HB3	1:C:1011:MET:HE2	2.01	0.41
2:D:102:ASN:N	2:D:102:ASN:HD22	2.19	0.41
1:A:222:THR:HA	1:A:224:PRO:HD3	2.01	0.40
1:A:486:LEU:N	1:A:486:LEU:HD12	2.36	0.40
1:B:14:VAL:HG21	1:C:890:ALA:HB2	2.03	0.40
1:B:370:ILE:O	1:B:374:VAL:HG23	2.21	0.40
1:B:753:ALA:O	1:B:775:SER:HB3	2.22	0.40
1:B:984:LEU:O	1:B:988:PRO:HD3	2.20	0.40
1:C:1031:ARG:O	1:C:1033:PHE:N	2.54	0.40
1:C:332:PHE:CA	1:C:335:ILE:HG22	2.48	0.40
1:A:1038:GLU:O	1:A:1039:ASP:HB3	2.22	0.40
1:A:158:VAL:CG2	1:A:177:LEU:HD11	2.51	0.40
1:A:545:TYR:O	1:A:549:VAL:HG23	2.20	0.40
1:A:693:GLU:H	1:A:693:GLU:CD	2.23	0.40
1:B:999:ALA:O	1:B:1003:VAL:HG13	2.21	0.40
1:B:144:ASN:ND2	1:B:148:THR:CG2	2.84	0.40
2:E:93:LEU:HB2	2:E:128:ILE:HD11	2.03	0.40
1:A:172:VAL:HG13	1:A:291:ILE:HG23	2.03	0.40
1:A:348:ILE:CG2	1:A:349:ILE:N	2.84	0.40
1:A:361:ASN:O	1:A:365:THR:HG22	2.22	0.40
1:A:448:VAL:C	1:A:451:ALA:HB2	2.41	0.40
1:A:960:LEU:HD13	1:A:1027:VAL:HA	2.03	0.40
1:B:115:MET:N	1:B:116:PRO:CD	2.84	0.40
1:B:143:ILE:HG22	1:B:286:ALA:CB	2.51	0.40
1:B:235:ILE:O	1:C:728:LYS:HD2	2.21	0.40
1:B:578:LEU:HD23	1:B:578:LEU:N	2.36	0.40
1:B:892:TYR:O	1:B:950:LYS:HE3	2.22	0.40
1:B:400:LEU:HD13	1:B:929:VAL:HG12	2.04	0.40
1:C:1031:ARG:C	1:C:1033:PHE:N	2.73	0.40
1:C:546:LEU:HA	1:C:546:LEU:HD12	1.91	0.40
1:C:671:ILE:HA	5:C:2080:HOH:O	2.22	0.40
2:D:96:VAL:HG21	2:D:128:ILE:HD13	2.03	0.40
2:E:73:VAL:O	2:E:73:VAL:HG22	2.21	0.40
1:A:188:MET:HE1	1:A:193:LEU:HD11	2.03	0.40
1:A:242:SER:OG	1:A:245:GLU:HG3	2.22	0.40
1:A:348:ILE:CD1	4:A:3049:LMU:H123	2.50	0.40
1:A:345:VAL:H	4:A:3049:LMU:H81	1.83	0.40
1:A:901:VAL:CG2	1:A:946:VAL:HG11	2.52	0.40
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.92	0.40
1:B:11:PHE:O	1:B:11:PHE:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:CG2	1:B:287:SER:HB3	2.51	0.40
1:B:883:VAL:O	3:B:3037:LMT:H122	2.21	0.40
1:B:872:GLN:O	1:B:873:ALA:C	2.60	0.40
1:B:44:THR:CG2	1:B:89:GLN:HG3	2.52	0.40
1:C:937:LEU:HB3	1:C:1011:MET:HE3	2.04	0.40
3:C:3042:LMT:C2B	3:C:3042:LMT:C3'	2.86	0.40
1:C:867:ARG:HG2	1:C:871:ASN:HD21	1.86	0.40
2:D:16:LYS:C	2:D:16:LYS:HD3	2.42	0.40
2:E:97:GLU:O	2:E:101:LYS:HG3	2.22	0.40
1:A:254:ASN:ND2	1:A:258:SER:HB2	2.22	0.40
1:A:451:ALA:CA	3:A:3047:LMT:C8	2.99	0.40
1:A:764:ASP:OD2	1:A:769:LYS:NZ	2.45	0.40
1:A:877:TYR:O	1:A:880:SER:HB3	2.22	0.40
1:B:538:THR:O	1:B:539:GLY:C	2.59	0.40
1:B:877:TYR:O	1:B:881:LEU:HB2	2.22	0.40
1:C:127:VAL:O	1:C:127:VAL:HG23	2.22	0.40
1:C:281:PHE:O	1:C:282:ASN:C	2.60	0.40
1:C:372:VAL:N	1:C:373:PRO:CD	2.85	0.40
1:C:360:GLN:NE2	1:C:513:PHE:HB3	2.36	0.40
1:C:640:GLU:N	1:C:640:GLU:CD	2.62	0.40
1:B:225:VAL:HG22	1:C:781:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1042/1055 (99%)	941 (90%)	74 (7%)	27 (3%)	7 9
1	B	1031/1055 (98%)	945 (92%)	73 (7%)	13 (1%)	15 25
1	C	1038/1055 (98%)	947 (91%)	80 (8%)	11 (1%)	17 30
2	D	154/169 (91%)	146 (95%)	6 (4%)	2 (1%)	15 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	E	151/169 (89%)	130 (86%)	17 (11%)	4 (3%)	7 9
All	All	3416/3503 (98%)	3109 (91%)	250 (7%)	57 (2%)	11 18

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	LYS
1	A	674	LEU
1	A	677	ALA
1	A	678	THR
1	A	959	GLY
1	A	1043	SER
1	B	510	LYS
1	B	921	LEU
1	B	994	GLY
1	C	510	LYS
1	C	994	GLY
1	A	507	GLU
1	A	538	THR
1	A	671	ILE
1	A	672	VAL
1	A	679	GLY
1	A	869	SER
1	A	957	GLY
1	A	994	GLY
1	A	1038	GLU
1	B	424	GLY
1	B	511	GLY
1	B	673	GLU
1	B	674	LEU
1	B	870	GLY
1	C	620	ARG
2	E	138	ASP
1	A	362	PHE
1	A	658	ILE
1	A	960	LEU
1	A	978	THR
1	B	617	PHE
1	C	1032	ARG
2	D	39	ASP
2	E	78	THR
2	E	137	ALA

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Mol	Chain	Res	Type
1	A	37	THR
1	A	427	PRO
1	A	439	GLN
1	A	1036	LYS
1	B	353	LEU
1	B	563	PHE
1	B	671	ILE
1	C	282	ASN
1	C	435	MET
1	C	804	PHE
2	D	135	TYR
2	E	36	ASN
1	A	979	SER
1	A	995	ALA
1	A	1034	SER
1	B	861	GLY
1	C	436	GLY
1	C	504	ASP
1	C	51	GLY
1	C	36	PRO
1	A	961	ILE

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	850/861 (99%)	799 (94%)	51 (6%)	24	41
1	B	839/861 (97%)	775 (92%)	64 (8%)	16	29
1	C	846/861 (98%)	790 (93%)	56 (7%)	21	36
2	D	120/132 (91%)	114 (95%)	6 (5%)	30	51
2	E	118/132 (89%)	109 (92%)	9 (8%)	16	29
All	All	2773/2847 (97%)	2587 (93%)	186 (7%)	20	35

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	30	LEU
1	A	48	SER
1	A	49	TYR
1	A	60	THR
1	A	64	VAL
1	A	85	THR
1	A	111	LEU
1	A	121	GLU
1	A	144	ASN
1	A	214	VAL
1	A	224	PRO
1	A	229	GLN
1	A	262	LEU
1	A	293	LEU
1	A	310	LEU
1	A	337	ILE
1	A	341	VAL
1	A	351	VAL
1	A	361	ASN
1	A	362	PHE
1	A	376	LEU
1	A	414	GLU
1	A	431	THR
1	A	452	VAL
1	A	470	PHE
1	A	473	THR
1	A	566	ASP
1	A	577	GLN
1	A	634	TRP
1	A	659	LYS
1	A	673	GLU
1	A	687	GLN
1	A	695	LEU
1	A	711	ASP
1	A	714	THR
1	A	716	VAL
1	A	767	ARG
1	A	801	PHE
1	A	867	ARG
1	A	919	ARG
1	A	935	ILE
1	A	946	VAL

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Mol	Chain	Res	Type
1	A	961	ILE
1	A	962	GLU
1	A	971	ARG
1	A	1019	ILE
1	A	1030	ARG
1	A	1038	GLU
1	A	1041	GLU
1	A	1042	HIS
1	B	3	ASN
1	B	11	PHE
1	B	38	ILE
1	B	49	TYR
1	B	75	LEU
1	B	78	MET
1	B	108	GLN
1	B	111	LEU
1	B	163	LYS
1	B	172	VAL
1	B	194	ASN
1	B	197	GLN
1	B	213	GLN
1	B	222	THR
1	B	224	PRO
1	B	240	LEU
1	B	250	LEU
1	B	267	LYS
1	B	270	LEU
1	B	278	ILE
1	B	293	LEU
1	B	306	ILE
1	B	307	ARG
1	B	355	MET
1	B	361	ASN
1	B	365	THR
1	B	429	GLU
1	B	483	LEU
1	B	495	THR
1	B	500	ILE
1	B	519	MET
1	B	528	THR
1	B	540	ARG
1	B	577	GLN

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Mol	Chain	Res	Type
1	B	587	THR
1	B	610	PHE
1	B	632	LYS
1	B	662	MET
1	B	668	LEU
1	B	674	LEU
1	B	687	GLN
1	B	695	LEU
1	B	705	GLU
1	B	711	ASP
1	B	713	LEU
1	B	714	THR
1	B	778	LYS
1	B	784	ASP
1	B	801	PHE
1	B	850	LYS
1	B	862	MET
1	B	871	ASN
1	B	881	LEU
1	B	888	LEU
1	B	914	LEU
1	B	921	LEU
1	B	937	LEU
1	B	955	LYS
1	B	956	GLU
1	B	960	LEU
1	B	965	LEU
1	B	1022	VAL
1	B	1030	ARG
1	B	1033	PHE
1	C	10	ILE
1	C	11	PHE
1	C	34	GLN
1	C	49	TYR
1	C	55	LYS
1	C	88	VAL
1	C	113	LEU
1	C	125	GLN
1	C	127	VAL
1	C	153	ASP
1	C	158	VAL
1	C	177	LEU

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Mol	Chain	Res	Type
1	C	194	ASN
1	C	213	GLN
1	C	224	PRO
1	C	229	GLN
1	C	239	ARG
1	C	243	THR
1	C	289	LEU
1	C	310	LEU
1	C	324	VAL
1	C	344	LEU
1	C	383	LEU
1	C	394	THR
1	C	404	LEU
1	C	425	LEU
1	C	450	SER
1	C	482	VAL
1	C	518	ARG
1	C	519	MET
1	C	571	VAL
1	C	575	MET
1	C	601	LYS
1	C	645	GLU
1	C	674	LEU
1	C	684	LEU
1	C	693	GLU
1	C	695	LEU
1	C	702	LEU
1	C	717	ARG
1	C	750	LEU
1	C	792	ARG
1	C	859	TRP
1	C	902	MET
1	C	950	LYS
1	C	952	LEU
1	C	966	ASP
1	C	968	VAL
1	C	986	VAL
1	C	987	MET
1	C	993	THR
1	C	1011	MET
1	C	1019	ILE
1	C	1032	ARG

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Mol	Chain	Res	Type
1	C	1036	LYS
1	C	1037	ASN
2	D	36	ASN
2	D	48	TRP
2	D	86	LEU
2	D	94	GLU
2	D	123	ARG
2	D	152	ILE
2	E	26	ARG
2	E	29	GLU
2	E	34	MET
2	E	48	TRP
2	E	119	LEU
2	E	123	ARG
2	E	154	ILE
2	E	160	ASP
2	E	166	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	81	ASN
1	A	191	ASN
1	A	194	ASN
1	A	229	GLN
1	A	254	ASN
1	A	338	HIS
1	A	361	ASN
1	A	415	ASN
1	A	505	HIS
1	A	526	HIS
1	A	577	GLN
1	A	687	GLN
1	A	865	GLN
1	A	872	GLN
1	A	923	ASN
1	A	941	ASN
1	A	1000	GLN
1	A	1001	ASN
1	A	1037	ASN
1	A	1042	HIS

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Mol	Chain	Res	Type
1	B	3	ASN
1	B	67	GLN
1	B	104	GLN
1	B	124	GLN
1	B	125	GLN
1	B	176	GLN
1	B	191	ASN
1	B	194	ASN
1	B	197	GLN
1	B	213	GLN
1	B	360	GLN
1	B	361	ASN
1	B	592	ASN
1	B	687	GLN
1	B	701	GLN
1	B	733	GLN
1	B	871	ASN
1	B	941	ASN
1	B	1000	GLN
1	C	3	ASN
1	C	34	GLN
1	C	67	GLN
1	C	125	GLN
1	C	194	ASN
1	C	197	GLN
1	C	213	GLN
1	C	218	GLN
1	C	231	ASN
1	C	254	ASN
1	C	361	ASN
1	C	415	ASN
1	C	517	ASN
1	C	569	GLN
1	C	604	ASN
1	C	692	HIS
1	C	737	GLN
1	C	830	GLN
1	C	871	ASN
1	C	1037	ASN
2	D	36	ASN
2	D	102	ASN
2	D	122	ASN

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Mol	Chain	Res	Type
2	E	36	ASN
2	E	89	HIS
2	E	92	HIS
2	E	142	GLN
2	E	158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	LMT	A	3046	-	36,36,36	1.14	3 (8%)	47,47,47	1.37	6 (12%)
3	LMT	A	3047	-	36,36,36	0.62	1 (2%)	47,47,47	1.75	9 (19%)
3	LMT	A	3048	-	36,36,36	1.43	5 (13%)	47,47,47	1.41	6 (12%)
4	LMU	A	3049	-	36,36,36	0.51	0	47,47,47	1.22	4 (8%)
3	LMT	B	3035	-	36,36,36	0.47	0	47,47,47	1.19	5 (10%)
3	LMT	B	3036	-	36,36,36	0.49	0	47,47,47	1.62	9 (19%)
3	LMT	B	3037	-	36,36,36	0.69	1 (2%)	47,47,47	2.06	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	LMT	C	3042	-	36,36,36	0.50	0	47,47,47	1.47	6 (12%)
3	LMT	C	3043	-	36,36,36	1.67	5 (13%)	47,47,47	1.81	10 (21%)
3	LMT	C	3044	-	36,36,36	0.42	0	47,47,47	1.65	5 (10%)
3	LMT	C	3046	-	36,36,36	0.61	1 (2%)	47,47,47	1.32	7 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	A	3046	-	-	0/21/61/61	0/2/2/2
3	LMT	A	3047	-	-	0/21/61/61	0/2/2/2
3	LMT	A	3048	-	-	0/21/61/61	0/2/2/2
4	LMU	A	3049	-	-	0/21/61/61	0/2/2/2
3	LMT	B	3035	-	-	0/21/61/61	0/2/2/2
3	LMT	B	3036	-	-	0/21/61/61	0/2/2/2
3	LMT	B	3037	-	-	0/21/61/61	0/2/2/2
3	LMT	C	3042	-	-	0/21/61/61	0/2/2/2
3	LMT	C	3043	-	-	0/21/61/61	0/2/2/2
3	LMT	C	3044	-	-	0/21/61/61	0/2/2/2
3	LMT	C	3046	-	-	0/21/61/61	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3048	LMT	C2-C1	-5.14	1.28	1.51
3	A	3048	LMT	O1B-C1B	2.06	1.47	1.41
3	A	3047	LMT	O1'-C1'	2.14	1.44	1.40
3	A	3046	LMT	O1'-C1'	2.15	1.44	1.40
3	A	3048	LMT	O5B-C5B	2.35	1.50	1.44
3	A	3046	LMT	O5B-C1B	2.39	1.48	1.41
3	C	3046	LMT	O1'-C1'	2.41	1.44	1.40
3	A	3048	LMT	O5B-C1B	2.52	1.48	1.41
3	B	3037	LMT	O1'-C1'	2.56	1.44	1.40
3	C	3043	LMT	O5B-C5B	3.08	1.52	1.44
3	C	3043	LMT	O5B-C1B	3.13	1.49	1.41
3	C	3043	LMT	O1'-C1'	3.18	1.45	1.40
3	C	3043	LMT	O1B-C1B	3.24	1.50	1.41
3	A	3046	LMT	O5B-C5B	3.30	1.52	1.44
3	A	3048	LMT	O1'-C1'	3.44	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3043	LMT	C2-C1	6.38	1.78	1.51

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3043	LMT	O1'-C1-C2	-5.83	92.85	109.63
3	B	3036	LMT	C1-O1'-C1'	-5.53	104.33	114.00
3	B	3037	LMT	O5B-C5B-C4B	-5.08	99.97	109.67
3	C	3044	LMT	C1-O1'-C1'	-4.76	105.68	114.00
3	B	3037	LMT	O5'-C1'-C2'	-4.67	100.56	110.28
4	A	3049	LMU	C3'-C4'-C5'	-4.62	100.28	110.85
3	B	3037	LMT	C1'-O5'-C5'	-4.60	104.72	113.74
3	C	3042	LMT	C1B-O1B-C4'	-4.34	106.46	118.00
3	C	3046	LMT	C3'-C4'-C5'	-4.17	101.33	110.85
3	C	3044	LMT	C1'-O5'-C5'	-4.08	105.73	113.74
3	B	3037	LMT	C1B-O5B-C5B	-3.91	106.08	113.74
3	B	3037	LMT	C1B-O1B-C4'	-3.87	107.70	118.00
3	C	3043	LMT	C3'-C4'-C5'	-3.71	102.37	110.85
3	B	3036	LMT	C6B-C5B-C4B	-3.57	104.04	112.99
3	A	3047	LMT	C3'-C4'-C5'	-3.29	103.34	110.85
3	A	3046	LMT	C3'-C4'-C5'	-3.20	103.53	110.85
3	C	3042	LMT	C1-O1'-C1'	-3.18	108.45	114.00
3	B	3037	LMT	O1B-C4'-C5'	-3.15	100.94	109.33
3	C	3042	LMT	C4B-C3B-C2B	-3.09	105.09	110.79
3	A	3047	LMT	O5'-C1'-C2'	-3.08	103.88	110.28
3	B	3037	LMT	O1B-C1B-O5B	-2.83	103.31	110.69
3	A	3048	LMT	C3B-C4B-C5B	-2.70	105.41	110.23
3	C	3042	LMT	C6'-C5'-C4'	-2.70	105.32	113.25
3	C	3043	LMT	O5'-C5'-C6'	-2.67	99.47	106.38
3	B	3035	LMT	O5'-C1'-C2'	-2.65	104.78	110.28
3	C	3043	LMT	C6B-C5B-C4B	-2.64	106.38	112.99
3	A	3047	LMT	C1B-O1B-C4'	-2.59	111.12	118.00
3	C	3046	LMT	C1'-O5'-C5'	-2.51	108.81	113.74
3	C	3046	LMT	O5B-C5B-C4B	-2.46	104.96	109.67
3	A	3047	LMT	C6B-C5B-C4B	-2.37	107.06	112.99
3	C	3044	LMT	O5'-C1'-C2'	-2.36	105.37	110.28
3	B	3035	LMT	C1B-O1B-C4'	-2.33	111.81	118.00
3	C	3046	LMT	C1-O1'-C1'	-2.28	110.01	114.00
3	B	3036	LMT	C1'-O5'-C5'	-2.22	109.39	113.74
3	B	3035	LMT	C1'-O5'-C5'	-2.19	109.45	113.74
3	C	3046	LMT	C1B-O5B-C5B	-2.15	109.52	113.74
3	C	3046	LMT	C1B-O1B-C4'	-2.08	112.47	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3042	LMT	C6B-C5B-C4B	-2.06	107.83	112.99
3	B	3035	LMT	O5'-C1'-O1'	-2.01	105.16	109.99
4	A	3049	LMU	O1B-C1B-O5B	-2.01	105.44	110.69
3	A	3046	LMT	C1-O1'-C1'	-2.01	110.48	114.00
3	B	3036	LMT	O1B-C1B-O5B	2.08	116.12	110.69
3	C	3043	LMT	C1B-O5B-C5B	2.11	117.88	113.74
3	A	3046	LMT	O3B-C3B-C4B	2.16	115.23	110.36
3	B	3036	LMT	O5'-C5'-C6'	2.16	111.98	106.38
3	A	3048	LMT	C2'-C3'-C4'	2.19	114.47	109.63
3	A	3048	LMT	C1'-C2'-C3'	2.22	114.39	109.98
3	A	3046	LMT	O5B-C5B-C6B	2.33	112.42	106.38
3	C	3043	LMT	O1B-C1B-O5B	2.41	116.98	110.69
3	B	3036	LMT	O1B-C4'-C3'	2.43	113.53	107.18
4	A	3049	LMU	C1'-C2'-C3'	2.45	114.84	109.98
3	B	3037	LMT	O5'-C5'-C6'	2.48	112.81	106.38
3	B	3035	LMT	O1B-C1B-C2B	2.54	114.44	108.12
3	B	3036	LMT	O1'-C1'-C2'	2.55	111.13	108.00
3	A	3048	LMT	C1B-O5B-C5B	2.58	118.81	113.74
3	A	3047	LMT	O1'-C1-C2	2.66	117.29	109.63
3	A	3046	LMT	C1B-O5B-C5B	2.69	119.02	113.74
3	C	3046	LMT	C1B-C2B-C3B	2.76	115.45	109.98
3	A	3048	LMT	O1'-C1'-C2'	2.87	111.54	108.00
3	C	3044	LMT	O5B-C5B-C6B	2.90	113.90	106.38
3	C	3043	LMT	O1'-C1'-C2'	2.97	111.65	108.00
3	A	3047	LMT	C1B-O5B-C5B	3.04	119.70	113.74
4	A	3049	LMU	O5'-C1'-C2'	3.26	117.06	110.28
3	B	3036	LMT	C1B-C2B-C3B	3.38	116.69	109.98
3	C	3043	LMT	O1B-C4'-C3'	3.67	116.76	107.18
3	C	3042	LMT	O1B-C4'-C3'	3.67	116.77	107.18
3	A	3047	LMT	O5B-C5B-C4B	3.76	116.85	109.67
3	B	3036	LMT	O5B-C1B-C2B	3.84	118.27	110.28
3	C	3043	LMT	O5'-C5'-C4'	3.96	118.22	109.78
3	A	3046	LMT	O5B-C5B-C4B	4.17	117.63	109.67
3	A	3047	LMT	O5B-C1B-C2B	4.24	119.09	110.28
3	C	3043	LMT	O5B-C5B-C6B	4.41	117.82	106.38
3	A	3048	LMT	O1'-C1-C2	5.15	124.44	109.63
3	A	3047	LMT	O1'-C1'-C2'	6.56	116.07	108.00
3	C	3044	LMT	O1'-C1'-C2'	6.77	116.33	108.00
3	B	3037	LMT	O1'-C1'-C2'	7.40	117.11	108.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 238 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3046	LMT	10	0
3	A	3047	LMT	48	0
3	A	3048	LMT	26	0
4	A	3049	LMU	50	0
3	B	3035	LMT	3	0
3	B	3036	LMT	18	0
3	B	3037	LMT	29	0
3	C	3042	LMT	17	0
3	C	3043	LMT	15	0
3	C	3044	LMT	12	0
3	C	3046	LMT	16	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1044/1055 (98%)	0.12	79 (7%) 17 19	13, 43, 87, 106	0
1	B	1033/1055 (97%)	-0.02	36 (3%) 48 54	14, 40, 66, 89	0
1	C	1040/1055 (98%)	-0.04	28 (2%) 58 63	16, 36, 62, 94	0
2	D	156/169 (92%)	-0.05	0 100 100	25, 39, 63, 75	0
2	E	153/169 (90%)	0.43	12 (7%) 16 18	28, 54, 76, 81	0
All	All	3426/3503 (97%)	0.04	155 (4%) 37 43	13, 40, 73, 106	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1035	ARG	8.0
1	C	1034	SER	6.5
1	A	1035	ARG	5.4
1	A	918	PHE	5.0
2	E	33	LEU	4.9
1	A	511	GLY	4.8
1	A	512	PHE	4.7
2	E	34	MET	4.6
1	A	870	GLY	4.6
1	A	869	SER	4.5
1	A	1044	HIS	4.4
1	A	868	LEU	4.4
1	C	506	GLY	4.4
1	A	515	TRP	4.2
1	C	1036	LYS	4.1
1	A	510	LYS	4.1
1	A	362	PHE	3.9
1	C	511	GLY	3.9
1	C	1040	ILE	3.9
1	A	712	MET	3.9

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Mol	Chain	Res	Type	RSRZ
2	E	35	ALA	3.8
1	A	541	TYR	3.7
1	A	675	GLY	3.7
1	C	741	VAL	3.7
1	B	638	PRO	3.7
1	C	515	TRP	3.6
1	A	459	PHE	3.6
1	A	543	VAL	3.5
1	B	512	PHE	3.4
1	A	509	LYS	3.4
1	A	873	ALA	3.4
1	C	739	LEU	3.4
1	B	874	PRO	3.3
1	B	515	TRP	3.3
1	A	513	PHE	3.3
1	C	28	LEU	3.3
1	A	538	THR	3.2
1	B	513	PHE	3.2
1	A	871	ASN	3.2
1	B	871	ASN	3.2
1	A	832	ALA	3.2
1	A	546	LEU	3.1
1	B	554	TYR	3.1
1	C	510	LYS	3.1
1	B	678	THR	3.1
1	A	518	ARG	3.0
1	A	500	ILE	3.0
1	C	1033	PHE	3.0
1	C	554	TYR	3.0
1	A	1036	LYS	3.0
1	A	866	GLU	2.9
1	B	657	GLN	2.9
1	B	991	ILE	2.9
1	C	1038	GLU	2.9
1	A	404	LEU	2.9
1	A	835	LYS	2.9
2	E	32	ILE	2.9
1	C	933	THR	2.9
2	E	99	LEU	2.9
1	A	534	ILE	2.9
1	A	833	PRO	2.9
1	C	811	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	426	PRO	2.9
1	A	1034	SER	2.8
1	B	557	VAL	2.8
2	E	139	VAL	2.8
1	A	937	LEU	2.8
1	A	407	ASP	2.8
1	A	876	LEU	2.8
1	C	3	ASN	2.8
1	C	403	GLY	2.7
1	A	501	ALA	2.7
1	B	563	PHE	2.7
1	A	674	LEU	2.7
1	A	955	LYS	2.7
1	C	519	MET	2.7
1	A	713	LEU	2.7
1	B	511	GLY	2.7
1	A	425	LEU	2.7
1	C	937	LEU	2.7
1	A	957	GLY	2.7
1	B	255	GLN	2.7
2	E	38	ALA	2.7
1	A	424	GLY	2.6
1	A	993	THR	2.6
1	B	508	GLY	2.6
1	A	255	GLN	2.6
1	B	653	ARG	2.6
1	A	1037	ASN	2.6
1	A	1042	HIS	2.6
1	A	936	GLY	2.6
1	A	872	GLN	2.6
1	C	707	ALA	2.5
1	A	498	LYS	2.5
1	A	514	GLY	2.5
1	B	319	SER	2.5
1	A	554	TYR	2.5
1	A	516	PHE	2.5
1	A	432	ARG	2.5
1	A	558	ARG	2.5
1	C	255	GLN	2.5
2	E	37	GLY	2.5
1	A	411	VAL	2.5
1	A	385	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	14	LEU	2.4
1	B	558	ARG	2.4
1	A	556	PHE	2.4
1	B	666	PHE	2.4
1	B	641	GLU	2.4
1	A	403	GLY	2.4
1	A	670	ALA	2.4
1	B	25	LEU	2.4
1	A	935	ILE	2.4
1	B	509	LYS	2.4
1	B	501	ALA	2.4
1	B	642	ASN	2.3
1	A	933	THR	2.3
1	A	496	MET	2.3
1	A	1033	PHE	2.3
1	A	406	VAL	2.3
1	C	29	LYS	2.3
1	A	932	LEU	2.3
1	C	404	LEU	2.3
1	A	1040	ILE	2.2
1	B	28	LEU	2.2
1	A	940	LYS	2.2
1	A	555	LEU	2.2
1	B	134	SER	2.2
1	A	934	THR	2.2
1	C	501	ALA	2.2
1	B	518	ARG	2.2
1	A	960	LEU	2.2
1	B	256	ASP	2.1
1	C	401	ALA	2.1
1	B	516	PHE	2.1
1	A	405	LEU	2.1
1	B	519	MET	2.1
1	A	939	ALA	2.1
1	A	942	ALA	2.1
1	B	659	LYS	2.1
1	B	674	LEU	2.1
1	B	866	GLU	2.1
1	C	503	GLY	2.1
1	B	873	ALA	2.1
2	E	150	PHE	2.1
1	A	1038	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	933	THR	2.0
1	A	408	ASP	2.0
1	B	941	ASN	2.0
2	E	166	GLN	2.0
1	A	11	PHE	2.0
1	A	429	GLU	2.0
1	C	955	LYS	2.0
2	E	26	ARG	2.0
1	A	542	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	LMT	C	3046	35/35	0.81	0.47	8.99	103,106,110,111	0
4	LMU	A	3049	35/35	0.78	0.40	6.73	90,98,121,121	0
3	LMT	B	3037	35/35	0.88	0.58	5.53	124,128,147,149	0
3	LMT	C	3043	35/35	0.81	0.41	4.76	64,70,112,113	0
3	LMT	C	3042	35/35	0.85	0.37	4.66	94,97,104,105	0
3	LMT	A	3047	35/35	0.85	0.32	3.43	75,83,117,118	0
3	LMT	C	3044	35/35	0.73	0.34	3.31	57,84,94,95	0
3	LMT	B	3036	35/35	0.81	0.27	2.39	65,78,86,87	0
3	LMT	B	3035	35/35	0.88	0.26	2.37	56,67,69,71	0
3	LMT	A	3046	35/35	0.86	0.20	0.99	48,59,69,70	0
3	LMT	A	3048	35/35	0.83	0.29	0.50	90,92,116,117	0

6.5 Other polymers (i)

There are no such residues in this entry.